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[Continued on next page]

(54) **Title**: STING CRYSTALS AND MODULATORS

Figure 1A

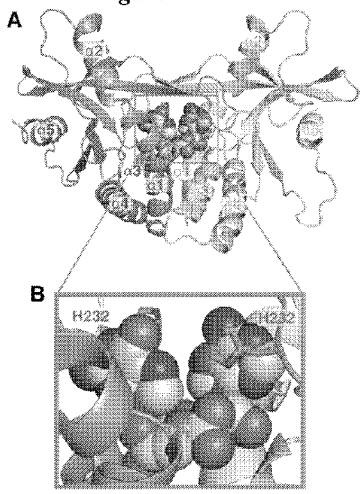


Figure 1B

Figure 1C

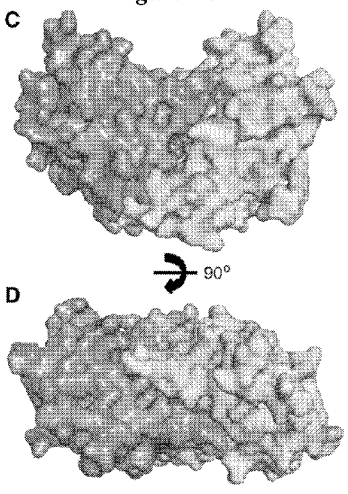


Figure 1D

(57) **Abstract**: The present invention provides STING crystals. The present invention also provides STING modulators that interact with sites present in and/or defined by such crystals. The present invention also provides methods of making and using such crystals and modulators. Other aspects and/or features of the present invention will be apparent to those skilled in the art, reading the present specification.

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STING CRYSTALS AND MODULATORS

Cross Reference to Related Applications

[0001] The present invention claims priority to United States provisional patent application no. 61/860,818, filed July 31, 2013, the entire contents of which is hereby incorporated by reference herein.

Background

[0002] The protein TMEM173/STING (stimulator of interferon genes) (Ishikawa and Barber, 2008; Zhong et al. 2008; Sun et al. 2009; Burdette et al. 2011) is a central player in the innate immune response to nucleic acids, particularly cytosolic dsDNA (reviewed in Burdette and Vance, 2013). STING responds to various pathogens, as well as to mitochondrial damage, and its overactivation may contribute or possibly even trigger the onset of autoimmune disorders such as systemic lupus erythematosus. Drug discovery requires a mechanistic understanding of the cytosolic DNA-sensing pathway. Such discovery is desperately needed for development of agonists and antagonists of innate immunity, and will have a profound impact on anti-cancer and vaccine development, as well as therapies for autoimmune disorders.

Summary

[0003] The present disclosure provides insights into STING structure and function; such insights define agents useful as modulators of human STING, and provide methods and compositions related thereto.

[0004] Among other things, the present invention identifies the source of one or more probems with prior efforts to modulate (agonist or antagonist) human STING, and provides solutions to such problems. The present invention also identifies the source of one or more problems with prior efforts to define or determine hSTING structure, or relevant aspects of hSTING-interacting agents, based on comparisons with STING orthologs. The present invention provides solutions to such problems. Thus, among other things, the present invention provides STING polypeptides, STING crystal (and/or crystallizable) compositions, STING binding

agents, systems that tangibly embody or otherwise contrain or utilize information about such polypeptides, compositions, and/or binding agents, and methods of generating and/or using each of these.

[0005] The present invention provides, among other things, a STING modulator whose structure is an analog of c[G(2',5')pA(3',5')p], 5,6-dimethylxanthenone-4-acetic acid (DMXAA), or 10-carboxymethyl-9-acridine (CMA), and includes a moiety that interacts with a residue corresponding to Ser162 and/or Ile165 of hSTING. In some embodiments, a STING modulator whose structure is an analog of c[G(2',5')pA(3',5')p], 5,6-dimethylxanthenone-4-acetic acid (DMXAA), or 10-carboxymethyl-9-acridine (CMA), includes a moiety that interacts with a residue corresponding Gly230, Gln266, Ser162, or Ile165 of hSTING, or a combination thereof. In some embodiments, a provided STING modulator includes a moiety that interacts with a residue corresponding to Gln266 of hSTING. In some embodiments, a provided STING modulator includes a moiety that interacts with a residue corresponding to Gly230 of hSTING. In some embodiments, a provided STING modulator includes a moiety that interacts with a residue corresponding to Ser162 of hSTING.

[0006] In some embodiments, provided STING modulators, upon binding hSTING, an antiparallel β-pleated sheet forms over the binding pocket indicative of formation of a closed STING conformation.

[0007] In some embodiments, a STING modulator comprises one or more of the following features:

i.) direct hydrogen bonds to the side chain of Thr267 of hSTING;

ii.) direct hydrogen bonds to the side chain of Arg238 of hSTING; and

iii.) direct hydrogen bonds to the side chain of Thr263 of hSTING.

[0008] In some embodiments, a STING modulator comprises one or more of the following features:

i) direct hydrogen bonds to the side chain of Arg238 of hSTING; and

ii) water-mediated hydrogen bonds to Tyr240 of hSTING.

[0009] In some embodients, a STING modulator comprises one or more of the following features:

i) hydrophobic interactions with a residue corresponding to Leu170 of hSTING;

ii) hydrophobic interactions with a residue corresponding to Ile235 of hSTING; and

iii) hydrophobic interactions with a residue corresponding to Ile165 of hSTING.

[0010] In certain embodiments, the one or more features of provided STING modulators include at least one feature selected from the group consisting of: spatial separation between the moiety and the potential interaction site; energy of the potential moiety-interaction site interaction, and/or combinations thereof.

[0011] In some embodiments, provided STING agents modulate hSTING.

[0012] In some embodiments, provided STING agents are specific to hSTING as compared with mSTING.

[0013] In some embodiments, the present invention provides methods of designing or characterizing a STING modulator comprising providing an image of a STING crystal that includes at least one potential interaction site; docking in the image at least one moiety that is a potential STING modulator structural element; and assessing one or more features of a potential moiety-interaction site interaction.

[0014] In some embodiments, the at least one potential interaction site includes a site of hSTING selected from the group consisting of Ser162, Ile165, R238, T263, T267, and combinations thereof. In some embodiments, the at least one potential interaction site includes a site of hSTING selected from the group consisting of Ser162, Ile165, Arg238, Thr263, Thr267, and combinations thereof. In some embodiments, the at least one potential interaction site includes a site of hSTING selected from the group consisting of Gly230, Gln266, Tyr240, Leu170, Ile235, and combinations thereof.

[0015] In some embodiments, the at least one potential interaction site is Ser162 of hSTING.

[0016] In some embodiments, the at least one potential interaction site is Ile165 of hSTING.

[0017] In some embodiments, the at least one potential interaction site is Gly230 of hSTING.

[0018] In some embodiments, provided methods further comprise a step of providing an image of a potential STING modulator comprising the moiety docked with the image of the STING crystal.

[0019] In some embodiments, provided methods further comprise further comprising a step of comparing the image with that of a STING crystal including a bound known modulator.

[0020] In some embodiments, the present invention provides a system comprising a computer or computer readable medium in which a STING crystal structure, or coordinates thereof, is embedded and/or displayed.

[0021] One feature of the present invention is that it permits assessment of potential and/or actual STING modulators based on both structural and functional attributes. For example, in some embodiments, the present invention provides methods of designing and/or characterizing a STING modulator, which methods comprise steps of (i) using a system comprising a computer or computer readable medium in which a STING crystal structure, or coordinates thereof, is embedded and/or displayed to assess one or more structural features of the STING modulator; and (ii) performing one or more *in vitro, in vivo* or cell-based assays to characterize the STING modulator. In some embodiments, the one or more structure features of the STING modulator comprise a moiety that interacts with a residue corresponding to Ser162 and/or Ile165 of hSTING. In some embodiments, the one or more structure features of the STING modulator comprise a moiety that interacts with a residue corresponding to Gly230 of hSTING. In some embodiments, the one or more structure features of the STING modulator comprise a moiety that interacts with a residue corresponding to Arg238, Thr263, Thr267, Gln266, Tyr240, Leu170, Ile235 of hSTING, or a combination thereof.

[0022] In some embodiments, the present invention provides a method of designing and/or characterizing a STING modulator, which method comprises steps of (i) determining the

STING modulator binds in the binding pocket having a three-dimensional structure characterized by the structure coordinates of any one of Tables 1, 2, 3, 4, 5, 6, 7, 8, and/or 9; and (ii) assessing one or more structure features of the STING modulator. In some embodiments, the method further comprises the step of defining the three-dimensional shape of the modulator. In some embodiments, the three-dimensional shape of the modulator includes a moiety that interacts with a residue corresponding to Ser162 and/or Ile165 of hSTING. In certain embodiments, the three-dimensional shape of the modulator includes a moiety that interacts with a residue corresponding to Gly230 of hSTING. In some embodiments, the three-dimensional shape of the modulator includes a moiety that interacts with a residue corresponding to Arg238, Thr263, Thr267, Gln266, Tyr240, Leu170, Ile235 of hSTING, or a combination thereof.

[0023] In some embodiments, the present invention provides a modulator of STING characterized in that it binds in the binding pocket having a three-dimensional structure characterized by the structure coordinates of any one of Tables 1, 2, 3, 4, 5, 6, 7, 8, and/or 9.

[0024] In some embodiments, the present invention provides a designed STING modulator, comprising the crystallography coordinates of any one of Tables 1, 2, 3, 4, 5, 6, 7, 8, and/or 9, wherein the crystallography coordinates are within about a root mean square deviation of not more than about 1.5 Å from the backbone atoms of the amino acids according to Tables 1, 2, 3, 4, 5, 6, 7, 8, and/or 9.

[0025] In some embodiments, the present invention provides a computer system containing a set of information to perform a design or characterization of a STING modulator having a user interface comprising a display unit, the set of information comprising: (i) logic for inputting an information regarding a binding of a STING protein to a moiety known to bind STING protein; (ii) logic for designing a candidate STING modulator based on the binding of the STING protein to the moiety known to bind STING protein; (iii) logic for determing an information regarding a binding of the STING protein to the candidate STING modulator; and logic for making a conclusion regarding a STING agonist or antagonist properties of the candidate STING modulator based on the determination of step (iii).

[0026] In some embodiments, the present invention provides a computer-readable storage medium containing a set of information for a general purpose computer having a user interface

comprising, a display unit, the set of information comprising: (i) logic for inputting an information regarding a binding of a STING protein to a chemical known to binding STING protein; (ii) logic for design a candidate STING modulator based on the binding of the STING protein to the chemical known to bind STING protein; (iii) logic for determining an information regarding a binding of the STING protein to the candidate STING modulator; and (iv) logic for making a conclusion regarding a STING agonist or antagonist properties of the candidate STING modulator based on the determination step of step (iii).

[0027] In some embodiments, the present invention provides an electronic signal or carrier wave that is propagated over the internet between computers comprising a set of information for a general purpose computer having a user interface comprising a display unit, the set of information comprising a computer-readable storage medium containing a set of information for a general purpose computer having a user interface comprising a display unit, the set of information comprising: (i) logic for inputting an information regarding a binding of a STING protein to an agent known to bind STING protein; (ii) logic for designing a candidate STING modulator based on the binding of the STING protein to the agent known to bind STING protein; (iii) logic for determining an information regarding a binding of the STING protein to the candidate STING modulator; and (iv) logic for making a conclusion regarding a STING agonist or antagonist properties of the candidate STING modulator based on the determination of step (iii).

[0028] In some embodiments, the present invention provides a crystalline or crystallizable composition comprising or consisting of a STING polypeptide. In some embodiments, the present invention provides methods of making and using such crystalline or crystallizable compositions.

Brief Description of the Drawings

[0029] The Figures described below, that together make up the Drawings, are for illustration purposes only, not for limitation.

[0030] **Figure 1** depicts an exemplary crystal structure of c[G(2',5')pA(3',5')p] bound to hSTING^{H232} and exemplary details of intermolecular contacts in the complex. **FIG. 1A** depicts an exemplary 2.25 Å crystal structure of cyclic [G(2',5')pA(3',5')p] bound to hSTING^{H232} (aa 155-341). The symmetrical hSTING^{H232} dimer is shown in a ribbon representation, with individual monomers colored in magenta and yellow. α-helices are labeled from α 1 to α 5. The c[G(2',5')pA(3',5')p] in a space-filling representation is bound in the central cavity at the interface between the two monomers. **FIG. 1B** depicts an exemplary expanded view of the c[G(2',5')pA(3',5')p] binding pocket in the complex. The position of H232 (in green) in a stick representation is labeled in this panel. **FIG. 1C** depicts an exemplary surface representation of the structure of the complex shown in panel A. **FIG. 1D** depicts an exemplary view in panel C rotated through 90°. **FIG. 1E, FIG. 1F** and **FIG. 1G** depict exemplary intermolecular contacts in the complex of c[G(2',5')pA(3',5')p] bound to hSTING^{H232}. The bound c[G(2',5')pA(3',5')p] is shown in biscuit color, with individual STING subunits in the symmetrical dimer shown in magenta and yellow. The bracketing of the purine rings of c[G(2',5')pA(3',5')p] by Y167 is shown in panel E, and intermolecular contacts to the base edges and backbone phosphates of the ligand by the subunits of STING are shown in panels F and G, respectively.

[0031] **Figure 2** depicts an exemplary comparison of hSTING^{H232} complexes bound to c[G(2',5')pA(3',5')p] and c[di-GMP]. **FIG. 2A** depicts exemplary Details related to alignment and hydrogen-bonding patterns within the four-stranded anti-parallel β-sheet that forms a cap over the binding pocket on formation of the c[G(2',5')pA(3',5')p]-hSTING^{H232} complex. **FIG. 2B** depicts an exemplary superposition of the c[G(2',5')pA(3',5')p] bound structure of hSTING^{H232} (aa 155-341) with both subunits in green and c-[d-GMP] bound structure of hSTING^{H232} (aa 139-379) with both subunits in beige (PDB: 4EF4). **FIG. 2C** depicts an exemplary superposition of the c[G(2',5')pA(3',5')p] in green and c[di-GMP] in orange (PDB: 4EF4) in their complexes with hSTING^{H232}. **FIG. 2D** depicts an exemplary expanded view in stereo of the top right segment of panel B following superposition of the c[G(2',5')pA(3',5')p] bound structure of hSTING^{H232} (both subunits in green) and c[di-GMP] bound structure of hSTING^{H232} (both subunits in orange) (PDB: 4EF4).

[0032] **Figure 3** depicts an exemplary crystal structure of c[G(2',5')pA(3',5')p] bound to mSting^{R231} and an exemplary comparison of its complex with the same ligand bound to hSTING^{H23}. **FIG. 3A** depicts an exemplary 1.77 Å crystal structure of c[G(2',5')pA(3',5')p] bound to mSting^{R231} (aa 154-340). **FIG. 3B** depicts exemplary intermolecular contacts to the cyclic dinucleotide ring system of the ligand by the subunits of mSting^{R231}. **FIG. 3C** depicts an exemplary superposition of the c[G(2',5')pA(3',5')p] bound structures of hSTING^{H232} (both subunits in green) and mSTING^{R231} (both subunits in magenta). **FIG. 3D** depicts an exemplary superposition of the c[G(2',5')pA(3',5')p] in its complexes with hSTING^{H232} in green and mSTING^{R231} in magenta. **FIG. 3E** depicts an exemplary 1.9 Å crystal structure of c[G(2',5')pA(2',5')p] bound to hSTING^{H232} (aa 155-341). **FIG. 3F** depicts an exemplary 2.1 Å crystal structure of c[G(3',5')pA(3',5')p] bound to mSting^{R231} (aa 154-340).

[0033] **Figure 4** depicts exemplary ITC data on binding of cGAMP linkage isomers to hSTING^{H232} and hSTING^{H232} mutants, as well as to hSTING^{R232}, hSTING$^{A230/R232}$, mSting^{R231} and mSting^{A231}. **FIG. 4A** and **FIG. 4B** depicts exemplary ITC binding curves for complex formation between cGAMP linkage isomers bound to hSTING^{H232} (aa 140-379) (panel A) and binding of c[G(2',5')pA(3',5')p] to mutants of hSTING^{H232} (panel B). **FIG. 4C** depicts exemplary ITC binding curves for complex formation between cGAMP linkage isomers bound to hSTING^{R232} (aa 140-379). **FIG. 4D** depicts exemplary ITC binding curves for complex formation between cGAMP linkage isomers bound to hSTING$^{A230/R232}$ (aa 140-379). **FIG. 4E** depicts exemplary ITC binding curves for complex formation between cGAMP linkage isomers bound to mSting^{R231} (aa 139-378). **FIG. 4F** depicts exemplary ITC binding curves for complex formation between cGAMP linkage isomers bound to mSting^{A231} (aa 139-378).

[0034] **Figure 5** depicts an exemplary crystal structure of DMXAA ligand bound to mSting^{R231}. **FIG. 5A** depicts exemplary chemical formulas of dimethylxanthenone-4-acetic acid (DMXAA). **FIG. 5B** depicts an exemplary 2.4 Å crystal structure of two molecules of DMXAA bound to mSting^{R231} (aa 154-340). **FIG. 5C** depicts exemplary intermolecular contacts in the complex of DMXAA bound to mSting^{R231}. The two bound DMXAA molecules are shown in biscuit color, with individual mSting subunits in the symmetrical dimer shown in magenta and yellow. The intermolecular contacts to the polar and nonpolar edges of the DMXAA by the

mSting subunits are shown in two alternate views. **FIG. 5D** depicts an exemplary superposition of the 2.4 Å DMXAA bound structure of $mSting^{R231}$ (both subunits in biscuit) and of the 1.77 Å structure of c[G(2',5')pA(3',5')p] of $mSting^{R231}$ (both subunits in magenta). For dose dependence: Data points were determined in triplicate and are depicted as means ± SEM.

[0035] **Figure 6** depicts exemplary results of cGAMP stimulation of the IFN pathway in mouse and human cells. **FIG. 6A** depicts an exemplary result showing BMDMs (1×10^6) from C57B/6 mice were treated with increasing concentrations (5, 10 and 20 μM) of cGAMP linkage isomers, c[G(2',5')pA(2',5')p], c[G(2',5')pA(3',5')p] and c[G(3',5')pA(3',5')p], and cells were collected at 4 h post-treatment. cGAMP linkage isomers were provided by addition into media. Mock treatment control was included. qPCR analyses of Ifnb1, Il6 and Ccl5 mRNAs were performed. **FIG. 6B** depicts an exemplary result showing BMDMs from $IRF3^{-/-}$ and age-matched wild-type control mice were generated. Cells (1×10^6) were treated with cGAMP linkage isomers, c[G(2',5')pA(2',5')p], c[G(2',5')pA(3',5')p] and c[G(3',5')pA(3',5')p] at a final concentration of 15 μM. cGAMP linkage isomers were provided by addition into media. qPCR analysis of Ifnb1, Il6 and Ccl5 mRNAs were performed. **FIG. 6C** depicts an exemplary result illustrating murine BMDMs were incubated in media supplemented with indicated concentrations of cGAMP isomers for 18 h (left panel), or for 30 min with and without Digitonin-mediated permeabilization (right panel). 18 h later, IFN-α concentrations in the supernatant were determined by ELISA. **FIG. 6D** depicts an exemplary result showing THP1 cells were incubated in media supplemented with indicated concentrations of cGAMP linkage isomers for 18 h (left panel), or for 30 min with and without Digitonin-mediated permeabilization (right panel). CXCL10 concentrations were determined by ELISA after 18 h. **FIG. 6E** depicts an exemplary time-course of STING-dependent IFN pathway activation by cGAMP linkage isomers. THP1 cells were incubated in media supplemented with cGAMP linkage isomers from 0 to 12 h without permeabilization. IFNB1 and CXCL10 transcriptional activation was measured by RT-PCR, normalized against TUBA1B and vehicle control. For bar graphs: Data points were determined in triplicate and are depicted as means ± SEM.

[0036] **Figure 7** depicts an exemplary mouse and human STING mutational analysis. **FIG. 7A** depicts an exemplary experiment where HEK293T cells were transfected with reporter

constructs and human or murine STING expression plasmids as indicated. After 12 h, cells were digitonin permeabilized to deliver cGAMP linkage isomers (5 μM concentration, 30 min permeabilization) and incubated for an additional 12 h, followed by luciferase-reporter assay. **FIG. 7B** depicts an exemplary experiment where, to gauge STING mutant stimulation by murine cGAS compared to the inactive cGAS mutant E211A, plasmids containing the indicated human or murine STING variants were cotransfected with either cGAS form and luciferase reporter constructs. Luciferase induction was determined after 30 h. In this setting, the transfected plasmids provide the dsDNA stimulus for cGAS activation. Activation is expressed as fold induction in relation to control plasmid pMAX-GFP. **FIG. 7C** depicts exemplary results where HEK293T cells were transfected as in panel A and stimulated with cyclic di-GMP (5 and 10 μM) following digitonin permeabilization. Luciferase activity was determined 12 h after stimulation. As negative and positive controls, HEK293T cells transfected with $hSTING^{H232}$ were mock-treated (white bar) or stimulated with 5 μM c[G(2',5')pA(3',5')p] following digitonin permeabilization (green bar), respectively. **FIG. 7D** depicts an exemplary experiment where HEK293T cells were transfected as in panel C and after 12 h stimulated with medium containing DMXAA (136 and 266 μM). Luciferase activity was measured after additional 12 h. **FIG. 7E** depicts exemplary ITC binding curves for complex formation between DMAXX and $mSting^{R231}$. **FIG. 7F** depicts exemplary ITC binding curves for complex formation between DMAXX and $hSTING^{R232/A162}$ and$hSTING^{R232/V162}$. **FIG. 7G** depicts exemplary ITC binding curves for complex formation between DMAXX and $hSTING^{H232/A162}$ and$hSTING^{H232/V162}$. **FIG. 7H** depicts

[0037] **Figure 8** depicts exemplary surface views of the crystral structure of c[di-GMP] bound to $hSTING^{H232}$ and exemplary details of intermolecular contacts in the complex. **FIG. 8A** depicts an exemplary 2.15 Å crystal structure of c[di-GMP] bound to $hSTING^{H232}$ (aa 139-379) (PDB: 4EF4). The representations and color codes are the same as used in Figure 1A. Note that the two loops that protrude over the binding pocket are disordered for about half their lengths as one proceeds towards the tips of these loops. **FIG. 8B** depicts an exemplary expanded view of the c[di-GMP] binding pocket in the complex. **FIG. 8C** depicts an exemplary surface representation of an exemplary structure of a complex of c[di-GMP] bound to human $STING^{H232}$ (aa 139-379) (PDB: 4EF4) with the same color-coding as in Figure 1A. **FIG. 8D** depicts an

exemplary view in panel C rotated through 90°. **FIG. 8E** and **FIG. 8F** depicts exemplary intermolecular contacts in the complex of c[di-GMP] bound to hSTING^{H232}. The bound cyclic c[di-GMP] is shown in biscuit color, with individual STING subunits in the symmetrical dimer shown in magenta and yellow. The intermolecular contacts to the base edges of the ligand by the magenta and yellow subunits of STING are shown in panel E, while the intermolecular contacts to the backbone phosphates of the ligand by STING are shown in panel F.

[0038] **Figure 9** depicts exemplary details of c[G(2',5')pA(2',5')p]-hSTING^{H232} and c[G(3',5')pA(3',5')p]-mSting^{R231} complexes. **FIG. 9A** depicts an exemplary superposition of the c[G(2',5')pA(2',5')p] (both subunits in red) and c[G(2',5')pA(3',5')p] (both subunits in green) bound structures of hSTING^{H232} (aa 155-341). **FIG. 9B** depicts exemplary details of hydrogen-bonding interactions in the structure of the c[G(2',5')pA(2',5')p]-hSTING^{H232} complex. Note the water-mediated hydrogen bonds between the 3'-OH groups and side chains of S162 and T267. **FIG. 9C** depicts an exemplary superposition of the c[G(3',5')pA(3',5')p] (both subunits in cyan) and c[G(2',5')pA(3',5')p] (both subunits in magenta) bound structures of mSting^{R231} (aa 154-340). **FIG. 9D** depicts exemplary details of hydrogen-bonding interactions in the structure of the c[G(3',5')pA(3',5')p]-mSting^{R231} complex. Note the direct hydrogen bonds between the 2'-OH groups and the side chains of T262. **FIG. 9E** depicts an exemplary superposition of the c[G(2',5')pA(2',5')p] in its complex with hSTING^{H232} in red and c[G(3',5')pA(3',5')p] in its complex with mSTING^{R231} in cyan. The c[G(2',5')pA(2',5')p] is positioned deeper in the binding pocket than is its c[G(3',5')pA(3',5')p] counterpart.

[0039] **Figure 10** depicts exemplary an exemplary crystal structure of CMA ligand bound to mSting^{R231}. **FIG. 10A** depicts an exemplary chemical formula of 10-carboxymethyl-9-acridine (CMA). **FIG. 10B** depicts an exemplary superposition of the 2.90 Å DMXAA-bound structure of mSting^{R231} (aa 154-340) with both subunits in biscuit and 2.75 Å CMA-bound structure of mSting^{R231} (aa 149-348) with both subunits in yellow (PDB: 4JC5).

[0040] **Figure 11** depicts an exemplary experiment of cGAMP stimulation of BMDMs from wild-type and mutant STING mice. BMDMs from wild-type mice (Sting$^{+/+}$) and the N-ethyl-N-nitrosourea (ENU)-induced *Goldenticket* (*Gt*) mutant mice (Sting$^{Gt/Gt}$) were generated. Cells (1 x 10^6) were treated with cGAMP linkage isomers, c[G(2',5')pA(2',5')p],

c[G(2',5')pA(3',5')p] and c[G(3',5')pA(3',5')p] at a final concentration of 15 μM. As before, cGAMP linkage isomers were provided by addition into media. Cells were collected at 2, 4, and 8 h post-treatment. Mock treatment controls were included (0 h). Western blot analysis was performed with anti-phosphoserine-396 of IRF3 or anti-IRF3, anti-phosphoserine-172 of TBK1 and anti-TBK1. Glyceraldehyde 3-phosphate dehydrogenase (Gapdh) was used as a loading control.

[0041] **Figure 12** depicts exemplary results showing that STING point mutants and natural STING variants display distinct dose-responses to cGAMP linkage isomers. The dotted line indicates the 5 μM cGAMP dose, whose corresponding values are that shown in Figure 7. For dose dependence: Data points were determined in triplicate and are depicted as means ± SEM. **FIG. 12A, FIG. 12B, FIG. 12C, FIG. 12D, FIG. 12E, FIG. 12F and FIG. 12G** depicts exemplary results showing HEK293T cells were transfected with human (panels A-F) or murine (panel G) STING variants for 12 h and cGAMP isomers delivered by Digitonin permeabilization (30 min) were titrated as indicated. Luciferase values were determined 12 h after stimulation.

[0042] **Figure 13** depicts exemplary results showing that the S162A point mutation acquires DMXAA responsiveness in both $hSTING^{H232}$ and $hSTING^{R232}$ variants. HEK293T cells were transfected with human STING variants and murine STING as indicated, and 12 h later incubated with DMXAA without permeabilization or stimulated with c[di-GMP] and cGAMP isomers following digitonin permeabilization (30 min). Luciferase values were determined 12 h after stimulation. Panels A and B show human $STING^{H232}$ and $STING^{R232}$, panels C and D show the respective S162A mutants. In panel E responsiveness of murine Sting to DMXAA, c[di-GMP] and cGAMP isomers is shown for comparison. For dose dependence: Data points were determined in triplicate and are depicted as means ± SEM.

[0043] **Figure 14** depicts exemplary results of hSTING position 162 variants and their sensitivity to cyclic dinucleaotides and DMXAA. 293T cells were transfected with reporter plasmids and hSTING variants as indicated. 12 h after transfection, cells were stimulated by incubation with 75 μg/ml DMXAA (panel A) or Digitonin-permeabilized for 30 min in the presence of cyclic dinucleotides (5μM) as indicated (panel B). After another 12h, cells were lysed and luciferase assay was performed. For bar graphs: Data points were determined in

triplicate and are depicted as means ± SEM. **FIG. 14A** depicts an exemplary result showing conversion of S162 to Ala in H232 or R232 hSTING background renders the protein sensitive to DMXAA stimulation. However, substitution by V162 or I162 does not yield similar results with DMXAA. **FIG. 14B** depicts an exemplary result showing conversion of S162 to Ala in H232 or R232 hSTING background does not significantly affect the respective protein sensitivities to cGAMP linkage isomers or c-[di-GMP]. Substitution by V162 or I162 reduces/eliminates stimulation by any cyclic dinucleotide.

[0044] **Figure 15** depicts exemplary results of how the replacement of non-conserved residues of hSTING with its murine counterparts enables recognition of DMXAA, as well as a crystal structure of DMXAA bound to $hSTING^{group2}$ and details of intermolecular interactions in the complex. **FIG. 15A** depicts the chemical formula of 5,6-dimethyl-xanthenone-4-acetic acid (DMXAA). **FIGS. 15C-D** depict isothermal titration calorimetry (ITC) binding curves for complex formation between DMXAA bound to $hSTING^{group1234}$ (aa 140-379) (panel B) and $hSTING^{group2}$ (panel C). **FIG. 15D** depicts 293T cells were transfected with IFN-β reporter constructs and STING variants as indicated. 12 hours after transfection, cells were stimulated with 0.18 mM DMXAA (50 μg/ml). Luciferase activity was determined after another 12 hours. Dotted lines separate (from left to right) wt controls, single group mutants, $hSTING^{group1234}$ and triple group mutants. Shown are raw values of Gaussia luciferase activity normalized to constitutive Firefly luciferase values. Values depicted are the means of triplicates +SEM and representative of 3 independent experiments. **FIG. 15E** depicts the 1.88 Å crystal structure of DMXAA bound to $hSTING^{group2}$ (aa 155-341). The symmetrical $hSTING^{group2}$ dimer is shown in a ribbon representation. The DMXAA in a space-filling representation is bound in the central cavity at the interface between the two monomers. **FIG. 15F** depicts intermolecular contacts in the complex. The bound DMXAA is shown with individual STING subunits in the symmetrical dimer. **FIG. 15G** depicts two expanded views of the hydrophobic interactions of the G230I substitution in the complex (box region in panel E). Other residues lining the hydrophobic pocket are shown in a lighter shade.

[0045] **Figure 16** depicts that G230 in hSTING and I229 in mSTING are relevant for DMXAA species selectivity. **FIG. 16A** depicts results where 293T cells were transfected with

IFN-β reporter constructs and STING variants as indicated. 12 hours after transfection, cells were stimulated with ascending concentrations of DMXAA. Luciferase activity was determined after another 12 hours. Shown are the means of triplicates +SEM, representative of 3 independent experiments. **FIG. 16B** depicts results where 293T cells were transfected with mSTING variants and reporter constructs. Stimulation and luciferase assay was performed as described in panel A. Dose-responses are representative of 2 independent experiments. **FIG. 16C** depicts the 2.51 Å crystal structure of DMXAA bound to hSTINGG230I (aa 155-341). The representations are the same as used in Figure 15E. **FIG. 16D** depicts detailed hydrophobic interactions in the complex of DMXAA bound to hSTINGG230I, with the same representations as in Figure 15G.

[0046] **Figure 17** depicts exemplary results showing S162A and Q266I substitutions render hSTING sensitive to DMXAA. **FIG. 17A** depicts results where A293T cells were transfected with reporter constructs and indicated hSTING variants. 12 hours after transfection, cells were stimulated with 0.18 mM DMXAA for another 12 hours, followed by luciferase assay. Shown are means of triplicates +SEM, representative of 3 independent experiments. **FIG. 17B** depicts DMXAA dose-response curves of 293T cells transfected with indicated STING variants and illustrating one representative of 3 independent experiments. **FIG. 17C** depicts an ITC binding curve for complex formation between DMXAA bound to hSTINGS162A/Q266I (aa 140-379). **FIG. 17D** depicts natural variants of hSTING (Yi et al., 2013). Five hSTING variants (shown in the left column) were studied in this work. The amino acid variations are shown in the right column. **FIG. 17E** depicts results where 293T cells were transfected and stimulated as in (A). Shown are S162A and Q266I mutants of major human STING alleles. WT denotes the respective allele in this context. Shown are the means of triplicates +SEM, representative of 3 independent experiments. **FIG. 17F** depicts the 2.42 Å crystal structure of DMXAA bound to hSTINGS162A/Q266I (aa 155-341). The representations are the same as used in Figure 15E. **FIG. 17G** depicts two alternate views of the hydrophobic interactions of DMXAA with hSTINGS162A/Q266I. The two bound DMXAA molecules are shown in space-filling representation, with surrounded hydrophobic side chains shown in stick and dot representations.

[0047] **Figure 18** depicts findings that triple substitution of G230I/S162A/Q266I yields an hSTING Variant with higher affinity to DMXAA compared to mSTING, and robust stimulation of cytokines/chemokines in mouse cells. **FIG. 18A** depicts an ITC binding curve for complex formation between DMXAA bound to $hSTING^{S162A/G230I/Q266I}$ (aa 140-379). **FIG. 18B** depicts results where 293T cells were transfected with reporter constructs and indicated STING variants. After 12 hours, cells were stimulated with ascending concentrations of DMXAA for another 12 hours, followed by luciferase assay. Individual data points are means of triplicates ±SEM. Representative of 3 independent experiments. **FIG. 18C** depicts the 2.37 Å crystal structure of DMXAA bound to $hSTING^{S162A/G230I/Q266I}$ (aa 155-341). The representations are the same as used in Figure 15E. **FIG. 18D** depicts hydrophobic interactions of G230I substitution in the complex of DMXAA bound to $hSTING^{S162A/G230I/Q266I}$. The representations are the same as used in Figure 15G. **FIG. 18E** depicts hydrophobic interactions of DMXAA in the ligand-binding pocket, with the same representations as Figure 17G. **FIG. 18F** depicts results where BMDCs ($1x10^6$) from $STING^{Gt/Gt}$ mouse were transduced with retroviruses expressing wt and various hSTING mutants. Two days afterviral infection, BMDCs were treated with 50μg/ml of DMXAA for 3 hours and cells were collected for real-time PCR to measure IFN-β, CXCL10, CCL5 and IL-6 mRNA levels. Data shown are means ± SEM (n=3), representative of two independent experiments. **FIG. 18G** depicts results where BMDCs were transfected with retroviruses expressing wt hSTING and various hSTING mutants. Cells were collected 2 days after retroviral infection, and the levels of hSTING were determined by Western blot analysis.

[0048] **Figure 19** depicts sequence alignment of STING from mouse and human and the design of group substituents. The transmembrane domain (1-139 of hSTING; 1-138 of mSTING) and C-terminal domian (140-379 of hSTING; 139-378 of mSTING) are shown in gray and black, respectively. The group substituents are indicated in boxes. Arrows indicate the mutated residues within the ligand-binding pocket.

[0049] **Figure 20** depicts ITC binding assays for DMXAA with hSTING group1, group3, and group4 mutants and structural comparison of DMXAA Bound to hSTINGgroup2 and mSTING. **FIG. 20A** depicts ITC binding curves for complex formation between DMXAA bound to hSTINGgroup1 (aa 140-379) (left), hSTINGgroup3 (middle), and hSTINGgroup4

(right). **FIG. 20B** depicts superposed structures of the complex of DMXAA bound with mSTING (PDB: 4LOL) and hSTINGgroup2 (aa 155-341). **FIG. 20C** depicts hydrophobic interactions of I229 with surrounding residues in the mSTING-DMXAA complex, with the same representations used in Figure 15G.

[0050] **Figure 21** depicts a structural comparison of DMXAA Bound to $hSTING^{G230I}$ and $hSTING^{group2}$, as well as ITC-based DMXAA-binding assays for hSTING S162A and Q266I Mutants. **FIG. 21A** depicts exemplary intermolecular contacts in the complex of DMXAA bound to $hSTING^{G230I}$ (aa 155-341). The bound DMXAA is shown with individual STING subunits in the symmetrical dimer. **FIG. 21B** depicts superposed structures of the complex of DMXAA bound with $hSTING^{G230I}$ (aa 155-341) and $hSTING^{group2}$ (aa 155-341). **FIGS. 21C-D** depict ITC binding curves for complex formation between DMXAA bound to $hSTING^{S162A}$ (aa 140-379) (panel C) and $hSTING^{Q266I}$ (panel D).

[0051] **Figure 22** depicts dose-responses of hSTING Variants and their respective S162A, Q266I Mutants to DMXAA and the structural comparison of DMXAA bound to $hSTING^{G230I}$ and $hSTING^{S162A/Q266I}$, as well as DMXAA stimulation of cytokines/chemokines in mouse cells. 293T cells were transfected with reporter constructs and indicated STING variants. After 12 hours, cells were stimulated with ascending concentration of DMXAA (A and B) directly added to medium. Luciferase assay was performed after another 12 hours. Dose-responses shown are representative of 2 independent experiments. **FIG. 22A** depicts DMXAA dose-response of hSTING variants with S162A, Q266I double substituent. For improved clarity, only $hSTING^{H232}$ is shown as a representative for the corresponding wt variants. Circle refers to magnified view in (B). **FIG. 22B** depicts DMXAA dose-responses of $hSTING^{HAQ}$ and $hSTING^{HAQ}$ S162A, Q266I on a magnified scale (circle denotes corresponding $hSTING^{HAQ}$ S162A, Q266I curve in (A)). **FIG. 22C** depicts superposed structures of the complex of DMXAA bound with $hSTING^{G230I}$ (aa 155-341) and $hSTING^{S162A/Q266I}$ (aa 155-341). **FIG. 22D** depicts exemplary intermolecular contacts in the complex of DMXAA bound to $hSTING^{S162A/Q266I}$ (aa 155-341). The bound DMXAA is shown with individual STING subunits in the symmetrical dimer. **FIG. 22E** depicts results where BMDCs were infected with retroviruses (same as in Figure 18F). Cells were incubated with 50 μg/ml of DMXAA and

supernatants were collected 18 hours after treatment. CXCL10 protein levels were determined by ELISA. Data shown are means ± SEM (n=3), representative of two independent experiments.

[0052] **Figure 23** depicts an exemplary block diagram of a computing device and a mobile computing device.

[0053] **Figure 24** depicts an exemplary block diagram of a network environment for establishing a multi-channel context aware communication environment.

Definitions

[0054] Compounds of this invention include those described generally above, and are further illustrated by the classes, subclasses, and species disclosed herein. As used herein, the following definitions shall apply unless otherwise indicated. For purposes of this invention, the chemical elements are identified in accordance with the Periodic Table of the Elements, CAS version, Handbook of Chemistry and Physics, 75th Ed. Additionally, general principles of organic chemistry are described in "Organic Chemistry", Thomas Sorrell, University Science Books, Sausalito: 1999, and "March's Advanced Organic Chemistry", 5th Ed., Ed.: Smith, M.B. and March, J., John Wiley & Sons, New York: 2001, the entire contents of which are hereby incorporated by reference.

[0055] The abbreviations used herein have their conventional meaning within the chemical and biological arts. The chemical structures and formulae set forth herein are constructed according to the standard rules of chemical valency known in the chemical arts.

[0056] Unless otherwise stated, structures depicted herein are also meant to include all isomeric (e.g., enantiomeric, diastereomeric, and geometric (or conformational)) forms of the structure; for example, the R and S configurations for each asymmetric center, Z and E double bond isomers, and Z and E conformational isomers. Therefore, single stereochemical isomers as well as enantiomeric, diastereomeric, and geometric (or conformational) mixtures of the present compounds are within the scope of the invention. Unless otherwise stated, all tautomeric forms of the compounds of the invention are within the scope of the invention. Additionally, unless otherwise stated, structures depicted herein are also meant to include compounds that differ only

in the presence of one or more isotopically enriched atoms. For example, compounds having the present structures including the replacement of hydrogen by deuterium or tritium, or the replacement of a carbon by a ^{13}C- or ^{14}C-enriched carbon are within the scope of this invention. Such compounds are useful, for example, as analytical tools, as probes in biological assays, or as therapeutic agents in accordance with the present invention.

[0057] *Administration:* As used herein, the term "administration" refers to the administration of a composition to a subject. Administration may be by any appropriate route. For example, in some embodiments, administration may be bronchial (including by bronchial instillation), buccal, enteral, interdermal, intra-arterial, intradermal, intragastric, intramedullary, intramuscular, intranasal, intraperitoneal, intrathecal, intravenous, intraventricular, mucosal, nasal, oral, rectal, subcutaneous, sublingual, topical, tracheal (including by intratracheal instillation), transdermal, vaginal and vitreal.

[0058] *Aliphatic:* As used herein, the term "aliphatic" or "aliphatic group" means a straight-chain (i.e., unbranched) or branched, substituted or unsubstituted hydrocarbon chain that is completely saturated or that contains one or more units of unsaturation, or a monocyclic hydrocarbon or bicyclic hydrocarbon that is completely saturated or that contains one or more units of unsaturation, but which is not aromatic (also referred to herein as "carbocycle," "cycloaliphatic" or "cycloalkyl"), that has a single point of attachment to the rest of the molecule. Unless otherwise specified, aliphatic groups contain 1-6 aliphatic carbon atoms. In some embodiments, aliphatic groups contain 1-5 aliphatic carbon atoms. In some embodiments, aliphatic groups contain 1-4 aliphatic carbon atoms. In some embodiments, aliphatic groups contain 1-3 aliphatic carbon atoms, and in yet other embodiments, aliphatic groups contain 1-2 aliphatic carbon atoms. In some embodiments, "cycloaliphatic" (or "carbocycle" or "cycloalkyl") refers to a monocyclic C_3-C_6 hydrocarbon that is completely saturated or that contains one or more units of unsaturation, but which is not aromatic, that has a single point of attachment to the rest of the molecule. Suitable aliphatic groups include, but are not limited to, linear or branched, substituted or unsubstituted alkyl, alkenyl, alkynyl groups and hybrids thereof such as (cycloalkyl)alkyl, (cycloalkenyl)alkyl or (cycloalkyl)alkenyl.

[0059] *Alkyl:* As used herein, the term "alkyl" refers to saturated, straight– or branched–chain hydrocarbon radicals derived from an aliphatic moiety containing between one and six carbon atoms by removal of a single hydrogen atom. Unless otherwise specified, alkyl groups contain 1–12 carbon atoms. In certain embodiments, alkyl groups contain 1–8 carbon atoms. In certain embodiments, alkyl groups contain 1–6 carbon atoms. In some embodiments, alkyl groups contain 1–5 carbon atoms, in some embodiments, alkyl groups contain 1–4 carbon atoms, in some embodiments alkyl groups contain 1–3 carbon atoms, and in some embodiments alkyl groups contain 1–2 carbon atoms. Examples of alkyl radicals include, but are not limited to, methyl, ethyl, n–propyl, isopropyl, n–butyl, iso–butyl, sec–butyl, sec–pentyl, iso–pentyl, tert–butyl, n–pentyl, neopentyl, n–hexyl, sec–hexyl, n–heptyl, n–octyl, n–decyl, n–undecyl, dodecyl, and the like.

[0060] *Amino acid:* As used herein, the term "amino acid," in its broadest sense, refers to any compound and/or substance that can be incorporated into a polypeptide chain, e.g., through formation of one or more peptide bonds. In some embodiments, an amino acid has the general structure H2N–C(H)(R)–COOH. In some embodiments, an amino acid is a naturally-occurring amino acid. In some embodiments, an amino acid is a synthetic amino acid; in some embodiments, an amino acid is a D-amino acid; in some embodiments, an amino acid is an L-amino acid. "Standard amino acid" refers to any of the twenty standard L-amino acids commonly found in naturally occurring peptides. "Nonstandard amino acid" refers to any amino acid, other than the standard amino acids, regardless of whether it is prepared synthetically or obtained from a natural source. In some embodiments, an amino acid, including a carboxy- and/or amino-terminal amino acid in a polypeptide, can contain a structural modification as compared with the general structure above. For example, in some embodiments, an amino acid may be modified by methylation, amidation, acetylation, and/or substitution as compared with the general structure. In some embodiments, such modification may, for example, alter the circulating half life of a polypeptide containing the modified amino acid as compared with one containing an otherwise identical unmodified amino acid. In some embodiments, such modification does not significantly alter a relevant activity of a polypeptide containing the modified amino acid, as compared with one containing an otherwise identical unmodified amino acid. As will be clear from context, in some embodiments, the term "amino acid" is used to refer

to a free amino acid; in some embodiments it is used to refer to an amino acid residue of a polypeptide.

[0061] *Analog:* As used herein, the term "analog" refers to a substance that shares one or more particular structural features, elements, components, or moieties with a reference substance. Typically, an "analog" shows significant structural similarity with the reference substance, for example sharing a core or consensus structure, but also differs in certain discrete ways. In some embodiments, an analog a substance that can be generated from the reference substance by chemical manipulation of the reference substance. In some embodiemnts, an analog is a substance that can be generated through performance of a synthetic process substantially similar to (e.g., sharing a plurality of steps with) one that generates the reference substance. In some embodiments, an analog is or can be generated through performance of a synthetic process different from that used to generate the reference substance.

[0062] *Animal:* As used herein, the term "animal" refers to any member of the animal kingdom. In some embodiments, "animal" refers to humans, at any stage of development. In some embodiments, "animal" refers to non-human animals, at any stage of development. In some embodiments, the non-human animal is a mammal (e.g., a rodent, a mouse, a rat, a rabbit, a monkey, a dog, a cat, a sheep, cattle, a primate, and/or a pig). In some embodiments, animals include, but are not limited to, mammals, birds, reptiles, amphibians, fish, and/or worms. In some embodiments, an animal may be a transgenic animal, genetically-engineered animal, and/or a clone.

[0063] *Approximately:* As used herein, the term "approximately" and "about" is intended to encompass normal statistical variation as would be understood by those of ordinary skill in the art as appropriate to the relevant context. In certain embodiments, the term "approximately" or "about" refers to a range of values that fall within 25%, 20%, 19%, 18%, 17%, 16%, 15%, 14%, 13%, 12%, 11%, 10%, 9%, 8%, 7%, 6%, 5%, 4%, 3%, 2%, 1%, or less in either direction (greater than or less than) of the stated reference value unless otherwise stated or otherwise evident from the context (except where such number would exceed 100% of a possible value).

[0064] *Associated with:* Two events or entities are "associated" with one another, as that term is used herein, if the presence, level and/or form of one is correlated with that of the other. For example, a particular entity (e.g., polypeptide) is considered to be associated with a particular disease, disorder, or condition, if its presence, level and/or form correlates with incidence of and/or susceptibility of the disease, disorder, or condition (e.g., across a relevant population). In some embodiments, two or more entities are physically "associated" with one another if they interact, directly or indirectly, so that they are and remain in physical proximity with one another. In some embodiments, two or more entities that are physically associated with one another are covalently linked to one another; in some embodiments, two or more entities that are physically associated with one another are not covalently linked to one another but are non-covalently associated, for example by means of hydrogen bonds, van der Waals interaction, hydrophobic interactions, magnetism, and combinations thereof.

[0065] *Characteristic sequence element:* As used herein, the phrase "characteristic sequence element" refers to a sequence element found in a polymer (e.g., in a polypeptide or nucleic acid) that represents a characteristic portion of that polymer. In some embodiments, presence of a characteristic sequence element correlates with presence or level of a particular activity or property of the polymer. In some embodiments, presence (or absence) of a characteristic sequence element defines a particular polymer as a member (or not a member) of a particular family or group of such polymers. A characteristic sequence element typically comprises at least two monomers (e.g., amino acids or nucleotides). In some embodiments, a characteristic sequence element includes at least 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 20, 25, 30, 35, 40, 45, 50, or more monomers (e.g., contiguously linked monomers). In some embodiments, a characteristic sequence element includes at least first and second stretches of continguous monomers spaced apart by one or more spacer regions whose length may or may not vary across polymers that share the sequence element. In certain embodiments, particular characteristic sequence elements may be referred to as "motifs".

[0066] *Combination therapy:* As used herein, the term "combination therapy" refers to those situations in which a subject is simultaneously exposed to two or more therapeutic agents. In some embodiments, such agents are administered simultaneously; in some embodiments, such

agents are administered sequentially; in some embodiments, such agents are administered in overlapping regimens.

[0067] *Comparable:* The term "comparable", as used herein, refers to two or more agents, entities, situations, sets of conditions, etc that may not be identical to one another but that are sufficiently similar to permit comparison therebetween so that conclusions may reasonably be drawn based on differences or similarities observed. Those of ordinary skill in the art will understand, in context, what degree of identity is required in any given circumstance for two or more such agents, entities, situations, sets of conditions, etc to be considered comparable.

[0068] *Computer-readable medium:* The term "computer-readable medium", as used herein, refers to non-volatile (i.e. secondary storage) computer data storage and/or memory to retain digital data even when not powered. Examples of computer-readable medium include, but are not limited to hard disk, floppy disk, flash memory(i.e. solid state memory), Ferroelectric RAM (F-RAM), Magnetoresistive RAM (MRAM), optical disc, standalone RAM disks, ZIP drives, magenetic tape and holographic memory.

[0069] *Computer system:* The term "computer system" or "computer", as used herein, refers to a computing device that can be used to implement the techniques described in this disclosure. An exemplary computing device 2500 and a mobile computing device are shown in FIG. 25.

[0070] *Corresponding to*: As used herein, the term "corresponding to" is often used to designate the position/identity of a residue in a polymer, such as an amino acid residue in a polypeptide or a nucleotide residue in a nucleic acid. Those of ordinary skill will appreciate that, for purposes of simplicity, residues in such a polymer are often designated using a canonical numbering system based on a reference related polymer, so that a residue in a first polymer "corresponding to" a residue at position 190 in the reference polymer, for example, need not actually be the 190th residue in the first polymer but rather corresponds to the residue found at the 190th position in the reference polymer; those of ordinary skill in the art readily appreciate how to identify "corresponding" amino acids, including through use of one or more commercially-available algorithms specifically designed for polymer sequence comparisons.

[0071] *Crystal structure:* As used herein, the term "crystal structure" of a composition shall mean a computer readable medium in which is stored a representation of three dimensional positional information (i.e. coordinates) for atoms of the composition.

[0072] *Derivative:* As used herein, the term "derivative" refers to a structural analogue of a reference substance. That is, a "derivative" is a substance that shows significant structural similarity with the reference substance, for example sharing a core or consensus structure, but also differs in certain discrete ways. In some embodiments, a derivative is a substance that can be generated from the reference substance by chemical manipulation. In some embodiemnts, a derivative is a substance that can be generated through performance of a synthetic process substantially similar to (e.g., sharing a plurality of steps with) one that generates the reference substance.

[0073] *Docking:* As used herein, the term "docking" refers to orienting, rotating, translating a chemical entity in the binding pocket, domain, molecule or molecular complex or portion thereof based on distance geometry or energy. Docking may be performed by distance geometry methods that find sets of atoms of a chemical entity that match sets of sphere centers of the binding pocket, domain, molecule or molecular complex or portion thereof. See Meng et al. J. Comp. Chem. 4: 505-524 (1992). Sphere centers are generated by providing an extra radius of given length from the atoms (excluding hydrogen atoms) in the binding pocket, domain, molecule or molecular complex or portion thereof. Real-time interaction energy calculations, energy minimizations or rigid-body minimizations (Gschwend et al., J. Mol. Recognition 9:175-186 (1996)) can be performed while orienting the chemical entity to facilitate docking. For example, interactive docking experiments can be designed to follow the path of least resistance. If the user in an interactive docking experiment makes a move to increase the energy, the system will resist that move. However, if that user makes a move to decrease energy, the system will favor that move by increased responsiveness. (Cohen et al., J. Med. Chem. 33:889-894 (1990)). Docking can also be performed by combining a Monte Carlo search technique with rapid energy evaluation using molecular affinity potentials. See Goodsell and Olson, Proteins: Structure, Function and Genetics 8:195-202 (1990). Software programs that carry out docking functions

include but are not limited to MATCHMOL (Cory et al., J. Mol. Graphics 2: 39 (1984); MOLFIT (Redington, Comput. Chem. 16: 217 (1992)) and DOCK (Meng et al., supra).

[0074] *Dosage form:* As used herein, the term "dosage form" refers to a physically discrete unit of a therapeutic agentfor administration to a subject. Each unit contains a predetermined quantity of active agent. In some embodiments, such quantity is a unit dosage amount (or a whole fraction thereof) appropriate for administration in accordance with a dosing regimen that has been determined to correlate with a desired or beneficial outcome when administered to a relevant population (i.e., with a therapeutic dosing regimen).

[0075] *Designed:* As used herein, the term "designed" refers to an agent (i) whose structure is or was selected by the hand of man; (ii) that is produced by a process requiring the hand of man; and/or (iii) that is distinct from natural substances and other known agents.

[0076] *Dosing regimen:* As used herein, the term "dosing regimen" refers to a set of unit doses (typically more than one) that are administered individually to a subject, typically separated by periods of time. In some embodiments, a given therapeutic agent has a recommended dosing regimen, which may involve one or more doses. In some embodiments, a dosing regimen comprises a plurality of doses each of which are separated from one another by a time period of the same length; in some embodiments, a dosing regimen comprises a plurality of doses and at least two different time periods separating individual doses. In some embodiments, a dosing regimen is correlated with a desired or beneficial outcome when administered across a relevant population (i.e., is a therapeutic dosing regimen).

[0077] *Engineered:* In general, the term "engineered" refers to the aspect of having been manipulated by the hand of man. For example, a polynucleotide is considered to be "engineered" when two or more sequences, that are not linked together in that order in nature, are manipulated by the hand of man to be directly linked to one another in the engineered polynucleotide. For example, in some embodiments of the present invention, an engineered polynucleotide comprises a regulatory sequence that is found in nature in operative association with a first coding sequence but not in operative association with a second coding sequence, is linked by the hand of man so that it is operatively associated with the second coding sequence. Comparably, a cell or organism is considered to be "engineered" if it has been manipulated so

that its genetic information is altered (*e.g.*, new genetic material not previously present has been introduced, for example by transformation, mating, somatic hybridization, transfection, transduction, or other mechanism, or previously present genetic material is altered or removed, for example by substitution or deletion mutation, or by mating protocols). As is common practice and is understood by those in the art, progeny of an engineered polynucleotide or cell are typically still referred to as "engineered" even though the actual manipulation was performed on a prior entity.

[0078] *Fragment:* A "fragment" of a material or entity as described herein has a structure that includes a discrete portion of the whole, but lacks one or more moieties found in the whole. In some embodiments, a fragment consists of such a discrete portion. In some embodiments, a fragment consists of or comprises a characteristic structural element or moiety found in the whole. In some embodiments, a polymer fragment comprises or consists of at least 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 25, 30, 35, 40, 45, 50, 55, 60, 65, 70, 75, 80, 85, 90, 95, 100, 110, 120, 130, 140, 150, 160, 170, 180, 190, 200, 210, 220, 230, 240, 250, 275, 300, 325, 350, 375, 400, 425, 450, 475, 500 or more monomeric units (e.g., residues) as found in the whole polymer. In some embodiments, a polymer fragment comprises or consists of at least about 5%, 10%, 15%, 20%, 25%, 30%, 25%, 40%, 45%, 50%, 55%, 60%, 65%, 70%, 75%, 80%, 85%, 90%, 95%, 96%, 97%, 98%, 99% or more of the monomeric units (e.g., residues) found in the whole polymer. The whole material or entity may in some embodiments be referred to as the "parent" of the whole.

[0079] *Homology:* As used herein, the term "homology" refers to the overall relatedness between polymeric molecules, e.g., between nucleic acid molecules (*e.g.*, DNA molecules and/or RNA molecules) and/or between polypeptide molecules. In some embodiments, polymeric molecules are considered to be "homologous" to one another if their sequences are at least 25%, 30%, 35%, 40%, 45%, 50%, 55%, 60%, 65%, 70%, 75%, 80%, 85%, 90%, 95%, or 99% identical. In some embodiments, polymeric molecules are considered to be "homologous" to one another if their sequences are at least 25%, 30%, 35%, 40%, 45%, 50%, 55%, 60%, 65%, 70%, 75%, 80%, 85%, 90%, 95%, or 99% similar (e.g., containing residues with related chemical properties at corresponding positions). For example, as is well known by those of ordinary skill

in the art, certain amino acids are typically classified as similar to one another as "hydrophobic" or "hydrophilic"amino acids, and/or as having "polar" or "non-polar" side chains. Substitution of one amino acid for another of the same type may often be considered a "homologous" substitution. Typical amino acid categorizations are summarized below:

Alanine	Ala	A	nonpolar	neutral	1.8
Arginine	Arg	R	polar	positive	-4.5
Asparagine	Asn	N	polar	neutral	-3.5
Aspartic acid	Asp	D	polar	negative	-3.5
Cysteine	Cys	C	nonpolar	neutral	2.5
Glutamic acid	Glu	E	polar	negative	-3.5
Glutamine	Gln	Q	polar	neutral	-3.5
Glycine	Gly	G	nonpolar	neutral	-0.4
Histidine	His	H	polar	positive	-3.2
Isoleucine	Ile	I	nonpolar	neutral	4.5
Leucine	Leu	L	nonpolar	neutral	3.8
Lysine	Lys	K	polar	positive	-3.9
Methionine	Met	M	nonpolar	neutral	1.9
Phenylalanine	Phe	F	nonpolar	neutral	2.8
Proline	Pro	P	nonpolar	neutral	-1.6
Serine	Ser	S	polar	neutral	-0.8
Threonine	Thr	T	polar	neutral	-0.7
Tryptophan	Trp	W	nonpolar	neutral	-0.9
Tyrosine	Tyr	Y	polar	neutral	-1.3

Valine	Val	V	nonpolar	neutral	4.2

Ambiguous Amino Acids	3-Letter	1-Letter
Asparagine or aspartic acid	Asx	B
Glutamine or glutamic acid	Glx	Z
Leucine or Isoleucine	Xle	J
Unspecified or unknown amino acid	Xaa	X

[0080] As will be understood by those skilled in the art, a variety of algorithms are available that permit comparison of sequences in order to determine their degree of homology, including by permitting gaps of designated length in one sequence relative to another when considering which residues "correspond" to one another in different sequences. Calculation of the percent homology between two nucleic acid sequences, for example, can be performed by aligning the two sequences for optimal comparison purposes (e.g., gaps can be introduced in one or both of a first and a second nucleic acid sequences for optimal alignment and non-corresponding sequences can be disregarded for comparison purposes). In certain embodiments, the length of a sequence aligned for comparison purposes is at least 30%, at least 40%, at least 50%, at least 60%, at least 70%, at least 80%, at least 90%, at least 95%, or substantially 100% of the length of the reference sequence. The nucleotides at corresponding nucleotide positions are then compared. When a position in the first sequence is occupied by the same nucleotide as the corresponding position in the second sequence, then the molecules are identical at that position; when a position in the first sequence is occupied by a similar nucleotide as the corresponding position in the second sequence, then the molecules are similar at that position. The percent homology between the two sequences is a function of the number of identical and similar positions shared by the sequences, taking into account the number of gaps, and the length of each gap, which needs to be introduced for optimal alignment of the two sequences. Representative algorithms and computer programs useful in determining the percent homology between two nucleotide sequences include, for example, the algorithm of Meyers and Miller (CABIOS, 1989, 4: 11-17), which has been incorporated into the ALIGN program (version 2.0)

using a PAM120 weight residue table, a gap length penalty of 12 and a gap penalty of 4. The percent homology between two nucleotide sequences can, alternatively, be determined for example using the GAP program in the GCG software package using an NWSgapdna.CMP matrix.

[0081] *Homology model:* As used herein, the term "homology model" refers to a set of coordinates derived from known three-dimensional structure used as template. Generation of the homology model, termed "homology modeling", involves sequence alignment, residue replacement and residue conformation adjustment through energy minimization.

[0082] *Human*: In some embodiments, a human is an embryo, a fetus, an infant, a child, a teenager, an adult, or a senior citizen.

[0083] *Hydrophilic:* As used herein, the term "hydrophilic" and/or "polar" refers to a tendency to mix with, or dissolve easily in, water.

[0084] *Hydrophobic:* As used herein, the term "hydrophobic" and/or "non-polar", refers to a tendency to repel, *not* combine with, or an inability to dissolve easily in, water.

[0085] *Identity:* As used herein, the term "identity" refers to the overall relatedness between polymeric molecules, *e.g.*, between nucleic acid molecules (e.g., DNA molecules and/or RNA molecules) and/or between polypeptide molecules. In some embodiments, polymeric molecules are considered to be "substantially identical" to one another if their sequences are at least 25%, 30%, 35%, 40%, 45%, 50%, 55%, 60%, 65%, 70%, 75%, 80%, 85%, 90%, 95%, or 99% identical. As will be understood by those skilled in the art, a variety of algorithms are available that permit comparison of sequences in order to determine their degree of homology, including by permitting gaps of designated length in one sequence relative to another when considering which residues "correspond" to one another in different sequences. Calculation of the percent identity between two nucleic acid sequences, for example, can be performed by aligning the two sequences for optimal comparison purposes (e.g., gaps can be introduced in one or both of a first and a second nucleic acid sequences for optimal alignment and non-corresponding sequences can be disregarded for comparison purposes). In certain embodiments, the length of a sequence aligned for comparison purposes is at least 30%, at least 40%, at least

50%, at least 60%, at least 70%, at least 80%, at least 90%, at least 95%, or substantially 100% of the length of the reference sequence. The nucleotides at corresponding nucleotide positions are then compared. When a position in the first sequence is occupied by the same nucleotide as the corresponding position in the second sequence, then the molecules are identical at that position. The percent identity between the two sequences is a function of the number of identical positions shared by the sequences, taking into account the number of gaps, and the length of each gap, which needs to be introduced for optimal alignment of the two sequences. Representative algorithms and computer programs useful in determinng the percent identity between two nucleotide sequences include, for example, the algorithm of Meyers and Miller (CABIOS, 1989, 4: 11-17), which has been incorporated into the ALIGN program (version 2.0) using a PAM120 weight residue table, a gap length penalty of 12 and a gap penalty of 4. The percent identity between two nucleotide sequences can, alternatively, be determined for example using the GAP program in the GCG software package using an NWSgapdna.CMP matrix.

[0086] *Inhibition model:* As used herein, the term "inhibition model" refers to a region or regions of proteins that can associate with another chemical entity or compound. Such regions are of significant utility in fields such as drug discovery. These regions are formed by amino acid residues key for ligand binding or may be residues that are spatially related and define a three-dimensional shape of the binding pocket. In some embodiments, the amino acid residues may be contiguous or non-contiguous in primary sequence. In some embodiments, the region or regions may be embodied as a dataset (e.g. an array of structure coordinates) recorded on computer readable media.

[0087] *Isolated:* As used herein, the term "isolated" refers to a substance and/or entity that has been (1) separated from at least some of the components with which it was associated when initially produced (whether in nature and/or in an experimental setting), and/or (2) designed, produced, prepared, and/or manufactured by the hand of man. Isolated substances and/or entities may be separated from about 10%, about 20%, about 30%, about 40%, about 50%, about 60%, about 70%, about 80%, about 90%, about 91%, about 92%, about 93%, about 94%, about 95%, about 96%, about 97%, about 98%, about 99%, or more than about 99% of the other components with which they were initially associated. In some embodiments, isolated

agents are about 80%, about 85%, about 90%, about 91%, about 92%, about 93%, about 94%, about 95%, about 96%, about 97%, about 98%, about 99%, or more than about 99% pure. As used herein, a substance is "pure" if it is substantially free of other components. In some embodiments, as will be understood by those skilled in the art, a substance may still be considered "isolated" or even "pure", after having been combined with certain other components such as, for example, one or more carriers or excipients (*e.g.*, buffer, solvent, water, etc.); in such embodiments, percent isolation or purity of the substance is calculated without including such carriers or excipients. In some embodiments, isolation involves or requires disruption of covalent bonds (e.g., to isolate a polypeptide domain from a longer polypeptide and/or to isolate a nucleotide sequence element from a longer oligonucleotide or nucleic acid).

[0088] *Modulator:* The term "modulator" is used to refer to an entity whose presence in a system in which an activity of interest is observed correlates with a change in level and/or nature of that activity as compared with that observed under otherwise comparable conditions when the modulator is absent. In some embodiments, a modulator is an activator, in that activity is increased in its presence as compared with that observed under otherwise comparable conditions when the modulator is absent. In some embodiments, a modulator is an inhibitor, in that activity is reduced in its presence as compared with otherwise comparable conditions when the modulator is absent. In some embodiments, a modulator interacts directly with a target entity whose activity is of interest. In some embodiments, a modulator interacts indirectly (i.e., directly with an intermediate agent that interacts with the target entity) with a target entity whose activity is of interest. In some embodiments, a modulator affects level of a target entity of interest; alternatively or additionally, in some embodiments, a modulator affects activity of a target entity of interest without affecting level of the target entity. In some embodiments, a modulator affects both level and activity of a target entity of interest, so that an observed difference in activity is not entirely explained by or commensurate with an observed difference in level.

[0089] *Nucleic acid:* As used herein, the term "nucleic acid," in its broadest sense, refers to any compound and/or substance that is or can be incorporated into an oligonucleotide chain. In some embodiments, a nucleic acid is a compound and/or substance that is or can be incorporated into an oligonucleotide chain via a phosphodiester linkage. As will be clear from

context, in some embodiments, "nucleic acid" refers to individual nucleic acid residues (*e.g.*, nucleotides and/or nucleosides); in some embodiments, "nucleic acid" refers to an oligonucleotide chain comprising individual nucleic acid residues. In some embodiments, a "nucleic acid" is or comprises RNA; in some embodiments, a "nucleic acid" is or comprises DNA. In some embodiments, a nucleic acid is, comprises, or consists of one or more natural nucleic acid residues. In some embodiments, a nucleic acid is, comprises, or consists of one or more nucleic acid analogs. In some embodiments, a nuclic acid analog differs from a nucleic acid in that it does not utilize a phosphodiester backbone. For example, in some embodiments, a nucleic acid is, comprises, or consists of one or more "peptide nucleic acids", which are known in the art and have peptide bonds instead of phosphodiester bonds in the backbone, are considered within the scope of the present invention. Alternatively or additionally, in some embodiments, a nucleic acid has one or more phosphorothioate and/or 5'-N-phosphoramidite linkages rather than phosphodiester bonds. In some embodiments, a nucleic acid is, comprises, or consists of one or more natural nucleosides (e.g., adenosine, thymidine, guanosine, cytidine, uridine, deoxyadenosine, deoxythymidine, deoxyguanosine, and deoxycytidine). In some embodiments, a nucleic acid is, comprises, or consists of one or more nucleoside analogs (e.g., 2-aminoadenosine, 2-thiothymidine, inosine, pyrrolo-pyrimidine, 3-methyl adenosine, 5-methylcytidine, C-5 propynyl-cytidine, C-5 propynyl-uridine, 2-aminoadenosine, C5-bromouridine, C5-fluorouridine, C5-iodouridine, C5-propynyl-uridine, C5-propynyl-cytidine, C5-methylcytidine, 2-aminoadenosine, 7-deazaadenosine, 7-deazaguanosine, 8-oxoadenosine, 8-oxoguanosine, O(6)-methylguanine, 2-thiocytidine, methylated bases, intercalated bases, and combinations thereof). In some embodiments, a nucleic acid comprises one or more modified sugars (e.g., 2'-fluororibose, ribose, 2'-deoxyribose, arabinose, and hexose) as compared with those in natural nucleic acids. In some embodiments, a nucleic acid has a nucleotide sequence that encodes a functional gene product such as an RNA or protein. In some embodiments, a nucleic acid includes one or more introns. In some embodiments, nucleic acids are prepared by one or more of isolation from a natural source, enzymatic synthesis by polymerization based on a complementary template (*in vivo* or *in vitro*), reproduction in a recombinant cell or system, and chemical synthesis. In some embodiments, a nucleic acid is at least 3, 4, 5, 6, 7, 8, 9, 10, 15, 20, 25, 30, 35, 40, 45, 50, 55, 60, 65, 70, 75, 80, 85, 90, 95, 100, 110, 120, 130, 140, 150, 160, 170,

180, 190, 20, 225, 250, 275, 300, 325, 350, 375, 400, 425, 450, 475, 500, 600, 700, 800, 900, 1000, 1500, 2000, 2500, 3000, 3500, 4000, 4500, 5000 or more residues long.

[0090] *Patient:* As used herein, the term "patient" or "subject" refers to a human or any non-human animal (e.g., mouse, rat, rabbit, dog, cat, cattle, swine, sheep, horse or primate) to whom therapy is administered. In many embodiments, a patient is a human being. In some embodiments, a patient is a human presenting to a medical provider for diagnosis or treatment of a disease, disorder or condition. In some embodiments, a patient displays one or more symptoms or characteristics of a disease, disorder or condition. In some embodiments, a patient does not display any symptom or characteristic of a disease, disorder, or condition. In some embodiments, a patient is someone with one or more features characteristic of susceptibility to or risk of a disease, disorder, or condition.

[0091] *Pharmaceutically acceptable:* The term "pharmaceutically acceptable" as used herein, refers to agents that, within the scope of sound medical judgment, are suitable for use in contact with tissues of human beings and/or animals without excessive toxicity, irritation, allergic response, or other problem or complication, commensurate with a reasonable benefit/risk ratio.

[0092] *Polypeptide:* The term "polypeptide", as used herein, generally has its art-recognized meaning of a polymer of at least three amino acids, linked to one another by peptide bonds. In some embodiments, the term is used to refer to specific functional classes of polypeptides, such as, for example, autoantigen polypeptides, nicotinic acetylcholine receptor polypeptides, alloantigen polypeptides, etc. For each such class, the present specification provides several examples of amino acid sequences of known exemplary polypeptides within the class; in some embodiments, such known polypeptides are reference polypeptides for the class. In such embodiments, the term "polypeptide" refers to any member of the class that shows significant sequence homology or identity with a relevant reference polypeptide. In many embodiments, such member also shares significant activity with the reference polypeptide. For example, in some embodiments, a member polypeptide shows an overall degree of sequence homology or identity with a reference polypeptide that is at least about 30-40%, and is often greater than about 50%, 60%, 70%, 80%, 90%, 91%, 92%, 93%, 94%, 95%, 96%, 97%, 98%,

99% or more and/or includes at least one region (i.e., a conserved region, often including a characteristic sequence element) that shows very high sequence identity, often greater than 90% or even 95%, 96%, 97%, 98%, or 99%. Such a conserved region usually encompasses at least 3-4 and often up to 20 or more amino acids; in some embodiments, a conserved region encompasses at least one stretch of at least 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15 or more contiguous amino acids. In some embodiments, a useful polypeptide as described herein may comprise or consist of a fragment of a parent polypeptide. In some embodiments, a useful polypeptide as described herein may comprise or consist of a plurality of fragments, each of which is found in the same parent polypeptide in a different spatial arrangement relative to one another than is found in the polypeptide of interest (e.g., fragments that are directly linked in the parent may be spatially separated in the polypeptide of interest or vice versa, and/or fragments may be present in a different order in the polypeptide of interest than in the parent), so that the polypeptide of interest is a derivative of its parent polypeptide.

[0093] *Protein:* As used herein, the term "protein" refers to a polypeptide (*i.e.*, a string of at least two amino acids linked to one another by peptide bonds). Proteins may include moieties other than amino acids (*e.g.*, may be glycoproteins, proteoglycans, etc.) and/or may be otherwise processed or modified. Those of ordinary skill in the art will appreciate that a "protein" can be a complete polypeptide chain as produced by a cell (with or without a signal sequence), or can be a characteristic portion thereof. Those of ordinary skill will appreciate that a protein can sometimes include more than one polypeptide chain, for example linked by one or more disulfide bonds or associated by other means. Polypeptides may contain L-amino acids, D-amino acids, or both and may contain any of a variety of amino acid modifications or analogs known in the art. Useful modifications include, *e.g.*, terminal acetylation, amidation, methylation, etc. In some embodiments, proteins may comprise natural amino acids, non-natural amino acids, synthetic amino acids, and combinations thereof. The term "peptide" is generally used to refer to a polypeptide having a length of less than about 100 amino acids, less than about 50 amino acids, less than 20 amino acids, or less than 10 amino acids. In some embodiments, proteins are antibodies, antibody fragments, biologically active portions thereof, and/or characteristic portions thereof.

[0094] *Reference*: The term "reference" is often used herein to describe a standard or control agent or value against which an agent or value of interest is compared. In some embodiments, a reference agent is tested and/or a reference value is determined substantially simultaneously with the testing or determination of the agent or value of interest. In some embodiments, a reference agent or value is a historical reference, optionally embodied in a tangible medium. Typically, as would be understood by those skilled in the art, a reference agent or value is determined or characterized under conditions comparable to those utilized to determine or characterize the agent or value of interest.

[0095] *Small molecule:* As used herein, the term "small molecule" means a low molecular weight organic compound that may serve as an enzyme substrate or regulator of biological processes. In general, a "small molecule" is a molecule that is less than about 5 kilodaltons (kD) in size. In some embodiments, provided nanoparticles further include one or more small molecules. In some embodiments, the small molecule is less than about 4 kD, 3 kD, about 2 kD, or about 1 kD. In some embodiments, the small molecule is less than about 800 daltons (D), about 600 D, about 500 D, about 400 D, about 300 D, about 200 D, or about 100 D. In some embodiments, a small molecule is less than about 2000 g/mol, less than about 1500 g/mol, less than about 1000 g/mol, less than about 800 g/mol, or less than about 500 g/mol. In some embodiments, one or more small molecules are encapsulated within the nanoparticle. In some embodiments, small molecules are non-polymeric. In some embodiments, in accordance with the present invention, small molecules are not proteins, polypeptides, oligopeptides, peptides, polynucleotides, oligonucleotides, polysaccharides, glycoproteins, proteoglycans, *etc.* In some embodiments, a small molecule is a therapeutic. In some embodiments, a small molecule is an adjuvant. In some embodiments, a small molecule is a drug.

[0096] *Specific:* The term "specific", when used herein with reference to an agent or entity having an activity, is understood by those skilled in the art to mean that the agent or entity discriminates between potential targets or states. For example, an agent is said to bind "specifically" to its target if it binds preferentially with that target in the presence of competing alternative targets. In some embodiments, the agent or entity does not detectably bind to the competing alternative target under conditions of binding to its target. In some embodiments, the

agent or entity binds with higher on-rate, lower off-rate, increased affinity, decreased dissociation, and/or increased stability to its target as compared with the competing alternative target(s).

[0097] *Storage environment:* As used herein, the term "storage environment" comprises any environment comprising secondary storage, i.e. long-term persistent storage. In some embodiments, a storage environment comprises computer-readable medium. In some embodiments, a storage environment comprises a network environment for establishing a multi-channel context aware communication environment (i.e. cloud computing). For example, FIG. 23 is a block diagram of a network environment for establishing a multi-channel context aware communication environment.

[0098] *Subject:* As used herein, the term "subject" refers to a human or any non-human animal (e.g., mouse, rat, rabbit, dog, cat, cattle, swine, sheep, horse or primate). A human includes pre and post natal forms. In many embodiments, a subject is a human being. A subject can be a patient, which refers to a human presenting to a medical provider for diagnosis or treatment of a disease. A subject can be afflicted with or is susceptible to a disease or disorder but may or may not display symptoms of the disease or disorder.

[0099] *Substantially:* As used herein, the term "substantially" refers to the qualitative condition of exhibiting total or near-total extent or degree of a characteristic or property of interest. One of ordinary skill in the biological arts will understand that biological and chemical phenomena rarely, if ever, go to completion and/or proceed to completeness or achieve or avoid an absolute result. The term "substantially" is therefore used herein to capture the potential lack of completeness inherent in many biological and chemical phenomena.

[0100] *Suffering from:* An individual who is "suffering from" a disease, disorder, or condition has been diagnosed with and/or exhibits or has exhibited one or more symptoms or characteristics of the disease, disorder, or condition.

[0101] *Susceptible to:* An individual who is "susceptible to" a disease, disorder, or condition is at risk for developing the disease, disorder, or condition. In some embodiments, an individual who is susceptible to a disease, disorder, or condition does not display any symptoms

of the disease, disorder, or condition. In some embodiments, an individual who is susceptible to a disease, disorder, or condition has not been diagnosed with the disease, disorder, and/or condition. In some embodiments, an individual who is susceptible to a disease, disorder, or condition is an individual who has been exposed to conditions associated with development of the disease, disorder, or condition. In some embodiments, a risk of developing a disease, disorder, and/or condition is a population-based risk (*e.g.*, family members of individuals suffering from allergy, *etc.*

[0102] *Symptoms are reduced:* According to the present invention, "symptoms are reduced" when one or more symptoms of a particular disease, disorder or condition is reduced in magnitude (*e.g.*, intensity, severity, *etc.*) and/or frequency. For purposes of clarity, a delay in the onset of a particular symptom is considered one form of reducing the frequency of that symptom.

[0103] *Therapeutic agent:* As used herein, the phrase "therapeutic agent" refers to any agent that has a therapeutic effect and/or elicits a desired biological and/or pharmacological effect, when administered to a subject. In some embodiments, an agent is considered to be a therapeutic agent if its administration to a relevant population is statistically correlated with a desired or beneficial therapeutic outcome in the population, whether or not a particular subject to whom the agent is administered experiences the desired or beneficial therapeutic outcome.

[0104] *Therapeutically effective amount:* As used herein, the term "therapeutically effective amount" means an amount that is sufficient, when administered to a population suffering from or susceptible to a disease, disorder, and/or condition in accordance with a therapeutic dosing regimen, to treat the disease, disorder, and/or condition (*e.g.*, allergy). In some embodiments, a therapeutically effective amount is one that reduces the incidence and/or severity of, and/or delays onset of, one or more symptoms of the disease, disorder, and/or condition. Those of ordinary skill in the art will appreciate that the term "therapeutically effective amount" does not in fact require successful treatment be achieved in a particular individual. Rather, a therapeutically effective amount may be that amount that provides a particular desired pharmacological response in a significant number of subjects when administered to patients in need of such treatment. It is specifically understood that particular subjects may, in fact, be "refractory" to a "therapeutically effective amount." To give but one

example, a refractory subject may have a low bioavailability such that clinical efficacy is not obtainable. In some embodiments, reference to a therapeutically effective amount may be a reference to an amount as measured in one or more specific tissues (e.g., a tissue affected by the disease, disorder or condition) or fluids (e.g., blood, saliva, serum, sweart, tears, urine, etc). Those of ordinary skill in the art will appreciate that, in some embodiments, a therapeutically effective agent may be formulated and/or administered in a single dose. In some embodiments, a therapeutically effective agent may be formulated and/or administered in a plurality of doses, for example, as part of a dosing regimen.

[0105] *Therapeutic regimen*: A "therapeutic regimen", as that term is used herein, refers to a dosing regimen whose administration across a relevant population is correlated with a desired or beneficial therapeutic outcome.

[0106] *Treatment:* As used herein, the term "treatment" (also "treat" or "treating") refers to any administration of a substance that partially or completely alleviates, ameliorates, relives, inhibits, delays onset of, reduces severity of, and/or reduces frequency, incidence or severity of one or more symptoms, features, and/or causes of a particular disease, disorder, and/or condition. Such treatment may be of a subject who does not exhibit signs of the relevant disease, disorder and/or condition and/or of a subject who exhibits only early signs of the disease, disorder, and/or condition. Alternatively or additionally, such treatment may be of a subject who exhibits one or more established signs of the relevant disease, disorder and/or condition. In some embodiments, treatment may be of a subject who has been diagnosed as suffering from the relevant disease, disorder, and/or condition. In some embodiments, treatment may be of a subject known to have one or more susceptibility factors that are statistically correlated with increased risk of development of the relevant disease, disorder, and/or condition.

[0107] *Three dimensional representation*: As used herein, the term " three dimensional representation" refers to converting the lists of structure coordinates into structural models or graphical representation in three-dimensional space. In some embodiments, the three dimensional structure may be displayed or used to performing computer modeling or fitting operations. In some embodiments, the structure coordinates themselves, without the displayed model, may be used to perform computer-based modeling and fitting operations.

[0108] *Unsaturated:* As used herein, the term "unsaturated" means that a moiety has one or more units of unsaturation.

[0109] As used herein, the term "pharmaceutically acceptable salt" refers to those salts which are, within the scope of sound medical judgment, suitable for use in contact with the tissues of humans and lower animals without undue toxicity, irritation, allergic response and the like, and are commensurate with a reasonable benefit/risk ratio. Pharmaceutically acceptable salts are well known in the art. For example, S. M. Berge et al., describe pharmaceutically acceptable salts in detail in J. Pharmaceutical Sciences, 1977, 66, 1–19, incorporated herein by reference. Pharmaceutically acceptable salts of the compounds of this invention include those derived from suitable inorganic and organic acids and bases. Examples of pharmaceutically acceptable, nontoxic acid addition salts are salts of an amino group formed with inorganic acids such as hydrochloric acid, hydrobromic acid, phosphoric acid, sulfuric acid and perchloric acid or with organic acids such as acetic acid, oxalic acid, maleic acid, tartaric acid, citric acid, succinic acid or malonic acid or by using other methods used in the art such as ion exchange. Other pharmaceutically acceptable salts include adipate, alginate, ascorbate, aspartate, benzenesulfonate, benzoate, bisulfate, borate, butyrate, camphorate, camphorsulfonate, citrate, cyclopentanepropionate, digluconate, dodecylsulfate, ethanesulfonate, formate, fumarate, glucoheptonate, glycerophosphate, gluconate, hemisulfate, heptanoate, hexanoate, hydroiodide, 2–hydroxy–ethanesulfonate, lactobionate, lactate, laurate, lauryl sulfate, malate, maleate, malonate, methanesulfonate, 2–naphthalenesulfonate, nicotinate, nitrate, oleate, oxalate, palmitate, pamoate, pectinate, persulfate, 3–phenylpropionate, phosphate, pivalate, propionate, stearate, succinate, sulfate, tartrate, thiocyanate, p–toluenesulfonate, undecanoate, valerate salts, and the like.

[0110] Salts derived from appropriate bases include alkali metal, alkaline earth metal, ammonium and $N^+(C_{1-4}alkyl)_4$ salts. Representative alkali or alkaline earth metal salts include sodium, lithium, potassium, calcium, magnesium, and the like. Further pharmaceutically acceptable salts include, when appropriate, nontoxic ammonium, quaternary ammonium, and amine cations formed using counterions such as halide, hydroxide, carboxylate, sulfate, phosphate, nitrate, loweralkyl sulfonate and aryl sulfonate.

[0111] In certain embodiments, neutral forms of the compounds are regenerated by contacting the salt with a base or acid and isolating the parent compound in the conventional manner. In some embodiments, the parent form of the compound differs from the various salt forms in certain physical properties, such as solubility in polar solvents.

[0112] The symbol "〰", except when used as a bond to depict unknown or mixed stereochemistry, denotes the point of attachment of a chemical moiety to the remainder of a molecule or chemical formula.

Detailed Description of Certain Embodiments

STING

[0113] The protein TMEM173/STING (stimulator of interferon genes) (Ishikawa and Barber, 2008; Zhong et al. 2008; Sun et al. 2009; Burdette et al. 2011; Ishikawa et al., 2009; Jin et al., 2008) is a central player in the innate immune response to nucleic acids, particularly cytosolic dsDNA (reviewed in Burdette and Vance, 2013; Cai et al., 2014; Danilchanka and Mekalanos, 2013; O'Neill, 2013; Paludan and Bowie, 2013; Xiao and Fitzgerald, 2013). STING responds to various pathogens, as well as to mitochondrial damage, and its overactivation may contribute or possibly even trigger the onset of autoimmune disorders such as systemic lupus erythematosus (Gall et al. 2012; Gehrke et al., 2013). STING's role in the immune system is consistent with its higher expression in certain organs such as the thymus, spleen and placenta. STING is also expressed in THP1 human monocytic cells.

[0114] An initial screen designed to discover potential regulators of the type I interferon (IFN) antiviral response identified cyclic GMP-AMP (cGAMP) synthase (MB21D1/cGAS) as a gene with broad antiviral effect (Schoggins et al. 2011). Independently, biochemical fractionation identified cGAS as the metazoan cytosolic DNA sensor and synthase of cGAMP, the endogenous second messenger that activates the type I IFN pathway (Sun et al. 2013; Wu et al. 2013). A structure-function study demonstrated that only one specific isomer of cGAMP, namely c[G(2',5')pA(3',5')p] was produced by cGAS (Gao et al. 2013). This isomer of the second messenger contained an unanticipated 2',5'-linkage at the GpA step, a feature

subsequently validated by several independent studies (Diner et al. 2013; Ablasser et al. 2013; Zhang et al. 2013). Structures of dsDNA-bound cGAS with ATP and GTP (Gao et al. 2013; Civril et al. 2013), pppGpA dinucleotide intermediate (Gao et al. 2013), and the product c[G(2',5')pA(3',5')p] (Gao et al. 2013), along with biochemical analysis of reaction intermediates, provided insights into the stepwise conversion of GTP and ATP in the first step to pppGpA (Gao et al. 2013; Ablasser et al. 2013) and subsequent cyclization to c[G(2',5')pA(3',5')p] (Gao et al. 2013; Ablasser et al. 2013).

[0115] The identification of c[G(2',5')pA(3',5')p] as a novel second messenger generated by dsDNA-bound cGAS in the presence of GTP and ATP (Gao et al., 2013) has prompted studies of the role of c[G(2',5')pA(3',5')p] in activating the IFN pathway via the downstream receptor STING (Diner et al. 2013; Ablasser et al. 2013; Zhang et al. 2013). Binding of c[G(2',5')pA(3',5')p] to STING activates a cascade of events whereby STING recruits and activates IκB kinase (IKK) and TANK-binding kinase (TBK1), which following their phosphorylation, respectively activate nuclear transcription factor κB (NF-κB) and interferon regulatory factor 3 (IRF3). These activated proteins translocate to the nucleus to induce transcription of the genes encoding type I IFN and cytokines for promoting intercellular host immune defense (reviewed in Keating et al. 2011; Paludan and Bowie, 2013). STING is a direct sensor of bacterial cyclic dinucleotides (CDNs) such as c[di-GMP] (Burdette et al., 2011), although it was subsequently demonstrated that the host-encoded cytosolic DNA-binding sensor cyclic GMP-AMP synthase (cGAS) (Sun et al., 2013) and its product cyclic GMP-AMP (cGAMP) (Wu et al., 2013) acted as the second messenger binding to STING in response to cells exposed to DNA.

[0116] In the human population, there are several STING variants, which may influence the responsiveness to cGAMP, its linkage isomers and other CDNs (Diner et al., 2013; Yi et al., 2013). Among them, R71/G230/R232/R293 (referred to as $hSTING^{R232}$) appears to be the most common variant (Yi et al., 2013). Thus, unless specified otherwise, the experiments described in the ensuing exemplification were based on this variant.

[0117] Human (h) and mouse (m) STING exhibit 68% amino acid identity and 81% similarity, with distinct sequence alleles reported in humans (Diner et al. 2013). Established

numbering systems of human and mouse STING are offset by one residue, with hSTING^{R232} and mSTING^{R231} occupying corresponding positions. The amino acid sequences of hSTING (accession no. NP_938023.1; SEQ ID NO.: 1) and mSTING (accession no.; SEQ ID NO.: 2) are shown in Table A.

[0118] Table A. Human and Mouse Stimulator of Interferon Genes Protein (STING)

Human STING **Accession number: NP_938023.1**	MPHSSLHPSIPCPRGHGAQKAALVLLSACLVTLWGLGEPPEHTLRYLVLHLASLQL GLLLNGVCSLAEELRHIHSRYRGSYWRTVRACLGCPLRRGALLLLSIYFYYSLPNA VGPPFTWMLALLGLSQALNILLGLKGLAPAEISAVCEKGNFNVAHGLAWSYYIGYL RLILPELQARIRTYNQHYNNLLRGAVSQRLYILLPLDCGVPDNLSMADPNIRFLDK LPQQTGDHAGIKDRVYSNSIYELLENGQRAGTCVLEYATPLQTLFAMSQYSQAGFS REDRLEQAKLFCRTLEDILADAPESQNNCRLIAYQEPADDSSFSLSQEVLRHLRQE EKEEVTVGSLKTSAVPSTSTMSQEPELLISGMEKPLPLRTDFS **(SEQ ID NO:1)**
Mouse STING **Accession number: NP_082537.1**	MPYSNLHPAIPRPRGHRSKYVALIFLVASLMILWVAKDPPNHTLKYLALHLASHEL GLLLKNLCCLAEELCHVQSRYQGSYWKAVRACLGCPIHCMAMILLSSYFYFLQNTA DIYLSWMFGLLVLYKSLSMLLGLQSLTPAEVSAVCEEKKLNVAHGLAWSYYIGYLR LILPGLQARIRMFNQLHNNMLSGAGSRRLYILFPLDCGVPDNLSVVDPNIRFRDML PQQNIDRAGIKNRVYSNSVYEILENGQPAGVCILEYATPLQTLFAMSQDAKAGFSR EDRLEQAKLFCRTLEEILEDVPESRNNCRLIVYQEPTDGNSFSLSQEVLRHIRQEE KEEVTMNAPMTSVAPPPSVLSQEPRLLISGMDQPLPLRTDLI **(SEQ ID NO:2)**

[0119] hSTING is composed of a N-terminal transmembrane domain (aa 1-154), a central globular domain (aa 155-341) and a C-terminal tail (aa 342-379). Distinct sequence variants of either mouse or human STING have been studied with different functional assays and outcomes, complicating interpretation. Diner et al (2013) identified natural variant alleles of STING, namely the R232H variant to the genome reference of human STING (hSTING^{H232}, reference sequence) and the R231A variant of mouse Sting (mSTING^{A231}), which were activated by c[G(2',5')pA(3',5')p] but not by c[di-GMP] or c[G(3',5')pA(3',5')p]. By contrast, Zhang et al (2013) proposed based on structural, calorimetric-based binding and cellular assays that c[G(2',5')pA(3',5')p] is the highest affinity ligand for hSTING^{R232}, even though their in vitro calorimetric binding measurements did not support their results seen with IFN induction cellular assays. Ablasser et al (2013) investigated the contribution of 2',5'- and 3',5'-linkages in cGAMP

and concluded that c[G(2',5')pA(3',5')p] was more potent than c[G(3',5')pA(3',5')] in activating hSTING from human fibroblasts and THP1 cells, and wild-type mSTING^{R231}.

[0120] Structural studies have been reported on hSTING^{H232} in the free and c[di-GMP] bound states. STING forms a symmetrical dimer in both states with c[di-GMP] bound in a pocket within the dimer interface and anchored by a network of intermolecular hydrogen bonds (reviewed in Burdette and Vance, 2013). For all but one of the c[di-GMP]-hSTING^{H232} complexes, the STING dimer adopts the same V-shaped conformation independent of the presence of the ligand and also does not completely surround the bound ligand. In the one exception, c[di-GMP]-bound hSTING$^{A230/R232}$ forms an anti-parallel β-pleated sheet cap over the binding pocket on complex formation and this conformational change further sequesters the bound ligand (Huang et al. 2012). More recently, the same conformational transition has been reported on formation of the complex between mSTING^{R231} and the anti-viral drug CMA (Cavlar et al. 2013) and on formation of the complex between hSTING^{R232} and c[G(2',5')pA(3',5')p] (Zhang et al. 2013).

[0121] The present disclosure provides valuable insights into the structural basis and functional output of ligand-binding by hSTING and mSTING. Given STING's central role in immunoregulation of the anti-viral response and in eliciting a macrophage-dependent tumoricidal program (Kim et al. 2013), such insights permit design, production, and or characterization of useful STING modulators. In some embodiments, such modulators are useful in medicine (e.g., in therapy and/or in prophylaxis) of one or more diseases, disorders, or conditions.

[0122] The present disclosure provides insights relevant to selectivity of hSTING^{R232} for [G(2',5')pA(3',5')p], as well as its ability to recognize, bind to and/or discriminate between its linkage isomers.

[0123] The present disclosure also assesses the extent to which distinct STING alleles (e.g., hSTING^{H232} and mSTING^{A231}) and/or variants differentially respond to particular modulator agents.

[0124] Among other things, the present disclosure provides crystal structures of various STING alleles and/or variants alone or complexed with one or more modulator or candidate

modulator agents. Such crystal structures are useful, for example, to guide design of modulator agents, including modulator agents whose structures include moieties that can and/or do make specified interactions with complementary STING moieties. In some embodiments, such complementary STING moieties are present in some STING alleles or variants but not others. The present disclosure, therefore, among other things, provides technologies for designing, identifying and/or characterizing STING modulators that discriminate between or among STING alleles and/or variants.

STING Function

[0125] It is generally believed that STING coordinates multiple immune responses to infection, including the induction of interferons and STAT6-dependent response and selective autophagy response. STING plays an important role in innate immunity and mediates type I interferon production in response to intracellular DNA and a variety of intracellular pathogens, such as viruses, mycobacteria and intracellular parasites. For example, STING binds directly to cyclic di-GMP, and this recognition leads to the production of cytokines, such as type I interferon. Type I interferon protects infected cells and nearby cells from local infection in an autocrine and paracrine manner.

[0126] For example, binding of c[G(2',5')pA(3',5')p] to STING activates a cascade of events whereby STING recruits and activates IκB kinase (IKK) and TANK-binding kinase (TBK1), which following their phosphorylation, respectively activate nuclear transcription factor κB (NF-κB) and interferon regulatory factor 3 (IRF3). These activated proteins translocate to the nucleus to induce transcription of the genes encoding type I IFN and cytokines for promoting intercellular host immune defense (reviewed in Keating et al. 2011; Paludan and Bowie, 2013).

[0127] STING plays an important role in antiviral immunity and elicits powerful type I interferon immunity against viral infection. After viral entry, viral nucleic acids will be present in the cytosol of infected cells. Several DNA sensors, such as DAI, RNA polymerase III, IFI16, DDX41 and cGAS, can detect foreign nucleic acids. After recognizing viral DNA, DNA sensors initiate the downstream signaling pathways by activating STING-mediated interferon response. Viruses that activate a STING-depenent innate immune response include, but are not limited to,

adenovirus, *herpes simplex virus* (e.g., HSV-1 and HSV-2), negative-stranded RNA virus-*vesicular stomatitis virus* (VSV), and combinations thereof.

[0128] A variety of assays are known to one of skill in the art that detect and/or characterize STING activities. In some embodiments, STING activity is or comprises interacting with a particular binding partner or partners. In some embodiments, STING activity is or comprises discriminating between potential partners. In some embodiments, STING activity is or comprises hSTING activity. In some embodiments, STING activity is or comprises mSTING activity.

[0129] In some embodiments, STING activity is or comprises phosphorylation of a particular substrate or substrates. In some embodiments, STING activity is or comprises phosphorylation of TBK1, IKK, IRF3, STAT6 and/or combinations thereof.

[0130] In some embodiments, STING activity is or comprises upregulation of gene expression of of IFN-β, CCL2, CCL20, and/or combinations thereof.

[0131] In some embodiments, a STING polypeptide shares at least one of these activites with a reference STING polypeptide, such as a wild type STING. In some embodiments, a STING polypeptide is considered to "share" an activity with a reference if it shows an acivity that would be recognized by those skilled in the art as comparable to, or not significiantly different from, that of a relevant reference in an appropriate assay that detects and/or characterizes the activity. While the kinase activity of a STING polypeptide compared to a reference may be significantly lower, it can be recognized by its ability to phosphorylate STING-specific sites in bona-fide STING substrates such as IKK and TBK1.

STING Crystal Structure

[0132] Among other things, the present invention provides a crystalline (i.e., containing at least one crystal) or crystallizable composition comprising a STING polypeptide. In some embodiments, such a provided composition consists of or consists essentially of the STING polypeptide. In some embodiments, a composition is considered to "consist of" a STING polypeptide if it includes only the polypeptide, one or more solvents, and optionally salts and/or metals. In some embodiments, such a provided composition includes one or more other agents

such as one or more other polypeptides (e.g., one or more potential or actual STING binding partner polypeptides) and/or one or more interacting agents (e.g., small molecules).

[0133] In some embodiments, such a provided composition comprises a wild-type STING polypeptide. Exemplary wild-type STING polypeptides include, but are not limited to, hSTING (SEQ ID NO: 1) and mSTING (SEQ ID NO: 2). In some embodiments, such a provided composition comprises a STING polypeptide comprising an N-terminal truncation. In some embodiments, a STING polypeptide comprises an N-terminal truncation of hSTING comprising a truncation of amino acid residues 1-139 ($hSTING^{140-379}$). In some embodiments, a STING polypeptide comprises an N-terminal truncation of mSTING comprising a truncation of amino acid residues 1-138 ($mSTING^{139-378}$).

[0134] In some embodiments, a STING polypeptide comprises a C-terminal truncation.

[0135] In some embodiments, a STING polypeptide comprises both an N-terminal truncation *and* a C-terminal truncation. In some embodiments, a STING polypeptide comprises both an N-terminal truncation *and* a C-terminal truncation of hSTING comprising a trunctation of N-terminal residues 1-154 and C-terminal residues 342-379 ($hSTING^{H232}$ comprising residues 155-341). In some embodiments, a STING polypeptide comprises both an N-terminal truncation *and* a C-terminal truncation of mSTING comprising a trunctation of N-terminal residues 1-153 and C-terminal residues 341-378 ($mSTING^{R231}$ comprising residues 154-340).

[0136] In some embodiments, a STING polypeptide comprises both an N-terminal truncation *and* one or more internal deletions. In some embodiments, a STING polypeptide comprises an N-terminal truncation, a C-terminal truncation, one or more internal deletions, and/or combinations thereof.

[0137] Without wishing to be bound by any particular theory, truncation and/or internal deletion of the STING polypeptide favors crystallization because it can reduce flexibility, can result in more compact shape, and eliminate undesirable events like aggregation, if for example, the deleted region has a hydrophobic binding site for a protein-binding partner.

[0138] In some embodiments, provided compositions comprise a STING polypeptide bound to one or more binding partners. In some embodiments, such a provided composition

comprises a STING polypeptide bound to c[G(2',5')pA(3',5')p] (see, e.g., Table 1: c[G(2',5')pA(3',5')p]-hSTING^{H232} complex (4LOH) coordinates; and Table 3: c[G(2',5')pA(3',5')p]-mSting^{R231} complex (4LOJ) coordinates).

[0139] In some embodiments, such a provided composition comprises a STING polypeptide bound to c[G(2',5')pA(2',5')p] (see, e.g., Table 2: c[G(2',5')pA(2',5')p]-hSTING^{H232} complex (4LOI) coordinates).

[0140] In some embodiments, such a provided composition comprises a STING polypeptide bound to c[G(3',5')pA(3',5')p] (see, e.g., Table 4: c[G(3',5')pA(3',5')p]-mSting^{R231} complex (4LOK) coordinates).

[0141] In some embodiments, such a provided composition comprises a STING polypeptide bound to DMXAA (see, e.g., Table 5: DMXAA-mSting^{R231} complex (4LOL) coordinates).

[0142] In some embodiments, such a provided composition comprises a STING polypeptide bound to DMXAA (see, e.g., Table 6: DMXAA-hSting^{group2} complex (4QXO) coordinates).

[0143] In some embodiments, such a provided composition comprises a STING polypeptide bound to DMXAA (see, e.g., Table 7: DMXAA-hSTING^{G230I} complex (4QXP) coordinates).

[0144] In some embodiments, such a provided composition comprises a STING polypeptide bound to DMXAA (see, e.g., Table 8: DMXAA-hSTING$^{S162A/Q266I}$ complex (4QXQ) coordinates).

[0145] In some embodiments, such a provided composition comprises a STING polypeptide bound to DMXAA (see, e.g., Table 9: DMXAA-hSTING$^{S162A/G230I/Q266I}$ complex (4QXR) coordinates).

[0146] In some embodiments, provided composition comprise an STING polypeptide bound to one or more STING modulators. In some embodiments, provided composition comprises a STING polypeptide bound to one or more exemplary STING modulators including,

but not limited to, analogs of of c[G(2',5')pA(3',5')p], DMXAA, CMA, and/or combinations thereof.

[0147] The present invention also provides structural information and/or analyses of STING polypeptide crystals and/or sets thereof. In some embodiments, such structural information includes, but is not limited to, diffraction patterns, and/or coordinates, as well as any data sets, images, models, and/or graphical representations thereof or generated therefrom. In some embodiments, such graphical representations may include, for example, space-filling models, molecular surface representations, shell or boundary models, ribbon models, stick models; and/or combinations thereof.

[0148] In some embodiments, provided information is or comprises differences observed between or among structures that differ from one another in the presence or absence of one or more binding partners and/or interacting agents. In some embodiments, provided information is or comprises differences observed between or among structures that differ from one another in the presence or absence of one or more binding partners and/or one or more modulators.

[0149] In some embodiments, such structural information and/or analyses may be embodied in a tangible medium (e.g., a computer-readable medium) or a storage environment. Thus, the present invention provides tangible embodiments of STING polypeptide crystal structure information, as well as its use, for example, by or with a computer system, in any of a variety of applications. For example, in some embodiments, such structural information and/or analyses may be accessed by, transported to or from, and/or otherwise utilized by a computer system or program running thereon.

STING Modulators

[0150] As discussed herein, among other things, the present disclosure defines and/or provides certain STING modulators. In some embodiments, the present disclosure provides technologies for identifying, designing, and/or characterizing STING modulators. In some embodiments, STING modulators are specific STING modulators. In some embodiments, STING modulators are specific modulators of one or more STING alleles or variants; in some

such embodiments, STING modulators have differential effects on different STING alleles or variants and/or discriminate between or among such alleles or variants.

[0151] In some embodiments, the present disclosure provides STING modulators that are DMXAA analogs. DMXAA (5,6-dimethylxanthenone-4-acetic acid, Vadimezan) was initially identified as a small molecule exhibiting immune modulatory activities through induction of cytokines, and disrupting tumor vascularization in mouse xenotransplantation models (Baguley and Ching, 2002). The induction of interferon (IFN) β expression by DMXAA also slowed the growth of tumors *in vivo* (Head and Jameson, 2010; Roberts et al., 2008). DMXAA, in combination with paclitaxel and carboplatin showed promising efficacy, and was therefore evaluated in a phase II clinical trial against non-small-cell lung cancer, but subsequently failed in human phase III trials (Lara et al. 2011). Recently, it has been demonstrated that DMXAA-induced IFN production by murine macrophages was impaired by the absence of STING (Prantner et al. 2012), suggesting that DMXAA targets the STING pathway. Despite high sequence identity between mSting and hSTING, DMXAA, which only activates mSting and has no effect on hSTING (Conlon et al. 2013; Kim et al., 2013), which presumably hampered further therapeutic development of DMXAA as a human drug.

[0152] In some embodiments, DMXAA analogs include substitutions at position 1 and/or position 2 (Fig. 5A). In some embodiments, the H at position 1 and/or 2 is replaced by an OH or O-methyl group. In some embodiments, positions 1 and/or 2 could also be replaced by F, Cl, NO_2 groups to facilitate hydrogen bond formation with Ser162 of hSTING. Without wishing to be bound to a particular theory, hydrogen replacement by either an OH or O-methyl group facilitates hydrogen bond formation with Ser162 of hSTING.

[0153] In some embodiments, DMXAA analogs include substitutions at position 7 and/or position 8 (Fig. 5A). In some embodiments, the H at position 7 and/or 8 is replaced by methyl and/or larger alkyl groups. Without wishing to be bound to a particular theory, hydrogen replacement by methyl and/or larger alkyl groups facilitates hydrophobic contacts with Ile165 of hSTING. In some embodiments, the H at position 7 is replaced by polar groups (OH, OCH_3, F, Cl, NO_2). Without wishing to be bound to a particular theory, hydrogen replacement by polar groups facilitates hydrogen bond formation with Gln266 of hSTING.

[0154] The present disclosure describes systematic structure-function studies of mouse and human STING interaction with DMXAA. The present disclosure specifically defines interaction points between STING modulator compounds and STING moieties. In one example, the present disclosure specifically defines interaction points between DMXAA moieties and STING moieties. Moreover, the present disclosure describes modifications of hSTING and/or DMXAA structure (i.e., mutations of hSTING and analogs of DMXAA) that permit interaction between them. Thus, the present disclosure defines DMXAA analogs that can act as hSTING modulators, including as specific hSTING modulators (even relative to mSting).

[0155] The present disclosure also describes cyclic dinucleotide compounds (e.g., cGAMP-analogs and/or isomers) active as STING modulators, and particularly as hSTING modulators (e.g., specific hSTING modulators). Among other things, the present disclosure demonstrates that hSTING was more discriminating towards 2',5'-linkage-containing isomers versus those isomers containing all 3',5'-linkages.

[0156] The present disclosure also describes 10-carboxymethyl-9-acridine (CMA) analogs that are active as STING modulators, and particularly as hSTING modulators (e.g., specific hSTING modulators). In certain embodiments, alternative CMA analogs are provided and tested for STING modulatory activity as described herein.

[0157] In some embodiments, provided STING modulators are compounds whose structure include one or more moieties that interact with a residue corresponding to Ser162 and/or Ile165 of hSTING. In some embodiments, provided STING modulators are compounds whose structure include one or more moieties that interact with a residue corresponding to Gly230, Gln266, Ser162, and/or Ile165 of hSTING. In some embodiments, provided STING modulators are compounds whose structure include one or more moieties that interact with a residue corresponding to Gly230, Gln266, and/or Ser162 of hSTING. In some embodiments, provided STING modulators are compounds whose structures include one or more moieties that interact with a residue corresponding to Leu170, Ile235, Ile165, Thr267, Arg238, Tyr240, and/or Thr263 of hSTING. In some embodiments, provided STING modulators are compounds whose structures include one or more moieties that interact with a residue corresponding to Gly230,

Gln266, Ser162, Ile165, Leu170, Ile235, Ile165, Thr267, Arg238, Tyr240, and/or Thr263 of hSTING.

[0158] In some embodiments, provided STING modulators are characterized by variety well understood and known by those skilled in the art including, but not limited to cGAMP stimulation of cells, ELISA, Isothermal Titration Calorimetry (ITC) Binding Assay, and/or combinations thereof. For example, in some embodiments, provided STING modulators show activity in an ITC binding assay such as is described in the Examples.

[0159] In some embodiments, in accordance with the present invention, STING modulators, and particularly hSTING modulators (e.g., specific hSTING modulators) are useful as agonists or antagonists of innate immunity. In some embodiments, in accordance with the present invention, STING modulators, and particularly hSTING modulators (e.g., specific hSTING modulators) are useful as anti-cancer agents. In some embodiments, in accordance with the present invention, STING modulators, and particularly hSTING modulators (e.g., specific hSTING modulators) are useful in vaccine development. In some embodiments, in accordance with the present invention, STING modulators, and particularly hSTING modulators (e.g., specific hSTING modulators) are useful as therapies for autoimmune disorders.

[0160] In some embodiments, a STING modulator is a compound described in International Patent Application No. PCT/US14/35909, the entire contents of which is hereby incorporated by reference.

STING Species Selectivity

[0161] In one aspect, the present invention defines the molecular basis underlying DMXAA species selectivity. The small molecule drug DMXAA specifically activates the STING nucleic acid-sensing pathway in a species-dependent manner. Functional and structural studies demonstrate that DMXAA activates mouse but not human STING (Conlon et al., 2013; Kim et al., 2013). DMXAA showed great promise in mouse cancer models, underscoring its potential for human application, notwithstanding the outcome of a phase III clinical trial for non-small cell lung carcinoma (Lara et al., 2011). Hence it is important to recognize that while

DMXAA itself is apparently not a viable drug, pharmacological modulation of STING remains an ideal therapeutic strategy.

[0162] One model recently suggested that DMXAA species-selectivity might be due to non-conserved residues within mSTING that could directly bind to DMXAA (Conlon et al., 2013). However, previous structural studies established that DMXAA binds to mSTING within the same pocket as cGAMP and that DMXAA binding involves interactions with identical amino acids in both mSTING and hSTING (Gao et al., 2013b). Therefore, although the non-conserved residues do not participate in direct interaction with DMXAA, they potentially play alternative roles in DMXAA recognition. Results disclosed herein on ITC binding (Figures 15B, 15C and 20A) and IFN induction (Figure 15D) studies established that the non-conserved residues located within the lid region of the ligand-binding pocket (group2) are important for the species-specific response to DMXAA. Furthermore, the structural studies described herein reveal the same 'closed' conformation for the complexes of DMXAA bound to $hSTING^{group2}$ (Figure 15E) and mSTING (Figure 20B), confirming the important role of group2 residues in DMXAA recognition and complex formation.

[0163] Moreover, the present disclosure identifies a hydrophobic interaction between the substituted I230 and the residues from both the lid region and other parts of the protein in the $hSTING^{group2}$-DMXAA complex (Figure 15G), a distinctive feature that was also found in the structure of the mSTING-DMXAA complex (Figure 20C). All residues that form the hydrophobic pocket that contains I230 are conserved in both human and mouse STING proteins. The gain of function of $hSTING^{G230I}$ and inversely the loss of function of $mSTING^{I229G}$ or $mSTING^{I229A}$ in their abilities to induce IFN gene expression in response to DMXAA, further confirmed the role of this residue in species-specific recognition of DMXAA (Figure 16A, B). A crystal structure of the $hSTING^{G230I}$-DMXAA complex also exhibited the active 'closed' conformation (Figures 16C, D), further supporting the conclusion that this single point substitution outside of the binding pocket of hSTING modulates sensitivity to the otherwise mouse-selective DMXAA ligand. Hydrophobic interactions could help facilitate formation of the lid region and other parts of the protein, allowing mSTING to form the 'closed' conformation more readily than hSTING in response to DMXAA.

[0164] The disclosed structural studies indicate that mSTING is induced more readily to assume the 'closed' conformation than hSTING in response to CDNs and their analogs. Due to this 'intrinsic disadvantage' of hSTING, better fitting DMXAA analogs need to be designed to allow hSTING to overcome the energy barrier of transitioning from an 'open' to a 'closed' state. To enable the rational design of suitable DMXAA modifications, the ensuing Examples systematically introduced hSTING substitutions within the binding pocket and tested their influence on DMXAA-induced IFN-β production. Following this strategy and guided by co-crystal structures of STING substituents with DMXAA, the present invention identifies two point substitutions within the ligand-binding pocket, S162A reported previously (Gao et al., 2013b) and Q266I, each of which strongly promote DMXAA recognition (Figure 17A). These data suggest that modestly-altered DMXAA derivatives might be sufficient to bind and activate hSTING. By introducing the above substitutions into the predominant hSTING alleles, a dose-dependent response to DMXAA is restored in all cases (Figures 22A, B). However, the Q293-carrying hSTING variants still responded poorly to DMXAA (Figure 17E), in line with previous reports showing an impaired CDN response by $hSTING^{Q293}$ and $hSTING^{HAQ}$ (Jin et al., 2011; Yi et al., 2013). This general effect of Q293 will most likely also affect the responsiveness to human-active DMXAA derivatives, suggesting a need for STING-genotyping in patients and possible adjustment of drug dosing in future studies.

[0165] The S162A/G230I/Q266I triple substitution of hSTING showed an order of magnitude higher activity than mSTING (Figure 18B), indicating that all three substitutions confer a substantial synergistic effect to DMXAA recognition. $hSTING^{S162A/G230I/Q266I}$ might therefore be used as a benchmark hSTING synthetic allele in future drug development studies using humanized mouse models. In addition to the luciferase reporter assays in human 293T cells, the ensuing Examples describe IFN and proinflammatory cytokine/chemokine production for hSTING substitutions in BMDCs from the $STING^{Gt/Gt}$ mouse and similar results (Figure 18F and 22E).

[0166] The ensuing Examples also show DMXAA-induced type I IFN and proinflammatory cytokine/chemokine production in STING-deficient bone marrow-derived dendritic cells (BMDCs) reconstituted with the hSTING mutants by retroviral transduction. In

some embodiments, reconstitution with hSTING$^{S162A/G230I/Q266I}$ resulted in the highest responsiveness to DMXAA stimulation in primary DCs with the induction of IFNB, IL-6, CCL5 and CXCL10 gene expression. These findings provide a guide for future rational drug design of DMXAA variants with potential IFN-β-stimulating activity in humans that are needed for the development of anti-cancer therapies and vaccine adjuvants

[0167] Thus the present invention provides, among other things, a comprehensive structural, biophysical, and functional analysis of DMXAA association with select substitutions within hSTING. The present invention highlights the role of the lid residue at position 230 (229 in mSTING) and unveils the structural basis for the mSTING-selectivity of DMXAA. Provided structural and functional results also shed light on strategies to restore an efficient DMXAA-response of hSTING based on the binding pocket S162A and Q266I substitutions. Imitating the effects of these amino acid substitutions by rational design of reciprocal DMXAA derivatives should lead to the development of human-active STING agonists for anti-tumor, anti-viral, and vaccine adjuvant applications. The same principles may apply to generation of analogs of CMA, the other small molecule that to date can target mSTING but not hSTING (Cavlar et al., 2013).

Structure-Based Drug Design

[0168] In some embodiments, the present disclosure provides systems for identifying and/or characterizing STING modulators. In some embodiments, the present disclosure provides a method of designing, identifying and/or characterizing a STING modulator comprising the steps of: a) providing an image of a STING crystal that includes at least one potential interaction site; b) docking in the image at least one moiety that is a potential STING modulator structural element; and c) assessing one or more features of a potential moiety-interaction site interaction.

[0169] In some embodiments, the at least one potential interaction site includes a site selected from the group consisting of Ser162, Ile165, and combinations thereof. In some embodiments, the at least one potential interaction site includes a site selected from the group consisting of Ser162, Ile165, Gly230, Gln266, and combinations thereof. In some embodiments, the at least one potential interaction site includes Ser162. In some embodiments, the at least one potential interaction site includes Ile165. In some embodiments, the at least one potential interaction site includes Gly230. In some embodiments, the at least one potential

interaction site includes Gln266. In some embodiments, the modulator is a compound disclosed herein.

[0170] In some embodiments, the one or more features include at least one feature selected from the group consisting of: spatial separation between the moiety and the potential interaction site; energy of the potential moiety-interaction site interaction, and/or combinations thereof.

[0171] In some embodiments, a method further comprises a step of providing an image of a potential STING modulator comprising the moiety docked with the image of the STING crystal. In some embodiments, a method further comprises a step of comparing the image with that of a STING crystal including a bound known modulator, substrate, or product.

Computer Systems

[0172] As will be appreciated by those skilled in the art, reading the present disclosure, in some aspects, the present invention is ideally suited for use in computer-implemented inventions. FIG. 24 shows but one example of a computing device 2500 and a mobile computing device 2550 that can be used to implement certain techniques described in this disclosure. The computing device 2500 depicted in FIG. 24 is intended to represent any of a variety forms of digital computers, such as laptops, desktops, workstations, personal digital assistants, servers, blade servers, mainframes, and other appropriate computers. The depicted mobile computing device 2550 is intended to represent any appropriate form of mobile devices, such as personal digital assistants, cellular telephones, smart-phones, tablet computers, and other similar computing devices. Moreover, the components shown in FIG. 24 and elsewhere in the Figures, their connections and relationships, and their functions, are meant to be examples only, and are not meant to be limiting.

[0173] The computing device depicted in FIG. 24 2500 includes a processor 2502, a memory 2504, a storage device 2506, a high-speed interface 2508 connecting to the memory 2504 and multiple high-speed expansion ports 2510, and a low-speed interface 2512 connecting to a low-speed expansion port 2514 and the storage device 2506. Each of the processor 2502, the memory 2504, the storage device 2506, the high-speed interface 2508, the high-speed

expansion ports 2510, and the low-speed interface 2512, are interconnected using various busses, and may be mounted on a common motherboard or in other manners as appropriate. The processor 2502 can process instructions for execution within the computing device 2500, including instructions stored in the memory 2504 or on the storage device 2506 to display graphical information for a GUI on an external input/output device, such as a display 2516 coupled to the high-speed interface 2508. In some implementations, multiple processors and/or multiple buses may be used, as appropriate, along with multiple memories and types of memory. Also, multiple computing devices may be connected, with each device providing portions of the necessary operations (e.g., as a server bank, a group of blade servers, or a multi-processor system).

[0174] The memory 2504 depicted in FIG. 24 stores information within the computing device 2500. In some implementations, the memory 2504 is a volatile memory unit or units. In some implementations, the memory 2504 is a non-volatile memory unit or units. The memory 2504 may also be another form of computer-readable medium, such as a magnetic or optical disk.

[0175] The storage device 2506 depicted in FIG. 24 is capable of providing mass storage for the computing device 2500. In some implementations, the storage device 2506 may be or contain a computer-readable medium, such as a floppy disk device, a hard disk device, an optical disk device, or a tape device, a flash memory or other similar solid state memory device, or an array of devices, including devices in a storage area network or other configurations. Instructions can be stored in an information carrier. The instructions, when executed by one or more processing devices (for example, processor 2502), perform one or more methods, such as those described above. The instructions can also be stored by one or more storage devices such as computer- or machine-readable mediums (for example, the memory 2504, the storage device 2506, or memory on the processor 2502).

[0176] The high-speed interface 2508 manages bandwidth-intensive operations for the computing device 2500, while the low-speed interface 2512 manages lower bandwidth-intensive operations. Such allocation of functions is an example only. In some implementations, the high-speed interface 2508 is coupled to the memory 2504, the display 2516 (e.g., through a graphics

processor or accelerator), and to the high-speed expansion ports 2510, which may accept various expansion cards (not shown). In the implementation, the low-speed interface 2512 is coupled to the storage device 2506 and the low-speed expansion port 2514. The low-speed expansion port 2514, which may include various communication ports (e.g., USB, Bluetooth®, Ethernet, wireless Ethernet) may be coupled to one or more input/output devices, such as a keyboard, a pointing device, a scanner, or a networking device such as a switch or router, e.g., through a network adapter.

[0177] The computing device 2500 may be implemented in a number of different forms, as shown in the figure. For example, it may be implemented as a standard server 2520, or multiple times in a group of such servers. In addition, it may be implemented in a personal computer such as a laptop computer 2522. It may also be implemented as part of a rack server system 2524. Alternatively, components from the computing device 2500 may be combined with other components in a mobile device (not shown), such as a mobile computing device 2550. Each of such devices may contain one or more of the computing device 2500 and the mobile computing device 2550, and an entire system may be made up of multiple computing devices communicating with each other.

[0178] The mobile computing device 2550 depicted in FIG. 24 includes a processor 2552, a memory 2564, an input/output device such as a display 2554, a communication interface 2566, and a transceiver 2568, among other components. The mobile computing device 2550 may also be provided with a storage device, such as a micro-drive or other device, to provide additional storage. Each of the processor 2552, the memory 2564, the display 2554, the communication interface 2566, and the transceiver 2568, are interconnected using various buses, and several of the components may be mounted on a common motherboard or in other manners as appropriate.

[0179] The processor 2552 depicted in FIG. 24 can execute instructions within the mobile computing device 2550, including instructions stored in the memory 2564. The processor 2552 may be implemented as a chipset of chips that include separate and multiple analog and digital processors. The processor 2552 may provide, for example, for coordination of the other components of the mobile computing device 2550, such as control of user interfaces,

applications run by the mobile computing device 2550, and wireless communication by the mobile computing device 2550.

[0180] The processor 2552 may communicate with a user through a control interface 2558 and a display interface 2556 coupled to the display 2554. The display 2554 depicted in FIG. 24 may be, for example, a TFT (Thin-Film-Transistor Liquid Crystal Display) display or an OLED (Organic Light Emitting Diode) display, or other appropriate display technology. The display interface 2556 may comprise appropriate circuitry for driving the display 2554 to present graphical and other information to a user. The control interface 2558 may receive commands from a user and convert them for submission to the processor 2552. In addition, an external interface 2562 may provide communication with the processor 2552, so as to enable near area communication of the mobile computing device 2550 with other devices. The external interface 2562 may provide, for example, for wired communication in some implementations, or for wireless communication in other implementations, and multiple interfaces may also be used.

[0181] The memory 2564 depicted in FIG. 24 stores information within the mobile computing device 2550. The memory 2564 can be implemented as one or more of a computer-readable medium or media, a volatile memory unit or units, or a non-volatile memory unit or units. An expansion memory 2574 may also be provided and connected to the mobile computing device 2550 through an expansion interface 2572, which may include, for example, a SIMM (Single In Line Memory Module) card interface. The expansion memory 2574 may provide extra storage space for the mobile computing device 2550, or may also store applications or other information for the mobile computing device 2550. Specifically, the expansion memory 2574 may include instructions to carry out or supplement the processes described above, and may include secure information also. Thus, for example, the expansion memory 2574 may be provide as a security module for the mobile computing device 2550, and may be programmed with instructions that permit secure use of the mobile computing device 2550. In addition, secure applications may be provided via the SIMM cards, along with additional information, such as placing identifying information on the SIMM card in a non-hackable manner.

[0182] The memory may include, for example, flash memory and/or NVRAM memory (non-volatile random access memory), as discussed below. In some implementations,

instructions are stored in an information carrier. that the instructions, when executed by one or more processing devices (for example, processor 2552), perform one or more methods, such as those described above. The instructions can also be stored by one or more storage devices, such as one or more computer- or machine-readable mediums (for example, the memory 2564, the expansion memory 2574, or memory on the processor 2552). In some implementations, the instructions can be received in a propagated signal, for example, over the transceiver 2568 or the external interface 2562.

[0183] The mobile computing device 2550 depicted in FIG. 24 may communicate wirelessly through the communication interface 2566, which may include digital signal processing circuitry where necessary. The communication interface 2566 may provide for communications under various modes or protocols, such as GSM voice calls (Global System for Mobile communications), SMS (Short Message Service), EMS (Enhanced Messaging Service), or MMS messaging (Multimedia Messaging Service), CDMA (code division multiple access), TDMA (time division multiple access), PDC (Personal Digital Cellular), WCDMA (Wideband Code Division Multiple Access), CDMA2000, or GPRS (General Packet Radio Service), among others. Such communication may occur, for example, through the transceiver 2568 using a radio-frequency. In addition, short-range communication may occur, such as using a Bluetooth®, Wi-Fi™, or other such transceiver (not shown). In addition, a GPS (Global Positioning System) receiver module 2570 may provide additional navigation- and location-related wireless data to the mobile computing device 2550, which may be used as appropriate by applications running on the mobile computing device 2550.

[0184] The mobile computing device 2550 depicted in FIG. 24 may also communicate audibly using an audio codec 2560, which may receive spoken information from a user and convert it to usable digital information. The audio codec 2560 may likewise generate audible sound for a user, such as through a speaker, e.g., in a handset of the mobile computing device 2550. Such sound may include sound from voice telephone calls, may include recorded sound (e.g., voice messages, music files, etc.) and may also include sound generated by applications operating on the mobile computing device 2550.

[0185] The mobile computing device 2550 may be implemented in a number of different forms, as shown in FIG. 24. For example, it may be implemented as a cellular telephone 2580. It may also be implemented as part of a smart-phone 2582, personal digital assistant, or other similar mobile device.

[0186] Various implementations of the systems and techniques described here can be realized in digital electronic circuitry, integrated circuitry, specially designed ASICs (application specific integrated circuits), computer hardware, firmware, software, and/or combinations thereof. These various implementations can include implementation in one or more computer programs that are executable and/or interpretable on a programmable system including at least one programmable processor, which may be special or general purpose, coupled to receive data and instructions from, and to transmit data and instructions to, a storage system, at least one input device, and at least one output device.

[0187] These computer programs (also known as programs, software, software applications or code) include machine instructions for a programmable processor, and can be implemented in a high-level procedural and/or object-oriented programming language, and/or in assembly/machine language. As used herein, the terms machine-readable medium and computer-readable medium refer to any computer program product, apparatus and/or device (e.g., magnetic discs, optical disks, memory, Programmable Logic Devices (PLDs)) used to provide machine instructions and/or data to a programmable processor, including a machine-readable medium that receives machine instructions as a machine-readable signal. The term machine-readable signal refers to any signal used to provide machine instructions and/or data to a programmable processor.

[0188] To provide for interaction with a user, the systems and techniques described here can be implemented on a computer having a display device (e.g., a CRT (cathode ray tube) or LCD (liquid crystal display) monitor) for displaying information to the user and a keyboard and a pointing device (e.g., a mouse or a trackball) by which the user can provide input to the computer. Other kinds of devices can be used to provide for interaction with a user as well; for example, feedback provided to the user can be any form of sensory feedback (e.g., visual

feedback, auditory feedback, or tactile feedback); and input from the user can be received in any form, including acoustic, speech, or tactile input.

[0189] The systems and techniques described here can be implemented in a computing system that includes a back end component (e.g., as a data server), or that includes a middleware component (e.g., an application server), or that includes a front end component (e.g., a client computer having a graphical user interface or a Web browser through which a user can interact with an implementation of the systems and techniques described here), or any combination of such back end, middleware, or front end components. The components of the system can be interconnected by any form or medium of digital data communication (e.g., a communication network). Examples of communication networks include a local area network (LAN), a wide area network (WAN), and the Internet.

[0190] The computing system can include clients and servers. A client and server are generally remote from each other and typically interact through a communication network. The relationship of client and server arises by virtue of computer programs running on the respective computers and having a client-server relationship to each other.

[0191] In some embodiments, there is provided an implementation of an exemplary cloud computing environment for subscription management in a multi-channel context aware communication environment. As shown in FIG. 23, the cloud computing environment 2400 may include one or more resource providers 2402a, 2402b, 2402c (collectively, 2402). Each resource provider 2402 may include computing resources. In some implementations, computing resources may include any hardware and/or software used to process data. For example, computing resources may include hardware and/or software capable of executing algorithms, computer programs, and/or computer applications. In some implementations, exemplary computing resources may include application servers and/or databases with storage and retrieval capabilities. Each resource provider 2402 may be connected to any other resource provider 2402 in the cloud computing environment 2400. In some implementations, the resource providers 2402 may be connected over a computer network 2408. Each resource provider 2402 may be connected to one or more computing device 2404a, 2404b, 2404c (collectively, 2404), over the computer network 2408.

[0192] The cloud computing environment 2400 depicted in FIG. 23 may include a resource manager 2406. The resource manager 2406 may be connected to the resource providers 2402 and the computing devices 2404 over the computer network 2408. In some implementations, the resource manager 2406 may facilitate the provision of computing resources by one or more resource providers 2402 to one or more computing devices 2404. The resource manager 2406 may receive a request for a computing resource from a particular computing device 2404. The resource manager 2406 may identify one or more resource providers 2402 capable of providing the computing resource requested by the computing device 2404. The resource manager 2406 may select a resource provider 2402 to provide the computing resource. The resource manager 2406 may facilitate a connection between the resource provider 2402 and a particular computing device 2404. In some implementations, the resource manager 2406 may establish a connection between a particular resource provider 2402 and a particular computing device 2404. In some implementations, the resource manager 2406 may redirect a particular computing device 2404 to a particular resource provider 2402 with the requested computing resource.

[0193] As will be appreciated by those skilled in the art, reading the present disclosure in some embodiments, the present invention provides a computer system comprising one or more of (a) atomic coordinate data as disclosed herein [+/- a root mean square deviation from the Ca atoms of note more than 1.5Å (or 1.0 Å or 0.5 Å)]; (b) structure factor data (where a structure factor comprises the amplitude and phase of the diffracted wave) for STING, said structure factor data being derivable from the atomic coordinate data of Tables 1-5 +/- a root mean square deviation from the Ca atoms of note more than 1.5 Å (or 1.0 Å or 0.5 Å); (c) atomic coordinate data of a STING modulator protein generated by homology modeling of the target based on the data disclosed herein +/- a root mean square deviation from the Ca atoms of not more than 1.5Å (or 1.0 Å or 0.5 Å); (d) atomic coordinate data of a STING modulator protein generated by interpreting X-ray crystallographic data or NMR data by reference to the data disclosed herein +/- a root mean square deviation from the Ca atoms of note more than 1.5Å (or 1.0 Å or 0.5 Å); or (e) structure factor data a derivable from the atomic coordinate data of (c) or (d). In certain embodiments, a computer system comprises: a computer-readable data storage medium comprising data storage material encoded with the computer-readable data; (a) a working

memory for storing instructions for processing said computer-readable data; and (b) a central-processing unit coupled to said working memory and to said computer-readable data storage medium for processing said computer-readable data and thereby generating structures, characterizing structures and/or performing rational drug design.

[0194] In some embodiments, there is provided a machine-readable data storage medium, comprising a data storage material encoded with machine-readable data, wherein said data comprises all or part of a c[G(2',5')pA(3',5')p]-hSTING^{H232} complex defined by structure coordinates of hSTING^{H232}amino acids (SEQ ID NO.:1), according Table 1; or a molecule or molecular complex comprising all or part of a c[G(2',5')pA(3',5')p]-hSTING^{H232} complex defined by structure coordinates of corresponding amino acids that are identical to said hSTING^{H232} amino acids, wherein the root mean square deviation of the backbone atoms between said corresponding amino acids and said hSTING^{H232} amino acids is not more than about 3.0Å, 2.5 Å, 2.0 Å, 1.5 Å, 1.0 Å; or a molecule or molecular complex comprising all or part of a c[G(2',5')pA(3',5')p]-hSTING^{H232} complex defined by structure coordinates of a set of corresponding amino acids, wherein the root mean square deviation of the backbone atoms between said set of corresponding amino acids and said hSTING^{H232} amino acids is not more than about 1.1, 0.9, 0.7, or 0.5 Å, and wherein at least one of said corresponding amino acids is not identical to the hSTING^{H232} amino acid to which it corresponds.

[0195] In some embodiments, there is provided a machine-readable data storage medium, comprising a data storage material encoded with machine-readable data, wherein said data comprises all or part of a c[G(2',5')pA(2',5')p]-hSTING^{H232} complex defined by structure coordinates of hSTING^{H232} amino acids (SEQ ID NO.:1), according Table 2; or a molecule or molecular complex comprising all or part of a c[G(2',5')pA(2',5')p]-hSTING^{H232} complex defined by structure coordinates of corresponding amino acids that are identical to said hSTING^{H232} amino acids, wherein the root mean square deviation of the backbone atoms between said corresponding amino acids and said hSTING^{H232} amino acids is not more than about 3.0Å, 2.5 Å, 2.0 Å, 1.5 Å, 1.0 Å; or a molecule or molecular complex comprising all or part of a c[G(2',5')pA(2',5')p]-hSTING^{H232} complex defined by structure coordinates of a set of corresponding amino acids, wherein the root mean square deviation of the backbone atoms

between said set of corresponding amino acids and said hSTING^{H232} amino acids is not more than about 1.1, 0.9, 0.7, or 0.5 Å, and wherein at least one of said corresponding amino acids is not identical to the hSTING^{H232} amino acid to which it corresponds.

[0196] In some embodiments, there is provided a machine-readable data storage medium, comprising a data storage material encoded with machine-readable data, wherein said data comprises all or part of a c[G(2',5')pA(3',5')p]-mSting^{R231} complex defined by structure coordinates of mSting^{R231} amino acids (SEQ ID NO.:2), according Table 3; or a molecule or molecular complex comprising all or part of a c[G(2',5')pA(3',5')p]-mSting^{R231} complex defined by structure coordinates of corresponding amino acids that are identical to said mSting^{R231} amino acids, wherein the root mean square deviation of the backbone atoms between said corresponding amino acids and said mSting^{R231} amino acids is not more than about 3.0Å, 2.5 Å, 2.0 Å, 1.5 Å, 1.0 Å; or a molecule or molecular complex comprising all or part of a c[G(2',5')pA(3',5')p]-mSting^{R231} complex defined by structure coordinates of a set of corresponding amino acids, wherein the root mean square deviation of the backbone atoms between said set of corresponding amino acids and said mSting^{R231} amino acids is not more than about 1.1, 0.9, 0.7, or 0.5 Å, and wherein at least one of said corresponding amino acids is not identical to the mSting^{R231} amino acid to which it corresponds.

[0197] In some embodiments, there is provided a machine-readable data storage medium, comprising a data storage material encoded with machine-readable data, wherein said data comprises all or part of a c[G(3',5')pA(3',5')p]-mSting^{R231} complex defined by structure coordinates of mSting^{R231} amino acids (SEQ ID NO.:2), according Table 4; or a molecule or molecular complex comprising all or part of a c[G(3',5')pA(3',5')p]-mSting^{R231} complex defined by structure coordinates of corresponding amino acids that are identical to said mSting^{R231} amino acids, wherein the root mean square deviation of the backbone atoms between said corresponding amino acids and said mSting^{R231} amino acids is not more than about 3.0Å, 2.5 Å, 2.0 Å, 1.5 Å, 1.0 Å; or a molecule or molecular complex comprising all or part of a c[G(2',5')pA(3',5')p]-mSting^{R231} complex defined by structure coordinates of a set of corresponding amino acids, wherein the root mean square deviation of the backbone atoms between said set of corresponding amino acids and said mSting^{R231} amino acids is not more than

about 1.1, 0.9, 0.7, or 0.5 Å, and wherein at least one of said corresponding amino acids is not identical to the $mSting^{R231}$ amino acid to which it corresponds.

[0198] In some embodiments, there is provided a machine-readable data storage medium, comprising a data storage material encoded with machine-readable data, wherein said data comprises all or part of a DMXAA-$mSting^{R231}$ complex defined by structure coordinates of $mSting^{R231}$ amino acids (SEQ ID NO.:2), according Table 5; or a molecule or molecular complex comprising all or part of a DMXAA-$mSting^{R231}$ complex defined by structure coordinates of corresponding amino acids that are identical to said $mSting^{R231}$ amino acids, wherein the root mean square deviation of the backbone atoms between said corresponding amino acids and said $mSting^{R231}$ amino acids is not more than about 3.0Å, 2.5 Å, 2.0 Å, 1.5 Å, 1.0 Å; or a molecule or molecular complex comprising all or part of a DMXAA-$mSting^{R231}$ complex defined by structure coordinates of a set of corresponding amino acids, wherein the root mean square deviation of the backbone atoms between said set of corresponding amino acids and said $mSting^{R231}$ amino acids is not more than about 1.1, 0.9, 0.7, or 0.5 Å, and wherein at least one of said corresponding amino acids is not identical to the $mSting^{R231}$ amino acid to which it corresponds.

[0199] In some embodiments, there is provided a machine-readable data storage medium, comprising a data storage material encoded with machine-readable data, wherein said data comprises all or part of a DMXAA-$hSTING^{group2}$ complex defined by structure coordinates of $hSTING^{group2}$ amino acids, according Table 6; or a molecule or molecular complex comprising all or part of a DMXAA-$hSTING^{group2}$ complex defined by structure coordinates of corresponding amino acids that are identical to said $hSTING^{group2}$ amino acids, wherein the root mean square deviation of the backbone atoms between said corresponding amino acids and said $hSTING^{group2}$ amino acids is not more than about 3.0Å, 2.5 Å, 2.0 Å, 1.5 Å, 1.0 Å; or a molecule or molecular complex comprising all or part of a DMXAA-$hSTING^{group2}$ complex defined by structure coordinates of a set of corresponding amino acids, wherein the root mean square deviation of the backbone atoms between said set of corresponding amino acids and said $hSTING^{group2}$ amino acids is not more than about 1.1, 0.9, 0.7, or 0.5 Å, and wherein at least one of said corresponding amino acids is not identical to the $hSTING^{group2}$ amino acid to which it corresponds.

[0200] In some embodiments, there is provided a machine-readable data storage medium, comprising a data storage material encoded with machine-readable data, wherein said data comprises all or part of a DMXAA-hSTING^{G230I} complex defined by structure coordinates of hSTING^{G230I} amino acids, according Table 7; or a molecule or molecular complex comprising all or part of a DMXAA-hSTING^{G230I} complex defined by structure coordinates of corresponding amino acids that are identical to said hSTING^{G230I} amino acids, wherein the root mean square deviation of the backbone atoms between said corresponding amino acids and said hSTING^{G230I} amino acids is not more than about 3.0Å, 2.5 Å, 2.0 Å, 1.5 Å, 1.0 Å; or a molecule or molecular complex comprising all or part of a DMXAA-hSTING^{G230I} complex defined by structure coordinates of a set of corresponding amino acids, wherein the root mean square deviation of the backbone atoms between said set of corresponding amino acids and said hSTING^{G230I} amino acids is not more than about 1.1, 0.9, 0.7, or 0.5 Å, and wherein at least one of said corresponding amino acids is not identical to the hSTING^{G230I} amino acid to which it corresponds.

[0201] In some embodiments, there is provided a machine-readable data storage medium, comprising a data storage material encoded with machine-readable data, wherein said data comprises all or part of a DMXAA-hSTING$^{S162A/Q266I}$ complex defined by structure coordinates of hSTING$^{S162A/Q266I}$ amino acids, according Table 8; or a molecule or molecular complex comprising all or part of a DMXAA-hSTING$^{S162A/Q266I}$ complex defined by structure coordinates of corresponding amino acids that are identical to said hSTING$^{S162A/Q266I}$ amino acids, wherein the root mean square deviation of the backbone atoms between said corresponding amino acids and said hSTING$^{S162A/Q266I}$ amino acids is not more than about 3.0Å, 2.5 Å, 2.0 Å, 1.5 Å, 1.0 Å; or a molecule or molecular complex comprising all or part of a DMXAA-hSTING$^{S162A/Q266I}$ complex defined by structure coordinates of a set of corresponding amino acids, wherein the root mean square deviation of the backbone atoms between said set of corresponding amino acids and said hSTING$^{S162A/Q266I}$ amino acids is not more than about 1.1, 0.9, 0.7, or 0.5 Å, and wherein at least one of said corresponding amino acids is not identical to the hSTING$^{S162A/Q266I}$ amino acid to which it corresponds.

[0202] In some embodiments, there is provided a machine-readable data storage medium, comprising a data storage material encoded with machine-readable data, wherein said data comprises all or part of a DMXAA-hSTING$^{S162A/G230I/Q266I}$ complex defined by structure coordinates of hSTING$^{S162A/G230I/Q266I\ /Q266I}$ amino acids, according Table 9; or a molecule or molecular complex comprising all or part of a DMXAA-hSTING$^{S162A/G230I/Q266I}$ complex defined by structure coordinates of corresponding amino acids that are identical to said hSTING$^{S162A/G230I/Q266I}$ amino acids, wherein the root mean square deviation of the backbone atoms between said corresponding amino acids and said hSTING$^{S162A/G230I/Q266I}$ amino acids is not more than about 3.0Å, 2.5 Å, 2.0 Å, 1.5 Å, 1.0 Å; or a molecule or molecular complex comprising all or part of a DMXAA-hSTING$^{S162A/G230I/Q266I}$ complex defined by structure coordinates of a set of corresponding amino acids, wherein the root mean square deviation of the backbone atoms between said set of corresponding amino acids and said hSTING$^{S162A/G230I/Q266I}$ amino acids is not more than about 1.1, 0.9, 0.7, or 0.5 Å, and wherein at least one of said corresponding amino acids is not identical to the hSTING$^{S162A/G230I/Q266I}$ amino acid to which it corresponds.

[0203] In some embodiments, the data storage material is encoded with machine-readable data comprising all or part of a superposition of a STING complex with one or more additional molecules and/or complexes. In some embodiments, data storage material is encoded with machine-readable data comprising all or part of a superposition of a STING protein and STING modulator complex. In some embodiments, one or more domain(s) of STING are superposed with one or more molecules and/or complexes. In some embodiments, the cyclic dinucleotide cleft domain of STING and DMXAA are superpositioned. In some embodiments, the cyclic dinucleotide cleft domain of STING and a candidate STING modulator are superpositioned.

[0204] In some embodiments, the present invention provides a computer system comprising executable code for computer-aided and/or structure-based drug design of STING modulators. In some embodiments, the present invention provides a computer system comprising executable code for docking STING modulators in at least one potential STING interaction site (e.g., dinucleotide cleft domain, ligand-binding pocket). In some embodiments,

said executable code comprises instructions for providing an image of a STRING crystal that includes at least one potential interaction site; docking in the image at least one moiety that is a potential STING modulator structural element; and assessing one or more features of a potential moiety-interaction site interaction.

[0205] In some embodiments, said executable code comprises a determining step, wherein said determining step comprises a prediction of 1.) whether said moiety will bind to at least one potential STING interaction site; 2.) calculates the strength of binding affinity; and 3.) calculates moiety specificity. In some embodiments, the determining step further comprises predicting the conformation of the moiety when bound to at least one potential interaction site. In some embodiments, the determining step further comprises one or more predictions of conformational changes in a STING polypeptide when said moiety binds at least one potential interaction site.

[0206] In some embodiments, provided computer system comprise executable code for superimposing all or part of a STING crystal or crystallizable composition with another crystal or crystallizable composition.

[0207] In some embodiments, provided computer systems comprise executable code for modeling interactions with a STING crystal or crystallizable composition.

Identifying, Designing and/or Characterizing STING modulators

[0208] As described herein, the present disclosure describes systems useful in the identification, design, and/or characterization of STING modulators and/or STING modulator candidates. In some embodiments, such systems are or comprise structure based drug design systems. In some embodiments, such systems are or comprise one or more activity assays.

[0209] In some embodiments, candidate STING modulator compounds are tested in accordance with systems described herein in order to identify and/or characterize those with desirable structural and/or functional attributes. In some embodiments, a population of candidate STING modulator compounds is provided through structure-based drug design predictions of interacting moieties. In some embodiments, a population of candidate STING modulator

compounds is or comprises analogs of a reference compound selected from the group consisting of cyclic dinucleotides, DMXAA, CMA, and combinations thereof.

Pharmaceutical Compositions

[0210] The pharmaceutical compositions can be in a variety of forms including oral dosage forms, topic creams, topical patches, iontophoresis forms, suppository, nasal spray and inhaler, eye drops, intraocular injection forms, depot forms, as well as injectable and infusible solutions. Methods for preparing pharmaceutical composition are well known in the art.

[0211] Pharmaceutical compositions typically contain the active agent described herein (e.g. STING modulators) in an amount effective to achieve the desired therapeutic effect while avoiding or minimizing adverse side effects. Pharmaceutically acceptable preparations and salts of the active agent are provided herein and are well known in the art. For the administration of STING modulators and the like, the amount administered desirably is chosen that is therapeutically effective with few to no adverse side effects. The amount of the therapeutic or pharmaceutical composition which is effective in the treatment of a particular disease, disorder or condition depends on the nature and severity of the disease, the target site of action, the subject's weight, special diets being followed by the subject, concurrent medications being used, the administration route and other factors that are recognized by those skilled in the art. The dosage can be adapted by the clinician in accordance with conventional factors such as the extent of the disease and different parameters from the subject. Effective doses may be extrapolated from dose-response curves derived from *in vitro* or animal model test systems (e.g., as described by the U.S. Department of Health and Human Services, Food and Drug Administration, and Center for Drug Evaluation and Research in "Guidance for Industry: Estimating Maximum Safe Starting Dose in Initial Clinical Trials for Therapeutics in Adult Healthy Volunteers", *Pharmacology and Toxicology*, July 2005, the entire contents of which are incorporated herein by reference).

[0212] Various delivery systems are known and can be used to administer active agent described herein (e.g. STING modulators) or a pharmaceutical composition comprising the same. The pharmaceutical compositions described herein can be administered by any suitable route including, intravenous or intramuscular injection, intraventricular or intrathecal injection (for

central nervous system administration), orally, topically, subcutaneously, intrapulmonary (*e.g.*, inhalation), subconjunctivally, intraocularly, or via intranasal, intradermal, sublingual, vaginal, rectal or epidural routes.

[0213] Other delivery systems well known in the art can be used for delivery of the pharmaceutical compositions described herein, for example via aqueous solutions, encapsulation in microparticules, or microcapsules. The pharmaceutical compositions of the present invention can also be delivered in a controlled release system. For example, a polymeric material can be used (see, e.g., Smolen and Ball, Controlled Drug Bioavailability, Drug product design and performance, 1984, John Wiley & Sons; Ranade and Hollinger, Drug Delivery Systems, pharmacology and toxicology series, 2003, 2nd edition, CRRC Press). Alternatively, a pump may be used (Saudek et al., *N. Engl. J. Med.* 321:574 (1989)). The compositions described herein may also be coupled to a class of biodegradable polymers useful in achieving controlled release of the drug, for example, polylactic acid, polyorthoesters, cross-linked amphipathic block copolymers and hydrogels, polyhydroxy butyric acid, and polydihydropyrans.

[0214] As described above, pharmaceutical compositions desirably include a pharmaceutically acceptable carrier. The term carrier refers to diluents, adjuvants, excipients or vehicles with which STING modulators are administered. Such pharmaceutical carriers include sterile liquids such as water and oils including mineral oil, vegetable oil (e.g., soybean oil or corn oil), animal oil or oil of synthetic origin. Aqueous glycerol and dextrose solutions as well as saline solutions may also be employed as liquid carriers of the pharmaceutical compositions of the present invention. The choice of the carrier depends on factors well recognized in the art, such as the nature of the peptide, peptide derivative or peptidomimetic, its solubility and other physiological properties as well as the target site of delivery and application. Examples of suitable pharmaceutical carriers are described in Remington: The Science and Practice of Pharmacy by Alfonso R. Gennaro, 2003, 21th edition, Mack Publishing Company. Moreover, suitable carriers for oral administration are known in the art and are described, for example, in U.S. Patent Nos. 6,086,918, 6,673,574, 6,960,355, and 7,351,741 and in WO2007/131286, the disclosures of which are hereby incorporated by reference.

[0215] Further pharmaceutically suitable materials that may be incorporated in pharmaceutical preparations include absorption enhancers including those intended to increase paracellular absorption, pH regulators and buffers, osmolarity adjusters, preservatives, stabilizers, antioxidants, surfactants, thickeners, emollient, dispersing agents, flavoring agents, coloring agents, and wetting agents.

[0216] Examples of suitable pharmaceutical excipients include, water, glucose, sucrose, lactose, glycol, ethanol, glycerol monostearate, gelatin, starch flour (e.g., rice flour), chalk, sodium stearate, malt, sodium chloride, and the like. The pharmaceutical compositions comprising STING modulators can take the form of solutions, capsules, tablets, creams, gels, powders sustained release formulations and the like. The composition can be formulated as a suppository, with traditional binders and carriers such as triglycerides (see Remington: The Science and Practice of Pharmacy by Alfonso R. Gennaro, 2003, 21th edition, Mack Publishing Company). Such compositions contain a therapeutically effective amount of the therapeutic composition, together with a suitable amount of carrier so as to provide the form for proper administration to the subject. The formulations are designed to suit the mode of administration and the target site of action (e.g., a particular organ or cell type).

[0217] The pharmaceutical compositions comprising the active agent described herein (e.g. STING modulators) also include compositions formulated as neutral or salt forms. Pharmaceutically acceptable salts include those that form with free amino groups and those that react with free carboxyl groups. Non-toxic alkali metal, alkaline earth metal, and ammonium salts commonly used in the pharmaceutical industry include sodium, potassium, lithium, calcium, magnesium, barium, ammonium, and protamine zinc salts, which are prepared by methods well known in the art. Also included are non-toxic acid addition salts, which are generally prepared by reacting the compounds of the present invention with suitable organic or inorganic acid. Representative salts include the hydrobromide, hydrochloride, valerate, oxalate, oleate, laureate, borate, benzoate, sulfate, bisulfate, acetate, phosphate, tysolate, citrate, maleate, fumarate, tartrate, succinate, napsylate salts, and the like.

[0218] Examples of fillers or binders that may be used in accordance with the present invention include acacia, alginic acid, calcium phosphate (dibasic), carboxymethylcellulose,

carboxymethylcellulose sodium, hydroxyethylcellulose, hydroxypropylcellulose, hydroxypropylmethylcellulose, dextrin, dextrates, sucrose, tylose, pregelatinized starch, calcium sulfate, amylose, glycine, bentonite, maltose, sorbitol, ethylcellulose, disodium hydrogen phosphate, disodium phosphate, disodium pyrosulfite, polyvinyl alcohol, gelatin, glucose, guar gum, liquid glucose, compressible sugar, magnesium aluminum silicate, maltodextrin, polyethylene oxide, polymethacrylates, povidone, sodium alginate, tragacanth microcrystalline cellulose, starch, and zein. In certain embodiments, a filler or binder is microcrystalline cellulose.

[0219] Examples of disintegrating agents that may be used include alginic acid, carboxymethylcellulose, carboxymethylcellulose sodium, hydroxypropylcellulose (low substituted), microcrystalline cellulose, powdered cellulose, colloidal silicon dioxide, sodium croscarmellose, crospovidone, methylcellulose, polacrilin potassium, povidone, sodium alginate, sodium starch glycolate, starch, disodium disulfite, disodium edathamil, disodium edetate, disodiumethylenediaminetetraacetate (EDTA) crosslinked polyvinylpyrrolidones, pregelatinized starch, carboxymethyl starch, sodium carboxymethyl starch, microcrystalline cellulose.

[0220] Examples of lubricants include calcium stearate, canola oil, glyceryl palmitostearate, hydrogenated vegetable oil (type I), magnesium oxide, magnesium stearate, mineral oil, poloxamer, polyethylene glycol, sodium lauryl sulfate, sodium stearate fumarate, stearic acid, talc and, zinc stearate, glyceryl behapate, magnesium lauryl sulfate, boric acid, sodium benzoate, sodium acetate, sodium benzoate/sodium acetate (in combination), DL-leucine.

[0221] Examples of silica flow conditioners include colloidal silicon dioxide, magnesium aluminum silicate and guar gum. Another most preferred silica flow conditioner consists of silicon dioxide.

[0222] Examples of stabilizing agents include acacia, albumin, polyvinyl alcohol, alginic acid, bentonite, dicalcium phosphate, carboxymethylcellulose, hydroxypropylcellulose, colloidal silicon dioxide, cyclodextrins, glyceryl monostearate, hydroxypropyl methylcellulose, magnesium trisilicate, magnesium aluminum silicate, propylene glycol, propylene glycol alginate, sodium alginate, carnauba wax, xanthan gum, starch, stearate(s), stearic acid, stearic monoglyceride and stearyl alcohol.

[0223] In some embodiments, the present invention contemplates oral formulations containing the active agent described herein (e.g. STING modulators). For example, pharmaceutical compositions described herein may include a cyclodextrin or cyclodextrin derivative. Cyclodextrins are generally made up of five or more α-D-glycopyranoside unites linked 1->4. Typically, cyclodextrins contain a number of glucose monomers ranging from six to eight units in a ring, creating a cone shape (α-cyclodextrin: six membered sugar ring molecule, β-cyclodextrin: seven sugar ring molecule, γ-cyclodextrin: eight sugar ring molecule). Exemplary cyclodextrins and cyclodextrin derivatives are disclosed in U.S. Patent No. 7,723,304, U.S. Publication No. 2010/0196452, and U.S. Publication No. 2010/0144624, the entire contents of each of which are incorporated herein by reference. For example, in some embodiments, a cyclodextrin in accordance with the present invention is an alkylated cyclodextrin, hydroxyalkylated cyclodextrin, or acylated cyclodextrin. In some embodiments, a cyclodextrin is a hydroxypropyl β-cyclodextrin. Exemplary cyclodextrin derivatives are disclosed in Szejtli, J. Chem Rev, (1998), 98, 1743-1753; and Szente, L and Szejtli, J., Advance Drug Delivery Reviews, 36 (1999) 17-28, the entire contents of each of which are hereby incorporated by reference. Examples of cyclodextin derivatives include methylated cyclodextrins (e.g., RAMEB; randomly methylated β-cyclodextrin); hydroxyalkylated cyclodextrins (hydroxypropyl-β-cyclodextrin and hydroxypropyl γ-cyclodextrin); acetylated cyclodextrins (acetyl-γ-cyclodextrin); reactive cyclodextrins (chlorotriazinyl β- cyclodextrin); and branched cyclodextrins (glucosyl- and maltosyl β-cyclodextrin); acetyl-γ-cyclodextrin; acetyl-β-cyclodextrin, sulfobutyl-β cyclodextrin, sulfated α-, β- and γ-cyclodextrins; sulfoalkylated cyclodextrins; and hydroxypropyl β-cyclodextrin.

Dosing

[0224] Typically, active agent described herein (e.g. STING modulators) in an amount ranging from 0.001 to 100 mg/kg/day is administered to the subject. For example, in some embodiments, about 0.01 mg/kg/day to about 25 mg/kg/day, about 1 mg/kg/day to about 20 mg/kg/day, 0.2 mg/kg/day to about 10 mg/kg/day, about 0.02 mg/kg/day to about 0.1 mg/kg/day, or about 1 mg/kg/day to about 100 mg/kg/day is administered to the subject. In some embodiments, active agent described herein (e.g. STING modulators) in an amount of about 10

μg/kg/day, 50 μg/kg/day, 100 μg/kg/day, 200 μg/kg/day, 300 μg/kg/day, 400 μg/kg/day, 500 μg/kg/day, 600 μg/kg/day, 700 μg/kg/day, 800 μg/kg/day, 900 μg/kg/day, or 1000 μg/kg/day is administered to the subject.

[0225] In some embodiments, the STING modulator is administered at an effective dose ranging from about 1-1,000 μg/kg/day (e.g., ranging from about 1-900 μg/kg/day, 1-800 μg/kg/day, 1-700 μg/kg/day, 1-600 μg/kg/day, 1-500 μg/kg/day, 1-400 μg/kg/day, 1-300 μg/kg/day, 1-200 μg/kg/day, 1-100 μg/kg/day, 1-90 μg/kg/day, 1-80 μg/kg/day, 1-70 μg/kg/day, 1-60 μg/kg/day, 1-50 μg/kg/day, 1-40 μg/kg/day, 1-30 μg/kg/day, 1-20 μg/kg/day, 1-10 μg/kg/day). In some embodiments, the STING modulator is administered at an effective dose ranging from about 1-500 μg/kg/day. In some embodiments, the STING modulator is administered at an effective dose ranging from about 1-100 μg/kg/day. In some embodiments, the STING modulator is administered at an effective dose ranging from about 1-60 μg/kg/day. In some embodiments, the STING modulator is administered at an effective dose selected from about 1, 2, 4, 6, 8, 10, 15, 20, 25, 30, 35, 40, 45, 50, 75, 100, 150, 200, 250, 300, 350, 400, 450, 500, 550, 600, 650, 700, 750, 800, 850, 900, 950, or 1,000 ug/kg/day.

[0226] In some embodiments, a therapeutically effective amount of an STING modulator may be an amount ranging from about 10-1,000 mg (e.g., about 20 mg – 1,000 mg, 30 mg – 1,000 mg, 40 mg – 1,000 mg, 50 mg – 1,000 mg, 60 mg – 1,000 mg, 70 mg – 1,000 mg, 80 mg – 1,000 mg, 90 mg – 1,000 mg, about 10-900 mg, 10-800 mg, 10-700 mg, 10-600 mg, 10-500 mg, 100-1000 mg, 100-900 mg, 100-800 mg, 100-700 mg, 100-600 mg, 100-500 mg, 100-400 mg, 100-300 mg, 200-1000 mg, 200-900 mg, 200-800 mg, 200-700 mg, 200-600 mg, 200-500 mg, 200-400 mg, 300-1000 mg, 300-900 mg, 300-800 mg, 300-700 mg, 300-600 mg, 300-500 mg, 400 mg – 1,000 mg, 500 mg – 1,000 mg, 100 mg - 900 mg, 200 mg – 800 mg, 300 mg – 700 mg, 400 mg – 700 mg, and 500 mg – 600 mg). In some embodiments, an STING modulator is present in an amount of or greater than about 10 mg, 50 mg, 100 mg, 150 mg, 200 mg, 250 mg, 300 mg, 350 mg, 400 mg, 450 mg, 500 mg, 550 mg, 600 mg, 650 mg, 700 mg, 750 mg, 800 mg. In some embodiments, an STING modulator is present in an amount of or less than about 1000 mg, 950 mg, 900 mg, 850 mg, 800 mg, 750 mg, 700 mg, 650 mg, 600 mg, 550 mg, 500 mg, 450 mg, 400 mg, 350 mg, 300 mg, 250 mg, 200 mg, 150 mg, or 100 mg. In some embodiments, the

therapeutically effective amount described herein is provided in one dose. In some embodiments, the therapeutically effective amount described herein is provided in one day.

[0227] In other embodiments, a therapeutically effective amount may be, for example, about 0.001 mg/kg weight to 500 mg/kg weight, e.g., from about 0.001 mg/kg weight to 400 mg/kg weight, from about 0.001 mg/kg weight to 300 mg/kg weight, from about 0.001 mg/kg weight to 200 mg/kg weight, from about 0.001 mg/kg weight to 100 mg/kg weight, from about 0.001 mg/kg weight to 90 mg/kg weight, from about 0.001 mg/kg weight to 80 mg/kg weight, from about 0.001 mg/kg weight to 70 mg/kg weight, from about 0.001 mg/kg weight to 60 mg/kg weight, from about 0.001 mg/kg weight to 50 mg/kg weight, from about 0.001 mg/kg weight to 40 mg/kg weight, from about 0.001 mg/kg weight to 30 mg/kg weight, from about 0.001 mg/kg weight to 25 mg/kg weight, from about 0.001 mg/kg weight to 20 mg/kg weight, from about 0.001 mg/kg weight to 15 mg/kg weight, from about 0.001 mg/kg weight to 10 mg/kg weight. In some embodiments, the therapeutically effective amount described herein is provided in one dose. In some embodiments, the therapeutically effective amount described herein is provided in one day.

[0228] In still other embodiments, a therapeutically effective amount may be, for example, about 0.0001 mg/kg weight to 0.1 mg/kg weight, e.g. from about 0.0001 mg/kg weight to 0.09 mg/kg weight, from about 0.0001 mg/kg weight to 0.08 mg/kg weight, from about 0.0001 mg/kg weight to 0.07 mg/kg weight, from about 0.0001 mg/kg weight to 0.06 mg/kg weight, from about 0.0001 mg/kg weight to 0.05 mg/kg weight, from about 0.0001 mg/kg weight to about 0.04 mg/kg weight, from about 0.0001 mg/kg weight to 0.03 mg/kg weight, from about 0.0001 mg/kg weight to 0.02 mg/kg weight, from about 0.0001 mg/kg weight to 0.019 mg/kg weight, from about 0.0001 mg/kg weight to 0.018 mg/kg weight, from about 0.0001 mg/kg weight to 0.017 mg/kg weight, from about 0.0001 mg/kg weight to 0.016 mg/kg weight, from about 0.0001 mg/kg weight to 0.015 mg/kg weight, from about 0.0001 mg/kg weight to 0.014 mg/kg weight, from about 0.0001 mg/kg weight to 0.013 mg/kg weight, from about 0.0001 mg/kg weight to 0.012 mg/kg weight, from about 0.0001 mg/kg weight to 0.011 mg/kg weight, from about 0.0001 mg/kg weight to 0.01 mg/kg weight, from about 0.0001 mg/kg weight to 0.009 mg/kg weight, from about 0.0001 mg/kg weight to 0.008 mg/kg weight, from about 0.0001

mg/kg weight to 0.007 mg/kg weight, from about 0.0001 mg/kg weight to 0.006 mg/kg weight, from about 0.0001 mg/kg weight to 0.005 mg/kg weight, from about 0.0001 mg/kg weight to 0.004 mg/kg weight, from about 0.0001 mg/kg weight to 0.003 mg/kg weight, from about 0.0001 mg/kg weight to 0.002 mg/kg weight. In some embodiments, the therapeutically effective dose may be 0.0001 mg/kg weight, 0.0002 mg/kg weight, 0.0003 mg/kg weight, 0.0004 mg/kg weight, 0.0005 mg/kg weight, 0.0006 mg/kg weight, 0.0007 mg/kg weight, 0.0008 mg/kg weight, 0.0009 mg/kg weight, 0.001 mg/kg weight, 0.002 mg/kg weight, 0.003 mg/kg weight, 0.004 mg/kg weight, 0.005 mg/kg weight, 0.006 mg/kg weight, 0.007 mg/kg weight, 0.008 mg/kg weight, 0.009 mg/kg weight, 0.01 mg/kg weight, 0.02 mg/kg weight, 0.03 mg/kg weight, 0.04 mg/kg weight, 0.05 mg/kg weight, 0.06 mg/kg weight, 0.07 mg/kg weight, 0.08 mg/kg weight, 0.09 mg/kg weight, or 0.1 mg/kg weight. The effective dose for a particular individual can be varied (e.g., increased or decreased) over time, depending on the needs of the individual. In some embodiments, the therapeutically effective amount described herein is provided in one dose. In some embodiments, the therapeutically effective amount described herein is provided in one day.

[0229] In some embodiments, a provided composition is provided as a pharmaceutical formulation. In some embodiments, a pharmaceutical formulation is or comprises a unit dose amount for administration in accordance with a dosing regimen correlated with achievement of the reduced incidence or risk of cancer. In some embodiments, a pharmaceutical formulation is or comprises a unit dose amount for administration in accordance with a dosing regimen correlated with achievement of the reduced incidence or risk of infectious disease (i.e., vaccine). In some embodiments, a pharmaceutical formulation is or comprises a unit dose amount for administration in accordance with a dosing regimen correlated with achievement of the reduced incidence or risk of autoimmune disorders.

[0230] In some embodiments, a formulation comprising a STING modulator as described herein administered as a single dose. In some embodiments, a formulation comprising a STING modulator as described herein is administered at regular intervals. Administration at an "interval," as used herein, indicates that the therapeutically effective amount is administered periodically (as distinguished from a one-time dose). The interval can be determined by standard

clinical techniques. In some embodiments, a formulation comprising a STING modulator as described herein is administered bimonthly, monthly, twice monthly, triweekly, biweekly, weekly, twice weekly, thrice weekly, daily, twice daily, or every six hours. The administration interval for a single individual need not be a fixed interval, but can be varied over time, depending on the needs of the individual.

[0231] As used herein, the term "bimonthly" means administration once per two months (*i.e.,* once every two months); the term "monthly" means administration once per month; the term "triweekly" means administration once per three weeks (*i.e.*, once every three weeks); the term "biweekly" means administration once per two weeks (*i.e.*, once every two weeks); the term "weekly" means administration once per week; and the term "daily" means administration once per day.

[0232] In some embodiments, a formulation comprising a STING modulator as described herein is administered at regular intervals indefinitely. In some embodiments, a formulation comprising a STING modulator as described herein is administered at regular intervals for a defined period. In some embodiments, a formulation comprising a STING modulator as described herein is administered at regular intervals for 5 years, 4, years, 3, years, 2, years, 1 year, 11 months, 10 months, 9 months, 8 months, 7 months, 6 months, 5 months, 4 months, 3 months, 2 months, a month, 3 weeks, 2, weeks, a week, 6 days, 5 days, 4 days, 3 days, 2 days or a day.

Combination Therapy

[0233] In some embodiments, the present invention provides STING modulator agents for use in combination with one or more additional therapeutic and/or diagnostic agents and/or modalities. In some embodiments, provided agents are useful in combination with one or more other therapeutic agents or modalities known to be useful in the treatment or prevention of one or more STING -associated diseases, disorders, or conditions, and/or with the relief of one or more symptoms of such diseases, disorders, or conditions. For example, in some embodiments, provided agents are useful in combination with one or more chemotherapeutic, autoimmune medications and/or infectious disease agents. In some embodiments, provided agents are useful

in combination with one or more other agents or modalities that is or are approved by the United States Food and Drug Administration or one or more other non-US agencies.

[0234] In some embodiments, agents utilized in combination may be included in a single pharmaceutical compositions. More commonly, however, agents utilized in combination are administered in accordance with overlapping regimens so that a subject is simultaneously exposed to both (or all) agents, and/or is exposed to individual agents in a predetermined order and/or with a predetermined timing.

[0235] For purposes of the present disclosure, the term "palliative" refers to treatment that is focused on the relief of symptoms of a disease and/or side effects of a therapeutic regimen, but is not curative. For example, in some embodiments, palliative treatment encompasses painkillers and antinausea medications. Alternatively or additionally, in some embodiments, chemotherapy, radiotherapy, and surgery can all be used palliatively (that is, to reduce symptoms without going for cure; e.g., for shrinking tumors and reducing pressure, bleeding, pain, and/or other symptoms or signs of cancer).

[0236] In some embodiments, a STING modulator is administered in combination with one or more known therapeutic agents (e.g., autoimmune medications) currently used for treatment of autoimmune disorders (e.g., systemic lupus erythematosus).

[0237] In some embodiments, a STING modulator is administered in combination with one or more known therapeutic agents (e.g., anti-viral medications) currently used for treatment of infectious disease (e.g., pathogenic infection).

[0238] In some embodiments, the known therapeutic agent(s) is/are administered according to its standard or approved dosing regimen and/or schedule. In some embodiments, the known therapeutic agent(s) is/are administered according to a regimen that is altered as compared with its standard or approved dosing regimen and/or schedule. In some embodiments, such an altered regimen differs from the standard or approved dosing regimen in that one or more unit doses is altered (e.g., reduced or increased) in amount, and/or in that dosing is altered in frequency (e.g., in that one or more intervals between unit doses is expanded, resulting in lower frequency, or is reduced, resulting in higher frequency).

Applications for STING modulators

[0239] In certain embodiments provided modulators are useful in medicine. In some embodiments, provided modulators are useful in treating immune disease, disorders, or conditions. In some embodiments, the present invention provides a method for the treatment or prevention of an immune disease, disorder, or condition comprising administering to a subject in need thereof a provided modulator or a pharmaceutical composition thereof.

[0240] In some embodiments, the immune disease, disorder, or condition is an autoimmune disease, disorder, or condition. In certain embodiments, the immune disease, disorder, or condition is selected from the group consisting of any of a variety of diseases, disorders, and/or conditions, including but not limited to one or more of the following: autoimmune disorders (*e.g.* diabetes, lupus, multiple sclerosis, psoriasis, rheumatoid arthritis); inflammatory disorders (*e.g.* arthritis, pelvic inflammatory disease); infectious diseases (*e.g.* viral infections (*e.g.*, HIV, HCV, RSV), bacterial infections, fungal infections, sepsis); neurological disorders (*e.g.* Alzheimer's disease, Huntington's disease; autism; Duchenne muscular dystrophy); cardiovascular disorders (*e.g.* atherosclerosis, hypercholesterolemia, thrombosis, clotting disorders, angiogenic disorders such as macular degeneration); proliferative disorders (*e.g.* cancer, benign neoplasms); respiratory disorders (*e.g.* chronic obstructive pulmonary disease); digestive disorders (*e.g.* inflammatory bowel disease, ulcers); musculoskeletal disorders (*e.g.* fibromyalgia, arthritis); endocrine, metabolic, and nutritional disorders (*e.g.* diabetes, osteoporosis); urological disorders (*e.g.* renal disease); psychological disorders (*e.g.* depression, schizophrenia); skin disorders (*e.g.* wounds, eczema); blood and lymphatic disorders (*e.g.* anemia, hemophilia); *etc.* In some embodiments, the immune disease, disorder, or condition is characterized by inflammation. In some embodiments, the immune disease, disorder, or condition is caused by, sustained by, or related to cGAS activation. In some embodiments, the immune disease, disorder, or condition is caused by, sustained by, or related to STING activation.

[0241] In some embodiments the autoimmune disorder or disease is selected from Acute disseminated encephalomyelitis (ADEM), Addison's disease, Agammaglobulinemia, Alopecia

areata, Amyotrophic lateral sclerosis (Also Lou Gehrig's disease; Motor Neuron Disease), Ankylosing Spondylitis, Antiphospholipid syndrome, Antisynthetase syndrome, Atopic allergy, Atopic dermatitis, Autoimmune aplastic anemia, Autoimmune cardiomyopathy, Autoimmune enteropathy, Autoimmune hemolytic anemia, Autoimmune hepatitis, Autoimmune inner ear disease, Autoimmune lymphoproliferative syndrome, Autoimmune peripheral neuropathy, Autoimmune pancreatitis, Autoimmune polyendocrine syndrome, Autoimmune progesterone dermatitis, Autoimmune thrombocytopenic purpura, Autoimmune urticarial, Autoimmune uveitis, Balo disease/Balo concentric sclerosis, Behçet's disease, Berger's disease, Bickerstaff's encephalitis, Blau syndrome, Bullous pemphigoid Cancer, Castleman's disease, Celiac disease, Chagas disease, Chronic inflammatory demyelinating polyneuropathy, Chronic recurrent multifocal osteomyelitis, Chronic obstructive pulmonary disease, Churg-Strauss syndrome, Cicatricial pemphigoid Cogan syndrome, Cold agglutinin disease, Complement component 2 deficiency, Contact dermatitis, Cranial arteritis, CREST syndrome, Crohn's disease (idiopathic inflammatory bowel disease "IBD"), Cushing's Syndrome, Cutaneous leukocytoclastic angiitis, Dego's disease, Dermatitis herpetiformis, Dermatomyositis, Diabetes mellitus type 1, Diffuse cutaneous systemic sclerosis, Dressler's syndrome, Drug-induced lupus, Discoid lupus erythematosus, Eczema, Endometriosis, Enthesitis-related arthritis, Eosinophilic fasciitis, Eosinophilic gastroenteritis, Epidermolysis bullosa acquisita, Erythema nodosum, Erythroblastosis fetalis, Essential mixed cryoglobulinemia, Evan's syndrome, Fibrodysplasia ossificans progressiva, Fibrosing alveolitis (or Idiopathic pulmonary fibrosis), Gastritis, Gastrointestinal pemphigoid, Glomerulonephritis, Goodpasture's syndrome, Graves' disease, Guillain-Barré syndrome (GBS), Hashimoto's encephalopathy, Hashimoto's thyroiditis, Henoch-Schonlein purpura, Herpes gestationis aka Gestational Pemphigoid, Hidradenitis suppurativa, Hughes-Stovin syndrome, Hypogammaglobulinemia, Idiopathic inflammatory demyelinating diseases, Idiopathic pulmonary fibrosis, Idiopathic thrombocytopenic purpura, IgA nephropathy, Inclusion body myositis, Chronic inflammatory demyelinating polyneuropathy, Interstitial cystitis, Juvenile idiopathic arthritis aka Juvenile rheumatoid arthritis, Kawasaki's disease, Lambert-Eaton myasthenic syndrome, Leukocytoclastic vasculitis, Lichen planus, Lichen sclerosus, Linear IgA disease (LAD), Lupoid hepatitis aka Autoimmune hepatitis, Lupus erythematosus, Majeed syndrome, Ménière's disease, Microscopic polyangiitis, Miller-Fisher

syndrome see Guillain-Barre Syndrome, Mixed connective tissue disease, Morphea, Mucha-Habermann disease aka Pityriasis lichenoides et varioliformis acuta, Multiple sclerosis, Myasthenia gravis, Myositis, Narcolepsy, Neuromyelitis optica (also Devic's disease), Neuromyotonia, Occular cicatricial pemphigoid, Opsoclonus myoclonus syndrome, Ord's thyroiditis, Palindromic rheumatism, PANDAS (pediatric autoimmune neuropsychiatric disorders associated with streptococcus), Paraneoplastic cerebellar degeneration, Paroxysmal nocturnal hemoglobinuria (PNH), Parry Romberg syndrome, Parsonage-Turner syndrome, Pars planitis, Pemphigus vulgaris, Pernicious anaemia, Perivenous encephalomyelitis, POEMS syndrome, Polyarteritis nodosa, Polymyalgia rheumatica, Polymyositis, Primary biliary cirrhosis, Primary sclerosing cholangitis, Progressive inflammatory neuropathy, Psoriasis, Psoriatic arthritis, Pyoderma gangrenosum, Pure red cell aplasia, Rasmussen's encephalitis, Raynaud phenomenon, Relapsing polychondritis, Reiter's syndrome, Restless leg syndrome, Retroperitoneal fibrosis, Rheumatoid arthritis, Rheumatic fever, Sarcoidosis, Schizophrenia, Schmidt syndrome, Schnitzler syndrome, Scleritis, Scleroderma, Serum Sickness, Sjögren's syndrome, Spondyloarthropathy, Still's disease, Subacute bacterial endocarditis (SBE), Susac's syndrome, Sweet's syndrome, Sydenham chorea see PANDAS, Sympathetic ophthalmia, Systemic lupus erythematosis, Takayasu's arteritis, Temporal arteritis (also known as "giant cell arteritis"), Thrombocytopenia, Tolosa-Hunt syndrome, Transverse myelitis, Ulcerative colitis (one of two types of idiopathic inflammatory bowel disease "IBD"), Undifferentiated connective tissue disease different from Mixed connective tissue disease, Undifferentiated spondyloarthropathy, Urticarial vasculitis, Vasculitis, Vitiligo, and Wegener's granulomatosis.

[0242] In certain embodiments, administration of a STING modulator to a patient in need thereof results in a decrease of cGAS activity. In some embodiments, administration of a STING modulator to a patient in need thereof results in a decrease of STING activity. In some embodiments, compounds used in the provided methods are prepared by chemical synthesis.

[0243] In certain embodiments, the present invention provides a method of inhibiting STING comprising contacting STING with a provided modulator.

[0244] In certain embodiments, the present invention provides a method of modulating activity of an STING polypeptide, the method comprising contacting the STING polypeptide

with a STING modulator designed by the methods disclosed herein, which modulating agent is not a known modulator, substrate, or product of STING.

Kits

[0245] The invention provides a variety of kits for conveniently and/or effectively carrying out methods of the present invention. Typically kits will comprise sufficient amounts and/or numbers of components to allow a user to perform multiple treatments of a subject(s) and/or to perform multiple experiments.

[0246] In one aspect, the present invention provides kits comprising the molecules (compounds and compositions as described above) of the invention. In one embodiment, the kit comprises one or more functional antibodies or function fragments thereof.

[0247] Kits of the invention may comprise one or more STING parent molecules, or any mimic, analog or variant thereof. Kits may also comprise any of the STING variants, analogs or mutants described herein. The kit may further comprise packaging and instructions and/or a delivery agent to form a formulation composition. The delivery agent may comprise a saline, a buffered solution, a lipid or any delivery agent disclosed herein.

[0248] In one embodiment, the buffer solution may include sodium chloride, calcium chloride, phosphate and/or EDTA. In another embodiment, the buffer solution may include, but is not limited to, saline, saline with 2mM calcium, 5% sucrose, 5% sucrose with 2mM calcium, 5% Mannitol, 5% Mannitol with 2mM calcium, Ringer's lactate, sodium chloride, sodium chloride with 2mM calcium and mannose (See e.g., U.S. Pub. No. 20120258046; herein incorporated by reference in its entirety). In a futher embodiment, the buffer solutions may be precipitated or it may be lyophilized. The amount of each component may be varied to enable consistent, reproducible higher concentration saline or simple buffer formulations. The components may also be varied in order to increase the stability of the compound or composition in the buffer solution over a period of time and/or under a variety of conditions. In one aspect, the present invention provides kits for research applications related to STING activity or cGAMP signaling, provided in an amount effective to study the concomitant signaling pathways when

introduced into a target cell. The kits may further comprise a second or further modulator or composition described herein. Such second or further molecules may modulate the immune response or an inflammatory process or comprise one or more therapeutic molecules. In one embodiment, a kit comprises at least one STING polypeptide and at least one cGAMP molecule. In one embodiment, the kits of the present invention comprise packaging and instructions.

Exemplification

[0249] Unless otherwise described in a particular Example, the reagents, protocols and constructs used in each Example are as described below. In each case, one of skill in the art will recognize that variations of particular reagents or procedures would be acceptable equivalents and it is contemplated that these alternatives are considered as part of the present description. The Examples below are intended only to provide specific exemplary enbodiments, and are not limiting.

[0250] The following coordinates have been deposited in the RCSB Protein Data Bank, with which the skilled artisan will be familiar, and correspond to Tables 1-9 incorporated by reference herein. With respect to Tables 1-5, see also Gao, P., et al. *Cell* 154, 748-762 (2013), including supplementary materials, the entire contents of which are hereby incorporated by reference herein. Furthermore, in the context of Figures 1-3, 5, and 8-10, the data presented in Tables 1-5 of United States provisional patent application no. 61/860,818, filed July 31, 2013, are hereby incorporated by reference.

Sample	**PDB code[1]**	**Table**
c[G(2',5')pA(3',5')p]-hSTING^{H232} complex	4LOH	1
c[G(2',5')pA(2',5')p]-hSTING^{H232} complex	4LOI	2
c[G(2',5')pA(3',5')p]-mSting^{R231} complex	4LOJ	3
c[G(3',5')pA(3',5')p]-mSting^{R231} complex	4LOK	4
DMXAA-mSting^{R231} complex	4LOL	5
DMXAA-hSTING^{group2} complex	4QXO	6
DMXAA-hSTING^{G230I} complex	4QXP	7

DMXAA-hSTING$^{S162A/Q266I}$ complex	4QXQ	8
DMXAA-hSTING$^{S162A/G230I/Q266I}$ complex	4QXR	9

[1] One method of accessing the RCSB Protein Data Bank is online at www.rcsb.org.

[0251] Tables 6-9 are found at the end of the specification and are hereby incorporated by reference herein in their entirety. Table 6 lists atomic structure coordinates for a DMXAA-hSTING^{group2} complex as derived from X-ray diffraction from the corresponding crystal. Table 7 lists atomic structure coordinates for a DMXAA-hSTING^{G230I} complex as derived from X-ray diffraction from the corresponding crystal. Table 8 lists atomic structure coordinates for a DMXAA-hSTING$^{S162A/Q266I}$ complex as derived from X-ray diffraction from the corresponding crystal. Table 9 lists atomic structure coordinates for a DMXAA-hSTING$^{S162A/G230I/Q266I}$ complex as derived from X-ray diffraction from the corresponding crystal.

Plasmid Construction

[0252] The human and murine STING sequences (reference sequences) used in the following Examples were inserted into a modified pMAX-cloning (Amaxa, Cologne, Germany) by standard cloning techniques, in frame with a N-terminal FLAG-tag. Site-directed mutagenesis was performed by the Quikchange method (Agilent, Santa Clara, CA) using Pfu Ultra Hot Start DNA Polymerase (Agilent) or Phusion Polymerase (NEB, Ipswich, MA). Luciferase reporter constructs were as described (Gao et al., 2013). Constructs (Figure 147) were verified by restriction digest and Sanger sequencing (Seqlab, Göttingen, Germany).

Table S7. Primer sequences for STING cloning and mutagenesis

Primer Name	Sequence (5'-3')	SEQ ID NO.
mSTINGfwSalI	ATATATGTCGACATGCCATACTCCAACCTGCATCCA	3
mSTINGrevNotI	ATATATGCGGCCGCTCAGATGAGGTCAGTGCGGAGT	4
hSTINGfwSalI	ATATATGTCGACACCATGCCCCACTCCAGCCTGCA	5
hSTINGrevNotI	ATATATGCGGCCGCTCAAGAGAAATCCGTGCGGAGA	6

hSTINGfw-39bpFlag-GibA	GCCACCATGGATTACAAGGATGACGACGATAAGGTCG ACATGCCCCACTCCAGCCTGCA	7
hSTINGrev458-GibA	AAATTCCCTTTTTCACACACTGCAG	8
hSTINGfw420-GibA	CCCAGCTGAGATCTCTGCA	9
hSTINGrev-40bp-GibA	TGTGGTTTGTCCAAACTCATCGAGCTCGATGCGGCCG CGGTCAAGAGAAATCCGTGCGGAGA	10
mmSTING t481g_antisense	CCCAATGTAGTATGCCCAGGCCAGCCCG	11
mmSTING t481g	CGGGCTGGCCTGGGCATACTACATTGGG	12
mmSTING t496g_a497c	CTGGTCATACTACATTGGGGCCTTGCGGTTGATCTTACCA	13
mmSTING t496g_a497c_antisense	TGGTAAGATCAACCGCAAGGCCCCAATGTAGTATGACCAG	14
mmSTING c709g_g710c	CGACCGTGCTGGCATCAAGAATGCGGTTTATTCCAACAG	15
mmSTING c709g_g710c_antisense	CTGTTGGAATAAACCGCATTCTTGATGCCAGCACGGTCG	16
mmSTING t715g_a716c_antisense	TCGTAGACGCTGTTGGAAGCAACCCGATTCTTGATGCCAG	17
mmSTING t715g_a716c	CTGGCATCAAGAATCGGGTTGCTTCCAACAGCGTCTACGA	18
mmSTING a721g_a722c_antisense	CAGAATCTCGTAGACGCTGGCGGAATAAACCCGATTCTTG	19
mmSTING a721g_a722c	CAAGAATCGGGTTTATTCCGCCAGCGTCTACGAGATTCTG	20
mmSTING a776c_antisense	GGGGGTGGCGTACGCCAGGATACAGAC	21
mmSTING a776c	GTCTGTATCCTGGCGTACGCCACCCCC	22
mmSTING a784g	CCTGGAGTACGCCGCCCCCTTGCAGAC	23
mmSTING a784g_antisense	GTCTGCAAGGGGGCGGCGTACTCCAGG	24
mmSTING a796g_antisense	CATGGCAAACAGGGCCTGCAAGGGGGTGG	25
mmSTING a796g	CCACCCCCTTGCAGGCCCTGTTTGCCATG	26
hSTING t484g_c485g_antisense	AGATATCCGATGTAATATCCCCATGCCAGCCCATGGGC	27

hSTING t484g_c485g	GCCCATGGGCTGGCATGGGGATATTACATCGGATATCT	28
hSTING t484a_a486g	GCCCATGGGCTGGCATGGACGTATTACATCGGATATCTG	29
hSTING t484a_a486g_antisense	CAGATATCCGATGTAATACGTCCATGCCAGCCCATGGGC	30
hSTING c485t	CCATGGGCTGGCATGGTTATATTACATCGGATATC	31
hSTING c485t_antisense	GATATCCGATGTAATATAACCATGCCAGCCCATGG	32
hSTINGfw-39bpFlag-GibA	GCCACCATGGATTACAAGGATGACGACGATAAGGTCGACAT GCCCCACTCCAGCCTGCA	33
hSTINGrev458-GibA	AAATTCCCTTTTTCACACACTGCAG	34
hSTINGfw420-GibA	CCCAGCTGAGATCTCTGCA	35
hSTINGrev-40bp-GibA	TGTGGTTTGTCCAAACTCATCGAGCTCGATGCGGCCGCGGT CAAGAGAAATCCGTGCGGAGA	36
revbefgroup1	TGGCAGGATCAGCCGCAG	37
fwbefgroup1	CTGCGGCTGATCCTGCCA	38
revbefgroup2	ACAGTCCAATGGGAGGAGAATATACAG	39
fwbefgroup2	CTGTATATTCTCCTCCCATTGGACTGT	40
revbefgroup3	TGGCGTACTCCAGGACACAGG	41
fwbefgroup3	CCTGTGTCCTGGAGTACGCCA	42
revbefgroup4	ACAGCGAGAAGCTGCTGTCAT	43
fwbefgroup4	ATGACAGCAGCTTCTCGCTGT	44
revbeforore266	TGGCGTACTCCAGGACACAG	45
fwbefore266	AGCTTCTGGAGAACGGGCAG	46
fwafter266	TGCCATGTCACAATACAGTCAAGCT	47
revafter266	GGCCTGCTCAAGCCTATCCTC	48
G230R232fw	CTGCCCCAGCAGACCGGTGACCGTGCTGGCATCAAGGATC	49
G230R232rev	GATCCTTGATGCCAGCACGGTCACCGGTCTGCTGGGGCAG	50

A230R232fw	CTGCCCCAGCAGACCGCTGACCGTGCTGGCATCAAGGATC	51
A230R232rev	GATCCTTGATGCCAGCACGGTCAGCGGTCTGCTGGGGCAG	52
G230H232fw	CTGCCCCAGCAGACCGGTGACCATGCTGGCATCAAGGATC	53
G230H232rev	GATCCTTGATGCCAGCATGGTCACCGGTCTGCTGGGGCAG	54
group2toGfw	CTGCCCCAGCAGAACGGTGACCGTGCTGGCATCAAGAATC	55
group2toGrev	GATTCTTGATGCCAGCACGGTCACCGTTCTGCTGGGGCAG	56
Q266Ifw	GTGACATGGCAAACAAAGTTATCAAGGGGGTGGCGTACTCC	57
Q266Irev	GGAGTACGCCACCCCCTTGATAACTTTGTTTGCCATGTCAC	58
S162Afw	CCCATGGGCTGGCATGGGCATATTACATCGGATATC	59
S162Arev	GATATCCGATGTAATATGCCCATGCCAGCCCATGGG	60
G230I 232H_fw	CTGCCCCAGCAGACCATTGACCATGCTGGCAT	61
G230I 232H_rev	ATGCCAGCATGGTCAATGGTCTGCTGGGGCAG	62
G230I 232R_fw	TCCTTGATGCCAGCACGGTCAATGGTCTGCTGGGGCAG	63
G230I 232R_rev	CTGCCCCAGCAGACCATTGACCGTGCTGGCATCAAGGA	64
I165Afw	GGGCTGGCATGGTCATATTACGCCGGATATCTGCGGCT	65
I165Arev	AGCCGCAGATATCCGGCGTAATATGACCATGCCAGCCC	66
G166Sfw	CTGGCATGGTCATATTACATCAGCTATCTGCGGCTGATCC	67
G166Srev	GGATCAGCCGCAGATAGCTGATGTAATATGACCATGCCAG	68
I235Lfw	AGACCGGTGACCGTGCTGGCCTCAAGGATCGGG	69
I235Lrev	CCCGATCCTTGAGGCCAGCACGGTCACCGGTCT	70
Q266Ifw	GGAGTACGCCACCCCCTTGATAACTTTGTTTGCCATGTCAC	71
Q266Irev	GTGACATGGCAAACAAAGTTATCAAGGGGGTGGCGTACTCC	72
Q266Lfw	CGCCACCCCCTTGCTGACTTTGTTTGCCAT	73
Q266Lrev	ATGGCAAACAAAGTCAGCAAGGGGGTGGCG	74
Q266Vfw	GTACGCCACCCCCTTGGTGACTTTGTTTGCCATGT	75

Q266Vrev	ACATGGCAAACAAAGTCACCAAGGGGGTGGCGTAC	76
mSTING_I229Gfw	ATGCTGCCCCAGCAAAACGGCGACCGTGCTGG	77
mSTING_I229Grev	CCAGCACGGTCGCCGTTTTGCTGGGGCAGCAT	78
mSTING_I229Afw	ATGCTGCCCCAGCAAAACGCCGACCGTGCTGG	79
mSTING_I229Arev	CCAGCACGGTCGGCGTTTTGCTGGGGCAGCAT	80

[0253] Human STING mutants were assembled from C-terminal mutated constructs (140-C) and N-terminal reference sequence by Gibson Assembly (NEB) and confirmed by Sanger sequencing. $STING^{THP1}$ and $STING^{R232}$ cDNAs were cloned from THP1 cells and Peripheral Blood Mononuclear Cells of a voluntary human donor with informed consent, respectively.

Protein Expression and Purification

[0254] Unless otherwise specified, sequences used in the following Examples corresponding to residues aa 140-379 and 155-341 of $hSTING^{H232}$, $hSTING^{R232}$, $hSTING^{A230/R232}$, $hSTING^{group2}$, $hSTING^{G230I}$, $hSTING^{S162A/Q266I}$, and $hSTING^{S162A/G230I/Q266I}$; and residues 139-378 and 154-340 of $mSTING^{R231}$ were inserted into a modified pRSFDuet-1 vector (Novagen), in which the target protein was separated from the preceding His_6-SUMO tag by an ubiquitin-like protease (ULP1) cleavage site. The gene sequences were subsequently confirmed by sequencing. The fusion proteins were expressed in BL21 (DE3) RIL cell strain. The cells were grown at 37 °C until OD600 reached approx. 0.6. The temperature was then shifted to 18 °C and the cells were induced by addition of isopropyl β-D-1-thiogalactopyranoside (IPTG) to the culture medium at a final concentration of 0.3 mM. After induction, the cells were grown overnight. The fusion proteins were purified over a Ni-NTA affinity column. The His_6-SUMO tag was removed by ULP1 cleavage during dialysis against buffer containing 40 mM Tris-HCl, 300 mM NaCl, pH 7.5. After dialysis, the His_6-SUMO tag was removed by Ni-NTA affinity column and the sample was further fractionated over a gel filtration 16/60 G200 Superdex column. The final sample of $hSTING^{H232}$, $hSTING^{R232}$ and $hSTING^{A230/R232}$, $mSTING^{R231}$, $hSTING^{group2}$, $hSTING^{G230I}$, $hSTING^{S162A/Q266I}$, and $hSTING^{S162A/G230I/Q266I}$ contain

about 13-16 mg/ml protein, 20 mM Tris-HCl, 150 mM NaCl, pH 7.5. All the mutants were cloned and purified using the same protocol as used for preparation of the wild-type protein.

Crystallization

[0255] Crystals were grown in the following Examples using the sitting drop vapor diffusion method and diffraction data collected at synchrotron beam lines. For crystallization of $hSTING^{H232}$ (155-341) with c[G(2',5')pA(3',5')p] and c[G(2',5')pA(2',5')p], the protein was incubated with c[G(2',5')pA(3',5')p] (2 mM) or c[G(2',5')pA(2',5')p] (2 mM) and $MgCl_2$ (5 mM) for 0.5 h at room temperature. The crystals were generated by sitting drop vapor diffusion method at 20 °C, by mixing equal volume reservoir solution (for c[G(2',5')pA(3',5')p]: 0.01 M $NiCl_2$, 0.1 M Tris, 20% PEG2000, pH 8.5; for c[G(2',5')pA(2',5')p]: 1.6 M NaH_2PO_4, 0.4 M Na_2HPO_4, 0.1 M phosphate-citrate, pH 4.2) with the sample.

[0256] For crystallization of $mSTING^{R231}$ (154-340) with c[G(2',5')pA(3',5')p], c[G(3',5')pA(3',5')p] and DMXAA, the protein was incubated with c[G(2',5')pA(3',5')p] (2 mM) or c[G(3',5')pA(3',5')p] (2 mM) or DMXAA (4 mM) for 0.5 h at room temperature. The crystals were generated by sitting drop vapor diffusion method at 20 °C, by mixing equal volume reservoir solution (for c[G(2',5')pA(3',5')p]: 0.2 M di-ammonium tartrate, 20% PEG3350; for c[G(3',5')pA(3',5')p]: 0.2 M sodium formate, 20% PEG3350; for DMXAA: 1.6 M ammonium sulfate, 0.1 M Tris-HCl, pH 8.0) with the samples.

[0257] For crystallization of DMXAA with hSTING mutants (aa 155-341), the protein samples were mixed and incubated with DMXAA (1:2 molar ratio) for 0.5 h at room temperature before setting up crystals. The crystals were generated by sitting drop vapor diffusion method at 20 °C, by mixing equal volume reservoir solution with the sample. The detailed conditions are listed below: DMXAA-$hSTING^{group2}$: 2 M LiCl, 10% PEG6000, 0.01 M $CaCl_2$, 0.1 M Tris, pH 7.8; DMXAA-$hSTING^{G230I}$: 0.2 M Li_2SO_4, 20% PEG 3350, 0.015 mM CYMAL®-7, 0.1 M Tris, pH 8.1; DMXAA-$hSTING^{S162A/Q266I}$: 0.2 M $Ca(Ac)_2$, 15% PEG3000, 0.01 M L-Proline, 0.1 M NaAc, pH 5.1; DMXAA-$hSTING^{S162A/G230I/Q266I}$: 0.2 M $Ca(Ac)_2$, 15% PEG3000, 0.1 M LiCl, 0.1 M NaAc, pH 5.1. All structures were solved using PHASER, COOT, PHENIX, and REFMAC programs.

Structure Determination

[0258] All the diffraction data sets (except mSTING^{R231} with DMXAA) in the following Examples were collected at the Brookhaven National Laboratory, and were indexed, integrated and scaled using the HKL2000 program (Otwinowski and Minor, 1997). The data set for mSTING^{R231}, hSTING^{group2}, hSTING^{G230I}, hSTING$^{S162A/Q266I}$, and hSTING$^{S162A/G230I/Q266I}$ with DMXAA were collected at Argonne National Laboratory and was indexed, integrated and scaled using the RAPD online server. The structure of hSTING^{H232} with c[G(2',5')pA(3',5')p] or c[G(2',5')pA(2',5')p] was solved using molecular replacement method in PHASER (McCoy et al., 2007) using the complex structure of hSTING$^{A230/R232}$ and c[di-GMP] (PDB: 4F5D) as the search model. For mSTING^{R231} with c[G(2',5')pA(3',5')p], c[G(3',5')pA(3',5')p] and DMXAA, the structure of mSTING^{R231} and CMA (PDB: 4JC5) was used as the search model. For the cGAMP-STING binary structures, two STING molecules in the STING dimer have equal probability to bind with either G or A moiety of the cGAMP isomers. The electron density also clearly indicated that the cGAMP isomers adopt two alternative conformations. We therefore assigned two conformations with 0.5 occupancy for bound cGAMP isomers.

[0259] The structures of DMXAA-hSTING^{group2}, DMXAA-hSTING^{G230I}, DMXAA-hSTING$^{S162A/Q266I}$, and DMXAA-hSTING$^{S162A/G230I/Q266I}$ were solved using molecular replacement method in PHASER (McCoy et al., 2007) using the structure of hSTING^{H232} complex bound to c[G(2',5')pA(3',5')p] (PDB: 4LOH) as the search model.

[0260] The model building was conducted using the program COOT (Emsley et al., 2010) and structural refinement was conducted using the program REFMAC (Murshudov et al., 1997). The statistics of the data collection and refinement are shown in Table S1, S2, and S7.

Isothermal Titration Calorimetry

[0261] The dissociation constants (Kd) and thermodynamic parameters of binding reactions of hSTING^{H232} (aa 140-379), hSTING^{R232} (aa 140-379), hSTING$^{A230/R232}$ (aa 140-379), mSting^{R231} (aa 139-378), mSting^{A231} (aa 139-378), hSTING^{H232} (aa 140-379), hSTING^{group2} (aa 140-379), hSTING^{G230I} (aa 140-379), hSTING$^{S162A/Q266I}$ (aa 140-379), and hSTING$^{S162A/G230I/Q266I}$

(aa 140-379), mutants with different cGAMP isomers or DMXAA were measured in the following Examples by isothermal titration calorimetry using a MicroCal ITC200 calorimeter at 25°C. First, wild-type and mutant protein samples were dialyzed overnight against working buffer (100 mM NaCl, 30 mM HEPES, pH 7.5) at 4 °C. Then, the protein samples were diluted with working buffer and the lyophilized cGAMP isomers or DMXAA were dissolved in working buffer. The titration was carried out with 16 successive injections of 2.4 μL cGAMP isomers or DMXAA, spaced 180s apart, into the sample cell containing the protein solution. The data for $mSting^{R231}$ (aa 139-378) and $hSTING^{S162}$ (aa 140-379) mutants with DMXAA were collected using the same protocol as used for STING with cGAMP isomers. The detailed concentration for different titrations was listed in Table S3, S4 and S6. The data were fit using the program Origin 7.0 software.

[0262] We observe a mixture of exothermic and endothermic transitions for complex formation of hSTING/mSting complexes with c[G(3',5')pA(3',5')p] (green triangles, Figure 4, and Table S3), primarily endothermic transitions for complex formation of hSTING/mSting complexes with c[G(2',5')pA(2',5')p] (red circles, Figure 4, and Table S3), and exclusively endothermic transitions for hSTING/mSting complexes bound to c[G(2',5')pA(3',5')p] (black squares, Figure 4, and Table S3). Endothermic binding events are not uncommon and may reflect ligand-induced conformational changes in STING that yield significant solvent reorganization/displacement, often resulting in 'melting' (an endothermic event) and release (an entropically favorable event) of 'restricted' (bound) solvent (Table S3). The distinct thermodynamic outcome (exothermic versus endothermic) could possibly relate to very subtle structural differences or alternately to the use of distinct folding pathways with defined energy parameters to arrive at the same or a distinct endpoint.

Mice

[0263] Female C57B/6 mice between 6 and 10 weeks of age were purchased from the Jackson Laboratory and were used for the preparation of bone marrow-derived macrophages in the following Examples. These mice were maintained in the animal facility at the Sloan-Kettering Cancer Institute. All procedures were performed in strict accordance with the recommendations in the Guide for the Care and Use of Laboratory Animals of the National

Institute of Health. The protocol was approved by the Committee on the Ethics of Animal Experiments of Sloan-Kettering Cancer Institute (protocol number 96-04-017). $IRF3^{-/-}$ and $STING^{Gt/Gt}$ mice were generated in the laboratories of Drs. Tadatsugu Taniguchi (University of Tokyo) and Russell Vance (University of California, Berkeley).

Generation of Bone-Marrow-Derived Macrophages

[0264] Female $IRF3^{-/-}$, $STING^{Gt/Gt}$ and WT C57B/6 mice were used for the preparation of bone marrow-derived macrophages in the following Examples. These mice were maintained in the animal facility at the Sloan-Kettering Cancer Institute. Bone marrow cells were cultured in complete medium (CM) in the presence of 5% of supernatant of L929 mouse fibroblasts as conditioned medium providing macrophage colony-stimulating factor (M-CSF) for 7 days. CM is RPMI 1640 medium supplemented with 10% heat-inactivated fetal bovine serum (FBS), 100 U/ml penicillin, 100 μg/ml streptomycin, 0.1mM essential and nonessential amino acids, 2 mM L-glutamine, 1 mM sodium pyruvate, and 10 mM HEPES-KOH buffer. Cells were fed at day 4 by replacing 50% of the old medium with fresh medium. Cells were plated into 6-well plate (1 million cells per well) at day 7, the day before stimulation.

Generation of Bone Marrow-derived Dendritic Cells

[0265] The protocol for generation of bone marrow-derived dendritic cells was described before (Dai et al., 2014). Bone marrow-derived dendritic cells were generated by culturing bone marrow cells from the tibia and femur of $STING^{Gt/Gt}$ mice in complete medium (CM) in the presence of GM-CSF (30 ng/ml, produced by the Monoclonal Antibody Core facility at the Sloan Kettering Institute) for 10 days. CM is RPMI 1640 medium supplemented with 10% heat-inactivated fetal bovine serum (FBS), 100 U/ml penicillin, 100 μg/ml streptomycin, 0.1 mM essential and nonessential amino acids, 2 mM L-glutamine, 1 mM sodium pyruvate, and 10 mM HEPES buffer. Cells were fed every 2-3 days by replacing 50% of the old medium with fresh medium. Cells were plated into 6-well plate (1×10^6 cells per well) at day 10, the day before retroviral infection. BMDCs ($1x10^6$ cells/well) were infected with retroviruses expressing hSTING (wt and various substitution mutants). 48 hours after retroviral infection, cells were stimulated with DMXAA.

Retroviruses Transduction and DMXAA Treatment

[0266] hSTING cDNAs were cloned into pQCXIP-HA vector. In vitro packaging system was used to generate retroviruses according to protocol (Clontech). BMDCs ($1x10^6$ cells/well) were seeded into 6-well plates and infected with retroviruses. 48 hours after retroviral infection, cells were stimulated with DMXAA at a final concentration of 50 μg/ml (Sigma). For real-time PCR analysis, cells were collected at 3 hours post DMXAA treatment. Supernatants were collected at 18 hours post DMXAA treatment. CXCL10 protein level was determined by ELISA.

THP1 Cell Culture

[0267] Human THP1 cells were cultured in RPMI1640 (Life Technologies) containing 10% FBS, 2 mM glutamine (Life Technologies), 1 mM sodium pyruvate (Life Technologies), and 100 U/ml penicillin/streptomycin (Life Technologies).

cGAMP Stimulation of Cells

[0268] Bone marrow derived murine macrophages and THP-1 cells were stimulated by incubation with cGAMP isomers at indicated concentrations for 18 hrs, or by Digitonin permeabilization (30 minutes) at indicated concentrations as described (Woodward et al., 2010). Cytokines in supernatants were determined after 18 hrs by ELISA. THP1 cells were plated at $8x10^4$ cells per 96-well and treated as described above.

RT-PCR analysis of THP1 Cells

[0269] For RT-PCR analyses in the following Examples, $5x10^5$ THP1 cells were plated in 12-well dishes and incubated overnight. 12.5 μM of cGAMP isomers were applied to the media and cells were harvested at indicated times. RNA samples were isolated and cDNA libraries were generated. KOD Polymerase was used to PCR amplify regions of IFNB1 and CXCL10 and normalized against TUBA1B.

RNA Isolation and Real-time PCR

[0270] Total RNA was extracted from whole-cell lystates with an RNeasy Mini kit (Qiagen) and reverse transcribed with the First Strand cDNA synthesis kit (Fermentas) in the following Examples. Quantitative real-time PCR was performed in triplicate with the Applied

Biosystem 7500 Real-Time PCR Detection System (Life Technologies) using Fast SYBR Green Master Mix and gene-specific primers. Relative expression was normalized to the levels of glyceraldehyde-3-phosphate dehydrogenase (GADPH).

RT-PCR Analysis

[0271] RNA was extracted and isolated from each sample in the following Examples using TRIzol (Life Technologies), per manufacturer's instructions. Superscript III RT-PCR Kit (Life Technologies) was used for generating cDNA libraries, using oligo-dT primers, per manufacturer's instructions. The following primers were used for PCR:

IFNB1

5'-GGACCATAGTCAGAGTGGAAATCCTAAG-3' (SEQ ID NO.:33)

5'-CACTTAAACAGCATCTGCTGGTTGAAG-3' (SEQ ID NO.:34)

5'-TGGAGATGACGGAGAAGATG-3' (SEQ ID NO.:81)

5'-TTGGATGGCAAAGGCAGT-3' (SEQ ID NO.:82)

TUBA1B

5'-ACCTTAACCGCCTTATTAGCCA-3' (SEQ ID NO.:35)

5'-ACATTCAGGGCTCCATCAAATC-3' (SEQ ID NO.:36)

CXCL10

5'-GCTACCTACATACAATTCCAAACACATAC-3' (SEQ ID NO.:37)

5'-GTACTTAATTACATGTTATTCCATGTACACTGAAAAC-3' (SEQ ID NO.:38)

5'-GTCAGGTTGCCTCTGTCTCA-3' (SEQ ID NO.:83)

5'-TCAGGGAAGAGTCTGGAAAG-3' (SEQ ID NO.:84)

CCL5

5'-GCCCACGTCAAGGAGTATTTCTA-3' (SEQ ID NO.:85)

5'-ACACACTTGGCGGTTCCTTC-3' (SEQ ID NO.:86)

IL-6

5'-AGGCATAACGCACTAGGTTT-3' (SEQ ID NO.:87)

5'-AGCTGGAGTCACAGAAGGAG-3' (SEQ ID NO.:88)

GAPDH

5'-ATCAAGAAGGTGGTGAAGCA-3' (SEQ ID NO.:89)

5'-AGACAACCTGGTCCTCAGTGT-3' (SEQ ID NO.:90)

PCR was accomplished using KOD Hot Start DNA polymerase (EMD Millipore) according to manufacturer's instructions. ImageJ (v1.47q) was used for quantitation of amplicons using TUBA1B for normalization.

Cell Culture

[0272] 293T cells (Life Technologies, Carlsbad, CA) were grown in DMEM supplemented with 10% fetal bovine serum (FBS), 1 mM sodium pyruvate, 1x MEM non-essential amino acids and 100 U/ml Penicillin/Streptomycin (Life Technologies).

Luciferase Assay

[0273] HEK293T cells in the following Examples were reverse-transfected with STING expression plasmids and reporter constructs. 12 hrs later, DMXAA was added directly, while cGAMP isomers and c[di-GMP] were delivered with digitonin permeabilization. Luciferase expression was determined after another 12 hrs, or 30 hrs when transfected together with a cGAS-expression plasmid.

[0274] For cGAMP Luciferase Assays, $3x10^4$ HEK293T cells (Life Technologies, Carlsbad, CA) per 96-well were reverse-transfected with a mix of pGL3-IFNB1-Gluc (50ng), pLenti-EF1-Fluc (10ng), pMAX-Flag-STING (5ng) and 35 ng empty plasmid (pMAX-cloning; Amaxa, Cologne, Germany) using Trans-IT LT1 Reagent (MirusBio, Madison, WI). 12h after transfection, cGAMP isomers (synthesized by Roger Jones) and c[di-GMP] (Invivogen, San Diego, CA) were delivered with digitonin permeabilization as described (Woodward et al., 2010). DMXAA (Sigma) was diluted in fresh medium added to transfected cells. Luciferase expression was determined after 12 h. For stimulation by cGAS, cells were transfected as described above, but instead of empty plasmid pLenti(p)-EF1-Flag-mm-cGAS (WT or non-functional E211A mutation) was used, and Luciferase expression was determined 30 h after transfection. In this setting, expression plasmid served as cGAS stimulus at the same time. Cells were lysed in Passive Lysis Buffer. Firefly and gaussia luciferase activities were determined on an EnVision reader (Perkin Elmer, Waltham, MA) using their respective substrates (D-Luciferin

and coelenterazine, PJK GmbH, Kleinblittersdorf, Germany) according to standard protocols. IFNB1-Gluc values were normalized to constitutive firefly luciferase values and fold induction was calculated in relation to control-plasmid pMAX-GFP.

[0275] Luciferase assays for DMXAA experiments were performed as described above. Briefly, $3x10^4$ 293T cells were reverse-transfected with STING constructs (5 ng per 96-well) and reporter constructs (50 ng pIFNβ-Gluc, 10 ng pLenti-EF1-Fluc for normalization, 35 ng pMAX-empty as stuffer, delivered with TransIT-LT1, MirusBio, Madison WI). 12 hours after transfection, medium was replaced with fresh Medium containing DMXAA. 12 hours after stimulation with STING-ligands, cells were resuspended in passive lysis buffer and luciferase activity was determined using the respective substrates Coelenterazine and D-Luciferin (PJK, Kleinblittersdorf, Germany). Gaussia Luciferase values were then normalized to constitutive Firefly Luciferase values (resulting in Relative Light Units, RLU).

ELISA

[0276] CXCL10 was measured using the BD Opteia human IP-10 ELISA Set according to manufacturer's recommendations. Murine IFN-α was determined by ELISA using antibody RMMA-1 for capture and rabbit-anti-murine IFN-α polyclonal antibody for detection (PBL Interferon Source, Piscataway, NJ). Dose-response curves were fitted and EC_{50} values were determined with Graphpad Prism (Graph Pad Software Inc., San Diego, CA).

Western Blot Analysis

[0277] BMDMs (1×10^6) were treated with cGAMP linkage isomers. At various times post-stimulation, the medium was removed and cells were collected. Whole-cell lysates were prepared at 2, 4, and 8 h post-treatment. Equal amounts of proteins were subjected to SDS-PAGE and transferred to a nitrocellulose membrane. Phosphorylation of IRF3 was determined using a rabbit polyclonal antibody specific for phosphoserine-396 of IRF3 (Cell signaling). The level of IRF3 was determined by using a rabbit polyclonal antibody against IRF3. Phosphorylation of TBK1 was determined using a rabbit monoclonal antibody specific for phosphoserine-172 of TBK1 (Cell Signaling). The level of TBK1 was determined by using a rabbit monoclonal

antibody against TBK1 (Cell Signaling). Anti-glyceraldehyde-3-phosphate dehydrogenase (GADPH) was used as loading controls.

[0278] BMDCs (1 x 10^6 cells) were infected with retroviruses carrying WT hSTING and various hSTING mutants. Cells were collected at 2 days post retroviral infection. Whole-cell lysates were prepared by lysing cells in RIPA buffer. Equal amounts of proteins were subjected to SDS-PAGE and transferred to a nitrocellulose membrane. The levels of HA-hSTING in transduced cells were determined by using a mouse monoclonal antibody specific for HA tag (Covance). Anti-glyceraldehyde-3-phosphate dehydrogenase (GAPDH) was used as a loading control, and was detected using a polyclonal antibody against GAPDH (Cell Signaling).

Example 1: Crystal Structure of c[G(2',5')pA(3',5')p] Bound to hSTING^{H232}

[0279] The present Example presents the 2.25 Å crystal structure of an ~186 amino acid human STING polypeptide bound to c[G(2',5')pA(3',5')p].

[0280] The 2.25 Å crystal structure of c[G(2',5')pA(3',5')p] bound to the symmetrical dimer of human STING (G230/H232; aa 155-341; termed hSTING^{H232}) is shown in Figure 1A (x-ray statistics in Table S1). The individual symmetry-related subunits of STING in a ribbon representation are color-coded in magenta and yellow, while the bound c[G(2',5')pA(3',5')p] is shown in a space-filling representation. The bound ligand is positioned in a deep U-shaped cleft between subunits, with the cyclic sugar-phosphate backbone at the base and the purine rings pointing upwards in a parallel alignment (expanded view in Figure 1B). The bound U-shaped ligand is further anchored in place by an overhead cap element formed on complex formation by an anti-parallel four-stranded β-pleated sheet (Figure 2A), such that the hSTING dimer completely envelops the bound ligand (Figure 1C, D).

Table S1. X-ray Statistics for cGAMP Linkage Isomers with hSTING^{H232}

Data collection and refinement statistics of hSTING with Ligands		
Crystal	**hSTING^{H232} + c[G(2',5')pA(3',5')p]**	**hSTING^{H232} + c[G(2',5')pA(2',5')p]**
Beam line	NSLS-X29A	NSLS-X29A
Wavelength	1.075	1.075
Space group	*P*1	$P2_12_12$
Unit cell		
a, b, c (Å)	36.5, 59.2, 59.2	94.1, 116.7, 36.2
α, β, γ (°)	84.0, 85.8, 85.9	90.0, 90.0, 90.0
Resolution (Å)	50-2.3 (2.33-2.25)[a]	50-1.9 (1.97-1.90)[a]
R_{merge}	0.026 (0.284)	0.060 (0.382)
I/ σ (I)	45.4 (5.1)	40.8 (5.8)
Completeness (%)	97.9 (97.1)	99.8 (100)
Redundancy	3.9 (3.9)	6.7 (6.5)
Number of unique reflections	22653	32537
Wilson B factors (Å^2)	22.24	20.11
R_{work}/R_{free} (%)	18.63/21.53	17.6/19.9
Number of non-H atoms		
Protein	2960	2914
Water	127	227
Ligands(molecule)	1	1
Average B factors (Å^2)		
Protein	36.09	31.42
Water	32.08	37.06
ligands	16.35	19.01
R.m.s. deviations		
Bond lengths (Å)	0.020	0.018

[a] Highest resolution shell (in Å) shown in parentheses.

[0281] Relates to Figure 1, 2 and 3.

[0282] The binding pocket is uncharged at its base, while both positive- and negative-charged residues line its walls. The bound c[G(2',5')pA(3',5')p] is anchored by its purine bases being bracketed on either side by Y167 (Figure 1E) and by R238 (whose position is buttressed by Y240), with R238 aligned in the plane and hydrogen bonds to the N7 of one purine, while its guanidinium group stacks over the other purine of the bound cyclic dinucleotide (Figure 1E, F, G). The bound ligand is further stabilized through a network of direct and water-mediated hydrogen bonds to the base edges from side chains of hSTING^{H232} (Figure 1F, G). Amino acids

participating in this network and positioned above the bound ligand include N242, S241 and V239 which form water-mediated hydrogen bonds to the O6 of guanosine, while Y163, E260, and Y261 form water-mediated hydrogen bonds together with a direct hydrogen bond from T263 to the NH_2 group of guanosine (Figure 1F). The edges of the adenosine base are not involved in hydrogen-bond formation (Figure 1F).

[0283] The phosphate backbone and ribose hydroxyls of the cyclic dinucleotide ring system are additionally stabilized through hydrogen bonds. Amino acids participating in this network and positioned below the bound ligand include S162 and T267 (Figure 1G), with the 3'-OH group of the guanosine hydrogen-bonded to the side chain hydroxyl of S162, while no hydrogen-bonding is observed to the 2'-OH of adenosine of c[G(2',5')pA(3',5')p] in the complex (Figure 1G). The backbone phosphates of the bound cyclic dinucleotide are recognized by direct contacts from the guanidinium groups of R238 and through water-mediated hydrogen bonds from the hydroxyl groups of T267 and Y240 (Figure 1G).

[0284] The four-stranded anti-parallel β-sheet that forms upon c[G(2',5')pA(3',5')p]-hSTING^{H232} complex formation (Figure 2A) caps the top of the binding pocket and restricts access to it (Figure 1A). In addition to hydrogen-bonding between strands across the four-stranded β-pleated sheet, anchoring at either end of the sheet is achieved by salt bridges (Figure 2A). It should be noted that G230 forms part of the outer β-strand of this four-stranded β-sheet (Figure 2A).

Example 2: Comparison of Crystal Structures of c[G(2',5')pA(3',5')p] and c[di-GMP] Bound to hSTING^{H232}

[0285] The present Example describes the binding cleft of human STING and presents "open" and "closed" STING complex structure.

[0286] An exemplary crystal structures of c[di-GMP] bound to the symmetrical dimer of hSTING^{H232} (aa 139-379) (PDB: 4EF4; 2.15 Å resolution) is shown in Figure 8A, with an expanded view of the ligand binding pocket shown in Figure 8B. Note that the loops protruding over the binding pockets are disordered over half their lengths in the direction of their tips, while

the symmetry-related α2-helices form a larger angle in the V-shaped c[di-GMP] complex (Figure 8A), as compared to the U-shaped c[G(2',5')pA(3',5')p] complex (Figure 1A) with hSTING^{H232}. Indeed, space filling views of the c[di-GMP] complex indicate that the hSTING^{H232} dimer does not encapsulate the bound c[di-GMP] in its complex (Figure 10C, D; termed the 'open' STING complex), as it does in space filling views of the c[G(2',5')pA(3',5')p] complex (Figure 1C, D; termed the 'closed' STING complex) with hSTING^{H232}.

[0287] The intermolecular hydrogen bonds stabilizing complex formation in the exemplary structure of the complex of c[di-GMP] with hSTING^{H232} (PDB: 4EF4) are shown in Figure 8E, F. Notably, the side chains of R238 are disordered, unlike the key recognition role they play in the complex of c[G(2',5')pA(3',5')p] with hSTING^{H232} (Figure 1F, G).

[0288] The superposition of c[di-GMP] bound to the 'open' hSTING complex (both subunits in beige) with that for c[G(2',5')pA(3',5')p] bound to the 'closed' hSTING complex (both subunits in green) shows large conformational differences in STING between the two complexes (Figure 2B; rmsd = 3.11 Å). Indeed, the separation between the tips of the symmetry related α2-helices decreases from approx. 60 Å in the 'open' complex to approx. 38 Å in the 'closed' complex. Furthermore, superposition of the bound c[di-GMP] in beige with that of bound c[G(2',5')pA(3',5')p] in green establishes that the purine bases are further apart in the former complex compared to the latter complex (Figure 2C), and presumably facilitate switching of the hSTING^{H232} from an 'open' and more flexible (partly disordered loops positioned over the binding pocket) conformation in the c[di-GMP] complex (Figure 8A) to a 'closed' and more compact (well defined four-stranded β-sheet cap over the binding pocket) conformation in the c[G(2',5')pA(3',5')p] complex (Figure 1A). Furthermore, the bound c[G(2',5')pA(3',5')p] (in green) is positioned slightly deeper in the binding cleft than its bound c[di-GMP] counterpart (in beige) (Figure 2C, top panel). Importantly, the conformational changes propagate to the surface of the STING protein as shown in a stereo view (Figure 2D) highlighting the upper right segment of Figure 2B.

Example 3: Similar 'Closed' Conformations Adopted by c[G(2',5')pA(3',5')p] Bound to mSting^{R231} and hSTING^{H232}

[0289] The present Example describes the 1.77 Å crystal structure of an ~186 amino acid mouse STING polypeptide bound to c[G(2',5')pA(3',5')p].

[0290] We have solved the 1.77 Å crystal structure of c[G(2',5')pA(3',5')p] bound to the symmetrical dimer of mSting^{R231} (aa 154-340) (Figure 3A and Table S2). The side chain of R231 of mSting^{R231} is shown in green in a stick representation (Figure 3A). Given the high resolution of this complex, the network of hydrogen bonds are clearly visible; the 3'-OH of guanosine of bound c[G(2',5')pA(3',5')p] makes hydrogen bonds with the side chain of S161 and two water molecules (Figure 3B). The guanidinium group of R231 interacts with the backbone phosphates of c[G(2',5')pA(3',5')p] through a bridging water molecule (Figure 3B). Formation of the four-stranded anti-parallel β-pleated sheet acts as a cap over the bound ligand in the complex (Figure 3A).

Table S2. X-ray Statistics for cGAMP Linkage Isomers and DMXAA with mSting^{231}

Data collection and refinement statistics of mSting with Ligands			
Crystal	**mSting^{R231} + c[G(2',5')pA(3',5')p]**	**mSting^{R231} + c[G(3',5')pA(3',5')p]**	**mSting^{R231} + DMXAA**
Beam line	NSLS-X29A	NSLS-X29A	APS-24ID-E
Wavelength	1.075	1.075	0.9792
Space group	$P2_12_12_1$	$P2_12_12_1$	$H3$
Unit cell			
a, b, c (Å)	46.2, 46.5, 157.9 0.	46.4, 47.4, 156.2	108.4, 108.4, 101.2
α, β, γ (°)	90.0, 90.0, 90.0	90.0, 90.0, 90.0	90.0, 90.0, 120.0
Resolution (Å)	50-1.8 (1.83-1.77)[a]	50-2.1 (2.14-2.07)[a]	50-2.4 (2.57-2.43)[a]
R_{merge}	0.050 (0.351)	0.075 (0.542)	0.046 (0.397)
I/ σ (I)	38.6 (4.5)	29.8 (3.4)	18.2 (3.4)
Completeness (%)	96.5 (94.0)	97.5 (94.3)	99.5 (100)
Redundancy	7.2 (7.2)	8.0 (8.1)	4.7 (4.8)
Number of unique reflections	31300	20191	15773
Wilson B factors (Å^2)	17.73	28.34	49.02
R_{work}/R_{free} (%)	19.1/21.2	17.7/23.6	16.1/18.9
Number of non-H atoms			
Protein	2889	2908	2870
Water	218	139	41
Ligands(molecule)	1	1	2
Average B factors (Å^2)			
Protein	24.94	42.95	63.36
Water	30.18	37.91	44.66
ligands	15.29	37.60	43.34
R.m.s. deviations			
Bond lengths (Å)	0.018	0.015	0.014
Bond angles (°)	2.005	1.843	1.741

[a] Highest resolution shell (in Å) shown in parentheses.

Relates to Figure 3 and 5.

[0291] We observe excellent superposition of hSTING^{H232} (both subunits in green) and mSting^{R231} (both subunits in magenta) in its complexes with c[G(2',5')pA(3',5')p] as shown in Figure 3C (rmsd = 0.84 Å). The separation between the tips of symmetry related α2-helices are approx. 38 Å for both complexes (Figure 3C). We also observe excellent superposition of the c[G(2',5')pA(3',5')p] dinucleotide in its complexes with hSTING^{H232} and mSting^{R231} (Figure 3D). Thus, the same c[G(2',5')pA(3',5')p]-STING complex is observed whether a His or Arg occupies this key position. Indeed, the R238, S162 and T267 in hSTING^{H232} (Figure 1H) and their conserved counterparts R237, S161 and T266 in mSting^{R231} (Figure 3B) are involved in similar hydrogen-bonding interactions with the backbone phosphates and sugar hydroxyl groups in both complexes.

Example 4: c[G(2',5')pA(2',5')p]- and c[G(3',5')pA(3',5')p]-Bound STING Complexes Both Adopt 'Closed' Conformations

[0292] The present Example describes the 1.9 Å crystal structure of an ~186 amino acid human STING polypeptide bound to c[G(2',5')pA(2',5')p]. The present Example also describes the 2.1 Å crystal structure of an ~186 amino acid mouse STING polypeptide bound to c[G(3',5')pA(3',5')p].

[0293] We also crystallized the two other cGAMP linkage isomers c[G(2',5')pA(2',5')p] and c[G(3',5')pA(3',5')p] with hSTING^{H232} and mSting^{R231}, respectively. We solved a 1.9 Å crystal structure of c[G(2',5')pA(2',5')p] with hSTING^{H232} (aa 155-341) (Figure 3E and Table S1) and a 2.1 Å crystal structure of c[G(3',5')pA(3',5')p] with mSting^{R231} (aa 154-340) (Figure 3F and Table S2). The structures of both complexes adopt the 'closed' conformation as reflected by the positioning of the ligands in the binding pocket, the separation between the tips of the α2-helices by approx. 38 Å, and the formation of the four-stranded anti-parallel β-sheet cap over the bound ligands (Figure 3E, F).

[0294] The crystal structures of c[G(2',5')pA(2',5')p] (in red) and c[G(2',5')pA(3',5')p] (in green) in their bound complexes with hSTING^{H232} superimpose with an rmsd of 0.59 Å (Figure 9A), with the 3'-OH groups of bound c[G(2',5')pA(2',5')p] forming water-mediated hydrogen bonds to the hydroxyls of S162 and T267 (Figure 9B). The crystal structures of c[G(3',5')pA(3',5')p] (in cyan) and c[G(2',5')pA(3',5')p] (in magenta) in their bound complexes with mSting^{R231} superimpose with an rmsd of 0.25 Å (Figure 9C), with the 2'-OH groups of bound c[G(3',5')pA(3',5')p] forming direct hydrogen bonds to the hydroxyls of T262 (Figure 9D). The bound c[G(2',5')pA(2',5')p] (in red) is positioned somewhat deeper in the binding pocket than c[G(3',5')pA(3',5')p] (in cyan) (Figure 9E).

Example 5: ITC Binding Studies of hSTING^{H232} and its Mutants with Linkage Isomers of cGAMP

[0295] The present Example describes isothermal titration calorimetric (ITC) binding curves for a human STING polypeptide bound with various linkage isomers of cGAMP including c[G(2',5')pA(2',5')p], c[G(3',5')pA(3',5')p], or c[G(2',5')pA(3',5')p].

[0296] We recorded the isothermal titration calorimetric (ITC) binding curves for hSTING^{H232} (aa 140-379) with three linkage isomers of cGAMP as shown in Figure 4A. The binding curves are exothermic for complex formation with c[G(2',5')pA(2',5')p] (red circles) and c[G(3',5')pA(3',5')p] (green triangles), and endothermic for complex formation with c[G(2',5')pA(3',5')p] (black squares; K_D = 5.3 μM). The thermodynamic K_D, ΔG, ΔH and TΔS parameters for these complexes are listed in Table S3.

Table S3. ITC Parameters for Binding of cGAMP Linkage Isomers to hSTING and mSting Alleles

hSTING^{H232} with cGAMP Isomers					
Protein: 0.2 mM; Ligands: 1 mM; Buffer: 30 mM HEPES, 100 mM NaCl, pH 7.5; T: 25 °C					
	N	K_D (μM)	ΔG (Kcal/mol)	ΔH (Kcal/mol)	TΔS (Kcal/mol)
c[G(3',5')pA(3',5')p]	0.61	5.4 ± 0.1	-7.01	-10.62	-3.61

c[G(2',5')pA(2',5')p]	0.62	2.5 ± 0.1	-7.52	-7.15	+0.37
c[G(2',5')pA(3',5')p]	0.54	5.3 ± 0.5	-7.19	+2.62	+9.81

hSTING^{R232} with cGAMP Isomers					
Protein: 0.2 mM; Ligands: 0.9 mM; Buffer: 30 mM HEPES, 100 mM NaCl, pH 7.5; T: 25 °C					
	N	K_D (μM)	ΔG (Kcal/mol)	ΔH (Kcal/mol)	TΔS (Kcal/mol)
c[G(3',5')pA(3',5')p]	0.61	1.4 ± 0.1	-7.99	-1.13	+6.86
c[G(2',5')pA(2',5')p]	0.54	0.17 ± 0.02	-9.25	+5.63	+14.88
c[G(2',5')pA(3',5')p]	0.52	0.11 ± 0.01	-9.50	+2.78	+12.28

hSTING$^{A230/R232}$ with cGAMP Isomers					
Protein: 0.2 mM; Ligands: 0.9 mM; Buffer: 30 mM HEPES, 100 mM NaCl, pH 7.5; T: 25 °C					
	N	K_D (μM)	ΔG (Kcal/mol)	ΔH (Kcal/mol)	TΔS (Kcal/mol)
c[G(3',5')pA(3',5')p]	0.57	0.16 ± 0.02	-9.26	+4.93	+14.19
c[G(2',5')pA(2',5')p]	0.53	0.13 ± 0.02	-9.39	+4.74	+14.13
c[G(2',5')pA(3',5')p]	0.56	0.16 ± 0.01	-9.28	+1.39	+10.67

mSting^{R231} with cGAMP Isomers					
Protein: 0.2 mM; Ligands: 0.9 mM; Buffer: 30 mM HEPES, 100 mM NaCl, pH 7.5; T: 25 °C					
	N	K_D (μM)	ΔG (Kcal/mol)	ΔH (Kcal/mol)	TΔS (Kcal/mol)
c[G(3',5')pA(3',5')p]	0.55	0.26 ± 0.03	-8.99	+3.95	+12.94
c[G(2',5')pA(2',5')p]	0.52	0.18 ± 0.02	-9.20	+3.92	+13.12
c[G(2',5')pA(3',5')p]	a				

mSTING^{A231} with cGAMP Isomers					
Protein: 0.2 mM; Ligands: 1.0 mM; Buffer: 30 mM HEPES, 100 mM NaCl, pH 7.5; T: 25 °C					
	N	K_D (μM)	ΔG (Kcal/mol)	ΔH (Kcal/mol)	TΔS (Kcal/mol)

c[G(3',5')pA(3',5')p]	0.42	1.34 ± 0.14	-8.01	-7.36	+0.65
c[G(2',5')pA(2',5')p]	a				
c[G(2',5')pA(3',5')p]	0.41	0.34 ± 0.04	-8.80	+3.63	+12.43

[a] Values could not be measured due to precipitation of complex

Relates to Figure 4.

[0297] We also recorded ITC binding curves for complex formation of c[G(2',5')pA(3',5')p] with mutants of hSTING^{H232} that participate in intermolecular contacts on complex formation. For this linkage isomer, cGAMP binding is completely lost (Figure 4B and Table S4) for the R238A mutant involved in cyclic dinucleotide base N7 and backbone phosphate recognition (Figure 1E, F, G), as well as for the Y240A, N242A and E260A (significantly reduced) mutants involved in water-mediated guanosine base edge recognition (Figure 1F). The impact of mutating the polar Thr and Ser residues involved in intermolecular hydrogen bond formation is more nuanced, with no effect on binding affinity for the T267A mutant, a modest reduction for the S162A mutant and a more pronounced reduction for the T263A mutant (Figure 1B). The thermodynamic parameters are listed in Table S4.

Table S4. ITC Parameters for Binding of c[G(2',5')pA(3',5')p] to hSTING^{H232} Mutants

hSTING^{H232} Mutants with c[G(2',5')pA(3',5')p]					
Protein: 0.3 mM; Ligands: 1.5 mM; Buffer: 30 mM HEPES, 100 mM NaCl, pH 7.5; T: 25 °C					
	N	K_D (μM)	ΔG (Kcal/mol)	ΔH (Kcal/mol)	TΔS (Kcal/mol)
T267A	0.43	2.91 ± 0.35	-7.59	+2.25	+9.84
T263A	0.52	41.67 ± 2.29	-5.97	+4.76	+10.73
E260A	UD	UD; >200			
N242A	UD	UD; >200			
Y240A	UD	UD; >200			
R238A	UD	UD; >200			
S162A	0.55	10.66 ± 0.48	-7.20	+5.59	+12.79
WT	0.47	4.39 ± 0.23	-7.29	+2.28	+9.57

Relates to Figure 4.

ITC Binding Studies of hSTING^{R232} and hSTING$^{A230/R232}$ With Linkage Isomers of cGAMP

[0298] The corresponding ITC-based thermodynamic parameters were also recorded for complex formation of cGAMP linkage isomers with hSTING^{R232} and hSTING$^{A230/R232}$ (aa 140-379) (Figure 4C, D, respectively). The 2',5'-containing linkage isomers of cGAMP exhibited increased binding affinity by about an order of magnitude for STING variants with R232 compared to H232, while the corresponding binding affinity increase was about 4-fold for the all-3',5' linkage isomer of cGAMP (Table S3), with endothermic titration patterns observed for all binding curves, except for an exothermic titration pattern for c[G(3',5')pA(3',5')p] with hSTING^{R232} (Figure 4C). The dissociation constants for c[G(2',5')pA(3',5')p] bound to hSTING^{R232} and hSTING$^{A230/R232}$ were K_D = 0.11 μM and 0.16 μM, respectively (Table S3).

ITC Binding Studies of mSting^{R231} and mSting^{A231} with Linkage Isomers of cGAMP

[0299] The corresponding ITC-based thermodynamic parameters for complex formation of cGAMP linkage isomers with mouse Sting^{R231} (I229/R231; aa 139-378) are plotted in Figure 4E, with observed K_D values similar to those observed for hSTING$^{A230/R232}$ (Table S3). The ITC titrations for mSting^{A231} with the various cGAMP linkage isomers are plotted in Figure 4F, with the observed K_D values listed in Table S3. The dissociation constants for c[G(2',5')pA(3',5')p] bound to mSting^{A231} was K_D = 0.34 μM (Table S3).

Example 6: Crystal Structure of DMXAA Bound to mSting^{R231}

[0300] The present Example describes a 2.4 Å crystal structure of an ~186 amino acid mouse STING polypeptide bound to 5,6-dimethylxanthenone-4-acetic acid (DMXAA).

[0301] Reported antiviral small molecules reported to date that target mSting include 5,6-dimethylxanthenone-4-acetic acid (DMXAA) (Figure 5A) (Conlon et al. 2013; Kim et al. 2013) and 10-carboxymethyl-9-acridine (CMA) (Figure 10A) (Cavlar et al. 2013), with DMXAA and CMA showing species specificity for mouse but not human STING. The mode of binding of

DMXAA and CMA to mSting is of interest for structure-based design of agonists and antagonists of hSTING with value as anti-cancer/anti-viral vaccine adjuvants and anti-inflammatory compounds, respectively.

[0302] We solved the 2.4 Å crystal structure of DMXAA bound to $mSting^{R231}$ (aa 154-340) (x-ray statistics in Table S2), with the complex containing two molecules of DMXAA per $mSting^{R231}$ dimer (Figure 5B). The aromatic rings of the two DMXAA moieties are aligned in parallel but are not stacked on each other. The details of the intermolecular contacts in the complex are shown in Figure 5C, with the ketone groups of DMXAA forming direct hydrogen bonds to the side chain of T266, while the carboxylate moieties of the ligand are anchored through direct hydrogen bonds to the side chains of R237 and T262. In addition, the adjacent aromatic methyl groups of DMXAA form a hydrophobic patch with side chains of L169 and I234 of mSting, while the non-substituted aromatic edges (positions 7 and 8) of DMXAA are positioned opposite I164 (Figure 5C). A four-stranded anti-parallel β-pleated sheet forms a cap over the binding pocket indicative of formation of a 'closed' conformation on complex formation, consistent also with DMXAA exposure leading to type I IFN pathway activation via mSting (Conlon et al. 2013; Kim et al. 2013).

[0303] Finally, the mSting moieties bound to DMXAA (both subunits in biscuit) and to CMA (both subunits in yellow) (PDB: 4JC5) superpose well on each other (rmsd = 0.75 Å) representing the 'closed' conformation for both complexes (Figure 10B). By contrast, the mSting moieties bound to DMXAA (both subunits in biscuit) and to c[G(2',5')pA(3',5')p] (both subunits in magenta) show differences upon superposition despite both adopting the 'closed' conformation (rmsd = 2.21 Å) with the separation between the tips of the α2-helices increasing from approx. 42 Å in the former complex to approx. 38 Å in the latter complex (Figure 5D). Superposition of the $mSting^{R231}$-bound DMXAA (in salmon) and c[G(2',5')pA(2',5')p] (in magenta) ligands emphasize the different orientations adopted by these bound ligands within the same binding pocket (Figure 5E).

Example 7: cGAMP Isomers Activate Type I IFN Pathway Through the STING/IRF3 Pathway

[0304] The present Example describes a requirement for STING activation by cGAMP isomers to induce phosphorylation of Tbk1 and Irf3.

[0305] To test whether cGAMP isomers elicit an innate immune response in murine macrophages, we recorded simple dose-response of cultured bone-marrow-derived macrophages (BMDMs) by addition of increasing concentrations of c[G(2',5')pA(2',5')p], c[G(2',5')pA(3',5')p] and c[G(3',5')pA(3',5')p] to the medium, and assaying 4 h post-treatment. Using real-time reverse transcription PCR (qPCR) analysis to monitor induction of Ifnb1, Il6, and Ccl5, we determined that exposure of BMDMs to 20 μM c[G(3',5')pA(3',5')p] elicited the strongest induction among the three isomers, with Ifnb1, Il6 and Ccl5 mRNA levels increased by 1024-, 2624-, and 38-fold, respectively, relative to mock-treatment (Figure 6A). While c[G(3',5')pA(3',5')p] was the most potent compound, the differences between it and the other two isomers did not exceed three-fold. BMDMs isolated from $Irf3^{-/-}$ mice had reduced induction of Ifnb1, Il6, and Ccl5 upon exposure to cGAMP isomers, thereby indicating the involvement of Irf3-dependent type I IFN response pathway (Figure 6B).

[0306] Western blot analysis further demonstrated that cGAMP isomers induced phosphorylation of Tbk1 and Irf3 at 2 and 4 h post-treatment of BMDMs (Figure 11). Consistent with our qPCR results, incubation of BMDMs with c[G(3',5')pA(3',5')p] also showed the highest levels of Tbk1 and Irf3 protein phosphorylation compared to the two other isomers (Figure 11). To test whether mSting is required for cGAMP-induced Tbk1 and Irf3 phosphorylation, we compared type I IFN response in BMDMs derived from wild-type and *Goldenticket* (*Gt*) mutant mice ($Sting^{Gt/Gt}$), which carry a I199R missense mutation in exon 6 of the mSting gene resulting in no detectable protein by Western blot analysis of BMDMs (Rasmussen et al. 2011). We observed that cGAMP-induced Tbk1 and Irf3 phosphorylation was absent from mSting-deficient cells (Figure 11). We conclude that cGAMP treatment of BMDMs triggers type I IFN and pro-inflammatory cytokine/chemokine via the mSting/Irf3-dependent pathway. The strongest responses for mSting were seen for cGAMP derivatives comprising the non-metazoan all-3',5'-linkage isomer produced by bacteria, which was unexpected, considering

the recent report suggesting that the natural c[G(2',5')pA(3',5')p] was the highest affinity ligand for hSTING (Zhang et al. 2013).

[0307] Therefore, we also evaluated hSTING activation and its dependence on cGAMP isomer concentration. We assayed type I IFN and chemokine production in human THP1 cells by ELISA and RT-PCR analysis delivering cGAMP isomers by addition to the medium without or with Digitonin (Dig) permeabilization. In comparison to the murine system, which slightly favored the bacterial c[G(3',5')pA(3',5')p], the non-natural c[G(2',5')pA(2',5')p] stimulated THP1 cells 2.9- or 4.8-fold more effectively than the metazoan second messenger c[G(2',5')pA(3',5')p] or c[G(3',5')pA(3',5')p], respectively (Figure 6C and D, left panels, Table S5). Measuring transcriptional activation of hSTING-dependent IFN response genes by the various cGAMP linkage isomers (Figure 6E) confirmed the ELISA results. As early as 2 h, we detected by RT-PCR that c[G(2',5')pA(2',5')p] stimulated expression of IFNB1 and CXCL10 the most. Digitonin-mediated cell permeabilization significantly increased and enhanced sensitivity to all cGAMP isomer in BMDM and THP1 cells (Fig. 6C and D, right panels, Table S5). In THP1 cells, there was no difference in the EC_{50} values obtained for c[G(2',5')pA(2',5')p] and c[G(2',5')pA(3',5')p] exposure.

Table S5. Effective concentration (EC_{50}) values of ELISA dose response curves for BMDM and THP1 stimulation with cGAMP linkage isomers

BMDM – Ifna, unpermeabilized (refers to Fig. 6C left panel)			
	c[G(2',5')pA(2',5')p]	**c[G(2',5')pA(3',5')p]**	**c[G(3',5')pA(3',5')p]**
EC_{50} (μM)	12.5	12.5	8.4
95% CI (μM)	9.7 – 16.2	10.1 – 15.2	7.7 – 9.2
BMDM – Ifna, +Digitonin (refers to Fig. 6C right panel)			
EC_{50} (μM)	0.80	0.29	0.42
95% CI (μM)	0.2 – 3.2	0.2 – 0.4	0.3 – 0.6
THP1 – CXCL10, unpermeabilized (refers to Fig. 6D left panel)			
EC_{50} (μM)	1.2	3.4	5.7
95% CI (μM)	1.0 – 1.4	2.9 – 3.8	5.0 – 6.4

THP1 – CXCL10, +Digitonin (refers to Fig. 6D right panel)			
EC_{50} (μM)	0.12	0.14	0.33
95% CI (μM)	0.09 – 0.16	0.12 – 0.16	0.28 – 0.39

Related to Figure 6.

Example 8: Mutagenesis of hSTING and mSting Identified Amino Acids Important for Its Ligand-Binding-Induced IFN Pathway Activation

[0308] The present Example describes human STING amino acid residues important for ligand binding and IFN pathway activation.

[0309] To determine the functional importance of individual amino acids that interacted with c[G(2',5')pA(3',5')p] in the crystal structure, we generated Ala point mutants of specific residues within $hSTING^{H232}$, as well as of the corresponding mutations in $mSting^{R231}$, and tested their activities in human HEK293T cells using an IFN-sensitive luciferase reporter assay (Burdette et al. 2011; Gao et al. 2013). STING expression plasmids and IFNB1 luciferase reporter constructs were co-transfected followed by Dig-mediated delivery of cGAMP isomers (Figure 7A), or co-transfected with wild-type or catalytic mutant (E211A) cGAS in the absence of exogenous cGAMP addition (Figure 7B) (Gao et al. 2013). Human mutant STING variants with amino acid substitutions of either of Y167A, R238A, Y240A, or E260A, as well as their murine counterparts, were no longer able to stimulate the IFN-pathway. Notably, $hSTING^{H232/N242A}$ induced no measurable IFN reporter activity, whereas $mSTING^{R231/N241A}$ was only slightly impaired in its response. Mutants S162A and T267A of $hSTING^{H232}$ largely retained their normal function, whereas $hSTING^{H232/T263A}$ showed reduced activation (Figure 7A). Dose-response studies of $hSTING^{H232}$ (Figure 12) revealed no significant differences in stimulation between c[G(2',5')pA(2',5')p] and c[G(2',5')pA(3',5')p] and a lesser response to c[G(3',5')pA(3',5')p]. However, the $hSTING^{H232/T263A}$ mutant shows a gain in sensitivity to c[G(3',5')pA(3',5')p] compared to its response to 2',5' linkage isomers. The S162A and T267A $hSTING^{H232}$ mutants respond similarly to $hSTING^{H232}$, also showing a weaker response to c[G(3',5')pA(3',5')p].

[0310] Given the recent report of mSting and hSTING variants with distinct responsiveness (Diner et al. 2013), we sequenced hSTING DNAs derived from 8 Caucasians and our THP1 cells. All samples encoded R232 in both alleles; additionally $hSTING^{THP1}$ contained three additional point mutations (H72R, G230A, and R293Q) as reported before. We compared the cGAMP-dependent IFN-response for $hSTING^{H232}$, $hSTING^{R232}$, $hSTING^{THP1}$ and $mSting^{R231}$, and found that the prevalent $hSTING^{R232}$ was several-fold more responsive to all cGAMP isomers when compared to $hSTING^{H232}$, with the order of cGAMP isomer sensitivity remaining the same (Figure 7 and 12E, F). $hSTING^{THP1}$ and wild-type $mSting^{R231}$ displayed slightly reduced overall cGAMP sensitivity compared to $hSTING^{R232}$.

[0311] To complement our mutagenesis study of the cGAMP isomer response, we tested c[di-GMP] and DMXAA (Fig. 7C and D). While both ligands stimulated mSting, nearly all hSTING variants were non-responsive except for $hSTING^{R232}$ and $hSTING^{THP-1}$, which showed a residual response to high concentrations of c-di-GMP) (Fig. 7C and 12). Moreover, mSting mutants defective for recognition of all cGAMP isomers also failed to recognize c[di-GMP] and DMXAA. Mutants N241A and T262A of mSting were less responsive to c[di-GMP] and DMXAA compared to cGAMPs, whereas mSting (T266A) showed a moderately enhanced recognition of c[di-GMP] over DMXAA.

Example 9: S162A Mutant by hSTING is Activated by DMXAA

[0312] The present Example describes a point mutation in human STING that renders it sensitive to DMXAA.

[0313] Strikingly, we found that the single point mutant S162A enabled recognition of DMXAA by human STING (Figure 7D, left panel), while not restoring c[di-GMP] responsiveness (Figure 7C, left panel). In both $hSTING^{H232}$ and $hSTING^{R232}$ background, the S162A mutation enabled DMXAA recognition with near-identical dose-responses (Figure 13C, D). In contrast, the differences in recognition of cGAMP isomers and c[di-GMP] were only slightly altered or unchanged compared to the respective S162 variants (Figure 14B). Noticeably, IFN induction was not observed in cellular assays for the S162V and S162I mutants of

hSTING^{H232} or hSTING^{R132}, which contain bulkier hydrophobic amino acids compared to Ala at position 162 (Figure 14A).

[0314] ITC-based binding studies confirmed that mSting^{R231} bound DMXAA as reported previously (Figure 14E) (Kim et al., 2013), as did S162A (and S162V) mutants in a hSTING^{R232} and hSTING^{H232} context bound DMXAA (Figure 7F, G).

[0315] Table S6. ITC Parameters for Binding of DMXAA to hSTING Containing S162A and S162V Mutants in a R232 and H232 context

hSTING and its S162 Mutants with DMXAA					
Protein: 0.08 mM; Ligands: 0.8 mM; Buffer: 30 mM HEPES, 180 mM NaCl, pH 7.5; T: 25 °C					
	N	K_D (μM)	ΔG (Kcal/mol)	ΔH (Kcal/mol)	TΔS (Kcal/mol)
hSTING$^{R232/A162}$	1.49	0.86 ± 0.20	-8.29	+0.36	+8.65
hSTING$^{R232/V162}$	0.77	2.63 ± 0.45	-7.61	+0.32	+7.93
hSTING$^{H232/A162}$	1.52	2.88 ± 0.48	-7.55	+0.44	+7.99
hSTING$^{H232/V162}$	0.79	3.47 ± 0.39	-7.45	+0.39	+7.84
mSting^{R231}	1.23	0.49 ± 0.05	-8.61	-2.86	+5.75

Relates to Figure 7E, F and G.

Example 10: The Lid Region of the Ligand-Binding Pocket Is Important for DMXAA Recognition

[0316] Within STING, DMXAA (Figure 15A) and c[G(2',5')pA(3',5')p] share the same ligand binding pocket (Gao et al., 2013b), which in human and mouse proteins is composed of identical amino acids. Despite the fact that human and mouse STING C-terminal domains (CTD, aa 140-379) exhibit ~76% amino acid identity (Figure 19), DMXAA only binds and activates mSTING and has no effect on hSTING (Conlon et al., 2013; Kim et al., 2013). Therefore, the non-conserved residues between the two species that are located outside the DMXAA-binding pocket must play a role for distinct DMXAA recognition. We subdivided the non-conserved

residues located in the STING CTD into four groups (labeled as group1 to group4, hSTING$^{group1-4}$). We then substituted hSTING residues with their mSTING counterparts for each of the four groups (Figure 19). These residues are located either along the dimer interface or within the regions that undergo large conformational changes during the 'open' to 'closed' transition associated with complex formation. We also generated a construct containing the combined substitution in all four groups (hSTING^{group1234}).

[0317] We performed isothermal titration calorimetry (ITC) experiments to measure the DMXAA-binding affinity of hSTING CTD (aa 140-379) containing various group substitutions. hSTING^{group1234} showed a comparable exothermic binding curve and binding affinity (K_D: 0.69 μM) (Figure 15B) to mSTING (K_D: 0.49 μM) (Gao et al., 2013b). Similar to wild-type (wt) hSTING protein, no detectable binding to DMXAA was observed for the isolated group1, group3, or group4 substitutions of hSTING (Figure 20A). Only group2 substitutions of hSTING exhibited detectable endothermic binding with DMXAA (K_D: 3.12 μM; Figure 15C).

[0318] To validate the binding results, we used an IFN-β luciferase reporter assay to further test the responsiveness of hSTING group substitutions to DMXAA stimulation in human 293T cells, which lack endogenous STING expression. Full-length hSTING (wt and substitutions) and mSTING (wt) constructs were used for this cellular assay, and were expressed at moderate levels allowing ligand-dependent activation of IFN-β promoter. We confirmed that mSTING-transfected 293T cells responded to DMXAA, while hSTING-transfected cells did not (Figure 15D, left panel). Consistent with the ITC results among the individual group substitutions, only the hSTING^{group2} substitutions showed responsiveness to DMXAA (Figure 15D, middle panel). Inversely, removing the group2 substitutions from the combined group1234 substitutions (hSTING^{group134}) strongly diminished DMXAA activation, while loss of any of the other groups was tolerated (Figure 15D, right panel). These results indicate that group2 residues from mSTING, which are located within the lid region of the binding pocket, play an a role in DMXAA recognition.

Example 11: Crystal Structure of DMXAA Bound to hSTING^{group2}

[0319] We proceeded to solve the crystal structure of DMXAA bound to hSTING^{group2} (aa 155-341) at 1.88 Å resolution (x-ray statistics in Table S1) with the complex containing two molecules of DMXAA per hSTING^{group2} dimer (Figure 15E). The results were similar to what we observed for the complex of mSTING and DMXAA, described above. The four-stranded antiparallel β-pleated sheet formed a lid covering the binding pocket, indicative of formation of a 'closed' conformation of STING on complex formation, which is consistent with the conclusions drawn from our ITC (Figure 15B, C) and IFN-β-dependent luciferase reporter (Figure 15D) results. Rather than being stacked on each other, the aromatic rings of the two DMXAA moieties are aligned in parallel, with complex formation mediated by both intermolecular van der Waals contacts and hydrogen bond interactions. The details of the intermolecular contacts in the complex are shown in Figure 15F, with the ketone and ether groups of DMXAA forming direct hydrogen bonds to the side chain of T267 and T263, respectively. The carboxylate moieties are anchored through direct hydrogen bonds to the side chains of R238 and T263 and through water-mediated hydrogen bonds to Y240. In addition, the adjacent aromatic methyl groups (positions 5 and 6) of DMXAA form a hydrophobic patch with side chains of L170 and I235, whereas the non-substituted aromatic edges (positions 7 and 8) of DMXAA are positioned opposite I165. We observed excellent superposition of hSTING^{group2} and mSTING in their complexes with DMXAA as shown in Figure 20B (rmsd: 0.95 Å).

[0320] To elucidate the molecular basis underlying DMXAA species selectivity, we compared the structure of the hSTING^{group2}-DMXAA complex with those of the hSTING-c[G(2',5')pA(3',5')p] (Gao et al., 2013a) and mSTING-DMXAA (Gao et al., 2013b) complexes. We found that in the hSTING^{group2}-DMXAA structure, the side chain of the substituted residue I230 (G230 in wt protein) is located in a hydrophobic pocket composed of residues from both the four-stranded antiparallel β-sheet region (R232, I235, R238, and Y240) and the adjacent long α-helix (L170 and I171) (Figure 15G). The amino acids that form the hydrophobic pocket are identical between human and mouse proteins. This same structural feature was also found in the mSTING-DMXAA structure (Figure 20C). In the structure of the hSTING-c[G(2',5')pA(3',5')p] complex, the corresponding position to I230 (or I229 in mSTING) is G230, which results in the

loss of the hydrophobic interactions found in the other two structures. This isoleucine-mediated hydrophobic interaction may help stabilize the β-sheet and other parts of the protein, facilitating DMXAA-mediated formation of the 'closed' conformation by mSTING or hSTING^{group2}, thereby explaining the absence of complex formation by wt hSTING with a glycine at this position.

Example 12: G230 of hSTING and I229 of mSTING are Contributors to Differential DMXAA Recognition

[0321] To support our conclusions based on our structural findings above, we generated the G230I single substitution in hSTING and tested its IFN-β induction activity using the luciferase assay. Indeed, hSTING^{G230I} alone was sufficient to mimic the effects observed for hSTING^{group2}, resulting in almost identical IFN-β induction as hSTING^{group2} (Figure 16A). Using the same method, reverse substitutions on mSTING (I229G or I229A) were also generated and tested. As expected, mSTING^{I229G} and mSTING^{I229A} showed a significant decrease in DMXAA-mediated IFN-β induction (Figure 16B).

[0322] We also solved the crystal structure of DMXAA bound to hSTING^{G230I} (aa 155-341) at 2.51 Å resolution (x-ray statistics in Table S1), with hSTING^{G230I} in the complex forming a 'closed' conformation (Figure 16C). The detailed intermolecular contacts in the complex (Figure 21A) are similar to those observed for the hSTING^{group2}-DMXAA structure (Figure 15F). We observed excellent superposition of hSTING^{G230I} and hSTING^{group2} in their complexes with DMXAA, as shown in Figure 21B (rmsd: 0.61 Å). The I230 residue, which is positioned within a hydrophobic pocket (Figure 16D), forms the same intramolecular contacts as observed in the structures of the hSTING^{group2}-DMXAA (Figure 15G) and mSTING-DMXAA (Figure 20C) complexes. Taken together, our structural and functional data strongly demonstrate that the substitution of Gly with Ile at aa 230 results in the gain of function of hSTING for DMXAA recognition.

Example 13: hSTING^{Q266I} is Activated by DMXAA

[0323] Examples 1-8 identify a point substitution (S162A) placed within the cyclic-dinucleotide-binding site of hSTING that confers partial sensitivity to the otherwise mouse-specific drug DMXAA (Gao et al., 2013b). Guided by the structures of complexes of hSTING substitutions with DMXAA, we next tested additional substitutions within the ligand-binding pocket to identify more constraints that would help in the design of future modifications on DMXAA. We generated five new substitutions (G166S, I235L, Q266I, Q266L, Q266V) in hSTING (Figure 19) to either enhance the hydrophobic interaction or introduce additional hydrogen bonds with DMXAA. Initial IFN-β induction results showed that only the Q266I substitution in hSTING conferred DMXAA sensitivity at a level similar to that observed for the S162A substitution (Figure 17A). Q266L resulted in a less pronounced gain of DMXAA-mediated IFN-β induction, while G166S, I235L and Q266V showed no effects (Figure 17A). It should be noted that neither S162A nor Q266I substitutions alone were able to introduce IFN-β responsiveness to DMXAA at a level comparable to mSTING (Figure 17B). We therefore tested whether the S162A/Q266I double substitution would augment DMXAA recognition, and indeed observed an enhanced DMXAA-induced IFN-β induction similar to mSTING (Figure 17B). We further validated the luciferase reporter results by testing the binding affinity for hSTING^{S162A}, hSTING^{Q266I} and hSTING$^{S162A/Q266I}$ (aa 140-379) with DMXAA using ITC. These results confirmed that hSTING$^{S162A/Q266I}$ binds to DMXAA with higher affinity (K_D: 1.99 μM) (Figure 18C) when compared to either hSTING^{S162A} (Figure 21C) or hSTING^{Q266I} (Figure 21D).

[0324] Besides the prevalent allelic hSTING variant (R71/G230/R232/R293, hSTING^{R232}), four major non-synonymous variants are found in high frequencies with R71H/G230A/R293Q (hSTING^{HAQ}) is present in 20.4%, R232H (hSTING^{H232}) in 13.7%, G230A/R293Q (hSTING^{AQ}) in 5.2%, and R293Q (hSTING^{Q293}) in 1.5% of the human population (Yi et al., 2013). To determine whether the S162A and Q266I substitutions were effective in all natural human STING variants, we generated the respective single and double substitutions for all major hSTING alleles (listed in Figure 17D) and tested them for DMXAA recognition (Figure 17E). The S162A/Q266I double substitution was able to induce DMXAA responsiveness in all hSTING alleles, whereas single substitutions were only effective in

hSTING^{R232} and hSTING^{H232}. This was further validated by titration of DMXAA concentrations (Figure 17B for hSTING^{R232}, Figures 22A and 22B for other hSTING alleles), which showed a variable maximal IFN-β induction for different alleles, but clear sigmoidal dose-responses that diverges by less than one order of magnitude in their EC_{50}. Taken together, the Q266I substitution renders hSTING responsive to DMXAA. Further, hSTING containing Q266I and S162A substitutions led to a DMXAA-dependent IFN-β reporter response close to that observed for mSTING.

Example 14: Crystal Structure of DMXAA Bound to hSTING$^{S162A/Q266I}$

[0325] To better understand how S162A and Q266I substitutions facilitate the IFN induction of hSTING by DMXAA, we solved the co-crystal complex of DMXAA with hSTING$^{S162A/Q266I}$ (aa 155-341) at 2.42 Å resolution (x-ray statistics in Table S1). The complex adopts the 'closed' conformation as reflected by the positioning of two DMXAA in the binding pocket and the formation of the four-stranded antiparallel β-sheet lid over the bound ligands (Figure 17F). The crystal structures of hSTING$^{S162A/Q266I}$ and hSTING^{G230I} in their bound complexes with DMXAA superimpose with an rmsd of 0.70 Å (Figure 22C). The details of the intermolecular contacts in the complex are shown in Figure 22D, with the same intermolecular hydrogen bonding interaction network as observed in hSTING^{group2}-DMXAA (Figure 15F) and hSTING^{G230I}-DMXAA (Figure 21A) complexes. The substituted I266 side chain forms a hydrophobic patch together with the side chains of I165, L170 and I235, which fully covers the aromatic methyl groups (positions 5 and 6) and the non-substituted aromatic edges (positions 7 and 8) of DMXAA (Figure 17G). The substituted A162 side chain is juxtaposed to the aromatic edges lining the other side (positions 1 and 2) of DMXAA, forming additional hydrophobic interactions (Figure 17G). S162A and Q266I substitutions increase the binding affinity between hSTING and DMXAA and apparently assist hSTING to overcome the energy barrier from an 'open' to a 'closed' conformation. Based on the information on these two point substitutions in hSTING, it should be feasible to apply structure-guided approaches to design DMXAA analogs targeting hSTING.

Example 15: hSTING$^{S162A/G230I/Q266I}$ is more Sensitive to DMXAA than mSTING in IFN-β Induction

[0326] We next tested whether combining the G230I substitution with the binding-pocket substitutions S162A/Q266I would further enhance hSTING sensitivity to DMXAA. We generated the triple mutant of hSTING and tested its binding to DMXAA by ITC, as well as IFN induction by DMXAA in transfected cells. The ITC titration for hSTING$^{S162A/G230I/Q266I}$ with added DMXAA is plotted in Figure 18A, and showed a higher binding affinity (K_D: 0.99 μM) than that observed for hSTING^{group2} (K_D: 3.12 μM) (Figure 15C) or hSTING$^{S162A/Q266I}$ (K_D: 1.99 μM) (Figure 17C), indicating that all three substitutions individually contribute to an increased DMXAA sensitivity. This increase in affinity translates to synergistic functional effects based on our luciferase reporter assays in which hSTING$^{S162A/G230I/Q266I}$ showed approximately two orders of magnitude higher sensitivity than hSTING^{G230I}, as well as an order of magnitude higher than either hSTING$^{S162A/Q266I}$ or mSTING for the IFN-β induction by DMXAA (Figure 18B).

[0327] We also solved the crystal structure of DMXAA bound to hSTING$^{S162A/G230I/Q266I}$ (aa 155-341) at 2.37 Å resolution (x-ray statistics in Table S1) in the 'closed' conformation (Figure 18C). As expected, we observed both the hydrophobic pocket surrounding I230 (Figure 18D), which is the same as in the hSTING^{G230I}-DMXAA complex (Figure 16D), as well as the hydrophobic interactions within the DMXAA binding pocket (Figure 18E), which is the same as in the hSTING$^{S162A/Q266I}$-DMXAA complex (Figure 17G).

Table S7. X-ray Statistics for DMXAA with hSTING Mutants

Crystal	hSTING^{group2} + DMXAA	hSTING^{G230I} + DMXAA	hSTING$^{S162A/Q266I}$ + DMXAA	hSTING$^{S162A/G230I/Q266I}$ + DMXAA
Beam line	APS-ID24C	APS-ID24C	APS-ID24C	APS-ID24C
Wavelength	1.550	1.550	1.550	1.550
Space group	$P6_122$	$P2_1$	$P6$	$P6$
Unit cell				
a, b, c (Å)	62.9, 62.9, 196.1	36.6, 77.9, 79.6	148.0, 148.0, 36.1	148.6, 148.6, 36.2
α, β, γ (°)	90.0, 90.0, 120.0	90.0, 99.0, 90.0	90.0, 90.0, 120.0	90.0, 90.0, 120.0
Resolution (Å)	50-1.88 (1.92-1.88)[a]	50-2.51 (2.61-2.51)[a]	50-2.42 (2.55-2.42)[a]	50-2.37 (2.50-2.37)[a]
R_{merge}	0.077 (0.785)	0.102 (0.643)	0.118 (1.017)	0.115 (1.104)
I/ σ (I)	15.2 (2.4)	12.1 (2.3)	15.4 (2.3)	25.9 (3.1)
Completeness (%)	97.6 (93.7)	94.6 (89.5)	100.0 (100.0)	100.0 (100.0)
Redundancy	5.8 (6.0)	3.8 (3.7)	9.4 (9.0)	9.1 (8.7)
Number of unique reflections	19022	14320	17687	19048
R_{work}/R_{free} (%)	17.4/21.8	19.7/23.9	18.2/22.8	18.7/23.1
Number of non-H atoms				
Protein	1499	2932	2920	2928
Water	137	55	71	58
Ligands(molecule)	1	2	2	2
Average B factors (Å^2)				
Protein	38.68	68.70	56.51	68.13
Water	45.73	44.55	51.55	63.79
ligands	21.53	49.91	28.21	38.75
R.m.s. deviations				
Bond lengths (Å)	0.013	0.007	0.014	0.007
Bond angles (°)	1.580	1.262	1.613	1.203

[a] Highest resolution shell (in Å) shown in parentheses.

Example 16: DMXAA Activates Type I IFN and Proinflammatory Cytokine/Chemokine Production in mSTING-Deficient BMDCs reconstituted with hSTING Substitutions

[0328] Examples 1-8 show that c[G(2',5')pA(3',5')p] and its linkage analogs induce type I IFN and proinflammatory cytokine/chemokine production in a STING-dependent manner in bone marrow-derived macrophages. To test whether various hSTING substitutions can rescue the deficiency of type I IFN and proinflammatory cytokine/chemokine production in response to DMXAA in mSTING-deficient bone marrow-derived dendritic cells (BMDCs), we generated BMDCs from homozygous functional null STING mice (*Goldenticket, STING$^{Gt/Gt}$*) (Sauer et al., 2011). Retroviruses carrying wt hSTING or hSTING mutants (hSTING^{G230I}, hSTING$^{S162A/Q266I}$, hSTING$^{S162A/G230I/Q266I}$, hSTING^{S162A}) were used to transduce these BMDCs. Although wt hSTING did not induce the up-regulation of IFN-β mRNA after DMXAA treatment, we observed 2.6, 3.1, 4.2, and 2.2-fold increases in IFN-β mRNA levels in BMDCs expressing hSTING^{G230I}, hSTING$^{S162A/Q266I}$, hSTING$^{S162A/G230I/Q266I}$ and hSTING^{S162A}, respectively. Similar to the results obtained from the luciferase reporter assays, we found that STING$^{Gt/Gt}$-derived BMDCs expressing hSTING$^{S162A/G230I/Q266I}$ had the highest IFN-β mRNA induction after DMXAA treatment, corroborating that G230I substitution and the pocket substitutions S162A/Q226I lead to synergistic effects on hSTING sensitivity to DMXAA. We also observed up-regulation of CXCL10, CCL5 and IL-6 mRNAs in BMDCs expressing various hSTING mutants (Figure 18F), with hSTING$^{S162A/G230I/Q266I}$ eliciting the strongest induction among the four mutants after DMXAA treatment. We also collected supernatants at 18 h post DMXAA treatment. At this time point, hSTING$^{S162A/G230I/Q266I}$ induced the highest level of CXCL10 production compared with the other hSTING substituents (Figure 22E). We confirmed hSTING protein expression in transduced cells by Western blot analysis (Figure 18G).

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Table 6. DMXAA-hSTING^{group2} complex

```
REMARK   3
REMARK   3 REFINEMENT.
REMARK   3  PROGRAM     : PHENIX (phenix.refine: 1.8.2_1309)
REMARK   3  AUTHORS     : Adams,Afonine,Burnley,Chen,Davis,Echols,Gildea,
REMARK   3              : Gopal,Gros,Grosse-Kunstleve,Headd,Hung,Immormino,
REMARK   3              : Ioerger,McCoy,McKee,Moriarty,Pai,Read,Richardson,
REMARK   3              : Richardson,Romo,Sacchettini,Sauter,Smith,Storoni,
REMARK   3              : Terwilliger,Zwart
REMARK   3
REMARK   3  REFINEMENT TARGET : ML
REMARK   3
REMARK   3  DATA USED IN REFINEMENT.
REMARK   3  RESOLUTION RANGE HIGH (ANGSTROMS) : 1.880
REMARK   3  RESOLUTION RANGE LOW  (ANGSTROMS) : 54.491
REMARK   3  MIN(FOBS/SIGMA_FOBS)           : 1.37
REMARK   3  COMPLETENESS FOR RANGE       (%) : 96.91
REMARK   3  NUMBER OF REFLECTIONS           : 19022
REMARK   3  NUMBER OF REFLECTIONS (NON-ANOMALOUS) : 19022
REMARK   3
REMARK   3  FIT TO DATA USED IN REFINEMENT.
REMARK   3  R VALUE     (WORKING + TEST SET) : 0.1765
REMARK   3  R VALUE           (WORKING SET) : 0.1743
REMARK   3  FREE R VALUE                    : 0.2185
REMARK   3  FREE R VALUE TEST SET SIZE   (%) : 5.14
REMARK   3  FREE R VALUE TEST SET COUNT     : 977
REMARK   3
REMARK   3  FIT TO DATA USED IN REFINEMENT (IN BINS).
REMARK   3  BIN  RESOLUTION RANGE  COMPL.   NWORK NFREE   RWORK
RFREE
REMARK   3    1 54.5141 -  3.5962    0.98    2865   140  0.1574 0.1997
REMARK   3    2  3.5962 -  2.8544    0.99    2698   112  0.1674 0.1953
REMARK   3    3  2.8544 -  2.4936    0.98    2588   146  0.1813 0.2280
REMARK   3    4  2.4936 -  2.2656    0.98    2537   160  0.1775 0.2272
REMARK   3    5  2.2656 -  2.1032    0.97    2507   144  0.1899 0.2259
REMARK   3    6  2.1032 -  1.9792    0.95    2455   131  0.2010 0.2427
REMARK   3    7  1.9792 -  1.8801    0.93    2395   144  0.2943 0.3815
REMARK   3
REMARK   3  BULK SOLVENT MODELLING.
REMARK   3  METHOD USED        : FLAT BULK SOLVENT MODEL
REMARK   3  SOLVENT RADIUS     : 1.11
REMARK   3  SHRINKAGE RADIUS   : 0.90
REMARK   3  GRID STEP FACTOR   : 4.00
REMARK   3
REMARK   3  ERROR ESTIMATES.
REMARK   3  COORDINATE ERROR (MAXIMUM-LIKELIHOOD BASED)     : 0.22
REMARK   3  PHASE ERROR (DEGREES, MAXIMUM-LIKELIHOOD BASED) :
20.66
REMARK   3
REMARK   3  STRUCTURE FACTORS CALCULATION ALGORITHM : FFT
REMARK   3
REMARK   3  DEVIATIONS FROM IDEAL VALUES.
REMARK   3              RMSD     MAX  COUNT
REMARK   3  BOND      : 0.013   0.073  1551
REMARK   3  ANGLE     : 1.580  11.179  2109
REMARK   3  CHIRALITY : 0.113   0.543   225
REMARK   3  PLANARITY : 0.007   0.049   281
REMARK   3  DIHEDRAL  : 16.214  68.227   593
REMARK   3  MIN NONBONDED DISTANCE : 1.748
REMARK   3
REMARK   3  MOLPROBITY STATISTICS.
REMARK   3  ALL-ATOM CLASHSCORE : 4.68
REMARK   3  RAMACHANDRAN PLOT:
REMARK   3    OUTLIERS : 0.00 %
REMARK   3    ALLOWED  : 4.35 %
REMARK   3    FAVORED  : 95.65 %
REMARK   3  ROTAMER OUTLIERS : 3.07 %
REMARK   3  CBETA DEVIATIONS : 1
REMARK   3
REMARK   3  ATOMIC DISPLACEMENT PARAMETERS.
REMARK   3  WILSON B : 31.20
REMARK   3  RMS(B_ISO_OR_EQUIVALENT_BONDED) : 6.85
REMARK   3  ATOMS        NUMBER OF ATOMS
REMARK   3                ISO.  ANISO.
REMARK   3  ALL       :  1650   1494
REMARK   3  ALL (NO H) :  1650   1494
REMARK   3  SOLVENT    :  135      0
REMARK   3  NON-SOLVENT :  1515   1494
REMARK   3  HYDROGENS  :    0      0
REMARK   3
REMARK   3  TLS DETAILS.
REMARK   3  NUMBER OF TLS GROUPS: 7
REMARK   3  ORIGIN: CENTER OF MASS
REMARK   3  TLS GROUP : 1
REMARK   3   SELECTION: chain 'A' and (resid  154  through  167 )
REMARK   3   ORIGIN FOR THE GROUP (A): -13.4260  50.6427   4.3207
REMARK   3   T TENSOR
REMARK   3     T11:  0.1683 T22:  0.1103
REMARK   3     T33:  0.1207 T12:  -0.0135
REMARK   3     T13: -0.0096 T23:  -0.0277
REMARK   3   L TENSOR
REMARK   3     L11:  4.8802 L22:  3.2007
REMARK   3     L33:  6.2531 L12:  0.5545
REMARK   3     L13: -3.1583 L23:  -0.6229
REMARK   3   S TENSOR
REMARK   3     S11:  0.0931 S12:  -0.6224 S13:  0.0424
REMARK   3     S21:  0.2192 S22:  -0.0965 S23:  -0.1503
REMARK   3     S31: -0.0048 S32:  0.5314 S33:  -0.0194
REMARK   3  TLS GROUP : 2
REMARK   3   SELECTION: chain 'A' and (resid  168  through  185 )
REMARK   3   ORIGIN FOR THE GROUP (A): -32.7374  41.7922   9.1633
REMARK   3   T TENSOR
REMARK   3     T11:  0.3021 T22:  0.2444
REMARK   3     T33:  0.3426 T12:  -0.0595
REMARK   3     T13:  0.0922 T23:  -0.0478
REMARK   3   L TENSOR
REMARK   3     L11:  3.4374 L22:  2.9964
REMARK   3     L33:  3.1918 L12:  2.4360
REMARK   3     L13:  1.3854 L23:  2.0523
REMARK   3   S TENSOR
REMARK   3     S11:  0.5743 S12:  -1.1553 S13:  0.5744
REMARK   3     S21:  0.6347 S22:  -0.7613 S23:  0.8717
REMARK   3     S31:  0.1473 S32:  -0.3896 S33:  0.0968
REMARK   3  TLS GROUP : 3
REMARK   3   SELECTION: chain 'A' and (resid  186  through  211 )
REMARK   3   ORIGIN FOR THE GROUP (A): -27.1904  34.9528  -0.7246
REMARK   3   T TENSOR
REMARK   3     T11:  0.2543 T22:  0.1132
REMARK   3     T33:  0.2799 T12:  0.0289
REMARK   3     T13:  0.0152 T23:  -0.0043
REMARK   3   L TENSOR
REMARK   3     L11:  9.8039 L22:  4.3916
REMARK   3     L33:  2.9025 L12:  5.7740
REMARK   3     L13: -3.0538 L23:  -1.9563
REMARK   3   S TENSOR
REMARK   3     S11: -0.0078 S12:  0.1178 S13:  0.0817
REMARK   3     S21: -0.0786 S22:  -0.0580 S23:  0.0132
REMARK   3     S31:  0.0919 S32:  0.0047 S33:  -0.0013
REMARK   3  TLS GROUP : 4
REMARK   3   SELECTION: chain 'A' and (resid  212  through  280 )
REMARK   3   ORIGIN FOR THE GROUP (A): -25.5020  42.8838  -4.1159
REMARK   3   T TENSOR
REMARK   3     T11:  0.2173 T22:  0.1850
REMARK   3     T33:  0.1792 T12:  0.0218
REMARK   3     T13: -0.0241 T23:  -0.0111
REMARK   3   L TENSOR
REMARK   3     L11:  2.6912 L22:  1.9708
REMARK   3     L33:  1.7012 L12:  0.7989
REMARK   3     L13: -0.5883 L23:  -0.0806
REMARK   3   S TENSOR
REMARK   3     S11:  0.0125 S12:  0.0312 S13:  0.0124
REMARK   3     S21: -0.0313 S22:  -0.0579 S23:  0.1528
REMARK   3     S31:  0.0124 S32:  -0.1562 S33:  0.0446
REMARK   3  TLS GROUP : 5
REMARK   3   SELECTION: chain 'A' and (resid  281  through  299 )
REMARK   3   ORIGIN FOR THE GROUP (A): -7.1814  43.5461  -1.4472
REMARK   3   T TENSOR
REMARK   3     T11:  0.1952 T22:  0.1940
REMARK   3     T33:  0.2378 T12:  0.0443
REMARK   3     T13: -0.0485 T23:  -0.0102
REMARK   3   L TENSOR
REMARK   3     L11:  9.1414 L22:  4.6808
REMARK   3     L33:  6.3324 L12:  1.0083
REMARK   3     L13: -6.9440 L23:  -0.5677
REMARK   3   S TENSOR
REMARK   3     S11: -0.1423 S12:  -0.1738 S13:  -0.4257
REMARK   3     S21:  0.0344 S22:  0.0534 S23:  -0.4990
REMARK   3     S31:  0.5858 S32:  0.9638 S33:  0.2796
REMARK   3  TLS GROUP : 6
REMARK   3   SELECTION: chain 'A' and (resid  300  through  314 )
REMARK   3   ORIGIN FOR THE GROUP (A): -18.7157  39.1351   8.9537
REMARK   3   T TENSOR
REMARK   3     T11:  0.4995 T22:  0.3964
REMARK   3     T33:  0.2781 T12:  0.0221
REMARK   3     T13: -0.0514 T23:  0.0212
REMARK   3   L TENSOR
REMARK   3     L11:  4.8044 L22:  4.6243
REMARK   3     L33:  3.0810 L12:  -0.7724
REMARK   3     L13: -1.9557 L23:  3.4708
REMARK   3   S TENSOR
REMARK   3     S11: -0.0010 S12:  -0.9497 S13:  -0.1092
REMARK   3     S21:  1.1162 S22:  0.0813 S23:  -0.3287
REMARK   3     S31:  0.4353 S32:  -0.1031 S33:  0.1316
REMARK   3  TLS GROUP : 7
REMARK   3   SELECTION: chain 'A' and (resid  315  through  335 )
REMARK   3   ORIGIN FOR THE GROUP (A): -16.9164  28.0917  -5.8168
REMARK   3   T TENSOR
REMARK   3     T11:  0.3475 T22:  0.3288
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REMARK   3    T33:  0.3348 T12:  0.0762
REMARK   3    T13: -0.0345 T23:  0.0252
REMARK   3   L TENSOR
REMARK   3    L11:  3.4482 L22:  5.1152
REMARK   3    L33:  4.7731 L12:  2.2134
REMARK   3    L13: -4.0510 L23: -2.1278
REMARK   3   S TENSOR
REMARK   3    S11: -0.2271 S12: -0.1756 S13: -0.6768
REMARK   3    S21: -0.3089 S22: -0.2971 S23: -0.3644
REMARK   3    S31:  1.0155 S32:  0.9738 S33:  0.4937
REMARK   3
CRYST1  62.921  62.921 196.054 90.00 90.00 120.00 P 61 2 2
SCALE1      0.015893 0.009176 0.000000        0.00000
SCALE2      0.000000 0.018352 0.000000        0.00000
SCALE3      0.000000 0.000000 0.005101        0.00000
ATOM      1  N   SER A 154      -3.015  53.192   1.851  1.00 48.06           N
ANISOU    1  N   SER A 154     4854   7355   6050   -705   -138   -354       N
ATOM      2  CA  SER A 154      -3.281  52.521   0.590  1.00 39.52           C
ANISOU    2  CA  SER A 154     3932   5969   5113   -442     -2   -225       C
ATOM      3  CB  SER A 154      -2.946  51.028   0.690  1.00 43.14           C
ANISOU    3  CB  SER A 154     4273   6556   5563    -73    -34     16       C
ATOM      4  OG  SER A 154      -4.052  50.302   1.173  1.00 38.49           O
ANISOU    4  OG  SER A 154     3913   5780   4930     82    -81     78       O
ATOM      5  C   SER A 154      -4.739  52.703   0.174  1.00 25.77           C
ANISOU    5  C   SER A 154     2572   3800   3418   -416     56   -282       C
ATOM      6  O   SER A 154      -5.618  52.958   0.989  1.00 26.82           O
ANISOU    6  O   SER A 154     2833   3874   3483   -486    -14   -356       O
ATOM      7  N   VAL A 155      -4.997  52.549  -1.127  1.00 23.93           N
ANISOU    7  N   VAL A 155     2502   3308   3283   -308    189   -240       N
ATOM      8  CA  VAL A 155      -6.369  52.608  -1.607  1.00 21.08           C
ANISOU    8  CA  VAL A 155     2442   2628   2939   -259    219   -260       C
ATOM      9  CB  VAL A 155      -6.419  52.379  -3.125  1.00 23.46           C
ANISOU    9  CB  VAL A 155     2874   2750   3291   -158    351   -209       C
ATOM     10  CG1 VAL A 155      -7.832  52.019  -3.525  1.00 23.12           C
ANISOU   10  CG1 VAL A 155     3072   2495   3219    -72    330   -200       C
ATOM     11  CG2 VAL A 155      -5.958  53.669  -3.848  1.00 27.32           C
ANISOU   11  CG2 VAL A 155     3375   3176   3828   -342    478   -263       C
ATOM     12  C   VAL A 155      -7.284  51.616  -0.884  1.00 22.97           C
ANISOU   12  C   VAL A 155     2768   2836   3123   -109    121   -202       C
ATOM     13  O   VAL A 155      -8.384  51.959  -0.434  1.00 22.48           O
ANISOU   13  O   VAL A 155     2846   2660   3037   -163     83   -260       O
ATOM     14  N   ALA A 156      -6.812  50.382  -0.740  1.00 22.07           N
ANISOU   14  N   ALA A 156     2568   2817   3000     91    112    -73       N
ATOM     15  CA  ALA A 156      -7.594  49.312  -0.102  1.00 18.74           C
ANISOU   15  CA  ALA A 156     2251   2329   2539    237     69     10       C
ATOM     16  CB  ALA A 156      -6.768  48.036  -0.063  1.00 24.84           C
ANISOU   16  CB  ALA A 156     2928   3179   3333    489    125    186       C
ATOM     17  C   ALA A 156      -7.988  49.642   1.329  1.00 29.73           C
ANISOU   17  C   ALA A 156     3598   3873   3826    142    -58    -15       C
ATOM     18  O   ALA A 156      -9.069  49.262   1.804  1.00 24.94           O
ANISOU   18  O   ALA A 156     3139   3149   3188    164    -76     -9       O
ATOM     19  N   HIS A 157      -7.057  50.249   2.054  1.00 23.60           N
ANISOU   19  N   HIS A 157     2597   3396   2973     29   -138    -43       N
ATOM     20  C   HIS A 157      -8.467  51.558   3.555  1.00 30.39           C
ANISOU   20  C   HIS A 157     3620   4236   3692   -272   -216   -278       C
ATOM     21  O   HIS A 157      -9.351  51.389   4.384  1.00 28.20           O
ANISOU   21  O   HIS A 157     3443   3937   3334   -269   -245   -286       O
ATOM     22  CA AHIS A 157      -7.327  50.575   3.458  0.55 25.53           C
ANISOU   22  CA AHIS A 157     2798   3839   3063    -90   -256    -92       C
ATOM     23  CB AHIS A 157      -6.100  51.149   4.148  0.55 28.32           C
ANISOU   23  CB AHIS A 157     3072   4607   3296   -250   -357   -138       C
ATOM     24  CG AHIS A 157      -5.042  50.140   4.409  0.55 33.78           C
ANISOU   24  CG AHIS A 157     3283   5620   3931    -19   -424     99       C
ATOM     25  ND1AHIS A 157      -3.714  50.355   4.105  0.55 49.79           N
ANISOU   25  ND1AHIS A 157     4999   7946   5973    -53   -440    126       N
ATOM     26  CE1AHIS A 157      -3.015  49.285   4.440  0.55 49.57           C
ANISOU   26  CE1AHIS A 157     4756   8181   5897    246   -487    397       C
ATOM     27  NE2AHIS A 157      -3.838  48.387   4.945  0.55 40.13           N
ANISOU   27  NE2AHIS A 157     3761   6828   4660    459   -486    544       N
ATOM     28  CD2AHIS A 157      -5.117  48.893   4.935  0.55 32.78           C
ANISOU   28  CD2AHIS A 157     3148   5560   3748    277   -452    348       C
ATOM     29  CA BHIS A 157      -7.288  50.581   3.457  0.45 26.09           C
ANISOU   29  CA BHIS A 157     2862   3918   3134    -91   -257    -92       C
ATOM     30  CB BHIS A 157      -6.010  51.192   4.037  0.45 28.72           C
ANISOU   30  CB BHIS A 157     2897   4654   3359   -255   -349   -142       C
ATOM     31  CG BHIS A 157      -5.912  51.095   5.521  0.45 32.23           C
ANISOU   31  CG BHIS A 157     3220   5452   3574   -313   -500   -123       C
ATOM     32  ND1BHIS A 157      -5.892  49.888   6.198  0.45 29.79           N
ANISOU   32  ND1BHIS A 157     2854   5303   3160    -45   -570    129       N
ATOM     33  CE1BHIS A 157      -5.776  50.119   7.495  0.45 33.98           C
ANISOU   33  CE1BHIS A 157     3274   6195   3440   -169   -710    105       C
ATOM     34  NE2BHIS A 157      -5.719  51.418   7.690  0.45 24.55           N
ANISOU   34  NE2BHIS A 157     2074   5065   2190   -533   -722   -192       N
ATOM     35  CD2BHIS A 157      -5.794  52.058   6.476  0.45 47.22           C
ANISOU   35  CD2BHIS A 157     5053   7590   5297   -619   -579   -325       C
ATOM     36  N   GLY A 158      -8.466  52.579   2.687  1.00 24.89           N
ANISOU   36  N   GLY A 158     2990   3364   3102   -407   -121   -402       N
ATOM     37  CA  GLY A 158      -9.583  53.534   2.652  1.00 25.79           C
ANISOU   37  CA  GLY A 158     3307   3232   3260   -509    -41   -530       C
ATOM     38  C   GLY A 158     -10.898  52.868   2.270  1.00 24.90           C
ANISOU   38  C   GLY A 158     3352   2916   3193   -336    -25   -443       C
ATOM     39  O   GLY A 158     -11.920  53.116   2.899  1.00 23.56           O
ANISOU   39  O   GLY A 158     3276   2680   2997   -355    -11   -492       O
ATOM     40  N   LEU A 159     -10.877  52.021   1.243  1.00 22.28           N
ANISOU   40  N   LEU A 159     3043   2501   2921   -191    -11   -332       N
ATOM     41  CA  LEU A 159     -12.100  51.337   0.773  1.00 20.10           C
ANISOU   41  CA  LEU A 159     2897   2071   2670    -90      1   -280       C
ATOM     42  CB  LEU A 159     -11.835  50.527  -0.496  1.00 21.10           C
ANISOU   42  CB  LEU A 159     3064   2118   2834      7     43   -216       C
ATOM     43  CG  LEU A 159     -11.502  51.366  -1.739  1.00 27.15           C
ANISOU   43  CG  LEU A 159     3856   2820   3641    -28    109   -239       C
ATOM     44  CD1 LEU A 159     -11.225  50.461  -2.926  1.00 24.38           C
ANISOU   44  CD1 LEU A 159     3561   2419   3284     56    165   -199       C
ATOM     45  CD2 LEU A 159     -12.634  52.303  -2.094  1.00 26.58           C
ANISOU   45  CD2 LEU A 159     3805   2722   3571    -49     94   -235       C
ATOM     46  C   LEU A 159     -12.656  50.419   1.854  1.00 19.40           C
ANISOU   46  C   LEU A 159     2819   2038   2514    -42    -44   -230       C
ATOM     47  O   LEU A 159     -13.868  50.344   2.060  1.00 19.64           O
ANISOU   47  O   LEU A 159     2927   1992   2545    -52    -33   -245       O
ATOM     48  N   ALA A 160     -11.776  49.674   2.541  1.00 16.49           N
ANISOU   48  N   ALA A 160     2359   1823   2083     26    -84   -140       N
ATOM     49  CA  ALA A 160     -12.257  48.750   3.579  1.00 19.37           C
ANISOU   49  CA  ALA A 160     2758   2233   2370     93   -102    -44       C
ATOM     50  CB  ALA A 160     -11.093  47.886   4.114  1.00 20.08           C
ANISOU   50  CB  ALA A 160     2729   2506   2395    243   -132    127       C
ATOM     51  C   ALA A 160     -12.917  49.517   4.721  1.00 18.78           C
ANISOU   51  C   ALA A 160     2691   2251   2195    -30   -133   -136       C
ATOM     52  O   ALA A 160     -13.970  49.109   5.244  1.00 19.81           O
ANISOU   52  O   ALA A 160     2908   2320   2299    -26   -100   -114       O
ATOM     53  N   TRP A 161     -12.272  50.598   5.184  1.00 18.80           N
ANISOU   53  N   TRP A 161     2605   2409   2128   -162   -174   -254       N
ATOM     54  CA  TRP A 161     -12.856  51.359   6.295  1.00 18.71           C
ANISOU   54  CA  TRP A 161     2635   2471   2003   -298   -163   -382       C
ATOM     55  CB  TRP A 161     -11.852  52.340   6.892  1.00 20.35           C
ANISOU   55  CB  TRP A 161     2740   2899   2094   -491   -207   -532       C
ATOM     56  CG  TRP A 161     -10.927  51.647   7.810  1.00 22.45           C
ANISOU   56  CG  TRP A 161     2841   3531   2158   -465   -342   -418       C
ATOM     57  CD1 TRP A 161      -9.643  51.258   7.534  1.00 22.96           C
ANISOU   57  CD1 TRP A 161     2699   3817   2206   -406   -432   -306       C
ATOM     58  NE1 TRP A 161      -9.106  50.626   8.664  1.00 26.80           N
ANISOU   58  NE1 TRP A 161     3040   4687   2457   -347   -559   -164       N
ATOM     59  CE2 TRP A 161     -10.067  50.558   9.637  1.00 20.31           C
ANISOU   59  CE2 TRP A 161     2364   3860   1493   -378   -540   -188       C
ATOM     60  CD2 TRP A 161     -11.234  51.191   9.133  1.00 27.12           C
ANISOU   60  CD2 TRP A 161     3440   4341   2524   -455   -396   -358       C
ATOM     61  CE3 TRP A 161     -12.374  51.245   9.948  1.00 29.02           C
ANISOU   61  CE3 TRP A 161     3833   4517   2675   -488   -324   -411       C
ATOM     62  CZ3 TRP A 161     -12.312  50.688  11.239  1.00 30.61           C
ANISOU   62  CZ3 TRP A 161     4006   5022   2603   -469   -394   -304       C
ATOM     63  CH2 TRP A 161     -11.137  50.066  11.706  1.00 29.95           C
ANISOU   63  CH2 TRP A 161     3724   5323   2333   -386   -553   -115       C
ATOM     64  CZ2 TRP A 161     -10.011  49.986  10.931  1.00 22.60           C
ANISOU   64  CZ2 TRP A 161     2606   4479   1504   -328   -630    -49       C
ATOM     65  C   TRP A 161     -14.129  52.080   5.862  1.00 21.56           C
ANISOU   65  C   TRP A 161     3126   2583   2482   -323   -51   -481       C
ATOM     66  O   TRP A 161     -15.098  52.169   6.601  1.00 21.19           O
ANISOU   66  O   TRP A 161     3143   2520   2386   -337     2   -518       O
ATOM     67  N   SER A 162     -14.160  52.585   4.639  1.00 16.81           N
ANISOU   67  N   SER A 162     2551   1809   2028   -304    -4   -498       N
ATOM     68  CA  SER A 162     -15.357  53.322   4.246  1.00 19.51           C
ANISOU   68  CA  SER A 162     2945   1996   2473   -257    84   -510       C
ATOM     69  CB  SER A 162     -15.122  54.165   2.988  1.00 22.27           C
ANISOU   69  CB  SER A 162     3270   2261   2932   -211    109   -462       C
ATOM     70  OG  SER A 162     -14.791  53.302   1.937  1.00 29.53           O
ANISOU   70  OG  SER A 162     4168   3172   3882   -152     57   -384       O
ATOM     71  C   SER A 162     -16.536  52.367   4.057  1.00 19.48           C
ANISOU   71  C   SER A 162     2962   1950   2490   -170    -79   -425       C
ATOM     72  O   SER A 162     -17.683  52.731   4.317  1.00 19.92           O
ANISOU   72  O   SER A 162     3018   1978   2572   -143    141   -433       O
ATOM     73  N   TYR A 163     -16.268  51.157   3.587  1.00 16.74           N
ANISOU   73  N   TYR A 163     2621   1603   2137   -130     24   -339       N
ATOM     74  CA  TYR A 163     -17.350  50.178   3.382  1.00 15.57           C
ANISOU   74  CA  TYR A 163     2492   1416   2008   -105     35   -277       C
ATOM     75  CB  TYR A 163     -16.787  49.009   2.570  1.00 19.52           C
ANISOU   75  CB  TYR A 163     3026   1864   2527    -71     15   -209       C
ATOM     76  CG  TYR A 163     -17.816  47.972   2.152  1.00 20.68           C
ANISOU   76  CG  TYR A 163     3181   1980   2696   -110     46   -185       C
ATOM     77  CD1 TYR A 163     -18.877  48.315   1.297  1.00 20.58           C
ANISOU   77  CD1 TYR A 163     3118   1991   2711   -158     29   -227       C
ATOM     78  CE1 TYR A 163     -19.828  47.341   0.870  1.00 21.84           C
ANISOU   78  CE1 TYR A 163     3300   2133   2866   -268     50   -251       C
ATOM     79  CZ  TYR A 163     -19.685  46.034   1.331  1.00 21.63           C
ANISOU   79  CZ  TYR A 163     3343   2039   2836   -300    121   -217       C
ATOM     80  OH  TYR A 163     -20.579  45.055   0.933  1.00 25.03           O
ANISOU   80  OH  TYR A 163     3796   2449   3266   -443    170   -261       O
ATOM     81  CE2 TYR A 163     -18.625  45.678   2.173  1.00 26.54           C
ANISOU   81  CE2 TYR A 163     4032   2604   3447   -199    158   -135       C
ATOM     82  CD2 TYR A 163     -17.697  46.655   2.580  1.00 26.00           C
ANISOU   82  CD2 TYR A 163     3947   2575   3356   -110    105   -121       C
ATOM     83  C   TYR A 163     -17.903  49.705   4.723  1.00 22.80           C
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ANISOU  83 C  TYR A 163    3420  2401  2843  -131    67  -257      C
ATOM    84 O  TYR A 163     -19.100 49.451  4.884  1.00 22.77      O
ANISOU  84 O  TYR A 163    3407  2385  2859  -156   118  -251      O
ATOM    85 N  TYR A 164     -17.032 49.607  5.713  1.00 18.80      N
ANISOU  85 N  TYR A 164    2912  2007  2223  -133    39  -237      N
ATOM    86 CA TYR A 164     -17.478 49.264  7.064  1.00 17.85      C
ANISOU  86 CA TYR A 164    2817  1990  1975  -157    75  -204      C
ATOM    87 CB TYR A 164     -16.284 48.963  7.957  1.00 18.02      C
ANISOU  87 CB TYR A 164    2810  2207  1829  -133     0  -129      C
ATOM    88 CG TYR A 164     -16.714 48.809  9.406  1.00 23.37      C
ANISOU  88 CG TYR A 164    3523  3040  2316  -168    36  -100      C
ATOM    89 CD1 TYR A 164     -17.613 47.812  9.783  1.00 27.45      C
ANISOU  89 CD1 TYR A 164    4115  3485  2829  -134   128    27      C
ATOM    90 CE1 TYR A 164     -18.018 47.704 11.122  1.00 33.52      C
ANISOU  90 CE1 TYR A 164    4928  4408  3401  -168   183    66      C
ATOM    91 CZ  TYR A 164     -17.504 48.597 12.056  1.00 39.32      C
ANISOU  91 CZ  TYR A 164    5635  5387  3919  -246   130   -50      C
ATOM    92 OH  TYR A 164     -17.860 48.519 13.362  1.00 39.13      O
ANISOU  92 OH  TYR A 164    5666  5548  3654  -291   187   -27      O
ATOM    93 CE2 TYR A 164     -16.619 49.576 11.700  1.00 32.31      C
ANISOU  93 CE2 TYR A 164    4674  4570  3034  -314    36  -208      C
ATOM    94 CD2 TYR A 164     -16.234 49.680 10.371  1.00 28.56      C
ANISOU  94 CD2 TYR A 164    4152  3919  2781  -269    -3  -220      C
ATOM    95 C  TYR A 164     -18.288 50.438  7.662  1.00 18.86      C
ANISOU  95 C  TYR A 164    2950  2135  2080  -223   155  -347      C
ATOM    96 O  TYR A 164     -19.432 50.279  8.053  1.00 24.10      O
ANISOU  96 O  TYR A 164    3621  2783  2752  -230   243  -341      O
ATOM    97 N  ILE A 165     -17.698 51.623  7.673  1.00 18.20      N
ANISOU  97 N  ILE A 165    2866  2062  1987  -277   157  -481      N
ATOM    98 CA ILE A 165     -18.314 52.796  8.311  1.00 18.05      C
ANISOU  98 CA ILE A 165    2898  2010  1950  -335   289  -640      C
ATOM    99 CB ILE A 165     -17.304 53.978  8.362  1.00 20.17      C
ANISOU  99 CB ILE A 165    3160  2289  2213  -426   285  -760      C
ATOM   100 CG1 ILE A 165     -16.109 53.611  9.240  1.00 24.29      C
ANISOU 100 CG1 ILE A 165    3654  3068  2507  -556   170  -805      C
ATOM   101 CD1 ILE A 165     -16.524 53.402 10.683  1.00 27.09      C
ANISOU 101 CD1 ILE A 165    4048  3601  2642  -612   202  -840      C
ATOM   102 CG2 ILE A 165     -17.941 55.281  8.938  1.00 22.09      C
ANISOU 102 CG2 ILE A 165    3446  2450  2497  -445   441  -857      C
ATOM   103 C  ILE A 165     -19.561 53.238  7.533  1.00 21.76      C
ANISOU 103 C  ILE A 165    3353  2313  2603  -234   396  -623      C
ATOM   104 O  ILE A 165     -20.594 53.601  8.128  1.00 23.47      O
ANISOU 104 O  ILE A 165    3576  2516  2823  -207   534  -664      O
ATOM   105 N  GLY A 166     -19.460 53.210  6.215  1.00 20.23      N
ANISOU 105 N  GLY A 166    3117  2029  2540  -167   337  -549      N
ATOM   106 CA GLY A 166     -20.499 53.788  5.360  1.00 19.98      C
ANISOU 106 CA GLY A 166    3037  1904  2650   -51   410  -502      C
ATOM   107 C  GLY A 166     -21.514 52.776  4.821  1.00 24.12      C
ANISOU 107 C  GLY A 166    3447  2512  3206   -17   351  -387      C
ATOM   108 O  GLY A 166     -22.444 53.168  4.129  1.00 24.34      O
ANISOU 108 O  GLY A 166    3375  2554  3318    79   380  -324      O
ATOM   109 N  TYR A 167     -21.397 51.504  5.175  1.00 23.68      N
ANISOU 109 N  TYR A 167    3396  2523  3077   -101   287  -352      N
ATOM   110 CA TYR A 167     -22.426 50.533  4.765  1.00 19.81      C
ANISOU 110 CA TYR A 167    2816  2096  2616   -143   272  -288      C
ATOM   111 CB TYR A 167     -22.052 49.872  3.422  1.00 23.35      C
ANISOU 111 CB TYR A 167    3267  2518  3086   -176   164  -258      C
ATOM   112 CG TYR A 167     -23.121 48.879  2.961  1.00 23.88      C
ANISOU 112 CG TYR A 167    3247  2666  3161   -296   156  -245      C
ATOM   113 CD1 TYR A 167     -24.425 49.308  2.704  1.00 19.55      C
ANISOU 113 CD1 TYR A 167    2505  2278  2646   -287   165  -226      C
ATOM   114 CE1 TYR A 167     -25.424 48.411  2.321  1.00 22.32      C
ANISOU 114 CE1 TYR A 167    2733  2762  2987   -457   151  -240      C
ATOM   115 CZ  TYR A 167     -25.105 47.061  2.165  1.00 24.77      C
ANISOU 115 CZ  TYR A 167    3178  2967  3267   -649   163  -292      C
ATOM   116 OH  TYR A 167     -26.079 46.168  1.785  1.00 20.89      O
ANISOU 116 OH  TYR A 167    2588  2587  2763   -885   176  -349      O
ATOM   117 CE2 TYR A 167     -23.815 46.608  2.424  1.00 21.50      C
ANISOU 117 CE2 TYR A 167    2991  2339  2840   -605   186  -285      C
ATOM   118 CD2 TYR A 167     -22.832 47.524  2.818  1.00 22.85      C
ANISOU 118 CD2 TYR A 167    3220  2456  3008   -423   162  -252      C
ATOM   119 C  TYR A 167     -22.700 49.471  5.808  1.00 26.51      C
ANISOU 119 C  TYR A 167    3702  2978  3391   -236   325  -262      C
ATOM   120 O  TYR A 167     -23.812 49.378  6.349  1.00 21.01      O
ANISOU 120 O  TYR A 167    2925  2356  2702   -269   419  -255      O
ATOM   121 N  LEU A 168     -21.682 48.664  6.117  1.00 20.15      N
ANISOU 121 N  LEU A 168    3350  1833  2474   -240   126  -203      N
ATOM   122 CA LEU A 168     -21.900 47.511  7.002  1.00 19.16      C
ANISOU 122 CA LEU A 168    3184  1907  2190   -260   151  -138      C
ATOM   123 CB LEU A 168     -20.650 46.651  7.142  1.00 22.03      C
ANISOU 123 CB LEU A 168    3570  2512  2289   -278    21     1      C
ATOM   124 CG LEU A 168     -20.227 46.018  5.808  1.00 24.77      C
ANISOU 124 CG LEU A 168    3919  2788  2703   -124   -156   158      C
ATOM   125 CD1 LEU A 168     -18.963 45.224  6.058  1.00 25.63      C
ANISOU 125 CD1 LEU A 168    4007  3139  2591   -127   -287   228      C
ATOM   126 CD2 LEU A 168     -21.337 45.096  5.188  1.00 22.93      C
ANISOU 126 CD2 LEU A 168    3673  2390  2650    27   -217   288      C
ATOM   127 C  LEU A 168     -22.399 47.929  8.363  1.00 22.35      C
ANISOU 127 C  LEU A 168    3549  2418  2526   -419   346   -335      C
ATOM   128 O  LEU A 168     -23.295 47.323  8.944  1.00 25.48      O
ANISOU 128 O  LEU A 168    3902  2857  2922   -451   424   -349      O
ATOM   129 N  ARG A 169     -21.807 48.982  8.898  1.00 20.85      N
ANISOU 129 N  ARG A 169    3373  2291  2260   -554   442   -509      N
ATOM   130 CA ARG A 169     -22.216 49.460 10.196  1.00 27.08      C
ANISOU 130 CA ARG A 169    4117  3204  2969   -735   648   -741      C
ATOM   131 CB ARG A 169     -21.316 50.632 10.607  1.00 31.16      C
ANISOU 131 CB ARG A 169    4665  3783  3392   -877   719   -916      C
ATOM   132 CG ARG A 169     -21.420 50.911 12.029  1.00 57.57      C
ANISOU 132 CG ARG A 169    7975  7349  6550  -1103   913  -1129      C
ATOM   133 CD ARG A 169     -20.118 51.483 12.519  1.00 58.51      C
ANISOU 133 CD ARG A 169    8147  7661  6422  -1265   913  -1186      C
ATOM   134 NE ARG A 169     -20.103 52.913 12.341  1.00 57.53      N
ANISOU 134 NE ARG A 169    8006  7342  6512  -1281   997  -1396      N
ATOM   135 CZ ARG A 169     -19.256 53.726 12.961  1.00 59.53      C
ANISOU 135 CZ ARG A 169    8229  7721  6667  -1415  1034  -1459      C
ATOM   136 NH1 ARG A 169     -18.340 53.230 13.791  1.00 52.23      N
ANISOU 136 NH1 ARG A 169    7280  7099  5465  -1536   981  -1345      N
ATOM   137 NH2 ARG A 169     -19.322 55.035 12.747  1.00 45.52      N
ANISOU 137 NH2 ARG A 169    6446  5742  5109  -1409  1091  -1614      N
ATOM   138 C  ARG A 169     -23.674 49.912 10.190  1.00 32.27      C
ANISOU 138 C  ARG A 169    4672  3651  3938   -679   782   -940      C
ATOM   139 O  ARG A 169     -24.351 49.890 11.224  1.00 30.74      O
ANISOU 139 O  ARG A 169    4401  3589  3691  -823  968  -1129      O
ATOM   140 N  LEU A 170     -24.160 50.326  9.023  1.00 29.54      N
ANISOU 140 N  LEU A 170    4317  2989  3917  -486   680   -913      N
ATOM   141 CA LEU A 170     -25.530 50.812  8.902  1.00 30.35      C
ANISOU 141 CA LEU A 170    4297  2856  4379  -390   756  -1118      C
ATOM   142 CB LEU A 170     -25.699 51.677  7.648  1.00 31.20      C
ANISOU 142 CB LEU A 170    4430  2642  4781  -201   558  -1045      C
ATOM   143 CG LEU A 170     -24.803 52.909  7.572  1.00 43.17      C
ANISOU 143 CG LEU A 170    6037  4110  6257  -266   508  -1083      C
ATOM   144 CD1 LEU A 170     -25.163 53.707  6.324  1.00 42.70      C
ANISOU 144 CD1 LEU A 170    6043  3818  6363  -103   255   -927      C
ATOM   145 CD2 LEU A 170     -24.964 53.755  8.811  1.00 45.81      C
ANISOU 145 CD2 LEU A 170    6273  4542  6593  -396   709  -1381      C
ATOM   146 C  LEU A 170     -26.486 49.654  8.789  1.00 30.84      C
ANISOU 146 C  LEU A 170    4281  2952  4483  -318   750  -1015      C
ATOM   147 O  LEU A 170     -27.567 49.667  9.356  1.00 32.74      O
ANISOU 147 O  LEU A 170    4379  3206  4855  -318   903  -1203      O
ATOM   148 N  ILE A 171     -26.077 48.644  8.049  1.00 24.55      N
ANISOU 148 N  ILE A 171    3571  2181  3578  -230   576  -706      N
ATOM   149 CA ILE A 171     -27.024 47.620  7.594  1.00 27.28      C
ANISOU 149 CA ILE A 171    3860  2472  4034  -123   523  -585      C
ATOM   150 CB ILE A 171     -26.692 47.227  6.136  1.00 23.98      C
ANISOU 150 CB ILE A 171    3522  1881  3706   64   285  -323      C
ATOM   151 CG1 ILE A 171     -27.912 46.639  5.442  1.00 41.39      C
ANISOU 151 CG1 ILE A 171    5641  3956  6129   204   216  -269      C
ATOM   152 CD1 ILE A 171     -28.780 47.742  4.831  1.00 42.71      C
ANISOU 152 CD1 ILE A 171    5731  4079  6417   290   140  -358      C
ATOM   153 CG2 ILE A 171     -25.572 46.211  6.072  1.00 28.53      C
ANISOU 153 CG2 ILE A 171    4204  2656  3982   35   173   -82      C
ATOM   154 C  ILE A 171     -27.046 46.421  8.531  1.00 29.39      C
ANISOU 154 C  ILE A 171    4145  3018  4005  -281   593   -494      C
ATOM   155 O  ILE A 171     -28.076 45.781  8.758  1.00 27.90      O
ANISOU 155 O  ILE A 171    3878  2850  3872  -310   668   -525      O
ATOM   156 N  LEU A 172     -25.912 46.114  9.145  1.00 27.87      N
ANISOU 156 N  LEU A 172    4061  3046  3483  -409   561   -385      N
ATOM   157 CA LEU A 172     -25.867 44.907  9.974  1.00 26.16      C
ANISOU 157 CA LEU A 172    3910  2776  3256  -563   555   -241      C
ATOM   158 CB LEU A 172     -24.426 44.468 10.243  1.00 22.14      C
ANISOU 158 CB LEU A 172    3526  2717  2168  -608   395   -52      C
ATOM   159 CG LEU A 172     -23.609 44.006  9.042  1.00 28.10      C
ANISOU 159 CG LEU A 172    4321  3362  2993  -386   156   157      C
ATOM   160 CD1 LEU A 172     -22.179 43.700  9.507  1.00 25.83      C
ANISOU 160 CD1 LEU A 172    4105  3279  2430  -445    16   258      C
ATOM   161 CD2 LEU A 172     -24.218 42.787  8.379  1.00 31.53      C
ANISOU 161 CD2 LEU A 172    4768  3685  3527  -258    30   350      C
ATOM   162 C  LEU A 172     -26.706 44.887 11.280  1.00 31.38      C
ANISOU 162 C  LEU A 172    4518  3905  3501  -830   793   -439      C
ATOM   163 O  LEU A 172     -27.306 43.832 11.605  1.00 30.65      O
ANISOU 163 O  LEU A 172    4456  3893  3297  -977   868   -525      O
ATOM   164 N  PRO A 173     -26.755 46.004 12.044  1.00 30.45      N
ANISOU 164 N  PRO A 173    4326  3868  3376  -974   997   -743      N
ATOM   165 CA PRO A 173     -27.489 45.944 13.322  1.00 30.58      C
ANISOU 165 CA PRO A 173    4285  4118  3216  -1278  1246  -963      C
ATOM   166 CB PRO A 173     -27.504 47.400 13.792  1.00 34.05      C
ANISOU 166 CB PRO A 173    4608  4557  3774  -1341  1448  -1346      C
ATOM   167 CG PRO A 173     -26.014 47.937 13.299  1.00 36.01      C
ANISOU 167 CG PRO A 173    4964  4726  3994  -1214  1275  -1213      C
ATOM   168 CD PRO A 173     -26.014 47.266 11.913  1.00 28.01      C
ANISOU 168 CD PRO A 173    4008  3488  3148  -926  1012  -893      C
ATOM   169 C  PRO A 173     -28.915 45.448 13.222  1.00 37.33      C
ANISOU 169 C  PRO A 173    5010  4928  4245  -1293  1362  -1062      C
ATOM   170 O  PRO A 173     -29.357 44.789 14.159  1.00 41.16      O
ANISOU 170 O  PRO A 173    5523  5650  4468  -1486  1594  -1276      O
ATOM   171 N  GLU A 174     -31.053 45.322 12.137  1.00 35.66      C
ANISOU 171 N  GLU A 174    4502  4425  4622  -1053  1443  -1275      C
ATOM   172 CA GLU A 174     -32.016 46.487 11.920  1.00 47.44      C
ANISOU 172 CA GLU A 174    5892  5892  6240  -1121  1648  -1600      C
ATOM   173 CB GLU A 174
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ANISOU  173  CB  GLU A 174     5731   5744   6552   -922   1585  -1692       C
ATOM    174  CG  GLU A 174     -31.962  47.512  13.043  1.00 52.98           C
ANISOU  174  CG  GLU A 174     6333   6609   7187  -1133   1840  -2087       C
ATOM    175  CD  GLU A 174     -33.172  48.437  13.100  1.00 78.95           C
ANISOU  175  CD  GLU A 174     9307   9786  10904  -1062   1944  -2481       C
ATOM    176  OE1 GLU A 174     -33.548  49.025  12.056  1.00 77.51           O
ANISOU  176  OE1 GLU A 174     9026   9295  11130   -744   1739  -2438       O
ATOM    177  OE2 GLU A 174     -33.748  48.583  14.208  1.00 96.52           O
ANISOU  177  OE2 GLU A 174    11394  12249  13032  -1344   2136  -2736       O
ATOM    178  C   GLU A 174     -31.328  44.214  11.152  1.00 30.54           C
ANISOU  178  C   GLU A 174     3913   3634   4055   -883   1239   -960       C
ATOM    179  O   GLU A 174     -32.481  43.861  10.892  1.00 30.14           O
ANISOU  179  O   GLU A 174     3720   3533   4199   -860   1304  -1059       O
ATOM    180  N   LEU A 175     -30.260  43.653  10.597  1.00 26.19           N
ANISOU  180  N   LEU A 175     3556   3031   3364   -766    993   -608       N
ATOM    181  CA  LEU A 175     -30.424  42.636   9.557  1.00 23.01           C
ANISOU  181  CA  LEU A 175     3209   2474   3059   -583    786   -327       C
ATOM    182  CB  LEU A 175     -29.067  42.170   9.066  1.00 25.85           C
ANISOU  182  CB  LEU A 175     3753   2810   3260   -468    537    -18       C
ATOM    183  CG  LEU A 175     -29.171  41.063   8.012  1.00 33.37           C
ANISOU  183  CG  LEU A 175     4760   3616   4304   -291    327    245       C
ATOM    184  CD1 LEU A 175     -29.764  41.625   6.726  1.00 29.74           C
ANISOU  184  CD1 LEU A 175     4179   2906   4216   -45    276    176       C
ATOM    185  CD2 LEU A 175     -27.795  40.514   7.759  1.00 35.69           C
ANISOU  185  CD2 LEU A 175     5205   3940   4417   -217    104    488       C
ATOM    186  C   LEU A 175     -31.176  41.428  10.074  1.00 27.04           C
ANISOU  186  C   LEU A 175     3751   3116   3407   -785    843   -241       C
ATOM    187  O   LEU A 175     -32.043  40.857   9.392  1.00 29.08           O
ANISOU  187  O   LEU A 175     3939   3253   3858   -688    805   -200       O
ATOM    188  N   GLN A 176     -30.817  40.996  11.276  1.00 32.36           N
ANISOU  188  N   GLN A 176     4555   4040   3702  -1092    915   -194       N
ATOM    189  CA  GLN A 176     -31.454  39.816  11.872  1.00 35.78           C
ANISOU  189  CA  GLN A 176     5076   4606   3914  -1358    954    -78       C
ATOM    190  CB  GLN A 176     -30.847  39.578  13.243  1.00 42.72           C
ANISOU  190  CB  GLN A 176     6135   5759   4336  -1721    999    -16       C
ATOM    191  CG  GLN A 176     -31.457  38.427  13.985  1.00 67.24           C
ANISOU  191  CG  GLN A 176     9381   9015   7153  -2075   1034    116       C
ATOM    192  CD  GLN A 176     -30.502  37.853  15.002  1.00 74.59           C
ANISOU  192  CD  GLN A 176    10517  10063   7760  -2195    791    308       C
ATOM    193  OE1 GLN A 176     -30.917  37.196  15.953  1.00 73.42           O
ANISOU  193  OE1 GLN A 176    10445  10043   7407  -2464    781    310       O
ATOM    194  NE2 GLN A 176     -29.205  38.093  14.802  1.00 83.07           N
ANISOU  194  NE2 GLN A 176    11665  11082   8818  -2001    587    451       N
ATOM    195  C   GLN A 176     -32.983  39.967  11.980  1.00 35.25           C
ANISOU  195  C   GLN A 176     4782   4576   4037  -1472   1211   -383       C
ATOM    196  O   GLN A 176     -33.768  39.034  11.713  1.00 36.10           O
ANISOU  196  O   GLN A 176     4889   4653   4174  -1525   1195   -289       O
ATOM    197  N   ALA A 177     -33.409  41.148  12.419  1.00 33.69           N
ANISOU  197  N   ALA A 177     4373   4453   3974  -1521   1453   -781       N
ATOM    198  CA  ALA A 177     -34.840  41.420  12.612  1.00 35.51           C
ANISOU  198  CA  ALA A 177     4327   4746  4418  -1625   1715  -1162       C
ATOM    199  CB  ALA A 177     -35.042  42.763  13.316  1.00 40.04           C
ANISOU  199  CB  ALA A 177     4690   5428  5096  -1705   1974  -1628       C
ATOM    200  C   ALA A 177     -35.577  41.396  11.264  1.00 36.04           C
ANISOU  200  C   ALA A 177     4230   4523  4940  -1269   1584  -1160       C
ATOM    201  O   ALA A 177     -36.722  40.937  11.165  1.00 32.93           O
ANISOU  201  O   ALA A 177     3678   4161  4673  -1342   1688  -1292       O
ATOM    202  N   ARG A 178     -34.922  41.903  10.226  1.00 33.09           N
ANISOU  202  N   ARG A 178     3894   3882  4795   -912   1353  -1018       N
ATOM    203  CA  ARG A 178     -35.522  41.929   8.895  1.00 31.30           C
ANISOU  203  CA  ARG A 178     3548   3376  4969   -587   1189   -984       C
ATOM    204  CB  ARG A 178     -34.660  42.750   7.917  1.00 24.32           C
ANISOU  204  CB  ARG A 178     2734   2235  4273   -273    964   -865       C
ATOM    205  CG  ARG A 178     -34.729  44.226   8.210  1.00 29.40           C
ANISOU  205  CG  ARG A 178     3226   2808  5136   -216   1072  -1210       C
ATOM    206  CD  ARG A 178     -33.594  44.968   7.492  1.00 36.68           C
ANISOU  206  CD  ARG A 178     4302   3535  6101   -19    865  -1043       C
ATOM    207  NE  ARG A 178     -33.780  44.953   6.045  1.00 32.58           N
ANISOU  207  NE  ARG A 178     3797   2827  5754   232    575   -811       N
ATOM    208  CZ  ARG A 178     -32.785  44.927   5.164  1.00 32.73           C
ANISOU  208  CZ  ARG A 178     4012   2847  5577   323    340   -503       C
ATOM    209  NH1 ARG A 178     -31.534  44.928   5.602  1.00 31.02           N
ANISOU  209  NH1 ARG A 178     3951   2630  5206   260    376   -438       N
ATOM    210  NH2 ARG A 178     -33.045  44.914   3.848  1.00 28.33           N
ANISOU  210  NH2 ARG A 178     3507   2332  4927   427    123   -318       N
ATOM    211  C   ARG A 178     -35.662  40.522   8.387  1.00 30.06           C
ANISOU  211  C   ARG A 178     3523   3198  4701   -598   1045   -659       C
ATOM    212  O   ARG A 178     -36.644  40.166   7.756  1.00 33.78           O
ANISOU  212  O   ARG A 178     3854   3576  5407   -511   1026   -707       O
ATOM    213  N   ILE A 179     -34.654  39.710   8.661  1.00 24.53           N
ANISOU  213  N   ILE A 179     3091   2575  3654   -699    922   -335       N
ATOM    214  CA  ILE A 179     -34.688  38.327   8.216  1.00 25.44           C
ANISOU  214  CA  ILE A 179     3356   2641  3668   -707    758    -23       C
ATOM    215  CB  ILE A 179     -33.300  37.686   8.390  1.00 29.09           C
ANISOU  215  CB  ILE A 179     4101   3124  3829   -719    552    312       C
ATOM    216  CG1 ILE A 179     -32.378  38.220   7.289  1.00 27.69           C
ANISOU  216  CG1 ILE A 179     3936   2757  3828   -381    349    408       C
ATOM    217  CD1 ILE A 179     -30.955  37.759   7.426  1.00 29.97           C
ANISOU  217  CD1 ILE A 179     4433   3081  3872   -361    154    658       C
ATOM    218  CG2 ILE A 179     -33.384  36.176   8.333  1.00 29.16           C
ANISOU  218  CG2 ILE A 179     4286   3109  3680   -817    407    598       C
ATOM    219  C   ILE A 179     -35.768  37.559   8.954  1.00 33.00           C
ANISOU  219  C   ILE A 179     4272   3772  4496  -1030    945   -113       C
ATOM    220  O   ILE A 179     -36.510  36.755   8.374  1.00 25.64           O
ANISOU  220  O   ILE A 179     3307   2758  3677  -1004    893    -36       O
ATOM    221  N   ARG A 180     -35.889  37.850  10.245  1.00 28.95           N
ANISOU  221  N   ARG A 180     3748   3516  3734  -1365   1180   -304       N
ATOM    222  CA  ARG A 180     -36.908  37.212  11.055  1.00 31.42           C
ANISOU  222  CA  ARG A 180     4020   4047  3872  -1753   1401   -431       C
ATOM    223  CB  ARG A 180     -36.792  37.742  12.471  1.00 34.30           C
ANISOU  223  CB  ARG A 180     4389   4716  3926  -2127   1657   -657       C
ATOM    224  CG  ARG A 180     -37.479  36.940  13.528  1.00 70.91           C
ANISOU  224  CG  ARG A 180     9115   9608  8220  -2543   1773   -696       C
ATOM    225  CD  ARG A 180     -36.682  37.111  14.819  1.00 77.83           C
ANISOU  225  CD  ARG A 180    10196  10686  8689  -2768   1741   -672       C
ATOM    226  NE  ARG A 180     -35.440  36.333  14.769  1.00 80.32           N
ANISOU  226  NE  ARG A 180    10839  10896  8783  -2704   1411   -205       N
ATOM    227  CZ  ARG A 180     -34.258  36.749  15.214  1.00 78.79           C
ANISOU  227  CZ  ARG A 180    10774  10734  8427  -2671   1290   -107       C
ATOM    228  NH1 ARG A 180     -34.132  37.963  15.747  1.00 74.38           N
ANISOU  228  NH1 ARG A 180    10072  10310  7878  -2722   1489   -424       N
ATOM    229  NH2 ARG A 180     -33.201  35.942  15.121  1.00 78.07           N
ANISOU  229  NH2 ARG A 180    10929  10527  8206  -2559    950    277       N
ATOM    230  C   ARG A 180     -38.285  37.538  10.482  1.00 36.27           C
ANISOU  230  C   ARG A 180     4292   4608  4880  -1646   1546   -759       C
ATOM    231  O   ARG A 180     -39.166  36.679  10.371  1.00 33.43           O
ANISOU  231  O   ARG A 180     3896   4287  4520  -1795   1592   -745       O
ATOM    232  N   THR A 181     -38.469  38.806  10.116  1.00 32.13           N
ANISOU  232  N   THR A 181     3516   3982  4710  -1387   1598  -1064       N
ATOM    233  CA  THR A 181     -39.744  39.239   9.556  1.00 35.78           C
ANISOU  233  CA  THR A 181     3624   4365  5604  -1237   1687  -1404       C
ATOM    234  CB  THR A 181     -39.755  40.754   9.341  1.00 42.70           C
ANISOU  234  CB  THR A 181     4270   5103  6849   -967   1707  -1733       C
ATOM    235  OG1 THR A 181     -39.657  41.397  10.618  1.00 39.05           O
ANISOU  235  OG1 THR A 181     3741   4894  6200  -1247   1987  -2046       O
ATOM    236  CG2 THR A 181     -41.032  41.173   8.650  1.00 41.92           C
ANISOU  236  CG2 THR A 181     3810   4869  7250   -755   1715  -2055       C
ATOM    237  C   THR A 181     -39.999  38.515   8.224  1.00 34.84           C
ANISOU  237  C   THR A 181     3538   3999  5701   -968   1426  -1136       C
ATOM    238  O   THR A 181     -41.077  37.968   7.993  1.00 33.78           O
ANISOU  238  O   THR A 181     3242   3899  5696  -1037   1491  -1244       O
ATOM    239  N   TYR A 182     -38.983  38.485   7.376  1.00 28.75           N
ANISOU  239  N   TYR A 182     2972   3007  4943   -694   1143   -802       N
ATOM    240  CA  TYR A 182     -39.100  37.790   6.088  1.00 32.60           C
ANISOU  240  CA  TYR A 182     3512   3275  5597   -458    892   -545       C
ATOM    241  CB  TYR A 182     -37.766  37.890   5.372  1.00 27.90           C
ANISOU  241  CB  TYR A 182     3149   2507  4946   -222    632   -232       C
ATOM    242  CG  TYR A 182     -37.732  37.200   4.022  1.00 26.03           C
ANISOU  242  CG  TYR A 182     2981   2064  4845     4   377    21       C
ATOM    243  CD1 TYR A 182     -38.106  37.899   2.868  1.00 34.42           C
ANISOU  243  CD1 TYR A 182     3907   3020  6151   258   224   -44       C
ATOM    244  CE1 TYR A 182     -38.052  37.287   1.632  1.00 28.77           C
ANISOU  244  CE1 TYR A 182     3300   2446  5185   322    10   131       C
ATOM    245  CZ  TYR A 182     -37.623  35.966   1.548  1.00 26.95           C
ANISOU  245  CZ  TYR A 182     3246   2262  4732   266   -48   321       C
ATOM    246  OH  TYR A 182     -37.569  35.346   0.309  1.00 30.13           O
ANISOU  246  OH  TYR A 182     3725   2806  4919   308   -162   363       O
ATOM    247  CE2 TYR A 182     -37.249  35.254   2.681  1.00 26.36           C
ANISOU  247  CE2 TYR A 182     3294   2093  4630   105    40   458       C
ATOM    248  CD2 TYR A 182     -37.310  35.878   3.908  1.00 28.15           C
ANISOU  248  CD2 TYR A 182     3466   2338  4889   -76   262   321       C
ATOM    249  C   TYR A 182     -39.485  36.318   6.273  1.00 31.32           C
ANISOU  249  C   TYR A 182     3480   3209  5210   -700   903   -351       C
ATOM    250  O   TYR A 182     -40.404  35.777   5.626  1.00 28.21           O
ANISOU  250  O   TYR A 182     2964   2751  5002   -858   1584  -1028       O
ATOM    251  N   ASN A 183     -38.809  35.660   7.207  1.00 26.72           N
ANISOU  251  N   ASN A 183     3153   2779  4221   -978   937   -161       N
ATOM    252  CA  ASN A 183     -39.072  34.248   7.446  1.00 27.59           C
ANISOU  252  CA  ASN A 183     3447   2942  4094  -1235   907    63       C
ATOM    253  CB  ASN A 183     -37.931  33.627   8.220  1.00 29.61           C
ANISOU  253  CB  ASN A 183     4050   3258  3943  -1420   798   369       C
ATOM    254  CG  ASN A 183     -36.733  33.420   7.346  1.00 29.71           C
ANISOU  254  CG  ASN A 183     4233   3046  4009  -1084   482   667       C
ATOM    255  OD1 ASN A 183     -36.901  33.319   6.147  1.00 28.72           O
ANISOU  255  OD1 ASN A 183     4027   2729  4158   -799   344   710       O
ATOM    256  ND2 ASN A 183     -35.528  33.372   7.916  1.00 27.65           N
ANISOU  256  ND2 ASN A 183     4190   2823  3492  -1123   366   849       N
ATOM    257  C   ASN A 183     -40.419  33.884   8.058  1.00 41.63           C
ANISOU  257  C   ASN A 183     5059   4924  5836  -1582  1173  -185       C
ATOM    258  O   ASN A 183     -40.760  32.687   8.225  1.00 33.33           O
ANISOU  258  O   ASN A 183     4166   3906  4591  -1835  1153    -4       O
ATOM    259  N   GLN A 184     -41.218  34.891   8.374  1.00 33.78           N
ANISOU  259  N   GLN A 184     3734   4060  5042  -1607  1419   -621       N
ATOM    260  CA  GLN A 184     -42.591  34.608   8.785  1.00 36.01           C
ANISOU  260  CA  GLN A 184     3776   3660  6246  -1910  1951  -1472       C
ATOM    261  CB  GLN A 184     -43.284  35.867   9.291  1.00 58.73           C
ANISOU  261  CB  GLN A 184     6273   7583  8460  -1910  1951  -1472       C
ATOM    262  CG  GLN A 184     -42.728  36.349  10.615  1.00 60.83           C
ANISOU  262  CG  GLN A 184     6683   8078  8352  -2147   2095  -1570       C
ATOM    263  CD  GLN A 184     -43.342  37.664  11.059  1.00 84.00           C
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ANISOU  263  CD  GLN A 184     9307  11098  11513  -2056   2272  -2104       C
ATOM    264  OE1 GLN A 184     -44.275  38.172  10.428  1.00 89.57           O
ANISOU  264  OE1 GLN A 184     9700  11690  12642  -1817   2267  -2403       O
ATOM    265  NE2 GLN A 184     -42.815  38.230  12.150  1.00 85.62           N
ANISOU  265  NE2 GLN A 184     9617  11472  11444  -2240   2385  -2226       N
ATOM    266  C   GLN A 184     -43.391  33.995   7.648  1.00 35.18           C
ANISOU  266  C   GLN A 184     3550   4272   5544  -1720   1547   -880       C
ATOM    267  O   GLN A 184     -44.429  33.365   7.853  1.00 39.10           O
ANISOU  267  O   GLN A 184     3925   4916   6016  -1991   1706  -1023       O
ATOM    268  N   HIS A 185     -42.918  34.165   6.426  1.00 34.54           N
ANISOU  268  N   HIS A 185     3503   3899   5720  -1286   1258   -683       N
ATOM    269  CA  HIS A 185     -43.628  33.576   5.312  1.00 38.32           C
ANISOU  269  CA  HIS A 185     3884   4224   6452  -1120   1113   -622       C
ATOM    270  CB  HIS A 185     -43.552  34.501   4.109  1.00 46.28           C
ANISOU  270  CB  HIS A 185     4729   4983   7873   -650    901   -670       C
ATOM    271  CG  HIS A 185     -44.340  35.745   4.301  1.00 61.63           C
ANISOU  271  CG  HIS A 185     6293   6976  10149   -552   1046  -1126       C
ATOM    272  ND1 HIS A 185     -43.782  36.920   4.762  1.00 71.04           N
ANISOU  272  ND1 HIS A 185     7448   8161  11385   -457   1098  -1282       N
ATOM    273  CE1 HIS A 185     -44.727  37.836   4.875  1.00 65.56           C
ANISOU  273  CE1 HIS A 185     6373   7492  11044   -377   1217  -1729       C
ATOM    274  NE2 HIS A 185     -45.882  37.291   4.534  1.00 65.05           N
ANISOU  274  NE2 HIS A 185     6125   7471  11120   -423   1233  -1862       N
ATOM    275  CD2 HIS A 185     -45.671  35.975   4.189  1.00 63.20           C
ANISOU  275  CD2 HIS A 185     6112   7240  10661   -554   1159  -1501       C
ATOM    276  C   HIS A 185     -43.087  32.218   4.955  1.00 39.55           C
ANISOU  276  C   HIS A 185     4384   4268   6377  -1184    915   -189       C
ATOM    277  O   HIS A 185     -43.547  31.588   3.992  1.00 37.89           O
ANISOU  277  O   HIS A 185     4142   3918   6335  -1060    774   -94       O
ATOM    278  N   TYR A 186     -42.103  31.772   5.730  1.00 29.89           N
ANISOU  278  N   TYR A 186     3484   2875   4999   -392    741   -719       N
ATOM    279  CA  TYR A 186     -41.445  30.502   5.470  1.00 27.72           C
ANISOU  279  CA  TYR A 186     3439   2716   4378   -443    530   -640       C
ATOM    280  CB  TYR A 186     -40.013  30.711   4.941  1.00 24.61           C
ANISOU  280  CB  TYR A 186     3168   2280   3902   -352    436   -574       C
ATOM    281  CG  TYR A 186     -40.085  31.397   3.601  1.00 35.70           C
ANISOU  281  CG  TYR A 186     4444   3650   5472   -212    350   -414       C
ATOM    282  CD1 TYR A 186     -40.142  32.795   3.513  1.00 36.79           C
ANISOU  282  CD1 TYR A 186     4395   3660   5923   -105    462   -380       C
ATOM    283  CE1 TYR A 186     -40.266  33.422   2.277  1.00 41.78           C
ANISOU  283  CE1 TYR A 186     4854   4294   6725     -5    346   -120       C
ATOM    284  CZ  TYR A 186     -40.357  32.643   1.127  1.00 35.61           C
ANISOU  284  CZ  TYR A 186     4111   3717   5704    -81    124    -48       C
ATOM    285  OH  TYR A 186     -40.492  33.220  -0.110  1.00 35.86           O
ANISOU  285  OH  TYR A 186     3955   3862   5810    -80    -26    353       O
ATOM    286  CE2 TYR A 186     -40.331  31.260   1.194  1.00 35.84           C
ANISOU  286  CE2 TYR A 186     4348   3852   5417   -213     74    -85       C
ATOM    287  CD2 TYR A 186     -40.198  30.642   2.432  1.00 28.35           C
ANISOU  287  CD2 TYR A 186     3548   2827   4399   -244    185   -287       C
ATOM    288  C   TYR A 186     -41.478  29.609   6.706  1.00 35.09           C
ANISOU  288  C   TYR A 186     4500   3752   5081   -645    574   -743       C
ATOM    289  O   TYR A 186     -40.482  28.984   7.063  1.00 30.89           O
ANISOU  289  O   TYR A 186     4120   3263   4352   -706    490   -682       O
ATOM    290  N   ASN A 187     -42.643  29.527   7.337  1.00 27.12           N
ANISOU  290  N   ASN A 187     3389   2793   4123   -760    699   -845       N
ATOM    291  CA  ASN A 187     -42.794  28.596   8.443  1.00 32.10           C
ANISOU  291  CA  ASN A 187     4123   3570   4504   -997    714   -889       C
ATOM    292  CB  ASN A 187     -44.129  28.803   9.139  1.00 33.18           C
ANISOU  292  CB  ASN A 187     4113   3761   4734  -1136    920  -1062       C
ATOM    293  CG  ASN A 187     -44.186  30.076   9.900  1.00 44.34           C
ANISOU  293  CG  ASN A 187     5414   5135   6299  -1233   1237  -1340       C
ATOM    294  OD1 ASN A 187     -43.181  30.537  10.448  1.00 46.16           O
ANISOU  294  OD1 ASN A 187     5743   5420   6375  -1358   1298  -1441       O
ATOM    295  ND2 ASN A 187     -45.368  30.680   9.949  1.00 42.48           N
ANISOU  295  ND2 ASN A 187     4944   4791   6407  -1203   1482  -1480       N
ATOM    296  C   ASN A 187     -42.733  27.160   7.941  1.00 32.36           C
ANISOU  296  C   ASN A 187     4275   3605   4415   -991    516   -702       C
ATOM    297  O   ASN A 187     -42.530  26.226   8.716  1.00 35.90           O
ANISOU  297  O   ASN A 187     4813   4131   4698  -1154    474   -618       O
ATOM    298  N   ASN A 188     -42.969  26.969   6.644  1.00 28.11           N
ANISOU  298  N   ASN A 188     3715   2990   3974   -851    418   -629       N
ATOM    299  CA  ASN A 188     -42.731  25.654   6.064  1.00 25.78           C
ANISOU  299  CA  ASN A 188     3551   2642   3601   -884    318   -542       C
ATOM    300  CB  ASN A 188     -43.693  25.358   4.926  1.00 24.28           C
ANISOU  300  CB  ASN A 188     3295   2502   3427   -919    268   -548       C
ATOM    301  CG  ASN A 188     -43.418  24.021   4.254  1.00 25.69           C
ANISOU  301  CG  ASN A 188     3626   2594   3541  -1023    259   -566       C
ATOM    302  OD1 ASN A 188     -42.536  23.233   4.657  1.00 25.99           O
ANISOU  302  OD1 ASN A 188     3787   2461  3626  -1015    306   -531       O
ATOM    303  ND2 ASN A 188     -44.182  23.740   3.175  1.00 25.74           N
ANISOU  303  ND2 ASN A 188     3590   2717  3472  -1159    223   -608       N
ATOM    304  C   ASN A 188     -41.316  25.707   5.544  1.00 33.14           C
ANISOU  304  C   ASN A 188     4581   3462  4549   -764    273   -480       C
ATOM    305  O   ASN A 188     -41.037  26.402   4.564  1.00 30.13           O
ANISOU  305  O   ASN A 188     4165   3070  4212   -654    243   -490       O
ATOM    306  N   LEU A 189     -40.434  24.967   6.215  1.00 30.50           N
ANISOU  306  N   LEU A 189     4329   3059  4202   -800    264   -365       N
ATOM    307  CA  LEU A 189     -39.003  25.000   5.934  1.00 31.07           C
ANISOU  307  CA  LEU A 189     4444   3018  4343   -685    240   -264       C
ATOM    308  CB  LEU A 189     -38.266  24.108   6.923  1.00 35.06           C
ANISOU  308  CB  LEU A 189     4943   3482  4896   -761    209   -141       C
ATOM    309  CG  LEU A 189     -38.389  24.575   8.368  1.00 44.00           C
ANISOU  309  CG  LEU A 189     6019   4880  5818   -959    164    -65       C
ATOM    310  CD1 LEU A 189     -37.542  23.658   9.241  1.00 50.94           C
ANISOU  310  CD1 LEU A 189     6832   5783  6739  -1074    68    457       C
ATOM    311  CD2 LEU A 189     -37.967  26.036   8.508  1.00 40.10           C
ANISOU  311  CD2 LEU A 189     5505   4522  5208   -947   190    -84       C
ATOM    312  C   LEU A 189     -38.709  24.500   4.541  1.00 29.90           C
ANISOU  312  C   LEU A 189     4355   2708  4296   -612    282   -334       C
ATOM    313  O   LEU A 189     -37.707  24.852   3.954  1.00 31.73           O
ANISOU  313  O   LEU A 189     4603   2870  4581   -504    291   -328       O
ATOM    314  N   LEU A 190     -39.576  23.640   4.025  1.00 25.63           N
ANISOU  314  N   LEU A 190     3849   2131  3758   -727    336   -430       N
ATOM    315  CA  LEU A 190     -39.349  23.098   2.701  1.00 27.45           C
ANISOU  315  CA  LEU A 190     4149   2257  4025   -781    436   -578       C
ATOM    316  CB  LEU A 190     -40.332  21.985   2.399  1.00 34.17           C
ANISOU  316  CB  LEU A 190     5045   3073  4864   -995    531   -707       C
ATOM    317  CG  LEU A 190     -40.206  20.736   3.260  1.00 35.46           C
ANISOU  317  CG  LEU A 190     5235   2973  5266  -1022    640   -606       C
ATOM    318  CD1 LEU A 190     -41.180  19.706   2.762  1.00 32.07           C
ANISOU  318  CD1 LEU A 190     4864   2493  4827  -1268    773   -797       C
ATOM    319  CD2 LEU A 190     -38.796  20.135   3.206  1.00 38.04           C
ANISOU  319  CD2 LEU A 190     5563   2952  5937   -898    795   -515       C
ATOM    320  C   LEU A 190     -39.455  24.188   1.621  1.00 31.04           C
ANISOU  320  C   LEU A 190     4563   2915  4317   -777    359   -646       C
ATOM    321  O   LEU A 190     -38.982  23.996   0.510  1.00 35.79           O
ANISOU  321  O   LEU A 190     5219   3502  4878   -858    437   -766       O
ATOM    322  N   ARG A 191     -40.115  25.289   1.926  1.00 25.57           N
ANISOU  322  N   ARG A 191     3748   2404   3565   -719    237   -563       N
ATOM    323  CA  ARG A 191     -40.192  26.402   0.967  1.00 33.48           C
ANISOU  323  CA  ARG A 191     4643   3571   4508   -695    145   -506       C
ATOM    324  CB  ARG A 191     -41.468  27.225   1.148  1.00 35.97           C
ANISOU  324  CB  ARG A 191     4746   4044   4876   -693     61   -387       C
ATOM    325  CG  ARG A 191     -42.702  26.523   0.569  1.00 35.39           C
ANISOU  325  CG  ARG A 191     4606   4163   4677   -929     9   -380       C
ATOM    326  CD  ARG A 191     -43.983  27.372   0.580  1.00 41.69           C
ANISOU  326  CD  ARG A 191     5103   5126   5609   -919   -83   -174       C
ATOM    327  NE  ARG A 191     -44.403  27.612   1.952  1.00 52.43           N
ANISOU  327  NE  ARG A 191     6414   5237   7267   -803   -107   -743       N
ATOM    328  CZ  ARG A 191     -44.256  28.778   2.580  1.00 60.39           C
ANISOU  328  CZ  ARG A 191     7293   7222  8431   -606   -213   -213       C
ATOM    329  NH1 ARG A 191     -43.734  29.804   1.900  1.00 53.66           N
ANISOU  329  NH1 ARG A 191     6331   6343  7714   -485    -79   -65       N
ATOM    330  NH2 ARG A 191     -44.631  28.918   3.878  1.00 41.67           N
ANISOU  330  NH2 ARG A 191     4900   4757  6176   -593   -297   -358       N
ATOM    331  C   ARG A 191     -38.954  27.308   0.972  1.00 41.40           C
ANISOU  331  C   ARG A 191     5656   4494   5581   -514   -139   -454       C
ATOM    332  O   ARG A 191     -38.836  28.231   0.141  1.00 35.58           O
ANISOU  332  O   ARG A 191     4829   3864   4824   -491    -67   -369       O
ATOM    333  N   GLY A 192     -38.037  27.058   1.906  1.00 36.92           N
ANISOU  333  N   GLY A 192     5168   3768   5093   -417   -196   -454       N
ATOM    334  CA  GLY A 192     -36.747  27.728   1.907  1.00 32.93           C
ANISOU  334  CA  GLY A 192     4677   3201   4635   -287   -196   -408       C
ATOM    335  C   GLY A 192     -36.715  29.055   2.625  1.00 33.35           C
ANISOU  335  C   GLY A 192     4641   3300   4729   -371   -257   -371       C
ATOM    336  O   GLY A 192     -36.784  30.132   2.001  1.00 30.23           O
ANISOU  336  O   GLY A 192     4157   2938   4389   -146   -148   -338       O
ATOM    337  N   ALA A 193     -36.606  28.991   3.958  1.00 29.09           N
ANISOU  337  N   ALA A 193     4110   2770   4173   -258   -205   -371       N
ATOM    338  CA  ALA A 193     -36.398  30.179   4.784  1.00 27.07           C
ANISOU  338  CA  ALA A 193     3796   2559   3930   -278   -265   -429       C
ATOM    339  CB  ALA A 193     -36.478  29.816   6.261  1.00 27.16           C
ANISOU  339  CB  ALA A 193     3823   2690   3806   -476   -304   -448       C
ATOM    340  C   ALA A 193     -35.002  30.723   4.479  1.00 26.33           C
ANISOU  340  C   ALA A 193     3732   2434   3840   -200   -237   -374       C
ATOM    341  O   ALA A 193     -34.071  29.947   4.192  1.00 29.22           O
ANISOU  341  O   ALA A 193     4152   2760   4189   -159   -180   -263       O
ATOM    342  N   VAL A 194     -34.826  32.027   4.598  1.00 28.87           N
ANISOU  342  N   VAL A 194     3995   2740   4234   -186   -313   -454       N
ATOM    343  CA  VAL A 194     -33.507  32.580   4.289  1.00 26.56           C
ANISOU  343  CA  VAL A 194     3727   2580   3784   -129   -284   -403       C
ATOM    344  CB  VAL A 194     -33.595  34.032   3.772  1.00 26.20           C
ANISOU  344  CB  VAL A 194     3592   2280   4082   -50   -371   -458       C
ATOM    345  CG1 VAL A 194     -33.885  35.012   4.895  1.00 31.89           C
ANISOU  345  CG1 VAL A 194     4267   2972   4888   -198   -583   -667       C
ATOM    346  CG2 VAL A 194     -32.296  34.413   3.085  1.00 29.79           C
ANISOU  346  CG2 VAL A 194     4080   2720  4518    30   -308   -370       C
ATOM    347  C   VAL A 194     -32.559  32.436   5.478  1.00 31.50           C
ANISOU  347  C   VAL A 194     4382  3195  4394   -302   -274   -373       C
ATOM    348  O   VAL A 194     -32.950  32.657   6.615  1.00 27.07           O
ANISOU  348  O   VAL A 194     3806  2759  3719   -522   -358   -485       O
ATOM    349  N   SER A 195     -31.310  32.046   5.187  1.00 27.84           N
ANISOU  349  N   SER A 195     3929   2739   3910   -242   -177   -202       N
ATOM    350  CA  SER A 195     -30.240  31.954   6.193  1.00 36.11           C
ANISOU  350  CA  SER A 195     4935   3974   4811   -422   -111   -50       C
ATOM    351  CB  SER A 195     -28.925  31.482   5.552  1.00 34.33           C
ANISOU  351  CB  SER A 195     4663   3678   4703   -270    -26   -180       C
ATOM    352  OG  SER A 195     -29.075  30.159   5.074  1.00 44.08           O
ANISOU  352  OG  SER A 195     5886   4749   6113   -136    -18   -310       O
ATOM    353  C   SER A 195     -29.996  33.305   6.879  1.00 33.36           C
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ANISOU  353  C   SER A 195     4582   3759   4334   -635    214   -243       C
ATOM    354  O   SER A 195   -30.309  34.356   6.327  1.00 25.85           O
ANISOU  354  O   SER A 195     3643   2654   3526   -543    345   -444       O
ATOM    355  N   GLN A 196   -29.375  33.260   8.052  1.00 30.11           N
ANISOU  355  N   GLN A 196     4127   3644   3670   -957    163   -150       N
ATOM    356  CA  GLN A 196   -29.196  34.455   8.896  1.00 30.39           C
ANISOU  356  CA  GLN A 196     4170   3864   3511  -1304    323   -415       C
ATOM    357  CB  GLN A 196   -28.852  34.034  10.322  1.00 39.79           C
ANISOU  357  CB  GLN A 196     5301   5514   4301  -1790    232   -273       C
ATOM    358  CG  GLN A 196   -29.887  33.163  10.929  1.00 53.31           C
ANISOU  358  CG  GLN A 196     7015   7321   5920  -1905    219   -236       C
ATOM    359  CD  GLN A 196   -31.135  33.950  11.222  1.00 62.60           C
ANISOU  359  CD  GLN A 196     8262   8396   7126  -2031    543   -734       C
ATOM    360  OE1 GLN A 196   -31.083  35.178  11.359  1.00 71.86           O
ANISOU  360  OE1 GLN A 196     9460   9517   8327  -2185    806  -1105       O
ATOM    361  NE2 GLN A 196   -32.267  33.261  11.316  1.00 71.46           N
ANISOU  361  NE2 GLN A 196     9394   9452   8306  -1968    566   -752       N
ATOM    362  C   GLN A 196   -28.135  35.468   8.510  1.00 43.01           C
ANISOU  362  C   GLN A 196     5763   5433   5144  -1295    359   -470       C
ATOM    363  O   GLN A 196   -28.114  36.566   9.069  1.00 61.02           O
ANISOU  363  O   GLN A 196     8067   7780   7340  -1580    573   -781       O
ATOM    364  N   ARG A 197   -27.181  35.131   7.662  1.00 32.24           N
ANISOU  364  N   ARG A 197     4363   3985   3901  -1036    194   -202       N
ATOM    365  CA  ARG A 197   -26.090  36.112   7.505  1.00 27.46           C
ANISOU  365  CA  ARG A 197     3741   3425   3267  -1112    222   -243       C
ATOM    366  CB  ARG A 197   -24.732  35.438   7.456  1.00 27.83           C
ANISOU  366  CB  ARG A 197     3666   3643   3265  -1088     -6    163       C
ATOM    367  CG  ARG A 197   -24.551  34.315   8.411  1.00 49.05           C
ANISOU  367  CG  ARG A 197     6223   6622   5792  -1291   -194    526       C
ATOM    368  CD  ARG A 197   -23.871  34.789   9.622  1.00 59.22           C
ANISOU  368  CD  ARG A 197     7421   8389   6690  -1815   -263    603       C
ATOM    369  NE  ARG A 197   -22.605  34.096   9.835  1.00 81.90           N
ANISOU  369  NE  ARG A 197    10048  11498  9571  -1860   -527   1171       N
ATOM    370  CZ  ARG A 197   -22.459  33.042  10.633  1.00 91.78           C
ANISOU  370  CZ  ARG A 197    11095  13025  10752  -2040   -746   1669       C
ATOM    371  NH1 ARG A 197   -21.262  32.481  10.770  1.00 97.63           N
ANISOU  371  NH1 ARG A 197    11538  13940  11616  -2050   -976   2263       N
ATOM    372  NH2 ARG A 197   -23.505  32.555  11.293  1.00 89.88           N
ANISOU  372  NH2 ARG A 197    10911  12882  10359  -2213   -733   1619       N
ATOM    373  C   ARG A 197   -26.211  36.922   6.225  1.00 28.26           C
ANISOU  373  C   ARG A 197     3889   3180   3667   -792    330   -381       C
ATOM    374  O   ARG A 197   -26.835  36.491   5.282  1.00 30.08           O
ANISOU  374  O   ARG A 197     4140   3200   4091   -497    303   -332       O
ATOM    375  N   LEU A 198   -25.559  38.075   6.203  1.00 25.54           N
ANISOU  375  N   LEU A 198     3546   2823   3334   -906    439   -521       N
ATOM    376  CA  LEU A 198   -25.313  38.757   4.933  1.00 23.51           C
ANISOU  376  CA  LEU A 198     3292   2300   3340   -623    470   -506       C
ATOM    377  CB  LEU A 198   -25.141  40.253   5.196  1.00 26.85           C
ANISOU  377  CB  LEU A 198     3718   2617   3869   -811    711   -774       C
ATOM    378  CG  LEU A 198   -24.763  41.039   3.944  1.00 32.54           C
ANISOU  378  CG  LEU A 198     4412   3092   4861   -564    722   -683       C
ATOM    379  CD1 LEU A 198   -25.850  40.876   2.879  1.00 30.56           C
ANISOU  379  CD1 LEU A 198     4122   2608   4883   -252    692   -559       C
ATOM    380  CD2 LEU A 198   -24.580  42.502   4.286  1.00 27.59           C
ANISOU  380  CD2 LEU A 198     3769   2298  4416   -765   1005   -945       C
ATOM    381  C   LEU A 198   -24.033  38.164   4.317  1.00 31.06           C
ANISOU  381  C   LEU A 198     4207   3353   4241   -489    273   -219       C
ATOM    382  O   LEU A 198   -22.965  38.222   4.922  1.00 25.07           O
ANISOU  382  O   LEU A 198     3391   2826   3310   -692    203   -119       O
ATOM    383  N   TYR A 199   -24.139  37.577   3.139  1.00 21.95           N
ANISOU  383  N   TYR A 199     3058   2049   3232   -193    204    -89       N
ATOM    384  CA  TYR A 199   -23.001  36.985   2.487  1.00 20.99           C
ANISOU  384  CA  TYR A 199     2879   1961   3134   -71    111   116       C
ATOM    385  CB  TYR A 199   -23.357  35.639   1.862  1.00 26.01           C
ANISOU  385  CB  TYR A 199     3517   2495   3872   114    90   201       C
ATOM    386  CG  TYR A 199   -23.562  34.573   2.890  1.00 24.11           C
ANISOU  386  CG  TYR A 199     3220   2337   3605    38    27   336       C
ATOM    387  CD1 TYR A 199   -24.772  34.392   3.477  1.00 27.07           C
ANISOU  387  CD1 TYR A 199     3659   2722   3905   -42    39   225       C
ATOM    388  CE1 TYR A 199   -24.958  33.459   4.409  1.00 29.78           C
ANISOU  388  CE1 TYR A 199     3941   3172   4202   -150   -33   388       C
ATOM    389  CZ  TYR A 199   -23.926  32.679   4.785  1.00 35.83           C
ANISOU  389  CZ  TYR A 199     4542   4022   5052   -166   -132   730       C
ATOM    390  OH  TYR A 199   -24.105  31.720   5.719  1.00 44.14           O
ANISOU  390  OH  TYR A 199     5481   5186   6104   -285   -230  1003       O
ATOM    391  CE2 TYR A 199   -22.723  32.831   4.222  1.00 31.21           C
ANISOU  391  CE2 TYR A 199     3858   3399   4602   -60   -132   858       C
ATOM    392  CD2 TYR A 199   -22.542  33.786   3.287  1.00 30.62           C
ANISOU  392  CD2 TYR A 199     3886   3237   4511    29   -47   624       C
ATOM    393  C   TYR A 199   -22.489  37.949   1.447  1.00 24.55           C
ANISOU  393  C   TYR A 199     3345   2316   3668    13   159    76       C
ATOM    394  O   TYR A 199   -23.180  38.290   0.544  1.00 26.41           O
ANISOU  394  O   TYR A 199     3618   2414   4001   125   198    27       O
ATOM    395  N   ILE A 200   -21.259  38.372   1.626  1.00 20.52           N
ANISOU  395  N   ILE A 200     2774   1916   3106   -78   137   148       N
ATOM    396  CA  ILE A 200   -20.647  39.356   0.769  1.00 21.56           C
ANISOU  396  CA  ILE A 200     2913   1977   3303   -43   185   124       C
ATOM    397  CB  ILE A 200   -19.938  40.435   1.603  1.00 25.43           C
ANISOU  397  CB  ILE A 200     3373   2585   3702   -292   223    61       C
ATOM    398  CG1 ILE A 200   -20.923  41.148   2.490  1.00 31.11           C
ANISOU  398  CG1 ILE A 200     4107   3353   4241   -489   273   -219       C
ATOM    399  CD1 ILE A 200   -20.301  41.799   3.581  1.00 42.42           C
ANISOU  399  CD1 ILE A 200     5616   4410   6091   -434   529   -338       C
ATOM    400  CG2 ILE A 200   -19.276  41.450   0.733  1.00 24.16           C
ANISOU  400  CG2 ILE A 200     3217   2311   3651   -259    289    45       C
ATOM    401  C   ILE A 200   -19.654  38.723  -0.190  1.00 24.76           C
ANISOU  401  C   ILE A 200     3259   2398   3750   103   153   270       C
ATOM    402  O   ILE A 200   -18.661  38.222   0.198  1.00 24.51           O
ANISOU  402  O   ILE A 200     3112   2475   3724    86   109   420       O
ATOM    403  N   LEU A 201   -19.960  38.810  -1.461  1.00 24.18           N
ANISOU  403  N   LEU A 201     3231   2234   3722   209   194   244       N
ATOM    404  CA  LEU A 201   -19.136  38.263  -2.490  1.00 20.54           C
ANISOU  404  CA  LEU A 201     2726   1791   3286   282   247   287       C
ATOM    405  CB  LEU A 201   -19.991  37.908  -3.687  1.00 22.56           C
ANISOU  405  CB  LEU A 201     3056   2026   3489   293   293   213       C
ATOM    406  CG  LEU A 201   -21.179  36.989  -3.468  1.00 28.77           C
ANISOU  406  CG  LEU A 201     3893   2761   4276   318   289   147       C
ATOM    407  CD1 LEU A 201   -21.875  36.768  -4.737  1.00 28.76           C
ANISOU  407  CD1 LEU A 201     3945   2834   4148   230   324    86       C
ATOM    408  CD2 LEU A 201   -20.706  35.732  -2.910  1.00 30.85           C
ANISOU  408  CD2 LEU A 201     4213   2706   4805   -150   -150       N
ATOM    409  C   LEU A 201   -18.222  40.348  -3.163  1.00 20.60           O
ANISOU  409  O   LEU A 201     3729   1834   3264   170   243   334       O
ATOM    410  N   LEU A 202   -16.801  38.646  -2.937  1.00 20.66           N
ANISOU  410  N   LEU A 202     2572   1916   3360   259   301   419       N
ATOM    411  CA  LEU A 202   -15.604  39.345  -3.285  1.00 21.42           C
ANISOU  411  CA  LEU A 202     2597   2090   3450   320   477   477       C
ATOM    412  CB  LEU A 202   -14.726  39.606  -2.078  1.00 29.66           C
ANISOU  412  CB  LEU A 202     3504   3266   4498   108   227   626       C
ATOM    413  CG  LEU A 202   -15.343  40.555  -1.091  1.00 29.99           C
ANISOU  413  CG  LEU A 202     3647   3346   4402   -62   156   538       C
ATOM    414  CD1 LEU A 202   -15.779  39.820   0.047  1.00 39.48           C
ANISOU  414  CD1 LEU A 202     4777   4665   5560   -140   67   635       C
ATOM    415  CD2 LEU A 202   -14.366  41.537  -0.682  1.00 39.38           C
ANISOU  415  CD2 LEU A 202     4806   4646   5510   -263   151   532       C
ATOM    416  C   LEU A 202   -14.789  38.652  -4.371  1.00 22.57           C
ANISOU  416  C   LEU A 202     2661   2217   3698   272   484   453       C
ATOM    417  O   LEU A 202   -13.819  38.034  -4.105  1.00 23.93           O
ANISOU  417  O   LEU A 202     2646   2375   4070   338   551   564       O
ATOM    418  N   PRO A 203   -15.242  38.786  -5.601  1.00 26.16           N
ANISOU  418  N   PRO A 203     3222   2683   4034   218   569   322       N
ATOM    419  CA  PRO A 203   -14.472  38.328  -6.761  1.00 24.39           C
ANISOU  419  CA  PRO A 203     2946   2491   3830   170   788   210       C
ATOM    420  CB  PRO A 203   -15.421  38.581  -7.940  1.00 29.28           C
ANISOU  420  CB  PRO A 203     3713   3235   4179   -6   793   105       C
ATOM    421  CG  PRO A 203   -16.291  39.798  -7.482  1.00 23.44           C
ANISOU  421  CG  PRO A 203     3040   2510   3357   -8   536   288       C
ATOM    422  CD  PRO A 203   -16.476  39.522  -5.970  1.00 23.02           C
ANISOU  422  CD  PRO A 203     2963   2311   3472   144   461   313       C
ATOM    423  C   PRO A 203   -13.215  39.187  -6.866  1.00 27.35           C
ANISOU  423  C   PRO A 203     3222   2956   4214   130   780   314       C
ATOM    424  O   PRO A 203   -13.289  40.403  -6.946  1.00 28.27           O
ANISOU  424  O   PRO A 203     3403   3153   4185   42   643   397       O
ATOM    425  N   LEU A 204   -12.050  38.567  -6.848  1.00 26.69           N
ANISOU  425  N   LEU A 204     2949   2830   4364   198   945   333       N
ATOM    426  CA  LEU A 204   -10.850  39.361  -6.947  1.00 27.49           C
ANISOU  426  CA  LEU A 204     2936   3040   4468   145   934   441       C
ATOM    427  CB  LEU A 204   -9.647  38.626  -6.377  1.00 36.36           C
ANISOU  427  CB  LEU A 204     3759   4103   5955   269  1035   603       C
ATOM    428  CG  LEU A 204   -9.808  38.250  -4.913  1.00 45.00           C
ANISOU  428  CG  LEU A 204     4733   5188   7178   349   829   860       C
ATOM    429  CD1 LEU A 204   -8.455  37.867  -4.437  1.00 54.73           C
ANISOU  429  CD1 LEU A 204     5600   6454   8742   410   856  1158       C
ATOM    430  CD2 LEU A 204   -10.355  39.430  -4.106  1.00 50.15           C
ANISOU  430  CD2 LEU A 204     5555   6000   7501   198   550   900       C
ATOM    431  C   LEU A 204   -10.562  39.687  -8.390  1.00 32.86           C
ANISOU  431  C   LEU A 204     3867   3654   4964   -13   1107   280       C
ATOM    432  O   LEU A 204   -9.867  40.644  -8.667  1.00 32.01           O
ANISOU  432  O   LEU A 204     3548   3842  4772   -109   1057   363       O
ATOM    433  N   ASP A 205   -11.068  38.865  -9.304  1.00 36.91           N
ANISOU  433  N   ASP A 205     4262   4323  5441   -96  1329    40       N
ATOM    434  CA  ASP A 205   -10.725  39.039 -10.708  1.00 48.20           C
ANISOU  434  CA  ASP A 205     5731   5935  6648   -352  1538   -144       C
ATOM    435  CB  ASP A 205   -11.003  37.760 -11.486  1.00 52.93           C
ANISOU  435  CB  ASP A 205     6348  6477  7286   -479  1914   -505       C
ATOM    436  CG  ASP A 205   -10.152  36.586 -10.987  1.00 64.85           C
ANISOU  436  CG  ASP A 205     7619   7655  9365   -250  2244   -599       C
ATOM    437  OD1 ASP A 205   -8.914  36.771 -10.836  1.00 74.14           O
ANISOU  437  OD1 ASP A 205     8579   8785  10804   -150  2337   -486       O
ATOM    438  OD2 ASP A 205   -10.734  35.511 -10.715  1.00 49.64           O
ANISOU  438  OD2 ASP A 205     5690   5505   7667   -165  2397   -730       O
ATOM    439  C   ASP A 205   -11.462  40.226 -11.300  1.00 42.96           C
ANISOU  439  C   ASP A 205     5227   5511   5585   -561  1284    -1       C
ATOM    440  O   ASP A 205   -10.852  41.029 -12.005  1.00 54.14           O
ANISOU  440  O   ASP A 205     6568   7035   6968   -732  1238    -15       O
ATOM    441  N   CYS A 206   -12.759  40.359 -11.029  1.00 41.71           N
ANISOU  441  N   CYS A 206     5268  5428   5153   -559  1128    124       N
ATOM    442  CA  CYS A 206   -13.559  41.429 -11.615  1.00 41.82           C
ANISOU  442  CA  CYS A 206     5427  5654   4809   -737   1000    264       C
ATOM    443  CB  CYS A 206   -14.999  40.966 -11.836  1.00 43.61           C
ANISOU  443  CB  CYS A 206     5800  5923   4847   -777   1000    211       C
ATOM    444  SG  CYS A 206   -15.150  39.555 -12.955  1.00 52.93           S
ANISOU  444  SG  CYS A 206     6997  7116   5998   -966   1307   -124       S
ATOM    445  C   CYS A 206   -13.539  42.696 -10.772  1.00 39.39           C
ANISOU  445  C   CYS A 206     5116   5322   4529   -615   1000    511       C
ATOM    446  O   CYS A 206   -13.660  43.800 -11.300  1.00 42.96           O
ANISOU  446  O   CYS A 206     5618   5911   4795   -766   1000    643       O
ATOM    447  N   CYS A 206   -13.384  42.529  -9.463  1.00 34.71           N
ANISOU  447  N   CYS A 206     4471   4551   4167   -364   1013    572       N
ATOM    448  CA  CYS A 206   -13.103  43.670  -8.603  1.00 34.54           C
ANISOU  448  CA  CYS A 206     4429   4485   4211   -263   1045    766       C
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ANISOU  448  CA  CYS A 206     6722   7413   6434  -1058   1143    207       C
ATOM    449  CB  CYS A 206     -10.818  42.040 -14.430  1.00 60.90           C
ANISOU  449  CB  CYS A 206     7554   8592   6992  -1424   1323    125       C
ATOM    450  SG  CYS A 206     -11.670  41.292 -15.822  1.00140.36           S
ANISOU  450  SG  CYS A 206    17644  19019  16668  -1770   1000    565       S
ATOM    451  C   CYS A 206     -13.040  41.871 -13.333  1.00 57.09           C
ANISOU  451  C   CYS A 206     7192   7889   6610  -1167    942    336       C
ATOM    452  O   CYS A 206     -13.612  40.965 -13.954  1.00 53.89           O
ANISOU  452  O   CYS A 206     6844   7633   6000  -1373   1084    119       O
ATOM    453  N   GLY A 207     -13.661  42.937 -12.826  1.00 47.04           N
ANISOU  453  N   GLY A 207     5914   6521   5440  -1051    647    678       N
ATOM    454  CA  GLY A 207     -15.061  43.185 -13.105  1.00 47.98           C
ANISOU  454  CA  GLY A 207     6045   6737   5449  -1150    435    915       C
ATOM    455  C   GLY A 207     -15.933  42.560 -12.054  1.00 47.94           C
ANISOU  455  C   GLY A 207     6088   6473   5652   -890    400    808       C
ATOM    456  O   GLY A 207     -15.551  41.590 -11.382  1.00 44.85           O
ANISOU  456  O   GLY A 207     5734   5917   5391   -720    566    516       O
ATOM    457  N   VAL A 208     -17.103  43.166 -11.869  1.00 39.43           N
ANISOU  457  N   VAL A 208     4971   5343   4667   -854    186   1095       N
ATOM    458  CA  VAL A 208     -18.143  42.577 -11.057  1.00 40.20           C
ANISOU  458  CA  VAL A 208     5107   5266   4901   -679    149   1011       C
ATOM    459  CB  VAL A 208     -18.262  43.189 -9.619  1.00 53.25           C
ANISOU  459  CB  VAL A 208     6750   6544   6940   -384    114   1028       C
ATOM    460  CG1 VAL A 208     -17.191  44.251 -9.384  1.00 48.83           C
ANISOU  460  CG1 VAL A 208     6150   5876   6526   -358    142   1100       C
ATOM    461  CG2 VAL A 208     -19.648  43.744 -9.362  1.00 44.97           C
ANISOU  461  CG2 VAL A 208     5621   5365   6098   -325    -18   1268       C
ATOM    462  C   VAL A 208     -19.431  42.648 -11.858  1.00 45.85           C
ANISOU  462  C   VAL A 208     5754   6221   5447   -892    -23   1284       C
ATOM    463  O   VAL A 208     -19.775  43.691 -12.429  1.00 42.74           O
ANISOU  463  O   VAL A 208     5215   5930   5093  -1010   -200   1717       O
ATOM    464  N   PRO A 209     -20.098  41.497 -11.975  1.00 48.01           N
ANISOU  464  N   PRO A 209     6099   6609   5535   -980     33   1069       N
ATOM    465  CA  PRO A 209     -21.281  41.316 -12.806  1.00 43.92           C
ANISOU  465  CA  PRO A 209     5510   6423   4752  -1275   -121   1286       C
ATOM    466  CB  PRO A 209     -21.732  39.900 -12.456  1.00 41.75           C
ANISOU  466  CB  PRO A 209     5369   6102   4391  -1263     38    877       C
ATOM    467  CG  PRO A 209     -20.497  39.211 -12.109  1.00 45.60           C
ANISOU  467  CG  PRO A 209     5970   6395   4962  -1134    328    461       C
ATOM    468  CD  PRO A 209     -19.697  40.234 -11.333  1.00 48.95           C
ANISOU  468  CD  PRO A 209     6343   6553   5701   -837    264    620       C
ATOM    469  C   PRO A 209     -22.347  42.277 -12.375  1.00 44.75           C
ANISOU  469  C   PRO A 209     5440   6370   5193  -1108   -361   1744       C
ATOM    470  O   PRO A 209     -22.569  42.501 -11.182  1.00 46.70           O
ANISOU  470  O   PRO A 209     5698   6209   5837   -761   -326   1672       O
ATOM    471  N   ASP A 210     -23.023  42.816 -13.369  1.00 49.31           N
ANISOU  471  N   ASP A 210     5825   7293   5616  -1403   -585   2230       N
ATOM    472  CA  ASP A 210     -24.103  43.748 -13.164  1.00 60.92           C
ANISOU  472  CA  ASP A 210     7031   8619   7497  -1275   -801   2778       C
ATOM    473  CB  ASP A 210     -24.569  44.201 -14.531  1.00 86.00           C
ANISOU  473  CB  ASP A 210     9936  12294  10447  -1654  -1053   3211       C
ATOM    474  CG  ASP A 210     -24.805  43.028 -15.465  1.00104.03           C
ANISOU  474  CG  ASP A 210    12321  15155  12052  -2143  -1072   3002       C
ATOM    475  OD2 ASP A 210     -25.935  42.899 -15.990  1.00114.81           O
ANISOU  475  OD2 ASP A 210    13459  16819  13346  -2360  -1279   3232       O
ATOM    476  OD1 ASP A 210     -23.869  42.211 -15.628  1.00107.27           O
ANISOU  476  OD1 ASP A 210    13015  15694  12048  -2326   -825   2550       O
ATOM    477  C   ASP A 210     -25.248  43.022 -12.496  1.00 60.74           C
ANISOU  477  C   ASP A 210     7019   8480   7578  -1139   -805   2644       C
ATOM    478  O   ASP A 210     -25.984  43.570 -11.671  1.00 66.28           O
ANISOU  478  O   ASP A 210     7583   8810   8791   -846   -821   2813       O
ATOM    479  N   ASN A 211     -25.417  41.767 -12.865  1.00 46.27           N
ANISOU  479  N   ASN A 211     5346   6955   5280  -1383   -747   2307       N
ATOM    480  CA  ASN A 211     -26.540  41.033 -12.343  1.00 40.95           C
ANISOU  480  CA  ASN A 211     4676   6224   4658  -1311   -765   2204       C
ATOM    481  CB  ASN A 211     -27.502  40.675 -13.456  1.00 51.39           C
ANISOU  481  CB  ASN A 211     5850   8121   5557  -1790   -975   2512       C
ATOM    482  CG  ASN A 211     -28.758  40.088 -12.908  1.00 72.01           C
ANISOU  482  CG  ASN A 211     8413  10667   8283  -1705  -1027   2496       C
ATOM    483  OD1 ASN A 211     -28.847  38.879 -12.666  1.00 68.14           O
ANISOU  483  OD1 ASN A 211     8146  10187   7560  -1769   -856   1997       O
ATOM    484  ND2 ASN A 211     -29.736  40.951 -12.639  1.00 86.37           N
ANISOU  484  ND2 ASN A 211     9915  12351  10552  -1530  -1225   3044       N
ATOM    485  C   ASN A 211     -26.085  39.769 -11.660  1.00 33.26           C
ANISOU  485  C   ASN A 211     3992   5067   3579  -1190   -501   1554       C
ATOM    486  O   ASN A 211     -25.713  38.820 -12.314  1.00 34.24           O
ANISOU  486  O   ASN A 211     4258   5448   3303  -1483   -359   1231       O
ATOM    487  N   LEU A 212     -26.128  39.761 -10.332  1.00 28.70           N
ANISOU  487  N   LEU A 212     3643   3682   3281    68   -352   -279       N
ATOM    488  CA  LEU A 212     -25.600  38.636 -9.578  1.00 33.15           C
ANISOU  488  CA  LEU A 212     4526   4153   3916    53   -278   -314       C
ATOM    489  CB  LEU A 212     -25.863  38.877 -8.090  1.00 30.76           C
ANISOU  489  CB  LEU A 212     4186   3815  3686    82   -268   -261       C
ATOM    490  CG  LEU A 212     -24.998  38.114 -7.110  1.00 32.67           C
ANISOU  490  CG  LEU A 212     4451   3971  3990    92   -206   -238       C
ATOM    491  CD1 LEU A 212     -25.093  38.792 -5.756  1.00 32.43           C
ANISOU  491  CD1 LEU A 212     4396   3948  3980   118   -208   -176       C
ATOM    492  CD2 LEU A 212     -25.556  36.746 -7.000  1.00 30.16           C
ANISOU  492  CD2 LEU A 212     4133   3602  3724    33   -174   -285       C
ATOM    493  C   LEU A 212     -26.146  37.282 -10.051  1.00 31.55           C
ANISOU  493  C   LEU A 212     4332   3934   3724   -28   -258   -410       C
ATOM    494  O   LEU A 212     -25.398  36.333 -10.245  1.00 33.54           O
ANISOU  494  O   LEU A 212     4629   4110   4006   -44   -188   -461       O
ATOM    495  N   SER A 213     -27.456  37.192 -10.292  1.00 30.03           N
ANISOU  495  N   SER A 213     4087   3808   3514   -82   -316   -442       N
ATOM    496  CA  SER A 213     -28.034  35.904 -10.657  1.00 32.73           C
ANISOU  496  CA  SER A 213     4432   4129   3875   -179   -295   -545       C
ATOM    497  CB  SER A 213     -29.553  35.993 -10.673  1.00 30.08           C
ANISOU  497  CB  SER A 213     4008   3883   3537   -235   -370   -560       C
ATOM    498  OG  SER A 213     -29.950  36.788 -11.747  1.00 42.22           O
ANISOU  498  OG  SER A 213     5521   5551   4968   -238   -465   -551       O
ATOM    499  C   SER A 213     -27.516  35.415 -12.018  1.00 35.75           C
ANISOU  499  C   SER A 213     4880   4532   4172   -232   -276   -642       C
ATOM    500  O   SER A 213     -27.534  34.204 -12.316  1.00 30.55           O
ANISOU  500  O   SER A 213     4254   3808   3544   -309   -217   -751       O
ATOM    501  N   MET A 214     -27.046  36.346 -12.859  1.00 26.97           N
ANISOU  501  N   MET A 214     3793   3505   2950   -200   -313   -609       N
ATOM    502  CA  MET A 214     -26.566  35.934 -14.188  1.00 31.51           C
ANISOU  502  CA  MET A 214     4436   4123   3415   -263   -285   -707       C
ATOM    503  CB  MET A 214     -26.527  37.125 -15.153  1.00 35.37           C
ANISOU  503  CB  MET A 214     4934   4753   3753   -249   -363   -641       C
ATOM    504  CG  MET A 214     -27.866  37.465 -15.775  1.00 43.29           C
ANISOU  504  CG  MET A 214     5880   5906   4664   -308   -496   -631       C
ATOM    505  SD  MET A 214     -28.521  36.144 -16.823  1.00 52.64           S
ANISOU  505  SD  MET A 214     7087   7161   5751   -477   -503   -818       S
ATOM    506  CE  MET A 214     -27.746  36.529 -18.385  1.00 47.91           C
ANISOU  506  CE  MET A 214     6584   6690   4928   -524   -500   -845       C
ATOM    507  C   MET A 214     -25.153  35.337 -14.091  1.00 28.72           C
ANISOU  507  C   MET A 214     4145   3646   3123   -227   -155   -745       C
ATOM    508  O   MET A 214     -24.682  34.673 -15.001  1.00 33.83           O
ANISOU  508  O   MET A 214     4850   4285   3720   -281   -86   -860       O
ATOM    509  N   ALA A 215     -24.462  35.607 -12.989  1.00 30.46           N
ANISOU  509  N   ALA A 215     4348   3776   3502   -109   -232   -668       N
ATOM    510  CA  ALA A 215     -23.146  35.003 -12.775  1.00 31.76           C
ANISOU  510  CA  ALA A 215     4544   3823   3702   -89   -10   -668       C
ATOM    511  CB  ALA A 215     -22.561  35.502 -11.466  1.00 28.46           C
ANISOU  511  CB  ALA A 215     4087   3350   3377     3   -14   -539       C
ATOM    512  C   ALA A 215     -23.172  33.472 -12.803  1.00 33.12           C
ANISOU  512  C   ALA A 215     4740   3872   3972   -138    78   -781       C
ATOM    513  O   ALA A 215     -22.173  32.819 -13.164  1.00 40.56           O
ANISOU  513  O   ALA A 215     5714   4726   4969   -119   186   -844       O
ATOM    514  N   ASP A 216     -24.301  32.872 -12.432  1.00 29.15           N
ANISOU  514  N   ASP A 216     4217   3349   3508   -203    46   -811       N
ATOM    515  CA  ASP A 216     -24.357  31.408 -12.295  1.00 33.61           C
ANISOU  515  CA  ASP A 216     4807   3764   4198   -252   137   -904       C
ATOM    516  CB  ASP A 216     -23.886  31.020 -10.866  1.00 34.17           C
ANISOU  516  CB  ASP A 216     4854   3698   4431   -171   173   -780       C
ATOM    517  CG  ASP A 216     -23.770  29.485 -10.645  1.00 45.87           C
ANISOU  517  CG  ASP A 216     6365   4985   6078   -200   279   -842       C
ATOM    518  OD1 ASP A 216     -24.488  28.678 -11.267  1.00 45.93           O
ANISOU  518  OD1 ASP A 216     6401   4957   6093   -309   311   -980       O
ATOM    519  OD2 ASP A 216     -22.929  29.093 -9.812  1.00 47.89           O
ANISOU  519  OD2 ASP A 216     6612   5119   6465   -114   329   -742       O
ATOM    520  C   ASP A 216     -25.800  30.968 -12.504  1.00 26.10           C
ANISOU  520  C   ASP A 216     3839   2860   3219   -373    -83   -983       C
ATOM    521  O   ASP A 216     -26.701  31.529 -11.878  1.00 28.65           O
ANISOU  521  O   ASP A 216     4102   3257   3528   -376    -3   -902       O
ATOM    522  N   PRO A 217     -26.027  29.970 -13.378  1.00 33.30           N
ANISOU  522  N   PRO A 217     4795   3729   4127   -481    142   -1152       N
ATOM    523  CA  PRO A 217     -27.404  29.511 -13.623  1.00 35.75           C
ANISOU  523  CA  PRO A 217     5078   4094   4411   -618    87   -1241       C
ATOM    524  CB  PRO A 217     -27.262  28.468 -14.733  1.00 39.27           C
ANISOU  524  CB  PRO A 217     5597   4486   4839   -733    175   -1453       C
ATOM    525  CG  PRO A 217     -25.840  28.489 -15.169  1.00 39.99           C
ANISOU  525  CG  PRO A 217     5749   4513   4931   -648    280   -1476       C
ATOM    526  CD  PRO A 217     -25.033  29.157 -14.099  1.00 37.33           C
ANISOU  526  CD  PRO A 217     5377   4679   4679   -486    275   -1279       C
ATOM    527  C   PRO A 217     -27.965  28.806 -12.393  1.00 39.72           C
ANISOU  527  C   PRO A 217     5545   4467   5081   -629    113   -1181       C
ATOM    528  O   PRO A 217     -29.151  28.520 -12.345  1.00 35.26           O
ANISOU  528  O   PRO A 217     4934   3946   4516   -736    66   -1224       O
ATOM    529  N   ASN A 218     -27.121  28.502 -11.416  1.00 33.02           N
ANISOU  529  N   ASN A 218     4712   3465   4368   -529   187 -1076       N
ATOM    530  CA  ASN A 218     -27.651  27.869 -10.208  1.00 29.26           C
ANISOU  530  CA  ASN A 218     4209   2878   4029   -545   211   -993       C
ATOM    531  CB  ASN A 218     -26.784  26.705 -9.770  1.00 26.37           C
ANISOU  531  CB  ASN A 218     3898   2279   3845   -507   337   -979       C
ATOM    532  CG  ASN A 218     -26.863  25.557 -10.718  1.00 36.13           C
ANISOU  532  CG  ASN A 218     5190   3392   5144   -611   431 -1174       C
ATOM    533  OD1 ASN A 218     -27.948  25.115 -11.093  1.00 39.63           O
ANISOU  533  OD1 ASN A 218     5626   3862   5569   -756   415 -1288       O
ATOM    534  ND2 ASN A 218     -25.703  25.059 -11.142  1.00 40.30           N
ANISOU  534  ND2 ASN A 218     5772   3789   5753   -545   537 -1227       N
ATOM    535  C   ASN A 218     -27.826  28.836 -9.079  1.00 27.62           C
ANISOU  535  C   ASN A 218     3943   2753   3797   -466   140   -820       C
ATOM    536  O   ASN A 218     -28.078  28.433 -7.945  1.00 29.65           O
ANISOU  536  O   ASN A 218     4185   2933   4148   -464   166   -723       O
ATOM    537  N   ILE A 219     -27.691  30.127 -9.372  1.00 24.44           N
ANISOU  537  N   ILE A 219     3513   2505   3266   -405    59   -780       N
ATOM    538  CA  ILE A 219     -28.084  31.153 -8.407  1.00 22.26           C
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ANISOU  538  CA  ILE A 219     3177   2322   2958   -349     -7    -651       C
ATOM    539  CB  ILE A 219   -26.950  32.168  -8.194  1.00 24.06           C
ANISOU  539  CB  ILE A 219     3419   2581   3140   -228    -24    -558       C
ATOM    540  CG1 ILE A 219   -25.718  31.469  -7.587  1.00 26.28           C
ANISOU  540  CG1 ILE A 219     3742   2717   3526   -164     55    -497       C
ATOM    541  CD1 ILE A 219   -24.535  32.420  -7.342  1.00 30.86           C
ANISOU  541  CD1 ILE A 219     4321   3334   4069    -58     38    -410       C
ATOM    542  CG2 ILE A 219   -27.392  33.318  -7.295  1.00 23.28           C
ANISOU  542  CG2 ILE A 219     3265   2578   3002   -182    -84    -457       C
ATOM    543  C   ILE A 219   -29.255  31.890  -9.052  1.00 31.82           C
ANISOU  543  C   ILE A 219     4323   3697   4068   -404   -103    -699       C
ATOM    544  O   ILE A 219   -29.120  32.367 -10.185  1.00 33.03           O
ANISOU  544  O   ILE A 219     4490   3942   4119   -408   -150    -756       O
ATOM    545  N   ARG A 220   -30.398  31.968  -8.361  1.00 23.11           N
ANISOU  545  N   ARG A 220     3145   2640   2997   -447   -130    -669       N
ATOM    546  CA  ARG A 220   -31.577  32.616  -8.940  1.00 25.10           C
ANISOU  546  CA  ARG A 220     3307   3049   3181   -491   -226    -704       C
ATOM    547  CB  ARG A 220   -32.723  31.653  -9.178  1.00 28.33           C
ANISOU  547  CB  ARG A 220     3666   3464   3635   -635   -226    -801       C
ATOM    548  CG  ARG A 220   -32.331  30.216  -9.311  1.00 57.97           C
ANISOU  548  CG  ARG A 220     7500   7059   7466   -719   -131    -889       C
ATOM    549  CD  ARG A 220   -31.909  29.918 -10.719  1.00 67.27           C
ANISOU  549  CD  ARG A 220     8740   8257   8562   -768   -143   -1021       C
ATOM    550  NE  ARG A 220   -32.940  30.284 -11.683  1.00 82.63           N
ANISOU  550  NE  ARG A 220    10611  10384  10399   -858   -256   -1097       N
ATOM    551  CZ  ARG A 220   -32.738  30.330 -12.998  1.00 86.84           C
ANISOU  551  CZ  ARG A 220    11185  11006  10804   -909   -300   -1199       C
ATOM    552  NH1 ARG A 220   -33.730  30.671 -13.822  1.00 77.68           N
ANISOU  552  NH1 ARG A 220     9946  10032  9536   -995   -423   -1246       N
ATOM    553  NH2 ARG A 220   -31.536  30.039 -13.487  1.00 78.97           N
ANISOU  553  NH2 ARG A 220    10301   9922   9781   -875   -220   -1249       N
ATOM    554  C   ARG A 220   -32.105  33.631  -7.963  1.00 26.78           C
ANISOU  554  C   ARG A 220     3441   3327   3407   -424   -254    -601       C
ATOM    555  O   ARG A 220   -32.290  33.328  -6.779  1.00 24.58           O
ANISOU  555  O   ARG A 220     3149   2989   3200   -428   -193    -550       O
ATOM    556  N   PHE A 221   -32.405  34.816  -8.469  1.00 25.97           N
ANISOU  556  N   PHE A 221     3285   3346   3235   -368   -341    -573       N
ATOM    557  CA  PHE A 221   -33.000  35.840  -7.624  1.00 23.74           C
ANISOU  557  CA  PHE A 221     2919   3118   2983   -301   -357    -497       C
ATOM    558  CB  PHE A 221   -33.112  37.123  -8.424  1.00 32.34           C
ANISOU  558  CB  PHE A 221     3969   4311   4008   -227   -452    -459       C
ATOM    559  CG  PHE A 221   -33.861  38.188  -7.712  1.00 29.69           C
ANISOU  559  CG  PHE A 221     3533   4021   3727   -156   -465    -398       C
ATOM    560  CD1 PHE A 221   -33.302  38.805  -6.613  1.00 28.32           C
ANISOU  560  CD1 PHE A 221     3393   3786   3584    -82   -397    -347       C
ATOM    561  CE1 PHE A 221   -33.977  39.818  -5.945  1.00 28.57           C
ANISOU  561  CE1 PHE A 221     3337   3847   3672    -18   -388    -314       C
ATOM    562  CZ  PHE A 221   -35.240  40.230  -6.404  1.00 28.88           C
ANISOU  562  CZ  PHE A 221     3237   3977   3758    -10   -453    -315       C
ATOM    563  CE2 PHE A 221   -35.816  39.608  -7.511  1.00 34.53           C
ANISOU  563  CE2 PHE A 221     3905   4772   4441    -83   -542    -348       C
ATOM    564  CD2 PHE A 221   -35.118  38.578  -8.162  1.00 32.07           C
ANISOU  564  CD2 PHE A 221     3700   4433   4053   -165   -545    -399       C
ATOM    565  C   PHE A 221   -34.399  35.395  -7.227  1.00 27.59           C
ANISOU  565  C   PHE A 221     3293   3652   3539   -384   -355    -529       C
ATOM    566  O   PHE A 221   -35.156  34.912  -8.058  1.00 26.79           O
ANISOU  566  O   PHE A 221     3137   3615   3427   -474   -410    -600       O
ATOM    567  N   ARG A 222   -34.753  35.575  -5.963  1.00 23.13           N
ANISOU  567  N   ARG A 222     2687   3066   3035   -365   -290    -483       N
ATOM    568  CA  ARG A 222   -36.108  35.250  -5.540  1.00 22.96           C
ANISOU  568  CA  ARG A 222     2541   3098   3084   -443   -273    -511       C
ATOM    569  CB  ARG A 222   -36.133  34.381  -4.272  1.00 29.70           C
ANISOU  569  CB  ARG A 222     3427   3864   3994   -506   -154    -490       C
ATOM    570  CG  ARG A 222   -37.547  34.394  -3.681  1.00 33.28           C
ANISOU  570  CG  ARG A 222     3733   4393   4518   -567   -120    -506       C
ATOM    571  CD  ARG A 222   -37.753  33.656  -2.351  1.00 31.38           C
ANISOU  571  CD  ARG A 222     3511   4091   4320   -640     7    -471       C
ATOM    572  NE  ARG A 222   -37.248  32.289  -2.247  1.00 35.04           N
ANISOU  572  NE  ARG A 222     4081   4426   4806   -731     59    -465       N
ATOM    573  CZ  ARG A 222   -37.030  31.705  -1.068  1.00 39.92           C
ANISOU  573  CZ  ARG A 222     4759   4969   5438   -770    162    -391       C
ATOM    574  NH1 ARG A 222   -37.249  32.395   0.062  1.00 30.38           N
ANISOU  574  NH1 ARG A 222     3521   3823   4199   -735    221    -336       N
ATOM    575  NH2 ARG A 222   -36.568  30.456  -1.001  1.00 35.30           N
ANISOU  575  NH2 ARG A 222     4269   4247   4897   -841    208    -368       N
ATOM    576  C   ARG A 222   -36.896  36.541  -5.278  1.00 26.91           C
ANISOU  576  C   ARG A 222     2915   3698   3612   -359   -305    -475       C
ATOM    577  O   ARG A 222   -37.895  36.814  -5.940  1.00 29.21           O
ANISOU  577  O   ARG A 222     3078   4093   3927   -375   -384    -497       O
ATOM    578  N   ASP A 223   -36.468  37.317  -4.300  1.00 27.94           N
ANISOU  578  N   ASP A 223     3075   3796   3747   -274   -243    -422       N
ATOM    579  CA  ASP A 223   -37.145  38.569  -3.951  1.00 30.11           C
ANISOU  579  CA  ASP A 223     3239   4132   4069   -185   -245    -401       C
ATOM    580  CB  ASP A 223   -38.558  38.336  -3.413  1.00 36.93           C
ANISOU  580  CB  ASP A 223     3946   5062   5025   -243   -198    -434       C
ATOM    581  CG  ASP A 223   -38.596  37.424  -2.182  1.00 38.31           C
ANISOU  581  CG  ASP A 223     4162   5187   5208   -337    -68    -442       C
ATOM    582  OD1 ASP A 223   -37.523  36.987  -1.690  1.00 32.66           O
ANISOU  582  OD1 ASP A 223     3595   4387   4430   -347    -23    -411       O
ATOM    583  OD2 ASP A 223   -39.731  37.149  -1.715  1.00 44.40           O
ANISOU  583  OD2 ASP A 223     4807   6012   6052   -402    -11    -471       O
ATOM    584  C   ASP A 223   -36.335  39.355  -2.944  1.00 27.04           C
ANISOU  584  C   ASP A 223     2929   3685   3658   -107   -170    -365       C
ATOM    585  O   ASP A 223   -35.176  39.056  -2.724  1.00 29.55           O
ANISOU  585  O   ASP A 223     3379   3936   3913   -108   -150    -342       O
ATOM    586  N   MET A 224   -36.940  40.382  -2.343  1.00 26.04           N
ANISOU  586  N   MET A 224     2715   3587   3590    -39   -127    -367       N
ATOM    587  CA  MET A 224   -36.206  41.229  -1.410  1.00 27.28           C
ANISOU  587  CA  MET A 224     2948   3697   3722     22    -54    -357       C
ATOM    588  CB  MET A 224   -36.441  42.690  -1.750  1.00 30.33           C
ANISOU  588  CB  MET A 224     3270   4083   4171    143   -83    -348       C
ATOM    589  CG  MET A 224   -36.508  42.920  -3.231  1.00 48.94           C
ANISOU  589  CG  MET A 224     5593   6466   6534    187   -219    -305       C
ATOM    590  SD  MET A 224   -34.841  43.035  -3.895  1.00 58.51           S
ANISOU  590  SD  MET A 224     6982   7614   7634    207   -274    -261       S
ATOM    591  CE  MET A 224   -34.623  44.790  -3.628  1.00 71.47           C
ANISOU  591  CE  MET A 224     8618   9198   9339    334   -249    -233       C
ATOM    592  C   MET A 224   -36.625  41.043   0.033  1.00 29.38           C
ANISOU  592  C   MET A 224     3197   3973   3993    -30    79    -387       C
ATOM    593  O   MET A 224   -37.763  40.730   0.330  1.00 26.60           O
ANISOU  593  O   MET A 224     2728   3673   3705    -76   129    -418       O
ATOM    594  N   LEU A 225   -35.705  41.321   0.940  1.00 24.30           N
ANISOU  594  N   LEU A 225     2664   3293   3274    -26    138    -379       N
ATOM    595  CA  LEU A 225   -36.064  41.454   2.332  1.00 25.39           C
ANISOU  595  CA  LEU A 225     2794   3461   3392    -69    268    -413       C
ATOM    596  CB  LEU A 225   -34.796  41.685   3.159  1.00 25.55           C
ANISOU  596  CB  LEU A 225     2956   3454   3296    -78    294    -393       C
ATOM    597  CG  LEU A 225   -33.837  40.511   3.264  1.00 28.47           C
ANISOU  597  CG  LEU A 225     3438   3798   3581   -144   256   -315       C
ATOM    598  CD1 LEU A 225   -32.759  40.931   4.279  1.00 28.78           C
ANISOU  598  CD1 LEU A 225     3582   3845   3507   -154   284   -297       C
ATOM    599  CD2 LEU A 225   -34.576  39.280   3.811  1.00 22.90           C
ANISOU  599  CD2 LEU A 225     2707   3118   2877   -250   319   -291       C
ATOM    600  C   LEU A 225   -36.962  42.681   2.465  1.00 30.12           C
ANISOU  600  C   LEU A 225     3272   4080   4091    11   -322    -478       C
ATOM    601  O   LEU A 225   -37.012  43.518   1.556  1.00 29.91           O
ANISOU  601  O   LEU A 225     3200   4027   4138   110   247   -471       O
ATOM    602  N   PRO A 226   -37.650  42.819   3.610  1.00 35.06           N
ANISOU  602  N   PRO A 226     3848   4748   4724   -30   461   -537       N
ATOM    603  CA  PRO A 226   -38.235  44.144   3.895  1.00 30.32           C
ANISOU  603  CA  PRO A 226     3159   4138   4221    61   539   -614       C
ATOM    604  CB  PRO A 226   -38.843  43.988   5.286  1.00 29.40           C
ANISOU  604  CB  PRO A 226     3018   4084   4070   -22   714   -687       C
ATOM    605  CG  PRO A 226   -38.260  42.708   5.865  1.00 41.96           C
ANISOU  605  CG  PRO A 226     4729   5708   5505   -156   716   -624       C
ATOM    606  CD  PRO A 226   -37.893  41.836   4.684  1.00 36.60           C
ANISOU  606  CD  PRO A 226     4072   4994   4841   -179   609   -535       C
ATOM    607  C   PRO A 226   -37.131  45.210   3.951  1.00 35.67           C
ANISOU  607  C   PRO A 226     3952   4744   4859   129   522   -626       C
ATOM    608  O   PRO A 226   -35.966  44.912   4.288  1.00 29.81           O
ANISOU  608  O   PRO A 226     3355   3990   3983    77   496   -596       O
ATOM    609  N   GLN A 227   -37.495  46.451   3.633  1.00 33.23           N
ANISOU  609  N   GLN A 227     3568   4379   4678   243   538   -666       N
ATOM    610  CA  GLN A 227   -36.492  47.502   3.479  1.00 35.66           C
ANISOU  610  CA  GLN A 227     3975   4598   4976   307   512   -671       C
ATOM    611  CB  GLN A 227   -37.093  48.716   2.805  1.00 47.86           C
ANISOU  611  CB  GLN A 227     5504   6065   6707   448   504   -676       C
ATOM    612  CG  GLN A 227   -37.719  48.438   1.473  1.00 60.36           C
ANISOU  612  CG  GLN A 227     6883   7673   8380   511   367   -576       C
ATOM    613  CD  GLN A 227   -38.448  49.663   0.955  1.00 65.60           C
ANISOU  613  CD  GLN A 227     7417   8265   9242   660   366   -562       C
ATOM    614  OE1 GLN A 227   -39.151  50.354   1.712  1.00 52.17           O
ANISOU  614  OE1 GLN A 227     5630   6529   7663   708   505   -651       O
ATOM    615  NE2 GLN A 227   -38.258  49.964  -0.332  1.00 68.20           N
ANISOU  615  NE2 GLN A 227     7736   8569   9607   734   216   -446       N
ATOM    616  C   GLN A 227   -35.945  47.953   4.811  1.00 39.65           C
ANISOU  616  C   GLN A 227     4580   5100   5387   246   640   -768       C
ATOM    617  O   GLN A 227   -36.574  47.794   5.844  1.00 33.49           O
ANISOU  617  O   GLN A 227     3766   4378   4581   186   773   -848       O
ATOM    618  N   GLN A 228   -34.772  48.578   4.763  1.00 35.35           N
ANISOU  618  N   GLN A 228     4154   4492   4786   256   601   -766       N
ATOM    619  CA  GLN A 228   -34.188  49.174   5.941  1.00 30.17           C
ANISOU  619  CA  GLN A 228     3591   3834   4038   193   706   -870       C
ATOM    620  CB  GLN A 228   -32.763  48.635  6.082  1.00 31.98           C
ANISOU  620  CB  GLN A 228     3960   4095   4095   111   615   -806       C
ATOM    621  CG  GLN A 228   -31.923  49.342  7.144  1.00 28.30           C
ANISOU  621  CG  GLN A 228     3598   3635   3518    36   683   -904       C
ATOM    622  CD  GLN A 228   -32.417  49.013   8.515  1.00 38.59           C
ANISOU  622  CD  GLN A 228     4913   5047   4703   -71   813   -990       C
ATOM    623  OE1 GLN A 228   -32.424  47.845   8.900  1.00 45.26           O
ANISOU  623  OE1 GLN A 228     5776   5990   5430   -149   790   -913       O
ATOM    624  NE2 GLN A 228   -32.861  50.024   9.262  1.00 39.72           N
ANISOU  624  NE2 GLN A 228     5046   5166   4880    -78   962  -1150       N
ATOM    625  C   GLN A 228   -34.149  50.699   5.749  1.00 32.10           C
ANISOU  625  C   GLN A 228     3825   3950   4422   288   756   -946       C
ATOM    626  O   GLN A 228   -33.515  51.191   4.810  1.00 29.38           O
ANISOU  626  O   GLN A 228     3511   3519   4131   354   655   -877       O
ATOM    627  N   ASN A 229   -34.820  51.429   6.631  1.00 32.30           N
ANISOU  627  N   ASN A 229     3810   3954   4509   291   921  -1089       N
ATOM    628  CA  ASN A 229   -34.773  52.884   6.626  1.00 40.93           C
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ANISOU  628  CA  ASN A 229     4905   4902   5746    371    999  -1183       C
ATOM    629  CB  ASN A 229      -36.103  53.468   7.094  1.00 50.46           C
ANISOU  629  CB  ASN A 229     5978   6073   7123    438   1170  -1302       C
ATOM    630  CG  ASN A 229      -37.184  53.342   6.034  1.00 69.56           C
ANISOU  630  CG  ASN A 229     8221   8471   9738    575   1102  -1193       C
ATOM    631  OD1 ASN A 229      -37.415  54.274   5.258  1.00 85.07           O
ANISOU  631  OD1 ASN A 229    10121  10301  11901    713   1074  -1153       O
ATOM    632  ND2 ASN A 229      -37.831  52.178   5.973  1.00 71.20           N
ANISOU  632  ND2 ASN A 229     8350   8812   9891    530   1065  -1134       N
ATOM    633  C   ASN A 229      -33.639  53.364   7.518  1.00 45.38           C
ANISOU  633  C   ASN A 229     5620   5459   6162    261   1047  -1287       C
ATOM    634  O   ASN A 229      -33.495  52.917   8.663  1.00 39.60           O
ANISOU  634  O   ASN A 229     4948   4844   5254    131   1124  -1369       O
ATOM    635  N   ILE A 230      -32.832  54.270   6.985  1.00 35.87           N
ANISOU  635  N   ILE A 230     4477   4127   5025    303    999  -1277       N
ATOM    636  CA  ILE A 230      -31.712  54.814   7.738  1.00 28.23           C
ANISOU  636  CA  ILE A 230     3642   3148   3934    191   1032  -1380       C
ATOM    637  CB  ILE A 230      -30.396  54.600   7.004  1.00 31.07           C
ANISOU  637  CB  ILE A 230     4084   3504   4218    167    865  -1252       C
ATOM    638  CG1 ILE A 230      -30.119  53.114   6.857  1.00 34.74           C
ANISOU  638  CG1 ILE A 230     4553   4123   4523    115    744  -1116       C
ATOM    639  CD1 ILE A 230      -29.810  52.457   8.205  1.00 42.86           C
ANISOU  639  CD1 ILE A 230     5646   5307   5332    -35    789  -1181       C
ATOM    640  CG2 ILE A 230      -29.234  55.274   7.782  1.00 32.30           C
ANISOU  640  CG2 ILE A 230     4358   3649   4263     44    897  -1367       C
ATOM    641  C   ILE A 230      -31.911  56.298   7.931  1.00 39.52           C
ANISOU  641  C   ILE A 230     5074   4402   5540    244   1169  -1529       C
ATOM    642  O   ILE A 230      -32.109  57.030   6.965  1.00 40.28           O
ANISOU  642  O   ILE A 230     5122   4340   5844    376   1140  -1463       O
ATOM    643  N   ASP A 231      -31.871  56.734   9.191  1.00 38.78           N
ANISOU  643  N   ASP A 231     5039   4335   5361    135   1322  -1729       N
ATOM    644  CA  ASP A 231      -31.930  58.145   9.521  1.00 38.69           C
ANISOU  644  CA  ASP A 231     5051   4145   5504    157   1474  -1907       C
ATOM    645  CB  ASP A 231      -33.361  58.538   9.906  1.00 43.76           C
ANISOU  645  CB  ASP A 231     5574   4744   6308    243   1632  -1990       C
ATOM    646  CG  ASP A 231      -33.661  59.998   9.592  1.00 76.54           C
ANISOU  646  CG  ASP A 231     9695   8673  10713    351   1690  -2012       C
ATOM    647  OD2 ASP A 231      -33.685  60.837  10.532  1.00 86.05           O
ANISOU  647  OD2 ASP A 231    10945   9842  11908    275   1809  -2160       O
ATOM    648  OD1 ASP A 231      -33.874  60.301   8.395  1.00 88.58           O
ANISOU  648  OD1 ASP A 231    11151  10063  12444    508   1611  -1872       O
ATOM    649  C   ASP A 231      -30.962  58.462  10.669  1.00 54.88           C
ANISOU  649  C   ASP A 231     7238   6268   7344    -35   1516  -2056       C
ATOM    650  O   ASP A 231      -31.382  58.798  11.778  1.00 54.06           O
ANISOU  650  O   ASP A 231     7143   6220   7178   -115   1635  -2184       O
ATOM    651  N   ARG A 232      -29.666  58.360  10.385  1.00 50.25           N
ANISOU  651  N   ARG A 232     6745   5701   6647   -112   1388  -2001       N
ATOM    652  CA  ARG A 232      -28.629  58.666  11.356  1.00 50.55           C
ANISOU  652  CA  ARG A 232     6896   5823   6489   -297   1385  -2109       C
ATOM    653  CB  ARG A 232      -28.513  57.552  12.393  1.00 53.95           C
ANISOU  653  CB  ARG A 232     7362   6514   6625   -442   1364  -2117       C
ATOM    654  CG  ARG A 232      -27.882  56.281  11.846  1.00 52.47           C
ANISOU  654  CG  ARG A 232     7174   6457   6307   -446   1173  -1903       C
ATOM    655  CD  ARG A 232      -27.772  55.238  12.950  1.00 59.29           C
ANISOU  655  CD  ARG A 232     8077   7565   6887   -591   1157  -1893       C
ATOM    656  NE  ARG A 232      -27.302  53.946  12.452  1.00 63.91           N
ANISOU  656  NE  ARG A 232     8643   8256   7383   -573    977  -1658       N
ATOM    657  CZ  ARG A 232      -28.103  53.016  11.939  1.00 63.07           C
ANISOU  657  CZ  ARG A 232     8463   8166   7335   -480    952  -1524       C
ATOM    658  NH1 ARG A 232      -29.412  53.247  11.854  1.00 60.46           N
ANISOU  658  NH1 ARG A 232     8055   7768   7148   -396   1084  -1593       N
ATOM    659  NH2 ARG A 232      -27.600  51.855  11.516  1.00 54.53           N
ANISOU  659  NH2 ARG A 232     7375   7162   6180   -474    800  -1329       N
ATOM    660  C   ARG A 232      -27.309  58.791  10.610  1.00 49.47           C
ANISOU  660  C   ARG A 232     6820   5636   6340   -325   1241  -2022       C
ATOM    661  O   ARG A 232      -27.249  58.510   9.396  1.00 41.11           O
ANISOU  661  O   ARG A 232     5711   4514   5394   -201   1120  -1826       O
ATOM    662  N   ALA A 233      -26.255  59.173  11.342  1.00 48.73           N
ANISOU  662  N   ALA A 233     6811   5606   6098   -489   1217  -2109       N
ATOM    663  CA  ALA A 233      -24.918  59.411  10.776  1.00 52.66           C
ANISOU  663  CA  ALA A 233     7362   6063   6583   -546   1098  -2057       C
ATOM    664  CB  ALA A 233      -24.276  58.097  10.260  1.00 43.91           C
ANISOU  664  CB  ALA A 233     6226   5120   5337   -537   898  -1821       C
ATOM    665  C   ALA A 233      -24.964  60.438   9.651  1.00 44.36           C
ANISOU  665  C   ALA A 233     5294   4747   5816   -416   1122  -2016       C
ATOM    666  O   ALA A 233      -24.316  60.263   8.615  1.00 39.12           O
ANISOU  666  O   ALA A 233     4616   4048   5200   -363    989  -1837       O
ATOM    667  N   GLY A 234      -25.761  61.480   9.847  1.00 50.75           N
ANISOU  667  N   GLY A 234     7075   5404   6802   -349   1254  -2099       N
ATOM    668  CA  GLY A 234      -25.818  62.564   8.894  1.00 52.66           C
ANISOU  668  CA  GLY A 234     7304   5394   7310   -233   1278  -2045       C
ATOM    669  C   GLY A 234      -26.695  62.270   7.696  1.00 55.43           C
ANISOU  669  C   GLY A 234     7572   5640   7851    -26   1252  -1886       C
ATOM    670  O   GLY A 234      -27.012  63.172   6.925  1.00 58.34           O
ANISOU  670  O   GLY A 234     7911   5806   8449    95   1274  -1812       O
ATOM    671  N   ILE A 235      -27.100  61.019   7.517  1.00 46.88           N
ANISOU  671  N   ILE A 235     6438   4717   6659    14   1178  -1789       N
ATOM    672  CA  ILE A 235      -27.937  60.738   6.363  1.00 56.75           C
ANISOU  672  CA  ILE A 235     7588   5912   8064    200   1113  -1597       C
ATOM    673  CB  ILE A 235      -27.490  59.504   5.548  1.00 62.57           C
ANISOU  673  CB  ILE A 235     8305   7059   8412    -87   1210  -2056       C
ATOM    674  CG1 ILE A 235      -27.650  58.225   6.340  1.00 54.36           C
ANISOU  674  CG1 ILE A 235     7256   6002   7397    125   892  -1398       C
ATOM    675  CD1 ILE A 235      -26.913  57.078   5.675  1.00 60.49           C
ANISOU  675  CD1 ILE A 235     8037   6912   8034    107   718  -1217       C
ATOM    676  CG2 ILE A 235      -26.040  59.676   5.099  1.00 61.11           C
ANISOU  676  CG2 ILE A 235     8200   6613   8405    126   819  -1314       C
ATOM    677  C   ILE A 235      -29.397  60.734   6.767  1.00 61.97           C
ANISOU  677  C   ILE A 235     8151   6559   8836    297   1241  -1675       C
ATOM    678  O   ILE A 235      -29.803  60.244   7.835  1.00 56.45           O
ANISOU  678  O   ILE A 235     7449   5997   8002    216   1326  -1808       O
ATOM    679  N   LYS A 236      -30.179  61.389   5.933  1.00 58.00           N
ANISOU  679  N   LYS A 236     7566   5879   8592    470   1265  -1595       N
ATOM    680  CA  LYS A 236      -31.563  61.560   6.253  1.00 56.87           C
ANISOU  680  CA  LYS A 236     7306   5728   8575    569   1364  -1633       C
ATOM    681  CB  LYS A 236      -31.974  63.015   6.093  1.00 56.19           C
ANISOU  681  CB  LYS A 236     7195   5435   8719    657   1437  -1634       C
ATOM    682  CG  LYS A 236      -31.412  63.913   7.172  1.00 66.81           C
ANISOU  682  CG  LYS A 236     8641   6733  10010    516   1554  -1825       C
ATOM    683  CD  LYS A 236      -32.445  64.920   7.609  1.00 70.51           C
ANISOU  683  CD  LYS A 236     9039   7080  10671    592   1698  -1908       C
ATOM    684  CE  LYS A 236      -32.283  66.237   6.878  1.00 73.71           C
ANISOU  684  CE  LYS A 236     9457   7242  11306    682   1699  -1830       C
ATOM    685  NZ  LYS A 236      -31.008  66.973   7.199  1.00 60.28           N
ANISOU  685  NZ  LYS A 236     7897   5465  9544    534   1715  -1921       N
ATOM    686  C   LYS A 236      -32.347  60.673   5.320  1.00 51.03           C
ANISOU  686  C   LYS A 236     6441   5053   7894    702   1264  -1462       C
ATOM    687  O   LYS A 236      -32.147  60.702   4.102  1.00 66.07           O
ANISOU  687  O   LYS A 236     8328   6909   9867    789   1122  -1262       O
ATOM    688  N   ASN A 237      -33.181  59.844   5.925  1.00 43.83           N
ANISOU  688  N   ASN A 237     5451   4297   6903    684   1312  -1515       N
ATOM    689  CA  ASN A 237      -34.173  59.071   5.221  1.00 50.87           C
ANISOU  689  CA  ASN A 237     6199   5278   7850    791   1226  -1366       C
ATOM    690  CB  ASN A 237      -35.370  59.956   4.951  1.00 62.08           C
ANISOU  690  CB  ASN A 237     7474   6546   9569    964   1320  -1370       C
ATOM    691  CG  ASN A 237      -35.874  60.609   6.213  1.00 76.21           C
ANISOU  691  CG  ASN A 237     9270   8322  11366    905   1503  -1558       C
ATOM    692  OD1 ASN A 237      -36.404  59.932   7.102  1.00 81.73           O
ANISOU  692  OD1 ASN A 237     9933   9167  11954    830   1594  -1667       O
ATOM    693  ND2 ASN A 237      -35.673  61.923   6.330  1.00 77.96           N
ANISOU  693  ND2 ASN A 237     9543   8369  11707    925   1564  -1602       N
ATOM    694  C   ASN A 237      -33.667  58.433   3.944  1.00 48.25           C
ANISOU  694  C   ASN A 237     5877   5005   7451    817   1004  -1135       C
ATOM    695  O   ASN A 237      -34.087  58.754   2.835  1.00 58.60           O
ANISOU  695  O   ASN A 237     7108   6238   8920    953    918  -982       O
ATOM    696  N   ARG A 238      -32.727  57.533   4.101  1.00 29.46           N
ANISOU  696  N   ARG A 238     3599   2766   4829    683    916  -1110       N
ATOM    697  CA  ARG A 238      -32.293  56.720   3.001  1.00 27.71           C
ANISOU  697  CA  ARG A 238     3383   2621   4525    694   728  -918       C
ATOM    698  CB  ARG A 238      -30.811  56.514   3.080  1.00 31.28           C
ANISOU  698  CB  ARG A 238     3978   3100   4806    575    665  -911       C
ATOM    699  CG  ARG A 238      -30.119  56.413   1.754  1.00 45.66           C
ANISOU  699  CG  ARG A 238     5823   4933   6593    603    504  -729       C
ATOM    700  CD  ARG A 238      -28.621  56.449   1.919  1.00 35.81           C
ANISOU  700  CD  ARG A 238     4700   3689   5218    492    470  -740       C
ATOM    701  NE  ARG A 238      -28.039  57.711   1.553  1.00 33.42           N
ANISOU  701  NE  ARG A 238     4448   3209   5042    517    505  -745       N
ATOM    702  CZ  ARG A 238      -26.761  57.864   1.284  1.00 33.74           C
ANISOU  702  CZ  ARG A 238     4574   3234   5011    456   -713       C
ATOM    703  NH1 ARG A 238      -26.296  59.022   0.941  1.00 36.08           N
ANISOU  703  NH1 ARG A 238     4917   3362  5430    451   491  -707       N
ATOM    704  NH2 ARG A 238      -25.959  56.855   1.380  1.00 24.24           N
ANISOU  704  NH2 ARG A 238     3402   2182  3625    352   376  -682       N
ATOM    705  C   ARG A 238      -32.979  55.392   3.149  1.00 32.56           C
ANISOU  705  C   ARG A 238     3925   3416  5031    660   692  -891       C
ATOM    706  O   ARG A 238      -33.285  55.012   4.227  1.00 34.10           O
ANISOU  706  O   ARG A 238     4116   3692  5150    584   801  -1016       O
ATOM    707  N   VAL A 239      -33.214  54.691   2.059  1.00 27.39           N
ANISOU  707  N   VAL A 239     3213   2825   4369    708   549  -735       N
ATOM    708  CA  VAL A 239      -33.847  53.382   2.169  1.00 27.65           C
ANISOU  708  CA  VAL A 239     3180   3014   4311    662   515  -713       C
ATOM    709  CB  VAL A 239      -35.220  53.338   1.521  1.00 36.43           C
ANISOU  709  CB  VAL A 239     4120   4141   5582    770   489  -653       C
ATOM    710  CG1 VAL A 239      -35.798  51.929   1.653  1.00 38.27           C
ANISOU  710  CG1 VAL A 239     4293   4532   5715    695   458  -640       C
ATOM    711  CG2 VAL A 239      -36.140  54.349   2.152  1.00 33.68           C
ANISOU  711  CG2 VAL A 239     3674   3698   5427    855   643  -759       C
ATOM    712  C   VAL A 239      -32.944  52.388   1.482  1.00 28.59           C
ANISOU  712  C   VAL A 239     3378   3215   4272    598   372  -603       C
ATOM    713  O   VAL A 239      -32.579  52.590   0.325  1.00 27.41           O
ANISOU  713  O   VAL A 239     3240   3027   4149    652   262  -490       O
ATOM    714  N   TYR A 240      -32.538  51.330   2.207  1.00 22.82           N
ANISOU  714  N   TYR A 240     2703   2590   3376    482   380  -633       N
ATOM    715  CA  TYR A 240      -31.687  50.296   1.614  1.00 23.45           C
ANISOU  715  CA  TYR A 240     2850   2734   3326    427   261  -538       C
ATOM    716  CB  TYR A 240      -30.488  49.964   2.512  1.00 23.75           C
ANISOU  716  CB  TYR A 240     3005   2810   3210   319   279  -573       C
ATOM    717  CG  TYR A 240      -29.448  51.069   2.615  1.00 25.40           C
ANISOU  717  CG  TYR A 240     3294   2933   3422   315   291  -607       C
ATOM    718  CD1 TYR A 240      -29.650  52.174   3.463  1.00 34.26           C
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ANISOU  718  CD1 TYR A 240     4425   3990   4601    311    409    -733       C
ATOM    719  CE1 TYR A 240      -28.689  53.181   3.548  1.00 34.44           C
ANISOU  719  CE1 TYR A 240     4524   3926   4636    290    424    -775       C
ATOM    720  CZ  TYR A 240      -27.524  53.079   2.760  1.00 28.77           C
ANISOU  720  CZ  TYR A 240     3862   3196   3873    277    318    -678       C
ATOM    721  OH  TYR A 240      -26.537  54.046   2.799  1.00 29.68           O
ANISOU  721  OH  TYR A 240     4044   3228   4004    242    331    -714       O
ATOM    722  CE2 TYR A 240      -27.317  52.004   1.941  1.00 29.65           C
ANISOU  722  CE2 TYR A 240     3961   3378   3927    289    212    -557       C
ATOM    723  CD2 TYR A 240      -28.284  50.998   1.872  1.00 24.89           C
ANISOU  723  CD2 TYR A 240     3294   2852   3313    307    199    -527       C
ATOM    724  C   TYR A 240      -32.477  49.011   1.412  1.00 26.68           C
ANISOU  724  C   TYR A 240     3189   3243   3707    398    225    -499       C
ATOM    725  O   TYR A 240      -33.433  48.739   2.144  1.00 25.18           O
ANISOU  725  O   TYR A 240     2926   3100   3542    376    309    -559       O
ATOM    726  N   SER A 241      -32.025  48.196   0.460  1.00 27.20           N
ANISOU  726  N   SER A 241     3281   3339   3716    385    112    -409       N
ATOM    727  CA  SER A 241      -32.653  46.911   0.177  1.00 30.58           C
ANISOU  727  CA  SER A 241     3658   3846   4117    341     74    -380       C
ATOM    728  CB  SER A 241      -33.281  46.920  -1.212  1.00 31.87           C
ANISOU  728  CB  SER A 241     3740   4020   4350    403    -28    -316       C
ATOM    729  OG  SER A 241      -34.199  47.985  -1.336  1.00 51.40           O
ANISOU  729  OG  SER A 241     6108   6462   6961    496     -7    -323       O
ATOM    730  C   SER A 241      -31.619  45.814   0.181  1.00 29.71           C
ANISOU  730  C   SER A 241     3645   3759   3884    264     31    -341       C
ATOM    731  O   SER A 241      -30.433  46.081  -0.060  1.00 26.33           O
ANISOU  731  O   SER A 241     3303   3294   3406    268     -4    -312       O
ATOM    732  N   ASN A 242      -32.060  44.570   0.404  1.00 21.69           N
ANISOU  732  N   ASN A 242     2610   2795   2837    196     38    -335       N
ATOM    733  CA  ASN A 242      -31.138  43.438   0.208  1.00 20.43           C
ANISOU  733  CA  ASN A 242     2531   2634   2596    141     -6    -285       C
ATOM    734  CB  ASN A 242      -30.545  42.938   1.522  1.00 25.55           C
ANISOU  734  CB  ASN A 242     3247   3300   3161     70     53    -279       C
ATOM    735  CG  ASN A 242      -29.729  43.996   2.224  1.00 34.55           C
ANISOU  735  CG  ASN A 242     4443   4431   4256     82     80    -306       C
ATOM    736  OD1 ASN A 242      -30.267  44.771   3.008  1.00 31.48           O
ANISOU  736  OD1 ASN A 242     4028   4056   3875     79    157    -374       O
ATOM    737  ND2 ASN A 242      -28.420  44.060   1.920  1.00 25.65           N
ANISOU  737  ND2 ASN A 242     3385   3277   3086     91     23    -264       N
ATOM    738  C   ASN A 242      -31.906  42.336  -0.462  1.00 26.18           C
ANISOU  738  C   ASN A 242     3206   3388   3353    103    -40    -275       C
ATOM    739  O   ASN A 242      -33.114  42.207  -0.253  1.00 25.14           O
ANISOU  739  O   ASN A 242     2979   3296   3277     85     -6    -306       O
ATOM    740  N   SER A 243      -31.193  41.563  -1.282  1.00 20.70           N
ANISOU  740  N   SER A 243     2568   2671   2627     87    -100    -241       N
ATOM    741  CA  SER A 243      -31.815  40.594  -2.141  1.00 27.51           C
ANISOU  741  CA  SER A 243     3391   3549   3513     45    -140    -251       C
ATOM    742  CB  SER A 243      -31.215  40.694  -3.538  1.00 29.13           C
ANISOU  742  CB  SER A 243     3632   3745   3691     77    -222    -240       C
ATOM    743  OG  SER A 243      -31.640  41.898  -4.131  1.00 30.14           O
ANISOU  743  OG  SER A 243     3705   3903   3842    147    -270    -229       O
ATOM    744  C   SER A 243      -31.632  39.181  -1.608  1.00 25.19           C
ANISOU  744  C   SER A 243     3141   3224   3206     -39    -98    -240       C
ATOM    745  O   SER A 243      -30.565  38.827  -1.132  1.00 20.41           O
ANISOU  745  O   SER A 243     2619   2574   2562     -43    -80    -199       O
ATOM    746  N   VAL A 244      -32.672  38.363  -1.796  1.00 21.22           N
ANISOU  746  N   VAL A 244     2574   2741   2747    -107    -90    -270       N
ATOM    747  CA  VAL A 244      -32.644  36.958  -1.403  1.00 22.25           C
ANISOU  747  CA  VAL A 244     2742   2820   2890    -196    -44    -257       C
ATOM    748  CB  VAL A 244      -33.950  36.586  -0.721  1.00 24.58           C
ANISOU  748  CB  VAL A 244     2949   3157   3232    -272     17    -278       C
ATOM    749  CG1 VAL A 244      -33.926  35.109  -0.342  1.00 23.73           C
ANISOU  749  CG1 VAL A 244     2889   2979   3150    -372     70    -251       C
ATOM    750  CG2 VAL A 244      -34.138  37.453   0.502  1.00 24.35           C
ANISOU  750  CG2 VAL A 244     2901   3176   3177    -245     86    -264       C
ATOM    751  C   VAL A 244      -32.519  36.072  -2.640  1.00 19.66           C
ANISOU  751  C   VAL A 244     2435   2453   2580    -233    -92    -295       C
ATOM    752  O   VAL A 244      -33.279  36.219  -3.595  1.00 21.30           O
ANISOU  752  O   VAL A 244     2574   2718   2801    -249    -149    -348       O
ATOM    753  N   TYR A 245      -31.543  35.155  -2.636  1.00 19.50           N
ANISOU  753  N   TYR A 245     2507   2339   2563    -248    -69    -268       N
ATOM    754  CA  TYR A 245      -31.325  34.283  -3.786  1.00 21.54           C
ANISOU  754  CA  TYR A 245     2798   2544   2841    -287    -90    -327       C
ATOM    755  CB  TYR A 245      -29.903  34.467  -4.296  1.00 22.35           C
ANISOU  755  CB  TYR A 245     2982   2599   2910    -213    -105    -308       C
ATOM    756  CG  TYR A 245      -29.661  35.834  -4.853  1.00 20.09           C
ANISOU  756  CG  TYR A 245     2680   2396   2557    -137    -167    -307       C
ATOM    757  CD1 TYR A 245      -29.297  36.873  -4.021  1.00 24.02           C
ANISOU  757  CD1 TYR A 245     3175   2920   3030    -72    -165    -246       C
ATOM    758  CE1 TYR A 245      -29.087  38.121  -4.512  1.00 23.57           C
ANISOU  758  CE1 TYR A 245     3107   2913   2933     -7    -212    -241       C
ATOM    759  CZ  TYR A 245      -29.243  38.363  -5.876  1.00 27.94           C
ANISOU  759  CZ  TYR A 245     3653   3508   3454     -2    -270    -276       C
ATOM    760  OH  TYR A 245      -29.016  39.636  -6.356  1.00 30.92           O
ANISOU  760  OH  TYR A 245     4026   3926   3797     63    -315    -246       O
ATOM    761  CE2 TYR A 245      -29.619  37.337  -6.753  1.00 28.11           C
ANISOU  761  CE2 TYR A 245     3677   3531   3474    -74    -282    -340       C
ATOM    762  CD2 TYR A 245      -29.845  36.088  -6.224  1.00 22.22           C
ANISOU  762  CD2 TYR A 245     2940   2719   2784    -142    -227    -366       C
ATOM    763  C   TYR A 245      -31.476  32.827  -3.383  1.00 23.87           C
ANISOU  763  C   TYR A 245     3124   2734   3210    -376    -22    -325       C
ATOM    764  O   TYR A 245      -31.168  32.475  -2.244  1.00 24.04           O
ANISOU  764  O   TYR A 245     3178   2704   3251    -377     33    -238       O
ATOM    765  N   GLU A 246      -31.907  31.984  -4.328  1.00 22.81           N
ANISOU  765  N   GLU A 246     2986   2567   3114    -457    -26    -417       N
ATOM    766  CA  GLU A 246      -31.921  30.529  -4.156  1.00 22.71           C
ANISOU  766  CA  GLU A 246     3018   2415   3194    -544     47    -430       C
ATOM    767  CB  GLU A 246      -33.196  29.909  -4.772  1.00 23.99           C
ANISOU  767  CB  GLU A 246     3115   2606   3396    -679     41    -541       C
ATOM    768  CG  GLU A 246      -34.442  30.468  -4.113  1.00 31.00           C
ANISOU  768  CG  GLU A 246     3887   3613   4280    -715     30    -519       C
ATOM    769  CD  GLU A 246      -35.755  29.880  -4.614  1.00 49.61           C
ANISOU  769  CD  GLU A 246     6150   6014   6685    -857     19    -620       C
ATOM    770  OE1 GLU A 246      -36.740  29.963  -3.839  1.00 47.07           O
ANISOU  770  OE1 GLU A 246     5735   5749   6401    -907     52    -592       O
ATOM    771  OE2 GLU A 246      -35.800  29.347  -5.750  1.00 51.49           O
ANISOU  771  OE2 GLU A 246     6403   6239   6921    -926    -16    -731       O
ATOM    772  C   GLU A 246      -30.689  29.934  -4.807  1.00 28.55           C
ANISOU  772  C   GLU A 246     3851   3036   3961    -504     71    -452       C
ATOM    773  O   GLU A 246      -30.278  30.363  -5.898  1.00 27.96           O
ANISOU  773  O   GLU A 246     3791   3027   3807    -504     26    -452       O
ATOM    774  N   LEU A 247      -30.102  28.930  -4.149  1.00 23.76           N
ANISOU  774  N   LEU A 247     3304   2274   3450    -505    146    -384       N
ATOM    775  CA  LEU A 247      -28.939  28.242  -4.686  1.00 24.67           C
ANISOU  775  CA  LEU A 247     3494   2249   3630    -458    189    -403       C
ATOM    776  CB  LEU A 247      -27.834  28.146  -3.644  1.00 24.44           C
ANISOU  776  CB  LEU A 247     3500   2143   3643    -360    214    -241       C
ATOM    777  CG  LEU A 247      -27.530  29.467  -2.968  1.00 32.33           C
ANISOU  777  CG  LEU A 247     4468   4527   -282    148    -151       C
ATOM    778  CD1 LEU A 247      -26.464  29.230  -1.971  1.00 41.08           C
ANISOU  778  CD1 LEU A 247     5605   4332  5671    -209    161      4       C
ATOM    779  CD2 LEU A 247      -27.029  30.420  -4.025  1.00 35.98           C
ANISOU  779  CD2 LEU A 247     4924   3839  4909    -222     96    -232       C
ATOM    780  C   LEU A 247      -29.392  26.842  -5.050  1.00 32.38           C
ANISOU  780  C   LEU A 247     4501   3073  4729    -569    265    -489       C
ATOM    781  O   LEU A 247      -29.989  26.149  -4.228  1.00 31.07           O
ANISOU  781  O   LEU A 247     4330  2834  4641    -639    312    -427       O
ATOM    782  N   LEU A 248      -29.106  26.418  -6.286  1.00 25.92           N
ANISOU  782  N   LEU A 248     3719   2205  3925    -597    287    -638       N
ATOM    783  CA  LEU A 248      -29.552  25.102  -6.744  1.00 27.72           C
ANISOU  783  CA  LEU A 248     3981   2280  4271    -719    367    -758       C
ATOM    784  CB  LEU A 248      -30.257  25.192  -8.098  1.00 31.09           C
ANISOU  784  CB  LEU A 248     4391   2814  4607    -831    326    -962       C
ATOM    785  CG  LEU A 248      -31.263  26.318  -8.311  1.00 47.71           C
ANISOU  785  CG  LEU A 248     6402  5163  6562    -862    203    -970       C
ATOM    786  CD1 LEU A 248      -31.783  26.218  -9.732  1.00 48.11           C
ANISOU  786  CD1 LEU A 248     6447  5309  6525    -976    158   -1163       C
ATOM    787  CD2 LEU A 248      -32.417  26.193  -7.325  1.00 40.52           C
ANISOU  787  CD2 LEU A 248     5415  4278  5701    -937    199    -900       C
ATOM    788  C   LEU A 248      -28.361  24.168  -6.905  1.00 33.33           C
ANISOU  788  C   LEU A 248     4770   2770  5122    -656    470    -761       C
ATOM    789  O   LEU A 248      -27.233  24.605  -7.187  1.00 36.91           O
ANISOU  789  O   LEU A 248     5242   3231  5549    -535    468    -739       O
ATOM    790  N   GLU A 249      -28.640  22.891  -6.765  1.00 31.85           N
ANISOU  790  N   GLU A 249     4622   2383  5097    -740    565    -795       N
ATOM    791  CA  GLU A 249      -27.635  21.845  -6.886  1.00 38.51           C
ANISOU  791  CA  GLU A 249     5534   2976  6124    -683    682    -801       C
ATOM    792  CB  GLU A 249      -27.110  21.539  -5.496  1.00 37.38           C
ANISOU  792  CB  GLU A 249     5393   2716  6094    -586    702    -551       C
ATOM    793  CG  GLU A 249      -25.848  20.719  -5.443  1.00 58.08           C
ANISOU  793  CG  GLU A 249     8057   5104  8908    -467    796    -489       C
ATOM    794  CD  GLU A 249      -25.417  20.442  -4.002  1.00 68.73           C
ANISOU  794  CD  GLU A 249     9399   6366  10350    -380    788    -208       C
ATOM    795  OE1 GLU A 249      -26.257  19.927  -3.221  1.00 72.66           O
ANISOU  795  OE1 GLU A 249     9907   6808  10891    -475    804    -116       O
ATOM    796  OE2 GLU A 249      -24.253  20.764  -3.650  1.00 65.39           O
ANISOU  796  OE2 GLU A 249     8953   5948  9943    -227    760    -75       O
ATOM    797  C   GLU A 249      -28.379  20.644  -7.440  1.00 45.56           C
ANISOU  797  C   GLU A 249     6466   3706  7137    -847    775    -973       C
ATOM    798  O   GLU A 249      -29.413  20.267  -6.891  1.00 50.73           O
ANISOU  798  O   GLU A 249     7100  4346  7828    -965    775    -942       O
ATOM    799  N   ASN A 250      -27.881  20.058  -8.539  1.00 45.94           N
ANISOU  799  N   ASN A 250     6570   3640  7244    -867    861   -1167       N
ATOM    800  CA  ASN A 250      -28.553  18.931  -9.185  1.00 55.73           C
ANISOU  800  CA  ASN A 250     7843   4768  8563   -1022    937   -1346       C
ATOM    801  CB  ASN A 250      -28.425  17.654  -8.343  1.00 62.11           C
ANISOU  801  CB  ASN A 250     8676   5331  9592    -997   1029   -1209       C
ATOM    802  CG  ASN A 250      -27.000  17.385  -7.880  1.00 70.00           C
ANISOU  802  CG  ASN A 250     9694   6178  10725    -795   1085   -1051       C
ATOM    803  OD1 ASN A 250      -26.028  17.772  -8.536  1.00 71.45           O
ANISOU  803  OD1 ASN A 250     9880   6399  10867    -689   1097   -1112       O
ATOM    804  ND2 ASN A 250      -26.873  16.716  -6.731  1.00 73.18           N
ANISOU  804  ND2 ASN A 250    10101   6423  11282    -745   1115    -835       N
ATOM    805  C   ASN A 250      -30.042  19.183  -9.435  1.00 56.24           C
ANISOU  805  C   ASN A 250     7859   4998  8510   -1215    858   -1455       C
ATOM    806  O   ASN A 250      -30.866  18.295  -9.215  1.00 59.84           O
ANISOU  806  O   ASN A 250     8307   5377  9052   -1304    892   -1471       O
ATOM    807  N   GLY A 251      -30.381  20.402  -9.844  1.00 52.77           N
ANISOU  807  N   GLY A 251     7365   4825  7861   -1221    733   -1488       N
ATOM    808  CA  GLY A 251      -31.746  20.723 -10.222  1.00 53.96           C
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ANISOU  808  CA  GLY A 251     7442   5173   7887  -1384    635  -1586       C
ATOM    809  C   GLY A 251   -32.710  21.053  -9.092  1.00 66.52           C
ANISOU  809  C   GLY A 251     8942   6847   9484  -1411    576  -1422       C
ATOM    810  O   GLY A 251   -33.908  21.212  -9.336  1.00 67.45           O
ANISOU  810  O   GLY A 251     8978   7114   9535  -1550    507  -1499       O
ATOM    811  N   GLN A 252   -32.213  21.154  -7.857  1.00 60.21           N
ANISOU  811  N   GLN A 252     8151   5968   8760  -1284    604  -1198       N
ATOM    812  CA  GLN A 252   -33.083  21.373  -6.694  1.00 48.70           C
ANISOU  812  CA  GLN A 252     6619   4575   7308  -1318    579  -1045       C
ATOM    813  CB  GLN A 252   -33.271  20.070  -5.937  1.00 55.37           C
ANISOU  813  CB  GLN A 252     7512   5168   8358  -1403    704   -981       C
ATOM    814  CG  GLN A 252   -33.725  18.948  -6.827  1.00 65.46           C
ANISOU  814  CG  GLN A 252     8828   6296   9749  -1578    781  -1198       C
ATOM    815  CD  GLN A 252   -34.827  18.177  -6.198  1.00 86.42           C
ANISOU  815  CD  GLN A 252    11447   8873  12515  -1748    838  -1173       C
ATOM    816  OE1 GLN A 252   -35.840  17.856  -6.832  1.00 90.96           O
ANISOU  816  OE1 GLN A 252    11964   9539  13057  -1899    807  -1323       O
ATOM    817  NE2 GLN A 252   -34.652  17.874  -4.924  1.00 96.23           N
ANISOU  817  NE2 GLN A 252    12714   9993  13857  -1699    900   -948       N
ATOM    818  C   GLN A 252   -32.500  22.411  -5.746  1.00 45.33           C
ANISOU  818  C   GLN A 252     6171   4254   6797  -1147    523   -836       C
ATOM    819  O   GLN A 252   -31.282  22.524  -5.634  1.00 37.69           O
ANISOU  819  O   GLN A 252     5262   3213   5845  -1004    540   -758       O
ATOM    820  N   ARG A 253   -33.369  23.148  -5.052  1.00 40.98           N
ANISOU  820  N   ARG A 253     5532   3874   6165  -1167    465   -755       N
ATOM    821  CA  ARG A 253   -32.894  24.207  -4.172  1.00 41.24           C
ANISOU  821  CA  ARG A 253     5545   4021   6103  -1024    415   -588       C
ATOM    822  CB  ARG A 253   -34.024  25.098  -3.664  1.00 35.88           C
ANISOU  822  CB  ARG A 253     4753   3546   5333  -1061    359   -560       C
ATOM    823  CG  ARG A 253   -33.483  26.346  -2.958  1.00 31.49           C
ANISOU  823  CG  ARG A 253     4184   3117   4664   -915    307   -434       C
ATOM    824  CD  ARG A 253   -34.571  27.205  -2.347  1.00 36.84           C
ANISOU  824  CD  ARG A 253     4751   3971   5276   -941    281   -411       C
ATOM    825  NE  ARG A 253   -35.447  26.375  -1.544  1.00 45.19           N
ANISOU  825  NE  ARG A 253     5781   4974   6414  -1069    366   -370       N
ATOM    826  CZ  ARG A 253   -36.683  26.059  -1.912  1.00 54.51           C
ANISOU  826  CZ  ARG A 253     6868   6204   7639  -1206    372   -472       C
ATOM    827  NH1 ARG A 253   -37.180  26.538  -3.051  1.00 50.43           N
ANISOU  827  NH1 ARG A 253     6273   5805   7082  -1223    281   -609       N
ATOM    828  NH2 ARG A 253   -37.418  25.271  -1.145  1.00 56.92           N
ANISOU  828  NH2 ARG A 253     7151   6449   8025  -1331    463   -427       N
ATOM    829  C   ARG A 253   -32.129  23.587  -3.000  1.00 34.42           C
ANISOU  829  C   ARG A 253     4750   2991   5335   -961    491   -398       C
ATOM    830  O   ARG A 253   -32.591  22.638  -2.368  1.00 39.52           O
ANISOU  830  O   ARG A 253     5414   3507   6094  -1055    570   -338       O
ATOM    831  N   ALA A 254   -30.947  24.103  -2.740  1.00 34.10           N
ANISOU  831  N   ALA A 254     4746   2955   5254   -809    462   -297       N
ATOM    832  CA  ALA A 254   -30.088  23.540  -1.708  1.00 41.66           C
ANISOU  832  CA  ALA A 254     5762   3772   6295   -736    511   -104       C
ATOM    833  CB  ALA A 254   -28.793  22.995  -2.323  1.00 33.59           C
ANISOU  833  CB  ALA A 254     4800   2581   5380   -635    544   -120       C
ATOM    834  C   ALA A 254   -29.789  24.581  -0.629  1.00 32.23           C
ANISOU  834  C   ALA A 254     4541   2737   4966   -651    449    55       C
ATOM    835  O   ALA A 254   -29.318  24.257   0.449  1.00 31.77           O
ANISOU  835  O   ALA A 254     4516   2624   4932   -616    468   239       O
ATOM    836  N   GLY A 255   -30.110  25.831  -0.915  1.00 26.46           N
ANISOU  836  N   GLY A 255     3753   2208   4093   -627    374    -18       N
ATOM    837  CA  GLY A 255   -29.898  26.891   0.056  1.00 29.48           C
ANISOU  837  CA  GLY A 255     4112   2741   4347   -561    327    94       C
ATOM    838  C   GLY A 255   -30.615  28.138  -0.375  1.00 26.32           C
ANISOU  838  C   GLY A 255     3639   2530   3833   -562    267    -15       C
ATOM    839  O   GLY A 255   -31.012  28.283  -1.535  1.00 25.81           O
ANISOU  839  O   GLY A 255     3543   2493   3770   -585    237   -158       O
ATOM    840  N   THR A 256   -30.772  29.064   0.573  1.00 23.65           N
ANISOU  840  N   THR A 256     3271   2322   3391   -536    249    56       N
ATOM    841  CA  THR A 256   -31.410  30.344   0.301  1.00 22.76           C
ANISOU  841  CA  THR A 256     3084   2372   3191   -516    202   -29       C
ATOM    842  CB  THR A 256   -32.889  30.336   0.741  1.00 30.71           C
ANISOU  842  CB  THR A 256     4009   3455   4206   -619    246   -64       C
ATOM    843  OG1 THR A 256   -33.585  29.233   0.152  1.00 33.73           O
ANISOU  843  OG1 THR A 256     4375   3752   4690   -727    279   -129       O
ATOM    844  CG2 THR A 256   -33.586  31.647   0.363  1.00 28.54           C
ANISOU  844  CG2 THR A 256     3638   3332   3876   -581    197   -150       C
ATOM    845  C   THR A 256   -30.667  31.360   1.150  1.00 28.61           C
ANISOU  845  C   THR A 256     3844   3197   3831   -432    176    52       C
ATOM    846  O   THR A 256   -30.492  31.139   2.357  1.00 27.63           O
ANISOU  846  O   THR A 256     3750   3077   3671   -454    213    166       O
ATOM    847  N   CYS A 257   -30.229  32.465   0.554  1.00 23.84           N
ANISOU  847  N   CYS A 257     3225   2661   3172   -349    114    -1       N
ATOM    848  CA  CYS A 257   -29.446  33.420   1.335  1.00 21.24           C
ANISOU  848  CA  CYS A 257     2918   2400   2754   -283    92    62       C
ATOM    849  CB  CYS A 257   -28.009  32.962   1.443  1.00 29.26           C
ANISOU  849  CB  CYS A 257     3998   3337   3781   -228    70    152       C
ATOM    850  SG  CYS A 257   -27.290  32.878  -0.152  1.00 47.49           S
ANISOU  850  SG  CYS A 257     6318   5576   6148   -165    33    70       S
ATOM    851  C   CYS A 257   -29.497  34.828   0.785  1.00 26.04           C
ANISOU  851  C   CYS A 257     3486   3096   3486   -257    -16    -16       C
ATOM    852  O   CYS A 257   -29.819  35.058  -0.393  1.00 21.50           O
ANISOU  852  O   CYS A 257     2880   2525   2765   -203    6   -96       O
ATOM    853  N   VAL A 258   -29.160  35.764   1.659  1.00 20.23           N
ANISOU  853  N   VAL A 258     2757   2428   2500   -192    45    14       N
ATOM    854  CA  VAL A 258   -28.966  37.158   1.272  1.00 23.24           C
ANISOU  854  CA  VAL A 258     3119   2865   2848   -125    7   -42       C
ATOM    855  CB  VAL A 258   -29.117  38.083   2.466  1.00 27.42           C
ANISOU  855  CB  VAL A 258     3643   3471   3304   -134    45   -44       C
ATOM    856  CG1 VAL A 258   -29.060  39.550   2.003  1.00 28.03           C
ANISOU  856  CG1 VAL A 258     3696   3576   3380   -66    20   -111       C
ATOM    857  CG2 VAL A 258   -30.442  37.798   3.161  1.00 30.52           C
ANISOU  857  CG2 VAL A 258     3985   3908   3705   -204   121   -67       C
ATOM    858  C   VAL A 258   -27.556  37.317   0.741  1.00 26.76           C
ANISOU  858  C   VAL A 258     3615   3271   3283   -63   -44   -11       C
ATOM    859  O   VAL A 258   -26.611  37.090   1.464  1.00 24.60           O
ANISOU  859  O   VAL A 258     3381   2989   2977   -60   -48    64       O
ATOM    860  N   LEU A 259   -27.430  37.732  -0.531  1.00 20.03           N
ANISOU  860  N   LEU A 259     2751   2406   2454   -18   -85   -64       N
ATOM    861  CA  LEU A 259   -26.132  37.752 -1.180  1.00 22.36           C
ANISOU  861  CA  LEU A 259     3087   2662   2749    31   -116   -44       C
ATOM    862  CB  LEU A 259   -26.194  36.757 -2.345  1.00 24.21           C
ANISOU  862  CB  LEU A 259     3330   2835   3035    18   -115   -83       C
ATOM    863  CG  LEU A 259   -25.254  35.608 -2.526  1.00 40.60           C
ANISOU  863  CG  LEU A 259     5445   4816   5164    25   -91   -51       C
ATOM    864  CD1 LEU A 259   -24.920  34.948 -1.220  1.00 37.34           C
ANISOU  864  CD1 LEU A 259     5046   4369   4772    12   -67    50       C
ATOM    865  CD2 LEU A 259   -25.982  34.616 -3.438  1.00 34.53           C
ANISOU  865  CD2 LEU A 259     4678   3995   4447   -28   -69   -129       C
ATOM    866  C   LEU A 259   -25.929  39.103 -1.798  1.00 21.18           C
ANISOU  866  C   LEU A 259     2926   2550   2569    80   -150    -78       C
ATOM    867  O   LEU A 259   -26.867  39.673 -2.367  1.00 22.04           O
ANISOU  867  O   LEU A 259     2996   2692   2684    125   -166   -125       O
ATOM    868  N   GLU A 260   -24.704  39.621 -1.780  1.00 23.51           N
ANISOU  868  N   GLU A 260     3250   2840   2843   116   -166    -48       N
ATOM    869  CA  GLU A 260   -24.434  40.773 -2.643  1.00 25.73           C
ANISOU  869  CA  GLU A 260     3531   3136   3111   157   -192    -73       C
ATOM    870  CB  GLU A 260   -25.032  42.055 -2.061  1.00 25.76           C
ANISOU  870  CB  GLU A 260     3512   3172   3103   166   -188    -95       C
ATOM    871  CG  GLU A 260   -24.481  42.402 -0.730  1.00 26.16           C
ANISOU  871  CG  GLU A 260     3579   3242   3118   143   -167    -80       C
ATOM    872  CD  GLU A 260   -25.329  43.511 -0.074  1.00 46.27           C
ANISOU  872  CD  GLU A 260     6104   5811   5666   141   -133   -133       C
ATOM    873  OE1 GLU A 260   -26.576  43.404 -0.112  1.00 39.73           O
ANISOU  873  OE1 GLU A 260     5232   4994   4870   142   -112   -163       O
ATOM    874  OE2 GLU A 260   -24.754  44.479   0.449  1.00 42.71           O
ANISOU  874  OE2 GLU A 260     5673   5361   5193   137   -123   -153       O
ATOM    875  C   GLU A 260   -22.951  40.986 -2.888  1.00 26.03           C
ANISOU  875  C   GLU A 260     3595   3155   3140   182   -200    -42       C
ATOM    876  O   GLU A 260   -22.122  40.583 -2.102  1.00 22.38           O
ANISOU  876  O   GLU A 260     3137   2688   2679   175   -197     4       O
ATOM    877  N   TYR A 261   -22.624  41.632 -3.993  1.00 25.36           N
ANISOU  877  N   TYR A 261     3519   3071   3047   208   -214    -56       N
ATOM    878  CA  TYR A 261   -21.214  41.968 -4.227  1.00 22.95           C
ANISOU  878  CA  TYR A 261     3226   2755   2739   224   -210    -29       C
ATOM    879  CB  TYR A 261   -20.993  42.352 -5.678  1.00 20.10           C
ANISOU  879  CB  TYR A 261     2883   2396   2359   239   -210    -44       C
ATOM    880  CG  TYR A 261   -21.076  41.195 -6.634  1.00 23.37           C
ANISOU  880  CG  TYR A 261     3309   2797   2773   231   -190    -79       C
ATOM    881  CD1 TYR A 261   -20.113  40.202 -6.623  1.00 24.12           C
ANISOU  881  CD1 TYR A 261     3404   2851   2910   239   -149    -79       C
ATOM    882  CE1 TYR A 261   -20.179  39.131 -7.508  1.00 21.52           C
ANISOU  882  CE1 TYR A 261     3092   2491   2592   226   -112   -134       C
ATOM    883  CZ  TYR A 261   -21.227  39.070 -8.413  1.00 25.94           C
ANISOU  883  CZ  TYR A 261     3672   3086   3098   191   -130   -191       C
ATOM    884  OH  TYR A 261   -21.305  38.024 -9.287  1.00 28.34           O
ANISOU  884  OH  TYR A 261     4001   3366   3401   159   -90   -269       O
ATOM    885  CE2 TYR A 261   -22.197  40.039 -8.445  1.00 27.78           C
ANISOU  885  CE2 TYR A 261     3895   3378   3283   186   -190   -174       C
ATOM    886  CD2 TYR A 261   -22.117  41.111 -7.559  1.00 30.51           C
ANISOU  886  CD2 TYR A 261     4221   3731   3640   214   -212   -117       C
ATOM    887  C   TYR A 261   -20.804  43.135 -3.346  1.00 24.77           C
ANISOU  887  C   TYR A 261     3452   3003   2955   217   -218    -17       C
ATOM    888  O   TYR A 261   -21.569  44.050 -3.102  1.00 22.54           O
ANISOU  888  O   TYR A 261     3169   2726   2668   217   -219    -41       O
ATOM    889  N   ALA A 262   -19.558  43.108 -2.881  1.00 24.80           N
ANISOU  889  N   ALA A 262     3448   3015   2962   209   -221    16       N
ATOM    890  CA  ALA A 262   -18.990  44.245 -2.199  1.00 21.10           C
ANISOU  890  CA  ALA A 262     2976   2566   2474   183   -230    13       C
ATOM    891  CB  ALA A 262   -17.694  43.849 -1.540  1.00 22.62           C
ANISOU  891  CB  ALA A 262     3187   2790   2619   165   -250    59       C
ATOM    892  C   ALA A 262   -18.756  45.394 -3.183  1.00 26.11           C
ANISOU  892  C   ALA A 262     3626   3173   3121   194   -219    -1       C
ATOM    893  O   ALA A 262   -17.934  45.313 -4.114  1.00 23.10           O
ANISOU  893  O   ALA A 262     3242   2784   2751   206   -208    19       O
ATOM    894  N   THR A 263   -19.430  46.515 -2.945  1.00 22.72           N
ANISOU  894  N   THR A 263     3212   2724   2695   189   -212    -33       N
ATOM    895  CA  THR A 263   -19.363  47.633 -3.882  1.00 20.75           C
ANISOU  895  CA  THR A 263     2983   2429   2470   205   -201   -24       C
ATOM    896  CB  THR A 263   -20.320  48.754 -3.439  1.00 20.95           C
ANISOU  896  CB  THR A 263     3018   2410   2531   215   -186   -60       C
ATOM    897  OG1 THR A 263   -20.009  49.119 -2.086  1.00 24.23           O
ANISOU  897  OG1 THR A 263     3433   2836   2937   162   -168   -113       O
ATOM    898  CG2 THR A 263   -21.780  48.259 -3.504  1.00 23.24           C
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ANISOU  898  CG2 THR A 263     3287   2714   2830    254   -194    -70       C
ATOM    899  C   THR A 263    -17.986  48.257  -4.137  1.00 20.82           C
ANISOU  899  C   THR A 263     2994   2428   2489    172   -189     -5       C
ATOM    900  O   THR A 263    -17.764  48.807  -5.239  1.00 22.55           O
ANISOU  900  O   THR A 263     3234   2618   2717    184   -175     29       O
ATOM    901  N   PRO A 264    -17.079  48.233  -3.148  1.00 18.55           N
ANISOU  901  N   PRO A 264     2683   2172   2194    123   -196    -19       N
ATOM    902  CA  PRO A 264    -15.811  48.908  -3.478  1.00 18.56           C
ANISOU  902  CA  PRO A 264     2671   2166   2217     84   -183     -3       C
ATOM    903  CB  PRO A 264    -15.021  48.852  -2.174  1.00 21.66           C
ANISOU  903  CB  PRO A 264     3024   2616   2591     21   -212    -25       C
ATOM    904  CG  PRO A 264    -16.128  48.852  -1.075  1.00 19.83           C
ANISOU  904  CG  PRO A 264     2819   2395   2321     12   -220    -75       C
ATOM    905  CD  PRO A 264    -17.192  47.966  -1.690  1.00 20.43           C
ANISOU  905  CD  PRO A 264     2907   2456   2399     85   -215    -50       C
ATOM    906  C   PRO A 264    -15.024  48.214  -4.584  1.00 21.01           C
ANISOU  906  C   PRO A 264     2958   2493   2532    108   -166     43       C
ATOM    907  O   PRO A 264    -14.119  48.810  -5.162  1.00 20.72           O
ANISOU  907  O   PRO A 264     2912   2446   2516     79   -138     61       O
ATOM    908  N   LEU A 265    -15.358  46.976  -4.887  1.00 19.28           N
ANISOU  908  N   LEU A 265     2731   2294   2300    152   -171     53       N
ATOM    909  CA  LEU A 265    -14.728  46.348  -6.054  1.00 20.19           C
ANISOU  909  CA  LEU A 265     2834   2416   2420    174   -133     72       C
ATOM    910  CB  LEU A 265    -15.088  44.853  -6.132  1.00 23.60           C
ANISOU  910  CB  LEU A 265     3257   2853   2857    215   -131     63       C
ATOM    911  CG  LEU A 265    -14.629  44.051  -4.909  1.00 28.28           C
ANISOU  911  CG  LEU A 265     3797   3463   3486    220   -161     85       C
ATOM    912  CD1 LEU A 265    -15.138  42.638  -5.021  1.00 28.89           C
ANISOU  912  CD1 LEU A 265     3878   3514   3585    258   -150     82       C
ATOM    913  CD2 LEU A 265    -13.110  43.994  -4.758  1.00 32.78           C
ANISOU  913  CD2 LEU A 265     4289   4058   4107    214   -152    119       C
ATOM    914  C   LEU A 265    -15.103  47.054  -7.342  1.00 24.01           C
ANISOU  914  C   LEU A 265     3371   2879   2871    176   -105     83       C
ATOM    915  O   LEU A 265    -14.342  47.023  -8.328  1.00 22.26           O
ANISOU  915  O   LEU A 265     3148   2671   2639    167    -57     98       O
ATOM    916  N   GLN A 266    -16.293  47.668  -7.396  1.00 18.89           N
ANISOU  916  N   GLN A 266     2766   2206   2207    190   -132     85       N
ATOM    917  CA  GLN A 266    -16.656  48.442  -8.587  1.00 19.73           C
ANISOU  917  CA  GLN A 266     2918   2297   2281    195   -124    127       C
ATOM    918  CB  GLN A 266    -18.130  48.897  -8.513  1.00 27.88           C
ANISOU  918  CB  GLN A 266     3970   3305   3317    231   -169    135       C
ATOM    919  CG  GLN A 266    -19.079  47.726  -8.335  1.00 31.19           C
ANISOU  919  CG  GLN A 266     4372   3765   3715    255   -199     96       C
ATOM    920  CD  GLN A 266    -20.531  48.157  -8.207  1.00 36.84           C
ANISOU  920  CD  GLN A 266     5080   4467   4450    290   -240    102       C
ATOM    921  OE1 GLN A 266    -20.989  49.073  -8.886  1.00 39.49           O
ANISOU  921  OE1 GLN A 266     5431   4783   4791    314   -260    159       O
ATOM    922  NE2 GLN A 266    -21.252  47.491  -7.324  1.00 53.37           N
ANISOU  922  NE2 GLN A 266     7143   6574   6563    296   -251     55       N
ATOM    923  C   GLN A 266    -15.799  49.683  -8.714  1.00 20.57           C
ANISOU  923  C   GLN A 266     3035   2363   2418    155    -91    163       C
ATOM    924  O   GLN A 266    -15.507  50.169  -9.822  1.00 20.87           O
ANISOU  924  O   GLN A 266     3106   2400   2423    141    -62    217       O
ATOM    925  N   THR A 267    -15.422  50.238  -7.579  1.00 19.79           N
ANISOU  925  N   THR A 267     2914   2233   2374    124    -94    134       N
ATOM    926  CA  THR A 267    -14.516  51.374  -7.587  1.00 18.48           C
ANISOU  926  CA  THR A 267     2751   2022   2250     66    -59    152       C
ATOM    927  CB  THR A 267    -14.418  52.066  -6.199  1.00 22.79           C
ANISOU  927  CB  THR A 267     3282   2531   2847     20    -71     91       C
ATOM    928  OG1 THR A 267    -15.681  52.681  -5.921  1.00 20.99           O
ANISOU  928  OG1 THR A 267     3095   2235   2645     58    -80     76       O
ATOM    929  CG2 THR A 267    -13.391  53.195  -6.248  1.00 18.35           C
ANISOU  929  CG2 THR A 267     2719   1918   2335    -61    -30     97       C
ATOM    930  C   THR A 267    -13.124  50.960  -8.042  1.00 19.03           C
ANISOU  930  C   THR A 267     2774   2142   2313     27    -18    164       C
ATOM    931  O   THR A 267    -12.509  51.639  -8.887  1.00 22.68           O
ANISOU  931  O   THR A 267     3253   2586   2778    -11     32    210       O
ATOM    932  N   LEU A 268    -12.611  49.854  -7.525  1.00 17.28           N
ANISOU  932  N   LEU A 268     2490   1984   2093     38    -31    134       N
ATOM    933  CA  LEU A 268    -11.289  49.389  -8.016  1.00 17.76           C
ANISOU  933  CA  LEU A 268     2485   2091   2172     17     19    146       C
ATOM    934  CB  LEU A 268    -10.863  48.111  -7.301  1.00 24.15           C
ANISOU  934  CB  LEU A 268     3217   2951   3010     52    -7    126       C
ATOM    935  CG  LEU A 268    -10.521  48.300  -5.828  1.00 25.93           C
ANISOU  935  CG  LEU A 268     3387   3201   3264     15    -72    115       C
ATOM    936  CD1 LEU A 268    -10.199  46.937  -5.231  1.00 24.89           C
ANISOU  936  CD1 LEU A 268     3184   3117   3158     63   -105    131       C
ATOM    937  CD2 LEU A 268    -9.289  49.192  -5.715  1.00 29.21           C
ANISOU  937  CD2 LEU A 268     3740   3635   3722    -67   -54    119       C
ATOM    938  C   LEU A 268    -11.307  49.127  -9.522  1.00 20.11           C
ANISOU  938  C   LEU A 268     2823   2402   2417    35    83    171       C
ATOM    939  O   LEU A 268    -10.358  49.461 -10.250  1.00 20.70           O
ANISOU  939  O   LEU A 268     2877   2491   2495    -7    153    193       O
ATOM    940  N   PHE A 269    -12.383  48.537  -9.998  1.00 18.55           N
ANISOU  940  N   PHE A 269     2680   2208   2161    83    63    163       N
ATOM    941  CA  PHE A 269    -12.519  48.282 -11.440  1.00 21.81           C
ANISOU  941  CA  PHE A 269     3142   2654   2492    84   113    176       C
ATOM    942  CB  PHE A 269    -13.819  47.485 -11.692  1.00 23.92           C
ANISOU  942  CB  PHE A 269     3453   2936   2700    128    65    148       C
ATOM    943  CG  PHE A 269    -14.066  47.254 -13.165  1.00 35.27           C
ANISOU  943  CG  PHE A 269     4949   4428   4024    111    102    153       C
ATOM    944  CD1 PHE A 269    -13.336  46.303 -13.839  1.00 34.51           C
ANISOU  944  CD1 PHE A 269     4838   4373   3902    100    186     94       C
ATOM    945  CE1 PHE A 269    -13.544  46.071 -15.211  1.00 39.02           C
ANISOU  945  CE1 PHE A 269     5472   5012   4342     66    229     79       C
ATOM    946  CZ  PHE A 269    -14.470  46.823 -15.892  1.00 35.95           C
ANISOU  946  CZ  PHE A 269     5154   4659   3847     47    167    151       C
ATOM    947  CE2 PHE A 269    -15.208  47.801 -15.223  1.00 50.29           C
ANISOU  947  CE2 PHE A 269     6972   6421   5713     75     75    230       C
ATOM    948  CD2 PHE A 269    -15.002  48.011 -13.857  1.00 42.44           C
ANISOU  948  CD2 PHE A 269     5921   5350   4853    105     53    218       C
ATOM    949  C   PHE A 269    -12.525  49.605 -12.210  1.00 20.57           C
ANISOU  949  C   PHE A 269     3044   2475   2297     41    133    252       C
ATOM    950  O   PHE A 269    -11.804  49.793 -13.214  1.00 19.82           O
ANISOU  950  O   PHE A 269     2963   2414   2155     -1    209    281       O
ATOM    951  N   ALA A 270    -13.319  50.562 -11.779  1.00 21.86           N
ANISOU  951  N   ALA A 270     3244   2577   2486     49     77    291       N
ATOM    952  CA  ALA A 270    -13.330  51.861 -12.475  1.00 22.59           C
ANISOU  952  CA  ALA A 270     3394   2622   2568     15     97    383       C
ATOM    953  CB  ALA A 270    -14.408  52.798 -11.892  1.00 25.08           C
ANISOU  953  CB  ALA A 270     3741   2846   2944     50     35    415       C
ATOM    954  C   ALA A 270    -11.963  52.552 -12.447  1.00 24.08           C
ANISOU  954  C   ALA A 270     3552   2786   2810    -62   172    400       C
ATOM    955  O   ALA A 270    -11.532  53.125 -13.440  1.00 25.67           O
ANISOU  955  O   ALA A 270     3792   2991   2970   -108   230    474       O
ATOM    956  N   MET A 271    -11.269  52.526 -11.308  1.00 21.47           N
ANISOU  956  N   MET A 271     3150   2442   2567    -87   168    336       N
ATOM    957  CA  MET A 271    -9.940  53.165 -11.249  1.00 24.68           C
ANISOU  957  CA  MET A 271     3507   2837   3032   -174   233    344       C
ATOM    958  CB  MET A 271    -9.339  53.026 -9.841  1.00 25.82           C
ANISOU  958  CB  MET A 271     3561   2991   3257   -202   195    269       C
ATOM    959  CG  MET A 271    -10.162  53.827 -8.799  1.00 28.30           C
ANISOU  959  CG  MET A 271     3918   3221   3613   -206   135    237       C
ATOM    960  SD  MET A 271    -9.551  53.567 -7.101  1.00 27.06           S
ANISOU  960  SD  MET A 271     3668   3114   3501   -255    76    143       S
ATOM    961  CE  MET A 271    -7.959  54.385 -7.235  1.00 25.30           C
ANISOU  961  CE  MET A 271     3373   2896   3346   -383   134    149       C
ATOM    962  C   MET A 271    -9.008  52.520 -12.265  1.00 21.88           C
ANISOU  962  C   MET A 271     3116   2567   2629   -195    320    355       C
ATOM    963  O   MET A 271    -8.151  53.173 -12.845  1.00 24.73           O
ANISOU  963  O   MET A 271     3469   2925   3001   -269    398    398       O
ATOM    964  N   SER A 272    -9.151  51.222 -12.502  1.00 23.19           N
ANISOU  964  N   SER A 272     3259   2803   2750   -135    321    308       N
ATOM    965  CA  SER A 272    -8.237  50.583 -13.459  1.00 27.82           C
ANISOU  965  CA  SER A 272     3806   3461   3301   -152    427    294       C
ATOM    966  CB  SER A 272    -8.269  49.052 -13.316  1.00 24.65           C
ANISOU  966  CB  SER A 272     3354  3106  2907   -79    428    215       C
ATOM    967  OG  SER A 272    -9.504  48.520 -13.763  1.00 30.73           O
ANISOU  967  OG  SER A 272     4212   3881  3583    -33    386    200       O
ATOM    968  C   SER A 272    -8.551  51.032 -14.911  1.00 35.47           C
ANISOU  968  C   SER A 272     4879   4455  4143   -187    486    361       C
ATOM    969  O   SER A 272    -7.719  50.898 -15.821  1.00 33.43           O
ANISOU  969  O   SER A 272     4606   4255  3840   -234    599    363       O
ATOM    970  N   GLN A 273    -9.749  51.577 -15.132  1.00 28.28           N
ANISOU  970  N   GLN A 273     4067   3508  3170   -166    412    422       N
ATOM    971  CA  GLN A 273    -10.192  51.971 -16.479  1.00 28.10           C
ANISOU  971  CA  GLN A 273     4144   3525  3007   -194    437    509       C
ATOM    972  CB  GLN A 273    -11.718  51.842 -16.621  1.00 33.47           C
ANISOU  972  CB  GLN A 273     4893   4207  3616   -131    325    537       C
ATOM    973  CG  GLN A 273    -12.262  50.432 -16.461  1.00 36.41           C
ANISOU  973  CG  GLN A 273     5242   4638  3955    -77    291    425       C
ATOM    974  CD  GLN A 273    -11.631  49.481 -17.473  1.00 55.46           C
ANISOU  974  CD  GLN A 273     7658   7150  6262    -113    394    358       C
ATOM    975  OE1 GLN A 273    -11.878  49.593 -18.677  1.00 50.47           O
ANISOU  975  OE1 GLN A 273     7104   6598  5475    -156    418    402       O
ATOM    976  NE2 GLN A 273    -10.781  48.569 -16.994  1.00 60.68           N
ANISOU  976  NE2 GLN A 273     8235   7810  7009    -96    460    255       N
ATOM    977  C   GLN A 273    -9.837  53.413 -16.776  1.00 33.75           C
ANISOU  977  C   GLN A 273     4903   4175  3747    -262    471    631       C
ATOM    978  O   GLN A 273    -9.836  53.831 -17.917  1.00 30.52           O
ANISOU  978  O   GLN A 273     4566   3804  3225    -308    516    726       O
ATOM    979  N   TYR A 274    -9.617  54.201 -15.728  1.00 27.34           N
ANISOU  979  N   TYR A 274     4054   3257  3078    -275    444    630       N
ATOM    980  CA  TYR A 274    -9.406  55.641 -15.883  1.00 36.32           C
ANISOU  980  CA  TYR A 274     5239   4292  4271    -340    473    739       C
ATOM    981  CB  TYR A 274    -10.276  56.378 -14.883  1.00 33.04           C
ANISOU  981  CB  TYR A 274     4841   3781  3934    -295    384    741       C
ATOM    982  CG  TYR A 274    -11.732  56.134 -15.112  1.00 31.18           C
ANISOU  982  CG  TYR A 274     4664   3515  3669    -197    289    778       C
ATOM    983  CD1 TYR A 274    -12.210  55.809 -16.388  1.00 46.18           C
ANISOU  983  CD1 TYR A 274     6625   5507  5416    -182    280    864       C
ATOM    984  CE1 TYR A 274    -13.554  55.615 -16.611  1.00 40.99           C
ANISOU  984  CE1 TYR A 274     6001   4868  4704    -102    180    904       C
ATOM    985  CZ  TYR A 274    -14.417  55.736 -15.531  1.00 51.08           C
ANISOU  985  CZ  TYR A 274     7254   6063  6096    -28    105    853       C
ATOM    986  OH  TYR A 274    -15.758  55.552 -15.712  1.00 71.32           O
ANISOU  986  OH  TYR A 274     9825   8648  8625     51     8    890       O
ATOM    987  CE2 TYR A 274    -13.964  56.055 -14.270  1.00 39.21           C
ANISOU  987  CE2 TYR A 274     5698   4466  4734    -43    127    762       C
ATOM    988  CD2 TYR A 274    -12.635  56.256 -14.070  1.00 40.83           C
ANISOU  943  CG  PHE A 269     4949   4428   4024    111    102    153       C
ATOM    944  CD1 PHE A 269    -13.336  46.303 -13.839  1.00 34.51           C
ANISOU  944  CD1 PHE A 269     4838   4373   3902    100    186     94       C
ATOM    945  CE1 PHE A 269    -13.544  46.071 -15.211  1.00 39.02           C
ANISOU  945  CE1 PHE A 269     5472   5012   4342     66    229     79       C
ATOM    946  CZ  PHE A 269    -14.470  46.823 -15.892  1.00 35.95           C
ANISOU  946  CZ  PHE A 269     5154   4659   3847     47    167    151       C
ATOM    947  CE2 PHE A 269    -15.208  47.801 -15.223  1.00 50.29           C
ANISOU  947  CE2 PHE A 269     6972   6421   5713     75     75    230       C
ATOM    948  CD2 PHE A 269    -15.002  48.011 -13.857  1.00 42.44           C
ANISOU  948  CD2 PHE A 269     5921   5350   4853    105     53    218       C
ATOM    949  C   PHE A 269    -12.525  49.605 -12.210  1.00 20.57           C
ANISOU  949  C   PHE A 269     3044   2475   2297     41    133    252       C
ATOM    950  O   PHE A 269    -11.804  49.793 -13.214  1.00 19.82           O
ANISOU  950  O   PHE A 269     2963   2414   2155     -1    209    281       O
ATOM    951  N   ALA A 270    -13.319  50.562 -11.779  1.00 21.86           N
ANISOU  951  N   ALA A 270     3244   2577   2486     49     77    291       N
ATOM    952  CA  ALA A 270    -13.330  51.861 -12.475  1.00 22.59           C
ANISOU  952  CA  ALA A 270     3394   2622   2568     15     97    383       C
ATOM    953  CB  ALA A 270    -14.408  52.798 -11.892  1.00 25.08           C
ANISOU  953  CB  ALA A 270     3741   2846   2944     50     35    415       C
ATOM    954  C   ALA A 270    -11.963  52.552 -12.447  1.00 24.08           C
ANISOU  954  C   ALA A 270     3552   2786   2810    -62   172    400       C
ATOM    955  O   ALA A 270    -11.532  53.125 -13.440  1.00 25.67           O
ANISOU  955  O   ALA A 270     3792   2991   2970   -108   230    474       O
ATOM    956  N   MET A 271    -11.269  52.526 -11.308  1.00 21.47           N
ANISOU  956  N   MET A 271     3150   2442   2567    -87   168    336       N
ATOM    957  CA  MET A 271    -9.940  53.165 -11.249  1.00 24.68           C
ANISOU  957  CA  MET A 271     3507   2837   3032   -174   233    344       C
ATOM    958  CB  MET A 271    -9.339  53.026 -9.841  1.00 25.82           C
ANISOU  958  CB  MET A 271     3561   2991   3257   -202   195    269       C
ATOM    959  CG  MET A 271    -10.162  53.827 -8.799  1.00 28.30           C
ANISOU  959  CG  MET A 271     3918   3221   3613   -206   135    237       C
ATOM    960  SD  MET A 271    -9.551  53.567 -7.101  1.00 27.06           S
ANISOU  960  SD  MET A 271     3668   3114   3501   -255    76    143       S
ATOM    961  CE  MET A 271    -7.959  54.385 -7.235  1.00 25.30           C
ANISOU  961  CE  MET A 271     3373   2896   3346   -383    134    149       C
ATOM    962  C   MET A 271    -9.008  52.520 -12.265  1.00 21.88           C
ANISOU  962  C   MET A 271     3116   2567   2629   -195    320    355       C
ATOM    963  O   MET A 271    -8.151  53.173 -12.845  1.00 24.73           O
ANISOU  963  O   MET A 271     3469   2925   3001   -269    398    398       O
ATOM    964  N   SER A 272    -9.151  51.222 -12.502  1.00 23.19           N
ANISOU  964  N   SER A 272     3259   2803   2750   -135    321    308       N
ATOM    965  CA  SER A 272    -8.237  50.583 -13.459  1.00 27.82           C
ANISOU  965  CA  SER A 272     3806   3461   3301   -152    427    294       C
ATOM    966  CB  SER A 272    -8.269  49.052 -13.316  1.00 24.65           C
ANISOU  966  CB  SER A 272     3354  3106  2907   -79    428    215       C
ATOM    967  OG  SER A 272    -9.504  48.520 -13.763  1.00 30.73           O
ANISOU  967  OG  SER A 272     4212   3881  3583    -33    386    200       O
ATOM    968  C   SER A 272    -8.551  51.032 -14.911  1.00 35.47           C
ANISOU  968  C   SER A 272     4879   4455  4143   -187    486    361       C
ATOM    969  O   SER A 272    -7.719  50.898 -15.821  1.00 33.43           O
ANISOU  969  O   SER A 272     4606   4255  3840   -234    599    363       O
ATOM    970  N   GLN A 273    -9.749  51.577 -15.132  1.00 28.28           N
ANISOU  970  N   GLN A 273     4067   3508  3170   -166    412    422       N
ATOM    971  CA  GLN A 273    -10.192  51.971 -16.479  1.00 28.10           C
ANISOU  971  CA  GLN A 273     4144   3525  3007   -194    437    509       C
ATOM    972  CB  GLN A 273    -11.718  51.842 -16.621  1.00 33.47           C
ANISOU  972  CB  GLN A 273     4893   4207  3616   -131    325    537       C
ATOM    973  CG  GLN A 273    -12.262  50.432 -16.461  1.00 36.41           C
ANISOU  973  CG  GLN A 273     5242   4638  3955    -77    291    425       C
ATOM    974  CD  GLN A 273    -11.631  49.481 -17.473  1.00 55.46           C
ANISOU  974  CD  GLN A 273     7658   7150  6262    -113    394    358       C
ATOM    975  OE1 GLN A 273    -11.878  49.593 -18.677  1.00 50.47           O
ANISOU  975  OE1 GLN A 273     7104   6598  5475    -156    418    402       O
ATOM    976  NE2 GLN A 273    -10.781  48.569 -16.994  1.00 60.68           N
ANISOU  976  NE2 GLN A 273     8235   7810  7009    -96    460    255       N
ATOM    977  C   GLN A 273    -9.837  53.413 -16.776  1.00 33.75           C
ANISOU  977  C   GLN A 273     4903   4175  3747    -262    471    631       C
ATOM    978  O   GLN A 273    -9.836  53.831 -17.917  1.00 30.52           O
ANISOU  978  O   GLN A 273     4566   3804  3225    -308    516    726       O
ATOM    979  N   TYR A 274    -9.617  54.201 -15.728  1.00 27.34           N
ANISOU  979  N   TYR A 274     4054   3257  3078    -275    444    630       N
ATOM    980  CA  TYR A 274    -9.406  55.641 -15.883  1.00 36.32           C
ANISOU  980  CA  TYR A 274     5239   4292  4271    -340    473    739       C
ATOM    981  CB  TYR A 274    -10.276  56.378 -14.883  1.00 33.04           C
ANISOU  981  CB  TYR A 274     4841   3781  3934    -295    384    741       C
ATOM    982  CG  TYR A 274    -11.732  56.134 -15.112  1.00 31.18           C
ANISOU  982  CG  TYR A 274     4664   3515  3669    -197    289    778       C
ATOM    983  CD1 TYR A 274    -12.210  55.809 -16.388  1.00 46.18           C
ANISOU  983  CD1 TYR A 274     6625   5507  5416    -182    280    864       C
ATOM    984  CE1 TYR A 274    -13.554  55.615 -16.611  1.00 40.99           C
ANISOU  984  CE1 TYR A 274     6001   4868  4704    -102    180    904       C
ATOM    985  CZ  TYR A 274    -14.417  55.736 -15.531  1.00 51.08           C
ANISOU  985  CZ  TYR A 274     7254   6063  6096    -28    105    853       C
ATOM    986  OH  TYR A 274    -15.758  55.552 -15.712  1.00 71.32           O
ANISOU  986  OH  TYR A 274     9825  8648  8625     51     8    890       O
ATOM    987  CE2 TYR A 274    -13.964  56.055 -14.270  1.00 39.21           C
ANISOU  987  CE2 TYR A 274     5698   4466  4734    -43    127    762       C
ATOM    988  CD2 TYR A 274    -12.635  56.256 -14.070  1.00 40.83           C
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ANISOU  988  CD2 TYR A 274     5873   4662   4979   -130    210    727       C
ATOM    989  C   TYR A 274      -7.954  56.008 -15.653  1.00 35.57           C
ANISOU  989  C   TYR A 274     5067   4188   4261   -441    571    713       C
ATOM    990  O   TYR A 274      -7.429  55.832 -14.553  1.00 37.85           O
ANISOU  990  O   TYR A 274     5263   4464   4656   -451    551    617       O
ATOM    991  N   SER A 275      -7.295  56.493 -16.697  1.00 33.77           N
ANISOU  991  N   SER A 275     4871   3983   3976   -523    674    802       N
ATOM    992  CA  SER A 275      -5.847  56.662 -16.642  1.00 40.71           C
ANISOU  992  CA  SER A 275     5656   4886   4926   -625    785    770       C
ATOM    993  CB  SER A 275      -5.257  56.889 -18.035  1.00 46.55           C
ANISOU  993  CB  SER A 275     6440   5693   5554   -707    917    865       C
ATOM    994  OG  SER A 275      -5.041  58.260 -18.291  1.00 47.46           O
ANISOU  994  OG  SER A 275     6616   5697   5718   -802    962    992       O
ATOM    995  C   SER A 275      -5.406  57.759 -15.635  1.00 49.10           C
ANISOU  995  C   SER A 275     6682   5819   6157   -699    772    762       C
ATOM    996  O   SER A 275      -4.282  57.737 -15.114  1.00 44.36           O
ANISOU  996  O   SER A 275     5962   5245   5646   -773    818    693       O
ATOM    997  N   GLN A 276      -6.287  58.707 -15.330  1.00 42.88           N
ANISOU  997  N   GLN A 276     5985   4890   5418   -682    710    822       N
ATOM    998  CA  GLN A 276      -5.909  59.695 -14.327  1.00 51.79           C
ANISOU  998  CA  GLN A 276     7085   5888   6706   -759    706    780       C
ATOM    999  CB  GLN A 276      -6.823  60.933 -14.358  1.00 49.84           C
ANISOU  999  CB  GLN A 276     6960   5452   6525   -748    684    877       C
ATOM   1000  CG  GLN A 276      -8.258  60.701 -13.884  1.00 48.87           C
ANISOU 1000  CG  GLN A 276     6887   5288   6394   -610    571    857       C
ATOM   1001  CD  GLN A 276      -9.008  62.021 -13.631  1.00 68.61           C
ANISOU 1001  CD  GLN A 276     9474   7573   9023   -599    563    923       C
ATOM   1002  OE1 GLN A 276     -10.096  62.244 -14.167  1.00 73.21           O
ANISOU 1002  OE1 GLN A 276    10132   8103   9580   -502    518   1036       O
ATOM   1003  NE2 GLN A 276      -8.419  62.898 -12.814  1.00 65.72           N
ANISOU 1003  NE2 GLN A 276     9090   7078   8804   -700    608    849       N
ATOM   1004  C   GLN A 276      -5.809  59.086 -12.907  1.00 48.36           C
ANISOU 1004  C   GLN A 276     6549   5491   6335   -733    624    621       C
ATOM   1005  O   GLN A 276      -5.309  59.743 -11.983  1.00 46.50           O
ANISOU 1005  O   GLN A 276     6268   5189   6212   -820    619    552       O
ATOM   1006  N   ALA A 277      -6.286  57.844 -12.729  1.00 36.82           N
ANISOU 1006  N   ALA A 277     5056   4137   4796   -625    559    564       N
ATOM   1007  CA  ALA A 277      -6.128  57.149 -11.442  1.00 38.50           C
ANISOU 1007  CA  ALA A 277     5171   4405   5052   -602    482    440       C
ATOM   1008  CB  ALA A 277      -7.175  56.061 -11.272  1.00 34.08           C
ANISOU 1008  CB  ALA A 277     4635   3899   4416   -470    402    410       C
ATOM   1009  C   ALA A 277      -4.707  56.580 -11.194  1.00 52.09           C
ANISOU 1009  C   ALA A 277     6739   6240   6813   -664    519    386       C
ATOM   1010  O   ALA A 277      -4.350  56.286 -10.050  1.00 46.35           O
ANISOU 1010  O   ALA A 277     5918   5555   6136   -679    451    304       O
ATOM   1011  N   GLY A 278      -3.916  56.410 -12.259  1.00 47.00           N
ANISOU 1011  N   GLY A 278     6061   5656   6141   -700    625    435       N
ATOM   1012  CA  GLY A 278      -2.535  55.944 -12.142  1.00 50.39           C
ANISOU 1012  CA  GLY A 278     6326   6190   6632   -755    679    394       C
ATOM   1013  C   GLY A 278      -2.407  54.518 -11.617  1.00 52.27           C
ANISOU 1013  C   GLY A 278     6457   6533   6871   -653    622    328       C
ATOM   1014  O   GLY A 278      -1.446  54.156 -10.924  1.00 50.66           O
ANISOU 1014  O   GLY A 278     6095   6402   6751   -679    602    285       O
ATOM   1015  N   PHE A 279      -3.372  53.685 -11.987  1.00 39.00           N
ANISOU 1015  N   PHE A 279     4856   4860   5101   -537    597    328       N
ATOM   1016  CA  PHE A 279      -3.610  52.432 -11.303  1.00 35.20           C
ANISOU 1016  CA  PHE A 279     4313   4432   4627   -433    522    273       C
ATOM   1017  CB  PHE A 279      -5.042  52.516 -10.832  1.00 40.20           C
ANISOU 1017  CB  PHE A 279     5070   5000   5203   -374    422    270       C
ATOM   1018  CG  PHE A 279      -5.363  51.673 -9.664  1.00 29.70           C
ANISOU 1018  CG  PHE A 279     3689   3699   3895   -308    318    222       C
ATOM   1019  CD1 PHE A 279      -4.670  51.815 -8.468  1.00 34.05           C
ANISOU 1019  CD1 PHE A 279     4134   4285   4517   -358    252    193       C
ATOM   1020  CE1 PHE A 279      -5.017  51.071 -7.353  1.00 30.63           C
ANISOU 1020  CE1 PHE A 279     3666   3888   4083   -305    150    168       C
ATOM   1021  CZ  PHE A 279      -6.079  50.179 -7.423  1.00 29.15           C
ANISOU 1021  CZ  PHE A 279     3549   3684   3841   -202    122    166       C
ATOM   1022  CE2 PHE A 279      -6.803  50.043 -8.627  1.00 28.00           C
ANISOU 1022  CE2 PHE A 279     3504   3498   3635   -155    186    180       C
ATOM   1023  CD2 PHE A 279      -6.437  50.802 -9.732  1.00 28.03           C
ANISOU 1023  CD2 PHE A 279     3545   3483   3623   -209    278    210       C
ATOM   1024  C   PHE A 279      -3.492  51.317 -12.329  1.00 34.75           C
ANISOU 1024  C   PHE A 279     4246   4436   4523   -361    610    263       C
ATOM   1025  O   PHE A 279      -4.336  51.199 -13.208  1.00 45.87           O
ANISOU 1025  O   PHE A 279     5777   5828   5822   -328    636    281       O
ATOM   1026  N   SER A 280      -2.463  50.478 -12.222  1.00 31.76           N
ANISOU 1026  N   SER A 280     3715   4126   4227   -336    657    230       N
ATOM   1027  CA  SER A 280      -2.288  49.395 -13.195  1.00 26.67           C
ANISOU 1027  CA  SER A 280     3056   3523   3555   -269    766    195       C
ATOM   1028  CB  SER A 280      -0.843  48.922 -13.202  1.00 36.47           C
ANISOU 1028  CB  SER A 280     4102   4828   4926   -271    857    173       C
ATOM   1029  OG  SER A 280      -0.555  48.249 -12.000  1.00 32.54           O
ANISOU 1029  OG  SER A 280     3475   4344   4544   -205    751    166       O
ATOM   1030  C   SER A 280      -3.174  48.196 -12.871  1.00 29.69           C
ANISOU 1030  C   SER A 280     3476   3887   3919   -151    699    154       C
ATOM   1031  O   SER A 280      -3.796  48.128 -11.830  1.00 28.25           O
ANISOU 1031  O   SER A 280     3308   3674   3751   -118    570    161       O
ATOM   1032  N   ARG A 281      -3.222  47.210 -13.768  1.00 31.32           N
ANISOU 1032  N   ARG A 281     3507   5175   3217    104   1232   -276       N
ATOM   1033  C   ARG A 281      -3.418  45.225 -12.314  1.00 30.70           C
ANISOU 1033  C   ARG A 281     3522   4747   3395    146    947   -663       C
ATOM   1034  O   ARG A 281      -4.145  44.638 -11.502  1.00 26.26           O
ANISOU 1034  O   ARG A 281     3035   4053   2889    137    750   -706       O
ATOM   1035  CA AARG A 281      -4.011  46.014 -13.484  0.51 31.58           C
ANISOU 1035  CA AARG A 281     3682   5189   3127     39   1013   -490       C
ATOM   1036  CB AARG A 281      -4.120  45.147 -14.737  0.51 36.30           C
ANISOU 1036  CB AARG A 281     4441   6023   3330    -84   1150   -739       C
ATOM   1037  CG AARG A 281      -4.698  45.912 -15.913  0.51 36.81           C
ANISOU 1037  CG AARG A 281     4510   6566   2909   -165   1180   -504       C
ATOM   1038  CD AARG A 281      -5.305  45.005 -16.984  0.51 46.03           C
ANISOU 1038  CD AARG A 281     5822   8136   3531   -406   1185   -799       C
ATOM   1039  NE AARG A 281      -4.404  43.964 -17.487  0.51 40.95           N
ANISOU 1039  NE AARG A 281     5323   7329   2908   -485   1495  -1250       N
ATOM   1040  CZ AARG A 281      -3.483  44.147 -18.426  0.51 43.75           C
ANISOU 1040  CZ AARG A 281     5711   7738   3173   -446   1780  -1260       C
ATOM   1041  NH1AARG A 281      -3.299  45.347 -18.964  0.51 46.70           N
ANISOU 1041  NH1AARG A 281     5996   8353   3396   -335   1834   -859       N
ATOM   1042  NH2AARG A 281      -2.731  43.129 -18.821  0.51 49.21           N
ANISOU 1042  NH2AARG A 281     6532   8162   4002   -486   2042  -1618       N
ATOM   1043  CA BARG A 281      -4.019  46.022 -13.485  0.49 31.54           C
ANISOU 1043  CA BARG A 281     3677   5186   3121     39   1012   -487       C
ATOM   1044  CB BARG A 281      -4.154  45.161 -14.745  0.49 35.97           C
ANISOU 1044  CB BARG A 281     4399   5989   3278    -87   1145   -733       C
ATOM   1045  CG BARG A 281      -4.775  45.900 -15.939  0.49 36.87           C
ANISOU 1045  CG BARG A 281     4522   6596   2891   -174   1168   -502       C
ATOM   1046  CD BARG A 281      -6.094  46.605 -15.575  0.49 33.65           C
ANISOU 1046  CD BARG A 281     4034   6380   2370   -179    894   -150       C
ATOM   1047  NE BARG A 281      -6.653  47.387 -16.688  0.49 42.90           N
ANISOU 1047  NE BARG A 281     5143   8091   3067   -170    928    215       N
ATOM   1048  CZ BARG A 281      -7.751  47.057 -17.369  0.49 49.92           C
ANISOU 1048  CZ BARG A 281     6014   9414   3537   -311    696    223       C
ATOM   1049  NH1BARG A 281      -8.432  45.959 -17.045  0.49 50.52           N
ANISOU 1049  NH1BARG A 281     6146   9496   3555   -530    494   -161       N
ATOM   1050  NH2BARG A 281      -8.179  47.834 -18.366  0.49 45.31           N
ANISOU 1050  NH2BARG A 281     5329   9166   2719   -225    670    602       N
ATOM   1051  N   GLU A 282      -2.095  45.214 -12.221  1.00 28.82           N
ANISOU 1051  N   GLU A 282     3128   4411   3411    269   1126   -724       N
ATOM   1052  CA  GLU A 282      -1.444  44.528 -11.103  1.00 32.36           C
ANISOU 1052  CA  GLU A 282     3444   4666   4187    436   1054   -782       C
ATOM   1053  CB  GLU A 282       0.068  44.386 -11.297  1.00 31.88           C
ANISOU 1053  CB  GLU A 282     3150   4595   4367    589   1293   -841       C
ATOM   1054  CG  GLU A 282       0.415  43.269 -12.244  1.00 43.11           C
ANISOU 1054  CG  GLU A 282     4725   5902   5752    659   1605  -1039       C
ATOM   1055  CD  GLU A 282       1.914  43.029 -12.359  1.00 63.96           C
ANISOU 1055  CD  GLU A 282     7099   8500   8705    864   1878  -1060       C
ATOM   1056  OE1 GLU A 282       2.303  42.117 -13.130  1.00 60.73           O
ANISOU 1056  OE1 GLU A 282     6811   7934   8329    935   2231  -1231       O
ATOM   1057  OE2 GLU A 282       2.690  43.748 -11.679  1.00 73.40           O
ANISOU 1057  OE2 GLU A 282     7944   9831  10115    927   1770   -933       O
ATOM   1058  C   GLU A 282      -1.743  45.236 -9.813  1.00 30.21           C
ANISOU 1058  C   GLU A 282     3042   4388   4050    415    793   -630       C
ATOM   1059  O   GLU A 282      -2.002  44.580 -8.807  1.00 31.89           O
ANISOU 1059  O   GLU A 282     3267   4497   4353    504    617   -620       O
ATOM   1060  N   ASP A 283      -1.746  46.574 -9.838  1.00 27.88           N
ANISOU 1060  N   ASP A 283     2644   4180   3770    285    829   -513       N
ATOM   1061  CA  ASP A 283      -2.155  47.358 -8.667  1.00 30.45           C
ANISOU 1061  CA  ASP A 283     2889   4471   4209    184    667   -429       C
ATOM   1062  CB  ASP A 283      -2.114  48.863 -8.932  1.00 33.61           C
ANISOU 1062  CB  ASP A 283     3211   4871   4688     27    892   -322       C
ATOM   1063  CG  ASP A 283      -0.710  49.382 -9.198  1.00 49.77           C
ANISOU 1063  CG  ASP A 283     5000   6983   6929   -11   1147   -435       C
ATOM   1064  OD1 ASP A 283       0.251  48.701 -8.774  1.00 52.74           O
ANISOU 1064  OD1 ASP A 283     5167   7462   7409     75   1057   -587       O
ATOM   1065  OD2 ASP A 283      -0.586  50.463 -9.847  1.00 53.92           O
ANISOU 1065  OD2 ASP A 283     5511   7456   7518   -105   1472   -337       O
ATOM   1066  C   ASP A 283      -3.578  47.030 -8.259  1.00 30.85           C
ANISOU 1066  C   ASP A 283     3162   4433   4124    152   458   -349       C
ATOM   1067  O   ASP A 283      -3.904  46.950 -7.073  1.00 25.86           O
ANISOU 1067  O   ASP A 283     2520   3732   3573    138   278   -343       O
ATOM   1068  N   ARG A 284      -4.446  46.890 -9.254  1.00 23.24           N
ANISOU 1068  N   ARG A 284     2374   3530   2926    129   489   -286       N
ATOM   1069  CA  ARG A 284      -5.849  46.617 -8.950  1.00 22.39           C
ANISOU 1069  CA  ARG A 284     2419   3392   2696     59    301   -217       C
ATOM   1070  CB  ARG A 284      -6.679  46.520 -10.237  1.00 22.88           C
ANISOU 1070  CB  ARG A 284     2575   3700   2419    -12    325   -159       C
ATOM   1071  CG  ARG A 284      -8.154  46.846 -9.962  1.00 29.86           C
ANISOU 1071  CG  ARG A 284     3484   4646   3217    -83   161    -37       C
ATOM   1072  CD  ARG A 284      -9.144  45.712 -10.189  1.00 37.19           C
ANISOU 1072  CD  ARG A 284     4521   5680   3928   -202    5   -153       C
ATOM   1073  NE  ARG A 284      -8.592  44.431 -10.656  1.00 37.63           N
ANISOU 1073  NE  ARG A 284     4699   5698   3901   -251    98   -525       N
ATOM   1074  CZ  ARG A 284      -8.880  43.253 -10.082  1.00 37.19           C
ANISOU 1074  CZ  ARG A 284     4778   5392   3962   -294    89   -776       C
ATOM   1075  NH1 ARG A 284      -8.368  42.117 -10.558  1.00 30.72           N
ANISOU 1075  NH1 ARG A 284     4082   4463   3129   -331    300  -1106       N
ATOM   1076  NH2 ARG A 284      -9.721  43.214 -9.045  1.00 33.12           N
ANISOU 1076  NH2 ARG A 284     4287   4697   3599   -301   -61   -690       N
ATOM   1077  C   ARG A 284      -5.992  45.310 -8.182  1.00 23.57           C
ANISOU 1077  C   ARG A 284     2669   3376   2910    123   163   -384       C
ATOM   1078  O   ARG A 284      -6.709  45.226 -7.178  1.00 24.32           O
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ANISOU 1078 O  ARG A 284    2818  3344  3076   105    11   -332       O
ATOM  1079 N  LEU A 285     -5.326 44.270 -8.669  1.00 23.14           N
ANISOU 1079 N  LEU A 285    2658  3282  2854   212   287   -567       N
ATOM  1080 CA LEU A 285     -5.409 42.961 -8.013  1.00 22.03           C
ANISOU 1080 CA LEU A 285    2628  2907  2834   325   287   -676       C
ATOM  1081 CB LEU A 285     -4.683 41.899 -8.840  1.00 25.04           C
ANISOU 1081 CB LEU A 285    3074  3193  3248   409   576   -884       C
ATOM  1082 CG LEU A 285     -4.777 40.518 -8.185  1.00 32.57           C
ANISOU 1082 CG LEU A 285    4162  3807  4406   565   710   -950       C
ATOM  1083 CD1 LEU A 285    -6.212 40.009 -8.165  1.00 39.55           C
ANISOU 1083 CD1 LEU A 285    5279  4575  5172   344   674  -1095       C
ATOM  1084 CD2 LEU A 285    -3.883 39.577 -8.965  1.00 40.85           C
ANISOU 1084 CD2 LEU A 285    5250  4691  5580   682  1111  -1131       C
ATOM  1085 C  LEU A 285     -4.821 42.996 -6.590  1.00 26.28           C
ANISOU 1085 C  LEU A 285    3020  3376  3591   506   162   -532       C
ATOM  1086 O  LEU A 285     -5.395 42.442 -5.638  1.00 27.21           O
ANISOU 1086 O  LEU A 285    3236  3339  3763   567    64   -473       O
ATOM  1087 N  GLU A 286     -3.673 43.641 -6.453  1.00 24.82           N
ANISOU 1087 N  GLU A 286    2576  3357  3497   572   175   -481       N
ATOM  1088 CA GLU A 286     -2.997 43.764 -5.155  1.00 28.42           C
ANISOU 1088 CA GLU A 286    2802  3931  4064   692    22   -372       C
ATOM  1089 CB GLU A 286     -1.705 44.555 -5.327  1.00 36.43           C
ANISOU 1089 CB GLU A 286    3477  5203  5161   667    82   -408       C
ATOM  1090 CG GLU A 286     -0.926 44.728 -4.045  1.00 51.92           C
ANISOU 1090 CG GLU A 286    5108  7458  7160   725  -105   -345       C
ATOM  1091 CD GLU A 286      0.250 45.681 -4.199  1.00 77.63           C
ANISOU 1091 CD GLU A 286    7986 11011 10499   580   -34   -464       C
ATOM  1092 OE1 GLU A 286      0.885 45.690 -5.280  1.00 76.40           O
ANISOU 1092 OE1 GLU A 286    7770 10810 10447   625   197   -521       O
ATOM  1093 OE2 GLU A 286      0.517 46.438 -3.236  1.00 97.02           O
ANISOU 1093 OE2 GLU A 286   10206 13749 12908   377  -173   -541       O
ATOM  1094 C  GLU A 286     -3.905 44.473 -4.149  1.00 26.26           C
ANISOU 1094 C  GLU A 286    3095  3476  3720   517  -175   -313       C
ATOM  1095 O  GLU A 286     -4.055 44.041 -2.995  1.00 24.26           O
ANISOU 1095 O  GLU A 286    2340  3419  3457   614  -320   -222       O
ATOM  1096 N  GLN A 287     -4.550 45.553 -4.587  1.00 21.56           N
ANISOU 1096 N  GLN A 287    2060  3053  3076   283  -134   -329       N
ATOM  1097 CA GLN A 287     -5.466 46.292 -3.715  1.00 23.64           C
ANISOU 1097 CA GLN A 287    2399  3253  3330   111  -221   -276       C
ATOM  1098 CB GLN A 287     -5.783 47.691 -4.278  1.00 23.23           C
ANISOU 1098 CB GLN A 287    2323  3179  3324   -89   -40   -234       C
ATOM  1099 CG GLN A 287     -4.589 48.636 -4.307  1.00 24.62           C
ANISOU 1099 CG GLN A 287    2250  3489  3616  -205   129   -338       C
ATOM  1100 CD GLN A 287     -3.913 48.810 -2.942  1.00 31.58           C
ANISOU 1100 CD GLN A 287    2933  4546  4519  -323    15   -494       C
ATOM  1101 OE1 GLN A 287     -4.548 49.235 -1.975  1.00 26.76           O
ANISOU 1101 OE1 GLN A 287    2397  3873  3896  -487   -15   -523       O
ATOM  1102 NE2 GLN A 287     -2.616 48.440 -2.837  1.00 27.30           N
ANISOU 1102 NE2 GLN A 287    2107  4285  3980  -243   -51   -592       N
ATOM  1103 C  GLN A 287     -6.777 45.542 -3.438  1.00 23.58           C
ANISOU 1103 C  GLN A 287    2648  3042  3268   138  -312   -216       C
ATOM  1104 O  GLN A 287     -7.348 45.634 -2.345  1.00 24.31           O
ANISOU 1104 O  GLN A 287    2807  3062  3366    88  -405   -173       O
ATOM  1105 N  ALA A 288     -7.295 44.833 -4.431  1.00 21.19           N
ANISOU 1105 N  ALA A 288    2484  2668  2899   169  -258   -252       N
ATOM  1106 CA ALA A 288     -8.462 43.974 -4.186  1.00 19.98           C
ANISOU 1106 CA ALA A 288    2537  2331  2722   153  -305   -268       C
ATOM  1107 CB ALA A 288     -8.871 43.253 -5.462  1.00 21.80           C
ANISOU 1107 CB ALA A 288    2865  2584  2833    87  -205   -419       C
ATOM  1108 C  ALA A 288     -8.122 42.939 -3.085  1.00 22.48           C
ANISOU 1108 C  ALA A 288    2916  2492  3134   350  -324   -244       C
ATOM  1109 O  ALA A 288     -8.914 42.665 -2.175  1.00 24.69           O
ANISOU 1109 O  ALA A 288    3326  2617  3440   342  -378   -181       O
ATOM  1110 N  LYS A 289     -6.957 42.319 -3.193  1.00 19.61           N
ANISOU 1110 N  LYS A 289    2451  2168  2833   564  -240   -248       N
ATOM  1111 CA LYS A 289     -6.564 41.332 -2.162  1.00 21.60           C
ANISOU 1111 CA LYS A 289    2714  2318  3175   846  -220   -100       C
ATOM  1112 CB LYS A 289     -5.241 40.668 -2.536  1.00 27.58           C
ANISOU 1112 CB LYS A 289    3301  3129  4048  1130   -61   -53       C
ATOM  1113 CG LYS A 289     -5.376 39.556 -3.551  1.00 32.83           C
ANISOU 1113 CG LYS A 289    4165  3468  4842  1181   278  -213       C
ATOM  1114 CD LYS A 289     -3.985 39.074 -4.032  1.00 37.34           C
ANISOU 1114 CD LYS A 289    4540  4076  5573  1459   502   -166       C
ATOM  1115 CE LYS A 289     -4.095 37.966 -5.054  1.00 45.86           C
ANISOU 1115 CE LYS A 289    5850  4779  6797  1460   945   -395       C
ATOM  1116 NZ LYS A 289     -2.752 37.600 -5.643  1.00 45.51           N
ANISOU 1116 NZ LYS A 289    5617  4738  6939  1711  1229   -367       N
ATOM  1117 C  LYS A 289     -6.452 41.974 -0.769  1.00 29.57           C
ANISOU 1117 C  LYS A 289    3603  3540  4092   847   -441    57       C
ATOM  1118 O  LYS A 289     -6.889 41.426  0.255  1.00 27.87           O
ANISOU 1118 O  LYS A 289    3505  3228  3857   966   -471   206       O
ATOM  1119 N  LEU A 290     -5.810 43.131 -0.732  1.00 26.71           N
ANISOU 1119 N  LEU A 290    3003  3485  3662   691   -549    -1       N
ATOM  1120 CA LEU A 290     -5.609 43.829  0.521  1.00 23.66           C
ANISOU 1120 CA LEU A 290    2475  3373  3142   586   -719    34       C
ATOM  1121 CB LEU A 290     -4.632 44.993  0.316  1.00 28.24           C
ANISOU 1121 CB LEU A 290    2744  4280  3708   378  -731   -123       C
ATOM  1122 CG LEU A 290     -4.233 45.884  1.491  1.00 34.27           C
ANISOU 1122 CG LEU A 290    3294  5417  4310   132  -852  -232       C
ATOM  1123 CD1 LEU A 290     -3.648 45.054  2.647  1.00 39.60           C
ANISOU 1123 CD1 LEU A 290    3788  6488  4769   380  -1072   -40       C
ATOM  1124 CD2 LEU A 290     -3.151 46.875  1.008  1.00 36.66           C
ANISOU 1124 CD2 LEU A 290    3267  5982  4680   -88  -762  -448       C
ATOM  1125 C  LEU A 290     -6.956 44.341  1.066  1.00 26.87           C
ANISOU 1125 C  LEU A 290    3128  3568  3515   352  -726     5       C
ATOM  1126 O  LEU A 290     -7.141 44.412  2.282  1.00 24.10           O
ANISOU 1126 O  LEU A 290    2798  3327  3031   317  -821    59       O
ATOM  1127 N  PHE A 291     -7.888 44.698  0.173  1.00 19.53           N
ANISOU 1127 N  PHE A 291    2355  2384  2682   202  -617   -58       N
ATOM  1128 CA PHE A 291     -9.209 45.154  0.617  1.00 22.58           C
ANISOU 1128 CA PHE A 291    2927  2560  3093    23  -587   -39       C
ATOM  1129 CB PHE A 291    -10.063 45.543 -0.594  1.00 25.93           C
ANISOU 1129 CB PHE A 291    3402  2853  3598   -82  -488   -36       C
ATOM  1130 CG PHE A 291    -11.531 45.717 -0.273  1.00 22.05           C
ANISOU 1130 CG PHE A 291    3057  2150  3172  -194  -452    38       C
ATOM  1131 CD1 PHE A 291    -11.981 46.887  0.308  1.00 19.19           C
ANISOU 1131 CD1 PHE A 291    2672  1741  2877  -347  -328    83       C
ATOM  1132 CE1 PHE A 291    -13.339 47.065  0.575  1.00 21.29           C
ANISOU 1132 CE1 PHE A 291    2963  2017  3108  -318  -143   124       C
ATOM  1133 CZ PHE A 291    -14.250 46.054  0.269  1.00 17.04           C
ANISOU 1133 CZ PHE A 291    2460  1471  2542  -256  -182   131       C
ATOM  1134 CE2 PHE A 291    -13.818 44.896 -0.332  1.00 27.49           C
ANISOU 1134 CE2 PHE A 291    3847  2742  3854  -216  -331    77       C
ATOM  1135 CD2 PHE A 291    -12.454 44.723 -0.601  1.00 29.77           C
ANISOU 1135 CD2 PHE A 291    4165  2988  4160  -161  -468    30       C
ATOM  1136 C  PHE A 291     -9.873 44.041  1.394  1.00 24.77           C
ANISOU 1136 C  PHE A 291    3410  2648  3354  166  -615    56       C
ATOM  1137 O  PHE A 291    -10.386 44.235  2.485  1.00 21.94           O
ANISOU 1137 O  PHE A 291    3148  2246  2941   93  -634   100       O
ATOM  1138 N  CYS A 292     -9.809 42.838  0.831  1.00 21.83           N
ANISOU 1138 N  CYS A 292    3119  2135  3042  364  -551    72       N
ATOM  1139 C  CYS A 292     -9.750 41.340  2.826  1.00 29.97           C
ANISOU 1139 C  CYS A 292    4326  3056  4003  750  -532   387       C
ATOM  1140 O  CYS A 292    -10.453 41.060  3.812  1.00 28.68           O
ANISOU 1140 O  CYS A 292    4328  2960  3802  760  -492   497       O
ATOM  1141 CA ACYS A 292    -10.384 41.666  1.455  0.58 25.04           C
ANISOU 1141 CA ACYS A 292    3737  2274  3503  520  -462   165       C
ATOM  1142 CB ACYS A 292    -10.210 40.480  0.515  0.58 29.34           C
ANISOU 1142 CB ACYS A 292    4356  2611  4179  663  -265    87       C
ATOM  1143 SG ACYS A 292    -10.855 38.997  1.190  0.58 32.61           S
ANISOU 1143 SG ACYS A 292    4866  2767  4755  723   -15   161       S
ATOM  1144 CA BCYS A 292    -10.370 41.649  1.473  0.42 25.91           C
ANISOU 1144 CA BCYS A 292    3848  2385  3613  526  -462   168       C
ATOM  1145 CB BCYS A 292    -10.196 40.424  0.579  0.42 28.23           C
ANISOU 1145 CB BCYS A 292    4222  2462  4042  679  -260    99       C
ATOM  1146 SG BCYS A 292    -11.302 40.449 -0.818  0.42 36.65           S
ANISOU 1146 SG BCYS A 292    5369  3413  5143  362  -178   -181       S
ATOM  1147 N  ARG A 293     -8.418 41.348  2.892  1.00 23.70           N
ANISOU 1147 N  ARG A 293    3276  2607  3122   935  -622   474       N
ATOM  1148 CA ARG A 293     -8.050 42.153  5.231  1.00 23.90           C
ANISOU 1148 C  ARG A 293    3148  3253  2680   863  -912   648       C
ATOM  1149 O  ARG A 293     -8.215 41.823  6.410  1.00 26.07           O
ANISOU 1149 O  ARG A 293    3493  3668  2744   972  -960   844       O
ATOM  1150 CA AARG A 293     -7.715 41.123  4.157  0.50 28.76           C
ANISOU 1150 CA AARG A 293    3776  3601  3552  1158  -749   727       C
ATOM  1151 CB AARG A 293     -6.220 41.156  3.918  0.50 29.57           C
ANISOU 1151 CB AARG A 293    3495  4140  3600  1345  -850   798       C
ATOM  1152 CG AARG A 293     -5.647 39.789  3.818  0.50 45.43           C
ANISOU 1152 CG AARG A 293    5494  5984  5784  1686  -641  1027       C
ATOM  1153 CD AARG A 293     -4.313 39.750  4.500  0.50 56.11           C
ANISOU 1153 CD AARG A 293    6486  7862  6972  1832  -779  1208       C
ATOM  1154 NE AARG A 293     -3.313 40.477  3.722  0.50 64.85           N
ANISOU 1154 NE AARG A 293    7271  9263  8106  1744  -871  1041       N
ATOM  1155 CZ AARG A 293     -2.573 41.485  4.181  0.50 58.42           C
ANISOU 1155 CZ AARG A 293    6145  8977  7075  1510  -1094   912       C
ATOM  1156 NH1AARG A 293     -1.689 42.061  3.370  0.50 43.26           N
ANISOU 1156 NH1AARG A 293    3953  7233  5249  1410  -1096   738       N
ATOM  1157 NH2AARG A 293     -2.706 41.916  5.434  0.50 48.44           N
ANISOU 1157 NH2AARG A 293    4852  8044  5507  1340  -1263   916       N
ATOM  1158 CA BARG A 293     -7.717 41.112  4.172  0.50 28.54           C
ANISOU 1158 CA BARG A 293    3749  3572  3522  1162  -749   731       C
ATOM  1159 CB BARG A 293     -6.208 41.132  3.979  0.50 30.71           C
ANISOU 1159 CB BARG A 293    3637  4297  3736  1357  -854   813       C
ATOM  1160 CG BARG A 293     -5.693 40.027  3.113  0.50 38.39           C
ANISOU 1160 CG BARG A 293    4608  5003  4975  1634  -611   899       C
ATOM  1161 CD BARG A 293     -6.010 38.649  3.692  0.50 48.55           C
ANISOU 1161 CD BARG A 293    6096  5980  6372  1834  -379  1113       C
ATOM  1162 NE BARG A 293     -5.060 37.673  3.176  0.50 61.22           N
ANISOU 1162 NE BARG A 293    7586  7514  8160  2110  -157  1231       N
ATOM  1163 CZ BARG A 293     -5.336 36.394  2.934  0.50 65.64           C
ANISOU 1163 CZ BARG A 293    8349  7653  8937  2240   199  1280       C
ATOM  1164 NH1BARG A 293     -4.386 35.590  2.471  0.50 58.47           N
ANISOU 1164 NH1BARG A 293    7326  6696  8196  2490   440  1404       N
ATOM  1165 NH2BARG A 293     -6.551 35.921  3.161  0.50 68.43           N
ANISOU 1165 NH2BARG A 293    8999  7655  9347  2088   345  1191       N
ATOM  1166 N  THR A 294     -8.104 43.397  4.820  1.00 23.14           N
ANISOU 1166 N  THR A 294    2965  3225  2601   494  -939   369       N
ATOM  1167 CA THR A 294     -8.306 44.526  5.720  1.00 23.71           C
ANISOU 1167 CA THR A 294    3012  3509  2487   137  -983   199       C
ATOM  1168 CB THR A 294     -8.058 45.852  5.002  1.00 24.41           C
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ANISOU 1168 CB THR A 294 2954 3618 2702 -208 -892 -85 C
ATOM 1169 OG1 THR A 294 -6.707 45.837 4.495 1.00 27.60 O
ANISOU 1169 OG1 THR A 294 3023 4383 3079 -113 -987 -120 O
ATOM 1170 CG2 THR A 294 -8.175 47.040 6.016 1.00 22.45 C
ANISOU 1170 CG2 THR A 294 2683 3550 2297 -634 -820 -333 C
ATOM 1171 C THR A 294 -9.737 44.462 6.265 1.00 25.64 C
ANISOU 1171 C THR A 294 3603 3353 2784 38 -854 231 C
ATOM 1172 O THR A 294 -9.985 44.618 7.459 1.00 23.05 O
ANISOU 1172 O THR A 294 3359 3174 2226 -64 -872 245 O
ATOM 1173 N LEU A 295 -10.668 44.186 5.380 1.00 19.55 N
ANISOU 1173 N LEU A 295 3010 2125 2293 61 -719 238 N
ATOM 1174 CA LEU A 295 -12.070 44.118 5.782 1.00 27.49 C
ANISOU 1174 CA LEU A 295 4286 2753 3406 -39 -580 264 C
ATOM 1175 CB LEU A 295 -12.946 44.000 4.518 1.00 23.99 C
ANISOU 1175 CB LEU A 295 3783 2118 3214 -66 -421 194 C
ATOM 1176 CG LEU A 295 -14.439 44.027 4.824 1.00 26.60 C
ANISOU 1176 CG LEU A 295 3980 2471 3654 -120 -156 160 C
ATOM 1177 CD1 LEU A 295 -14.795 45.397 5.476 1.00 23.35 C
ANISOU 1177 CD1 LEU A 295 3524 2093 3254 -271 -90 113 C
ATOM 1178 CD2 LEU A 295 -15.279 43.771 3.546 1.00 25.45 C
ANISOU 1178 CD2 LEU A 295 3748 2331 3591 -132 -100 118 C
ATOM 1179 C LEU A 295 -12.327 42.936 6.742 1.00 26.13 C
ANISOU 1179 C LEU A 295 4309 2489 3129 211 -555 482 C
ATOM 1180 O LEU A 295 -13.095 43.015 7.727 1.00 28.42 O
ANISOU 1180 O LEU A 295 4792 2662 3346 119 -468 522 O
ATOM 1181 N GLU A 296 -11.705 41.808 6.434 1.00 23.16 N
ANISOU 1181 N GLU A 296 3891 2125 2782 545 -551 644 N
ATOM 1182 CA GLU A 296 -11.740 40.659 7.318 1.00 25.88 C
ANISOU 1182 CA GLU A 296 4254 2476 3104 772 -413 873 C
ATOM 1183 CB GLU A 296 -10.810 39.574 6.787 1.00 34.10 C
ANISOU 1183 CB GLU A 296 5148 3539 4269 1054 -361 1003 C
ATOM 1184 CG GLU A 296 -11.558 38.389 6.269 1.00 64.30 C
ANISOU 1184 CG GLU A 296 9052 6977 8403 1017 -104 899 C
ATOM 1185 CD GLU A 296 -10.662 37.329 5.640 1.00 92.01 C
ANISOU 1185 CD GLU A 296 12513 10415 12030 1277 34 968 C
ATOM 1186 OE1 GLU A 296 -9.438 37.569 5.472 1.00 96.61 O
ANISOU 1186 OE1 GLU A 296 12926 11261 12521 1486 -77 1096 O
ATOM 1187 OE2 GLU A 296 -11.205 36.248 5.314 1.00 97.93 O
ANISOU 1187 OE2 GLU A 296 13370 10877 12959 1262 285 882 O
ATOM 1188 C GLU A 296 -11.304 41.045 8.723 1.00 33.80 C
ANISOU 1188 C GLU A 296 5291 3878 3672 841 -590 1063 C
ATOM 1189 O GLU A 296 -11.938 40.680 9.731 1.00 31.61 O
ANISOU 1189 O GLU A 296 5157 3531 3322 843 -472 1181 O
ATOM 1190 N ASP A 297 -10.197 41.771 8.802 1.00 32.22 N
ANISOU 1190 N ASP A 297 4822 4229 3189 796 -846 1009 N
ATOM 1191 CA ASP A 297 -9.658 42.169 10.099 1.00 37.60 C
ANISOU 1191 CA ASP A 297 5365 5539 3381 726 -1027 1076 C
ATOM 1192 CB ASP A 297 -8.272 42.775 9.944 1.00 44.36 C
ANISOU 1192 CB ASP A 297 5780 7001 4073 616 -1252 921 C
ATOM 1193 CG ASP A 297 -7.233 41.739 9.555 1.00 66.67 C
ANISOU 1193 CG ASP A 297 8385 9874 7073 1016 -1250 1178 C
ATOM 1194 OD1 ASP A 297 -7.503 40.534 9.776 1.00 70.41 O
ANISOU 1194 OD1 ASP A 297 9017 10049 7688 1342 -1080 1480 O
ATOM 1195 OD2 ASP A 297 -6.158 42.129 9.028 1.00 73.49 O
ANISOU 1195 OD2 ASP A 297 8917 11044 7961 972 -1353 1051 O
ATOM 1196 C ASP A 297 -10.557 43.156 10.830 1.00 33.25 C
ANISOU 1196 C ASP A 297 5015 4913 2707 267 -941 799 C
ATOM 1197 O ASP A 297 -10.671 43.123 12.052 1.00 34.91 O
ANISOU 1197 O ASP A 297 5309 5427 2528 232 -967 896 O
ATOM 1198 N ILE A 298 -11.150 44.071 10.084 1.00 28.81 N
ANISOU 1198 N ILE A 298 4510 3979 2458 -74 -806 477 N
ATOM 1199 CA ILE A 298 -12.064 45.027 10.713 1.00 28.98 C
ANISOU 1199 CA ILE A 298 4725 3817 2469 -483 -614 237 C
ATOM 1200 CB ILE A 298 -12.577 46.047 9.680 1.00 27.53 C
ANISOU 1200 CB ILE A 298 4522 3234 2704 -754 -425 -8 C
ATOM 1201 CG1 ILE A 298 -11.447 46.978 9.281 1.00 31.04 C
ANISOU 1201 CG1 ILE A 298 4656 4056 3083 -975 -492 -260 C
ATOM 1202 CD1 ILE A 298 -11.771 47.768 7.965 1.00 27.07 C
ANISOU 1202 CD1 ILE A 298 4100 3166 3020 -1079 -299 -352 C
ATOM 1203 CG2 ILE A 298 -13.699 46.919 10.297 1.00 30.85 C
ANISOU 1203 CG2 ILE A 298 5165 3320 3237 -1095 -113 -172 C
ATOM 1204 C ILE A 298 -13.257 44.295 11.319 1.00 29.64 C
ANISOU 1204 C ILE A 298 5161 3480 2619 -349 -435 442 C
ATOM 1205 O ILE A 298 -13.645 44.516 12.477 1.00 31.48 O
ANISOU 1205 O ILE A 298 5562 3819 2579 -510 -343 416 O
ATOM 1206 N LEU A 299 -13.834 43.388 10.538 1.00 28.35 N
ANISOU 1206 N LEU A 299 5112 2850 2809 -85 -353 614 N
ATOM 1207 CA LEU A 299 -15.025 42.662 10.982 1.00 32.92 C
ANISOU 1207 CA LEU A 299 5823 3085 3601 6 -112 680 C
ATOM 1208 CB LEU A 299 -15.672 41.901 9.827 1.00 32.64 C
ANISOU 1208 CB LEU A 299 5418 2943 4042 93 -7 570 C
ATOM 1209 CG LEU A 299 -16.196 42.848 8.772 1.00 33.61 C
ANISOU 1209 CG LEU A 299 5250 3131 4390 -85 2 354 C
ATOM 1210 CD1 LEU A 299 -16.715 42.104 7.559 1.00 31.95 C
ANISOU 1210 CD1 LEU A 299 4916 2871 4352 -39 23 301 C
ATOM 1211 CD2 LEU A 299 -17.313 43.679 9.394 1.00 40.66 C
ANISOU 1211 CD2 LEU A 299 6172 4005 5271 -231 109 259 C
ATOM 1212 C LEU A 299 -14.793 41.726 12.149 1.00 38.69 C
ANISOU 1212 C LEU A 299 6669 3986 4045 270 -94 985 C
ATOM 1213 O LEU A 299 -15.705 41.484 12.936 1.00 38.48 O
ANISOU 1213 O LEU A 299 6751 3800 4071 227 93 983 O
ATOM 1214 N ALA A 300 -13.581 41.191 12.271 1.00 40.24 N
ANISOU 1214 N ALA A 300 6026 5491 3774 763 -1795 -692 N
ATOM 1215 CA ALA A 300 -13.261 40.311 13.377 1.00 43.79 C
ANISOU 1215 CA ALA A 300 6719 6087 3831 930 -2090 -539 C
ATOM 1216 CB ALA A 300 -11.841 39.830 13.268 1.00 46.61 C
ANISOU 1216 CB ALA A 300 6935 6377 4399 1113 -2462 -657 C
ATOM 1217 C ALA A 300 -13.471 41.036 14.708 1.00 56.03 C
ANISOU 1217 C ALA A 300 8381 7949 4961 975 -2163 -723 C
ATOM 1218 O ALA A 300 -13.824 40.430 15.710 1.00 72.09 O
ANISOU 1218 O ALA A 300 10734 10144 6513 1059 -2245 -509 O
ATOM 1219 N ASP A 301 -13.254 42.347 14.697 1.00 54.94 N
ANISOU 1219 N ASP A 301 7987 7878 5009 911 -2101 -1129 N
ATOM 1220 CA ASP A 301 -13.354 43.184 15.884 1.00 59.31 C
ANISOU 1220 CA ASP A 301 8566 8733 5237 936 -2162 -1410 C
ATOM 1221 CB ASP A 301 -12.391 44.356 15.738 1.00 73.05 C
ANISOU 1221 CB ASP A 301 9929 10474 7353 934 -2239 -1942 C
ATOM 1222 CG ASP A 301 -10.962 44.004 16.101 1.00 89.11 C
ANISOU 1222 CG ASP A 301 11823 12603 9432 1145 -2689 -2178 C
ATOM 1223 OD1 ASP A 301 -10.618 42.802 16.176 1.00 89.10 O
ANISOU 1223 OD1 ASP A 301 11996 12585 9273 1311 -2947 -1882 O
ATOM 1224 OD2 ASP A 301 -10.178 44.957 16.315 1.00 97.29 O
ANISOU 1224 OD2 ASP A 301 12548 13704 10713 1141 -2745 -2666 O
ATOM 1225 C ASP A 301 -14.741 43.798 16.075 1.00 55.68 C
ANISOU 1225 C ASP A 301 8205 8337 4614 756 -1783 -1368 C
ATOM 1226 O ASP A 301 -15.158 44.107 17.194 1.00 54.35 O
ANISOU 1226 O ASP A 301 8181 8438 4031 759 -1786 -1463 O
ATOM 1227 N ALA A 302 -15.422 44.061 14.986 1.00 44.64 N
ANISOU 1227 N ALA A 302 6706 6704 3551 614 -1467 -1265 N
ATOM 1228 CA ALA A 302 -16.572 44.919 15.014 1.00 49.48 C
ANISOU 1228 CA ALA A 302 7288 7346 4164 472 -1127 -1354 C
ATOM 1229 CB ALA A 302 -16.998 45.269 13.638 1.00 41.37 C
ANISOU 1229 CB ALA A 302 6111 6047 3561 394 -867 -1269 C
ATOM 1230 C ALA A 302 -17.726 44.394 15.810 1.00 54.00 C
ANISOU 1230 C ALA A 302 8150 8100 4268 407 -984 -1139 C
ATOM 1231 O ALA A 302 -18.061 43.256 15.724 1.00 53.72 O
ANISOU 1231 O ALA A 302 8331 8008 4070 402 -962 -784 O
ATOM 1232 N PRO A 303 -18.327 45.276 16.582 1.00 52.89 N
ANISOU 1232 N PRO A 303 8002 8152 3943 476 -1380 -1380 N
ATOM 1233 CA PRO A 303 -19.465 44.951 17.415 1.00 50.54 C
ANISOU 1233 CA PRO A 303 7968 8041 3195 243 -653 -1246 C
ATOM 1234 CB PRO A 303 -19.705 46.233 18.174 1.00 62.06 C
ANISOU 1234 CB PRO A 303 9313 9715 4553 192 -570 -1658 C
ATOM 1235 CG PRO A 303 -19.162 47.258 17.354 1.00 67.17 C
ANISOU 1235 CG PRO A 303 9607 10168 5747 207 -550 -1943 C
ATOM 1236 CD PRO A 303 -17.978 46.689 16.695 1.00 58.92 C
ANISOU 1236 CD PRO A 303 8502 8954 4932 325 -817 -1828 C
ATOM 1237 C PRO A 303 -20.685 44.565 16.619 1.00 53.93 C
ANISOU 1237 C PRO A 303 8405 8318 3769 106 -311 -1039 C
ATOM 1238 O PRO A 303 -21.444 43.768 17.109 1.00 60.62 O
ANISOU 1238 O PRO A 303 9498 9253 4283 16 -143 -852 O
ATOM 1239 N GLU A 304 -20.901 45.155 15.446 1.00 42.81 N
ANISOU 1239 N GLU A 304 6744 6699 2823 95 -193 -1091 N
ATOM 1240 CA GLU A 304 -22.109 44.852 14.678 1.00 60.92 C
ANISOU 1240 CA GLU A 304 9003 8908 5235 -3 99 -965 C
ATOM 1241 CB GLU A 304 -22.564 45.952 13.730 1.00 60.83 C
ANISOU 1241 CB GLU A 304 8716 8776 5621 21 251 -1161 C
ATOM 1242 CG GLU A 304 -21.537 46.827 13.166 1.00 65.41 C
ANISOU 1242 CG GLU A 304 9126 9176 6551 131 107 -1270 C
ATOM 1243 CD GLU A 304 -20.866 47.708 14.171 1.00 71.45 C
ANISOU 1243 CD GLU A 304 9828 10036 7283 146 17 -1599 C
ATOM 1244 OE1 GLU A 304 -21.430 48.734 14.578 1.00 63.77 O
ANISOU 1244 OE1 GLU A 304 8784 9152 6292 103 185 -1845 O
ATOM 1245 OE2 GLU A 304 -19.739 47.382 14.512 1.00 74.99 O
ANISOU 1245 OE2 GLU A 304 10272 10479 7742 204 -228 -1646 O
ATOM 1246 C GLU A 304 -22.184 43.470 14.059 1.00 61.21 C
ANISOU 1246 C GLU A 304 9130 8796 5331 -9 87 -632 C
ATOM 1247 O GLU A 304 -23.201 43.097 13.576 1.00 54.22 O
ANISOU 1247 O GLU A 304 8172 7846 4583 -79 298 -565 O
ATOM 1248 N SER A 305 -21.090 42.735 14.041 1.00 69.16 N
ANISOU 1248 N SER A 305 10274 9757 6246 73 -167 -459 N
ATOM 1249 CA SER A 305 -21.158 41.320 13.756 1.00 71.04 C
ANISOU 1249 CA SER A 305 10644 9852 6495 58 -162 -140 C
ATOM 1250 CB SER A 305 -20.544 41.117 12.405 1.00 59.16 C
ANISOU 1250 CB SER A 305 8912 8138 5428 117 -253 -116 C
ATOM 1251 OG SER A 305 -19.179 41.315 12.512 1.00 57.25 O
ANISOU 1251 OG SER A 305 8655 7847 5252 249 -570 -141 O
ATOM 1252 C SER A 305 -20.340 40.639 14.860 1.00 88.37 C
ANISOU 1252 C SER A 305 13115 12092 8370 164 -420 37 C
ATOM 1253 O SER A 305 -19.185 40.967 14.956 1.00103.54 O
ANISOU 1253 O SER A 305 14946 13987 10408 310 -730 -44 O
ATOM 1254 N GLN A 306 -20.792 39.670 15.657 1.00 91.87 N
ANISOU 1254 N GLN A 306 13899 12590 8417 118 -310 268 N
ATOM 1255 CA GLN A 306 -22.160 39.115 15.826 1.00 86.51 C
ANISOU 1255 CA GLN A 306 13372 11915 7582 -81 97 375 C
ATOM 1256 CB GLN A 306 -23.169 40.227 16.174 1.00 83.78 C
ANISOU 1256 CB GLN A 306 12897 11760 7178 -212 345 73 C
ATOM 1257 CG GLN A 306 -22.810 40.988 17.422 1.00 81.90 C
ANISOU 1257 CG GLN A 306 12788 11777 6555 -155 215 -99 C
ATOM 1258 CD GLN A 306 -24.027 41.364 18.238 1.00 92.08 C

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ANISOU 1258  CD  GLN A 306    14169 13244  7573  -339   570  -246       C
ATOM  1259  OE1 GLN A 306     -25.110 41.576 17.690  1.00 98.93           O
ANISOU 1259  OE1 GLN A 306    14846 14063  8681  -486   872  -366       O
ATOM  1260  NE2 GLN A 306     -23.862 41.433 19.558  1.00 95.02           N
ANISOU 1260  NE2 GLN A 306    14787 13838  7477  -309   523  -257       N
ATOM  1261  C   GLN A 306     -22.757 38.154 14.785  1.00 68.32           C
ANISOU 1261  C   GLN A 306    11024 9380  5553  -195   326   562       C
ATOM  1262  O   GLN A 306     -23.966 38.190 14.551  1.00 63.46           O
ANISOU 1262  O   GLN A 306    10370 8778  4965  -379   685   500       O
ATOM  1263  N   ASN A 307     -21.937 37.292 14.191  1.00 56.05           N
ANISOU 1263  N   ASN A 307    9461  7627  4209   -92   130   751       N
ATOM  1264  CA  ASN A 307     -22.425 36.170 13.380  1.00 58.66           C
ANISOU 1264  CA  ASN A 307    9758  7736  4793  -203   345   912       C
ATOM  1265  CB  ASN A 307     -23.004 35.045 14.237  1.00 68.96           C
ANISOU 1265  CB  ASN A 307    11451 8950  5800  -312   617  1182       C
ATOM  1266  CG  ASN A 307     -22.011 33.941 14.480  1.00 81.43           C
ANISOU 1266  CG  ASN A 307    13307 10325  7308  -153   405  1517       C
ATOM  1267  OD1 ASN A 307     -21.976 32.949 13.745  1.00 92.50           O
ANISOU 1267  OD1 ASN A 307    14667 11476  9003  -193   492  1658       O
ATOM  1268  ND2 ASN A 307     -21.178 34.111 15.500  1.00 80.70           N
ANISOU 1268  ND2 ASN A 307    13479 10348  6836    48   106  1620       N
ATOM  1269  C   ASN A 307     -23.490 36.667 12.423  1.00 57.58           C
ANISOU 1269  C   ASN A 307    9288  7637  4951  -342   597   675       C
ATOM  1270  O   ASN A 307     -24.595 36.113 12.339  1.00 55.42           O
ANISOU 1270  O   ASN A 307    9018  7334  4706  -520   942   668       O
ATOM  1271  N   ASN A 308     -23.133 37.736 11.730  1.00 52.50           N
ANISOU 1271  N   ASN A 308    8364  7059  4525  -246   427   464       N
ATOM  1272  CA  ASN A 308     -24.075 38.566 11.002  1.00 51.54           C
ANISOU 1272  CA  ASN A 308    7957  7026  4601  -294   596   217       C
ATOM  1273  CB  ASN A 308     -23.983 39.972 11.566  1.00 44.59           C
ANISOU 1273  CB  ASN A 308    7029  6303  3611  -227   520     5       C
ATOM  1274  CG  ASN A 308     -25.271 40.420 12.144  1.00 68.41           C
ANISOU 1274  CG  ASN A 308    10031 9476  6485  -350   804  -170       C
ATOM  1275  OD1 ASN A 308     -26.299 39.775 11.944  1.00 78.84           O
ANISOU 1275  OD1 ASN A 308    11317 10794 7844  -485  1067  -177       O
ATOM  1276  ND2 ASN A 308     -25.240 41.524 12.884  1.00 71.94           N
ANISOU 1276  ND2 ASN A 308    10478 10064  6793  -319   773  -360       N
ATOM  1277  C   ASN A 308     -23.700 38.671  9.546  1.00 38.43           C
ANISOU 1277  C   ASN A 308    6029  5263  3310  -208   485   175       C
ATOM  1278  O   ASN A 308     -24.503 39.025  8.668  1.00 31.35           O
ANISOU 1278  O   ASN A 308    4901  4413  2596  -213   612    26       O
ATOM  1279  N   CYS A 309     -22.436 38.403  9.299  1.00 32.05           N
ANISOU 1279  N   CYS A 309    5253  4329  2597  -107   232   289       N
ATOM  1280  CA  CYS A 309     -21.873 38.739  8.016  1.00 30.24           C
ANISOU 1280  CA  CYS A 309    4798  4010  2684   -20   121   223       C
ATOM  1281  CB  CYS A 309     -21.243 40.124  8.161  1.00 40.98           C
ANISOU 1281  CB  CYS A 309    6094  5408  4068    87   -9    58       C
ATOM  1282  SG  CYS A 309     -20.620 40.771  6.675  1.00 43.61           S
ANISOU 1282  SG  CYS A 309    6210  5613  4749   183   -59   -25       S
ATOM  1283  C   CYS A 309     -20.802 37.714  7.700  1.00 33.97           C
ANISOU 1283  C   CYS A 309    5314  4306  3288    12   -53   386       C
ATOM  1284  O   CYS A 309     -20.087 37.274  8.590  1.00 33.95           O
ANISOU 1284  O   CYS A 309    5503  4265  3130    56  -213   506       O
ATOM  1285  N   ARG A 310     -20.682 37.332  6.437  1.00 27.49           N
ANISOU 1285  N   ARG A 310    4312  3388  2742    10   -35   378       N
ATOM  1286  CA  ARG A 310     -19.639 36.403  6.028  1.00 27.36           C
ANISOU 1286  CA  ARG A 310    4292  3193  2912    37  -190   488       C
ATOM  1287  CB  ARG A 310     -20.220 35.011  5.845  1.00 31.43           C
ANISOU 1287  CB  ARG A 310    4844  3614  3483   -74   -29   619       C
ATOM  1288  CG  ARG A 310     -19.161 33.962  5.568  1.00 47.33           C
ANISOU 1288  CG  ARG A 310    6871  5412  5699   -37  -183   742       C
ATOM  1289  CD  ARG A 310     -18.592 33.453  6.871  1.00 69.84           C
ANISOU 1289  CD  ARG A 310    10016 8185  8336    42  -336   942       C
ATOM  1290  NE  ARG A 310     -17.935 32.159  6.714  1.00 89.65           N
ANISOU 1290  NE  ARG A 310    12580 10452 11032    74  -414  1105       N
ATOM  1291  CZ  ARG A 310     -18.543 30.988  6.886  1.00 99.47           C
ANISOU 1291  CZ  ARG A 310    13965 11542 12287   -23  -196  1280       C
ATOM  1292  NH1 ARG A 310     -17.866 29.854  6.726  1.00100.90           N
ANISOU 1292  NH1 ARG A 310    14193 11466 12680    29  -272  1425       N
ATOM  1293  NH2 ARG A 310     -19.829 30.951  7.224  1.00101.33           N
ANISOU 1293  NH2 ARG A 310    14286 11859 12355  -178   124  1288       N
ATOM  1294  C   ARG A 310     -19.074 36.889  4.688  1.00 25.08           C
ANISOU 1294  C   ARG A 310    3776 2848  2905    87  -236   363       C
ATOM  1295  O   ARG A 310     -19.835 37.176  3.778  1.00 26.01           O
ANISOU 1295  O   ARG A 310    3754 3040  3090    70   -85   281       O
ATOM  1296  N   LEU A 311     -17.744 36.995  4.588  1.00 28.48           N
ANISOU 1296  N   LEU A 311    4175 3161  3486   158  -439   331       N
ATOM  1297  CA  LEU A 311     -17.085 37.403  3.339  1.00 23.32           C
ANISOU 1297  CA  LEU A 311    3338 2421  3102   179  -439   214       C
ATOM  1298  CB  LEU A 311     -15.748 38.080  3.637  1.00 28.59           C
ANISOU 1298  CB  LEU A 311    3973 3002  3886   247  -619    82       C
ATOM  1299  CG  LEU A 311     -15.860 39.295  4.538  1.00 35.69           C
ANISOU 1299  CG  LEU A 311    4937 4006  4616   290  -630   -29       C
ATOM  1300  CD1 LEU A 311     -14.510 40.015  4.593  1.00 37.69           C
ANISOU 1300  CD1 LEU A 311    5085 4159  5074   333  -760  -246       C
ATOM  1301  CD2 LEU A 311     -16.935 40.205  4.008  1.00 29.42           C
ANISOU 1301  CD2 LEU A 311    4122 3293  3764   283  -399   -57       C
ATOM  1302  C   LEU A 311     -16.757 36.143  2.527  1.00 29.04           C
ANISOU 1302  C   LEU A 311    3971 3020  4043   129  -445   273       C
ATOM  1303  O   LEU A 311     -16.204 35.180  3.075  1.00 30.33           O
ANISOU 1303  O   LEU A 311    4206 3072  4248   136  -579   371       O
ATOM  1304  N   ILE A 312     -17.059 36.174  1.231  1.00 22.31           N
ANISOU 1304  N   ILE A 312    2970 2186  3322    98  -308   204       N
ATOM  1305  CA  ILE A 312     -16.758 35.049  0.353  1.00 23.57           C
ANISOU 1305  CA  ILE A 312    3005 2245  3706    35  -289   202       C
ATOM  1306  CB  ILE A 312     -18.021 34.471 -0.217  1.00 25.02           C
ANISOU 1306  CB  ILE A 312    3110 2553  3843   -35  -103   194       C
ATOM  1307  CG1 ILE A 312     -18.860 33.916  0.930  1.00 31.07           C
ANISOU 1307  CG1 ILE A 312    4017 3344  4444   -92   -42   308       C
ATOM  1308  CD1 ILE A 312     -20.200 33.372  0.495  1.00 32.02           C
ANISOU 1308  CD1 ILE A 312    4025 3592  4549  -186   178   230       C
ATOM  1309  CG2 ILE A 312     -17.687 33.299 -1.168  1.00 29.23           C
ANISOU 1309  CG2 ILE A 312    3483 2987  4637  -116   -67   142       C
ATOM  1310  C   ILE A 312     -15.877 35.557 -0.788  1.00 27.65           C
ANISOU 1310  C   ILE A 312    3390 2694  4422    51  -281    69       C
ATOM  1311  O   ILE A 312     -16.356 36.148 -1.761  1.00 24.50           O
ANISOU 1311  O   ILE A 312    2935 2395  3978    71  -141    10       O
ATOM  1312  N   ALA A 313     -14.583 35.397 -0.619  1.00 23.70           N
ANISOU 1312  N   ALA A 313    2854 2027  4125    60  -428    13       N
ATOM  1313  CA  ALA A 313     -13.637 35.934 -1.614  1.00 24.35           C
ANISOU 1313  CA  ALA A 313    2817 2013  4421    44  -376  -147       C
ATOM  1314  CB  ALA A 313     -12.417 36.462 -0.967  1.00 28.54           C
ANISOU 1314  CB  ALA A 313    3332 2420  5092    80  -526  -272       C
ATOM  1315  C   ALA A 313     -13.276 34.766 -2.529  1.00 28.76           C
ANISOU 1315  C   ALA A 313    3223 2487  5218   -35  -351  -195       C
ATOM  1316  O   ALA A 313     -13.185 33.636 -2.063  1.00 27.24           O
ANISOU 1316  O   ALA A 313    3015 2215  5120   -50  -461  -128       O
ATOM  1317  N   TYR A 314     -13.083 35.038 -3.828  1.00 24.14           N
ANISOU 1317  N   TYR A 314    2543 1908  4721   -80  -188  -307       N
ATOM  1318  CA  TYR A 314     -12.761 33.964 -4.788  1.00 21.36           C
ANISOU 1318  CA  TYR A 314    2022 1502  4593  -172  -138  -400       C
ATOM  1319  CB  TYR A 314     -13.976 33.154 -5.203  1.00 25.25           C
ANISOU 1319  CB  TYR A 314    2468 2156  4970  -206   -49  -350       C
ATOM  1320  CG  TYR A 314     -15.095 34.008 -5.714  1.00 22.95           C
ANISOU 1320  CG  TYR A 314    2243 2107  4370  -136   83  -324       C
ATOM  1321  CD1 TYR A 314     -15.961 34.616 -4.823  1.00 26.91           C
ANISOU 1321  CD1 TYR A 314    2879 2711  4633   -57   55  -207       C
ATOM  1322  CE1 TYR A 314     -16.994 35.388 -5.258  1.00 28.70           C
ANISOU 1322  CE1 TYR A 314    3146 3151  4606   40   149  -201       C
ATOM  1323  CZ  TYR A 314     -17.171 35.604 -6.616  1.00 28.95           C
ANISOU 1323  CZ  TYR A 314    3119 3314  4567    91   256  -284       C
ATOM  1324  OH  TYR A 314     -18.218 36.401 -6.993  1.00 31.00           O
ANISOU 1324  OH  TYR A 314    3432 3793  4553   248   305  -267       O
ATOM  1325  CE2 TYR A 314     -16.338 35.017 -7.551  1.00 28.08           C
ANISOU 1325  CE2 TYR A 314    2899 3129  4642     4   303  -391       C
ATOM  1326  CD2 TYR A 314     -15.266 34.229 -7.084  1.00 26.73           C
ANISOU 1326  CD2 TYR A 314    2656 2719  4783  -125   225  -424       C
ATOM  1327  C   TYR A 314     -12.033 34.510 -5.984  1.00 32.30           C
ANISOU 1327  C   TYR A 314    3339 2875  6057  -209    23  -547       C
ATOM  1328  O   TYR A 314     -12.129 35.713 -6.306  1.00 24.86           O
ANISOU 1328  O   TYR A 314    2510 1940  4997  -173   155  -550       O
ATOM  1329  N   GLN A 315     -11.193 33.657 -6.539  1.00 31.12           N
ANISOU 1329  N   GLN A 315    2353 5936  3534   449  -507   650       N
ATOM  1330  CA  GLN A 315     -10.335 34.001 -7.654  1.00 29.17           C
ANISOU 1330  CA  GLN A 315    1998 5780  3306   571  -354   631       C
ATOM  1331  CB  GLN A 315     -8.960 34.402 -7.146  1.00 31.75           C
ANISOU 1331  CB  GLN A 315    1897 6571  3597   542  -380   844       C
ATOM  1332  CG  GLN A 315     -8.030 34.958 -8.189  1.00 41.08           C
ANISOU 1332  CG  GLN A 315    2938 7866  4804   604  -206   814       C
ATOM  1333  CD  GLN A 315     -6.621 35.126 -7.662  1.00 53.35           C
ANISOU 1333  CD  GLN A 315    4236 9687  6348   561  -209  1016       C
ATOM  1334  OE1 GLN A 315     -6.233 34.519 -6.660  1.00 62.13           O
ANISOU 1334  OE1 GLN A 315    5239 10917  7451   601  -313  1238       O
ATOM  1335  NE2 GLN A 315     -5.840 35.955 -8.336  1.00 72.17           N
ANISOU 1335  NE2 GLN A 315    6513 12184  8725   476   -96   953       N
ATOM  1336  C   GLN A 315     -10.246 32.720 -8.454  1.00 37.56           C
ANISOU 1336  C   GLN A 315    3249 6549  4474   959  -169   672       C
ATOM  1337  O   GLN A 315     -10.024 31.651 -7.890  1.00 35.66           O
ANISOU 1337  O   GLN A 315    2973 6268  4307  1202  -138   872       O
ATOM  1338  N   GLU A 316     -10.457 32.833 -9.758  1.00 34.53           N
ANISOU 1338  N   GLU A 316    3010 5904  4207   930  -303   609       N
ATOM  1339  CA  GLU A 316     -10.470 31.691 -10.660  1.00 37.57           C
ANISOU 1339  CA  GLU A 316    3774 5988  4513  1274  -217   449       C
ATOM  1340  CB  GLU A 316     -11.659 31.805 -11.602  1.00 43.39           C
ANISOU 1340  CB  GLU A 316    4922 6419  5147  1086   192   167       C
ATOM  1341  CG  GLU A 316     -12.939 32.260 -10.968  1.00 53.58           C
ANISOU 1341  CG  GLU A 316    6279 7666  6413   799   -68    71       C
ATOM  1342  CD  GLU A 316     -14.055 32.388 -12.007  1.00 65.76           C
ANISOU 1342  CD  GLU A 316    8187 8974  7861   621  -116  -140       C
ATOM  1343  OE1 GLU A 316     -14.122 31.508 -12.909  1.00 62.88           O
ANISOU 1343  OE1 GLU A 316    8087 8374  7430   713    36  -236       O
ATOM  1344  OE2 GLU A 316     -14.849 33.365 -11.931  1.00 62.69           O
ANISOU 1344  OE2 GLU A 316    7717 8643  7460   376  -284  -189       O
ATOM  1345  C   GLU A 316     -9.208 31.693 -11.494  1.00 41.89           C
ANISOU 1345  C   GLU A 316    4180 6627  5109  1501   483   538       C
ATOM  1346  O   GLU A 316     -8.631 32.747 -11.763  1.00 43.79           O
ANISOU 1346  O   GLU A 316    4205 7125  5310  1374   468   522       O
ATOM  1347  N   PRO A 317     -8.761 30.500 -11.918  1.00 46.74           N
ANISOU 1347  N   PRO A 317    4934 6997  5829  1840   787   634       N
ATOM  1348  CA  PRO A 317     -7.609 30.417 -12.813  1.00 48.15           C
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ANISOU 1348 CA PRO A 317 5026 7180 6088 2080 1128 715 C
ATOM 1349 CB PRO A 317 -7.458 28.915 -13.058 1.00 57.84 C
ANISOU 1349 CB PRO A 317 6510 8017 7449 2438 1502 812 C
ATOM 1350 CG PRO A 317 -8.408 28.239 -12.100 1.00 59.58 C
ANISOU 1350 CG PRO A 317 6865 8104 7668 2396 1313 828 C
ATOM 1351 CD PRO A 317 -9.466 29.216 -11.785 1.00 57.23 C
ANISOU 1351 CD PRO A 317 6608 7940 7196 1974 897 608 C
ATOM 1352 C PRO A 317 -7.951 31.083 -14.144 1.00 40.30 C
ANISOU 1352 C PRO A 317 4356 6035 4922 1878 1207 410 C
ATOM 1353 O PRO A 317 -9.081 30.952 -14.606 1.00 38.43 O
ANISOU 1353 O PRO A 317 4529 5541 4533 1682 1120 170 O
ATOM 1354 N ALA A 318 -6.988 31.770 -14.751 1.00 44.03 N
ANISOU 1354 N ALA A 318 4634 6683 5412 1917 1367 442 N
ATOM 1355 CA ALA A 318 -7.240 32.476 -16.005 1.00 44.94 C
ANISOU 1355 CA ALA A 318 5049 6684 5344 1730 1447 189 C
ATOM 1356 CB ALA A 318 -6.022 33.297 -16.398 1.00 53.27 C
ANISOU 1356 CB ALA A 318 5786 7990 6463 1785 1624 275 C
ATOM 1357 C ALA A 318 -7.645 31.548 -17.161 1.00 49.91 C
ANISOU 1357 C ALA A 318 6253 6859 5852 1788 1737 -1 C
ATOM 1358 O ALA A 318 -8.307 31.986 -18.105 1.00 43.64 O
ANISOU 1358 O ALA A 318 5809 5951 4822 1547 1685 -229 O
ATOM 1359 N ASP A 319 -7.232 30.279 -17.093 1.00 44.29 N
ANISOU 1359 N ASP A 319 5646 5893 5289 2091 2064 110 N
ATOM 1360 CA ASP A 319 -7.416 29.347 -18.194 1.00 47.04 C
ANISOU 1360 CA ASP A 319 6573 5778 5522 2132 2459 -79 C
ATOM 1361 CB ASP A 319 -6.128 28.541 -18.421 1.00 55.85 C
ANISOU 1361 CB ASP A 319 7609 6717 6893 2562 3031 133 C
ATOM 1362 CG ASP A 319 -5.830 27.561 -17.274 1.00 70.31 C
ANISOU 1362 CG ASP A 319 9168 8528 9020 2888 3093 453 C
ATOM 1363 OD1 ASP A 319 -6.160 27.860 -16.100 1.00 70.90 O
ANISOU 1363 OD1 ASP A 319 8881 8913 9143 2844 2675 596 O
ATOM 1364 OD2 ASP A 319 -5.268 26.481 -17.558 1.00 88.04 O
ANISOU 1364 OD2 ASP A 319 11585 10444 11423 3058 3457 577 O
ATOM 1365 C ASP A 319 -8.564 28.361 -17.997 1.00 46.87 C
ANISOU 1365 C ASP A 319 6963 5443 5404 2013 2394 -225 C
ATOM 1366 O ASP A 319 -8.716 27.420 -18.776 1.00 58.24 O
ANISOU 1366 O ASP A 319 8915 6469 6745 2017 2765 -387 O
ATOM 1367 N ASP A 320 -9.350 28.535 -16.953 1.00 46.14 N
ANISOU 1367 N ASP A 320 6675 5518 5340 1886 1973 -179 N
ATOM 1368 CA ASP A 320 -10.400 27.559 -16.690 1.00 61.81 C
ANISOU 1368 CA ASP A 320 9013 7202 7269 1782 1936 -303 C
ATOM 1369 CB ASP A 320 -9.979 26.608 -15.560 1.00 71.44 C
ANISOU 1369 CB ASP A 320 10024 8352 8767 2132 2088 -28 C
ATOM 1370 CG ASP A 320 -10.789 25.314 -15.541 1.00 85.13 C
ANISOU 1370 CG ASP A 320 12237 9637 10472 2102 2284 -165 C
ATOM 1371 OD1 ASP A 320 -11.965 25.325 -15.971 1.00 90.43 O
ANISOU 1371 OD1 ASP A 320 13266 10181 10912 1717 2086 -459 O
ATOM 1372 OD2 ASP A 320 -10.235 24.285 -15.080 1.00 91.79 O
ANISOU 1372 OD2 ASP A 320 13076 10263 11536 2464 2649 48 O
ATOM 1373 C ASP A 320 -11.666 28.303 -16.327 1.00 53.37 C
ANISOU 1373 C ASP A 320 7908 6309 6062 1409 1417 -427 C
ATOM 1374 O ASP A 320 -11.617 29.373 -15.716 1.00 58.58 O
ANISOU 1374 O ASP A 320 8167 7318 6775 1342 1110 -319 O
ATOM 1375 N SER A 321 -12.806 27.750 -16.720 1.00 45.18 N
ANISOU 1375 N SER A 321 7292 5023 4853 1146 1348 -651 N
ATOM 1376 CA SER A 321 -14.077 28.398 -16.414 1.00 51.69 C
ANISOU 1376 CA SER A 321 8055 5995 5588 808 884 -730 C
ATOM 1377 CB SER A 321 -14.758 28.873 -17.706 1.00 48.40 C
ANISOU 1377 CB SER A 321 7942 5584 4865 461 759 -933 C
ATOM 1378 OG SER A 321 -14.893 27.794 -18.619 1.00 63.20 O
ANISOU 1378 OG SER A 321 10355 7122 6538 352 1051 -1142 O
ATOM 1379 C SER A 321 -14.990 27.442 -15.642 1.00 53.39 C
ANISOU 1379 C SER A 321 8411 5995 5879 745 820 -768 C
ATOM 1380 O SER A 321 -16.213 27.513 -15.748 1.00 65.39 O
ANISOU 1380 O SER A 321 10067 7489 7291 422 554 -902 O
ATOM 1381 N SER A 322 -14.391 26.538 -14.872 1.00 51.56 N
ANISOU 1381 N SER A 322 8130 5614 5847 1063 1077 -620 N
ATOM 1382 CA SER A 322 -15.164 25.517 -14.179 1.00 46.87 C
ANISOU 1382 CA SER A 322 7724 4758 5327 1036 1103 -655 C
ATOM 1383 CB SER A 322 -14.372 24.223 -14.094 1.00 58.70 C
ANISOU 1383 CB SER A 322 9422 5922 6959 1394 1618 -558 C
ATOM 1384 OG SER A 322 -13.158 24.461 -13.414 1.00 66.40 O
ANISOU 1384 OG SER A 322 9952 7129 8148 1792 1699 -218 O
ATOM 1385 C SER A 322 -15.577 25.939 -12.779 1.00 43.31 C
ANISOU 1385 C SER A 322 6900 4517 5037 1041 774 -486 C
ATOM 1386 O SER A 322 -16.247 25.189 -12.063 1.00 39.55 O
ANISOU 1386 O SER A 322 6541 3845 4639 1019 772 -493 O
ATOM 1387 N PHE A 323 -15.191 27.137 -12.360 1.00 34.26 N
ANISOU 1387 N PHE A 323 5340 3747 3930 1041 529 -347 N
ATOM 1388 CA PHE A 323 -15.562 27.540 -11.008 1.00 31.45 C
ANISOU 1388 CA PHE A 323 4692 3566 3692 999 268 -207 C
ATOM 1389 CB PHE A 323 -14.832 28.827 -10.649 1.00 29.78 C
ANISOU 1389 CB PHE A 323 4061 3760 3492 995 108 -64 C
ATOM 1390 CG PHE A 323 -15.370 29.501 -9.416 1.00 28.30 C
ANISOU 1390 CG PHE A 323 3648 3746 3360 820 -155 10 C
ATOM 1391 CD1 PHE A 323 -15.035 29.021 -8.159 1.00 31.41 C
ANISOU 1391 CD1 PHE A 323 3893 4210 3833 959 -163 211 C
ATOM 1392 CE1 PHE A 323 -15.508 29.639 -7.005 1.00 27.35 C
ANISOU 1392 CE1 PHE A 323 3227 3836 3328 756 -368 260 C
ATOM 1393 CZ PHE A 323 -16.326 30.757 -7.125 1.00 25.45 C
ANISOU 1393 CZ PHE A 323 2973 3629 3069 443 -514 114 C
ATOM 1394 CE2 PHE A 323 -16.674 31.257 -8.406 1.00 30.63 C
ANISOU 1394 CE2 PHE A 323 3732 4224 3683 348 -509 -43 C
ATOM 1395 CD2 PHE A 323 -16.198 30.620 -9.534 1.00 33.68 C
ANISOU 1395 CD2 PHE A 323 4281 4507 4008 519 -356 -100 C
ATOM 1396 C PHE A 323 -17.079 27.726 -10.920 1.00 37.58 C
ANISOU 1396 C PHE A 323 5608 4236 4436 653 19 -378 C
ATOM 1397 O PHE A 323 -17.685 28.373 -11.776 1.00 38.32 O
ANISOU 1397 O PHE A 323 5769 4375 4415 406 -125 -516 O
ATOM 1398 N SER A 324 -17.689 27.163 -9.878 1.00 34.34 N
ANISOU 1398 N SER A 324 5218 3694 4136 644 -24 -334 N
ATOM 1399 CA SER A 324 -19.121 27.351 -9.636 1.00 31.00 C
ANISOU 1399 CA SER A 324 4861 3176 3742 332 -240 -454 C
ATOM 1400 CB SER A 324 -19.806 26.004 -9.447 1.00 38.51 C
ANISOU 1400 CB SER A 324 6136 3765 4731 311 -94 -556 C
ATOM 1401 OG SER A 324 -21.013 26.174 -8.726 1.00 35.52 O
ANISOU 1401 OG SER A 324 5710 3328 4458 80 -283 -587 O
ATOM 1402 C SER A 324 -19.379 28.228 -8.407 1.00 25.05 C
ANISOU 1402 C SER A 324 3806 2608 3102 257 -430 -321 C
ATOM 1403 O SER A 324 -19.102 27.848 -7.288 1.00 26.21 O
ANISOU 1403 O SER A 324 3885 2753 3321 386 -388 -185 O
ATOM 1404 N LEU A 325 -19.947 29.406 -8.625 1.00 25.52 N
ANISOU 1404 N LEU A 325 3714 2815 3169 31 -613 -350 N
ATOM 1405 CA LEU A 325 -20.181 30.339 -7.530 1.00 26.25 C
ANISOU 1405 CA LEU A 325 3574 3039 3361 -79 -710 -250 C
ATOM 1406 CB LEU A 325 -20.634 31.693 -8.084 1.00 25.17 C
ANISOU 1406 CB LEU A 325 3290 3033 3241 -275 -813 -262 C
ATOM 1407 CG LEU A 325 -20.838 32.775 -7.030 1.00 25.13 C
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ATOM 1408 CD1 LEU A 325 -19.565 32.966 -6.204 1.00 24.63 C
ANISOU 1408 CD1 LEU A 325 2898 3280 3179 -328 -754 -91 C
ATOM 1409 CD2 LEU A 325 -21.197 34.069 -7.765 1.00 32.63 C
ANISOU 1409 CD2 LEU A 325 3921 4153 4324 -553 -838 -162 C
ATOM 1410 C LEU A 325 -21.231 29.782 -6.557 1.00 24.51 C
ANISOU 1410 C LEU A 325 3448 2590 3277 -184 -728 -261 C
ATOM 1411 O LEU A 325 -21.118 29.948 -5.330 1.00 26.39 O
ANISOU 1411 O LEU A 325 3599 2867 3560 -190 -715 -162 O
ATOM 1412 N SER A 326 -22.235 29.104 -7.091 1.00 27.07 N
ANISOU 1412 N SER A 326 3961 2682 3641 -298 -750 -383 N
ATOM 1413 CA SER A 326 -23.239 28.519 -6.217 1.00 26.94 C
ANISOU 1413 CA SER A 326 4037 2427 3771 -402 -737 -404 C
ATOM 1414 CB SER A 326 -24.389 27.888 -7.005 1.00 27.11 C
ANISOU 1414 CB SER A 326 4229 2249 3824 -605 -792 -553 C
ATOM 1415 OG SER A 326 -23.925 26.883 -7.894 1.00 33.76 O
ANISOU 1415 OG SER A 326 5339 2988 4499 -527 -679 -676 O
ATOM 1416 C SER A 326 -22.599 27.475 -5.299 1.00 29.26 C
ANISOU 1416 C SER A 326 4462 2607 4049 -176 -578 -333 C
ATOM 1417 O SER A 326 -22.928 27.388 -4.116 1.00 28.35 O
ANISOU 1417 O SER A 326 4338 2413 4021 -205 -555 -262 O
ATOM 1418 N GLN A 327 -21.699 26.655 -5.841 1.00 25.32 N
ANISOU 1418 N GLN A 327 4098 2077 3445 -58 -434 -329 N
ATOM 1419 CA GLN A 327 -21.010 25.678 -4.986 1.00 27.04 C
ANISOU 1419 CA GLN A 327 4398 2202 3674 335 -255 -178 C
ATOM 1420 CB GLN A 327 -20.126 24.744 -5.811 1.00 31.11 C
ANISOU 1420 CB GLN A 327 5086 2609 4126 606 -11 -171 C
ATOM 1421 CG GLN A 327 -20.915 23.655 -6.525 1.00 39.92 C
ANISOU 1421 CG GLN A 327 6596 3330 5241 498 171 -398 C
ATOM 1422 CD GLN A 327 -21.653 22.761 -5.532 1.00 45.24 C
ANISOU 1422 CD GLN A 327 7449 3709 6032 485 278 -389 C
ATOM 1423 OE1 GLN A 327 -21.034 22.145 -4.662 1.00 46.97 O
ANISOU 1423 OE1 GLN A 327 7673 3871 6303 780 445 -172 O
ATOM 1424 NE2 GLN A 327 -22.987 22.701 -5.641 1.00 40.65 N
ANISOU 1424 NE2 GLN A 327 6989 2957 5499 143 180 -595 N
ATOM 1425 C GLN A 327 -20.161 26.365 -3.906 1.00 28.99 C
ANISOU 1425 C GLN A 327 4363 2765 3887 432 -340 57 C
ATOM 1426 O GLN A 327 -20.047 25.904 -2.772 1.00 29.42 O
ANISOU 1426 O GLN A 327 4429 2794 3956 524 -303 215 O
ATOM 1427 N GLU A 328 -19.533 27.468 -4.278 1.00 25.60 N
ANISOU 1427 N GLU A 328 3693 2651 3384 384 -452 85 N
ATOM 1428 CA GLU A 328 -18.671 28.161 -3.332 1.00 32.77 C
ANISOU 1428 CA GLU A 328 4336 3902 4213 395 -537 282 C
ATOM 1429 CB GLU A 328 -17.942 29.292 -4.046 1.00 30.51 C
ANISOU 1429 CB GLU A 328 3824 3920 3850 337 -602 265 C
ATOM 1430 CG GLU A 328 -16.852 29.890 -3.206 1.00 38.72 C
ANISOU 1430 CG GLU A 328 4580 5356 4774 329 -675 465 C
ATOM 1431 CD GLU A 328 -15.697 28.907 -2.952 1.00 42.08 C
ANISOU 1431 CD GLU A 328 4893 5921 5175 683 -606 737 C
ATOM 1432 OE1 GLU A 328 -14.875 29.237 -2.093 1.00 43.17 O
ANISOU 1432 OE1 GLU A 328 4777 6424 5203 654 -711 954 O
ATOM 1433 OE2 GLU A 328 -15.593 27.836 -3.618 1.00 47.49 O
ANISOU 1433 OE2 GLU A 328 5736 6359 5948 974 -426 750 O
ATOM 1434 C GLU A 328 -19.508 28.720 -2.157 1.00 27.77 C
ANISOU 1434 C GLU A 328 3706 3240 3605 118 -621 269 C
ATOM 1435 O GLU A 328 -19.134 28.627 -0.980 1.00 30.45 O
ANISOU 1435 O GLU A 328 3994 3712 3863 116 -647 436 O
ATOM 1436 N VAL A 329 -20.667 29.266 -2.489 1.00 27.93 N
ANISOU 1436 N VAL A 329 3794 3737 3737 -121 -647 92 N
ATOM 1437 CA VAL A 329 -21.541 29.833 -1.451 1.00 28.45 C
ANISOU 1437 CA VAL A 329 3881 3051 3876 -381 -645 73 C
ATOM 1438 CB VAL A 329 -22.671 30.696 -2.074 1.00 29.21 C

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ANISOU 1439 CG1 VAL A 329 4738 3574 5026 -836 -563 -63 C
ATOM 1440 CG2 VAL A 329 -22.068 31.919 -2.727 1.00 25.08 C
ANISOU 1440 CG2 VAL A 329 3229 2749 3551 -660 -685 -55 C
ATOM 1441 C VAL A 329 -22.141 28.726 -0.603 1.00 28.84 C
ANISOU 1441 C VAL A 329 4142 2824 3990 -335 -568 99 C
ATOM 1442 O VAL A 329 -22.217 28.824 0.622 1.00 33.19 O
ANISOU 1442 O VAL A 329 4734 3382 4495 -441 -541 181 O
ATOM 1443 N LEU A 330 -22.520 27.627 -1.250 1.00 28.62 N
ANISOU 1443 N LEU A 330 4287 2547 4041 -194 -507 23 N
ATOM 1444 CA LEU A 330 -23.097 26.505 -0.513 1.00 28.99 C
ANISOU 1444 CA LEU A 330 4566 2289 4160 -144 -386 35 C
ATOM 1445 CB LEU A 330 -23.568 25.404 -1.462 1.00 33.47 C
ANISOU 1445 CB LEU A 330 5350 2565 4804 -69 -283 -111 C
ATOM 1446 CG LEU A 330 -24.898 25.699 -2.148 1.00 33.79 C
ANISOU 1446 CG LEU A 330 5389 2462 4987 -357 -342 -311 C
ATOM 1447 CD1 LEU A 330 -25.147 24.664 -3.247 1.00 32.28 C
ANISOU 1447 CD1 LEU A 330 5358 2136 4772 -339 -242 -464 C
ATOM 1448 CD2 LEU A 330 -26.029 25.637 -1.100 1.00 33.43 C
ANISOU 1448 CD2 LEU A 330 5203 2429 5069 -476 -174 -307 C
ATOM 1449 C LEU A 330 -22.106 25.926 0.509 1.00 40.33 C
ANISOU 1449 C LEU A 330 6015 3854 5457 82 -339 280 C
ATOM 1450 O LEU A 330 -22.501 25.497 1.603 1.00 38.52 O
ANISOU 1450 O LEU A 330 5923 3476 5234 47 -273 353 O
ATOM 1451 N ARG A 331 -20.829 25.890 0.138 1.00 34.46 N
ANISOU 1451 N ARG A 331 5114 3391 4591 318 -368 435 N
ATOM 1452 CA ARG A 331 -19.789 25.511 1.088 1.00 43.92 C
ANISOU 1452 CA ARG A 331 6213 4825 5649 526 -378 750 C
ATOM 1453 CB ARG A 331 -18.427 25.754 0.488 1.00 48.86 C
ANISOU 1453 CB ARG A 331 6566 5811 6188 739 -427 914 C
ATOM 1454 CG ARG A 331 -17.656 24.541 0.224 1.00 66.08 C
ANISOU 1454 CG ARG A 331 8778 7910 8420 1170 -240 1135 C
ATOM 1455 CD ARG A 331 -16.339 24.980 -0.310 1.00 72.85 C
ANISOU 1455 CD ARG A 331 9306 9155 9219 1338 -290 1306 C
ATOM 1456 NE ARG A 331 -16.178 24.508 -1.670 1.00 79.52 N
ANISOU 1456 NE ARG A 331 10270 9768 10177 1538 -72 1171 N
ATOM 1457 CZ ARG A 331 -15.371 23.507 -1.997 1.00 87.77 C
ANISOU 1457 CZ ARG A 331 11325 10712 11312 1951 192 1392 C
ATOM 1458 NH1 ARG A 331 -14.649 22.919 -1.050 1.00 82.48 N
ANISOU 1458 NH1 ARG A 331 10488 10201 10648 2237 224 1809 N
ATOM 1459 NH2 ARG A 331 -15.269 23.110 -3.263 1.00 94.50 N
ANISOU 1459 NH2 ARG A 331 12356 11309 12241 2075 442 1223 N
ATOM 1460 C ARG A 331 -19.869 26.326 2.382 1.00 50.48 C
ANISOU 1460 C ARG A 331 6971 5871 6336 245 -510 832 C
ATOM 1461 O ARG A 331 -19.793 25.779 3.483 1.00 50.95 O
ANISOU 1461 O ARG A 331 7122 5932 6307 290 -494 1026 O
ATOM 1462 N HIS A 332 -20.003 27.640 2.247 1.00 47.45 N
ANISOU 1462 N HIS A 332 6455 5661 5914 -59 -608 691 N
ATOM 1463 CA HIS A 332 -20.064 28.505 3.422 1.00 48.11 C
ANISOU 1463 CA HIS A 332 6525 5919 5835 -394 -667 724 C
ATOM 1464 CB HIS A 332 -19.932 29.970 3.030 1.00 39.01 C
ANISOU 1464 CB HIS A 332 5209 4969 4643 -677 -709 581 C
ATOM 1465 CG HIS A 332 -18.555 30.363 2.662 1.00 43.71 C
ANISOU 1465 CG HIS A 332 5519 6021 5067 -596 -836 716 C
ATOM 1466 ND1 HIS A 332 -17.677 30.932 3.573 1.00 43.01 N
ANISOU 1466 ND1 HIS A 332 5287 6358 4698 -816 -951 867 N
ATOM 1467 CE1 HIS A 332 -16.535 31.187 2.964 1.00 46.31 C
ANISOU 1467 CE1 HIS A 332 5413 7140 5041 -698 -1047 972 C
ATOM 1468 NE2 HIS A 332 -16.623 30.797 1.705 1.00 42.72 N
ANISOU 1468 NE2 HIS A 332 4945 6487 4801 -396 -975 892 N
ATOM 1469 CD2 HIS A 332 -17.882 30.271 1.489 1.00 43.95 C
ANISOU 1469 CD2 HIS A 332 5377 6163 5158 -349 -858 727 C
ATOM 1470 C HIS A 332 -21.368 28.329 4.173 1.00 48.81 C
ANISOU 1470 C HIS A 332 6891 5617 6040 -588 -535 603 C
ATOM 1471 O HIS A 332 -21.416 28.396 5.398 1.00 51.44 O
ANISOU 1471 O HIS A 332 7339 5992 6214 -767 -522 694 O
ATOM 1472 N LEU A 333 -22.438 28.126 3.426 1.00 39.92 N
ANISOU 1472 N LEU A 333 5866 4123 5179 -582 -437 404 N
ATOM 1473 CA LEU A 333 -23.730 27.960 4.049 1.00 44.01 C
ANISOU 1473 CA LEU A 333 6600 4258 5866 -761 -290 295 C
ATOM 1474 CB LEU A 333 -24.798 27.797 2.990 1.00 43.50 C
ANISOU 1474 CB LEU A 333 6496 3947 6084 -737 -223 99 C
ATOM 1475 CG LEU A 333 -25.796 28.932 2.854 1.00 51.50 C
ANISOU 1475 CG LEU A 333 7177 5114 7278 -810 -73 -40 C
ATOM 1476 CD1 LEU A 333 -25.136 30.243 3.047 1.00 62.55 C
ANISOU 1476 CD1 LEU A 333 8501 6724 8542 -953 -116 -7 C
ATOM 1477 CD2 LEU A 333 -26.388 28.887 1.480 1.00 46.78 C
ANISOU 1477 CD2 LEU A 333 6480 4543 6752 -755 -29 -153 C
ATOM 1478 C LEU A 333 -23.711 26.723 4.919 1.00 52.19 C
ANISOU 1478 C LEU A 333 7853 5136 6839 -599 -214 435 C
ATOM 1479 O LEU A 333 -24.203 26.722 6.042 1.00 59.27 O
ANISOU 1479 O LEU A 333 8930 5895 7697 -774 -117 459 O
ATOM 1480 N ARG A 334 -23.131 25.663 4.382 1.00 50.19 N
ANISOU 1480 N ARG A 334 7610 4879 6580 -255 -215 537 N
ATOM 1481 CA ARG A 334 -23.110 24.374 5.047 1.00 63.41 C
ANISOU 1481 CA ARG A 334 9504 6352 8237 -33 -85 696 C
ATOM 1482 CB ARG A 334 -22.873 23.277 4.019 1.00 58.91 C
ANISOU 1482 CB ARG A 334 8999 5600 7785 299 33 686 C
ATOM 1483 CG ARG A 334 -24.070 23.092 3.119 1.00 54.79 C
ANISOU 1483 CG ARG A 334 8612 4709 7496 142 128 364 C
ATOM 1484 CD ARG A 334 -23.716 22.301 1.879 1.00 58.47 C
ANISOU 1484 CD ARG A 334 9137 5073 8006 363 230 292 C
ATOM 1485 NE ARG A 334 -24.907 21.997 1.090 1.00 53.37 N
ANISOU 1485 NE ARG A 334 8380 4386 7511 127 233 -9 N
ATOM 1486 CZ ARG A 334 -24.871 21.562 -0.164 1.00 56.33 C
ANISOU 1486 CZ ARG A 334 8807 4709 7888 148 278 -152 C
ATOM 1487 NH1 ARG A 334 -23.695 21.404 -0.775 1.00 48.14 N
ANISOU 1487 NH1 ARG A 334 7901 3643 6748 417 372 -56 N
ATOM 1488 NH2 ARG A 334 -26.007 21.292 -0.808 1.00 47.87 N
ANISOU 1488 NH2 ARG A 334 7650 3629 6908 -76 229 -359 N
ATOM 1489 C ARG A 334 -22.075 24.282 6.164 1.00 75.37 C
ANISOU 1489 C ARG A 334 10961 8210 9465 59 -179 1037 C
ATOM 1490 O ARG A 334 -21.314 23.310 6.226 1.00 73.23 O
ANISOU 1490 O ARG A 334 10684 7996 9143 418 -138 1304 O
ATOM 1491 N GLN A 335 -22.066 25.287 7.043 1.00 82.10 N
ANISOU 1491 N GLN A 335 11779 9287 10129 -282 -281 1045 N
ATOM 1492 CA GLN A 335 -21.179 25.311 8.207 1.00 87.81 C
ANISOU 1492 CA GLN A 335 12461 10394 10508 -322 -415 1361 C
ATOM 1493 CB GLN A 335 -19.723 25.282 7.761 1.00 87.61 C
ANISOU 1493 CB GLN A 335 12085 10862 10339 -64 -609 1637 C
ATOM 1494 CG GLN A 335 -19.219 26.618 7.293 1.00 87.85 C
ANISOU 1494 CG GLN A 335 11852 11255 10271 -330 -765 1507 C
ATOM 1495 CD GLN A 335 -17.801 26.526 6.793 1.00100.41 C
ANISOU 1495 CD GLN A 335 13072 13311 11768 -59 -928 1783 C
ATOM 1496 OE1 GLN A 335 -17.369 27.322 5.953 1.00 97.19 O
ANISOU 1496 OE1 GLN A 335 12442 13096 11390 -124 -990 1657 O
ATOM 1497 NE2 GLN A 335 -17.058 25.540 7.302 1.00106.17 N
ANISOU 1497 NE2 GLN A 335 13716 14216 12405 270 -971 2194 N
ATOM 1498 C GLN A 335 -21.395 26.541 9.093 1.00 86.69 C
ANISOU 1498 C GLN A 335 12375 10417 10147 -832 -462 1256 C
ATOM 1499 O GLN A 335 -22.446 27.182 9.066 1.00 84.41 O
ANISOU 1499 O GLN A 335 12232 9813 10028 -1111 -302 969 O
TER 1500 GLN A 335
HETATM 1501 OAD DRG B 1 -16.913 52.085 -3.644 1.00 21.87 O
HETATM 1502 CAQ DRG B 1 -18.087 52.173 -3.207 1.00 18.29 C
HETATM 1503 CAS DRG B 1 -19.156 52.069 -4.081 1.00 18.47 C
HETATM 1504 CAJ DRG B 1 -18.968 51.880 -5.449 1.00 19.15 C
HETATM 1505 CAH DRG B 1 -20.089 51.757 -6.304 1.00 16.84 C
HETATM 1506 CAN DRG B 1 -21.395 51.829 -5.799 1.00 19.67 C
HETATM 1507 CAA DRG B 1 -22.520 51.711 -6.653 1.00 25.26 C
HETATM 1508 CAO DRG B 1 -21.592 52.036 -4.427 1.00 22.20 C
HETATM 1509 CAB DRG B 1 -22.866 52.116 -3.794 1.00 19.46 C
HETATM 1510 CAT DRG B 1 -20.465 52.177 -3.620 1.00 21.40 C
HETATM 1511 OAL DRG B 1 -20.706 52.339 -2.325 1.00 22.41 O
HETATM 1512 CAU DRG B 1 -19.692 52.388 -1.437 1.00 22.13 C
HETATM 1513 CAR DRG B 1 -18.353 52.319 -1.857 1.00 15.64 C
HETATM 1514 CAI DRG B 1 -17.334 52.372 -0.879 1.00 22.69 C
HETATM 1515 CAF DRG B 1 -17.712 52.519 0.460 1.00 18.38 C
HETATM 1516 CAG DRG B 1 -19.054 52.618 0.841 1.00 21.40 C
HETATM 1517 CAP DRG B 1 -20.066 52.548 -0.115 1.00 21.65 C
HETATM 1518 CAK DRG B 1 -21.433 52.639 0.231 1.00 25.61 C
HETATM 1519 CAM DRG B 1 -22.368 51.413 -0.084 1.00 32.80 C
HETATM 1520 OAE DRG B 1 -21.857 50.326 -0.472 1.00 22.31 O
HETATM 1521 OAC DRG B 1 -23.600 51.605 0.140 1.00 24.49 O
HETATM 1523 O HOH S 1 -28.626 34.785 4.215 1.00 27.03 O
HETATM 1524 O HOH S 2 -47.650 29.425 8.056 1.00 26.56 O
HETATM 1525 O HOH S 3 -24.245 53.450 2.078 1.00 23.35 O
HETATM 1526 O HOH S 4 -12.178 44.652 -8.731 1.00 28.37 O
HETATM 1527 O HOH S 5 -24.927 42.673 -5.489 1.00 28.51 O
HETATM 1528 O HOH S 6 -23.646 48.402 -0.574 1.00 26.00 O
HETATM 1529 O HOH S 7 -22.287 45.745 -0.729 1.00 29.09 O
HETATM 1530 O HOH S 8 -31.590 54.969 11.707 1.00 29.64 O
HETATM 1531 O HOH S 9 -28.418 41.765 -0.998 1.00 31.77 O
HETATM 1532 O HOH S 10 -30.530 45.924 8.039 1.00 29.84 O
HETATM 1533 O HOH S 11 -33.319 26.230 0.957 1.00 29.84 O
HETATM 1534 O HOH S 12 -35.646 26.330 5.040 1.00 34.11 O
HETATM 1535 O HOH S 13 -34.846 44.984 0.897 1.00 29.86 O
HETATM 1536 O HOH S 14 -27.499 41.332 -4.679 1.00 28.34 O
HETATM 1537 O HOH S 15 -45.238 30.820 6.608 1.00 43.53 O
HETATM 1538 O HOH S 16 -28.702 41.986 12.955 1.00 37.06 O
HETATM 1539 O HOH S 17 -31.558 42.751 14.241 1.00 35.37 O
HETATM 1540 O HOH S 18 -24.593 24.298 -7.345 1.00 34.03 O
HETATM 1541 O HOH S 19 -8.656 59.398 -16.700 1.00 36.28 O
HETATM 1542 O HOH S 20 -13.395 34.463 1.907 1.00 44.34 O
HETATM 1543 O HOH S 21 -40.903 35.861 0.075 1.00 42.86 O
HETATM 1544 O HOH S 22 -30.129 28.153 3.170 1.00 34.09 O
HETATM 1545 O HOH S 23 -12.878 28.829 -13.442 1.00 47.21 O
HETATM 1546 O HOH S 24 -41.253 37.066 3.047 1.00 36.72 O
HETATM 1547 O HOH S 25 1.987 48.116 -11.341 1.00 46.52 O
HETATM 1548 O HOH S 26 -9.801 45.800 -13.365 1.00 49.67 O
HETATM 1549 O HOH S 27 -20.039 30.304 -11.343 1.00 46.35 O
HETATM 1550 O HOH S 28 -0.095 44.565 -0.710 1.00 39.19 O
HETATM 1551 O HOH S 29 -0.804 42.091 -8.287 1.00 33.98 O
HETATM 1552 O HOH S 30 -13.241 42.472 -8.951 1.00 33.71 O
HETATM 1553 O HOH S 31 -41.235 40.094 3.813 1.00 48.03 O
HETATM 1554 O HOH S 33 -16.015 36.319 7.016 1.00 41.21 O
HETATM 1555 O HOH S 34 -20.404 23.105 -2.297 1.00 47.69 O
HETATM 1556 O HOH S 35 -2.053 42.697 -1.666 1.00 34.78 O
HETATM 1557 O HOH S 36 -39.542 41.578 -3.465 1.00 35.79 O
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HETATM 1558  O   HOH S  37     -17.528  50.479 -11.644  1.00 45.34           O
HETATM 1559  O   HOH S  38      -2.790  36.224  -7.911  1.00 42.91           O
HETATM 1560  O   HOH S  39     -40.194  28.680  -2.146  1.00 39.59           O
HETATM 1561  O   HOH S  40     -38.407  41.038  13.382  1.00 42.80           O
HETATM 1562  O   HOH S  41     -22.915  26.393 -10.704  1.00 51.77           O
HETATM 1563  O   HOH S  42     -38.845  41.788  -5.971  1.00 49.03           O
HETATM 1564  O   HOH S  43     -36.099  50.115   9.037  1.00 41.25           O
HETATM 1565  O   HOH S  44     -17.355  45.376 -13.697  1.00 44.10           O
HETATM 1566  O   HOH S  45      -1.162  40.678  -6.005  1.00 39.09           O
HETATM 1567  O   HOH S  46     -28.753  22.369 -10.777  1.00 55.50           O
HETATM 1568  O   HOH S  47      -0.975  52.746  -7.990  1.00 46.39           O
HETATM 1569  O   HOH S  48      -0.894  40.925  -3.330  1.00 51.81           O
HETATM 1570  O   HOH S  49     -38.793  44.872   0.338  1.00 48.00           O
HETATM 1571  O   HOH S  50      -4.562  44.866   5.976  1.00 44.49           O
HETATM 1572  O   HOH S  51      -8.838  52.510 -19.877  1.00 48.90           O
HETATM 1573  O   HOH S  52      -3.172  41.183   0.843  1.00 32.89           O
HETATM 1574  O   HOH S  53     -39.600  39.040  -6.706  1.00 44.50           O
HETATM 1575  O   HOH S  54     -25.008  47.181  -2.438  1.00 54.96           O
HETATM 1576  O   HOH S  55     -41.565  36.148  -3.772  1.00 49.33           O
HETATM 1577  O   HOH S  56     -16.996  30.410 -13.718  1.00 49.44           O
HETATM 1578  O   HOH S  57      -0.606  40.376 -10.330  1.00 47.80           O
HETATM 1579  O   HOH S  58     -34.434  26.234   7.374  1.00 53.47           O
HETATM 1580  O   HOH S  59     -35.799  24.448   0.839  1.00 54.83           O
HETATM 1581  O   HOH S  60      -4.278  32.309 -13.316  1.00 54.95           O
HETATM 1582  O   HOH S  61     -32.854  27.376   3.585  1.00 57.52           O
HETATM 1583  O   HOH S  62     -29.653  39.466  -9.483  1.00 30.72           O
HETATM 1584  O   HOH S  63     -38.448  44.245   9.663  1.00 41.03           O
HETATM 1585  O   HOH S  64     -12.664  36.441  -9.105  1.00 34.86           O
HETATM 1586  O   HOH S  65     -26.130  31.681   7.764  1.00 52.31           O
HETATM 1587  O   HOH S  66      -7.106  38.900   6.887  1.00 53.76           O
HETATM 1588  O   HOH S  67      -5.686  44.678   8.679  1.00 53.91           O
HETATM 1589  O   HOH S  68      -5.310  50.083 -15.622  1.00 48.56           O
HETATM 1590  O   HOH S  69     -12.151  44.755 -11.201  1.00 52.71           O
HETATM 1591  O   HOH S  70     -32.153  39.882 -10.835  1.00 52.92           O
HETATM 1592  O   HOH S  71     -40.912  45.254   8.515  1.00 57.89           O
HETATM 1593  O   HOH S  72      -2.684  33.749 -15.633  1.00 73.29           O
HETATM 1594  O   HOH S  73     -36.012  52.047  11.245  1.00 52.92           O
HETATM 1595  O   HOH S  74      -0.858  48.085  -5.158  1.00 40.90           O
HETATM 1596  O   HOH S  75     -21.507  55.180  10.249  1.00 38.22           O
HETATM 1597  O   HOH S  76     -29.020  37.926  11.432  1.00 58.69           O
HETATM 1598  O   HOH S  77     -36.997  40.484  15.741  1.00 54.77           O
HETATM 1599  O   HOH S  78      -7.288  40.043 -12.107  1.00 46.19           O
HETATM 1600  O   HOH S  79     -39.134  51.613   3.883  1.00 60.09           O
HETATM 1601  O   HOH S  80     -29.823  60.093   1.452  1.00 41.05           O
HETATM 1602  O   HOH S  81      -6.828  60.448  -9.582  1.00 38.94           O
HETATM 1603  O   HOH S  82     -20.347  50.897 -10.447  1.00 41.52           O
HETATM 1604  O   HOH S  83     -20.453  38.061  11.698  1.00 52.10           O
HETATM 1605  O   HOH S  84      -9.000  38.961 -14.050  1.00 55.93           O
HETATM 1606  O   HOH S  85     -13.476  38.546  10.079  1.00 45.40           O
HETATM 1607  O   HOH S  86      -1.261  50.399  -5.536  1.00 51.75           O
HETATM 1608  O   HOH S  87     -29.289  25.588   3.450  1.00 58.12           O
HETATM 1609  O   HOH S  88     -27.435  36.764  12.898  1.00 54.77           O
HETATM 1610  O   HOH S  89     -39.441  47.478   6.524  1.00 52.37           O
HETATM 1611  O   HOH S  90     -28.782  30.517   9.098  1.00 60.43           O
HETATM 1612  O   HOH S  91     -25.426  31.438  10.148  1.00 61.49           O
HETATM 1613  O   HOH S  92     -33.527  37.427 -12.120  1.00 49.18           O
HETATM 1614  O   HOH S  93      -6.868  50.707 -18.505  1.00 50.15           O
HETATM 1615  O   HOH S  94     -35.352  21.726  -2.285  1.00 61.43           O
HETATM 1616  O   HOH S  95     -15.812  25.105   4.715  1.00 63.37           O
HETATM 1617  O   HOH S  96     -29.866  61.685   9.944  1.00 65.49           O
HETATM 1618  O   HOH S  97     -27.164  42.367  -8.980  1.00 48.83           O
HETATM 1619  O   HOH S  98     -18.982  36.563  -9.603  1.00 29.51           O
HETATM 1620  O   HOH S  99     -11.189  32.358 -16.167  1.00 32.70           O
HETATM 1621  O   HOH S 100     -10.913  22.271 -12.926  1.00 68.19           O
HETATM 1622  O   HOH S 101     -28.185  47.430   0.578  1.00 38.10           O
HETATM 1623  O   HOH S 102     -35.456  47.332  10.106  1.00 56.92           O
HETATM 1624  O   HOH S 103     -17.914  47.101 -11.833  1.00 43.20           O
HETATM 1625  O   HOH S 104      -0.497  48.708  -0.679  1.00 42.44           O
HETATM 1626  O   HOH S 105      -3.385  38.402   0.448  1.00 46.11           O
HETATM 1627  O   HOH S 106      -5.480  37.289  -0.956  1.00 56.81           O
HETATM 1628  O   HOH S 107     -39.368  34.378  11.707  1.00 45.98           O
HETATM 1629  O   HOH S 108      -7.993  44.416 -14.099  1.00 57.03           O
HETATM 1630  O   HOH S 109     -26.188  21.362 -10.628  1.00 50.15           O
HETATM 1631  O   HOH S 110      -7.070  53.352 -21.857  1.00 51.73           O
HETATM 1632  O   HOH S 111     -27.759  45.038  -2.135  1.00 52.15           O
HETATM 1633  O   HOH S 112     -45.575  33.318  11.373  1.00 54.88           O
HETATM 1634  O   HOH S 113     -40.213  41.041   1.415  1.00 56.13           O
HETATM 1635  O   HOH S 114     -24.062  22.286  -9.305  1.00 56.30           O
HETATM 1636  O   HOH S 115     -29.751  62.184   3.214  1.00 59.44           O
HETATM 1637  O   HOH S 116     -36.144  21.864  -4.757  1.00 66.85           O
HETATM 1638  O   HOH S 117     -14.039  32.204   0.301  1.00 53.76           O
HETATM 1639  O   HOH S 118      -4.451  41.510 -15.804  1.00 56.62           O
HETATM 1640  O   HOH S 119     -40.947  31.934  -2.395  1.00 51.83           O
HETATM 1641  O   HOH S 120      -2.530  52.445  -3.131  1.00 32.81           O
HETATM 1643  O   HOH S 122     -18.008  51.050  14.806  1.00 46.96           O
HETATM 1644  O   HOH S 123     -29.579  48.175  10.569  1.00 36.92           O
HETATM 1645  O   HOH S 124     -30.555  50.195  12.051  1.00 43.32           O
HETATM 1646  O   HOH S 125     -35.450  33.626  11.031  1.00 35.19           O
HETATM 1647  O   HOH S 126     -33.049  36.196  11.934  1.00 54.98           O
HETATM 1648  O   HOH S 127     -42.986  29.868  -1.137  1.00 53.56           O
HETATM 1649  O   HOH S 128     -32.867  34.876 -11.501  1.00 34.67           O
HETATM 1650  O   HOH S 129     -29.358  32.427 -13.212  1.00 34.76           O
HETATM 1651  O   HOH S 130     -40.317  46.851   2.832  1.00 48.74           O
HETATM 1653  O   HOH S 132     -23.707  45.060  -4.522  1.00 44.38           O
HETATM 1654  O   HOH S 133      -5.646  53.727 -14.252  1.00 35.34           O
HETATM 1655  O   HOH S 135      -9.150  37.201   1.775  1.00 50.25           O
HETATM 1656  O   HOH S 136     -22.113  30.881   7.444  1.00 58.42           O
HETATM 1659  O   HOH S 138      -7.204  46.240   9.573  1.00 30.00           O
HETATM 1660  O   HOH S 139     -38.441  50.149   7.696  1.00 30.00           O
END
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Table 7. DMXAA-hSTING^{G230I} complex

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REMARK   3
REMARK   3 REFINEMENT.
REMARK   3  PROGRAM     : PHENIX (phenix.refine: 1.8.2_1309)
REMARK   3  AUTHORS     : Adams,Afonine,Burnley,Chen,Davis,Echols,Gildea,
REMARK   3              : Gopal,Gros,Grosse-Kunstleve,Headd,Hung,Immormino,
REMARK   3              : Ioerger,McCoy,McKee,Moriarty,Pai,Read,Richardson,
REMARK   3              : Richardson,Romo,Sacchettini,Sauter,Smith,Storoni,
REMARK   3              : Terwilliger,Zwart
REMARK   3
REMARK   3  REFINEMENT TARGET : ML
REMARK   3
REMARK   3  DATA USED IN REFINEMENT.
REMARK   3  RESOLUTION RANGE HIGH (ANGSTROMS) : 2.510
REMARK   3  RESOLUTION RANGE LOW  (ANGSTROMS) : 78.660
REMARK   3  MIN(FOBS/SIGMA_FOBS)              : 1.39
REMARK   3  COMPLETENESS FOR RANGE        (%) : 94.13
REMARK   3  NUMBER OF REFLECTIONS             : 14320
REMARK   3  NUMBER OF REFLECTIONS (NON-ANOMALOUS) : 14320
REMARK   3
REMARK   3  FIT TO DATA USED IN REFINEMENT.
REMARK   3  R VALUE     (WORKING + TEST SET) : 0.1995
REMARK   3  R VALUE           (WORKING SET) : 0.1975
REMARK   3  FREE R VALUE                    : 0.2391
REMARK   3  FREE R VALUE TEST SET SIZE   (%) : 5.03
REMARK   3  FREE R VALUE TEST SET COUNT      : 720
REMARK   3
REMARK   3  FIT TO DATA USED IN REFINEMENT (IN BINS).
REMARK   3  BIN  RESOLUTION RANGE  COMPL.    NWORK NFREE   RWORK
RFREE
REMARK   3     1 78.6985 -  4.2921    0.95     2803   147  0.1705 0.1929
REMARK   3     2  4.2921 -  3.4068    0.95     2763   123  0.1804 0.2261
REMARK   3     3  3.4068 -  2.9761    0.93     2678   149  0.2266 0.2915
REMARK   3     4  2.9761 -  2.7040    0.94     2706   156  0.2615 0.3201
REMARK   3     5  2.7040 -  2.5102    0.92     2650   145  0.2906 0.3356
REMARK   3
REMARK   3  BULK SOLVENT MODELLING.
REMARK   3  METHOD USED        : FLAT BULK SOLVENT MODEL
REMARK   3  SOLVENT RADIUS     : 1.11
REMARK   3  SHRINKAGE RADIUS   : 0.90
REMARK   3  GRID STEP FACTOR   : 4.00
REMARK   3
REMARK   3  ERROR ESTIMATES.
REMARK   3  COORDINATE ERROR (MAXIMUM-LIKELIHOOD BASED)     : 0.38
REMARK   3  PHASE ERROR (DEGREES, MAXIMUM-LIKELIHOOD BASED) :
28.36
REMARK   3
REMARK   3  STRUCTURE FACTORS CALCULATION ALGORITHM : FFT
REMARK   3
REMARK   3  DEVIATIONS FROM IDEAL VALUES.
REMARK   3              RMSD     MAX  COUNT
REMARK   3  BOND      : 0.007   0.050  3034
REMARK   3  ANGLE     : 1.262  16.566  4120
REMARK   3  CHIRALITY : 0.081   0.389   446
REMARK   3  PLANARITY : 0.005   0.043   544
REMARK   3  DIHEDRAL  : 20.446  89.486  1142
REMARK   3  MIN NONBONDED DISTANCE : 2.017
REMARK   3
REMARK   3  MOLPROBITY STATISTICS.
REMARK   3  ALL-ATOM CLASHSCORE : 14.50
REMARK   3  RAMACHANDRAN PLOT:
REMARK   3    OUTLIERS : 0.56 %
REMARK   3    ALLOWED  : 3.89 %
REMARK   3    FAVORED  : 95.56 %
REMARK   3  ROTAMER OUTLIERS : 14.15 %
REMARK   3  CBETA DEVIATIONS : 3
REMARK   3
REMARK   3  ATOMIC DISPLACEMENT PARAMETERS.
REMARK   3  WILSON B : None
REMARK   3  RMS(B_ISO_OR_EQUIVALENT_BONDED) : 8.54
REMARK   3  ATOMS         NUMBER OF ATOMS
REMARK   3                ISO.  ANISO.
REMARK   3  ALL       :  3020    2932
REMARK   3  ALL (NO H) :  3020    2932
REMARK   3  SOLVENT    :    46       0
REMARK   3  NON-SOLVENT :  2974    2932
REMARK   3  HYDROGENS  :     0       0
REMARK   3
REMARK   3  TLS DETAILS.
REMARK   3  NUMBER OF TLS GROUPS: 13
REMARK   3  ORIGIN: CENTER OF MASS
REMARK   3  TLS GROUP : 1
REMARK   3    SELECTION: chain 'A' and (resid  154  through  184 )
REMARK   3    ORIGIN FOR THE GROUP (A):  18.5649 -84.9417 -65.0832
REMARK   3    T TENSOR
REMARK   3      T11:  0.4393 T22:  0.3018
REMARK   3      T33:  0.4398 T12:  0.0825
REMARK   3      T13: -0.0564 T23: -0.0648
REMARK   3    L TENSOR
REMARK   3      L11:  0.5884 L22:  3.2436
REMARK   3      L33:  1.0127 L12: -0.3808
REMARK   3      L13:  0.0492 L23:  1.3981
REMARK   3    S TENSOR
REMARK   3      S11: -0.0732 S12: -0.1629 S13:  0.0759
REMARK   3      S21: -0.2078 S22:  0.5745 S23: -0.8923
REMARK   3      S31:  0.5100 S32:  0.4198 S33: -0.2551
REMARK   3  TLS GROUP : 2
REMARK   3    SELECTION: chain 'A' and (resid  185  through  203 )
REMARK   3    ORIGIN FOR THE GROUP (A):  15.0533 -97.1915 -72.8326
REMARK   3    T TENSOR
REMARK   3      T11:  0.4444 T22:  0.4429
REMARK   3      T33:  0.7942 T12:  0.0775
REMARK   3      T13:  0.1063 T23: -0.1346
REMARK   3    L TENSOR
REMARK   3      L11:  1.3482 L22:  3.5737
REMARK   3      L33:  1.1882 L12: -0.3929
REMARK   3      L13:  0.5508 L23:  0.1118
REMARK   3    S TENSOR
REMARK   3      S11: -0.1754 S12:  0.1904 S13: -0.9845
REMARK   3      S21: -0.1476 S22: -0.0773 S23: -0.9503
REMARK   3      S31:  0.5475 S32: -0.1593 S33:  0.2662
REMARK   3  TLS GROUP : 3
REMARK   3    SELECTION: chain 'A' and (resid  204  through  218 )
REMARK   3    ORIGIN FOR THE GROUP (A):  -0.0262 -86.6210 -74.0738
REMARK   3    T TENSOR
REMARK   3      T11:  0.4134 T22:  0.5352
REMARK   3      T33:  1.1526 T12:  0.0870
REMARK   3      T13:  0.0015 T23:  0.0352
REMARK   3    L TENSOR
REMARK   3      L11:  0.3197 L22:  2.3847
REMARK   3      L33:  1.9616 L12: -0.7523
REMARK   3      L13: -0.2715 L23:  1.7058
REMARK   3    S TENSOR
REMARK   3      S11: -0.1620 S12:  0.0679 S13: -1.4908
REMARK   3      S21: -0.4128 S22: -0.4686 S23:  2.4070
REMARK   3      S31:  0.1596 S32: -0.0763 S33:  0.3138
REMARK   3  TLS GROUP : 4
REMARK   3    SELECTION: chain 'A' and (resid  219  through  247 )
REMARK   3    ORIGIN FOR THE GROUP (A):  12.4963 -92.7353 -62.3817
REMARK   3    T TENSOR
REMARK   3      T11:  0.6214 T22:  0.4812
REMARK   3      T33:  0.6515 T12:  0.0930
REMARK   3      T13:  0.0352 T23:  0.0210
REMARK   3    L TENSOR
REMARK   3      L11:  2.3340 L22:  4.1461
REMARK   3      L33:  4.4152 L12: -1.2271
REMARK   3      L13: -1.0413 L23:  0.0238
REMARK   3    S TENSOR
REMARK   3      S11: -0.1280 S12: -0.6561 S13: -0.2175
REMARK   3      S21:  1.0992 S22:  0.2608 S23: -0.2951
REMARK   3      S31:  0.3088 S32: -0.4641 S33:  0.1404
REMARK   3  TLS GROUP : 5
REMARK   3    SELECTION: chain 'A' and (resid  248  through  262 )
REMARK   3    ORIGIN FOR THE GROUP (A):  8.4387 -94.2521 -79.3077
REMARK   3    T TENSOR
REMARK   3      T11:  0.6585 T22:  0.4111
REMARK   3      T33:  0.6599 T12:  0.1126
REMARK   3      T13: -0.0693 T23: -0.1355
REMARK   3    L TENSOR
REMARK   3      L11:  2.0873 L22:  1.5403
REMARK   3      L33:  0.4325 L12:  0.6038
REMARK   3      L13:  0.5988 L23: -0.0328
REMARK   3    S TENSOR
REMARK   3      S11:  0.1274 S12:  0.2224 S13: -0.5200
REMARK   3      S21: -0.6720 S22: -0.2759 S23:  0.6116
REMARK   3      S31:  0.0107 S32:  0.0571 S33: -0.0481
REMARK   3  TLS GROUP : 6
REMARK   3    SELECTION: chain 'A' and (resid  263  through  280 )
REMARK   3    ORIGIN FOR THE GROUP (A):  -0.0640 -71.1490 -64.7673
REMARK   3    T TENSOR
REMARK   3      T11:  0.2561 T22:  0.3183
REMARK   3      T33:  0.4491 T12: -0.0366
REMARK   3      T13:  0.0507 T23: -0.0720
REMARK   3    L TENSOR
REMARK   3      L11:  3.8910 L22:  3.4313
REMARK   3      L33:  2.8197 L12: -2.0277
REMARK   3      L13: -0.9236 L23:  0.2563
REMARK   3    S TENSOR
REMARK   3      S11: -0.1066 S12:  0.1651 S13:  0.0430
REMARK   3      S21:  0.1833 S22: -0.0732 S23:  0.6659
REMARK   3      S31:  0.3945 S32: -0.8557 S33:  0.0402
REMARK   3  TLS GROUP : 7
REMARK   3    SELECTION: chain 'A' and (resid  281  through  301 )
REMARK   3    ORIGIN FOR THE GROUP (A):  11.2863 -70.6978 -72.9476
REMARK   3    T TENSOR
REMARK   3      T11:  0.3233 T22:  0.2157
REMARK   3      T33:  0.3495 T12:  0.0468
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REMARK   3    T13:  0.0400 T23:  0.0147
REMARK   3   L TENSOR
REMARK   3    L11:  8.5718 L22:  4.6285
REMARK   3    L33:  3.2871 L12: -2.7268
REMARK   3    L13:  1.2567 L23:  0.1583
REMARK   3   S TENSOR
REMARK   3    S11:  0.4866 S12:  0.3128 S13:  1.2110
REMARK   3    S21: -0.5846 S22: -0.2970 S23: -0.6743
REMARK   3    S31: -0.0057 S32:  0.0562 S33: -0.0866
REMARK   3  TLS GROUP : 8
REMARK   3   SELECTION: chain 'A' and (resid  302  through  314 )
REMARK   3   ORIGIN FOR THE GROUP (A):  19.5103 -82.4342 -73.4070
REMARK   3   T TENSOR
REMARK   3    T11:  0.4366 T22:  0.4324
REMARK   3    T33:  0.9085 T12: -0.0064
REMARK   3    T13: -0.0121 T23: -0.1791
REMARK   3   L TENSOR
REMARK   3    L11:  5.0079 L22:  1.4371
REMARK   3    L33:  2.3589 L12:  0.3981
REMARK   3    L13:  1.8094 L23:  0.5328
REMARK   3   S TENSOR
REMARK   3    S11: -0.2832 S12: -0.0864 S13:  1.3536
REMARK   3    S21: -0.2094 S22:  0.2364 S23: -1.3952
REMARK   3    S31: -0.0630 S32:  0.4603 S33: -0.1243
REMARK   3  TLS GROUP : 9
REMARK   3   SELECTION: chain 'A' and (resid  315  through  335 )
REMARK   3   ORIGIN FOR THE GROUP (A):   5.9841 -84.6983 -84.8320
REMARK   3   T TENSOR
REMARK   3    T11:  0.8254 T22:  0.4773
REMARK   3    T33:  0.7360 T12:  0.0892
REMARK   3    T13: -0.2281 T23: -0.1026
REMARK   3   L TENSOR
REMARK   3    L11:  0.5859 L22:  3.6900
REMARK   3    L33:  3.4392 L12:  0.8135
REMARK   3    L13: -1.0849 L23:  0.4363
REMARK   3   S TENSOR
REMARK   3    S11:  0.1659 S12:  0.6695 S13:  0.4312
REMARK   3    S21: -1.8859 S22:  0.0194 S23:  0.7650
REMARK   3    S31: -1.3287 S32: -0.1047 S33:  0.1265
REMARK   3  TLS GROUP : 10
REMARK   3   SELECTION: chain 'B' and (resid  154  through  184 )
REMARK   3   ORIGIN FOR THE GROUP (A):   2.6989 -79.4016 -49.5127
REMARK   3   T TENSOR
REMARK   3    T11:  0.4055 T22:  0.5218
REMARK   3    T33:  0.4268 T12: -0.0439
REMARK   3    T13:  0.0964 T23:  0.1163
REMARK   3   L TENSOR
REMARK   3    L11:  0.8467 L22:  1.0167
REMARK   3    L33:  1.5333 L12:  0.1082
REMARK   3    L13:  0.4092 L23: -0.9415
REMARK   3   S TENSOR
REMARK   3    S11: -0.3737 S12: -0.2406 S13: -0.4167
REMARK   3    S21: -0.1505 S22:  0.5597 S23: -0.1553
REMARK   3    S31:  0.3988 S32: -0.8521 S33: -0.0941
REMARK   3  TLS GROUP : 11
REMARK   3   SELECTION: chain 'B' and (resid  185  through  197 )
REMARK   3   ORIGIN FOR THE GROUP (A):   4.3298 -89.0654 -31.6612
REMARK   3   T TENSOR
REMARK   3    T11:  0.8391 T22:  0.9093
REMARK   3    T33:  0.9086 T12: -0.0131
REMARK   3    T13:  0.1673 T23:  0.1257
REMARK   3   L TENSOR
REMARK   3    L11:  0.3021 L22:  2.2105
REMARK   3    L33:  0.2378 L12:  0.5587
REMARK   3    L13:  0.0275 L23:  0.7643
REMARK   3   S TENSOR
REMARK   3    S11: -0.3698 S12: -0.2731 S13: -0.2713
REMARK   3    S21:  1.3272 S22:  0.5413 S23: -0.7772
REMARK   3    S31: -0.2905 S32: -0.6279 S33: -0.0887
REMARK   3  TLS GROUP : 12
REMARK   3   SELECTION: chain 'B' and (resid  198  through  252 )
REMARK   3   ORIGIN FOR THE GROUP (A):  12.7528 -81.7477 -42.9709
REMARK   3   T TENSOR
REMARK   3    T11:  0.6197 T22:  0.7199
REMARK   3    T33:  0.5747 T12:  0.0259
REMARK   3    T13: -0.0478 T23:  0.1385
REMARK   3   L TENSOR
REMARK   3    L11:  1.7783 L22:  3.4469
REMARK   3    L33:  1.9528 L12:  0.4436
REMARK   3    L13: -0.9387 L23: -1.2119
REMARK   3   S TENSOR
REMARK   3    S11:  0.0497 S12: -0.4807 S13: -0.8641
REMARK   3    S21:  0.2895 S22: -0.1031 S23: -0.6763
REMARK   3    S31:  0.5541 S32:  0.3894 S33:  0.0559
REMARK   3  TLS GROUP : 13
REMARK   3   SELECTION: chain 'B' and (resid  253  through  335 )
REMARK   3   ORIGIN FOR THE GROUP (A):  12.4991 -68.6162 -46.0924
REMARK   3   T TENSOR
REMARK   3    T11:  0.3619 T22:  0.5606
REMARK   3    T33:  0.3032 T12:  0.0043
REMARK   3    T13: -0.0138 T23: -0.0069
REMARK   3   L TENSOR
REMARK   3    L11:  2.2900 L22:  3.5956
REMARK   3    L33:  3.1007 L12:  0.4476
REMARK   3    L13: -0.6791 L23: -1.4882
REMARK   3   S TENSOR
REMARK   3    S11:  0.1403 S12: -0.7469 S13:  0.0186
REMARK   3    S21:  0.7529 S22: -0.0615 S23:  0.0205
REMARK   3    S31: -0.3571 S32:  0.0704 S33: -0.0094
REMARK   3
CRYST1  36.570  77.919  79.634  90.00  98.97  90.00 P 1 21 1
SCALE1      0.027345  0.000000  0.004317        0.00000
SCALE2      0.000000  0.012834  0.000000        0.00000
SCALE3      0.000000  0.000000  0.012713        0.00000
ATOM      1  N   SER A 154      12.290 -62.777 -65.163  1.00 38.38           N
ANISOU    1  N   SER A 154     4119   4350   6113   -935    208   -285       N
ATOM      2  CA  SER A 154      11.396 -63.506 -66.054  1.00 25.17           C
ANISOU    2  CA  SER A 154     2763   2582   4220   -991    161   -112       C
ATOM      3  CB  SER A 154      12.123 -63.829 -67.354  1.00 30.71           C
ANISOU    3  CB  SER A 154     3671   3116   4882  -1071    398   -137       C
ATOM      4  OG  SER A 154      11.332 -64.604 -68.222  1.00 38.95           O
ANISOU    4  OG  SER A 154     5026   4061   5710  -1111    343     16       O
ATOM      5  C   SER A 154      10.920 -64.795 -65.403  1.00 36.48           C
ANISOU    5  C   SER A 154     4192   4114   5553   -883    -20    -45       C
ATOM      6  O   SER A 154      11.686 -65.464 -64.707  1.00 40.92           O
ANISOU    6  O   SER A 154     4592   4763   6193   -768    -27   -147       O
ATOM      7  N   VAL A 155       9.654 -65.141 -65.634  1.00 38.95           N
ANISOU    7  N   VAL A 155     4692   4404   5704   -917   -168    118       N
ATOM      8  CA  VAL A 155       9.066 -66.362 -65.094  1.00 30.23           C
ANISOU    8  CA  VAL A 155     3619   3370   4498   -838   -323    197       C
ATOM      9  CB  VAL A 155       7.565 -66.467 -65.416  1.00 34.83           C
ANISOU    9  CB  VAL A 155     4383   3908   4945   -903   -477    357       C
ATOM     10  CG1 VAL A 155       7.082 -67.913 -65.299  1.00 26.15           C
ANISOU   10  CG1 VAL A 155     3391   2817   3729   -855   -571    439       C
ATOM     11  CG2 VAL A 155       6.765 -65.560 -64.508  1.00 17.05           C
ANISOU   11  CG2 VAL A 155     1968   1754   2755   -901   -610    369       C
ATOM     12  C   VAL A 155       9.781 -67.590 -65.652  1.00 22.80           C
ANISOU   12  C   VAL A 155     2793   2367   3502   -802   -230    175       C
ATOM     13  O   VAL A 155      10.131 -68.517 -64.919  1.00 35.79           O
ANISOU   13  O   VAL A 155     4350   4095   5154   -688   -288    139       O
ATOM     14  N   ALA A 156       9.997 -67.576 -66.960  1.00 21.75           N
ANISOU   14  N   ALA A 156     2877   2081   3307   -895    -85    196       N
ATOM     15  CA  ALA A 156      10.641 -68.677 -67.665  1.00 30.61           C
ANISOU   15  CA  ALA A 156     4137   3123   4369   -877     24    176       C
ATOM     16  CB  ALA A 156      10.571 -68.456 -69.164  1.00 42.97           C
ANISOU   16  CB  ALA A 156     5999   4500   5826  -1001    167    229       C
ATOM     17  C   ALA A 156      12.095 -68.868 -67.247  1.00 39.65           C
ANISOU   17  C   ALA A 156     5066   4319   5682   -792    159    -10       C
ATOM     18  O   ALA A 156      12.624 -69.982 -67.245  1.00 48.24           O
ANISOU   18  O   ALA A 156     6166   5406   6756   -714    173    -50       O
ATOM     19  N   HIS A 157      12.751 -67.764 -66.923  1.00 33.82           N
ANISOU   19  N   HIS A 157     4124   3612   5116   -806    256   -135       N
ATOM     20  CA  HIS A 157      14.158 -67.781 -66.578  1.00 30.84           C
ANISOU   20  CA  HIS A 157     3512   3266   4941   -733    390   -345       C
ATOM     21  CB  HIS A 157      14.680 -66.351 -66.440  1.00 44.66           C
ANISOU   21  CB  HIS A 157     5077   5016   6877   -792    513   -466       C
ATOM     22  CG  HIS A 157      16.159 -66.254 -66.244  1.00 41.24           C
ANISOU   22  CG  HIS A 157     4392   4586   6690   -740    679   -708       C
ATOM     23  ND1 HIS A 157      17.059 -66.776 -67.134  1.00 43.00           N
ANISOU   23  ND1 HIS A 157     4684   4694   6960   -775    905   -806       N
ATOM     24  CE1 HIS A 157      18.292 -66.536 -66.707  1.00 40.67           C
ANISOU   24  CE1 HIS A 157     4095   4426   6932   -715   1012  -1047       C
ATOM     25  NE2 HIS A 157      18.214 -65.881 -65.569  1.00 35.86           N
ANISOU   25  NE2 HIS A 157     3242   3945   6436   -637    849  -1103       N
ATOM     26  CD2 HIS A 157      16.885 -65.684 -65.256  1.00 34.62           C
ANISOU   26  CD2 HIS A 157     3227   3848   6080   -654    648   -889       C
ATOM     27  C   HIS A 157      14.386 -68.557 -65.279  1.00 33.45           C
ANISOU   27  C   HIS A 157     3643   3745   5322   -555    203   -407       C
ATOM     28  O   HIS A 157      15.263 -69.426 -65.196  1.00 36.54           O
ANISOU   28  O   HIS A 157     3971   4136   5776   -459    237   -520       O
ATOM     29  N   GLY A 158      13.584 -68.249 -64.266  1.00 30.30           N
ANISOU   29  N   GLY A 158     3164   3462   4888   -508      4   -334       N
ATOM     30  CA  GLY A 158      13.659 -68.964 -63.006  1.00 25.57           C
ANISOU   30  CA  GLY A 158     2434   2991   4292   -341   -184   -367       C
ATOM     31  C   GLY A 158      13.309 -70.431 -63.176  1.00 30.72           C
ANISOU   31  C   GLY A 158     3285   3621   4766   -292   -277   -248       C
ATOM     32  O   GLY A 158      13.948 -71.304 -62.589  1.00 42.20           O
ANISOU   32  O   GLY A 158     4680   5128   6227   -144   -372   -310       O
ATOM     33  N   LEU A 159      12.288 -70.700 -63.984  1.00 24.37           N
ANISOU   33  N   LEU A 159     2729   2727   3804   -411   -260    -83       N
ATOM     34  CA  LEU A 159      11.844 -72.068 -64.235  1.00 25.17           C
ANISOU   34  CA  LEU A 159     3030   2791   3741   -385   -342     35       C
ATOM     35  CB  LEU A 159      10.560 -72.069 -65.067  1.00 36.37           C
ANISOU   35  CB  LEU A 159     4689   4120   5010   -524   -364    211       C
ATOM     36  CG  LEU A 159       9.251 -72.243 -64.293  1.00 35.53           C
ANISOU   36  CG  LEU A 159     4631   4067   4802   -530   -546    352       C
ATOM     37  CD2 LEU A 159       8.069 -71.768 -65.123  1.00 18.32           C
ANISOU   37  CD2 LEU A 159     2607   1802   2554   -672   -565    466       C
ATOM     38  CD1 LEU A 159       9.310 -71.503 -62.965  1.00 38.67           C
ANISOU   38  CD1 LEU A 159     4804   4608   5280   -452   -641    305       C
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ATOM    39  C   LEU A 159      12.917 -72.905 -64.928  1.00 29.35           C
ANISOU  39  C   LEU A 159      3607   3247   4297   -333   -227    -61       C
ATOM    40  O   LEU A 159      13.122 -74.070 -64.587  1.00 35.64           O
ANISOU  40  O   LEU A 159      4431   4062   5047   -220   -312    -66       O
ATOM    41  N   ALA A 160      13.598 -72.306 -65.900  1.00 37.83           N
ANISOU  41  N   ALA A 160      4701   4226   5446   -420    -23    -142      N
ATOM    42  CA  ALA A 160      14.657 -72.996 -66.627  1.00 31.63           C
ANISOU  42  CA  ALA A 160      3943   3361   4715   -388    128    -260      C
ATOM    43  CB  ALA A 160      15.168 -72.131 -67.769  1.00 25.03           C
ANISOU  43  CB  ALA A 160      3171   2401   3937   -526    387    -322      C
ATOM    44  C   ALA A 160      15.795 -73.362 -65.683  1.00 34.97           C
ANISOU  44  C   ALA A 160      4105   3868   5315   -217     89    -457      C
ATOM    45  O   ALA A 160      16.364 -74.450 -65.764  1.00 30.64           O
ANISOU  45  O   ALA A 160      3585   3304   4754   -112     53    -506      O
ATOM    46  N   TRP A 161      16.115 -72.437 -64.785  1.00 33.35           N
ANISOU  46  N   TRP A 161      3645   3743   5283   -183     84    -584      N
ATOM    47  CA  TRP A 161      17.152 -72.645 -63.787  1.00 26.02           C
ANISOU  47  CA  TRP A 161      2457   2894   4534     -5      4    -787      C
ATOM    48  CB  TRP A 161      17.634 -71.318 -63.223  1.00 35.89           C
ANISOU  48  CB  TRP A 161      3436   4209   5993     -6     36    -935      C
ATOM    49  CG  TRP A 161      18.635 -70.691 -64.132  1.00 43.81           C
ANISOU  49  CG  TRP A 161      4337   5114   7193   -105    312   -1104      C
ATOM    50  CD1 TRP A 161      18.423 -69.712 -65.065  1.00 27.79           C
ANISOU  50  CD1 TRP A 161      2394   2998   5168   -294    522   -1056      C
ATOM    51  NE1 TRP A 161      19.588 -69.438 -65.731  1.00 51.15           N
ANISOU  51  NE1 TRP A 161      5238   5863   8333   -345    782   -1256      N
ATOM    52  CE2 TRP A 161      20.580 -70.245 -65.240  1.00 44.33           C
ANISOU  52  CE2 TRP A 161      4188   5031   7625   -183    731   -1451      C
ATOM    53  CD2 TRP A 161      20.008 -71.056 -64.239  1.00 38.97           C
ANISOU  53  CD2 TRP A 161      3539   4463   6806    -22    425   -1354      C
ATOM    54  CE3 TRP A 161      20.819 -71.988 -63.576  1.00 38.53           C
ANISOU  54  CE3 TRP A 161      3342   4444   6853    177    294   -1516      C
ATOM    55  CZ3 TRP A 161      22.153 -72.074 -63.924  1.00 32.78           C
ANISOU  55  CZ3 TRP A 161      2415   3651   6388    212    460   -1783      C
ATOM    56  CH2 TRP A 161      22.696 -71.249 -64.926  1.00 48.47           C
ANISOU  56  CH2 TRP A 161      4352   5533   8531     36    788   -1884      C
ATOM    57  CZ2 TRP A 161      21.928 -70.333 -65.593  1.00 45.55           C
ANISOU  57  CZ2 TRP A 161      4152   5116   8039    -163    932   -1714      C
ATOM    58  C   TRP A 161      16.763 -73.609 -62.669  1.00 34.15           C
ANISOU  58  C   TRP A 161      3517   4010   5448    163   -254    -725      C
ATOM    59  O   TRP A 161      17.583 -74.406 -62.219  1.00 36.07           O
ANISOU  59  O   TRP A 161      3682   4262   5762    324   -327    -858      O
ATOM    60  N   SER A 162      15.518 -73.543 -62.214  1.00 39.41           N
ANISOU  60  N   SER A 162      4305   4727   5941    128   -389    -532      N
ATOM    61  CA  SER A 162      15.095 -74.397 -61.114  1.00 29.89           C
ANISOU  61  CA  SER A 162      3153   3589   4613    271   -605    -465      C
ATOM    62  C   SER A 162      14.876 -75.814 -61.623  1.00 23.85           C
ANISOU  62  C   SER A 162      2623   2742   3696    288   -621    -366      C
ATOM    63  O   SER A 162      15.062 -76.783 -60.892  1.00 28.93           O
ANISOU  63  O   SER A 162      3309   3402   4282    441   -761    -379      O
ATOM    64  CB  SER A 162      13.837 -73.867 -60.426  1.00 40.44           C
ANISOU  64  CB  SER A 162      4532   5000   5833    220   -717    -307      C
ATOM    65  OG  SER A 162      12.692 -74.127 -61.207  1.00 54.79           O
ANISOU  65  OG  SER A 162      6572   6752   7492     71   -685    -110      O
ATOM    66  N   TYR A 163      14.484 -75.931 -62.886  1.00 23.57           N
ANISOU  66  N   TYR A 163      2759   2608   3590    134   -484    -269      N
ATOM    67  CA  TYR A 163      14.335 -77.235 -63.506  1.00 28.48           C
ANISOU  67  CA  TYR A 163      3601   3140   4082    139   -483    -189      C
ATOM    68  CB  TYR A 163      13.719 -77.119 -64.892  1.00 34.72           C
ANISOU  68  CB  TYR A 163      4592   3821   4779    -44   -348     -71      C
ATOM    69  CG  TYR A 163      13.306 -78.446 -65.478  1.00 37.27           C
ANISOU  69  CG  TYR A 163      5162   4053   4945    -49   -378      39      C
ATOM    70  CD1 TYR A 163      12.506 -79.328 -64.749  1.00 39.18           C
ANISOU  70  CD1 TYR A 163      5509   4321   5057      9   -548     163      C
ATOM    71  CE1 TYR A 163      12.115 -80.546 -65.283  1.00 38.93           C
ANISOU  71  CE1 TYR A 163      5701   4198   4894      0   -574     259      C
ATOM    72  CZ  TYR A 163      12.524 -80.891 -66.564  1.00 35.64           C
ANISOU  72  CZ  TYR A 163      5409   3669   4463    -61   -438     232      C
ATOM    73  OH  TYR A 163      12.129 -82.103 -67.081  1.00 42.87           O
ANISOU  73  OH  TYR A 163      6546   4493   5251    -66   -474     322      O
ATOM    74  CE2 TYR A 163      13.322 -80.029 -67.308  1.00 32.75           C
ANISOU  74  CE2 TYR A 163      4957   3275   4211   -120   -257     111      C
ATOM    75  CD2 TYR A 163      13.707 -78.820 -66.762  1.00 37.16           C
ANISOU  75  CD2 TYR A 163      5288   3919   4911   -117   -223      16      C
ATOM    76  C   TYR A 163      15.697 -77.905 -63.614  1.00 25.39           C
ANISOU  76  C   TYR A 163      3120   2712   3814    269   -435    -381      C
ATOM    77  O   TYR A 163      15.836 -79.114 -63.453  1.00 36.60           O
ANISOU  77  O   TYR A 163      4646   4099   5159    374   -522    -369      O
ATOM    78  N   TYR A 164      16.707 -77.098 -63.892  1.00 50.12           N
ANISOU  78  N   TYR A 164      6049   5843   7153    259   -291    -569      N
ATOM    79  CA  TYR A 164      18.058 -77.593 -64.022  1.00 28.03           C
ANISOU  79  CA  TYR A 164      3119   3007   4525    373   -226    -791      C
ATOM    80  CB  TYR A 164      18.911 -76.586 -64.779  1.00 29.02           C
ANISOU  80  CB  TYR A 164      3078   3087   4860    270    -23    -960      C
ATOM    81  CG  TYR A 164      20.391 -76.807 -64.635  1.00 47.79           C
ANISOU  81  CG  TYR A 164      5214   5448   7495    401    -81   -1248      C
ATOM    82  CD1 TYR A 164      20.987 -77.963 -65.128  1.00 57.40           C
ANISOU  82  CD1 TYR A 164      6504   6586   8719    472    118   -1323      C
ATOM    83  CE1 TYR A 164      22.342 -78.174 -65.003  1.00 59.14           C
ANISOU  83  CE1 TYR A 164      6485   6786   9202    597    164   -1609      C
ATOM    84  CZ  TYR A 164      23.128 -77.219 -64.385  1.00 58.63           C
ANISOU  84  CZ  TYR A 164      6096   6777   9404    651    173   -1831      C
ATOM    85  OH  TYR A 164      24.481 -77.436 -64.264  1.00 64.14           O
ANISOU  85  OH  TYR A 164      6531   7445 10395    780    209   -2143      O
ATOM    86  CE2 TYR A 164      22.563 -76.054 -63.889  1.00 51.96           C
ANISOU  86  CE2 TYR A 164      5181   6012   8550    579    139   -1755      C
ATOM    87  CD2 TYR A 164      21.198 -75.860 -64.012  1.00 39.99           C
ANISOU  87  CD2 TYR A 164      3913   4519   6762    456     93   -1462      C
ATOM    88  C   TYR A 164      18.678 -77.923 -62.655  1.00 42.04           C
ANISOU  88  C   TYR A 164      4715   4866   6392    604   -440    -932      C
ATOM    89  O   TYR A 164      19.248 -78.997 -62.456  1.00 41.43           O
ANISOU  89  O   TYR A 164      4664   4757   6321    753   -528   -1012      O
ATOM    90  N   ILE A 165      18.548 -77.000 -61.711  1.00 34.21           N
ANISOU  90  N   ILE A 165      3560   3975   5463    641   -537    -964      N
ATOM    91  CA  ILE A 165      19.126 -77.164 -60.385  1.00 29.13           C
ANISOU  91  CA  ILE A 165      2761   3407   4900    865   -753   -1106      C
ATOM    92  CB  ILE A 165      19.170 -75.821 -59.620  1.00 28.86           C
ANISOU  92  CB  ILE A 165      2500   3471   4994    868   -791   -1188      C
ATOM    93  CG1 ILE A 165      20.057 -74.816 -60.346  1.00 29.74           C
ANISOU  93  CG1 ILE A 165      2376   3551   5372    769   -568   -1381      C
ATOM    94  CD1 ILE A 165      21.515 -75.304 -60.487  1.00 31.91           C
ANISOU  94  CD1 ILE A 165      2462   3773   5891    903   -531   -1665      C
ATOM    95  CG2 ILE A 165      19.674 -76.008 -58.192  1.00 29.77           C
ANISOU  95  CG2 ILE A 165      2493   3659   5158   1115   -1046   -1325      C
ATOM    96  C   ILE A 165      18.376 -78.203 -59.545  1.00 41.79           C
ANISOU  96  C   ILE A 165      4585   5029   6265    982   -975    -944      C
ATOM    97  O   ILE A 165      18.973 -78.957 -58.772  1.00 38.50           O
ANISOU  97  O   ILE A 165      4157   4613   5860   1192   -1149   -1050      O
ATOM    98  N   GLY A 166      17.058 -78.239 -59.691  1.00 42.72           N
ANISOU  98  N   GLY A 166      4911   5151   6171    845   -969    -694      N
ATOM    99  CA  GLY A 166      16.215 -79.045 -58.830  1.00 43.82           C
ANISOU  99  CA  GLY A 166      5253   5305   6091    922   -1145    -532      C
ATOM   100  C   GLY A 166      15.796 -80.370 -59.423  1.00 58.76           C
ANISOU  100  C   GLY A 166      7407   7099   7819    897   -1137    -396      C
ATOM   101  O   GLY A 166      15.092 -81.162 -58.791  1.00 62.85           O
ANISOU  101  O   GLY A 166      8120   7606   8155    948   -1257    -258      O
ATOM   102  N   TYR A 167      16.224 -80.621 -60.650  1.00 55.21           N
ANISOU  102  N   TYR A 167      6976   6568   7433    814   -982    -438      N
ATOM   103  CA  TYR A 167      15.887 -81.878 -61.286  1.00 49.20           C
ANISOU  103  CA  TYR A 167      6459   5708   6528    792   -973    -324      C
ATOM   104  CB  TYR A 167      14.620 -81.744 -62.120  1.00 25.58           C
ANISOU  104  CB  TYR A 167      3646   2676   3397    576   -881    -109      C
ATOM   105  CG  TYR A 167      14.215 -83.061 -62.711  1.00 35.84           C
ANISOU  105  CG  TYR A 167      5198   3870   4550    557   -890      6      C
ATOM   106  CD1 TYR A 167      13.920 -84.139 -61.874  1.00 49.68           C
ANISOU  106  CD1 TYR A 167      7095   5606   6174    676   -1044     79      C
ATOM   107  CE1 TYR A 167      13.564 -85.366 -62.379  1.00 46.91           C
ANISOU  107  CE1 TYR A 167      6973   5152   5700    661   -1055    178      C
ATOM   108  CZ  TYR A 167      13.495 -85.541 -63.750  1.00 51.83           C
ANISOU  108  CZ  TYR A 167      7683   5690   6319    533   -920    203      C
ATOM   109  OH  TYR A 167      13.130 -86.773 -64.236  1.00 67.21           O
ANISOU  109  OH  TYR A 167      9857   7533   8147    522   -941    297      O
ATOM   110  CE2 TYR A 167      13.790 -84.490 -64.620  1.00 44.14           C
ANISOU  110  CE2 TYR A 167      6591   4727   5454    417   -764    134      C
ATOM   111  CD2 TYR A 167      14.156 -83.253 -64.090  1.00 25.70           C
ANISOU  111  CD2 TYR A 167      4024   2492   3249    427   -744     37      C
ATOM   112  C   TYR A 167      16.995 -82.452 -62.152  1.00 46.60           C
ANISOU  112  C   TYR A 167      6095   5295   6317    838   -872    -482      C
ATOM   113  O   TYR A 167      17.515 -83.537 -61.874  1.00 51.43           O
ANISOU  113  O   TYR A 167      6770   5860   6910    995   -976    -543      O
ATOM   114  N   LEU A 168      17.346 -81.733 -63.211  1.00 43.65           N
ANISOU  114  N   LEU A 168      5634   4890   6060    701   -663    -551      N
ATOM   115  CA  LEU A 168      18.150 -82.314 -64.279  1.00 33.98           C
ANISOU  115  CA  LEU A 168      4437   3565   4910    690   -513    -660      C
ATOM   116  CB  LEU A 168      18.264 -81.365 -65.470  1.00 30.00           C
ANISOU  116  CB  LEU A 168      3900   3016   4483    497   -254    -687      C
ATOM   117  CG  LEU A 168      17.030 -81.352 -66.369  1.00 36.41           C
ANISOU  117  CG  LEU A 168      4980   3767   5086    307   -191    -450      C
ATOM   118  CD1 LEU A 168      17.256 -80.423 -67.544  1.00 31.34           C
ANISOU  118  CD1 LEU A 168      4342   3059   4507    137    -62    -491      C
ATOM   119  CD2 LEU A 168      16.681 -82.770 -66.851  1.00 28.35           C
ANISOU  119  CD2 LEU A 168      4213   2657   3903    329   -242    -346      C
ATOM   120  C   LEU A 168      19.526 -82.789 -63.834  1.00 44.16           C
ANISOU  120  C   LEU A 168      5539   4849   6390    895   -570    -916      C
ATOM   121  O   LEU A 168      19.971 -83.868 -64.215  1.00 45.07           O
ANISOU  121  O   LEU A 168      5746   4885   6493    972   -575    -966      O
ATOM   122  N   ARG A 169      20.125 -81.982 -62.989  1.00 46.34           N
ANISOU  122  N   ARG A 169      5549   5204   6852    995   -628    -1092     N
ATOM   123  CA  ARG A 169      21.377 -82.228 -62.347  1.00 62.71           C
ANISOU  123  CA  ARG A 169      7419   7265   9143   1199   -701   -1369     C
ATOM   124  CB  ARG A 169      21.669 -81.068 -61.445  1.00 63.72           C
ANISOU  124  CB  ARG A 169      7208   7451   9553   1217   -635   -1604     C
ATOM   125  CG  ARG A 169      22.895 -80.329 -61.807  1.00 55.08           C
ANISOU  125  CG  ARG A 169      6014   6468   8446   1314   -843   -1593     C
ATOM   126  CD  ARG A 169      22.684 -78.898 -61.490  1.00 55.94           C
ANISOU  126  CD  ARG A 169      5827   6620   8808   1243   -707   -1768     C
ATOM   127  NE  ARG A 169      22.761 -78.639 -60.078  1.00 70.61           N
ANISOU  127  NE  ARG A 169      7521   8579 10731   1388   -921   -1853      N
ATOM   128  CZ  ARG A 169      23.694 -77.870 -59.549  1.00 67.93           C
ANISOU  128  CZ  ARG A 169      6950   8281 10580   1357   -891   -2043      C
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ATOM 129 NH1 ARG A 169 24.611 -77.350 -60.327 1.00 60.38 N
ANISOU 129 NH1 ARG A 169 5836 7266 9841 1251 -668 -2212 N
ATOM 130 NH2 ARG A 169 23.710 -77.624 -58.262 1.00 68.38 N
ANISOU 130 NH2 ARG A 169 6991 8423 10568 1392 -1066 -2041 N
ATOM 131 C ARG A 169 21.331 -83.404 -61.453 1.00 65.45 C
ANISOU 131 C ARG A 169 7861 7631 9376 1428 -1003 -1347 C
ATOM 132 O ARG A 169 22.301 -84.093 -61.318 1.00 73.90 O
ANISOU 132 O ARG A 169 8813 8677 10587 1637 -1131 -1560 O
ATOM 133 N LEU A 170 20.244 -83.552 -60.735 1.00 64.80 N
ANISOU 133 N LEU A 170 8001 7580 9039 1391 -1117 -1095 N
ATOM 134 CA LEU A 170 20.068 -84.719 -59.939 1.00 77.52 C
ANISOU 134 CA LEU A 170 9794 9175 10487 1577 -1364 -1028 C
ATOM 135 CB LEU A 170 18.816 -84.557 -59.104 1.00 77.11 C
ANISOU 135 CB LEU A 170 9910 9181 10207 1518 -1455 -787 C
ATOM 136 CG LEU A 170 18.590 -83.230 -58.395 1.00 76.46 C
ANISOU 136 CG LEU A 170 9645 9214 10191 1503 -1485 -819 C
ATOM 137 CD1 LEU A 170 17.531 -83.409 -57.331 1.00 75.73 C
ANISOU 137 CD1 LEU A 170 9757 9158 9859 1492 -1601 -600 C
ATOM 138 CD2 LEU A 170 19.888 -82.769 -57.789 1.00 74.45 C
ANISOU 138 CD2 LEU A 170 9141 8996 10150 1724 -1622 -1101 C
ATOM 139 C LEU A 170 19.932 -85.961 -60.796 1.00 78.96 C
ANISOU 139 C LEU A 170 10203 9243 10555 1571 -1335 -950 C
ATOM 140 O LEU A 170 20.548 -86.963 -60.545 1.00 84.49 O
ANISOU 140 O LEU A 170 10994 9886 11221 1765 -1503 -1011 O
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ANISOU 141 N ILE A 171 8668 7563 8858 1354 -1129 -822 N
ATOM 142 CA ILE A 171 18.858 -87.025 -62.660 1.00 55.20 C
ANISOU 142 CA ILE A 171 7555 6085 7332 1316 -1108 -695 C
ATOM 143 CB ILE A 171 17.487 -86.897 -63.326 1.00 61.34 C
ANISOU 143 CB ILE A 171 8543 6854 7908 1095 -1029 -421 C
ATOM 144 CG1 ILE A 171 16.828 -88.256 -63.493 1.00 72.80 C
ANISOU 144 CG1 ILE A 171 10208 8304 9150 1150 -1212 -234 C
ATOM 145 CD1 ILE A 171 15.944 -88.669 -62.340 1.00 59.38 C
ANISOU 145 CD1 ILE A 171 8790 6488 7285 1115 -1224 -89 C
ATOM 146 CG2 ILE A 171 17.589 -86.242 -64.677 1.00 67.08 C
ANISOU 146 CG2 ILE A 171 9421 7477 8591 959 -864 -368 C
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ANISOU 147 C ILE A 171 7971 6470 7945 1317 -956 -861 C
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ANISOU 148 O ILE A 171 7531 5797 7301 1409 -1017 -867 O
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ANISOU 149 N LEU A 172 7108 5827 7477 1216 -749 -1004 N
ATOM 150 CA LEU A 172 21.427 -86.756 -65.464 1.00 56.08 C
ANISOU 150 CA LEU A 172 7363 6036 7910 1184 -551 -1162 C
ATOM 151 CB LEU A 172 21.790 -85.427 -66.135 1.00 35.51 C
ANISOU 151 CB LEU A 172 4615 3435 5442 996 -269 -1235 C
ATOM 152 CG LEU A 172 20.721 -84.809 -67.038 1.00 47.25 C
ANISOU 152 CG LEU A 172 6311 4912 6729 762 -154 -983 C
ATOM 153 CD1 LEU A 172 21.355 -83.886 -68.068 1.00 45.09 C
ANISOU 153 CD1 LEU A 172 5960 4596 6575 589 148 -1072 C
ATOM 154 CD2 LEU A 172 19.899 -85.893 -67.718 1.00 52.67 C
ANISOU 154 CD2 LEU A 172 7323 5514 7176 710 -190 -782 C
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ANISOU 155 C LEU A 172 8564 7354 9470 1409 -632 -1436 C
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ANISOU 156 O LEU A 172 8895 7506 9735 1413 -536 -1497 O
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ANISOU 159 CB PRO A 173 6808 6284 8800 2021 -1150 -2046 C
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ATOM 161 CD PRO A 173 23.117 -86.184 -63.203 1.00 66.33 C
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ANISOU 163 O PRO A 173 6867 5696 8336 2017 -988 -2017 O
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ATOM 166 CB GLU A 174 22.772 -91.793 -61.725 1.00 46.65 C
ANISOU 166 CB GLU A 174 6545 4652 6528 2284 -1710 -1403 C
ATOM 167 CG GLU A 174 23.793 -91.922 -60.607 1.00 67.59 C
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ATOM 169 OE1 GLU A 174 24.866 -94.028 -60.884 1.00 95.75 O
ANISOU 169 OE1 GLU A 174 12796 10769 12816 2682 -2074 -1704 O
ATOM 170 OE2 GLU A 174 26.013 -92.231 -61.409 1.00 99.33 O
ANISOU 170 OE2 GLU A 174 12676 11336 13730 2597 -1841 -2063 O
ATOM 171 C GLU A 174 22.550 -92.092 -64.201 1.00 50.45 C
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ANISOU 174 CA LEU A 175 7452 5040 6807 1489 -892 -967 C
ATOM 175 CB LEU A 175 20.475 -90.690 -66.885 1.00 49.50 C
ANISOU 175 CB LEU A 175 7266 4915 6626 1240 -666 -870 C
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ATOM 189 O GLN A 176 23.275 -95.977 -68.509 1.00 62.01 O
ANISOU 189 O GLN A 176 9205 6037 8319 1777 -809 -1325 O
ATOM 190 N ALA A 177 23.982 -94.836 -66.699 1.00 52.81 N
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ATOM 198 CG ARG A 178 19.826 -95.466 -62.986 1.00 50.64 C
ANISOU 198 CG ARG A 178 8195 4842 6203 2000 -1705 -586 C
ATOM 199 CD ARG A 178 19.115 -94.178 -62.637 1.00 54.80 C
ANISOU 199 CD ARG A 178 8617 5492 6711 1853 -1637 -485 C
ATOM 200 NE ARG A 178 17.667 -94.322 -62.492 1.00 51.78 N
ANISOU 200 NE ARG A 178 8469 5099 6104 1694 -1628 -203 N
ATOM 201 CZ ARG A 178 16.779 -93.470 -62.998 1.00 59.71 C
ANISOU 201 CZ ARG A 178 9446 6161 7080 1466 -1480 -73 C
ATOM 202 NH1 ARG A 178 17.194 -92.423 -63.697 1.00 59.37 N
ANISOU 202 NH1 ARG A 178 9182 6184 7193 1369 -1323 -182 N
ATOM 203 NH2 ARG A 178 15.480 -93.665 -62.813 1.00 63.18 N
ANISOU 203 NH2 ARG A 178 10080 6581 7343 1337 -1486 156 N
ATOM 204 C ARG A 178 20.099 -97.524 -66.207 1.00 57.11 C
ANISOU 204 C ARG A 178 9298 5393 7008 1812 -1379 -600 C
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ATOM 208 CB ILE A 179 20.028 -96.343 -69.692 1.00 47.63 C
ANISOU 208 CB ILE A 179 8052 4149 5898 1325 -730 -636 C
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ANISOU 209 CG1 ILE A 179 7383 3521 5076 1149 -715 -429 C
ATOM 210 CD1 ILE A 179 18.911 -94.151 -70.393 1.00 36.23 C
ANISOU 210 CD1 ILE A 179 6541 2818 4407 973 -478 -468 C
ATOM 211 CG2 ILE A 179 19.979 -96.914 -71.097 1.00 39.24 C
ANISOU 211 CG2 ILE A 179 7147 2973 4790 1227 -560 -644 C
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ANISOU 212 C ILE A 179 9041 4799 6674 1663 -1029 -731 C
ATOM 213 O ILE A 179 20.220 -99.668 -69.578 1.00 53.06 O
ANISOU 213 O ILE A 179 9173 4579 6410 1620 -1044 -606 O
ATOM 214 N ARG A 180 22.067 -98.649 -68.785 1.00 57.47 N
ANISOU 214 N ARG A 180 9248 5251 7336 1839 -1048 -1002 N
ATOM 215 CA ARG A 180 22.937 -99.800 -69.000 1.00 67.50 C
ANISOU 215 CA ARG A 180 10546 6415 8687 2014 -1114 -1171 C
ATOM 216 CB ARG A 180 24.378 -99.465 -68.630 1.00 75.66 C
ANISOU 216 CB ARG A 180 11251 7480 10018 2201 -1134 -1505 C
ATOM 217 CG ARG A 180 25.321 -99.335 -69.808 1.00 85.75 C
ANISOU 217 CG ARG A 180 12363 8714 11502 2147 -868 -1739 C
ATOM 218 CD ARG A 180 26.223 -98.120 -69.643 1.00102.62 C
ANISOU 218 CD ARG A 180 14129 10940 13921 2153 -742 -1983 C

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ATOM  219 NE  ARG A 180     26.758 -98.000 -68.289 1.00115.10           N
ANISOU 219 NE  ARG A 180    15526 12580 15629  2381 -1012 -2116       N
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ANISOU 220 CZ  ARG A 180    15238 12734 15875  2376  -968 -2269       C
ATOM  221 NH1 ARG A 180     27.567 -95.867 -68.604 1.00110.30           N
ANISOU 221 NH1 ARG A 180    14434 12099 15375  2215  -673 -2370       N
ATOM  222 NH2 ARG A 180     27.841 -96.903 -66.575 1.00118.89           N
ANISOU 222 NH2 ARG A 180    15530 13278 16366  2520 -1218 -2316       N
ATOM  223 C   ARG A 180     22.461-100.947 -68.134 1.00 65.71           C
ANISOU 223 C   ARG A 180    10565  6117  8286  2160 -1387 -1032       C
ATOM  224 O   ARG A 180     22.390-102.098 -68.575 1.00 63.24           O
ANISOU 224 O   ARG A 180    10454  5686  7889  2197 -1425  -996       O
ATOM  225 N   THR A 181     22.155-100.615 -66.885 1.00 66.20           N
ANISOU 225 N   THR A 181    10618  6244  8292  2244 -1570  -959       N
ATOM  226 CA  THR A 181     21.571-101.564 -65.960 1.00 74.70           C
ANISOU 226 CA  THR A 181    11946  7267  9168  2341 -1798  -793       C
ATOM  227 CB  THR A 181     21.175-100.898 -64.641 1.00 84.72           C
ANISOU 227 CB  THR A 181    13172  8655 10364  2364 -1925  -708       C
ATOM  228 OG1 THR A 181     22.351-100.429 -63.972 1.00 90.29           O
ANISOU 228 OG1 THR A 181    13600  9441 11266  2542 -2025  -959       O
ATOM  229 CG2 THR A 181     20.442-101.889 -63.747 1.00 84.99           C
ANISOU 229 CG2 THR A 181    13445  8701 10146  2342 -2058  -523       C
ATOM  230 C   THR A 181     20.337-102.168 -66.601 1.00 73.84           C
ANISOU 230 C   THR A 181    12126  7088  8842  2145 -1720  -531       C
ATOM  231 O   THR A 181     20.229-103.378 -66.744 1.00 65.69           O
ANISOU 231 O   THR A 181    11256  5999  7704  2155 -1773  -478       O
ATOM  232 N   TYR A 182     19.424-101.314 -67.037 1.00 74.70           N
ANISOU 232 N   TYR A 182    12245  7246  8890  1926 -1573  -379       N
ATOM  233 CA  TYR A 182     18.179-101.800 -67.602 1.00 62.64           C
ANISOU 233 CA  TYR A 182    10959  5665  7175  1729 -1513  -142       C
ATOM  234 CB  TYR A 182     17.217-100.669 -67.916 1.00 58.98           C
ANISOU 234 CB  TYR A 182    10461  5278  6672  1504 -1384     1       C
ATOM  235 CG  TYR A 182     15.879-101.195 -68.361 1.00 61.74           C
ANISOU 235 CG  TYR A 182    10951  5654  6853  1271 -1323   198       C
ATOM  236 CD1 TYR A 182     14.905-101.540 -67.428 1.00 58.52           C
ANISOU 236 CD1 TYR A 182    10537  5354  6343  1175 -1364   308       C
ATOM  237 CE1 TYR A 182     13.684-102.030 -67.827 1.00 59.84           C
ANISOU 237 CE1 TYR A 182    10743  5557  6437   968 -1284   414       C
ATOM  238 CZ  TYR A 182     13.431-102.193 -69.177 1.00 65.30           C
ANISOU 238 CZ  TYR A 182    11495  6197  7117   857 -1195   426       C
ATOM  239 OH  TYR A 182     12.217-102.683 -69.592 1.00 71.77           O
ANISOU 239 OH  TYR A 182    12322  7054  7895   677 -1141   498       O
ATOM  240 CE2 TYR A 182     14.383-101.862 -70.124 1.00 65.98           C
ANISOU 240 CE2 TYR A 182    11632  6183  7256   933 -1151   346       C
ATOM  241 CD2 TYR A 182     15.599-101.380 -69.713 1.00 63.55           C
ANISOU 241 CD2 TYR A 182    11273  5815  7057  1137 -1198   224       C
ATOM  242 C   TYR A 182     18.346-102.693 -68.831 1.00 65.69           C
ANISOU 242 C   TYR A 182    11475  5934  7552  1691 -1426  -173       C
ATOM  243 O   TYR A 182     17.645-103.693 -68.987 1.00 65.11           O
ANISOU 243 O   TYR A 182    11555  5854  7331  1596 -1446   -44       O
ATOM  244 N   ASN A 183     19.252-102.325 -69.722 1.00 68.48           N
ANISOU 244 N   ASN A 183    11672  6286  8060  1696 -1274  -366       N
ATOM  245 CA  ASN A 183     19.447-103.124 -70.921 1.00 66.45           C
ANISOU 245 CA  ASN A 183    11542  5917  7790  1659 -1172  -409       C
ATOM  246 CB  ASN A 183     20.246-102.360 -71.970 1.00 49.23           C
ANISOU 246 CB  ASN A 183    9175  3769  5763  1587  -927  -595       C
ATOM  247 CG  ASN A 183     19.437-101.253 -72.611 1.00 55.28           C
ANISOU 247 CG  ASN A 183    9949  4595  6460  1347  -757  -466       C
ATOM  248 OD1 ASN A 183     18.205-101.284 -72.589 1.00 53.34           O
ANISOU 248 OD1 ASN A 183    9882  4339  6046  1219  -814  -239       O
ATOM  249 ND2 ASN A 183     20.121-100.265 -73.183 1.00 54.63           N
ANISOU 249 ND2 ASN A 183    9675  4566  6518  1286  -548  -619       N
ATOM  250 C   ASN A 183     20.063-104.485 -70.629 1.00 75.19           C
ANISOU 250 C   ASN A 183    12745  6918  8906  1864 -1329  -498       C
ATOM  251 O   ASN A 183     19.620-105.500 -71.166 1.00 78.02           O
ANISOU 251 O   ASN A 183    13281  7220  9143  1798 -1332  -399       O
ATOM  252 N   GLN A 184     21.133-104.524 -69.856 1.00 80.73           N
ANISOU 252 N   GLN A 184    13264  7663  9747  2075 -1454  -680       N
ATOM  253 CA  GLN A 184     21.670-105.801 -69.444 1.00 91.89           C
ANISOU 253 CA  GLN A 184    14695  9048 11170  2244 -1610  -767       C
ATOM  254 CB  GLN A 184     23.058-105.634 -68.847 1.00100.74           C
ANISOU 254 CB  GLN A 184    15525 10227 12525  2453 -1686 -1048       C
ATOM  255 CG  GLN A 184     24.053-104.976 -69.772 1.00107.62           C
ANISOU 255 CG  GLN A 184    16153 11093 13644  2446 -1471 -1306       C
ATOM  256 CD  GLN A 184     25.196-104.357 -69.015 1.00112.72           C
ANISOU 256 CD  GLN A 184    16451 11843 14536  2597 -1536 -1557       C
ATOM  257 OE1 GLN A 184     25.187-104.318 -67.791 1.00116.08           O
ANISOU 257 OE1 GLN A 184    16843 12341 14921  2712 -1759 -1525       O
ATOM  258 NE2 GLN A 184     26.187-103.873 -69.734 1.00112.69           N
ANISOU 258 NE2 GLN A 184    16185 11851 14781  2581 -1328 -1808       N
ATOM  259 C   GLN A 184     20.809-106.581 -68.473 1.00 94.56           C
ANISOU 259 C   GLN A 184    15215  9417 11295  2246 -1797  -568       C
ATOM  260 O   GLN A 184     20.570-107.743 -68.667 1.00 97.43           O
ANISOU 260 O   GLN A 184    15759  9723 11537  2222 -1839  -487       O
ATOM  261 N   HIS A 185     20.265-105.961 -67.445 1.00108.20           N
ANISOU 261 N   HIS A 185    16282  9713 11915  1301  496  -276       N
ATOM  262 C   HIS A 185     18.122-107.285 -66.815 1.00116.07           C
ANISOU 262 C   HIS A 185    13619 10627 19856  1058  449  -161       C
ATOM  263 O   HIS A 185     17.560-108.043 -66.050 1.00113.01           O
ANISOU 263 O   HIS A 185    13385 10120 19433  984  344   -2       O
ATOM  264 CA  HIS A 185     19.486-106.707 -66.448 1.00113.33           C
ANISOU 264 CA  HIS A 185    13108 10222 19731  1250  299  -62       C
ATOM  265 CB  HIS A 185     19.352-105.927 -65.167 1.00119.64           C
ANISOU 265 CB  HIS A 185    13998 10228 19238  1259  -268  422       C
ATOM  266 CG  HIS A 185     20.518-106.076 -64.251 1.00127.12           C
ANISOU 266 CG  HIS A 185    14970 11991 21338  1368  -268  422       C
ATOM  267 ND1 HIS A 185     21.809-106.209 -64.711 1.00132.10           N
ANISOU 267 ND1 HIS A 185    15466 12534 22191  1435  -308  413       N
ATOM  268 CE1 HIS A 185     22.629-106.314 -63.682 1.00134.29           C
ANISOU 268 CE1 HIS A 185    15827 12752 22443  1483  -594  633       C
ATOM  269 NE2 HIS A 185     21.916-106.234 -62.571 1.00131.80           N
ANISOU 269 NE2 HIS A 185    15716 12492 21871  1451  -735  794       N
ATOM  270 CD2 HIS A 185     20.594-106.083 -62.900 1.00127.82           C
ANISOU 270 CD2 HIS A 185    15234 12072 21259  1378  -537  676       C
ATOM  271 O   TYR A 186     17.692-107.513 -70.296 1.00131.41           O
ANISOU 271 O   TYR A 186    15518 12941 21472  828 1210 -1011       O
ATOM  272 N   TYR A 186     17.551-106.872 -67.930 1.00122.21           N
ANISOU 272 N   TYR A 186    14368 11595 20470  974  689  -420       N
ATOM  273 CA  TYR A 186     16.276-107.410 -68.391 1.00126.62           C
ANISOU 273 CA  TYR A 186    15060 12219 20832  789  818  -538       C
ATOM  274 C   TYR A 186     16.776-108.044 -69.692 1.00130.67           C
ANISOU 274 C   TYR A 186    15514 12670 21466  773 1094  -857       C
ATOM  275 CB  TYR A 186     15.179-106.337 -68.236 1.00124.50           C
ANISOU 275 CB  TYR A 186    14870 12344 20091  670  778  -522       C
ATOM  276 CG  TYR A 186     15.431-105.545 -66.977 1.00119.70           C
ANISOU 276 CG  TYR A 186    14302 11897 19280  722  535  -265       C
ATOM  277 CD2 TYR A 186     14.842-105.879 -65.786 1.00112.09           C
ANISOU 277 CD2 TYR A 186    13496 10964 18128  629  413  -66       C
ATOM  278 CD1 TYR A 186     16.328-104.509 -66.971 1.00122.36           C
ANISOU 278 CD1 TYR A 186    14531 12369 19593  856  440  -233       C
ATOM  279 CE2 TYR A 186     15.110-105.182 -64.649 1.00109.74           C
ANISOU 279 CE2 TYR A 186    13261 10821 17613  687  197  153       C
ATOM  280 CE1 TYR A 186     16.594-103.809 -65.836 1.00118.54           C
ANISOU 280 CE1 TYR A 186    14097 12028 18915  908  205  -19       C
ATOM  281 CZ  TYR A 186     15.987-104.147 -64.683 1.00113.64           C
ANISOU 281 CZ  TYR A 186    13649 11436 18093  831   83  168       C
ATOM  282 OH  TYR A 186     16.268-103.428 -63.556 1.00114.20           O
ANISOU 282 OH  TYR A 186    13791 11648 17951  899  -149  368       O
ATOM  283 O   ASN A 187     15.356-110.153 -67.321 1.00112.92           O
ANISOU 283 O   ASN A 187    13708 10078 19117  297  984  -574       O
ATOM  284 N   ASN A 187     16.341-109.247 -70.046 1.00128.71           N
ANISOU 284 N   ASN A 187    15332 12168 21404  701 1202  -961       N
ATOM  285 CA  ASN A 187     15.120-109.938 -69.671 1.00123.40           C
ANISOU 285 CA  ASN A 187    14790 11282 20816  601 1098  -798       C
ATOM  286 C   ASN A 187     14.702-109.714 -68.258 1.00122.38           C
ANISOU 286 C   ASN A 187    14790 11412 20299  410 1041  -714       C
ATOM  287 CB  ASN A 187     15.753-111.299 -69.623 1.00125.83           C
ANISOU 287 CB  ASN A 187    15076 11274 21458  742  907  -544       C
ATOM  288 CG  ASN A 187     17.049-111.272 -68.863 1.00133.97           C
ANISOU 288 CG  ASN A 187    16134 11892 22878  753  968  -594       C
ATOM  289 OD1 ASN A 187     17.435-112.234 -68.206 1.00140.04           O
ANISOU 289 OD1 ASN A 187    16910 12592 23706  688 1172  -850       O
ATOM  290 ND2 ASN A 187     17.731-110.144 -68.937 1.00136.34           N
ANISOU 290 ND2 ASN A 187    16464 11981 23356  826  765  -346       N
ATOM  291 O   ASN A 188     13.481-106.429 -69.712 1.00137.31           O
ANISOU 291 O   ASN A 188    16554 13697 21921  422 1393 -1280       O
ATOM  292 N   ASN A 188     13.542-109.092 -68.123 1.00130.97           N
ANISOU 292 N   ASN A 188    15845 12870 21047  393 1051  -778       N
ATOM  293 CA  ASN A 188     12.752-108.698 -69.297 1.00132.44           C
ANISOU 293 CA  ASN A 188    16081 13338 20901  223 1149  -944       C
ATOM  294 C   ASN A 188     13.358-107.566 -70.145 1.00130.85           C
ANISOU 294 C   ASN A 188    15824 13056 20835  261 1346 -1247       C
ATOM  295 CB  ASN A 188     11.295-108.364 -68.869 1.00130.18           C
ANISOU 295 CB  ASN A 188    15771 13455 20238  234 1072  -907       C
ATOM  296 CG  ASN A 188     11.072-106.888 -68.574 1.00 87.73           C
ANISOU 296 CG  ASN A 188    10286  8220 14829  358 1154 -1080       C
ATOM  297 OD1 ASN A 188     10.563-106.151 -69.415 1.00 95.34           O
ANISOU 297 OD1 ASN A 188    11236  9184 15804  337 1333 -1343       O
ATOM  298 ND2 ASN A 188     11.425-106.457 -67.362 1.00 66.22           N
ANISOU 298 ND2 ASN A 188    7498  5624 12036  482 1017  -927       N
ATOM  299 O   LEU A 189     15.291-108.371 -73.265 1.00110.59           O
ANISOU 299 O   LEU A 189    13161 10540 18319  411 1754 -1836       O
ATOM  300 N   LEU A 189     13.651-107.852 -71.399 1.00124.07           N
ANISOU 300 N   LEU A 189    15016 12363 19764  123 1457 -1472       N
ATOM  301 CA  LEU A 189     13.405-109.124 -72.033 1.00121.52           C
ANISOU 301 CA  LEU A 189    14716 11891 19564   97 1639 -1767       C
ATOM  302 C   LEU A 189     14.470-109.263 -73.079 1.00113.32           C
ANISOU 302 C   LEU A 189    13596 10729 18730  285 1770 -1896       C
ATOM  303 CB  LEU A 189     12.016-109.176 -72.676 1.00125.08           C
ANISOU 303 CB  LEU A 189    15228 12615 19680  -58 1696 -1989       C
ATOM  304 CG  LEU A 189     10.756-108.647 -71.964 1.00127.32           C
ANISOU 304 CG  LEU A 189    15519 13229 19627  -170 1562 -1847       C
ATOM  305 CD1 LEU A 189      9.742-108.113 -72.961 1.00126.49           C
ANISOU 305 CD1 LEU A 189    15458 13351 19252  -307 1616 -2103       C
ATOM  306 CD2 LEU A 189     10.083-109.681 -71.086 1.00 74.54           C
ANISOU 306 CD2 LEU A 189    8872  6457 12993  -279 1447 -1584       C
ATOM  307 N   LEU A 190     14.457-110.396 -73.749 1.00104.26           N
ANISOU 307 N   LEU A 190    12479  9290 17846  303 1909 -2077       N
ATOM  308 CA  LEU A 190     15.388-110.668 -74.798 1.00 68.03           C
ANISOU 308 CA  LEU A 190    7820  4558 13472  476 2083 -2233       C
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ATOM 309 CB LEU A 190 15.224-112.066 -75.325 1.00 86.22 C
ANISOU 309 CB LEU A 190 10187 6536 16036 468 2203 -2408 C
ATOM 310 CG LEU A 190 15.519-113.176 -74.350 1.00 72.84 C
ANISOU 310 CG LEU A 190 8517 4533 14627 422 2063 -2213 C
ATOM 311 CD2 LEU A 190 16.779-112.852 -73.600 1.00 74.17 C
ANISOU 311 CD2 LEU A 190 8557 4616 15010 579 1925 -1920 C
ATOM 312 CD1 LEU A 190 15.676-114.429 -75.158 1.00 76.01 C
ANISOU 312 CD1 LEU A 190 8985 4720 15174 394 2140 -2358 C
ATOM 313 C LEU A 190 15.166-109.722 -75.900 1.00 75.09 C
ANISOU 313 C LEU A 190 8729 5745 14058 489 2221 -2447 C
ATOM 314 O LEU A 190 16.008-109.613 -76.735 1.00 73.82 O
ANISOU 314 O LEU A 190 8528 5572 13950 604 2379 -2565 O
ATOM 315 N ARG A 191 14.021-109.063 -75.948 1.00 82.50 N
ANISOU 315 N ARG A 191 9731 7004 14610 353 2136 -2457 N
ATOM 316 CA ARG A 191 13.870-107.966 -76.905 1.00 78.40 C
ANISOU 316 CA ARG A 191 9251 6783 13757 351 2228 -2643 C
ATOM 317 CB ARG A 191 12.721-108.193 -77.851 1.00 73.01 C
ANISOU 317 CB ARG A 191 8716 6199 12826 177 2242 -2875 C
ATOM 318 CG ARG A 191 12.137-109.591 -77.842 1.00 84.33 C
ANISOU 318 CG ARG A 191 10222 7343 14476 65 2237 -2946 C
ATOM 319 CD ARG A 191 13.170-110.689 -77.957 1.00 96.27 C
ANISOU 319 CD ARG A 191 11747 8494 16336 185 2409 -3086 C
ATOM 320 NE ARG A 191 12.594-111.811 -78.648 1.00104.48 N
ANISOU 320 NE ARG A 191 12917 9383 17398 66 2434 -3284 N
ATOM 321 CZ ARG A 191 11.832-112.709 -78.068 1.00112.51 C
ANISOU 321 CZ ARG A 191 13968 10191 18592 -76 2342 -3244 C
ATOM 322 NH1 ARG A 191 11.598-112.635 -76.778 1.00112.22 N
ANISOU 322 NH1 ARG A 191 13852 10166 18620 -125 2184 -2931 N
ATOM 323 NH2 ARG A 191 11.336-113.695 -78.774 1.00123.75 N
ANISOU 323 NH2 ARG A 191 15503 11492 20022 -177 2355 -3432 N
ATOM 324 C ARG A 191 13.791-106.573 -76.267 1.00 77.81 C
ANISOU 324 C ARG A 191 9103 7025 13435 371 2081 -2443 C
ATOM 325 O ARG A 191 12.924-106.312 -75.466 1.00 76.08 O
ANISOU 325 O ARG A 191 8909 6977 13022 256 1915 -2317 O
ATOM 326 N GLY A 192 14.718-105.704 -76.652 1.00 59.28 N
ANISOU 326 N GLY A 192 6666 4746 11113 519 2151 -2418 N
ATOM 327 CA GLY A 192 14.932-104.394 -76.064 1.00 83.82 C
ANISOU 327 CA GLY A 192 9701 8121 14024 558 2011 -2236 C
ATOM 328 C GLY A 192 14.800-103.329 -77.113 1.00 75.54 C
ANISOU 328 C GLY A 192 8697 7330 12675 570 2128 -2415 C
ATOM 329 O GLY A 192 13.950-103.488 -77.952 1.00 68.42 O
ANISOU 329 O GLY A 192 7930 6516 11549 470 2204 -2642 O
ATOM 330 N ALA A 193 15.641-102.290 -77.141 1.00 69.65 N
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ATOM 332 CB ALA A 193 17.937-102.384 -76.357 1.00 60.58 C
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ATOM 333 C ALA A 193 16.625-100.303 -76.117 1.00 63.09 C
ANISOU 333 C ALA A 193 6822 6084 11065 827 1914 -1975 C
ATOM 334 O ALA A 193 16.621 -99.703 -77.150 1.00 59.63 O
ANISOU 334 O ALA A 193 6439 5799 10417 825 2063 -2141 O
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ANISOU 335 N VAL A 194 5113 4518 9432 859 1672 -1727 N
ATOM 336 CA VAL A 194 16.514 -98.258 -74.765 1.00 55.43 C
ANISOU 336 CA VAL A 194 5783 5489 9791 857 1542 -1658 C
ATOM 337 CB VAL A 194 16.109 -97.925 -73.316 1.00 61.87 C
ANISOU 337 CB VAL A 194 6604 6400 10505 837 1244 -1419 C
ATOM 338 CG1 VAL A 194 15.228 -99.007 -72.759 1.00 58.98 C
ANISOU 338 CG1 VAL A 194 6323 5921 10166 738 1197 -1395 C
ATOM 339 CG2 VAL A 194 17.313 -97.777 -72.426 1.00 67.41 C
ANISOU 339 CG2 VAL A 194 7166 6950 11499 973 1097 -1193 C
ATOM 340 C VAL A 194 17.624 -97.312 -75.219 1.00 57.36 C
ANISOU 340 C VAL A 194 5898 5743 10153 979 1615 -1623 C
ATOM 341 O VAL A 194 18.776 -97.606 -75.061 1.00 60.20 O
ANISOU 341 O VAL A 194 6114 5859 10900 1089 1689 -1562 O
ATOM 342 N SER A 195 17.254 -96.152 -75.728 1.00 47.46 N
ANISOU 342 N SER A 195 4689 4763 8581 959 1594 -1660 N
ATOM 343 CA SER A 195 18.226 -95.156 -76.114 1.00 51.50 C
ANISOU 343 CA SER A 195 5087 5304 9176 1055 1658 -1613 C
ATOM 344 CB SER A 195 17.607 -94.112 -77.000 1.00 57.14 C
ANISOU 344 CB SER A 195 5918 6307 9484 1002 1713 -1738 C
ATOM 345 OG SER A 195 17.317 -94.673 -78.245 1.00 67.53 O
ANISOU 345 OG SER A 195 7372 7623 10664 948 1964 -1591 O
ATOM 346 C SER A 195 18.886 -94.536 -74.905 1.00 49.50 C
ANISOU 346 C SER A 195 4692 5018 9099 1137 1392 -1348 C
ATOM 347 O SER A 195 18.451 -94.742 -73.810 1.00 50.41 O
ANISOU 347 O SER A 195 4842 5148 9163 1115 1150 -1209 O
ATOM 348 N GLN A 196 19.997 -93.851 -75.108 1.00 59.41 N
ANISOU 348 N GLN A 196 5796 6223 10556 1231 1436 -1277 N
ATOM 349 CA GLN A 196 20.854 -93.405 -74.008 1.00 64.26 C
ANISOU 349 CA GLN A 196 6247 6731 11438 1327 1187 -1037 C
ATOM 350 CB GLN A 196 22.314 -93.372 -74.452 1.00 55.36 C
ANISOU 350 CB GLN A 196 4998 5459 10577 1350 1287 -961 C
ATOM 351 CG GLN A 196 22.888 -94.734 -74.727 1.00 76.79 C
ANISOU 351 CG GLN A 196 7686 7928 13564 1346 1450 -1011 C
ATOM 352 CD GLN A 196 22.736 -95.666 -73.538 1.00 97.02 C
ANISOU 352 CD GLN A 196 10235 10306 16323 1377 1248 -905 C
ATOM 353 OE1 GLN A 196 22.997 -95.283 -72.396 1.00 99.29 O
ANISOU 353 OE1 GLN A 196 10473 10568 16686 1419 952 -707 O
ATOM 354 NE2 GLN A 196 22.296 -96.893 -73.801 1.00104.02 N
ANISOU 354 NE2 GLN A 196 11193 11060 17271 1350 1394 -1034 N
ATOM 355 C GLN A 196 20.494 -92.059 -73.388 1.00 60.44 C
ANISOU 355 C GLN A 196 5796 6486 10684 1322 913 -906 C
ATOM 356 O GLN A 196 21.037 -91.690 -72.347 1.00 61.96 O
ANISOU 356 O GLN A 196 5894 6601 11045 1395 651 -707 O
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ANISOU 357 N ARG A 197 5209 6035 9543 1244 958 -1022 N
ATOM 358 CA ARG A 197 19.252 -89.991 -73.570 1.00 52.91 C
ANISOU 358 CA ARG A 197 5011 6031 9060 1248 720 -919 C
ATOM 359 CB ARG A 197 19.297 -88.979 -74.686 1.00 52.63 C
ANISOU 359 CB ARG A 197 5008 6164 8827 1225 887 -1034 C
ATOM 360 CG ARG A 197 20.442 -89.155 -75.621 1.00 48.63 C
ANISOU 360 CG ARG A 197 4354 5479 8644 1280 1160 -1068 C
ATOM 361 CD ARG A 197 20.454 -88.029 -76.617 1.00 68.47 C
ANISOU 361 CD ARG A 197 6930 8178 10908 1253 1288 -1143 C
ATOM 362 NE ARG A 197 21.664 -88.006 -77.426 1.00 82.41 N
ANISOU 362 NE ARG A 197 8614 9810 12890 1267 1533 -1128 N
ATOM 363 CZ ARG A 197 22.350 -86.910 -77.707 1.00 88.41 C
ANISOU 363 CZ ARG A 197 9287 10592 13713 1286 1513 -1013 C
ATOM 364 NH1 ARG A 197 23.428 -86.984 -78.443 1.00 80.56 N
ANISOU 364 NH1 ARG A 197 8238 9479 12891 1273 1741 -995 N
ATOM 365 NH2 ARG A 197 21.958 -85.735 -77.255 1.00 92.14 N
ANISOU 365 NH2 ARG A 197 9724 11202 14084 1314 1259 -921 N
ATOM 366 C ARG A 197 17.893 -89.926 -72.906 1.00 52.07 C
ANISOU 366 C ARG A 197 5072 6134 8577 1177 517 -911 C
ATOM 367 O ARG A 197 17.079 -90.807 -73.038 1.00 46.29 O
ANISOU 367 O ARG A 197 4447 5418 7722 1096 601 -1018 O
ATOM 368 N LEU A 198 17.678 -88.822 -72.200 1.00 36.02 N
ANISOU 368 N LEU A 198 3057 4257 6373 1208 255 -785 N
ATOM 369 CA LEU A 198 16.403 -88.550 -71.578 1.00 37.30 C
ANISOU 369 CA LEU A 198 3370 4656 6146 1152 83 -788 C
ATOM 370 CB LEU A 198 16.594 -87.940 -70.191 1.00 38.99 C
ANISOU 370 CB LEU A 198 3579 4903 6334 1231 -251 -582 C
ATOM 371 CG LEU A 198 15.318 -87.612 -69.413 1.00 39.89 C
ANISOU 371 CG LEU A 198 3827 5128 6199 1203 -428 -517 C
ATOM 372 CD1 LEU A 198 15.654 -87.013 -68.056 1.00 33.43 C
ANISOU 372 CD1 LEU A 198 3062 4481 5159 1267 -714 -405 C
ATOM 373 CD2 LEU A 198 14.427 -86.673 -70.212 1.00 32.49 C
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ATOM 374 C LEU A 198 15.754 -87.549 -72.515 1.00 35.15 C
ANISOU 374 C LEU A 198 3186 4640 5529 1095 167 -945 C
ATOM 375 O LEU A 198 16.266 -86.450 -72.727 1.00 44.16 O
ANISOU 375 O LEU A 198 4289 5851 6640 1137 129 -917 O
ATOM 376 N TYR A 199 14.625 -87.948 -73.079 1.00 42.52 N
ANISOU 376 N TYR A 199 4239 5703 6213 997 269 -1108 N
ATOM 377 CA TYR A 199 13.914 -87.150 -74.025 1.00 48.62 C
ANISOU 377 CA TYR A 199 5113 6714 6646 946 313 -1261 C
ATOM 378 CB TYR A 199 13.350 -88.023 -75.116 1.00 43.25 C
ANISOU 378 CB TYR A 199 4519 6028 5887 854 558 -1488 C
ATOM 379 CG TYR A 199 14.409 -88.469 -76.040 1.00 43.73 C
ANISOU 379 CG TYR A 199 4523 5886 6208 887 819 -1549 C
ATOM 380 CD1 TYR A 199 15.221 -89.522 -75.723 1.00 51.53 C
ANISOU 380 CD1 TYR A 199 5403 6600 7576 925 913 -1484 C
ATOM 381 CE1 TYR A 199 16.208 -89.931 -76.567 1.00 49.04 C
ANISOU 381 CE1 TYR A 199 5019 6095 7520 968 1168 -1545 C
ATOM 382 CZ TYR A 199 16.398 -89.274 -77.726 1.00 48.01 C
ANISOU 382 CZ TYR A 199 4945 6049 7248 968 1349 -1660 C
ATOM 383 OH TYR A 199 17.376 -89.659 -78.573 1.00 57.63 O
ANISOU 383 OH TYR A 199 6100 7079 8718 1015 1637 -1721 O
ATOM 384 CE2 TYR A 199 15.604 -88.221 -78.064 1.00 51.17 C
ANISOU 384 CE2 TYR A 199 5472 6714 7256 926 1248 -1714 C
ATOM 385 CD2 TYR A 199 14.625 -87.818 -77.215 1.00 46.97 C
ANISOU 385 CD2 TYR A 199 4989 6366 6489 890 976 -1661 C
ATOM 386 C TYR A 199 12.858 -86.362 -73.294 1.00 46.31 C
ANISOU 386 C TYR A 199 4899 6667 6030 933 69 -1222 C
ATOM 387 O TYR A 199 12.030 -86.881 -72.623 1.00 37.25 O
ANISOU 387 O TYR A 199 3797 5571 4785 884 4 -1220 O
ATOM 388 N ILE A 200 12.963 -85.066 -73.425 1.00 46.68 N
ANISOU 388 N ILE A 200 4954 6854 5928 983 -59 -1182 N
ATOM 389 CA ILE A 200 12.113 -84.154 -72.701 1.00 45.80 C
ANISOU 389 CA ILE A 200 4906 6963 5533 1000 -305 -1134 C
ATOM 390 CB ILE A 200 12.931 -83.100 -71.989 1.00 34.87 C
ANISOU 390 CB ILE A 200 3465 5556 4228 1107 -523 -954 C
ATOM 391 CG1 ILE A 200 13.804 -83.775 -70.937 1.00 32.54 C
ANISOU 391 CG1 ILE A 200 3080 5025 4257 1168 -599 -777 C
ATOM 392 CD1 ILE A 200 14.642 -82.817 -70.148 1.00 29.05 C
ANISOU 392 CD1 ILE A 200 2581 4530 3924 1276 -850 -598 C
ATOM 393 CG2 ILE A 200 12.015 -82.071 -71.347 1.00 37.87 C
ANISOU 393 CG2 ILE A 200 3931 6174 4284 1136 -769 -931 C
ATOM 394 C ILE A 200 11.143 -83.497 -73.653 1.00 41.34 C
ANISOU 394 C ILE A 200 4446 6631 4630 945 -279 -1310 C
ATOM 395 O ILE A 200 11.538 -82.887 -74.641 1.00 63.22 O
ANISOU 395 O ILE A 200 7239 9424 7357 951 -195 -1374 O
ATOM 396 N LEU A 201 9.865 -83.649 -73.358 1.00 33.16 N
ANISOU 396 N LEU A 201 3474 5762 3365 890 -349 -1387 N
ATOM 397 CA LEU A 201 8.831 -83.119 -74.214 1.00 36.22 C
ANISOU 397 CA LEU A 201 3949 6318 3495 820 -346 -1513 C
ATOM 398 CB LEU A 201 7.568 -83.962 -74.105 1.00 34.09 C
ANISOU 398 CB LEU A 201 3699 6049 3203 701 -302 -1545 C

ATOM 399 CG LEU A 201 7.658 -85.302 -74.816 1.00 40.99 C
ANISOU 399 CG LEU A 201 4586 6836 4154 636 -90 -1747 C
ATOM 400 CD1 LEU A 201 6.421 -86.121 -74.500 1.00 51.18 C
ANISOU 400 CD1 LEU A 201 5876 8155 5413 528 -88 -1788 C
ATOM 401 CD2 LEU A 201 7.783 -85.059 -76.308 1.00 47.57 C
ANISOU 401 CD2 LEU A 201 5509 7584 4982 571 20 -1780 C
ATOM 402 C LEU A 201 8.542 -81.681 -73.829 1.00 37.07 C
ANISOU 402 C LEU A 201 4076 6421 3588 840 -490 -1294 C
ATOM 403 O LEU A 201 8.344 -81.363 -72.650 1.00 29.14 O
ANISOU 403 O LEU A 201 3074 5387 2610 877 -585 -1154 O
ATOM 404 N LEU A 202 8.519 -80.814 -74.829 1.00 34.29 N
ANISOU 404 N LEU A 202 3777 6031 3221 801 -452 -1264 N
ATOM 405 CA LEU A 202 8.213 -79.416 -74.603 1.00 40.08 C
ANISOU 405 CA LEU A 202 4561 6690 3978 799 -512 -1097 C
ATOM 406 CB LEU A 202 9.460 -78.569 -74.788 1.00 31.05 C
ANISOU 406 CB LEU A 202 3404 5543 2851 885 -554 -1071 C
ATOM 407 CG LEU A 202 10.540 -78.866 -73.762 1.00 36.65 C
ANISOU 407 CG LEU A 202 4042 6260 3623 1002 -656 -1052 C
ATOM 408 CD1 LEU A 202 11.919 -78.657 -74.376 1.00 46.89 C
ANISOU 408 CD1 LEU A 202 5252 7623 4942 1104 -701 -1123 C
ATOM 409 CD2 LEU A 202 10.344 -77.972 -72.554 1.00 30.81 C
ANISOU 409 CD2 LEU A 202 3393 5357 2958 962 -723 -853 C
ATOM 410 C LEU A 202 7.102 -78.924 -75.515 1.00 44.85 C
ANISOU 410 C LEU A 202 5251 7236 4556 688 -470 -1073 C
ATOM 411 O LEU A 202 7.366 -78.236 -76.506 1.00 36.94 O
ANISOU 411 O LEU A 202 4292 6224 3518 681 -454 -1083 O
ATOM 412 N PRO A 203 5.855 -79.310 -75.198 1.00 45.03 N
ANISOU 412 N PRO A 203 5238 7305 4567 663 -469 -1097 N
ATOM 413 CA PRO A 203 4.694 -78.745 -75.887 1.00 39.17 C
ANISOU 413 CA PRO A 203 4470 6630 3783 662 -474 -1140 C
ATOM 414 CB PRO A 203 3.507 -79.484 -75.261 1.00 34.94 C
ANISOU 414 CB PRO A 203 3880 6149 3246 629 -469 -1175 C
ATOM 415 CG PRO A 203 4.016 -79.980 -73.920 1.00 41.04 C
ANISOU 415 CG PRO A 203 4651 6889 4055 648 -479 -1108 C
ATOM 416 CD PRO A 203 5.465 -80.327 -74.210 1.00 42.10 C
ANISOU 416 CD PRO A 203 4851 6935 4211 633 -467 -1096 C
ATOM 417 C PRO A 203 4.575 -77.263 -75.576 1.00 33.03 C
ANISOU 417 C PRO A 203 3663 5871 3017 762 -521 -1078 C
ATOM 418 O PRO A 203 4.496 -76.884 -74.404 1.00 29.27 O
ANISOU 418 O PRO A 203 3157 5392 2572 827 -542 -1023 O
ATOM 419 N LEU A 204 4.550 -76.439 -76.616 1.00 34.53 N
ANISOU 419 N LEU A 204 4868 5402 2849 967 -1660 593 N
ATOM 420 CA LEU A 204 4.412 -75.002 -76.445 1.00 44.90 C
ANISOU 420 CA LEU A 204 6331 6766 3965 763 -1569 611 C
ATOM 421 CB LEU A 204 4.730 -74.268 -77.743 1.00 39.38 C
ANISOU 421 CB LEU A 204 5789 6036 3137 554 -1615 386 C
ATOM 422 CG LEU A 204 6.178 -74.408 -78.192 1.00 41.48 C
ANISOU 422 CG LEU A 204 6112 6441 3209 287 -1336 442 C
ATOM 423 CD1 LEU A 204 6.389 -73.632 -79.468 1.00 37.62 C
ANISOU 423 CD1 LEU A 204 5844 5843 2607 375 -1443 197 C
ATOM 424 CD2 LEU A 204 7.122 -73.920 -77.101 1.00 30.08 C
ANISOU 424 CD2 LEU A 204 4768 4979 1683 105 -1007 597 C
ATOM 425 C LEU A 204 3.026 -74.601 -75.932 1.00 53.13 C
ANISOU 425 C LEU A 204 7149 7660 5379 993 -1806 552 C
ATOM 426 O LEU A 204 2.873 -73.560 -75.297 1.00 58.32 O
ANISOU 426 O LEU A 204 7870 8434 5857 914 -1652 687 O
ATOM 427 N ASP A 205 2.013 -75.416 -76.210 1.00 50.93 N
ANISOU 427 N ASP A 205 6480 7001 5869 1062 -1977 313 N
ATOM 428 CA ASP A 205 0.672 -75.116 -75.716 1.00 55.17 C
ANISOU 428 CA ASP A 205 6646 7285 7031 1099 -2013 207 C
ATOM 429 CB ASP A 205 -0.422 -75.845 -76.516 1.00 52.86 C
ANISOU 429 CB ASP A 205 6034 6567 7484 1199 -2403 -206 C
ATOM 430 CG ASP A 205 -0.287 -77.370 -76.471 1.00 62.05 C
ANISOU 430 CG ASP A 205 6881 7556 9138 1164 -2186 -191 C
ATOM 431 OD2 ASP A 205 -0.667 -78.010 -77.476 1.00 75.31 O
ANISOU 431 OD2 ASP A 205 8489 8979 11146 1244 -2568 -529 O
ATOM 432 OD1 ASP A 205 0.197 -77.923 -75.453 1.00 45.81 O
ANISOU 432 OD1 ASP A 205 4669 5611 7126 1067 -1649 149 O
ATOM 433 C ASP A 205 0.566 -75.434 -74.215 1.00 57.84 C
ANISOU 433 C ASP A 205 6622 7668 7688 1005 -1407 556 C
ATOM 434 O ASP A 205 -0.477 -75.211 -73.589 1.00 57.84 O
ANISOU 434 O ASP A 205 6284 7487 8205 1009 -1322 525 O
ATOM 435 N CYS A 206 1.647 -75.980 -73.662 1.00 42.18 N
ANISOU 435 N CYS A 206 4715 5916 5396 931 -992 871 N
ATOM 436 CA CYS A 206 1.754 -76.299 -72.237 1.00 45.96 C
ANISOU 436 CA CYS A 206 4940 6470 6052 858 -397 1236 C
ATOM 437 CB CYS A 206 1.669 -75.033 -71.378 1.00 43.88 C
ANISOU 437 CB CYS A 206 4782 6426 5465 825 -225 1444 C
ATOM 438 SG CYS A 206 3.051 -73.897 -71.628 1.00 51.52 S
ANISOU 438 SG CYS A 206 6362 7888 5326 788 -285 1600 S
ATOM 439 C CYS A 206 0.723 -77.325 -71.778 1.00 53.16 C
ANISOU 439 C CYS A 206 5323 6993 7884 854 -206 1170 C
ATOM 440 O CYS A 206 0.384 -77.396 -70.595 1.00 51.86 O
ANISOU 440 O CYS A 206 4904 6796 8005 804 236 1406 O
ATOM 441 N GLY A 207 0.219 -78.108 -72.725 1.00 57.04 N
ANISOU 441 N GLY A 207 5657 7181 8835 902 -536 837 N
ATOM 442 CA GLY A 207 -0.716 -79.171 -72.422 1.00 45.53 C
ANISOU 442 CA GLY A 207 3704 5334 8262 883 -372 730 C
ATOM 443 C GLY A 207 0.010 -80.436 -72.013 1.00 45.38 C
ANISOU 443 C GLY A 207 3619 5306 8315 842 31 955 C
ATOM 444 O GLY A 207 0.657 -81.093 -72.829 1.00 45.28 O
ANISOU 444 O GLY A 207 3769 5310 8126 876 -155 858 O
ATOM 445 N VAL A 208 -0.102 -80.773 -70.735 1.00 55.32 N
ANISOU 445 N VAL A 208 4658 6534 9826 778 586 1257 N
ATOM 446 CA VAL A 208 0.537 -81.952 -70.178 1.00 49.52 C
ANISOU 446 CA VAL A 208 3873 5774 9167 755 1021 1502 C
ATOM 447 CB VAL A 208 1.398 -81.585 -68.971 1.00 49.49 C
ANISOU 447 CB VAL A 208 4054 6105 8644 737 1511 1954 C
ATOM 448 CG1 VAL A 208 2.171 -82.810 -68.476 1.00 42.72 C
ANISOU 448 CG1 VAL A 208 3207 5240 7785 751 1915 2194 C
ATOM 449 CG2 VAL A 208 2.335 -80.438 -69.336 1.00 42.90 C
ANISOU 449 CG2 VAL A 208 3657 5713 6932 763 1279 2016 C
ATOM 450 C VAL A 208 -0.520 -82.949 -69.732 1.00 54.82 C
ANISOU 450 C VAL A 208 4076 5998 10757 703 1276 1420 C
ATOM 451 O VAL A 208 -1.303 -82.656 -68.829 1.00 67.74 O
ANISOU 451 O VAL A 208 5460 7512 12765 648 1566 1509 O
ATOM 452 N PRO A 209 -0.544 -84.129 -70.319 1.00 59.87 N
ANISOU 452 N PRO A 209 4596 6384 11767 712 1180 1239 N
ATOM 453 CA PRO A 209 -1.500 -85.151 -69.928 1.00 66.95 C
ANISOU 453 CA PRO A 209 5044 6826 13567 644 1412 1120 C
ATOM 454 CB PRO A 209 -1.468 -86.114 -71.088 1.00 56.90 C
ANISOU 454 CB PRO A 209 3736 5339 12546 681 1063 810 C
ATOM 455 CG PRO A 209 -1.048 -85.296 -72.218 1.00 79.05 C
ANISOU 455 CG PRO A 209 6956 8469 14609 775 565 708 C
ATOM 456 CD PRO A 209 -0.012 -84.401 -71.645 1.00 69.42 C
ANISOU 456 CD PRO A 209 6065 7689 12622 779 820 1092 C
ATOM 457 C PRO A 209 -1.161 -85.876 -68.658 1.00 67.95 C
ANISOU 457 C PRO A 209 5304 6905 13610 560 2004 1478 C
ATOM 458 O PRO A 209 -0.031 -85.933 -68.258 1.00 70.33 O
ANISOU 458 O PRO A 209 5919 7494 13307 611 2209 1785 O
ATOM 459 N ASP A 210 -2.184 -86.426 -68.032 1.00 77.10 N
ANISOU 459 N ASP A 210 6319 7680 15296 451 2202 1397 N
ATOM 460 CA ASP A 210 -2.050 -87.226 -66.834 1.00 85.13 C
ANISOU 460 CA ASP A 210 7534 8542 16270 429 2646 1652 C
ATOM 461 CB ASP A 210 -3.451 -87.651 -66.364 1.00 95.97 C
ANISOU 461 CB ASP A 210 8669 9456 18340 333 2782 1469 C
ATOM 462 CG ASP A 210 -3.567 -87.738 -64.853 1.00 99.87 C
ANISOU 462 CG ASP A 210 9401 9895 18649 369 3146 1710 C
ATOM 463 OD2 ASP A 210 -3.522 -88.871 -64.318 1.00102.43 O
ANISOU 463 OD2 ASP A 210 9807 10003 19107 409 3427 1813 O
ATOM 464 OD1 ASP A 210 -3.703 -86.678 -64.203 1.00 84.79 O
ANISOU 464 OD1 ASP A 210 7590 8161 16466 379 3121 1772 O
ATOM 465 C ASP A 210 -1.241 -88.438 -67.193 1.00 86.00 C
ANISOU 465 C ASP A 210 7701 8602 16374 475 2746 1727 C
ATOM 466 O ASP A 210 -0.401 -88.882 -66.447 1.00 82.91 O
ANISOU 466 O ASP A 210 7620 8312 15570 551 3002 2000 O
ATOM 467 N ASN A 211 -1.562 -88.957 -68.361 1.00 87.26 N
ANISOU 467 N ASN A 211 7565 8604 16985 463 2467 1429 N
ATOM 468 CA ASN A 211 -1.023 -90.153 -68.900 1.00 73.27 C
ANISOU 468 CA ASN A 211 5763 6706 15370 502 2516 1416 C
ATOM 469 CB ASN A 211 -2.201 -91.082 -69.108 1.00 83.13 C
ANISOU 469 CB ASN A 211 6699 7425 17461 390 2541 1133 C
ATOM 470 CG ASN A 211 -1.810 -92.473 -69.497 1.00106.96 C
ANISOU 470 CG ASN A 211 9721 10237 20681 408 2735 1185 C
ATOM 471 OD1 ASN A 211 -1.291 -92.708 -70.580 1.00110.81 O
ANISOU 471 OD1 ASN A 211 10025 10618 21460 446 2429 911 O
ATOM 472 ND2 ASN A 211 -2.125 -93.420 -68.646 1.00119.38 N
ANISOU 472 ND2 ASN A 211 11544 11741 22072 427 3195 1509 N
ATOM 473 C ASN A 211 -0.435 -89.819 -70.238 1.00 73.45 C
ANISOU 473 C ASN A 211 5743 6969 15196 645 2056 1231 C
ATOM 474 O ASN A 211 -1.135 -89.445 -71.143 1.00 85.46 O
ANISOU 474 O ASN A 211 7141 8397 16934 647 1566 860 O
ATOM 475 N LEU A 212 0.854 -90.013 -70.380 1.00 67.52 N
ANISOU 475 N LEU A 212 5355 6528 13772 734 2081 1443 N
ATOM 476 CA LEU A 212 1.511 -89.867 -71.655 1.00 68.19 C
ANISOU 476 CA LEU A 212 5692 6818 13400 815 1542 1226 C
ATOM 477 CB LEU A 212 3.009 -89.882 -71.446 1.00 63.81 C
ANISOU 477 CB LEU A 212 5547 6700 12000 900 1668 1525 C
ATOM 478 CG LEU A 212 3.920 -89.921 -72.654 1.00 67.58 C
ANISOU 478 CG LEU A 212 6323 7406 11950 982 1223 1355 C
ATOM 479 CD1 LEU A 212 3.256 -89.250 -73.828 1.00 75.08 C
ANISOU 479 CD1 LEU A 212 7292 8342 12894 980 629 983 C
ATOM 480 CD2 LEU A 212 5.229 -89.251 -72.287 1.00 47.46 C
ANISOU 480 CD2 LEU A 212 4146 5360 8525 1039 1382 1655 C
ATOM 481 C LEU A 212 1.114 -90.933 -72.641 1.00 79.56 C
ANISOU 481 C LEU A 212 6953 7887 15389 819 1309 908 C
ATOM 482 O LEU A 212 0.964 -90.683 -73.807 1.00 80.85 O
ANISOU 482 O LEU A 212 7131 8009 15580 855 767 554 O
ATOM 483 N SER A 213 0.991 -92.149 -72.159 1.00 86.18 N
ANISOU 483 N SER A 213 7639 8443 16661 786 1725 1033 N
ATOM 484 CA SER A 213 0.613 -93.255 -73.004 1.00 96.17 C
ANISOU 484 CA SER A 213 8738 9341 18461 780 1578 766 C
ATOM 485 CB SER A 213 0.726 -94.540 -72.224 1.00 97.60 C
ANISOU 485 CB SER A 213 8778 9212 19093 727 2166 983 C
ATOM 486 OG SER A 213 0.238 -95.598 -73.001 1.00 96.24 O
ANISOU 486 OG SER A 213 8738 9239 18591 728 2676 1408 O
ATOM 487 C SER A 213 -0.785 -93.166 -73.593 1.00105.94 C
ANISOU 487 C SER A 213 9639 10262 20350 727 1151 299 C
ATOM 488 O SER A 213 -0.983 -93.458 -74.760 1.00111.89 O
ANISOU 488 O SER A 213 10365 10864 21283 768 739 -24 O

ATOM 489 N MET A 214 -1.748 -92.797 -72.759 1.00103.52 N
ANISOU 489 N MET A 214 9076 9859 20399 646 1236 247 N
ATOM 490 CA MET A 214 -3.137 -92.766 -73.175 1.00107.12 C
ANISOU 490 CA MET A 214 9241 10089 21369 628 764 -218 C
ATOM 491 CB MET A 214 -4.041 -92.384 -72.002 1.00112.52 C
ANISOU 491 CB MET A 214 9590 10354 22808 416 1024 -361 C
ATOM 492 CG MET A 214 -5.212 -93.329 -71.788 1.00119.93 C
ANISOU 492 CG MET A 214 10266 10958 24342 370 549 -897 C
ATOM 493 SD MET A 214 -6.666 -92.865 -72.748 1.00179.49 S
ANISOU 493 SD MET A 214 17963 18728 31506 561 -300 -1277 S
ATOM 494 CE MET A 214 -6.734 -94.209 -73.930 1.00 80.71 C
ANISOU 494 CE MET A 214 5281 5856 19531 542 -695 -1742 C
ATOM 495 C MET A 214 -3.290 -91.764 -74.303 1.00112.71 C
ANISOU 495 C MET A 214 10105 11106 21612 686 399 -283 C
ATOM 496 O MET A 214 -4.050 -91.981 -75.246 1.00115.31 O
ANISOU 496 O MET A 214 10493 11641 21677 655 682 -10 O
ATOM 497 N ALA A 215 -2.567 -90.656 -74.192 1.00117.16 N
ANISOU 497 N ALA A 215 10732 11662 22120 774 -236 -667 N
ATOM 498 CA ALA A 215 -2.729 -89.573 -75.116 1.00118.83 C
ANISOU 498 CA ALA A 215 11145 12109 21896 861 -733 -836 C
ATOM 499 CB ALA A 215 -1.915 -88.381 -74.673 1.00114.08 C
ANISOU 499 CB ALA A 215 10838 11922 20585 857 -497 -454 C
ATOM 500 C ALA A 215 -2.407 -89.940 -76.555 1.00116.17 C
ANISOU 500 C ALA A 215 11128 11872 21141 976 -1228 -1030 C
ATOM 501 O ALA A 215 -3.025 -89.413 -77.456 1.00116.67 O
ANISOU 501 O ALA A 215 11388 12041 20902 1073 -1759 -1279 O
ATOM 502 N ASP A 216 -1.403 -90.778 -76.793 1.00102.02 N
ANISOU 502 N ASP A 216 9410 10043 19309 971 -1032 -903 N
ATOM 503 CA ASP A 216 -0.988 -91.053 -78.164 1.00 81.17 C
ANISOU 503 CA ASP A 216 6993 7411 16438 1070 -1460 -1122 C
ATOM 504 CB ASP A 216 0.430 -90.546 -78.449 1.00 68.17 C
ANISOU 504 CB ASP A 216 5853 6219 13831 1127 -1437 -842 C
ATOM 505 CG ASP A 216 0.872 -90.780 -79.881 1.00 75.45 C
ANISOU 505 CG ASP A 216 7062 7194 14411 1238 -1976 -1116 C
ATOM 506 OD1 ASP A 216 0.801 -91.903 -80.361 1.00 87.85 O
ANISOU 506 OD1 ASP A 216 8516 8516 16347 1264 -2073 -1291 O
ATOM 507 OD2 ASP A 216 1.311 -89.857 -80.550 1.00 70.57 O
ANISOU 507 OD2 ASP A 216 6802 6860 13153 1298 -2290 -1156 O
ATOM 508 C ASP A 216 -1.106 -92.517 -78.408 1.00 85.47 C
ANISOU 508 C ASP A 216 7279 7605 17592 1028 -1259 -1186 C
ATOM 509 O ASP A 216 -0.919 -93.307 -77.500 1.00 94.35 O
ANISOU 509 O ASP A 216 8316 8685 18848 950 -696 -869 O
ATOM 510 N PRO A 217 -1.499 -92.866 -79.704 1.00 83.09 N
ANISOU 510 N PRO A 217 7869 7037 17668 1086 -1712 -1600 N
ATOM 511 CA PRO A 217 -1.630 -94.312 -79.897 1.00 81.29 C
ANISOU 511 CA PRO A 217 6412 6473 18003 1042 -1521 -1664 C
ATOM 512 CB PRO A 217 -2.714 -94.438 -80.978 1.00 89.92 C
ANISOU 512 CB PRO A 217 7250 7246 19670 1029 -2027 -2197 C
ATOM 513 CG PRO A 217 -2.869 -93.094 -81.605 1.00 92.23 C
ANISOU 513 CG PRO A 217 7702 7726 19616 1114 -2532 -2410 C
ATOM 514 CD PRO A 217 -1.785 -92.233 -81.080 1.00 85.60 C
ANISOU 514 CD PRO A 217 7242 7313 17967 1197 -2395 -2034 C
ATOM 515 C PRO A 217 -0.343 -94.984 -80.347 1.00 72.50 C
ANISOU 515 C PRO A 217 5664 5552 16332 1119 -1524 -1504 C
ATOM 516 O PRO A 217 -0.236 -96.180 -80.307 1.00 74.21 O
ANISOU 516 O PRO A 217 5775 5545 16878 1095 -1312 -1480 O
ATOM 517 N ASN A 218 0.628 -94.196 -80.761 1.00 84.13 N
ANISOU 517 N ASN A 218 7567 7436 16963 1208 -1755 -1405 N
ATOM 518 CA ASN A 218 1.910 -94.711 -81.164 1.00 80.88 C
ANISOU 518 CA ASN A 218 7510 7257 15966 1281 -1748 -1256 C
ATOM 519 CB ASN A 218 2.374 -94.042 -82.429 1.00 65.84 C
ANISOU 519 CB ASN A 218 5956 5557 13503 1396 -2337 -1498 C
ATOM 520 CG ASN A 218 1.551 -94.437 -83.607 1.00 69.10 C
ANISOU 520 CG ASN A 218 6205 5617 14433 1460 -2869 -1984 C
ATOM 521 OD1 ASN A 218 1.218 -95.581 -83.755 1.00 71.77 O
ANISOU 521 OD1 ASN A 218 6308 5633 15328 1451 -2833 -2121 O
ATOM 522 ND2 ASN A 218 1.216 -93.493 -84.444 1.00 69.06 N
ANISOU 522 ND2 ASN A 218 6335 5661 14242 1536 -3375 -2258 N
ATOM 523 C ASN A 218 2.938 -94.558 -80.076 1.00 76.59 C
ANISOU 523 C ASN A 218 7193 7078 14829 1259 -1240 -771 C
ATOM 524 O ASN A 218 4.107 -94.714 -80.319 1.00 72.42 O
ANISOU 524 O ASN A 218 6993 6838 13685 1326 -1238 -633 O
ATOM 525 N ILE A 219 2.496 -94.208 -78.881 1.00 66.32 N
ANISOU 525 N ILE A 219 6081 9555 9561 -94 952 -404 N
ATOM 526 CA ILE A 219 3.393 -94.166 -77.738 1.00 65.72 C
ANISOU 526 CA ILE A 219 6212 9181 9579 -72 1048 -310 C
ATOM 527 CB ILE A 219 3.620 -92.745 -77.206 1.00 64.88 C
ANISOU 527 CB ILE A 219 6116 9124 9411 274 1156 -241 C
ATOM 528 CG1 ILE A 219 4.273 -91.873 -78.271 1.00 59.25 C
ANISOU 528 CG1 ILE A 219 5506 8318 8690 570 1152 -300 C
ATOM 529 CD1 ILE A 219 4.549 -90.458 -77.806 1.00 57.36 C
ANISOU 529 CD1 ILE A 219 5316 8071 8409 892 1271 -246 C
ATOM 530 CG2 ILE A 219 4.496 -92.778 -75.962 1.00 57.46 C
ANISOU 530 CG2 ILE A 219 5381 7903 8550 264 1212 -167 C
ATOM 531 C ILE A 219 2.808 -95.035 -76.641 1.00 58.39 C
ANISOU 531 C ILE A 219 5219 8293 8675 -380 1094 -229 C
ATOM 532 O ILE A 219 1.721 -94.769 -76.135 1.00 64.43 O
ANISOU 532 O ILE A 219 5734 9391 9357 -415 1164 -170 O
ATOM 533 N ARG A 220 3.532 -96.084 -76.286 1.00 54.92 N
ANISOU 533 N ARG A 220 5009 7508 8349 -588 1075 -216 N
ATOM 534 CA ARG A 220 3.020 -97.081 -75.372 1.00 60.48 C
ANISOU 534 CA ARG A 220 5708 8192 9078 -908 1133 -133 C
ATOM 535 CB ARG A 220 2.793 -98.388 -76.118 1.00 65.47 C
ANISOU 535 CB ARG A 220 6374 8710 9791 -1252 1048 -229 C
ATOM 536 CG ARG A 220 2.451 -99.550 -75.230 1.00 81.76 C
ANISOU 536 CG ARG A 220 8513 10642 11912 -1608 1130 -137 C
ATOM 537 CD ARG A 220 2.623-100.853 -75.977 1.00 92.84 C
ANISOU 537 CD ARG A 220 10080 11777 13417 -1910 1047 -246 C
ATOM 538 NE ARG A 220 1.405-101.301 -76.631 1.00104.97 N
ANISOU 538 NE ARG A 220 11345 13587 14950 -2224 994 -357 N
ATOM 539 CZ ARG A 220 0.412-101.905 -75.990 1.00108.81 C
ANISOU 539 CZ ARG A 220 11665 14209 15470 -2570 1095 -290 C
ATOM 540 NH1 ARG A 220 -0.673-102.298 -76.645 1.00108.87 N
ANISOU 540 NH1 ARG A 220 11384 14481 15499 -2875 1022 -416 N
ATOM 541 NH2 ARG A 220 0.508-102.109 -74.683 1.00111.49 N
ANISOU 541 NH2 ARG A 220 12124 14423 15815 -2611 1271 -98 N
ATOM 542 C ARG A 220 3.998 -97.283 -74.227 1.00 64.38 C
ANISOU 542 C ARG A 220 6483 8363 9614 -860 1184 -22 C
ATOM 543 O ARG A 220 5.192 -97.494 -74.448 1.00 69.74 O
ANISOU 543 O ARG A 220 7400 8711 10387 -767 1117 -53 O
ATOM 544 N PHE A 221 3.494 -97.200 -73.002 1.00 68.57 N
ANISOU 544 N PHE A 221 6979 9009 10066 -900 1304 109 N
ATOM 545 CA PHE A 221 4.340 -97.367 -71.836 1.00 61.90 C
ANISOU 545 CA PHE A 221 6408 7898 9214 -834 1333 218 C
ATOM 546 CB PHE A 221 3.572 -97.065 -70.555 1.00 51.11 C
ANISOU 546 CB PHE A 221 4981 6740 7699 -834 1490 356 C
ATOM 547 CG PHE A 221 4.291 -97.479 -69.311 1.00 53.73 C
ANISOU 547 CG PHE A 221 5621 6812 7982 -811 1512 479 C
ATOM 548 CD1 PHE A 221 5.260 -96.656 -68.751 1.00 50.85 C
ANISOU 548 CD1 PHE A 221 5425 6327 7567 -516 1440 471 C
ATOM 549 CE1 PHE A 221 5.933 -97.033 -67.600 1.00 47.34 C
ANISOU 549 CE1 PHE A 221 5264 5670 7052 -473 1420 575 C
ATOM 550 CZ PHE A 221 5.637 -98.259 -66.996 1.00 49.71 C
ANISOU 550 CZ PHE A 221 5714 5851 7323 -709 1505 716 C
ATOM 551 CE2 PHE A 221 4.670 -99.094 -67.552 1.00 51.54 C
ANISOU 551 CE2 PHE A 221 5792 6166 7625 -1029 1612 732 C
ATOM 552 CD2 PHE A 221 4.007 -98.700 -68.701 1.00 60.21 C
ANISOU 552 CD2 PHE A 221 6575 7499 8801 -1087 1599 602 C
ATOM 553 C PHE A 221 4.877 -98.786 -71.799 1.00 66.05 C
ANISOU 553 C PHE A 221 7175 8073 9846 -1074 1294 245 C
ATOM 554 O PHE A 221 4.125 -99.755 -71.951 1.00 69.47 O
ANISOU 554 O PHE A 221 7557 8526 10310 -1395 1343 257 O
ATOM 555 N LEU A 222 6.182 -98.915 -71.604 1.00 57.16 N
ANISOU 555 N LEU A 222 6308 6620 8788 -921 1209 252 N
ATOM 556 CA LEU A 222 6.797-100.226 -71.524 1.00 58.48 C
ANISOU 556 CA LEU A 222 6739 6428 9051 -1080 1177 293 C
ATOM 557 CB LEU A 222 8.097-100.261 -72.318 1.00 68.01 C
ANISOU 557 CB LEU A 222 8082 7360 10400 -902 1052 196 C
ATOM 558 CG LEU A 222 8.011-100.741 -73.758 1.00 67.43 C
ANISOU 558 CG LEU A 222 7975 7227 10420 -1017 1013 50 C
ATOM 559 CD2 LEU A 222 7.111-101.961 -73.861 1.00 61.70 C
ANISOU 559 CD2 LEU A 222 7286 6462 9693 -1394 1066 57 C
ATOM 560 CD1 LEU A 222 9.409-101.051 -74.244 1.00 60.29 C
ANISOU 560 CD1 LEU A 222 7274 5978 9655 -845 938 4 C
ATOM 561 C LEU A 222 7.092-100.595 -70.088 1.00 56.21 C
ANISOU 561 C LEU A 222 6675 6000 8680 -1060 1226 466 C
ATOM 562 O LEU A 222 6.644-101.627 -69.587 1.00 54.92 O
ANISOU 562 O LEU A 222 6641 5730 8495 -1301 1321 576 O
ATOM 563 N ASP A 223 7.851 -99.740 -69.422 1.00 55.33 N
ANISOU 563 N ASP A 223 6627 5882 8514 -772 1160 487 N
ATOM 564 CA ASP A 223 8.398-100.110 -68.138 1.00 55.70 C
ANISOU 564 CA ASP A 223 6935 5759 8469 -695 1147 631 C
ATOM 565 CB ASP A 223 9.437-101.219 -68.336 1.00 63.37 C
ANISOU 565 CB ASP A 223 8159 6343 9575 -702 1050 656 C
ATOM 566 CG ASP A 223 9.612-102.085 -67.108 1.00 79.65 C
ANISOU 566 CG ASP A 223 10524 8218 11521 -722 1083 848 C
ATOM 567 OD1 ASP A 223 8.656-102.172 -66.305 1.00 92.81 O
ANISOU 567 OD1 ASP A 223 12208 10034 13023 -854 1239 970 O
ATOM 568 OD2 ASP A 223 10.703-102.673 -66.952 1.00 79.79 O
ANISOU 568 OD2 ASP A 223 10763 7945 11608 -587 964 888 O
ATOM 569 C ASP A 223 9.042 -98.920 -67.452 1.00 58.61 C
ANISOU 569 C ASP A 223 7311 6205 8753 -391 1055 606 C
ATOM 570 O ASP A 223 9.082 -97.813 -67.990 1.00 57.58 O
ANISOU 570 O ASP A 223 6994 6227 8655 -251 1026 483 O
ATOM 571 N LYS A 224 9.553 -99.165 -66.255 1.00 56.49 N
ANISOU 571 N LYS A 224 7283 5817 8366 -289 1006 721 N
ATOM 572 CA LYS A 224 10.285 -98.164 -65.513 1.00 57.81 C
ANISOU 572 CA LYS A 224 7501 6018 8447 -20 876 680 C
ATOM 573 CB LYS A 224 9.728 -98.051 -64.105 1.00 52.80 C
ANISOU 573 CB LYS A 224 7028 5506 7528 17 964 813 C
ATOM 574 CG LYS A 224 8.361 -97.472 -64.055 1.00 60.84 C
ANISOU 574 CG LYS A 224 7864 6837 8417 -68 1183 828 C
ATOM 575 CD LYS A 224 8.252 -96.576 -62.852 1.00 72.80 C
ANISOU 575 CD LYS A 224 9494 8494 9670 134 1203 850 C
ATOM 576 CE LYS A 224 6.871 -96.013 -62.766 1.00 80.98 C
ANISOU 576 CE LYS A 224 10342 9852 10575 83 1452 880 C
ATOM 577 NZ LYS A 224 5.905 -96.904 -63.482 1.00 86.45 N
ANISOU 577 NZ LYS A 224 10843 10620 11384 -217 1618 949 N
ATOM 578 C LYS A 224 11.758 -98.513 -65.435 1.00 62.08 C
ANISOU 578 C LYS A 224 8190 6281 9115 136 658 659 C

ATOM 579 O LYS A 224 12.138 -99.685 -65.452 1.00 64.62 O
ANISOU 579 O LYS A 224 8681 6373 9501 73 633 750 O
ATOM 580 N LEU A 225 12.586 -97.481 -65.349 1.00 61.28 N
ANISOU 580 N LEU A 225 8020 6200 9064 343 506 537 N
ATOM 581 CA LEU A 225 14.001 -97.653 -65.072 1.00 60.96 C
ANISOU 581 CA LEU A 225 8073 5954 9135 514 276 512 C
ATOM 582 CB LEU A 225 14.741 -96.349 -65.340 1.00 63.08 C
ANISOU 582 CB LEU A 225 8165 6271 9529 664 156 332 C
ATOM 583 CG LEU A 225 15.092 -96.002 -66.780 1.00 63.22 C
ANISOU 583 CG LEU A 225 7960 6235 9824 646 202 206 C
ATOM 584 CD1 LEU A 225 15.547 -94.564 -66.830 1.00 62.08 C
ANISOU 584 CD1 LEU A 225 7679 6160 9749 766 146 51 C
ATOM 585 CD2 LEU A 225 16.190 -96.920 -67.288 1.00 58.08 C
ANISOU 585 CD2 LEU A 225 7327 5338 9403 688 99 219 C
ATOM 586 C LEU A 225 14.151 -98.022 -63.605 1.00 74.14 C
ANISOU 586 C LEU A 225 10011 7601 10559 610 182 645 C
ATOM 587 O LEU A 225 13.228 -97.771 -62.813 1.00 81.92 O
ANISOU 587 O LEU A 225 11087 8754 11286 575 306 718 O
ATOM 588 N PRO A 226 15.306 -98.602 -63.227 1.00 72.48 N
ANISOU 588 N PRO A 226 9932 7198 10411 757 -29 682 N
ATOM 589 CA PRO A 226 15.532 -98.814 -61.798 1.00 72.91 C
ANISOU 589 CA PRO A 226 10256 7253 10193 901 -159 796 C
ATOM 590 CB PRO A 226 16.926 -99.447 -61.745 1.00 64.66 C
ANISOU 590 CB PRO A 226 9267 5999 9301 1083 -415 811 C
ATOM 591 CG PRO A 226 17.583 -99.030 -63.029 1.00 61.65 C
ANISOU 591 CG PRO A 226 8577 5565 9282 1069 -446 640 C
ATOM 592 CD PRO A 226 16.464 -99.019 -64.032 1.00 62.04 C
ANISOU 592 CD PRO A 226 8513 5672 9386 835 -162 623 C
ATOM 593 C PRO A 226 15.533 -97.483 -61.051 1.00 82.38 C
ANISOU 593 C PRO A 226 11427 8651 11222 1020 -260 671 C
ATOM 594 O PRO A 226 15.944 -96.452 -61.596 1.00 80.06 O
ANISOU 594 O PRO A 226 10906 8411 11102 1052 -333 479 O
ATOM 595 N GLN A 227 15.063 -97.511 -59.811 1.00 82.90 N
ANISOU 595 N GLN A 227 11751 8807 10941 1084 -243 779 N
ATOM 596 CA GLN A 227 14.912 -96.295 -59.037 1.00 73.01 C
ANISOU 596 CA GLN A 227 10533 7735 9474 1194 -305 660 C
ATOM 597 CB GLN A 227 14.103 -96.565 -57.774 1.00 76.63 C
ANISOU 597 CB GLN A 227 11313 8290 9514 1237 -178 830 C
ATOM 598 CG GLN A 227 12.631 -96.757 -58.045 1.00 78.01 C
ANISOU 598 CG GLN A 227 11437 8589 9614 1038 208 950 C
ATOM 599 CD GLN A 227 11.925 -97.465 -56.914 1.00 85.04 C
ANISOU 599 CD GLN A 227 12655 9505 10151 1044 383 1186 C
ATOM 600 OE1 GLN A 227 12.523 -98.279 -56.208 1.00 90.72 O
ANISOU 600 OE1 GLN A 227 13660 10074 10737 1154 248 1321 O
ATOM 601 NE2 GLN A 227 10.647 -97.155 -56.729 1.00 83.42 N
ANISOU 601 NE2 GLN A 227 12412 9496 9787 943 700 1249 N
ATOM 602 C GLN A 227 16.246 -95.652 -58.695 1.00 70.38 C
ANISOU 602 C GLN A 227 10167 7359 9217 1379 -668 485 C
ATOM 603 O GLN A 227 17.304 -96.285 -58.747 1.00 73.10 O
ANISOU 603 O GLN A 227 10505 7557 9711 1469 -894 503 O
ATOM 604 N GLN A 228 16.181 -94.376 -58.354 1.00 72.46 N
ANISOU 604 N GLN A 228 10398 7750 9385 1433 -718 308 N
ATOM 605 CA GLN A 228 17.353 -93.619 -57.983 1.00 76.24 C
ANISOU 605 CA GLN A 228 10832 8202 9934 1562 -1060 104 C
ATOM 606 CB GLN A 228 17.630 -92.547 -59.036 1.00 75.48 C
ANISOU 606 CB GLN A 228 10419 8090 10171 1477 -1024 -111 C
ATOM 607 CG GLN A 228 18.600 -91.464 -58.613 1.00 80.08 C
ANISOU 607 CG GLN A 228 10950 8661 10815 1552 -1315 -359 C
ATOM 608 CD GLN A 228 19.823 -91.389 -59.504 1.00 83.98 C
ANISOU 608 CD GLN A 228 11126 9024 11758 1516 -1475 -480 C
ATOM 609 OE1 GLN A 228 19.787 -91.793 -60.667 1.00 80.28 O
ANISOU 609 OE1 GLN A 228 10459 8479 11564 1430 -1295 -417 O
ATOM 610 NE2 GLN A 228 20.920 -90.871 -58.960 1.00 89.67 N
ANISOU 610 NE2 GLN A 228 11792 9724 12553 1581 -1814 -660 N
ATOM 611 C GLN A 228 17.097 -92.998 -56.619 1.00 79.11 C
ANISOU 611 C GLN A 228 11488 8690 9882 1694 -1157 57 C
ATOM 612 O GLN A 228 15.951 -92.758 -56.242 1.00 81.95 O
ANISOU 612 O GLN A 228 11996 9170 9971 1674 -894 130 O
ATOM 613 N THR A 229 18.163 -92.757 -55.869 1.00 80.30 N
ANISOU 613 N THR A 229 11717 8820 9973 1838 -1536 -68 N
ATOM 614 CA THR A 229 18.037 -92.144 -54.563 1.00 79.90 C
ANISOU 614 CA THR A 229 11975 8877 9505 1980 -1676 -149 C
ATOM 615 CB THR A 229 18.344 -93.156 -53.457 1.00 79.87 C
ANISOU 615 CB THR A 229 12300 8873 9172 2163 -1875 32 C
ATOM 616 OG1 THR A 229 17.451 -94.266 -53.584 1.00 79.72 O
ANISOU 616 OG1 THR A 229 12409 8825 9056 2107 -1546 334 O
ATOM 617 CG2 THR A 229 18.171 -92.535 -52.077 1.00 80.85 C
ANISOU 617 CG2 THR A 229 12794 9118 8807 2330 -2013 -51 C
ATOM 618 C THR A 229 18.940 -90.923 -54.485 1.00 87.92 C
ANISOU 618 C THR A 229 12861 9884 10659 1994 -1974 -472 C
ATOM 619 O THR A 229 19.990 -90.871 -55.126 1.00 88.12 O
ANISOU 619 O THR A 229 12592 9820 11070 1947 -2183 -590 O
ATOM 620 N ILE A 230 18.523 -89.935 -53.704 1.00 97.10 N
ANISOU 620 N ILE A 230 14246 11131 11516 2051 -1974 -619 N
ATOM 621 CA ILE A 230 19.181 -88.645 -53.709 1.00103.59 C
ANISOU 621 CA ILE A 230 14967 11916 12478 2015 -2183 -947 C
ATOM 622 C ILE A 230 19.863 -88.320 -52.399 1.00113.84 C
ANISOU 622 C ILE A 230 16534 13262 13458 2162 -2601 -1118 C
ATOM 623 O ILE A 230 19.295 -88.510 -51.324 1.00121.58 O
ANISOU 623 O ILE A 230 17907 14339 13949 2317 -2584 -1029 O

ATOM 624 CB ILE A 230 18.179 -87.538 -53.982 1.00105.04 C
ANISOU 624 CB ILE A 230 15193 12122 12595 1958 -1845 -1041 C
ATOM 625 CG1 ILE A 230 17.152 -88.005 -55.010 1.00104.55 C
ANISOU 625 CG1 ILE A 230 14959 12086 12678 1863 -1408 -819 C
ATOM 626 CG2 ILE A 230 18.903 -86.301 -54.458 1.00105.54 C
ANISOU 626 CG2 ILE A 230 15063 12070 12969 1856 -1977 -1352 C
ATOM 627 CD1 ILE A 230 17.745 -88.229 -56.383 1.00104.69 C
ANISOU 627 CD1 ILE A 230 14579 11987 13209 1717 -1392 -826 C
ATOM 628 N ASP A 231 21.086 -87.838 -52.482 1.00115.91 N
ANISOU 628 N ASP A 231 16583 13462 13997 2110 -2974 -1372 N
ATOM 629 CA ASP A 231 21.641 -87.140 -51.355 1.00120.15 C
ANISOU 629 CA ASP A 231 17336 14052 14261 2219 -3418 -1602 C
ATOM 630 CB ASP A 231 22.261 -88.073 -50.356 1.00123.58 C
ANISOU 630 CB ASP A 231 17760 14547 14647 2373 -3831 -1503 C
ATOM 631 CG ASP A 231 21.380 -88.242 -49.187 1.00128.77 C
ANISOU 631 CG ASP A 231 18883 15309 14735 2606 -3803 -1258 C
ATOM 632 OD1 ASP A 231 20.737 -89.295 -49.084 1.00126.27 O
ANISOU 632 OD1 ASP A 231 18942 15052 13982 2675 -3670 -1305 O
ATOM 633 OD2 ASP A 231 21.278 -87.276 -48.411 1.00134.04 O
ANISOU 633 OD2 ASP A 231 19559 15984 15387 2731 -3885 -1010 O
ATOM 634 C ASP A 231 22.444 -85.889 -51.637 1.00125.72 C
ANISOU 634 C ASP A 231 17842 14665 15262 2056 -3605 -1975 C
ATOM 635 O ASP A 231 23.430 -85.578 -50.971 1.00130.82 O
ANISOU 635 O ASP A 231 18489 15333 15883 2074 -4069 -2215 O
ATOM 636 N ARG A 232 21.995 -85.170 -52.642 1.00126.23 N
ANISOU 636 N ARG A 232 17735 14620 15606 1893 -3243 -2024 N
ATOM 637 CA ARG A 232 22.454 -83.831 -52.862 1.00134.44 C
ANISOU 637 CA ARG A 232 18668 15529 16885 1731 -3322 -2364 C
ATOM 638 CB ARG A 232 22.190 -83.405 -54.301 1.00129.88 C
ANISOU 638 CB ARG A 232 17785 14814 16749 1563 -2921 -2323 C
ATOM 639 CG ARG A 232 22.414 -84.525 -55.308 1.00126.61 C
ANISOU 639 CG ARG A 232 17023 14405 16678 1532 -2808 -2070 C
ATOM 640 CD ARG A 232 23.728 -84.381 -56.055 1.00128.51 C
ANISOU 640 CD ARG A 232 16828 14531 17471 1374 -3003 -2217 C
ATOM 641 NE ARG A 232 23.583 -83.816 -57.393 1.00128.05 N
ANISOU 641 NE ARG A 232 16541 14324 17789 1222 -2636 -2228 N
ATOM 642 CZ ARG A 232 24.433 -84.032 -58.394 1.00126.77 C
ANISOU 642 CZ ARG A 232 15985 14070 18113 1112 -2596 -2206 C
ATOM 643 NH1 ARG A 232 24.232 -83.474 -59.579 1.00122.76 N
ANISOU 643 NH1 ARG A 232 15332 13425 17886 1000 -2241 -2206 N
ATOM 644 NH2 ARG A 232 25.489 -84.807 -58.209 1.00127.58 N
ANISOU 644 NH2 ARG A 232 15849 14219 18408 1141 -2899 -2176 N
ATOM 645 C ARG A 232 21.706 -82.977 -51.836 1.00142.51 C
ANISOU 645 C ARG A 232 20155 16571 17423 1824 -3281 -2523 C
ATOM 646 O ARG A 232 20.819 -83.484 -51.140 1.00144.75 O
ANISOU 646 O ARG A 232 20784 16981 17234 2009 -3143 -2342 O
ATOM 647 N ALA A 233 22.108 -81.716 -51.686 1.00143.11 N
ANISOU 647 N ALA A 233 20255 16505 17614 1696 -3381 -2861 N
ATOM 648 CA ALA A 233 21.492 -80.842 -50.695 1.00138.64 C
ANISOU 648 CA ALA A 233 20161 15926 16589 1791 -3377 -3062 C
ATOM 649 CB ALA A 233 22.207 -79.516 -50.625 1.00139.58 C
ANISOU 649 CB ALA A 233 20248 15843 16945 1594 -3582 -3476 C
ATOM 650 C ALA A 233 20.032 -80.612 -50.987 1.00130.68 C
ANISOU 650 C ALA A 233 19385 14939 15328 1911 -2826 -2876 C
ATOM 651 O ALA A 233 19.631 -80.498 -52.133 1.00123.83 O
ANISOU 651 O ALA A 233 18270 14018 14763 1838 -2447 -2725 O
ATOM 652 N GLY A 234 19.248 -80.601 -49.919 1.00129.16 N
ANISOU 652 N GLY A 234 19667 14839 14568 2113 -2787 -2890 N
ATOM 653 CA GLY A 234 17.868 -80.190 -49.930 1.00121.13 C
ANISOU 653 CA GLY A 234 18879 13827 13278 2253 -2280 -2750 C
ATOM 654 C GLY A 234 16.980 -81.324 -50.323 1.00115.06 C
ANISOU 654 C GLY A 234 18018 12721 15421 2346 -1955 -2335 C
ATOM 655 O GLY A 234 15.779 -81.266 -50.165 1.00112.28 O
ANISOU 655 O GLY A 234 17846 13024 11790 2485 -1551 -2175 O
ATOM 656 N ILE A 235 17.585 -82.392 -50.807 1.00118.14 N
ANISOU 656 N ILE A 235 18116 13712 13061 2265 -2126 -2162 N
ATOM 657 CA ILE A 235 16.837 -83.594 -51.079 1.00116.53 C
ANISOU 657 CA ILE A 235 17814 13643 12818 2307 -1838 -1784 C
ATOM 658 CB ILE A 235 16.631 -83.752 -52.586 1.00101.63 C
ANISOU 658 CB ILE A 235 15504 11702 11411 2149 -1532 -1668 C
ATOM 659 CG1 ILE A 235 16.041 -85.107 -52.909 1.00102.57 C
ANISOU 659 CG1 ILE A 235 15486 11937 11548 2141 -1318 -1311 C
ATOM 660 CD1 ILE A 235 15.510 -85.210 -54.320 1.00101.97 C
ANISOU 660 CD1 ILE A 235 15053 11840 11850 2011 -992 -1204 C
ATOM 661 CG2 ILE A 235 17.931 -83.537 -53.315 1.00102.37 C
ANISOU 661 CG2 ILE A 235 13989 10357 10749 1967 -1798 -1865 C
ATOM 662 C ILE A 235 17.544 -84.794 -50.449 1.00125.11 C
ANISOU 662 C ILE A 235 18914 14799 13821 2357 -2152 -1626 C
ATOM 663 O ILE A 235 18.695 -85.089 -50.748 1.00129.27 O
ANISOU 663 O ILE A 235 19162 15258 14699 2258 -2463 -1682 O
ATOM 664 N LYS A 236 16.859 -85.458 -49.540 1.00123.27 N
ANISOU 664 N LYS A 236 19029 14699 13109 2532 -2052 -1423 N
ATOM 665 CA LYS A 236 17.371 -86.669 -48.951 1.00114.92 C
ANISOU 665 CA LYS A 236 18078 13699 11888 2630 -2295 -1230 C
ATOM 666 CB LYS A 236 17.898 -86.421 -47.532 1.00113.45 C
ANISOU 666 CB LYS A 236 18312 13564 11228 2825 -2700 -1398 C
ATOM 667 CG LYS A 236 17.834 -84.968 -47.042 1.00111.53 C
ANISOU 667 CG LYS A 236 18275 13281 10820 2839 -2776 -1760 C
ATOM 668 CD LYS A 236 16.484 -84.624 -46.406 1.00105.27 C
ANISOU 668 CD LYS A 236 17892 12574 9531 3002 -2360 -1675 C

ATOM 669 CE LYS A 236 15.824 -83.402 -47.022 1.00 96.12 C
ANISOU 669 CE LYS A 236 16631 11335 8557 2914 -2029 -1841 C
ATOM 670 NZ LYS A 236 14.653 -83.764 -47.859 1.00 89.20 N
ANISOU 670 NZ LYS A 236 15528 10526 7838 2867 -1480 -1542 N
ATOM 671 C LYS A 236 16.249 -87.674 -48.930 1.00109.77 C
ANISOU 671 C LYS A 236 17539 13141 11027 2679 -1867 -852 C
ATOM 672 O LYS A 236 15.233 -87.479 -48.277 1.00102.98 O
ANISOU 672 O LYS A 236 16975 12377 9775 2790 -1565 -779 O
ATOM 673 N ASP A 237 16.466 -88.792 -49.587 1.00110.51 N
ANISOU 673 N ASP A 237 17388 13197 11406 2586 -1825 -621 N
ATOM 674 CA ASP A 237 15.513 -89.845 -49.453 1.00109.66 C
ANISOU 674 CA ASP A 237 17362 13143 11160 2582 -1453 -260 C
ATOM 675 CB ASP A 237 15.250 -90.027 -47.980 1.00114.61 C
ANISOU 675 CB ASP A 237 18502 13861 11186 2803 -1437 -107 C
ATOM 676 CG ASP A 237 16.439 -90.614 -47.285 1.00120.20 C
ANISOU 676 CG ASP A 237 19399 14525 11747 2960 -1900 -83 C
ATOM 677 OD2 ASP A 237 16.700 -91.804 -47.497 1.00127.13 O
ANISOU 677 OD2 ASP A 237 20476 15390 12438 3037 -1803 224 O
ATOM 678 OD1 ASP A 237 17.149 -89.895 -46.570 1.00119.09 O
ANISOU 678 OD1 ASP A 237 19201 14361 11686 3005 -2357 -367 O
ATOM 679 C ASP A 237 14.254 -89.705 -50.273 1.00102.04 C
ANISOU 679 C ASP A 237 16189 12237 10347 2439 -947 -162 C
ATOM 680 O ASP A 237 13.234 -90.305 -49.986 1.00102.84 O
ANISOU 680 O ASP A 237 16412 12426 10236 2442 -589 94 O
ATOM 681 N ARG A 238 14.347 -88.889 -51.300 1.00 86.07 N
ANISOU 681 N ARG A 238 13848 10170 8686 2319 -912 -359 N
ATOM 682 CA ARG A 238 13.368 -88.855 -52.333 1.00 68.71 C
ANISOU 682 CA ARG A 238 11364 8022 6720 2178 -502 -247 C
ATOM 683 CB ARG A 238 13.647 -87.688 -53.201 1.00 64.35 C
ANISOU 683 CB ARG A 238 10582 7425 6442 2125 -467 -495 C
ATOM 684 CG ARG A 238 12.534 -86.809 -53.351 1.00 80.76 C
ANISOU 684 CG ARG A 238 12705 9636 8344 2194 -74 -492 C
ATOM 685 CD ARG A 238 13.089 -85.485 -53.158 1.00 82.55 C
ANISOU 685 CD ARG A 238 13158 9808 8401 2328 -185 -781 C
ATOM 686 NE ARG A 238 12.328 -84.515 -53.878 1.00 75.31 N
ANISOU 686 NE ARG A 238 12048 8868 7697 2313 45 -895 N
ATOM 687 CZ ARG A 238 11.618 -83.563 -53.330 1.00 85.25 C
ANISOU 687 CZ ARG A 238 13495 10183 8714 2471 276 -981 C
ATOM 688 NH1 ARG A 238 11.037 -82.744 -54.147 1.00 68.92 N
ANISOU 688 NH1 ARG A 238 11813 8200 6173 2650 324 -978 N
ATOM 689 NH2 ARG A 238 11.244 -83.615 -52.068 1.00 92.77 N
ANISOU 689 NH2 ARG A 238 14266 11098 9883 2476 477 -1061 N
ATOM 690 C ARG A 238 13.680 -90.055 -53.152 1.00 67.66 C
ANISOU 690 C ARG A 238 10977 7805 6924 2025 -530 -73 C
ATOM 691 O ARG A 238 14.825 -90.420 -53.255 1.00 66.89 O
ANISOU 691 O ARG A 238 10808 7585 7023 2021 -874 -141 O
ATOM 692 N VAL A 239 12.675 -90.651 -53.757 1.00 62.98 N
ANISOU 692 N VAL A 239 10250 7281 6398 1903 -174 144 N
ATOM 693 CA VAL A 239 12.877 -91.768 -54.633 1.00 61.13 C
ANISOU 693 CA VAL A 239 9796 6947 6483 1742 -166 291 C
ATOM 694 CB VAL A 239 12.141 -92.992 -54.166 1.00 67.70 C
ANISOU 694 CB VAL A 239 10808 7802 7113 1693 51 596 C
ATOM 695 CG1 VAL A 239 12.298 -94.081 -55.154 1.00 61.52 C
ANISOU 695 CG1 VAL A 239 9805 6891 6680 1502 94 720 C
ATOM 696 CG2 VAL A 239 12.667 -93.440 -52.841 1.00 66.47 C
ANISOU 696 CG2 VAL A 239 11066 7606 6586 1883 -159 679 C
ATOM 697 C VAL A 239 12.354 -91.369 -55.966 1.00 71.40 C
ANISOU 697 C VAL A 239 10722 8277 8130 1582 50 245 C
ATOM 698 O VAL A 239 11.300 -90.834 -56.061 1.00 75.06 O
ANISOU 698 O VAL A 239 11115 8899 8507 1546 371 304 O
ATOM 699 N TYR A 240 13.108 -91.620 -57.012 1.00 72.90 N
ANISOU 699 N TYR A 240 10667 8328 8703 1505 -124 142 N
ATOM 700 CA TYR A 240 12.701 -91.220 -58.340 1.00 73.01 C
ANISOU 700 CA TYR A 240 10354 8359 9027 1378 57 94 C
ATOM 701 CB TYR A 240 13.734 -90.307 -58.944 1.00 58.93 C
ANISOU 701 CB TYR A 240 8405 6462 7525 1405 -133 -145 C
ATOM 702 CG TYR A 240 13.712 -88.916 -58.444 1.00 54.44 C
ANISOU 702 CG TYR A 240 7957 5939 6790 1525 -151 -332 C
ATOM 703 CD2 TYR A 240 13.063 -87.934 -59.138 1.00 52.37 C
ANISOU 703 CD2 TYR A 240 7573 5744 6583 1536 83 -409 C
ATOM 704 CE2 TYR A 240 13.052 -86.669 -58.701 1.00 52.09 C
ANISOU 704 CE2 TYR A 240 7687 5712 6393 1658 87 -584 C
ATOM 705 CZ TYR A 240 13.709 -86.364 -57.565 1.00 72.81 C
ANISOU 705 CZ TYR A 240 10584 8284 8797 1748 -166 -704 C
ATOM 706 OH TYR A 240 13.712 -85.101 -57.105 1.00 72.59 O
ANISOU 706 OH TYR A 240 10745 8232 8604 1859 -167 -903 O
ATOM 707 CE1 TYR A 240 14.370 -87.320 -56.860 1.00 74.81 C
ANISOU 707 CE1 TYR A 240 10945 8501 8977 1744 -427 -632 C
ATOM 708 CD1 TYR A 240 14.372 -88.573 -57.297 1.00 62.68 C
ANISOU 708 CD1 TYR A 240 9262 6952 7603 1644 -408 -436 C
ATOM 709 C TYR A 240 12.606 -92.382 -59.262 1.00 79.47 C
ANISOU 709 C TYR A 240 11021 9109 10066 1213 142 250 C
ATOM 710 O TYR A 240 13.258 -93.372 -59.087 1.00 78.87 O
ANISOU 710 O TYR A 240 11034 8889 10043 1207 -24 335 O
ATOM 711 N SER A 241 11.791 -92.245 -60.275 1.00 79.90 N
ANISOU 711 N SER A 241 10855 9264 10238 1092 395 282 N
ATOM 712 CA SER A 241 11.721 -93.257 -61.304 1.00 79.70 C
ANISOU 712 CA SER A 241 10667 9161 10453 919 458 370 C
ATOM 713 CB SER A 241 10.567 -94.228 -61.051 1.00 72.20 C
ANISOU 713 CB SER A 241 9773 8310 9349 769 699 579 C
ATOM 714 OG SER A 241 9.320 -93.568 -61.151 1.00 61.03 O
ANISOU 714 OG SER A 241 8221 7146 7820 747 953 583 O
ATOM 715 C SER A 241 11.537 -92.543 -62.635 1.00 66.75 C
ANISOU 715 C SER A 241 8740 7566 9055 879 546 244 C
ATOM 716 O SER A 241 11.049 -91.414 -62.683 1.00 57.48 O
ANISOU 716 O SER A 241 7501 6529 7811 965 648 154 O
ATOM 717 N ASN A 242 11.949 -93.201 -63.709 1.00 57.03 N
ANISOU 717 N ASN A 242 7369 6207 8091 773 514 243 N
ATOM 718 CA ASN A 242 11.715 -92.701 -65.045 1.00 46.44 C
ANISOU 718 CA ASN A 242 5787 4909 6949 737 613 152 C
ATOM 719 CB ASN A 242 13.020 -92.279 -65.702 1.00 51.82 C
ANISOU 719 CB ASN A 242 6391 5396 7900 812 451 12 C
ATOM 720 CG ASN A 242 13.734 -91.197 -64.936 1.00 53.93 C
ANISOU 720 CG ASN A 242 6736 5627 8130 959 310 -114 C
ATOM 721 OD1 ASN A 242 14.380 -91.464 -63.925 1.00 64.35 O
ANISOU 721 OD1 ASN A 242 8213 6875 9363 1012 121 -107 O
ATOM 722 ND2 ASN A 242 13.608 -89.958 -65.405 1.00 57.51 N
ANISOU 722 ND2 ASN A 242 7096 6121 8634 1028 395 -237 N
ATOM 723 C ASN A 242 11.060 -93.789 -65.861 1.00 50.51 C
ANISOU 723 C ASN A 242 6208 5441 7541 544 733 248 C
ATOM 724 O ASN A 242 11.251 -94.977 -65.592 1.00 51.19 O
ANISOU 724 O ASN A 242 6420 5397 7633 442 693 355 O
ATOM 725 N SER A 243 10.303 -93.386 -66.869 1.00 51.20 N
ANISOU 725 N SER A 243 6092 5679 7683 502 870 203 N
ATOM 726 CA SER A 243 9.513 -94.343 -67.618 1.00 61.98 C
ANISOU 726 CA SER A 243 7354 7105 9093 296 972 266 C
ATOM 727 CB SER A 243 8.031 -93.970 -67.572 1.00 56.65 C
ANISOU 727 CB SER A 243 6516 6753 8254 245 1164 310 C
ATOM 728 OG SER A 243 7.543 -94.042 -66.250 1.00 44.33 O
ANISOU 728 OG SER A 243 5081 5286 6475 248 1245 423 O
ATOM 729 C SER A 243 9.984 -94.510 -69.050 1.00 46.82 C
ANISOU 729 C SER A 243 5320 5070 7399 268 930 171 C
ATOM 730 O SER A 243 10.370 -93.549 -69.712 1.00 45.92 O
ANISOU 730 O SER A 243 5115 4959 7373 411 920 65 O
ATOM 731 N ILE A 244 9.922 -95.747 -69.518 1.00 45.57 N
ANISOU 731 N ILE A 244 5197 4797 7320 82 928 214 N
ATOM 732 CA ILE A 244 10.367 -96.107 -70.850 1.00 50.86 C
ANISOU 732 CA ILE A 244 5815 5334 8176 49 896 128 C
ATOM 733 CB ILE A 244 11.176 -97.394 -70.813 1.00 40.31 C
ANISOU 733 CB ILE A 244 4665 3694 6956 -32 818 174 C
ATOM 734 CG1 ILE A 244 12.437 -97.174 -69.992 1.00 40.12 C
ANISOU 734 CG1 ILE A 244 4764 3493 6988 156 682 191 C
ATOM 735 CD1 ILE A 244 12.776 -98.327 -69.103 1.00 61.33 C
ANISOU 735 CD1 ILE A 244 7677 5991 9635 106 622 321 C
ATOM 736 CG2 ILE A 244 11.525 -97.844 -72.214 1.00 43.76 C
ANISOU 736 CG2 ILE A 244 5074 3995 7556 -68 815 80 C
ATOM 737 C ILE A 244 9.170 -96.318 -71.745 1.00 45.97 C
ANISOU 737 C ILE A 244 5030 4923 7513 -112 992 100 C
ATOM 738 O ILE A 244 8.204 -96.977 -71.362 1.00 43.32 O
ANISOU 738 O ILE A 244 4671 4707 7083 -316 1064 176 O
ATOM 739 N TYR A 245 9.235 -95.767 -72.947 1.00 42.32 N
ANISOU 739 N TYR A 245 4450 4510 7118 -24 994 -8 N
ATOM 740 CA TYR A 245 8.122 -95.871 -73.861 1.00 45.39 C
ANISOU 740 CA TYR A 245 4667 5132 7446 -142 1043 -55 C
ATOM 741 CB TYR A 245 7.534 -94.497 -74.140 1.00 44.07 C
ANISOU 741 CB TYR A 245 4319 5248 7178 59 1104 -89 C
ATOM 742 CG TYR A 245 6.857 -93.926 -72.929 1.00 51.54 C
ANISOU 742 CG TYR A 245 5208 6396 7978 104 1183 -2 C
ATOM 743 CD1 TYR A 245 7.597 -93.313 -71.917 1.00 55.10 C
ANISOU 743 CD1 TYR A 245 5802 6720 8414 259 1173 26 C
ATOM 744 CE1 TYR A 245 6.981 -92.802 -70.799 1.00 51.82 C
ANISOU 744 CE1 TYR A 245 5380 6478 7833 317 1255 96 C
ATOM 745 CZ TYR A 245 5.601 -92.907 -70.679 1.00 57.80 C
ANISOU 745 CZ TYR A 245 5950 7551 8459 222 1374 157 C
ATOM 746 OH TYR A 245 4.968 -92.399 -69.568 1.00 62.60 O
ANISOU 746 OH TYR A 245 6555 8339 8893 302 1493 235 O
ATOM 747 CE2 TYR A 245 4.847 -93.517 -71.668 1.00 64.11 C
ANISOU 747 CE2 TYR A 245 6558 8501 9301 48 1375 132 C
ATOM 748 CD2 TYR A 245 5.478 -94.025 -72.778 1.00 62.26 C
ANISOU 748 CD2 TYR A 245 6367 8079 9210 -14 1267 45 C
ATOM 749 C TYR A 245 8.498 -96.575 -75.147 1.00 54.37 C
ANISOU 749 C TYR A 245 5856 6110 8693 -212 993 -149 C
ATOM 750 O TYR A 245 9.658 -96.594 -75.556 1.00 56.14 O
ANISOU 750 O TYR A 245 6204 6078 9050 -87 958 -190 O
ATOM 751 N GLU A 246 7.492 -97.170 -75.765 1.00 56.22 N
ANISOU 751 N GLU A 246 5987 6504 8871 -420 994 -191 N
ATOM 752 CA GLU A 246 7.652 -97.872 -77.011 1.00 49.56 C
ANISOU 752 CA GLU A 246 5209 5540 8084 -508 940 -304 C
ATOM 753 CB GLU A 246 6.878 -99.179 -76.942 1.00 68.75 C
ANISOU 753 CB GLU A 246 7660 7954 10507 -869 925 -309 C
ATOM 754 CG GLU A 246 6.783 -99.964 -78.227 1.00 89.25 C
ANISOU 754 CG GLU A 246 10325 10461 13123 -1013 855 -457 C
ATOM 755 CD GLU A 246 5.777-101.091 -78.101 1.00101.26 C
ANISOU 755 CD GLU A 246 11815 12024 14635 -1416 844 -478 C
ATOM 756 OE1 GLU A 246 5.414-101.693 -79.133 1.00101.76 O
ANISOU 756 OE1 GLU A 246 11895 12086 14686 -1586 766 -629 O
ATOM 757 OE2 GLU A 246 5.356-101.362 -76.960 1.00103.92 O
ANISOU 757 OE2 GLU A 246 12122 12391 14973 -1569 921 -347 O
ATOM 758 C GLU A 246 7.062 -96.962 -78.063 1.00 52.61 C
ANISOU 758 C GLU A 246 5411 6208 8371 -364 933 -393 C

ATOM 759 O GLU A 246 6.003 -96.373 -77.857 1.00 54.05 O
ANISOU 759 O GLU A 246 5370 6734 8433 -359 956 -369 O
ATOM 760 N LEU A 247 7.753 -96.813 -79.182 1.00 62.85 N
ANISOU 760 N LEU A 247 6808 7369 9705 -213 915 -483 N
ATOM 761 CA LEU A 247 7.251 -95.977 -80.257 1.00 65.99 C
ANISOU 761 CA LEU A 247 7082 8013 9980 -40 910 -555 C
ATOM 762 CB LEU A 247 8.272 -94.914 -80.637 1.00 59.12 C
ANISOU 762 CB LEU A 247 6299 7001 9161 288 994 -545 C
ATOM 763 CG LEU A 247 8.763 -93.951 -79.566 1.00 51.92 C
ANISOU 763 CG LEU A 247 5368 6045 8314 445 1069 -450 C
ATOM 764 CD1 LEU A 247 9.570 -92.884 -80.260 1.00 59.21 C
ANISOU 764 CD1 LEU A 247 6355 6858 9285 731 1164 -467 C
ATOM 765 CD2 LEU A 247 7.607 -93.333 -78.806 1.00 37.80 C
ANISOU 765 CD2 LEU A 247 3387 4591 6383 447 1086 -390 C
ATOM 766 C LEU A 247 6.959 -96.825 -81.473 1.00 71.10 C
ANISOU 766 C LEU A 247 7789 8653 10574 -178 822 -690 C
ATOM 767 O LEU A 247 7.789 -97.632 -81.888 1.00 75.37 O
ANISOU 767 O LEU A 247 8555 8876 11208 -229 817 -743 O
ATOM 768 N LEU A 248 5.786 -96.636 -82.057 1.00 50.61 N
ANISOU 768 N LEU A 248 7284 4303 7644 1327 -1322 -1910 N
ATOM 769 CA LEU A 248 5.417 -97.407 -83.225 1.00 63.20 C
ANISOU 769 CA LEU A 248 8970 5788 9254 1408 -1506 -2095 C
ATOM 770 CB LEU A 248 4.080 -98.126 -83.030 1.00 53.38 C
ANISOU 770 CB LEU A 248 7561 4367 8355 1396 -1666 -2195 C
ATOM 771 CG LEU A 248 3.995 -99.081 -81.841 1.00 70.24 C
ANISOU 771 CG LEU A 248 9460 6444 10785 1325 -1542 -2118 C
ATOM 772 CD1 LEU A 248 3.466 -98.353 -80.611 1.00 74.77 C
ANISOU 772 CD1 LEU A 248 9866 7062 11481 1228 -1454 -1983 C
ATOM 773 CD2 LEU A 248 3.126-100.277 -82.170 1.00 59.29 C
ANISOU 773 CD2 LEU A 248 7977 4870 9680 1350 -1709 -2263 C
ATOM 774 C LEU A 248 5.374 -96.533 -84.460 1.00 66.39 C
ANISOU 774 C LEU A 248 9601 6239 9384 1468 -1657 -2170 C
ATOM 775 O LEU A 248 5.017 -95.353 -84.403 1.00 56.00 O
ANISOU 775 O LEU A 248 8321 4967 7989 1445 -1709 -2109 O
ATOM 776 N GLU A 249 5.763 -97.123 -85.578 1.00 54.63 N
ANISOU 776 N GLU A 249 8266 4743 7749 1540 -1727 -2303 N
ATOM 777 CA GLU A 249 5.634 -96.486 -86.861 1.00 62.70 C
ANISOU 777 CA GLU A 249 9508 5802 8514 1590 -1898 -2391 C
ATOM 778 CB GLU A 249 6.985 -95.985 -87.347 1.00 66.32 C
ANISOU 778 CB GLU A 249 10151 6441 8607 1609 -1751 -2322 C
ATOM 779 CG GLU A 249 6.928 -95.243 -88.664 1.00 78.31 C
ANISOU 779 CG GLU A 249 11908 8025 9822 1644 -1917 -2385 C
ATOM 780 CD GLU A 249 8.275 -94.679 -89.066 1.00 80.93 C
ANISOU 780 CD GLU A 249 12407 8548 9796 1649 -1753 -2293 C
ATOM 781 OE1 GLU A 249 8.895 -95.232 -90.005 1.00 81.21 O
ANISOU 781 OE1 GLU A 249 12583 8641 9633 1699 -1738 -2407 O
ATOM 782 OE2 GLU A 249 8.710 -93.692 -88.430 1.00 71.64 O
ANISOU 782 OE2 GLU A 249 11215 7464 8543 1601 -1636 -2113 O
ATOM 783 C GLU A 249 5.113 -97.566 -87.775 1.00 62.38 C
ANISOU 783 C GLU A 249 9507 5637 8559 1651 -2077 -2604 C
ATOM 784 O GLU A 249 5.775 -98.583 -87.952 1.00 66.38 O
ANISOU 784 O GLU A 249 10018 6135 9070 1686 -1987 -2679 O
ATOM 785 N ASN A 250 3.917 -97.366 -88.322 1.00 68.95 N
ANISOU 785 N ASN A 250 10356 6361 9480 1662 -2333 -2705 N
ATOM 786 CA ASN A 250 3.277 -98.359 -89.181 1.00 61.19 C
ANISOU 786 CA ASN A 250 9405 5244 8601 1714 -2535 -2916 C
ATOM 787 CB ASN A 250 4.117 -98.620 -90.431 1.00 83.15 C
ANISOU 787 CB ASN A 250 12422 8120 11050 1776 -2544 -3038 C
ATOM 788 CG ASN A 250 4.124 -97.448 -91.382 1.00 86.63 C
ANISOU 788 CG ASN A 250 13086 8675 11153 1779 -2670 -3017 C
ATOM 789 OD1 ASN A 250 3.082 -96.863 -91.657 1.00 92.92 O
ANISOU 789 OD1 ASN A 250 13894 9400 12014 1765 -2895 -3029 O
ATOM 790 ND2 ASN A 250 5.304 -97.086 -91.878 1.00 87.05 N
ANISOU 790 ND2 ASN A 250 13313 8907 10856 1792 -2527 -2975 N
ATOM 791 C ASN A 250 2.972 -99.672 -88.461 1.00 61.23 C
ANISOU 791 C ASN A 250 9195 5102 8968 1706 -2492 -2968 C
ATOM 792 O ASN A 250 3.009-100.744 -89.063 1.00 62.74 O
ANISOU 792 O ASN A 250 9413 5211 9213 1756 -2560 -3133 O
ATOM 793 N GLY A 251 2.673 -99.573 -87.168 1.00 66.76 N
ANISOU 793 N GLY A 251 9679 5772 9913 1639 -2379 -2825 N
ATOM 794 CA GLY A 251 2.377-100.730 -86.346 1.00 64.09 C
ANISOU 794 CA GLY A 251 9119 5306 9925 1611 -2329 -2831 C
ATOM 795 C GLY A 251 3.636-101.509 -86.021 1.00 67.33 C
ANISOU 795 C GLY A 251 9515 5773 10293 1619 -2108 -2786 C
ATOM 796 O GLY A 251 3.580-102.656 -85.578 1.00 59.53 O
ANISOU 796 O GLY A 251 8376 4671 9571 1609 -2080 -2812 O
ATOM 797 N GLN A 252 4.777-100.865 -86.180 1.00 65.92 N
ANISOU 797 N GLN A 252 9486 5767 9794 1633 -1953 -2710 N
ATOM 798 CA GLN A 252 6.064-101.531 -86.188 1.00 65.93 C
ANISOU 798 CA GLN A 252 9510 5826 9713 1660 -1765 -2699 C
ATOM 799 CB GLN A 252 6.737-101.346 -87.536 1.00 69.09 C
ANISOU 799 CB GLN A 252 10162 6317 9773 1741 -1799 -2838 C
ATOM 800 CG GLN A 252 6.625-102.478 -88.537 1.00 67.68 C
ANISOU 800 CG GLN A 252 10027 6021 9669 1816 -1920 -3079 C
ATOM 801 CD GLN A 252 5.384-103.310 -88.378 1.00 87.92 C
ANISOU 801 CD GLN A 252 12457 8377 12570 1809 -2141 -3187 C
ATOM 802 OE1 GLN A 252 5.322-104.179 -87.540 1.00 97.73 O
ANISOU 802 OE1 GLN A 252 13490 9495 14148 1776 -2103 -3148 O
ATOM 803 NE2 GLN A 252 4.398-103.058 -89.199 1.00 88.08 N
ANISOU 803 NE2 GLN A 252 12597 8360 12510 1834 -2380 -3315 N

ATOM 804 C GLN A 252 7.020-101.031 -85.137 1.00 65.63 C
ANISOU 804 C GLN A 252 9409 5925 9604 1599 -1508 -2474 C
ATOM 805 O GLN A 252 6.782-100.044 -84.498 1.00 54.80 O
ANISOU 805 O GLN A 252 8018 4635 8168 1541 -1464 -2332 O
ATOM 806 N ARG A 253 8.057-101.820 -84.901 1.00 70.21 N
ANISOU 806 N ARG A 253 9946 6515 10215 1612 -1348 -2452 N
ATOM 807 CA ARG A 253 9.374-101.358 -84.511 1.00 68.31 C
ANISOU 807 CA ARG A 253 9743 6435 9778 1591 -1114 -2293 C
ATOM 808 CB ARG A 253 10.072-100.715 -85.693 1.00 80.53 C
ANISOU 808 CB ARG A 253 11539 8109 10951 1665 -1113 -2384 C
ATOM 809 CG ARG A 253 11.452-101.249 -85.953 1.00 85.88 C
ANISOU 809 CG ARG A 253 12258 8865 11508 1703 -922 -2378 C
ATOM 810 CD ARG A 253 12.140-100.483 -87.045 1.00 90.46 C
ANISOU 810 CD ARG A 253 13078 9605 11688 1752 -902 -2428 C
ATOM 811 NE ARG A 253 11.212-100.203 -88.116 1.00103.68 N
ANISOU 811 NE ARG A 253 14899 11248 13247 1790 -1133 -2594 N
ATOM 812 CZ ARG A 253 11.335 -99.208 -88.985 1.00112.47 C
ANISOU 812 CZ ARG A 253 16200 12488 14044 1790 -1193 -2575 C
ATOM 813 NH1 ARG A 253 10.435 -99.032 -89.942 1.00116.05 N
ANISOU 813 NH1 ARG A 253 16715 13105 14273 1757 -1031 -2400 N
ATOM 814 NH2 ARG A 253 12.370 -98.400 -88.907 1.00111.39 N
ANISOU 814 NH2 ARG A 253 16189 12311 13823 1818 -1424 -2721 N
ATOM 815 C ARG A 253 9.225-100.540 -83.242 1.00 68.11 C
ANISOU 815 C ARG A 253 9601 6490 9787 1489 -999 -2062 C
ATOM 816 O ARG A 253 8.715-101.110 -82.295 1.00 77.18 O
ANISOU 816 O ARG A 253 10549 7559 11218 1422 -968 -1983 O
ATOM 817 N ALA A 254 9.558 -99.248 -83.174 1.00 60.53 N
ANISOU 817 N ALA A 254 8745 5680 8572 1464 -933 -1950 N
ATOM 818 CA ALA A 254 10.476 -98.491 -83.983 1.00 51.67 C
ANISOU 818 CA ALA A 254 7844 4702 7088 1512 -896 -1956 C
ATOM 819 CB ALA A 254 9.738 -97.522 -84.860 1.00 52.21 C
ANISOU 819 CB ALA A 254 8049 4782 7008 1530 -1086 -2021 C
ATOM 820 C ALA A 254 11.462 -97.776 -83.143 1.00 49.89 C
ANISOU 820 C ALA A 254 7594 4622 6742 1451 -679 -1742 C
ATOM 821 O ALA A 254 12.436 -97.296 -83.637 1.00 75.75 O
ANISOU 821 O ALA A 254 11010 8027 9743 1475 -580 -1698 O
ATOM 822 N GLY A 255 11.158 -97.669 -81.866 1.00 52.73 N
ANISOU 822 N GLY A 255 7768 4960 7307 1364 -607 -1607 N
ATOM 823 CA GLY A 255 12.022 -97.059 -80.899 1.00 49.18 C
ANISOU 823 CA GLY A 255 7274 4640 6774 1291 -413 -1401 C
ATOM 824 C GLY A 255 11.620 -97.436 -79.506 1.00 49.13 C
ANISOU 824 C GLY A 255 7043 4592 7033 1191 -345 -1283 C
ATOM 825 O GLY A 255 10.499 -97.792 -79.263 1.00 46.52 O
ANISOU 825 O GLY A 255 6596 4150 6929 1168 -460 -1345 O
ATOM 826 N THR A 256 12.559 -97.318 -78.594 1.00 48.50 N
ANISOU 826 N THR A 256 6901 4610 6919 1126 -156 -1106 N
ATOM 827 CA THR A 256 12.338 -97.524 -77.181 1.00 47.91 C
ANISOU 827 CA THR A 256 6626 4536 7040 1011 -67 -963 C
ATOM 828 CB THR A 256 12.829 -98.910 -76.737 1.00 59.52 C
ANISOU 828 CB THR A 256 7965 5933 8718 992 1 -916 C
ATOM 829 OG1 THR A 256 12.020 -99.934 -77.332 1.00 78.80 O
ANISOU 829 OG1 THR A 256 10364 8208 11369 1049 -152 -1083 O
ATOM 830 CG2 THR A 256 12.765 -99.038 -75.241 1.00 52.86 C
ANISOU 830 CG2 THR A 256 6929 5123 8030 855 108 -731 C
ATOM 831 C THR A 256 13.165 -96.444 -76.499 1.00 50.47 C
ANISOU 831 C THR A 256 6983 5039 7054 1049 -47 -1047 C
ATOM 832 O THR A 256 14.373 -96.349 -76.726 1.00 56.24 O
ANISOU 832 O THR A 256 7800 5838 7728 969 197 -719 O
ATOM 833 N CYS A 257 12.531 -95.604 -75.692 1.00 45.32 N
ANISOU 833 N CYS A 257 6261 4420 6538 866 96 -727 N
ATOM 834 CA CYS A 257 13.264 -94.498 -75.098 1.00 40.42 C
ANISOU 834 CA CYS A 257 5682 3950 5728 806 226 -581 C
ATOM 835 CB CYS A 257 13.315 -93.305 -76.062 1.00 40.41 C
ANISOU 835 CB CYS A 257 5872 3997 5486 876 151 -642 C
ATOM 836 SG CYS A 257 11.737 -92.410 -76.245 1.00 72.72 S
ANISOU 836 SG CYS A 257 9955 8021 9656 882 -30 -767 S
ATOM 837 C CYS A 257 12.694 -94.067 -73.756 1.00 47.88 C
ANISOU 837 C CYS A 257 6469 4941 6781 683 289 -489 C
ATOM 838 O CYS A 257 11.531 -94.324 -73.444 1.00 58.45 O
ANISOU 838 O CYS A 257 7690 6201 8316 654 210 -560 O
ATOM 839 N VAL A 258 13.534 -93.413 -72.961 1.00 38.95 N
ANISOU 839 N VAL A 258 5335 3943 5520 607 435 -333 N
ATOM 840 CA VAL A 258 13.090 -92.801 -71.721 1.00 37.87 C
ANISOU 840 CA VAL A 258 5075 3881 5433 488 507 -256 C
ATOM 841 CB VAL A 258 14.215 -92.703 -70.696 1.00 49.08 C
ANISOU 841 CB VAL A 258 6453 5432 6763 386 683 -59 C
ATOM 842 CG2 VAL A 258 14.720 -94.092 -70.335 1.00 42.74 C
ANISOU 842 CG2 VAL A 258 5549 4589 6101 352 738 31 C
ATOM 843 CG1 VAL A 258 13.737 -91.958 -69.458 1.00 41.05 C
ANISOU 843 CG1 VAL A 258 5325 4508 5764 261 757 -3 C
ATOM 844 C VAL A 258 12.575 -91.413 -72.041 1.00 37.64 C
ANISOU 844 C VAL A 258 5133 3878 5289 516 438 -332 C
ATOM 845 O VAL A 258 13.303 -90.582 -72.590 1.00 37.22 O
ANISOU 845 O VAL A 258 5230 3886 5026 561 446 -305 O
ATOM 846 N LEU A 259 11.320 -91.164 -71.680 1.00 52.37 N
ANISOU 846 N LEU A 259 6893 5696 7309 486 369 -422 N
ATOM 847 CA LEU A 259 10.568 -90.044 -72.223 1.00 38.24 C
ANISOU 847 CA LEU A 259 5173 3874 5482 538 248 -536 C
ATOM 848 CB LEU A 259 9.706 -90.554 -73.378 1.00 39.42 C
ANISOU 848 CB LEU A 259 5368 3875 5735 643 54 -697 C

ATOM 849 CG LEU A 259 8.977 -89.616 -74.331 1.00 53.35 C
ANISOU 849 CG LEU A 259 7238 5572 7460 724 -126 -821 C
ATOM 850 CD1 LEU A 259 9.952 -88.891 -75.223 1.00 56.32 C
ANISOU 850 CD1 LEU A 259 7825 6009 7564 786 -142 -777 C
ATOM 851 CD2 LEU A 259 8.019 -90.435 -75.175 1.00 49.92 C
ANISOU 851 CD2 LEU A 259 6795 4988 7186 796 -305 -969 C
ATOM 852 C LEU A 259 9.683 -89.405 -71.159 1.00 42.59 C
ANISOU 852 C LEU A 259 5572 4457 6154 448 286 -557 C
ATOM 853 O LEU A 259 8.977 -90.102 -70.437 1.00 50.93 O
ANISOU 853 O LEU A 259 6459 5487 7404 380 315 -570 O
ATOM 854 N GLU A 260 9.708 -88.082 -71.058 1.00 37.71 N
ANISOU 854 N GLU A 260 5007 3893 5429 443 288 -563 N
ATOM 855 CA GLU A 260 8.866 -87.404 -70.083 1.00 57.14 C
ANISOU 855 CA GLU A 260 7322 6384 8006 364 328 -610 C
ATOM 856 CB GLU A 260 9.445 -87.537 -68.673 1.00 37.08 C
ANISOU 856 CB GLU A 260 4670 3987 5432 225 533 -477 C
ATOM 857 CG GLU A 260 10.743 -86.792 -68.432 1.00 49.66 C
ANISOU 857 CG GLU A 260 6373 5703 6791 196 639 -346 C
ATOM 858 CD GLU A 260 11.408 -87.203 -67.124 1.00 69.53 C
ANISOU 858 CD GLU A 260 8788 8356 9274 56 825 -196 C
ATOM 859 OE1 GLU A 260 11.289 -88.393 -66.741 1.00 69.55 O
ANISOU 859 OE1 GLU A 260 8687 8347 9392 7 864 -147 O
ATOM 860 OE2 GLU A 260 12.031 -86.331 -66.479 1.00 78.26 O
ANISOU 860 OE2 GLU A 260 9915 9576 10243 -9 921 -126 O
ATOM 861 C GLU A 260 8.607 -85.938 -70.419 1.00 49.86 C
ANISOU 861 C GLU A 260 6475 5451 7018 405 247 -678 C
ATOM 862 O GLU A 260 9.412 -85.282 -71.081 1.00 53.54 O
ANISOU 862 O GLU A 260 7107 5941 7294 457 216 -627 O
ATOM 863 N TYR A 261 7.465 -85.440 -69.962 1.00 40.46 N
ANISOU 863 N TYR A 261 5152 4220 6001 380 211 -793 N
ATOM 864 CA TYR A 261 7.144 -84.027 -70.083 1.00 41.00 C
ANISOU 864 CA TYR A 261 5253 4270 6054 407 142 -863 C
ATOM 865 CB TYR A 261 5.662 -83.785 -69.851 1.00 39.58 C
ANISOU 865 CB TYR A 261 4912 3997 6132 408 60 -1026 C
ATOM 866 CG TYR A 261 4.799 -84.140 -71.026 1.00 67.12 C
ANISOU 866 CG TYR A 261 8437 7318 9747 514 -161 -1135 C
ATOM 867 CD1 TYR A 261 4.609 -83.233 -72.064 1.00 41.08 C
ANISOU 867 CD1 TYR A 261 5267 3927 6413 607 -351 -1188 C
ATOM 868 CE1 TYR A 261 3.826 -83.546 -73.147 1.00 46.60 C
ANISOU 868 CE1 TYR A 261 6009 4481 7217 696 -566 -1282 C
ATOM 869 CZ TYR A 261 3.220 -84.791 -73.209 1.00 47.70 C
ANISOU 869 CZ TYR A 261 6059 4558 7509 698 -592 -1334 C
ATOM 870 OH TYR A 261 2.435 -85.114 -74.289 1.00 47.41 O
ANISOU 870 OH TYR A 261 6065 4373 7577 783 -817 -1433 O
ATOM 871 CE2 TYR A 261 3.402 -85.717 -72.192 1.00 51.22 C
ANISOU 871 CE2 TYR A 261 6370 5085 8005 609 -405 -1279 C
ATOM 872 CD2 TYR A 261 4.184 -85.386 -71.111 1.00 41.20 C
ANISOU 872 CD2 TYR A 261 5063 3969 6622 515 -193 -1176 C
ATOM 873 C TYR A 261 7.929 -83.193 -69.090 1.00 37.67 C
ANISOU 873 C TYR A 261 4821 3991 5500 318 306 -775 C
ATOM 874 O TYR A 261 8.149 -83.610 -67.954 1.00 41.68 O
ANISOU 874 O TYR A 261 5213 4608 6014 208 477 -713 O
ATOM 875 N ALA A 262 8.338 -82.004 -69.517 1.00 43.51 N
ANISOU 875 N ALA A 262 5680 4729 6122 359 246 -765 N
ATOM 876 CA ALA A 262 8.974 -81.065 -68.614 1.00 37.57 C
ANISOU 876 CA ALA A 262 4916 4093 5267 280 377 -707 C
ATOM 877 CB ALA A 262 9.635 -79.928 -69.378 1.00 36.69 C
ANISOU 877 CB ALA A 262 4975 3961 5003 341 284 -661 C
ATOM 878 C ALA A 262 7.918 -80.527 -67.660 1.00 46.72 C
ANISOU 878 C ALA A 262 5887 5251 6613 221 418 -845 C
ATOM 879 O ALA A 262 6.958 -79.880 -68.079 1.00 38.37 O
ANISOU 879 O ALA A 262 4794 4076 5709 282 278 -983 O
ATOM 880 N THR A 263 8.105 -80.801 -66.374 1.00 35.15 N
ANISOU 880 N THR A 263 5895 2823 4636 -587 750 -531 N
ATOM 881 CA THR A 263 7.187 -80.360 -65.329 1.00 32.79 C
ANISOU 881 CA THR A 263 5520 2526 4413 -679 858 -542 C
ATOM 882 CB THR A 263 7.637 -80.873 -63.949 1.00 40.95 C
ANISOU 882 CB THR A 263 6718 3485 5357 -581 995 -424 C
ATOM 883 OG1 THR A 263 8.964 -80.417 -63.674 1.00 50.25 O
ANISOU 883 OG1 THR A 263 7938 4709 6446 -336 891 -336 O
ATOM 884 CG2 THR A 263 7.627 -82.387 -63.945 1.00 26.95 C
ANISOU 884 CG2 THR A 263 5102 1599 3538 -666 1112 -400 C
ATOM 885 C THR A 263 6.883 -78.853 -65.249 1.00 35.95 C
ANISOU 885 C THR A 263 5671 3107 4881 -593 751 -542 C
ATOM 886 O THR A 263 5.768 -78.488 -64.874 1.00 53.48 O
ANISOU 886 O THR A 263 7716 5425 7180 -696 795 -584 O
ATOM 887 N PRO A 264 7.862 -77.972 -65.570 1.00 35.75 N
ANISOU 887 N PRO A 264 5606 3131 4845 -396 623 -483 N
ATOM 888 CA PRO A 264 7.516 -76.556 -65.415 1.00 25.13 C
ANISOU 888 CA PRO A 264 4021 1933 3596 -315 540 -477 C
ATOM 889 CB PRO A 264 8.826 -75.841 -65.726 1.00 34.16 C
ANISOU 889 CB PRO A 264 5168 3055 4757 -116 437 -400 C
ATOM 890 CG PRO A 264 9.877 -76.821 -65.342 1.00 32.72 C
ANISOU 890 CG PRO A 264 5238 2725 4471 -60 492 -362 C
ATOM 891 CD PRO A 264 9.314 -78.139 -65.771 1.00 30.82 C
ANISOU 891 CD PRO A 264 5140 2415 4156 -228 581 -409 C
ATOM 892 C PRO A 264 6.433 -76.066 -66.372 1.00 28.16 C
ANISOU 892 C PRO A 264 4169 2480 4052 -403 462 -535 C
ATOM 893 O PRO A 264 5.874 -74.988 -66.165 1.00 37.68 O
ANISOU 893 O PRO A 264 5171 3800 5346 -353 424 -533 O
ATOM 894 N LEU A 265 6.159 -76.822 -67.425 1.00 35.30 N
ANISOU 894 N LEU A 265 5100 3401 4910 -509 425 -596 N
ATOM 895 CA LEU A 265 5.080 -76.452 -68.332 1.00 46.00 C
ANISOU 895 CA LEU A 265 6226 4945 6307 -580 326 -673 C
ATOM 896 CB LEU A 265 5.082 -77.311 -69.588 1.00 36.83 C
ANISOU 896 CB LEU A 265 5139 3802 5053 -647 248 -764 C
ATOM 897 CG LEU A 265 6.321 -77.225 -70.467 1.00 41.47 C
ANISOU 897 CG LEU A 265 5865 4364 5529 -459 184 -678 C
ATOM 898 CD1 LEU A 265 6.036 -77.958 -71.741 1.00 51.11 C
ANISOU 898 CD1 LEU A 265 7124 5658 6636 -514 91 -806 C
ATOM 899 CD2 LEU A 265 6.727 -75.780 -70.770 1.00 25.97 C
ANISOU 899 CD2 LEU A 265 3749 2510 3607 -243 114 -533 C
ATOM 900 C LEU A 265 3.740 -76.575 -67.609 1.00 43.44 C
ANISOU 900 C LEU A 265 5748 4678 6079 -756 411 -756 C
ATOM 901 O LEU A 265 2.800 -75.829 -67.887 1.00 47.75 O
ANISOU 901 O LEU A 265 6037 5407 6699 -759 341 -791 O
ATOM 902 N GLN A 266 3.653 -77.533 -66.691 1.00 38.33 N
ANISOU 902 N GLN A 266 5255 3873 5434 -889 579 -770 N
ATOM 903 CA GLN A 266 2.468 -77.680 -65.849 1.00 41.70 C
ANISOU 903 CA GLN A 266 5549 4332 5963 -1047 719 -813 C
ATOM 904 C GLN A 266 2.248 -76.399 -65.077 1.00 50.69 C
ANISOU 904 C GLN A 266 6533 5587 7141 -893 725 -751 C
ATOM 905 O GLN A 266 1.128 -75.893 -64.974 1.00 45.72 O
ANISOU 905 O GLN A 266 5651 5107 6612 -948 738 -798 O
ATOM 906 CB GLN A 266 2.617 -78.825 -64.853 1.00 32.58 C
ANISOU 906 CB GLN A 266 4631 2961 4785 -1154 943 -776 C
ATOM 907 CG GLN A 266 2.163 -80.177 -65.355 1.00 46.50 C
ANISOU 907 CG GLN A 266 6465 4594 6611 -1406 1013 -879 C
ATOM 908 CD GLN A 266 2.512 -81.291 -64.382 1.00 56.89 C
ANISOU 908 CD GLN A 266 8067 5649 7899 -1464 1259 -793 C
ATOM 909 OE1 GLN A 266 1.787 -81.532 -63.421 1.00 59.31 O
ANISOU 909 OE1 GLN A 266 8626 5804 8106 -1393 1253 -753 O
ATOM 910 NE2 GLN A 266 3.615 -81.994 -64.644 1.00 50.56 N
ANISOU 910 NE2 GLN A 266 7217 4827 7166 -1544 1479 -733 N
ATOM 911 N THR A 267 3.341 -75.889 -64.524 1.00 36.15 N
ANISOU 911 N THR A 267 4838 3669 5230 -695 712 -663 N
ATOM 912 CA THR A 267 3.303 -74.644 -63.789 1.00 33.16 C
ANISOU 912 CA THR A 267 4342 3365 4891 -532 700 -635 C
ATOM 913 CB THR A 267 4.624 -74.358 -63.088 1.00 27.38 C
ANISOU 913 CB THR A 267 3802 2517 4085 -345 681 -577 C
ATOM 914 OG1 THR A 267 4.835 -75.338 -62.072 1.00 28.48 O
ANISOU 914 OG1 THR A 267 4168 2544 4108 -376 838 -553 O
ATOM 915 CG2 THR A 267 4.601 -72.954 -62.467 1.00 22.52 C
ANISOU 915 CG2 THR A 267 3046 1967 3542 -176 632 -593 C
ATOM 916 C THR A 267 2.894 -73.465 -64.677 1.00 24.06 C
ANISOU 916 C THR A 267 2932 2371 3839 -448 547 -643 C
ATOM 917 O THR A 267 2.053 -72.659 -64.291 1.00 35.64 O
ANISOU 917 O THR A 267 4202 3949 5390 -412 568 -666 O
ATOM 918 N LEU A 268 3.485 -73.368 -65.864 1.00 27.55 N
ANISOU 918 N LEU A 268 3384 2823 4262 -395 410 -611 N
ATOM 919 CA LEU A 268 3.108 -72.323 -66.814 1.00 30.13 C
ANISOU 919 CA LEU A 268 3491 3300 4659 -289 280 -584 C
ATOM 920 CB LEU A 268 3.935 -72.390 -68.107 1.00 22.85 C
ANISOU 920 CB LEU A 268 2642 2375 3667 -206 168 -519 C
ATOM 921 CG LEU A 268 5.362 -71.851 -68.073 1.00 32.15 C
ANISOU 921 CG LEU A 268 3939 3412 4864 -37 156 -405 C
ATOM 922 CD1 LEU A 268 6.010 -71.993 -69.439 1.00 25.64 C
ANISOU 922 CD1 LEU A 268 3169 2616 3959 44 82 -327 C
ATOM 923 CD2 LEU A 268 5.408 -70.385 -67.643 1.00 20.92 C
ANISOU 923 CD2 LEU A 268 2367 1980 3602 117 143 -346 C
ATOM 924 C LEU A 268 1.611 -72.387 -67.138 1.00 41.27 C
ANISOU 924 C LEU A 268 4661 4901 6119 -409 266 -670 C
ATOM 925 O LEU A 268 0.943 -71.358 -67.274 1.00 44.67 O
ANISOU 925 O LEU A 268 4868 5468 6636 -306 217 -653 O
ATOM 926 N PHE A 269 1.086 -73.601 -67.255 1.00 34.51 N
ANISOU 926 N PHE A 269 3839 4043 5229 -625 311 -769 N
ATOM 927 CA PHE A 269 -0.334 -73.774 -67.535 1.00 33.62 C
ANISOU 927 CA PHE A 269 3465 4110 5198 -723 301 -870 C
ATOM 928 CB PHE A 269 -0.671 -75.211 -67.913 1.00 30.59 C
ANISOU 928 CB PHE A 269 3144 3676 4801 -1028 313 -1010 C
ATOM 929 CG PHE A 269 -2.055 -75.365 -68.455 1.00 42.66 C
ANISOU 929 CG PHE A 269 4362 5412 6432 -1181 237 -1158 C
ATOM 930 CD1 PHE A 269 -2.317 -75.054 -69.782 1.00 37.97 C
ANISOU 930 CD1 PHE A 269 3620 5029 5778 -1100 2 -1225 C
ATOM 931 CE1 PHE A 269 -3.597 -75.163 -70.300 1.00 42.36 C
ANISOU 931 CE1 PHE A 269 3859 5812 6424 -1221 -107 -1383 C
ATOM 932 CZ PHE A 269 -4.651 -75.585 -69.475 1.00 49.01 C
ANISOU 932 CZ PHE A 269 4506 6656 7462 -1452 45 -1469 C
ATOM 933 CE2 PHE A 269 -4.405 -75.889 -68.135 1.00 41.41 C
ANISOU 933 CE2 PHE A 269 3702 5469 6564 -1533 319 -1375 C
ATOM 934 CD2 PHE A 269 -3.107 -75.768 -67.634 1.00 35.26 C
ANISOU 934 CD2 PHE A 269 3262 4483 5653 -1383 400 -1223 C
ATOM 935 C PHE A 269 -1.207 -73.343 -66.352 1.00 45.00 C
ANISOU 935 C PHE A 269 4751 5594 6753 -796 444 -882 C
ATOM 936 O PHE A 269 -2.189 -72.610 -66.518 1.00 44.41 O
ANISOU 936 O PHE A 269 4393 5710 6770 -753 398 -908 O
ATOM 937 N ALA A 270 -0.842 -73.809 -65.162 1.00 29.37 N
ANISOU 937 N ALA A 270 2963 3447 4748 -839 631 -848 N
ATOM 938 CA ALA A 270 -1.561 -73.462 -63.944 1.00 33.76 C
ANISOU 938 CA ALA A 270 3422 4037 5368 -831 809 -840 C

ATOM 939 CB ALA A 270 -0.896 -74.060 -62.726 1.00 29.89 C
ANISOU 939 CB ALA A 270 3218 3359 4778 -826 997 -782 C
ATOM 940 C ALA A 270 -1.659 -71.952 -63.795 1.00 39.87 C
ANISOU 940 C ALA A 270 4041 4918 6191 -595 735 -807 C
ATOM 941 O ALA A 270 -2.739 -71.413 -63.559 1.00 31.21 O
ANISOU 941 O ALA A 270 2691 3973 5193 -582 783 -838 O
ATOM 942 N MET A 271 -0.515 -71.285 -63.938 1.00 27.67 N
ANISOU 942 N MET A 271 2640 3277 4597 -409 629 -746 N
ATOM 943 CA MET A 271 -0.426 -69.837 -63.818 1.00 37.35 C
ANISOU 943 CA MET A 271 3754 4536 5901 -184 564 -716 C
ATOM 944 CB MET A 271 0.997 -69.357 -64.075 1.00 25.21 C
ANISOU 944 CB MET A 271 2389 2845 4345 -38 459 -652 C
ATOM 945 CG MET A 271 1.999 -69.856 -63.055 1.00 41.28 C
ANISOU 945 CG MET A 271 4689 4714 6283 -29 532 -663 C
ATOM 946 SD MET A 271 3.679 -69.322 -63.408 1.00 38.90 S
ANISOU 946 SD MET A 271 4528 4245 6007 122 400 -603 S
ATOM 947 CE MET A 271 3.540 -67.565 -63.054 1.00 24.01 C
ANISOU 947 CE MET A 271 2466 2346 4312 322 356 -628 C
ATOM 948 C MET A 271 -1.400 -69.136 -64.757 1.00 28.37 C
ANISOU 948 C MET A 271 2319 3596 4865 -135 460 -715 C
ATOM 949 O MET A 271 -1.980 -68.109 -64.417 1.00 33.88 O
ANISOU 949 O MET A 271 2847 4367 5661 5 479 -714 O
ATOM 950 N SER A 272 -1.574 -69.695 -65.947 1.00 34.24 N
ANISOU 950 N SER A 272 3006 4433 5572 -226 342 -722 N
ATOM 951 CA SER A 272 -2.434 -69.087 -66.946 1.00 30.27 C
ANISOU 951 CA SER A 272 2231 4150 5122 -146 209 -718 C
ATOM 952 CB SER A 272 -2.214 -69.725 -68.324 1.00 36.09 C
ANISOU 952 CB SER A 272 2998 4965 5749 -198 46 -729 C
ATOM 953 OG SER A 272 -2.716 -71.050 -68.375 1.00 31.80 O
ANISOU 953 OG SER A 272 2453 4451 5180 -464 70 -866 O
ATOM 954 C SER A 272 -3.903 -69.215 -66.546 1.00 32.65 C
ANISOU 954 C SER A 272 2252 4634 5519 -254 281 -812 C
ATOM 955 O SER A 272 -4.752 -68.492 -67.055 1.00 39.74 O
ANISOU 955 O SER A 272 2880 5732 6487 -141 194 -809 O
ATOM 956 N GLN A 273 -4.215 -70.115 -65.642 1.00 35.83 N
ANISOU 956 N GLN A 273 2710 4971 5933 -461 455 -881 N
ATOM 957 CA GLN A 273 -5.577 -70.399 -65.279 1.00 35.92 C
ANISOU 957 CA GLN A 273 2441 5143 6063 -610 560 -966 C
ATOM 958 CB GLN A 273 -5.818 -71.889 -65.233 1.00 37.14 C
ANISOU 958 CB GLN A 273 2652 5231 6229 -926 653 -1054 C
ATOM 959 CG GLN A 273 -5.391 -72.620 -66.466 1.00 61.16 C
ANISOU 959 CG GLN A 273 5766 8273 9199 -1028 454 -1122 C
ATOM 960 CD GLN A 273 -6.433 -72.667 -67.531 1.00 62.36 C
ANISOU 960 CD GLN A 273 5566 8699 9428 -1081 264 -1246 C
ATOM 961 OE1 GLN A 273 -6.305 -72.045 -68.567 1.00 69.29 O
ANISOU 961 OE1 GLN A 273 6211 9662 10453 -1313 328 -1371 O
ATOM 962 NE2 GLN A 273 -7.470 -73.429 -67.286 1.00 52.67 N
ANISOU 962 NE2 GLN A 273 4284 7619 8108 -857 34 -1207 N
ATOM 963 C GLN A 273 -5.968 -69.850 -63.961 1.00 36.39 C
ANISOU 963 C GLN A 273 2455 5191 6183 -514 770 -939 C
ATOM 964 O GLN A 273 -7.099 -69.851 -63.653 1.00 41.14 O
ANISOU 964 O GLN A 273 2782 5948 6900 -575 876 -985 O
ATOM 965 N TYR A 274 -5.024 -69.388 -63.177 1.00 37.13 N
ANISOU 965 N TYR A 274 2806 5107 6194 -359 830 -879 N
ATOM 966 CA TYR A 274 -5.325 -68.740 -61.907 1.00 35.08 C
ANISOU 966 CA TYR A 274 2537 4839 5952 -224 1009 -879 C
ATOM 967 CB TYR A 274 -4.444 -69.261 -60.781 1.00 34.04 C
ANISOU 967 CB TYR A 274 2741 4516 5678 -228 1156 -862 C
ATOM 968 CG TYR A 274 -4.632 -70.717 -60.499 1.00 53.48 C
ANISOU 968 CG TYR A 274 5302 6925 8094 -482 1319 -853 C
ATOM 969 CD1 TYR A 274 -5.865 -71.205 -60.091 1.00 61.20 C
ANISOU 969 CD1 TYR A 274 6070 8014 9168 -635 1524 -869 C
ATOM 970 CE1 TYR A 274 -6.050 -72.544 -59.832 1.00 66.25 C
ANISOU 970 CE1 TYR A 274 6799 8564 9810 -883 1705 -849 C
ATOM 971 CZ TYR A 274 -4.986 -73.418 -59.985 1.00 60.65 C
ANISOU 971 CZ TYR A 274 6409 7653 8982 -959 1670 -815 C
ATOM 972 OH TYR A 274 -5.150 -74.757 -59.733 1.00 63.90 O
ANISOU 972 OH TYR A 274 6930 7935 9416 -1196 1866 -784 O
ATOM 973 CE2 TYR A 274 -3.750 -72.958 -60.391 1.00 54.23 C
ANISOU 973 CE2 TYR A 274 5799 6753 8052 -794 1456 -803 C
ATOM 974 CD2 TYR A 274 -3.580 -71.616 -60.643 1.00 55.22 C
ANISOU 974 CD2 TYR A 274 5817 6966 8198 -569 1288 -821 C
ATOM 975 C TYR A 274 -5.178 -67.233 -62.001 1.00 41.43 C
ANISOU 975 C TYR A 274 3266 5659 6819 60 905 -859 C
ATOM 976 O TYR A 274 -4.122 -66.722 -62.405 1.00 35.34 O
ANISOU 976 O TYR A 274 2653 4752 6023 181 767 -816 O
ATOM 977 N SER A 275 -6.204 -66.525 -61.578 1.00 36.49 N
ANISOU 977 N SER A 275 2392 5179 6294 168 992 -885 N
ATOM 978 CA SER A 275 -6.271 -65.073 -61.646 1.00 39.77 C
ANISOU 978 CA SER A 275 2710 5599 6803 448 920 -870 C
ATOM 979 CB SER A 275 -7.688 -64.597 -61.343 1.00 39.32 C
ANISOU 979 CB SER A 275 2337 5746 6859 536 1040 -903 C
ATOM 980 OG SER A 275 -8.067 -64.994 -60.077 1.00 40.50 O
ANISOU 980 OG SER A 275 2529 5907 6952 459 1290 -953 O
ATOM 981 C SER A 275 -5.216 -64.398 -60.787 1.00 35.19 C
ANISOU 981 C SER A 275 2403 4793 6174 609 948 -897 C
ATOM 982 O SER A 275 -4.810 -63.313 -61.047 1.00 47.30 O
ANISOU 982 O SER A 275 3947 6225 7802 808 848 -882 O
ATOM 983 N GLN A 276 -4.830 -65.075 -59.739 1.00 42.25 N
ANISOU 983 N GLN A 276 3514 5608 6932 530 1088 -942 N
ATOM 984 CA GLN A 276 -3.760 -64.673 -58.863 1.00 42.55 C
ANISOU 984 CA GLN A 276 3805 5467 6895 683 1093 -1007 C
ATOM 985 CB GLN A 276 -3.732 -65.543 -57.653 1.00 34.61 C
ANISOU 985 CB GLN A 276 2998 4456 5696 622 1283 -1042 C
ATOM 986 CG GLN A 276 -4.081 -64.747 -56.456 1.00 60.34 C
ANISOU 986 CG GLN A 276 6277 7748 8903 833 1426 -1142 C
ATOM 987 CD GLN A 276 -3.112 -64.904 -55.350 1.00 65.48 C
ANISOU 987 CD GLN A 276 7248 8273 9357 942 1426 -1224 C
ATOM 988 OE1 GLN A 276 -2.957 -65.974 -54.819 1.00 74.85 O
ANISOU 988 OE1 GLN A 276 8618 9471 10350 859 1557 -1180 O
ATOM 989 NE2 GLN A 276 -2.489 -63.825 -54.962 1.00 65.53 N
ANISOU 989 NE2 GLN A 276 7323 8153 9422 1135 1275 -1345 N
ATOM 990 C GLN A 276 -2.363 -64.578 -59.457 1.00 35.73 C
ANISOU 990 C GLN A 276 3124 4415 6039 692 901 -976 C
ATOM 991 O GLN A 276 -1.577 -63.792 -59.024 1.00 39.31 O
ANISOU 991 O GLN A 276 3690 4713 6532 849 834 -1041 O
ATOM 992 N ALA A 277 -2.062 -65.441 -60.396 1.00 34.12 N
ANISOU 992 N ALA A 277 2938 4220 5806 522 818 -891 N
ATOM 993 CA ALA A 277 -0.841 -65.389 -61.124 1.00 28.62 C
ANISOU 993 CA ALA A 277 2401 3363 5112 527 665 -841 C
ATOM 994 CB ALA A 277 -0.651 -66.633 -61.947 1.00 33.53 C
ANISOU 994 CB ALA A 277 3099 4009 5631 320 634 -777 C
ATOM 995 C ALA A 277 -0.739 -64.163 -61.981 1.00 48.08 C
ANISOU 995 C ALA A 277 4728 5784 7755 680 537 -777 C
ATOM 996 O ALA A 277 0.345 -63.802 -62.357 1.00 48.44 O
ANISOU 996 O ALA A 277 4881 5665 7858 734 439 -732 O
ATOM 997 N GLY A 278 -1.852 -63.546 -62.328 1.00 36.07 N
ANISOU 997 N GLY A 278 2961 4411 6333 758 551 -755 N
ATOM 998 CA GLY A 278 -1.853 -62.397 -63.219 1.00 30.45 C
ANISOU 998 CA GLY A 278 2117 3668 5786 936 455 -660 C
ATOM 999 C GLY A 278 -1.139 -62.697 -64.521 1.00 41.10 C
ANISOU 999 C GLY A 278 3517 4992 7108 896 331 -524 C
ATOM 1000 O GLY A 278 -0.367 -61.887 -65.030 1.00 57.64 O
ANISOU 1000 O GLY A 278 5676 6937 9286 1010 272 -420 O
ATOM 1001 N PHE A 279 -1.405 -63.875 -65.062 1.00 30.09 N
ANISOU 1001 N PHE A 279 2125 3745 5564 717 302 -518 N
ATOM 1002 CA PHE A 279 -0.601 -64.445 -66.123 1.00 36.68 C
ANISOU 1002 CA PHE A 279 3073 4552 6311 658 204 -427 C
ATOM 1003 CB PHE A 279 0.062 -65.696 -65.570 1.00 39.04 C
ANISOU 1003 CB PHE A 279 3595 4765 6472 462 249 -500 C
ATOM 1004 CG PHE A 279 1.154 -66.257 -66.424 1.00 25.35 C
ANISOU 1004 CG PHE A 279 2028 2948 4654 425 174 -422 C
ATOM 1005 CD1 PHE A 279 2.365 -65.578 -66.567 1.00 31.27 C
ANISOU 1005 CD1 PHE A 279 2880 3510 5492 551 147 -335 C
ATOM 1006 CE1 PHE A 279 3.414 -66.114 -67.341 1.00 23.25 C
ANISOU 1006 CE1 PHE A 279 2010 2424 4402 530 104 -252 C
ATOM 1007 CZ PHE A 279 3.240 -67.355 -67.971 1.00 30.38 C
ANISOU 1007 CZ PHE A 279 2985 3438 5121 391 75 -275 C
ATOM 1008 CE2 PHE A 279 2.014 -68.051 -67.811 1.00 40.84 C
ANISOU 1008 CE2 PHE A 279 4215 4930 6374 245 88 -386 C
ATOM 1009 CD2 PHE A 279 0.994 -67.490 -67.035 1.00 25.44 C
ANISOU 1009 CD2 PHE A 279 2094 3054 4518 260 144 -449 C
ATOM 1010 C PHE A 279 -1.519 -64.819 -67.271 1.00 43.93 C
ANISOU 1010 C PHE A 279 3812 5722 7156 629 112 -393 C
ATOM 1011 O PHE A 279 -2.354 -65.709 -67.124 1.00 44.45 O
ANISOU 1011 O PHE A 279 3792 5943 7156 456 131 -497 O
ATOM 1012 N SER A 280 -1.391 -64.144 -68.407 1.00 29.85 N
ANISOU 1012 N SER A 280 1963 3988 5390 804 -252 N
ATOM 1013 CA SER A 280 -2.302 -64.403 -69.511 1.00 34.02 C
ANISOU 1013 CA SER A 280 2308 4797 5821 826 -107 -236 C
ATOM 1014 CB SER A 280 -2.506 -63.162 -70.385 1.00 35.78 C
ANISOU 1014 CB SER A 280 2400 5088 6106 1125 -169 -58 C
ATOM 1015 OG SER A 280 -1.302 -62.815 -71.036 1.00 57.27 O
ANISOU 1015 OG SER A 280 5303 7638 8818 1241 -170 112 O
ATOM 1016 C SER A 280 -1.837 -65.577 -70.364 1.00 36.98 C
ANISOU 1016 C SER A 280 2817 5227 6005 685 -197 -262 C
ATOM 1017 O SER A 280 -0.692 -66.025 -70.266 1.00 44.22 O
ANISOU 1017 O SER A 280 3974 5953 6875 620 -159 -237 O
ATOM 1018 N ARG A 281 -2.734 -66.061 -71.215 1.00 46.62 N
ANISOU 1018 N ARG A 281 5219 6006 6489 895 -525 -580 N
ATOM 1019 CA ARG A 281 -2.451 -67.205 -72.066 1.00 41.03 C
ANISOU 1019 CA ARG A 281 4752 5356 5482 820 -618 -360 C
ATOM 1020 CB ARG A 281 -3.716 -67.664 -72.783 1.00 33.20 C
ANISOU 1020 CB ARG A 281 3729 4550 4335 888 -819 -278 C
ATOM 1021 CG ARG A 281 -3.662 -69.087 -73.250 1.00 54.60 C
ANISOU 1021 CG ARG A 281 6606 7383 6756 751 -981 -206 C
ATOM 1022 CD ARG A 281 -4.263 -69.236 -74.634 1.00 84.05 C
ANISOU 1022 CD ARG A 281 10451 11138 10347 955 -1184 -65 C
ATOM 1023 NE ARG A 281 -4.000 -70.562 -75.185 1.00 96.97 N
ANISOU 1023 NE ARG A 281 12281 12830 11735 866 -1361 -56 N
ATOM 1024 CZ ARG A 281 -4.766 -71.627 -74.973 1.00104.06 C
ANISOU 1024 CZ ARG A 281 13075 13868 12593 678 -1580 -163 C
ATOM 1025 NH1 ARG A 281 -4.438 -72.796 -75.510 1.00111.91 N
ANISOU 1025 NH1 ARG A 281 14255 14839 13427 619 -1764 -188 N
ATOM 1026 NH2 ARG A 281 -5.857 -71.527 -74.226 1.00 99.41 N
ANISOU 1026 NH2 ARG A 281 12177 13434 12162 554 -1610 -246 N
ATOM 1027 C ARG A 281 -1.373 -66.849 -73.087 1.00 45.00 C
ANISOU 1027 C ARG A 281 5480 5578 6040 949 -522 -115 C
ATOM 1028 O ARG A 281 -0.584 -67.700 -73.514 1.00 48.57 O
ANISOU 1028 O ARG A 281 6134 6038 6282 884 -523 -7 O

ATOM 1029 N GLU A 282 -1.352 -65.581 -73.479 1.00 41.06 N
ANISOU 1029 N GLU A 282 4925 4827 5849 1146 -427 -7 N
ATOM 1030 CA GLU A 282 -0.326 -65.060 -74.373 1.00 40.60 C
ANISOU 1030 CA GLU A 282 5019 4491 5917 1269 -272 295 C
ATOM 1031 CB GLU A 282 -0.702 -63.666 -74.875 1.00 50.25 C
ANISOU 1031 CB GLU A 282 6147 5438 7509 1509 -210 484 C
ATOM 1032 CG GLU A 282 -2.110 -63.577 -75.439 1.00 65.32 C
ANISOU 1032 CG GLU A 282 8021 7523 9275 1707 -397 546 C
ATOM 1033 CD GLU A 282 -3.163 -63.389 -74.354 1.00 90.16 C
ANISOU 1033 CD GLU A 282 10897 10804 12557 1648 -503 168 C
ATOM 1034 OE1 GLU A 282 -4.143 -64.167 -74.322 1.00 93.93 O
ANISOU 1034 OE1 GLU A 282 11324 11610 12755 1608 -678 63 O
ATOM 1035 OE2 GLU A 282 -3.005 -62.461 -73.531 1.00102.42 O
ANISOU 1035 OE2 GLU A 282 12264 12137 14515 1649 -412 -40 O
ATOM 1036 C GLU A 282 1.021 -65.017 -73.662 1.00 39.51 C
ANISOU 1036 C GLU A 282 4859 4181 5974 1097 -114 187 C
ATOM 1037 O GLU A 282 2.054 -65.384 -74.232 1.00 50.21 O
ANISOU 1037 O GLU A 282 6367 5471 7241 1086 -6 387 O
ATOM 1038 N ASP A 283 1.002 -64.566 -72.411 1.00 36.25 N
ANISOU 1038 N ASP A 283 4234 3727 5813 989 -113 -157 N
ATOM 1039 CA ASP A 283 2.185 -64.585 -71.555 1.00 36.68 C
ANISOU 1039 CA ASP A 283 4228 3678 6030 827 -33 -354 C
ATOM 1040 CB ASP A 283 1.851 -64.123 -70.136 1.00 48.57 C
ANISOU 1040 CB ASP A 283 5494 5261 7701 774 -93 -808 C
ATOM 1041 CG ASP A 283 1.656 -62.635 -70.031 1.00 55.19 C
ANISOU 1041 CG ASP A 283 6135 5749 9085 925 -60 -932 C
ATOM 1042 OD1 ASP A 283 2.042 -61.920 -70.979 1.00 56.74 O
ANISOU 1042 OD1 ASP A 283 6374 5573 9614 1024 40 -615 O
ATOM 1043 OD2 ASP A 283 1.125 -62.188 -68.991 1.00 63.03 O
ANISOU 1043 OD2 ASP A 283 6924 6845 10179 959 -130 -1341 O
ATOM 1044 C ASP A 283 2.741 -65.994 -71.476 1.00 45.58 C
ANISOU 1044 C ASP A 283 5523 5048 6747 671 -74 -332 C
ATOM 1045 O ASP A 283 3.952 -66.207 -71.499 1.00 40.22 O
ANISOU 1045 O ASP A 283 4897 4256 6130 601 14 -285 O
ATOM 1046 N ARG A 284 1.869 -66.959 -71.371 1.00 33.93 N
ANISOU 1046 N ARG A 284 4102 3886 4903 617 -218 -366 N
ATOM 1047 CA ARG A 284 2.248 -68.323 -71.256 1.00 32.75 C
ANISOU 1047 CA ARG A 284 4097 3928 4419 467 -296 -352 C
ATOM 1048 CB ARG A 284 0.998 -69.163 -71.086 1.00 32.00 C
ANISOU 1048 CB ARG A 284 3983 4119 4059 390 -465 -385 C
ATOM 1049 CG ARG A 284 1.284 -70.549 -70.615 1.00 31.12 C
ANISOU 1049 CG ARG A 284 3976 4150 3696 207 -562 -380 C
ATOM 1050 CD ARG A 284 0.092 -71.437 -70.703 1.00 40.90 C
ANISOU 1050 CD ARG A 284 5166 5597 4778 114 -729 -354 C
ATOM 1051 NE ARG A 284 -0.469 -71.521 -72.026 1.00 38.29 N
ANISOU 1051 NE ARG A 284 4958 5209 4379 252 -858 -231 N
ATOM 1052 CZ ARG A 284 -1.676 -71.979 -72.260 1.00 36.50 C
ANISOU 1052 CZ ARG A 284 4641 5119 4109 230 -1031 -229 C
ATOM 1053 NH1 ARG A 284 -2.145 -72.040 -73.466 1.00 33.52 N
ANISOU 1053 NH1 ARG A 284 4384 4710 3642 395 -1187 -157 N
ATOM 1054 NH2 ARG A 284 -2.416 -72.357 -71.272 1.00 40.25 N
ANISOU 1054 NH2 ARG A 284 4882 5791 4621 56 -1048 -298 N
ATOM 1055 C ARG A 284 2.991 -68.830 -72.452 1.00 41.12 C
ANISOU 1055 C ARG A 284 5389 4882 5352 548 -254 -95 C
ATOM 1056 O ARG A 284 3.931 -69.559 -72.320 1.00 46.30 O
ANISOU 1056 O ARG A 284 6132 5532 5927 464 -230 -102 O
ATOM 1057 N LEU A 285 2.526 -68.480 -73.629 1.00 45.30 N
ANISOU 1057 N LEU A 285 6012 5366 5836 745 -248 130 N
ATOM 1058 CA LEU A 285 3.174 -68.906 -74.832 1.00 44.40 C
ANISOU 1058 CA LEU A 285 6118 5243 5510 886 -198 369 C
ATOM 1059 CB LEU A 285 2.326 -68.659 -76.062 1.00 36.97 C
ANISOU 1059 CB LEU A 285 5281 4384 4381 1138 -274 577 C
ATOM 1060 CG LEU A 285 2.967 -69.206 -77.328 1.00 44.36 C
ANISOU 1060 CG LEU A 285 6453 5404 4997 1346 -226 796 C
ATOM 1061 CD1 LEU A 285 3.658 -70.527 -77.133 1.00 35.41 C
ANISOU 1061 CD1 LEU A 285 5451 4394 3609 1230 -367 599 C
ATOM 1062 CD2 LEU A 285 2.013 -69.309 -78.475 1.00 30.95 C
ANISOU 1062 CD2 LEU A 285 4863 3868 3028 1632 -359 960 C
ATOM 1063 C LEU A 285 4.524 -68.300 -74.982 1.00 35.89 C
ANISOU 1063 C LEU A 285 5014 3936 4685 922 62 526 C
ATOM 1064 O LEU A 285 5.399 -68.920 -75.472 1.00 40.10 O
ANISOU 1064 O LEU A 285 5670 4496 5069 948 140 615 O
ATOM 1065 N GLU A 286 4.661 -67.051 -74.615 1.00 29.21 N
ANISOU 1065 N GLU A 286 3980 2848 4272 924 192 545 N
ATOM 1066 CA GLU A 286 5.924 -66.377 -74.715 1.00 31.14 C
ANISOU 1066 CA GLU A 286 4124 2812 4896 914 431 691 C
ATOM 1067 CB GLU A 286 5.706 -64.872 -74.513 1.00 49.55 C
ANISOU 1067 CB GLU A 286 6233 4813 7782 938 508 696 C
ATOM 1068 CG GLU A 286 6.776 -64.110 -73.740 1.00 62.59 C
ANISOU 1068 CG GLU A 286 7655 6146 9980 791 626 559 C
ATOM 1069 CD GLU A 286 6.272 -62.922 -72.952 1.00 76.20 C
ANISOU 1069 CD GLU A 286 9137 7589 12228 775 560 298 C
ATOM 1070 OE1 GLU A 286 5.630 -63.087 -71.901 1.00 69.51 O
ANISOU 1070 OE1 GLU A 286 8232 6938 11240 725 371 -106 O
ATOM 1071 OE2 GLU A 286 6.570 -61.795 -73.373 1.00 84.20 O
ANISOU 1071 OE2 GLU A 286 10008 8224 13761 811 695 499 O
ATOM 1072 C GLU A 286 6.975 -66.948 -73.784 1.00 35.15 C
ANISOU 1072 C GLU A 286 4566 3337 5453 711 419 433 C
ATOM 1073 O GLU A 286 8.086 -67.122 -74.148 1.00 35.76 O
ANISOU 1073 O GLU A 286 4654 3349 5586 712 572 571 O

ATOM 1074 N GLN A 287 6.575 -67.204 -72.566 1.00 40.86 N
ANISOU 1074 N GLN A 287 5208 4190 6127 561 240 77 N
ATOM 1075 CA GLN A 287 7.382 -67.796 -71.541 1.00 39.48 C
ANISOU 1075 CA GLN A 287 4964 4075 5962 397 186 -175 C
ATOM 1076 CB GLN A 287 6.702 -67.668 -70.190 1.00 27.45 C
ANISOU 1076 CB GLN A 287 3295 2703 4432 292 31 -538 C
ATOM 1077 CG GLN A 287 6.583 -66.272 -69.667 1.00 26.25 C
ANISOU 1077 CG GLN A 287 2905 2332 4738 327 66 -740 C
ATOM 1078 CD GLN A 287 7.887 -65.527 -69.587 1.00 50.78 C
ANISOU 1078 CD GLN A 287 5848 5110 8335 290 170 -788 C
ATOM 1079 OE1 GLN A 287 8.705 -65.835 -68.776 1.00 39.68 O
ANISOU 1079 OE1 GLN A 287 4370 3774 6932 190 106 -1002 O
ATOM 1080 NE2 GLN A 287 8.052 -64.518 -70.401 1.00 30.37 N
ANISOU 1080 NE2 GLN A 287 3183 2156 6198 371 324 -561 N
ATOM 1081 C GLN A 287 7.713 -69.233 -71.838 1.00 43.35 C
ANISOU 1081 C GLN A 287 5661 4769 6043 373 112 -110 C
ATOM 1082 O GLN A 287 8.672 -69.730 -71.372 1.00 32.72 O
ANISOU 1082 O GLN A 287 4291 3422 4721 300 116 -191 O
ATOM 1083 N ALA A 288 6.852 -69.923 -72.543 1.00 39.44 N
ANISOU 1083 N ALA A 288 5350 4430 5204 446 10 5 N
ATOM 1084 CA ALA A 288 7.118 -71.318 -72.840 1.00 37.04 C
ANISOU 1084 CA ALA A 288 5236 4264 4572 438 -105 20 C
ATOM 1085 CB ALA A 288 5.871 -72.015 -73.376 1.00 28.57 C
ANISOU 1085 CB ALA A 288 4303 3344 3206 479 -298 43 C
ATOM 1086 C ALA A 288 8.259 -71.390 -73.844 1.00 39.20 C
ANISOU 1086 C ALA A 288 5600 4458 4836 590 71 207 C
ATOM 1087 O ALA A 288 9.172 -72.209 -73.716 1.00 36.28 O
ANISOU 1087 O ALA A 288 5279 4109 4396 569 56 154 O
ATOM 1088 N LYS A 289 8.210 -70.522 -74.845 1.00 37.58 N
ANISOU 1088 N LYS A 289 5401 4178 4700 766 250 454 N
ATOM 1089 CA LYS A 289 9.275 -70.463 -75.833 1.00 34.60 C
ANISOU 1089 CA LYS A 289 5070 3775 4300 937 485 698 C
ATOM 1090 CB LYS A 289 8.956 -69.438 -76.902 1.00 28.34 C
ANISOU 1090 CB LYS A 289 4284 2936 3548 1144 680 1048 C
ATOM 1091 CG LYS A 289 7.756 -69.756 -77.731 1.00 49.65 C
ANISOU 1091 CG LYS A 289 7183 5839 5842 1331 508 1102 C
ATOM 1092 CD LYS A 289 7.327 -68.497 -78.430 1.00 47.13 C
ANISOU 1092 CD LYS A 289 6813 5427 5669 1502 672 1446 C
ATOM 1093 CE LYS A 289 6.463 -68.774 -79.624 1.00 58.72 C
ANISOU 1093 CE LYS A 289 8494 7159 6660 1797 555 1594 C
ATOM 1094 NZ LYS A 289 6.671 -67.664 -80.589 1.00 76.11 N
ANISOU 1094 NZ LYS A 289 10629 9329 8961 1971 824 2003 N
ATOM 1095 C LYS A 289 10.565 -70.066 -75.154 1.00 39.80 C
ANISOU 1095 C LYS A 289 5511 4257 5355 805 648 656 C
ATOM 1096 O LYS A 289 11.626 -70.656 -75.384 1.00 47.29 O
ANISOU 1096 O LYS A 289 6470 5248 6249 849 739 680 O
ATOM 1097 N LEU A 290 10.465 -69.057 -74.302 1.00 39.17 N
ANISOU 1097 N LEU A 290 5211 3978 5696 659 661 551 N
ATOM 1098 CA LEU A 290 11.622 -68.516 -73.609 1.00 27.14 C
ANISOU 1098 CA LEU A 290 3428 2250 4634 528 767 455 C
ATOM 1099 CB LEU A 290 11.245 -67.247 -72.854 1.00 35.91 C
ANISOU 1099 CB LEU A 290 4308 3114 6220 425 744 306 C
ATOM 1100 CG LEU A 290 12.348 -66.570 -72.048 1.00 41.42 C
ANISOU 1100 CG LEU A 290 4693 3562 7481 281 782 114 C
ATOM 1101 CD1 LEU A 290 13.412 -65.994 -72.970 1.00 47.28 C
ANISOU 1101 CD1 LEU A 290 5287 4065 8610 323 1096 488 C
ATOM 1102 CD2 LEU A 290 11.719 -65.480 -71.213 1.00 31.06 C
ANISOU 1102 CD2 LEU A 290 3196 2051 6553 217 667 -160 C
ATOM 1103 C LEU A 290 12.210 -69.542 -72.644 1.00 30.60 C
ANISOU 1103 C LEU A 290 3862 2825 4940 406 583 156 C
ATOM 1104 O LEU A 290 13.424 -69.618 -72.464 1.00 33.02 O
ANISOU 1104 O LEU A 290 4023 3062 5460 371 666 128 O
ATOM 1105 N PHE A 291 11.333 -70.321 -72.025 1.00 23.18 N
ANISOU 1105 N PHE A 291 3059 2079 3669 347 336 -36 N
ATOM 1106 CA PHE A 291 11.753 -71.416 -71.170 1.00 33.49 C
ANISOU 1106 CA PHE A 291 4400 3531 4793 257 150 -234 C
ATOM 1107 CB PHE A 291 10.535 -72.132 -70.586 1.00 32.68 C
ANISOU 1107 CB PHE A 291 4426 3624 4366 182 -78 -337 C
ATOM 1108 CG PHE A 291 10.868 -73.384 -69.840 1.00 19.36 C
ANISOU 1108 CG PHE A 291 2810 2074 2471 107 -265 -431 C
ATOM 1109 CD1 PHE A 291 11.378 -73.325 -68.546 1.00 19.60 C
ANISOU 1109 CD1 PHE A 291 2683 2181 2582 11 -355 -627 C
ATOM 1110 CE1 PHE A 291 11.688 -74.485 -67.844 1.00 19.29 C
ANISOU 1110 CE1 PHE A 291 2714 2274 2340 -34 -531 -649 C
ATOM 1111 CZ PHE A 291 11.499 -75.732 -68.459 1.00 18.74 C
ANISOU 1111 CZ PHE A 291 2867 2191 2062 -4 -624 -495 C
ATOM 1112 CE2 PHE A 291 10.988 -75.795 -69.769 1.00 18.54 C
ANISOU 1112 CE2 PHE A 291 2993 2076 1975 90 -557 -372 C
ATOM 1113 CD2 PHE A 291 10.679 -74.623 -70.438 1.00 26.49 C
ANISOU 1113 CD2 PHE A 291 3935 3021 3109 154 -375 -330 C
ATOM 1114 C PHE A 291 12.613 -72.419 -71.944 1.00 33.35 C
ANISOU 1114 C PHE A 291 4521 3558 4594 372 197 -110 C
ATOM 1115 O PHE A 291 13.635 -72.897 -71.452 1.00 33.02 O
ANISOU 1115 O PHE A 291 4398 3518 4628 343 161 -211 O
ATOM 1116 N CYS A 292 12.187 -72.735 -73.161 1.00 31.32 N
ANISOU 1116 N CYS A 292 4462 3356 4082 537 259 81 N
ATOM 1117 CA CYS A 292 12.887 -73.704 -73.990 1.00 34.89 C
ANISOU 1117 CA CYS A 292 5059 3886 4309 707 146 146 C
ATOM 1118 CB CYS A 292 12.064 -74.067 -75.228 1.00 31.63 C
ANISOU 1118 CB CYS A 292 4890 3596 3534 910 266 266 C

ATOM 1119 SG CYS A 292 10.588 -75.049 -74.872 1.00 46.81 S
ANISOU 1119 SG CYS A 292 7000 5595 5192 808 -118 85 S
ATOM 1120 C CYS A 292 14.261 -73.190 -74.405 1.00 39.97 C
ANISOU 1120 C CYS A 292 5519 4457 5210 793 585 283 C
ATOM 1121 O CYS A 292 15.255 -73.913 -74.362 1.00 43.56 O
ANISOU 1121 O CYS A 292 5948 4948 5655 849 587 216 O
ATOM 1122 N ARG A 293 14.332 -71.950 -74.824 1.00 38.08 N
ANISOU 1122 N ARG A 293 5128 4100 5243 806 836 500 N
ATOM 1123 CA ARG A 293 15.569 -71.334 -75.222 1.00 32.59 C
ANISOU 1123 CA ARG A 293 4194 3303 4886 853 1158 706 C
ATOM 1124 CB ARG A 293 15.294 -69.934 -75.705 1.00 31.49 C
ANISOU 1124 CB ARG A 293 3907 2972 5084 845 1399 1000 C
ATOM 1125 CG ARG A 293 14.937 -69.836 -77.145 1.00 60.24 C
ANISOU 1125 CG ARG A 293 7691 6753 8444 1114 1659 1413 C
ATOM 1126 CD ARG A 293 14.643 -68.403 -77.523 1.00 79.46 C
ANISOU 1126 CD ARG A 293 9982 8945 11264 1085 1846 1725 C
ATOM 1127 NE ARG A 293 13.263 -68.025 -77.228 1.00 91.40 N
ANISOU 1127 NE ARG A 293 11655 10449 12622 1068 1597 1600 N
ATOM 1128 CZ ARG A 293 12.805 -66.786 -77.160 1.00 81.75 C
ANISOU 1128 CZ ARG A 293 10328 8986 11745 1033 1644 1752 C
ATOM 1129 NH1 ARG A 293 11.543 -66.584 -76.881 1.00 71.09 N
ANISOU 1129 NH1 ARG A 293 9116 7682 10214 1046 1406 1607 N
ATOM 1130 NH2 ARG A 293 13.595 -65.761 -77.387 1.00 76.60 N
ANISOU 1130 NH2 ARG A 293 9407 8024 11672 984 1923 2049 N
ATOM 1131 C ARG A 293 16.548 -71.218 -74.100 1.00 42.13 C
ANISOU 1131 C ARG A 293 5131 4387 6489 667 1085 469 C
ATOM 1132 O ARG A 293 17.702 -71.448 -74.269 1.00 39.07 O
ANISOU 1132 O ARG A 293 4602 4024 6217 724 1213 498 O
ATOM 1133 N THR A 294 16.067 -70.816 -72.950 1.00 33.02 N
ANISOU 1133 N THR A 294 3883 3129 5532 471 874 218 N
ATOM 1134 CA THR A 294 16.905 -70.664 -71.776 1.00 31.76 C
ANISOU 1134 CA THR A 294 3458 2886 5724 315 746 -63 C
ATOM 1135 CB THR A 294 16.141 -70.023 -70.626 1.00 32.28 C
ANISOU 1135 CB THR A 294 3445 2895 5927 163 530 -349 C
ATOM 1136 OG1 THR A 294 15.627 -68.762 -71.055 1.00 40.41 O
ANISOU 1136 OG1 THR A 294 4377 3697 7280 150 692 -207 O
ATOM 1137 CG2 THR A 294 17.058 -69.820 -69.429 1.00 28.64 C
ANISOU 1137 CG2 THR A 294 2696 2388 5799 47 366 -687 C
ATOM 1138 C THR A 294 17.471 -72.006 -71.336 1.00 35.30 C
ANISOU 1138 C THR A 294 4000 3520 5890 354 554 -226 C
ATOM 1139 O THR A 294 18.638 -72.117 -70.957 1.00 41.67 O
ANISOU 1139 O THR A 294 4586 4299 6949 337 553 -327 O
ATOM 1140 N LEU A 295 16.645 -73.038 -71.408 1.00 30.04 N
ANISOU 1140 N LEU A 295 3646 3020 4746 411 376 -242 N
ATOM 1141 CA LEU A 295 17.078 -74.354 -70.975 1.00 31.77 C
ANISOU 1141 CA LEU A 295 3973 3360 4737 451 165 -365 C
ATOM 1142 CB LEU A 295 15.898 -75.304 -70.846 1.00 24.18 C
ANISOU 1142 CB LEU A 295 3314 2507 3369 439 -68 -381 C
ATOM 1143 CG LEU A 295 16.274 -76.627 -70.191 1.00 27.31 C
ANISOU 1143 CG LEU A 295 3803 2966 3609 448 -322 -478 C
ATOM 1144 CD1 LEU A 295 16.761 -76.378 -68.764 1.00 30.25 C
ANISOU 1144 CD1 LEU A 295 3965 3393 4135 323 -468 -648 C
ATOM 1145 CD2 LEU A 295 15.089 -77.570 -70.202 1.00 39.74 C
ANISOU 1145 CD2 LEU A 295 5644 4581 4875 414 -530 -438 C
ATOM 1146 C LEU A 295 18.111 -74.937 -71.942 1.00 42.33 C
ANISOU 1146 C LEU A 295 5314 4717 6051 651 334 -248 C
ATOM 1147 O LEU A 295 19.084 -75.571 -71.524 1.00 45.99 O
ANISOU 1147 O LEU A 295 5680 5205 6590 690 245 -359 O
ATOM 1148 N GLU A 296 17.876 -74.734 -73.235 1.00 39.62 N
ANISOU 1148 N GLU A 296 5081 4404 5570 811 572 -26 N
ATOM 1149 CA GLU A 296 18.799 -75.167 -74.278 1.00 38.91 C
ANISOU 1149 CA GLU A 296 4981 4404 5399 1056 795 97 C
ATOM 1150 CB GLU A 296 18.336 -74.648 -75.638 1.00 56.51 C
ANISOU 1150 CB GLU A 296 7322 6721 7429 1239 1076 382 C
ATOM 1151 CG GLU A 296 17.911 -75.707 -76.622 1.00 72.87 C
ANISOU 1151 CG GLU A 296 9719 8988 8981 1517 995 348 C
ATOM 1152 CD GLU A 296 17.130 -75.126 -77.792 1.00 82.94 C
ANISOU 1152 CD GLU A 296 11140 10393 9982 1691 1177 598 C
ATOM 1153 OE1 GLU A 296 17.325 -73.932 -78.113 1.00 76.19 O
ANISOU 1153 OE1 GLU A 296 10096 9491 9362 1667 1494 906 O
ATOM 1154 OE2 GLU A 296 16.311 -75.865 -78.377 1.00 87.35 O
ANISOU 1154 OE2 GLU A 296 11990 11083 10118 1856 978 489 O
ATOM 1155 C GLU A 296 20.185 -74.615 -73.978 1.00 51.23 C
ANISOU 1155 C GLU A 296 6154 5888 7425 1008 987 117 C
ATOM 1156 O GLU A 296 21.195 -75.337 -74.007 1.00 49.44 O
ANISOU 1156 O GLU A 296 5837 5730 7218 1132 991 39 O
ATOM 1157 N ASP A 297 20.220 -73.321 -73.670 1.00 43.34 N
ANISOU 1157 N ASP A 297 4897 4720 6851 827 1125 200 N
ATOM 1158 CA ASP A 297 21.464 -72.616 -73.372 1.00 34.60 C
ANISOU 1158 CA ASP A 297 3355 3478 6312 733 1293 213 C
ATOM 1159 CB ASP A 297 21.217 -71.120 -73.197 1.00 49.13 C
ANISOU 1159 CB ASP A 297 4958 5059 8651 538 1424 317 C
ATOM 1160 CG ASP A 297 20.822 -70.442 -74.477 1.00 64.44 C
ANISOU 1160 CG ASP A 297 6959 6974 10551 652 1793 760 C
ATOM 1161 OD1 ASP A 297 21.065 -71.025 -75.552 1.00 64.82 O
ANISOU 1161 OD1 ASP A 297 7143 7246 10239 898 2016 994 O
ATOM 1162 OD2 ASP A 297 20.271 -69.324 -74.408 1.00 84.97 O
ANISOU 1162 OD2 ASP A 297 9471 9344 13469 526 1851 869 O
ATOM 1163 C ASP A 297 22.155 -73.148 -72.129 1.00 39.94 C
ANISOU 1163 C ASP A 297 3876 4157 7141 638 979 -137 C
ATOM 1164 O ASP A 297 23.379 -73.300 -72.103 1.00 56.63 O
ANISOU 1164 O ASP A 297 5709 6280 9530 684 1060 -165 O
ATOM 1165 N ILE A 298 21.376 -73.405 -71.088 1.00 31.56 N
ANISOU 1165 N ILE A 298 2975 3118 5898 523 627 -383 N
ATOM 1166 CA ILE A 298 21.936 -73.891 -69.842 1.00 32.53 C
ANISOU 1166 CA ILE A 298 2975 3296 6087 463 305 -685 C
ATOM 1167 CB ILE A 298 20.870 -74.035 -68.763 1.00 35.43 C
ANISOU 1167 CB ILE A 298 3533 3746 6183 351 -16 -875 C
ATOM 1168 CG1 ILE A 298 20.304 -72.674 -68.385 1.00 38.63 C
ANISOU 1168 CG1 ILE A 298 3781 4020 6876 192 21 -970 C
ATOM 1169 CD1 ILE A 298 19.221 -72.759 -67.326 1.00 39.89 C
ANISOU 1169 CD1 ILE A 298 4096 4328 6733 115 -252 -1166 C
ATOM 1170 CG2 ILE A 298 21.451 -74.694 -67.525 1.00 38.88 C
ANISOU 1170 CG2 ILE A 298 3886 4317 6569 351 -350 -1124 C
ATOM 1171 C ILE A 298 22.574 -75.255 -70.065 1.00 39.86 C
ANISOU 1171 C ILE A 298 4025 4358 6760 657 220 -685 C
ATOM 1172 O ILE A 298 23.686 -75.532 -69.602 1.00 43.02 O
ANISOU 1172 O ILE A 298 4180 4781 7383 697 132 -817 O
ATOM 1173 N LEU A 299 21.858 -76.102 -70.793 1.00 38.83 N
ANISOU 1173 N LEU A 299 4259 4302 6195 793 223 -563 N
ATOM 1174 CA LEU A 299 22.257 -77.488 -70.971 1.00 40.23 C
ANISOU 1174 CA LEU A 299 4603 4555 6127 991 79 -609 C
ATOM 1175 CB LEU A 299 21.113 -78.307 -71.563 1.00 38.88 C
ANISOU 1175 CB LEU A 299 4848 4407 5518 1075 -20 -548 C
ATOM 1176 CG LEU A 299 19.925 -78.424 -70.620 1.00 56.16 C
ANISOU 1176 CG LEU A 299 7211 6584 7541 871 -299 -594 C
ATOM 1177 CD1 LEU A 299 18.853 -79.317 -71.219 1.00 63.09 C
ANISOU 1177 CD1 LEU A 299 8445 7449 8077 936 -425 -544 C
ATOM 1178 CD2 LEU A 299 20.394 -78.954 -69.273 1.00 54.97 C
ANISOU 1178 CD2 LEU A 299 6971 6463 7450 803 -595 -723 C
ATOM 1179 C LEU A 299 23.485 -77.595 -71.852 1.00 41.10 C
ANISOU 1179 C LEU A 299 4507 4707 6404 1204 353 -540 C
ATOM 1180 O LEU A 299 24.356 -78.429 -71.612 1.00 59.31 O
ANISOU 1180 O LEU A 299 6736 7048 8751 1344 226 -657 O
ATOM 1181 N ALA A 300 23.547 -76.745 -72.872 1.00 48.26 N
ANISOU 1181 N ALA A 300 5309 5624 7403 1246 743 -321 N
ATOM 1182 CA ALA A 300 24.686 -76.711 -73.780 1.00 52.76 C
ANISOU 1182 CA ALA A 300 5636 6290 8122 1454 1094 -187 C
ATOM 1183 CB ALA A 300 24.570 -75.543 -74.727 1.00 39.76 C
ANISOU 1183 CB ALA A 300 3858 4643 6605 1439 1534 147 C
ATOM 1184 C ALA A 300 26.010 -76.634 -73.031 1.00 55.46 C
ANISOU 1184 C ALA A 300 5548 6592 8932 1400 1047 -325 C
ATOM 1185 O ALA A 300 27.012 -77.207 -73.451 1.00 59.73 O
ANISOU 1185 O ALA A 300 5930 7246 9519 1621 1168 -338 O
ATOM 1186 N ASP A 301 26.002 -75.930 -71.908 1.00 65.09 N
ANISOU 1186 N ASP A 301 6564 7671 10495 1129 849 -467 N
ATOM 1187 CA ASP A 301 27.227 -75.630 -71.179 1.00 62.82 C
ANISOU 1187 CA ASP A 301 5808 7337 10724 1052 780 -627 C
ATOM 1188 CB ASP A 301 27.296 -74.133 -70.878 1.00 64.32 C
ANISOU 1188 CB ASP A 301 5643 7324 11473 778 905 -602 C
ATOM 1189 CG ASP A 301 28.156 -73.381 -71.866 1.00 84.37 C
ANISOU 1189 CG ASP A 301 7787 9799 14469 791 1395 -298 C
ATOM 1190 OD1 ASP A 301 27.634 -73.001 -72.936 1.00 83.28 O
ANISOU 1190 OD1 ASP A 301 7800 9672 14171 850 1754 51 O
ATOM 1191 OD2 ASP A 301 29.355 -73.182 -71.569 1.00 99.13 O
ANISOU 1191 OD2 ASP A 301 9307 11640 16719 714 1370 -375 O
ATOM 1192 C ASP A 301 27.410 -76.414 -69.881 1.00 55.33 C
ANISOU 1192 C ASP A 301 4899 6435 9687 1047 288 -942 C
ATOM 1193 O ASP A 301 28.436 -76.281 -69.214 1.00 57.65 O
ANISOU 1193 O ASP A 301 4812 6728 10364 1021 156 -1121 O
ATOM 1194 N ALA A 302 26.423 -77.218 -69.504 1.00 69.57 N
ANISOU 1194 N ALA A 302 6806 6124 10497 1194 N ALA A 302 26.471 -77.857 -68.192 1.00 73.72 C
ANISOU 1195 CA ALA A 302 5393 6890 15730 3 -1488 -3415 C
ATOM 1196 CB ALA A 302 25.071 -78.095 -67.648 1.00 63.73 C
ANISOU 1196 CB ALA A 302 4422 5807 13984 129 -1635 -3524 C
ATOM 1197 C ALA A 302 27.271 -79.153 -68.215 1.00 75.63 C
ANISOU 1197 C ALA A 302 5551 7340 15845 52 -1407 -3423 C
ATOM 1198 O ALA A 302 27.071 -79.982 -69.109 1.00 70.93 O
ANISOU 1198 O ALA A 302 5038 6845 15065 1 -1165 -3205 O
ATOM 1199 N PRO A 303 28.167 -79.336 -67.229 1.00 77.08 N
ANISOU 1199 N PRO A 303 5631 7597 16059 189 -1586 -3645 N
ATOM 1200 CA PRO A 303 28.966 -80.563 -67.195 1.00 74.85 C
ANISOU 1200 CA PRO A 303 5274 7504 15662 271 -1541 -3651 C
ATOM 1201 CB PRO A 303 29.811 -80.404 -65.924 1.00 72.35 C
ANISOU 1201 CB PRO A 303 4879 7215 15397 399 -1798 -3917 C
ATOM 1202 CG PRO A 303 29.051 -79.424 -65.075 1.00 73.64 C
ANISOU 1202 CG PRO A 303 5161 7326 15491 457 -2000 -4090 C
ATOM 1203 CD PRO A 303 28.400 -78.485 -66.053 1.00 69.99 C
ANISOU 1203 CD PRO A 303 4698 6635 15262 298 -1844 -3908 C
ATOM 1204 C PRO A 303 28.072 -81.797 -67.084 1.00 78.23 C
ANISOU 1204 C PRO A 303 5941 8201 15583 394 -1582 -3631 C
ATOM 1205 O PRO A 303 28.353 -82.837 -67.694 1.00 73.46 O
ANISOU 1205 O PRO A 303 5373 7702 14837 1703 -3477 O
ATOM 1206 N GLU A 304 26.987 -81.662 -66.328 1.00 73.82 N
ANISOU 1206 N GLU A 304 5627 7749 14673 467 -1782 -3745 N
ATOM 1207 CA GLU A 304 26.070 -82.766 -66.066 1.00 76.65 C
ANISOU 1207 CA GLU A 304 5157 8408 15583 394 -1396 -3474 C
ATOM 1208 CB GLU A 304 25.025 -82.358 -65.017 1.00 65.55 C
ANISOU 1208 CB GLU A 304 5084 7116 12707 656 -2072 -3862 C

ATOM 1209 CG GLU A 304 25.549 -82.274 -63.592 1.00 68.63 C
ANISOU 1209 CG GLU A 304 5448 7637 12992 806 -2291 -4066 C
ATOM 1210 CD GLU A 304 25.981 -80.870 -63.195 1.00 91.01 C
ANISOU 1210 CD GLU A 304 8101 10263 16214 797 -2337 -4236 C
ATOM 1211 OE1 GLU A 304 26.159 -80.622 -61.982 1.00 97.21 O
ANISOU 1211 OE1 GLU A 304 8879 11175 16882 918 -2509 -4429 O
ATOM 1212 OE2 GLU A 304 26.136 -80.014 -64.091 1.00 97.88 O
ANISOU 1212 OE2 GLU A 304 8834 10849 17509 665 -2202 -4161 O
ATOM 1213 C GLU A 304 25.352 -83.268 -67.318 1.00 65.33 C
ANISOU 1213 C GLU A 304 5140 6919 12762 511 -1515 -3371 C
ATOM 1214 O GLU A 304 24.963 -84.432 -67.407 1.00 66.79 O
ANISOU 1214 O GLU A 304 5599 7274 12504 603 -1465 -3244 O
ATOM 1215 N SER A 305 25.185 -82.383 -68.290 1.00 69.48 N
ANISOU 1215 N SER A 305 5632 7227 13539 349 -1289 -3207 N
ATOM 1216 CA SER A 305 24.188 -82.588 -69.331 1.00 71.53 C
ANISOU 1216 CA SER A 305 6224 7483 13473 279 -1019 -2913 C
ATOM 1217 CB SER A 305 23.281 -81.367 -69.399 1.00 82.68 C
ANISOU 1217 CB SER A 305 7670 8740 15004 172 -1081 -2926 C
ATOM 1218 OG SER A 305 23.949 -80.322 -70.084 1.00 92.08 O
ANISOU 1218 OG SER A 305 8593 9651 16742 1 -955 -2824 O
ATOM 1219 C SER A 305 24.763 -82.781 -70.718 1.00 71.52 C
ANISOU 1219 C SER A 305 6186 7391 13595 172 -630 -2618 C
ATOM 1220 O SER A 305 24.209 -82.259 -71.687 1.00 68.46 O
ANISOU 1220 O SER A 305 5909 6898 13204 32 -412 -2381 O
ATOM 1221 N GLN A 306 25.863 -83.512 -70.832 1.00 71.66 N
ANISOU 1221 N GLN A 306 6038 7471 13718 239 -546 -2634 N
ATOM 1222 CA GLN A 306 26.501 -83.664 -72.129 1.00 68.61 C
ANISOU 1222 CA GLN A 306 5559 7054 13457 140 -169 -2397 C
ATOM 1223 CB GLN A 306 28.007 -83.438 -72.006 1.00 85.92 C
ANISOU 1223 CB GLN A 306 7306 9193 16146 121 -167 -2516 C
ATOM 1224 CG GLN A 306 28.359 -82.185 -71.204 1.00 93.36 C
ANISOU 1224 CG GLN A 306 7950 9954 17570 32 -430 -2707 C
ATOM 1225 CD GLN A 306 28.188 -80.892 -71.995 1.00 95.94 C
ANISOU 1225 CD GLN A 306 8171 10053 18229 -222 -278 -2501 C
ATOM 1226 OE1 GLN A 306 28.299 -80.882 -73.222 1.00 91.63 O
ANISOU 1226 OE1 GLN A 306 7634 9511 17672 -362 68 -2201 O
ATOM 1227 NE2 GLN A 306 27.924 -79.795 -71.292 1.00100.57 N
ANISOU 1227 NE2 GLN A 306 8647 10447 19119 -282 -554 -2665 N
ATOM 1228 C GLN A 306 26.178 -85.017 -72.773 1.00 67.93 C
ANISOU 1228 C GLN A 306 5767 7143 12900 249 32 -2259 C
ATOM 1229 O GLN A 306 26.569 -86.069 -72.261 1.00 61.54 O
ANISOU 1229 O GLN A 306 4982 6447 11953 427 -87 -2389 O
ATOM 1230 N ASN A 307 25.434 -84.960 -73.878 1.00 75.55 N
ANISOU 1230 N ASN A 307 6956 8117 13633 141 310 -1998 N
ATOM 1231 CA ASN A 307 25.054 -86.128 -74.686 1.00 76.62 C
ANISOU 1231 CA ASN A 307 7372 8405 13336 216 535 -1860 C
ATOM 1232 CB ASN A 307 26.280 -86.935 -75.126 1.00 85.31 C
ANISOU 1232 CB ASN A 307 8255 9592 14568 307 704 -1915 C
ATOM 1233 CG ASN A 307 27.046 -86.269 -76.241 1.00101.69 C
ANISOU 1233 CG ASN A 307 10041 11662 16933 128 1045 -1756 C
ATOM 1234 OD1 ASN A 307 26.741 -86.462 -77.418 1.00108.66 O
ANISOU 1234 OD1 ASN A 307 11046 12647 17592 48 1362 -1549 O
ATOM 1235 ND2 ASN A 307 28.041 -85.466 -75.880 1.00102.27 N
ANISOU 1235 ND2 ASN A 307 9719 11640 17499 47 977 -1844 N
ATOM 1236 C ASN A 307 24.006 -87.070 -74.090 1.00 69.24 C
ANISOU 1236 C ASN A 307 6822 7574 11913 359 342 -1908 C
ATOM 1237 O ASN A 307 23.724 -88.126 -74.656 1.00 63.30 O
ANISOU 1237 O ASN A 307 6299 6923 10828 435 480 -1825 O
ATOM 1238 N ASN A 308 23.419 -86.693 -72.962 1.00 71.89 N
ANISOU 1238 N ASN A 308 7216 7898 12199 388 22 -2046 N
ATOM 1239 CA ASN A 308 22.476 -87.580 -72.290 1.00 67.52 C
ANISOU 1239 CA ASN A 308 6989 7484 11181 500 -180 -2082 C
ATOM 1240 CB ASN A 308 23.009 -87.952 -70.913 1.00 69.39 C
ANISOU 1240 CB ASN A 308 7092 7788 11486 637 -536 -2318 C
ATOM 1241 CG ASN A 308 23.457 -86.742 -70.126 1.00 71.01 C
ANISOU 1241 CG ASN A 308 6981 7913 12087 589 -731 -2519 C
ATOM 1242 OD1 ASN A 308 23.284 -85.603 -70.569 1.00 72.61 O
ANISOU 1242 OD1 ASN A 308 7082 7980 12527 451 -624 -2477 O
ATOM 1243 ND2 ASN A 308 24.039 -86.978 -68.954 1.00 67.54 N
ANISOU 1243 ND2 ASN A 308 6378 7550 11735 700 -1038 -2737 N
ATOM 1244 C ASN A 308 21.075 -87.012 -72.132 1.00 54.62 C
ANISOU 1244 C ASN A 308 5594 5880 9278 423 -253 -2027 C
ATOM 1245 O ASN A 308 20.317 -87.467 -71.281 1.00 43.18 O
ANISOU 1245 O ASN A 308 4336 4572 7499 492 -486 -2102 O
ATOM 1246 N CYS A 309 20.738 -86.021 -72.949 1.00 51.60 N
ANISOU 1246 N CYS A 309 5188 5379 9038 276 -63 -1886 N
ATOM 1247 CA CYS A 309 19.468 -85.320 -72.824 1.00 49.91 C
ANISOU 1247 CA CYS A 309 5149 5163 8650 211 -145 -1857 C
ATOM 1248 CB CYS A 309 19.565 -84.256 -71.733 1.00 45.05 C
ANISOU 1248 CB CYS A 309 4296 4471 8348 215 -444 -2114 C
ATOM 1249 SG CYS A 309 17.995 -83.510 -71.263 1.00 68.53 S
ANISOU 1249 SG CYS A 309 7450 7496 11091 199 -629 -2194 S
ATOM 1250 C CYS A 309 19.096 -84.664 -74.148 1.00 53.87 C
ANISOU 1250 C CYS A 309 5710 5547 9210 55 148 -1588 C
ATOM 1251 O CYS A 309 19.948 -84.083 -74.817 1.00 67.10 O
ANISOU 1251 O CYS A 309 7150 7087 11260 -49 323 -1488 O
ATOM 1252 N ARG A 310 17.828 -84.744 -74.532 1.00 44.79 N
ANISOU 1252 N ARG A 310 4862 4468 7688 26 197 -1455 N
ATOM 1253 CA ARG A 310 17.393 -84.127 -75.778 1.00 51.21 C
ANISOU 1253 CA ARG A 310 5747 5188 8522 -122 450 -1178 C
ATOM 1254 CB ARG A 310 17.333 -85.146 -76.916 1.00 40.81 C
ANISOU 1254 CB ARG A 310 4638 4006 6862 -133 758 -960 C
ATOM 1255 CG ARG A 310 17.206 -84.504 -78.287 1.00 71.63 C
ANISOU 1255 CG ARG A 310 8543 7848 10826 -304 1050 -653 C
ATOM 1256 CD ARG A 310 18.432 -83.658 -78.602 1.00 86.94 C
ANISOU 1256 CD ARG A 310 10110 9635 13289 -423 1153 -594 C
ATOM 1257 NE ARG A 310 18.067 -82.363 -79.169 1.00 97.63 N
ANISOU 1257 NE ARG A 310 11397 10810 14887 -604 1189 -370 N
ATOM 1258 CZ ARG A 310 18.057 -81.219 -78.489 1.00 93.75 C
ANISOU 1258 CZ ARG A 310 10728 10085 14808 -647 943 -470 C
ATOM 1259 NH1 ARG A 310 18.412 -81.198 -77.212 1.00 88.06 N
ANISOU 1259 NH1 ARG A 310 9866 9321 14271 -523 660 -807 N
ATOM 1260 NH2 ARG A 310 17.704 -80.091 -79.092 1.00 90.92 N
ANISOU 1260 NH2 ARG A 310 10325 9533 14688 -813 965 -236 N
ATOM 1261 C ARG A 310 16.047 -83.433 -75.613 1.00 49.00 C
ANISOU 1261 C ARG A 310 5636 4887 8096 -152 317 -1164 C
ATOM 1262 O ARG A 310 15.107 -84.003 -75.066 1.00 49.14 O
ANISOU 1262 O ARG A 310 5883 5076 7713 -66 182 -1254 O
ATOM 1263 N LEU A 311 15.963 -82.201 -76.102 1.00 46.61 N
ANISOU 1263 N LEU A 311 5207 4373 8130 -279 348 -1044 N
ATOM 1264 CA LEU A 311 14.762 -81.396 -75.967 1.00 41.12 C
ANISOU 1264 CA LEU A 311 4621 3612 7390 -295 199 -1053 C
ATOM 1265 CB LEU A 311 15.122 -79.942 -75.684 1.00 43.85 C
ANISOU 1265 CB LEU A 311 4673 3657 8331 -365 27 -1138 C
ATOM 1266 CG LEU A 311 15.935 -79.703 -74.419 1.00 45.22 C
ANISOU 1266 CG LEU A 311 4567 3786 8828 -276 -238 -1502 C
ATOM 1267 CD1 LEU A 311 16.209 -78.220 -74.230 1.00 48.19 C
ANISOU 1267 CD1 LEU A 311 4660 3827 9821 -356 -420 -1589 C
ATOM 1268 CD2 LEU A 311 15.205 -80.268 -73.216 1.00 55.42 C
ANISOU 1268 CD2 LEU A 311 5984 5333 9739 -105 -486 -1815 C
ATOM 1269 C LEU A 311 13.915 -81.479 -77.218 1.00 40.12 C
ANISOU 1269 C LEU A 311 4747 3521 6975 -389 437 -718 C
ATOM 1270 O LEU A 311 14.387 -81.228 -78.325 1.00 52.01 O
ANISOU 1270 O LEU A 311 6197 4942 8621 -527 685 -433 O
ATOM 1271 N ILE A 312 12.650 -81.827 -77.032 1.00 39.73 N
ANISOU 1271 N ILE A 312 4963 3628 6504 -324 356 -752 N
ATOM 1272 CA ILE A 312 11.711 -81.950 -78.132 1.00 40.98 C
ANISOU 1272 CA ILE A 312 5378 3849 6344 -398 546 -463 C
ATOM 1273 CB ILE A 312 11.097 -83.346 -78.166 1.00 42.85 C
ANISOU 1273 CB ILE A 312 5916 4373 5992 -323 621 -464 C
ATOM 1274 CG1 ILE A 312 12.200 -84.400 -78.173 1.00 42.28 C
ANISOU 1274 CG1 ILE A 312 5799 4383 5885 -280 747 -501 C
ATOM 1275 CD1 ILE A 312 11.700 -85.811 -78.345 1.00 43.53 C
ANISOU 1275 CD1 ILE A 312 6248 4766 5524 -219 822 -476 C
ATOM 1276 CG2 ILE A 312 10.204 -83.509 -79.382 1.00 49.83 C
ANISOU 1276 CG2 ILE A 312 7053 5333 6548 -406 830 -171 C
ATOM 1277 C ILE A 312 10.613 -80.893 -78.015 1.00 36.75 C
ANISOU 1277 C ILE A 312 4870 3196 5896 -407 364 -477 C
ATOM 1278 O ILE A 312 9.618 -81.089 -77.325 1.00 34.99 O
ANISOU 1278 O ILE A 312 4779 3126 5391 -307 187 -663 O
ATOM 1279 N ALA A 313 10.819 -79.761 -78.678 1.00 42.89 N
ANISOU 1279 N ALA A 313 5505 3706 7087 -531 397 -278 N
ATOM 1280 CA ALA A 313 9.888 -78.646 -78.601 1.00 48.70 C
ANISOU 1280 CA ALA A 313 6229 4262 8016 -531 193 -293 C
ATOM 1281 CB ALA A 313 10.636 -77.323 -78.512 1.00 43.37 C
ANISOU 1281 CB ALA A 313 5238 3208 8031 -616 56 -293 C
ATOM 1282 C ALA A 313 8.966 -78.652 -79.806 1.00 46.31 C
ANISOU 1282 C ALA A 313 6165 4004 6331 -644 366 -45 C
ATOM 1283 O ALA A 313 9.409 -78.861 -80.936 1.00 54.57 O
ANISOU 1283 O ALA A 313 7254 5065 7254 -643 406 -406 O
ATOM 1284 N TYR A 314 7.688 -78.465 -79.564 1.00 44.11 N
ANISOU 1284 N TYR A 314 6026 3776 6959 -539 201 -25 N
ATOM 1285 CA TYR A 314 6.729 -78.469 -80.639 1.00 51.97 C
ANISOU 1285 CA TYR A 314 7257 4843 7645 -607 340 293 C
ATOM 1286 CB TYR A 314 6.349 -79.905 -80.989 1.00 47.50 C
ANISOU 1286 CB TYR A 314 6967 4636 6445 -587 559 352 C
ATOM 1287 CG TYR A 314 5.843 -80.707 -79.831 1.00 46.11 C
ANISOU 1287 CG TYR A 314 6879 4707 5933 -435 398 -2 C
ATOM 1288 CD1 TYR A 314 6.712 -81.297 -78.958 1.00 37.13 C
ANISOU 1288 CD1 TYR A 314 5639 3647 4820 -370 359 -235 C
ATOM 1289 CE1 TYR A 314 6.258 -82.024 -77.900 1.00 40.74 C
ANISOU 1289 CE1 TYR A 314 6173 4353 4953 -256 200 -513 C
ATOM 1290 CZ TYR A 314 4.933 -82.164 -77.718 1.00 44.45 C
ANISOU 1290 CZ TYR A 314 6810 5015 5063 -211 94 -575 C
ATOM 1291 OH TYR A 314 4.501 -82.879 -76.688 1.00 40.93 O
ANISOU 1291 OH TYR A 314 6422 4852 4275 -129 -58 -817 O
ATOM 1292 CE2 TYR A 314 4.038 -81.598 -78.565 1.00 35.48 C
ANISOU 1292 CE2 TYR A 314 5770 3806 3904 -259 136 -378 C
ATOM 1293 CD2 TYR A 314 4.494 -80.876 -79.621 1.00 36.48 C
ANISOU 1293 CD2 TYR A 314 5833 3665 4363 -367 279 -86 C
ATOM 1294 C TYR A 314 5.477 -77.671 -80.361 1.00 52.57 C
ANISOU 1294 C TYR A 314 7377 4854 7742 -524 91 184 C
ATOM 1295 O TYR A 314 5.102 -77.476 -79.246 1.00 58.84 O
ANISOU 1295 O TYR A 314 8084 5687 8584 -378 -167 -205 O
ATOM 1296 N GLN A 315 4.813 -77.242 -81.416 1.00 78.48 N
ANISOU 1296 N GLN A 315 12340 6281 11200 1199 -1498 -400 N
ATOM 1297 CA GLN A 315 3.437 -76.773 -81.353 1.00 82.66 C
ANISOU 1297 CA GLN A 315 12853 6562 11992 1625 -1833 -279 C
ATOM 1298 CB GLN A 315 3.315 -75.315 -81.780 1.00 83.38 C
ANISOU 1298 CB GLN A 315 13620 6228 11830 1723 -1757 -56 C

ATOM 1299 CG GLN A 315 4.312 -74.862 -82.822 1.00 92.81 C
ANISOU 1299 CG GLN A 315 15444 7359 12459 1471 -1586 29 C
ATOM 1300 CD GLN A 315 3.692 -74.009 -83.911 1.00100.51 C
ANISOU 1300 CD GLN A 315 17125 7915 13148 1707 -1728 281 C
ATOM 1301 OE1 GLN A 315 2.573 -74.252 -84.334 1.00104.15 O
ANISOU 1301 OE1 GLN A 315 17605 8249 13719 2135 -2186 407 O
ATOM 1302 NE2 GLN A 315 4.434 -73.016 -84.385 1.00100.46 N
ANISOU 1302 NE2 GLN A 315 17708 7693 12771 1427 -1336 353 N
ATOM 1303 C GLN A 315 2.566 -77.648 -82.250 1.00 92.39 C
ANISOU 1303 C GLN A 315 13930 7932 13242 1924 -2368 -262 C
ATOM 1304 O GLN A 315 2.979 -77.990 -83.337 1.00 99.61 O
ANISOU 1304 O GLN A 315 15145 8925 13778 1857 -2492 -223 O
ATOM 1305 N GLU A 316 1.380 -78.034 -81.796 1.00 90.84 N
ANISOU 1305 N GLU A 316 13264 7769 13483 2228 -2668 -305 N
ATOM 1306 CA GLU A 316 0.488 -78.789 -82.653 1.00 86.85 C
ANISOU 1306 CA GLU A 316 12586 7385 13027 2517 -3204 -291 C
ATOM 1307 CB GLU A 316 -0.433 -79.685 -81.856 1.00 81.04 C
ANISOU 1307 CB GLU A 316 11087 6995 12709 2531 -3240 -459 C
ATOM 1308 CG GLU A 316 0.226 -80.498 -80.781 1.00 76.25 C
ANISOU 1308 CG GLU A 316 10098 6686 12187 2314 -3180 -685 C
ATOM 1309 CD GLU A 316 -0.679 -81.571 -80.240 1.00 81.39 C
ANISOU 1309 CD GLU A 316 10104 7675 13145 2186 -3040 -844 C
ATOM 1310 OE1 GLU A 316 -1.681 -81.883 -80.893 1.00 82.49 O
ANISOU 1310 OE1 GLU A 316 10041 7941 13360 2291 -3228 -829 O
ATOM 1311 OE2 GLU A 316 -0.386 -82.111 -79.167 1.00 84.72 O
ANISOU 1311 OE2 GLU A 316 10278 8213 13698 1952 -2720 -982 O
ATOM 1312 C GLU A 316 -0.366 -77.791 -83.360 1.00 92.02 C
ANISOU 1312 C GLU A 316 13622 7805 13535 2825 -3480 -54 C
ATOM 1313 O GLU A 316 -1.096 -77.062 -82.733 1.00 95.16 O
ANISOU 1313 O GLU A 316 13834 8162 14160 2954 -3383 8 O
ATOM 1314 N PRO A 317 -0.289 -77.772 -84.674 1.00 99.97 N
ANISOU 1314 N PRO A 317 15164 8694 14125 2909 -3774 81 N
ATOM 1315 CA PRO A 317 -0.969 -76.740 -85.454 1.00110.29 C
ANISOU 1315 CA PRO A 317 16878 9797 15230 3149 -3965 312 C
ATOM 1316 CB PRO A 317 -0.519 -77.025 -86.886 1.00112.90 C
ANISOU 1316 CB PRO A 317 17808 10049 15039 3138 -4246 416 C
ATOM 1317 CG PRO A 317 -0.242 -78.494 -86.899 1.00110.25 C
ANISOU 1317 CG PRO A 317 17070 10076 14746 2955 -4326 208 C
ATOM 1318 CD PRO A 317 0.342 -78.786 -85.534 1.00103.75 C
ANISOU 1318 CD PRO A 317 15752 9415 14254 2693 -3853 4 C
ATOM 1319 C PRO A 317 -2.477 -76.882 -85.353 1.00115.18 C
ANISOU 1319 C PRO A 317 16957 10648 16158 3381 -4236 303 C
ATOM 1320 O PRO A 317 -3.004 -77.992 -85.440 1.00114.75 O
ANISOU 1320 O PRO A 317 16448 10917 16233 3357 -4463 159 O
ATOM 1321 N ALA A 318 -3.162 -75.762 -85.149 1.00119.53 N
ANISOU 1321 N ALA A 318 17573 11021 16821 3581 -4170 451 N
ATOM 1322 CA ALA A 318 -4.611 -75.752 -85.183 1.00119.96 C
ANISOU 1322 CA ALA A 318 17214 11238 17127 3819 -4414 478 C
ATOM 1323 CB ALA A 318 -5.144 -74.414 -84.712 1.00111.78 C
ANISOU 1323 CB ALA A 318 16268 9955 16250 4024 -4215 642 C
ATOM 1324 C ALA A 318 -5.050 -76.031 -86.614 1.00132.46 C
ANISOU 1324 C ALA A 318 19062 12866 18403 3957 -4900 570 C
ATOM 1325 O ALA A 318 -6.016 -76.756 -86.854 1.00138.36 O
ANISOU 1325 O ALA A 318 19398 13877 19296 4023 -5182 494 O
ATOM 1326 N ASP A 319 -4.316 -75.458 -87.562 1.00139.08 N
ANISOU 1326 N ASP A 319 20628 13433 18783 3964 -4963 730 N
ATOM 1327 CA ASP A 319 -4.604 -75.619 -88.981 1.00147.58 C
ANISOU 1327 CA ASP A 319 22080 14508 19485 4067 -5395 834 C
ATOM 1328 CB ASP A 319 -3.747 -74.655 -89.808 1.00149.84 C
ANISOU 1328 CB ASP A 319 23260 14420 19252 4051 -5315 1034 C
ATOM 1329 CG ASP A 319 -4.309 -74.412 -91.195 1.00157.47 C
ANISOU 1329 CG ASP A 319 24644 15322 19867 4227 -5737 1190 C
ATOM 1330 OD2 ASP A 319 -3.516 -74.147 -92.124 1.00155.33 O
ANISOU 1330 OD2 ASP A 319 25108 14841 19068 4118 -5734 1292 O
ATOM 1331 OD1 ASP A 319 -5.547 -74.480 -91.357 1.00164.57 O
ANISOU 1331 OD1 ASP A 319 25149 16373 21005 4457 -6050 1209 O
ATOM 1332 C ASP A 319 -4.368 -77.052 -89.456 1.00152.05 C
ANISOU 1332 C ASP A 319 22482 15356 19934 3883 -5615 665 C
ATOM 1333 O ASP A 319 -3.304 -77.628 -89.216 1.00152.57 O
ANISOU 1333 O ASP A 319 22637 15443 19891 3648 -5418 560 O
ATOM 1334 N ASP A 320 -5.376 -77.619 -90.117 1.00153.32 N
ANISOU 1334 N ASP A 320 22404 15724 20126 3988 -6005 641 N
ATOM 1335 CA ASP A 320 -5.254 -78.896 -90.823 1.00146.21 C
ANISOU 1335 CA ASP A 320 21461 15053 19040 3825 -6248 510 C
ATOM 1336 CB ASP A 320 -4.260 -78.773 -91.990 1.00147.85 C
ANISOU 1336 CB ASP A 320 22484 15053 18638 3729 -6334 629 C
ATOM 1337 CG ASP A 320 -4.875 -78.151 -93.230 1.00152.59 C
ANISOU 1337 CG ASP A 320 23549 15507 18922 3915 -6686 819 C
ATOM 1338 OD2 ASP A 320 -4.107 -77.783 -94.143 1.00153.12 O
ANISOU 1338 OD2 ASP A 320 24366 15345 18468 3840 -6690 945 O
ATOM 1339 OD1 ASP A 320 -6.118 -78.047 -93.300 1.00156.73 O
ANISOU 1339 OD1 ASP A 320 23701 16144 19704 4122 -6940 843 O
ATOM 1340 C ASP A 320 -4.759 -79.929 -89.813 1.00132.77 C
ANISOU 1340 C ASP A 320 19246 13616 17584 3584 -5853 259 C
ATOM 1341 O ASP A 320 -5.434 -80.246 -88.830 1.00123.63 O
ANISOU 1341 O ASP A 320 17438 12703 16831 3565 -5998 107 O
ATOM 1342 N SER A 321 -3.571 -80.434 -90.063 1.00130.82 N
ANISOU 1342 N SER A 321 19344 13304 17059 3391 -5889 227 N
ATOM 1343 CA SER A 321 -3.034 -81.747 -89.714 1.00128.83 C
ANISOU 1343 CA SER A 321 18757 13306 16887 3161 -5789 8 C
ATOM 1344 CB SER A 321 -1.514 -81.762 -89.887 1.00120.53 C
ANISOU 1344 CB SER A 321 18232 12090 15472 3001 -5595 51 C
ATOM 1345 OG SER A 321 -0.960 -82.971 -89.394 1.00110.50 O
ANISOU 1345 OG SER A 321 16582 11082 14319 2792 -5451 -165 O
ATOM 1346 C SER A 321 -3.379 -82.273 -88.325 1.00127.96 C
ANISOU 1346 C SER A 321 17888 13424 17306 3077 -5524 -200 C
ATOM 1347 O SER A 321 -3.604 -81.510 -87.382 1.00125.70 O
ANISOU 1347 O SER A 321 17394 13052 17315 3145 -5290 -174 O
ATOM 1348 N SER A 322 -3.416 -83.597 -88.224 1.00127.79 N
ANISOU 1348 N SER A 322 17502 13686 17368 2902 -5526 -403 N
ATOM 1349 CA SER A 322 -3.370 -84.265 -86.937 1.00125.23 C
ANISOU 1349 CA SER A 322 16592 13562 17427 2736 -5193 -613 C
ATOM 1350 CB SER A 322 -4.329 -85.449 -86.871 1.00128.30 C
ANISOU 1350 CB SER A 322 16528 14228 17990 2634 -5236 -781 C
ATOM 1351 OG SER A 322 -5.262 -85.264 -85.819 1.00130.27 O
ANISOU 1351 OG SER A 322 16328 14544 18623 2644 -5043 -836 O
ATOM 1352 C SER A 322 -1.928 -84.692 -86.697 1.00114.89 C
ANISOU 1352 C SER A 322 15414 12253 15984 2572 -4992 -687 C
ATOM 1353 O SER A 322 -1.412 -85.622 -87.320 1.00114.32 O
ANISOU 1353 O SER A 322 15461 12308 15666 2456 -5089 -760 O
ATOM 1354 N PHE A 323 -1.299 -83.965 -85.788 1.00104.42 N
ANISOU 1354 N PHE A 323 14075 10778 14821 2565 -4693 -662 N
ATOM 1355 CA PHE A 323 0.123 -84.024 -85.526 1.00 92.32 C
ANISOU 1355 CA PHE A 323 12725 9228 13124 2328 -4312 -707 C
ATOM 1356 CB PHE A 323 0.442 -82.860 -84.583 1.00 86.87 C
ANISOU 1356 CB PHE A 323 12071 8324 12612 2307 -3944 -643 C
ATOM 1357 CG PHE A 323 1.744 -82.973 -83.863 1.00 84.24 C
ANISOU 1357 CG PHE A 323 11684 8096 12228 1945 -3391 -759 C
ATOM 1358 CD1 PHE A 323 2.919 -82.534 -84.453 1.00 81.08 C
ANISOU 1358 CD1 PHE A 323 11794 7624 11388 1697 -3085 -687 C
ATOM 1359 CE1 PHE A 323 4.123 -82.615 -83.774 1.00 67.68 C
ANISOU 1359 CE1 PHE A 323 10004 6048 9665 1362 -2588 -796 C
ATOM 1360 CZ PHE A 323 4.154 -83.130 -82.481 1.00 70.89 C
ANISOU 1360 CZ PHE A 323 9836 6632 10467 1283 -2411 -967 C
ATOM 1361 CE2 PHE A 323 2.978 -83.558 -81.879 1.00 74.76 C
ANISOU 1361 CE2 PHE A 323 9862 7166 11377 1525 -2698 -1036 C
ATOM 1362 CD2 PHE A 323 1.786 -83.474 -82.569 1.00 78.37 C
ANISOU 1362 CD2 PHE A 323 10384 7515 11878 1849 -3174 -938 C
ATOM 1363 C PHE A 323 0.519 -85.375 -84.940 1.00 85.93 C
ANISOU 1363 C PHE A 323 11443 8743 12464 2111 -4135 -952 C
ATOM 1364 O PHE A 323 -0.255 -85.999 -84.218 1.00 94.92 O
ANISOU 1364 O PHE A 323 12062 10045 13958 2138 -4179 -1092 O
ATOM 1365 N SER A 324 1.712 -85.845 -85.280 1.00 67.43 N
ANISOU 1365 N SER A 324 9311 6518 9791 1822 -3826 -1010 N
ATOM 1366 CA SER A 324 2.182 -87.103 -84.731 1.00 59.71 C
ANISOU 1366 CA SER A 324 7925 5829 8933 1631 -3631 -1229 C
ATOM 1367 CB SER A 324 2.670 -88.044 -85.824 1.00 57.13 C
ANISOU 1367 CB SER A 324 7854 5644 8210 1499 -3686 -1273 C
ATOM 1368 OG SER A 324 2.801 -89.359 -85.318 1.00 61.93 O
ANISOU 1368 OG SER A 324 8032 6516 8984 1395 -3599 -1483 O
ATOM 1369 C SER A 324 3.291 -86.853 -83.732 1.00 68.42 C
ANISOU 1369 C SER A 324 8901 6975 10118 1389 -3102 -1296 C
ATOM 1370 O SER A 324 4.389 -86.437 -84.100 1.00 78.78 O
ANISOU 1370 O SER A 324 10574 8248 11112 1183 -2791 -1240 O
ATOM 1371 N LEU A 325 2.993 -87.103 -82.464 1.00 72.69 N
ANISOU 1371 N LEU A 325 9322 7600 11087 1401 -3002 -1422 N
ATOM 1372 CA LEU A 325 3.979 -86.960 -81.410 1.00 68.75 C
ANISOU 1372 CA LEU A 325 8262 7169 10691 1168 -2541 -1500 C
ATOM 1373 CB LEU A 325 3.331 -87.207 -80.050 1.00 58.12 C
ANISOU 1373 CB LEU A 325 6381 5868 9833 1235 -2527 -1626 C
ATOM 1374 CG LEU A 325 4.100 -86.672 -78.850 1.00 58.26 C
ANISOU 1374 CG LEU A 325 6273 5869 9994 1036 -2108 -1663 C
ATOM 1375 CD1 LEU A 325 4.480 -85.235 -79.126 1.00 53.01 C
ANISOU 1375 CD1 LEU A 325 6057 4951 9135 994 -1956 -1486 C
ATOM 1376 CD2 LEU A 325 3.250 -86.769 -77.596 1.00 55.50 C
ANISOU 1376 CD2 LEU A 325 5593 5558 9937 997 -2039 -1715 C
ATOM 1377 C LEU A 325 5.078 -87.981 -81.669 1.00 61.37 C
ANISOU 1377 C LEU A 325 7708 6481 9528 935 -2312 -1615 C
ATOM 1378 O LEU A 325 6.270 -87.706 -81.527 1.00 57.75 O
ANISOU 1378 O LEU A 325 7702 6006 9635 1378 -2536 -1936 -1614 O
ATOM 1379 N SER A 326 4.675 -89.168 -82.055 1.00 57.01 N
ANISOU 1379 N SER A 326 6597 6089 8974 1004 -2541 -1717 N
ATOM 1380 CA SER A 326 5.605 -90.218 -82.325 1.00 58.67 C
ANISOU 1380 CA SER A 326 6789 6521 8981 831 -2353 -1831 C
ATOM 1381 CB SER A 326 4.863 -91.496 -82.546 1.00 63.95 C
ANISOU 1381 CB SER A 326 7302 7311 9685 946 -2675 -1937 C
ATOM 1382 OG SER A 326 4.079 -91.363 -83.677 1.00 78.93 O
ANISOU 1382 OG SER A 326 8856 9234 11900 999 -2516 -1957 O
ATOM 1383 C SER A 326 6.537 -89.917 -83.473 1.00 59.11 C
ANISOU 1383 C SER A 326 7350 6533 8578 681 -2172 -1734 C
ATOM 1384 O SER A 326 7.683 -90.242 -83.390 1.00 55.11 O
ANISOU 1384 O SER A 326 6830 6163 7947 473 -1805 -1796 O
ATOM 1385 N GLN A 327 6.068 -89.296 -84.541 1.00 61.56 N
ANISOU 1385 N GLN A 327 8105 6652 8635 789 -2430 -1585 N
ATOM 1386 CA GLN A 327 6.942 -88.928 -85.642 1.00 58.07 C
ANISOU 1386 CA GLN A 327 8208 6130 7727 641 -2262 -1489 C
ATOM 1387 CB GLN A 327 6.142 -88.368 -86.818 1.00 60.68 C
ANISOU 1387 CB GLN A 327 9025 6236 7793 810 -2653 -1323 C
ATOM 1388 CG GLN A 327 5.491 -89.452 -87.653 1.00 56.58 C
ANISOU 1388 CG GLN A 327 8536 5816 7147 904 -3015 -1380 C

ATOM 1389 CD GLN A 327 6.488 -90.527 -88.072 1.00 61.98 C
ANISOU 1389 CD GLN A 327 9272 6687 7591 691 -2731 -1510 C
ATOM 1390 OE1 GLN A 327 7.400 -90.268 -88.859 1.00 74.76 O
ANISOU 1390 OE1 GLN A 327 11335 8241 8827 525 -2482 -1455 O
ATOM 1391 NE2 GLN A 327 6.327 -91.736 -87.533 1.00 55.10 N
ANISOU 1391 NE2 GLN A 327 7954 6036 6947 696 -2742 -1686 N
ATOM 1392 C GLN A 327 7.970 -87.917 -85.169 1.00 56.30 C
ANISOU 1392 C GLN A 327 8105 5832 7456 443 -1833 -1435 C
ATOM 1393 O GLN A 327 9.128 -87.939 -85.582 1.00 56.11 O
ANISOU 1393 O GLN A 327 8297 5865 7156 217 -1491 -1450 O
ATOM 1394 N GLU A 328 7.530 -87.042 -84.276 1.00 47.72 N
ANISOU 1394 N GLU A 328 6865 4618 6649 519 -1841 -1384 N
ATOM 1395 CA GLU A 328 8.375 -85.995 -83.731 1.00 65.69 C
ANISOU 1395 CA GLU A 328 9256 6801 8903 323 -1458 -1334 C
ATOM 1396 CB GLU A 328 7.537 -85.047 -82.880 1.00 53.31 C
ANISOU 1396 CB GLU A 328 7575 5035 7646 478 -1566 -1262 C
ATOM 1397 CG GLU A 328 8.225 -83.757 -82.563 1.00 62.79 C
ANISOU 1397 CG GLU A 328 9056 6054 8749 296 -1228 -1172 C
ATOM 1398 CD GLU A 328 8.302 -82.845 -83.767 1.00 85.08 C
ANISOU 1398 CD GLU A 328 12553 8611 11163 310 -1268 -991 C
ATOM 1399 OE1 GLU A 328 9.137 -81.911 -83.750 1.00 85.59 O
ANISOU 1399 OE1 GLU A 328 12936 8549 11035 83 -921 -934 O
ATOM 1400 OE2 GLU A 328 7.525 -83.063 -84.728 1.00 95.00 O
ANISOU 1400 OE2 GLU A 328 14035 9783 12278 535 -1648 -909 O
ATOM 1401 C GLU A 328 9.492 -86.593 -82.879 1.00 63.08 C
ANISOU 1401 C GLU A 328 8547 6737 8684 75 -1064 -1491 C
ATOM 1402 O GLU A 328 10.668 -86.241 -83.013 1.00 59.40 O
ANISOU 1402 O GLU A 328 8252 6311 8006 -181 -695 -1490 O
ATOM 1403 N VAL A 329 9.108 -87.498 -81.990 1.00 54.87 N
ANISOU 1403 N VAL A 329 6988 5879 7981 153 -1150 -1627 N
ATOM 1404 CA VAL A 329 10.066 -88.135 -81.111 1.00 53.12 C
ANISOU 1404 CA VAL A 329 6382 5912 7889 -38 -833 -1769 C
ATOM 1405 CB VAL A 329 9.380 -89.004 -80.063 1.00 54.00 C
ANISOU 1405 CB VAL A 329 5972 6153 8391 90 -981 -1900 C
ATOM 1406 CG1 VAL A 329 10.420 -89.658 -79.161 1.00 32.72 C
ANISOU 1406 CG1 VAL A 329 2914 3716 5803 -96 -668 -2032 C
ATOM 1407 CG2 VAL A 329 8.426 -88.164 -79.248 1.00 35.27 C
ANISOU 1407 CG2 VAL A 329 3498 3587 6317 213 -1116 -1850 C
ATOM 1408 C VAL A 329 11.014 -88.986 -81.930 1.00 52.84 C
ANISOU 1408 C VAL A 329 6447 6060 7568 -162 -663 -1829 C
ATOM 1409 O VAL A 329 12.223 -89.004 -81.694 1.00 62.39 O
ANISOU 1409 O VAL A 329 7584 7419 8702 -386 -300 -1878 O
ATOM 1410 N LEU A 330 10.478 -89.670 -82.909 1.00 49.00 N
ANISOU 1410 N LEU A 330 6132 5563 6924 -19 -925 -1828 N
ATOM 1411 CA LEU A 330 11.275 -90.514 -83.735 1.00 54.01 C
ANISOU 1411 CA LEU A 330 6893 6344 7284 -114 -771 -1891 C
ATOM 1412 CB LEU A 330 10.408 -91.383 -84.626 1.00 54.45 C
ANISOU 1412 CB LEU A 330 7089 6373 7225 66 -1136 -1905 C
ATOM 1413 CG LEU A 330 9.927 -92.679 -84.014 1.00 47.37 C
ANISOU 1413 CG LEU A 330 5736 5657 6604 180 -1278 -2058 C
ATOM 1414 CD1 LEU A 330 8.817 -93.282 -84.823 1.00 40.73 C
ANISOU 1414 CD1 LEU A 330 5047 4751 5676 351 -1704 -2058 C
ATOM 1415 CD2 LEU A 330 11.042 -93.658 -83.827 1.00 37.71 C
ANISOU 1415 CD2 LEU A 330 4344 4664 5321 48 -930 -2184 C
ATOM 1416 C LEU A 330 12.286 -89.772 -84.546 1.00 60.61 C
ANISOU 1416 C LEU A 330 8188 7093 7749 -318 -478 -1805 C
ATOM 1417 O LEU A 330 13.396 -90.220 -84.696 1.00 57.78 O
ANISOU 1417 O LEU A 330 7807 6896 7251 -494 -140 -1877 O
ATOM 1418 N ARG A 331 11.901 -88.630 -85.074 1.00 60.96 N
ANISOU 1418 N ARG A 331 8657 6870 7636 -289 -600 -1651 N
ATOM 1419 CA ARG A 331 12.796 -87.887 -85.913 1.00 56.55 C
ANISOU 1419 CA ARG A 331 8602 6178 6708 -492 -323 -1561 C
ATOM 1420 CB ARG A 331 12.078 -86.673 -86.468 1.00 67.64 C
ANISOU 1420 CB ARG A 331 10456 7250 7993 -389 -540 -1379 C
ATOM 1421 CG ARG A 331 12.956 -85.480 -86.800 1.00 81.49 C
ANISOU 1421 CG ARG A 331 12809 8814 9338 -599 -263 -1275 C
ATOM 1422 CD ARG A 331 12.123 -84.291 -87.225 1.00 85.89 C
ANISOU 1422 CD ARG A 331 13751 9036 9848 -489 -434 -1096 C
ATOM 1423 NE ARG A 331 12.252 -83.133 -86.353 1.00 86.24 N
ANISOU 1423 NE ARG A 331 13631 9046 10091 -641 -151 -1097 N
ATOM 1424 CZ ARG A 331 13.405 -82.620 -85.942 1.00 88.99 C
ANISOU 1424 CZ ARG A 331 14228 9350 10233 -955 286 -1091 C
ATOM 1425 NH1 ARG A 331 14.552 -83.174 -86.290 1.00 95.44 N
ANISOU 1425 NH1 ARG A 331 15459 10150 10655 -1139 505 -1087 N
ATOM 1426 NH2 ARG A 331 13.409 -81.554 -85.160 1.00 77.36 N
ANISOU 1426 NH2 ARG A 331 12601 7849 8944 -1105 518 -1099 N
ATOM 1427 C ARG A 331 13.998 -87.503 -85.080 1.00 69.23 C
ANISOU 1427 C ARG A 331 9979 7930 8395 -768 147 -1628 C
ATOM 1428 O ARG A 331 15.111 -87.606 -85.529 1.00 76.31 O
ANISOU 1428 O ARG A 331 11007 8924 9062 -987 497 -1671 O
ATOM 1429 N HIS A 332 13.775 -87.057 -83.857 1.00 66.23 N
ANISOU 1429 N HIS A 332 9246 7572 8346 -766 157 -1643 N
ATOM 1430 CA HIS A 332 14.851 -86.724 -82.964 1.00 59.31 C
ANISOU 1430 CA HIS A 332 8107 6854 7574 -1034 553 -1712 C
ATOM 1431 CB HIS A 332 14.317 -86.150 -81.685 1.00 42.49 C
ANISOU 1431 CB HIS A 332 5715 4657 5772 -1008 490 -1699 C
ATOM 1432 CG HIS A 332 13.906 -84.728 -81.793 1.00 60.89 C
ANISOU 1432 CG HIS A 332 8476 6649 8008 -991 431 -1547 C
ATOM 1433 ND1 HIS A 332 12.862 -84.315 -82.580 1.00 70.24 N
ANISOU 1433 ND1 HIS A 332 9994 7582 9113 -727 74 -1425 N
ATOM 1434 CE1 HIS A 332 12.730 -83.012 -82.485 1.00 67.36 C
ANISOU 1434 CE1 HIS A 332 9987 6931 8677 -748 112 -1295 C
ATOM 1435 NE2 HIS A 332 13.652 -82.567 -81.662 1.00 62.85 N
ANISOU 1435 NE2 HIS A 332 9338 6416 8125 -1045 494 -1339 N
ATOM 1436 CD2 HIS A 332 14.397 -83.620 -81.210 1.00 54.31 C
ANISOU 1436 CD2 HIS A 332 7810 5682 7143 -1203 685 -1495 C
ATOM 1437 C HIS A 332 15.620 -87.942 -82.617 1.00 65.45 C
ANISOU 1437 C HIS A 332 8431 7973 8463 -1092 724 -1869 C
ATOM 1438 O HIS A 332 16.810 -87.905 -82.478 1.00 67.77 O
ANISOU 1438 O HIS A 332 8631 8437 8682 -1335 1093 -1928 O
ATOM 1439 N LEU A 333 14.897 -89.026 -82.413 1.00 74.14 N
ANISOU 1439 N LEU A 333 9248 9171 9751 -863 453 -1938 N
ATOM 1440 CA LEU A 333 15.481 -90.283 -81.956 1.00 72.04 C
ANISOU 1440 CA LEU A 333 8543 9204 9626 -862 573 -2082 C
ATOM 1441 CB LEU A 333 14.388 -91.334 -81.756 1.00 77.23 C
ANISOU 1441 CB LEU A 333 8982 9884 10476 -595 220 -2142 C
ATOM 1442 CG LEU A 333 14.047 -91.758 -80.332 1.00 75.86 C
ANISOU 1442 CG LEU A 333 8299 9832 10694 -523 144 -2229 C
ATOM 1443 CD1 LEU A 333 13.263 -93.058 -80.359 1.00 68.32 C
ANISOU 1443 CD1 LEU A 333 7162 8941 9854 -309 -108 -2321 C
ATOM 1444 CD2 LEU A 333 15.314 -91.918 -79.519 1.00 78.69 C
ANISOU 1444 CD2 LEU A 333 8326 10434 11141 -712 488 -2305 C
ATOM 1445 C LEU A 333 16.506 -90.842 -82.930 1.00 71.32 C
ANISOU 1445 C LEU A 333 8613 9236 9251 -976 845 -2126 C
ATOM 1446 O LEU A 333 17.533 -91.392 -82.531 1.00 72.07 O
ANISOU 1446 O LEU A 333 8388 9580 9415 -1085 1126 -2222 O
ATOM 1447 N ARG A 334 16.208 -90.712 -84.215 1.00 68.75 N
ANISOU 1447 N ARG A 334 8787 8728 8605 -941 756 -2054 N
ATOM 1448 CA ARG A 334 16.986 -91.378 -85.244 1.00 64.04 C
ANISOU 1448 CA ARG A 334 8394 8211 7727 -1017 984 -2103 C
ATOM 1449 CB ARG A 334 16.163 -91.522 -86.524 1.00 49.46 C
ANISOU 1449 CB ARG A 334 7065 6146 5580 -891 710 -2031 C
ATOM 1450 CG ARG A 334 15.062 -92.561 -86.366 1.00 54.21 C
ANISOU 1450 CG ARG A 334 7465 6781 6349 -634 316 -2083 C
ATOM 1451 CD ARG A 334 13.975 -92.462 -87.424 1.00 57.75 C
ANISOU 1451 CD ARG A 334 8382 7000 6560 -498 -73 -1991 C
ATOM 1452 NE ARG A 334 13.199 -93.699 -87.494 1.00 56.49 N
ANISOU 1452 NE ARG A 334 8054 6921 6489 -320 -356 -2080 N
ATOM 1453 CZ ARG A 334 11.980 -93.808 -88.014 1.00 59.56 C
ANISOU 1453 CZ ARG A 334 8637 7174 6819 -158 -802 -2031 C
ATOM 1454 NH1 ARG A 334 11.366 -92.741 -88.513 1.00 65.55 N
ANISOU 1454 NH1 ARG A 334 9767 7703 7438 -114 -1041 -1878 N
ATOM 1455 NH2 ARG A 334 11.369 -94.987 -88.030 1.00 54.39 N
ANISOU 1455 NH2 ARG A 334 7806 6614 6245 -40 -1014 -2137 N
ATOM 1456 C ARG A 334 18.330 -90.702 -85.487 1.00 85.34 C
ANISOU 1456 C ARG A 334 11215 10962 10248 -1313 1449 -2104 C
ATOM 1457 O ARG A 334 18.599 -90.201 -86.578 1.00 87.32 O
ANISOU 1457 O ARG A 334 11979 11049 10152 -1431 1581 -2042 O
ATOM 1458 N GLN A 335 19.149 -90.681 -84.433 1.00 99.41 N
ANISOU 1458 N GLN A 335 12525 12975 12272 -1441 1688 -2178 N
ATOM 1459 CA GLN A 335 20.533 -90.204 -84.463 1.00101.72 C
ANISOU 1459 CA GLN A 335 12776 13402 12471 -1740 2148 -2216 C
ATOM 1460 CB GLN A 335 20.625 -88.732 -84.877 1.00 96.70 C
ANISOU 1460 CB GLN A 335 12614 12522 11606 -1959 2269 -2109 C
ATOM 1461 CG GLN A 335 19.533 -87.844 -84.316 1.00 92.69 C
ANISOU 1461 CG GLN A 335 12220 11781 11215 -1861 1949 -1999 C
ATOM 1462 CD GLN A 335 18.812 -87.082 -85.410 1.00 97.37 C
ANISOU 1462 CD GLN A 335 13490 12016 11489 -1807 1783 -1858 C
ATOM 1463 OE1 GLN A 335 18.806 -85.853 -85.425 1.00 97.60 O
ANISOU 1463 OE1 GLN A 335 13843 11834 11405 -1946 1862 -1764 O
ATOM 1464 NE2 GLN A 335 18.211 -87.812 -86.346 1.00 99.42 N
ANISOU 1464 NE2 GLN A 335 13991 12199 11584 -1609 1552 -1840 N
ATOM 1465 C GLN A 335 21.198 -90.404 -83.104 1.00101.48 C
ANISOU 1465 C GLN A 335 12117 13664 12776 -1815 2281 -2304 C
ATOM 1466 O GLN A 335 21.642 -91.502 -82.776 1.00100.12 O
ANISOU 1466 O GLN A 335 11547 13741 12754 -1722 2346 -2404 O
TER 1467 GLN A 335
HETATM 1468 OAD DRG C 1 7.647 -76.692 -62.085 1.00 44.74 O
HETATM 1469 CAQ DRG C 1 8.003 -77.711 -61.497 1.00 55.27 C
HETATM 1470 CAS DRG C 1 7.089 -78.705 -61.199 1.00 51.55 C
HETATM 1471 CAJ DRG C 1 5.760 -78.535 -61.568 1.00 51.37 C
HETATM 1472 CAH DRG C 1 4.840 -79.541 -61.279 1.00 56.00 C
HETATM 1473 CAN DRG C 1 5.237 -80.711 -60.627 1.00 46.44 C
HETATM 1474 CAA DRG C 1 4.300 -81.703 -60.347 1.00 26.68 C
HETATM 1475 CAO DRG C 1 6.574 -80.882 -60.258 1.00 45.72 C
HETATM 1476 CAB DRG C 1 6.990 -82.043 -59.604 1.00 30.41 C
HETATM 1477 CAT DRG C 1 7.483 -79.863 -60.537 1.00 43.76 C
HETATM 1478 OAL DRG C 1 8.781 -80.059 -60.194 1.00 36.28 O
HETATM 1479 CAU DRG C 1 9.705 -79.109 -60.509 1.00 47.85 C
HETATM 1480 CAR DRG C 1 9.328 -77.933 -61.155 1.00 57.72 C
HETATM 1481 CAI DRG C 1 10.309 -76.990 -61.463 1.00 52.34 C
HETATM 1482 CAF DRG C 1 11.633 -77.232 -61.107 1.00 41.69 C
HETATM 1483 CAG DRG C 1 11.999 -78.407 -60.453 1.00 34.93 C
HETATM 1484 CAP DRG C 1 11.022 -79.346 -60.145 1.00 47.31 C
HETATM 1485 CAK DRG C 1 11.361 -80.525 -59.495 1.00 48.85 C
HETATM 1486 CAM DRG C 1 11.257 -81.740 -60.416 1.00 49.85 C
HETATM 1487 OAE DRG C 1 10.890 -81.531 -61.601 1.00 37.91 O
HETATM 1488 OAC DRG C 1 11.567 -82.840 -59.898 1.00 44.52 O
ATOM 1490 N SER B 154 8.907 -62.145 -63.562 1.00 35.71 N
ANISOU 1490 N SER B 154 4521 4617 4430 -347 455 -551 N

ATOM 1491 CA SER B 154 9.833 -62.192 -62.435 1.00 31.79 C
ANISOU 1491 CA SER B 154 4035 3980 4063 -129 429 -586 C
ATOM 1492 CB SER B 154 9.235 -61.519 -61.198 1.00 35.80 C
ANISOU 1492 CB SER B 154 4487 4624 4491 140 301 -507 C
ATOM 1493 OG SER B 154 9.521 -62.261 -60.029 1.00 31.17 O
ANISOU 1493 OG SER B 154 3897 3982 3964 270 328 -489 O
ATOM 1494 C SER B 154 10.256 -63.615 -62.083 1.00 39.11 C
ANISOU 1494 C SER B 154 4993 4785 5082 -197 562 -605 C
ATOM 1495 O SER B 154 9.475 -64.561 -62.177 1.00 39.55 O
ANISOU 1495 O SER B 154 5044 4922 5062 -334 640 -550 O
ATOM 1496 N VAL B 155 11.502 -63.749 -61.653 1.00 45.14 N
ANISOU 1496 N VAL B 155 5788 5352 6013 -99 579 -674 N
ATOM 1497 CA VAL B 155 12.072 -65.036 -61.294 1.00 34.34 C
ANISOU 1497 CA VAL B 155 4451 3838 4756 -138 702 -697 C
ATOM 1498 CB VAL B 155 13.593 -64.913 -61.080 1.00 30.21 C
ANISOU 1498 CB VAL B 155 3954 3094 4431 -39 710 -777 C
ATOM 1499 CG1 VAL B 155 14.130 -66.040 -60.217 1.00 23.59 C
ANISOU 1499 CG1 VAL B 155 3126 2129 3708 22 788 -771 C
ATOM 1500 CG2 VAL B 155 14.289 -64.898 -62.412 1.00 23.39 C
ANISOU 1500 CG2 VAL B 155 3138 2116 3634 -221 800 -865 C
ATOM 1501 C VAL B 155 11.395 -65.600 -60.054 1.00 35.98 C
ANISOU 1501 C VAL B 155 4617 4144 4908 -14 680 -604 C
ATOM 1502 O VAL B 155 11.068 -66.786 -59.981 1.00 30.48 O
ANISOU 1502 O VAL B 155 3936 3439 4206 -128 781 -573 O
ATOM 1503 N ALA B 156 11.189 -64.729 -59.076 1.00 37.45 N
ANISOU 1503 N ALA B 156 4757 4422 5048 222 545 -557 N
ATOM 1504 CA ALA B 156 10.560 -65.103 -57.820 1.00 27.62 C
ANISOU 1504 CA ALA B 156 3467 3290 3737 373 513 -463 C
ATOM 1505 CB ALA B 156 10.539 -63.933 -56.889 1.00 33.50 C
ANISOU 1505 CB ALA B 156 4188 4105 4437 645 359 -441 C
ATOM 1506 C ALA B 156 9.138 -65.589 -58.050 1.00 38.88 C
ANISOU 1506 C ALA B 156 4847 4930 4995 244 551 -360 C
ATOM 1507 O ALA B 156 8.670 -66.551 -57.434 1.00 43.76 O
ANISOU 1507 O ALA B 156 5441 5600 5585 227 602 -285 O
ATOM 1508 N HIS B 157 8.448 -64.880 -58.927 1.00 37.71 N
ANISOU 1508 N HIS B 157 4680 4911 4735 153 515 -346 N
ATOM 1509 CA HIS B 157 7.055 -65.140 -59.219 1.00 28.64 C
ANISOU 1509 CA HIS B 157 3473 3990 3418 31 528 -234 C
ATOM 1510 CB HIS B 157 6.568 -64.137 -60.258 1.00 41.84 C
ANISOU 1510 CB HIS B 157 5132 5768 4998 -49 472 -237 C
ATOM 1511 CG HIS B 157 5.092 -64.144 -60.475 1.00 46.26 C
ANISOU 1511 CG HIS B 157 5611 6591 5376 -132 456 -102 C
ATOM 1512 ND1 HIS B 157 4.196 -63.819 -59.488 1.00 47.33 N
ANISOU 1512 ND1 HIS B 157 5655 6934 5395 65 389 20 N
ATOM 1513 CE1 HIS B 157 2.965 -63.908 -59.967 1.00 44.73 C
ANISOU 1513 CE1 HIS B 157 5252 6823 4919 -69 391 139 C
ATOM 1514 NE2 HIS B 157 3.036 -64.268 -61.228 1.00 40.72 N
ANISOU 1514 NE2 HIS B 157 4795 6251 4425 -352 448 94 N
ATOM 1515 CD2 HIS B 157 4.357 -64.425 -61.576 1.00 44.55 C
ANISOU 1515 CD2 HIS B 157 5387 6470 5071 -393 496 -61 C
ATOM 1516 C HIS B 157 6.889 -66.560 -59.754 1.00 36.70 C
ANISOU 1516 C HIS B 157 4531 4956 4456 -233 661 -224 C
ATOM 1517 O HIS B 157 5.980 -67.295 -59.357 1.00 40.73 O
ANISOU 1517 O HIS B 157 4996 5604 4878 -287 685 -111 O
ATOM 1518 N GLY B 158 7.784 -66.943 -60.655 1.00 32.57 N
ANISOU 1518 N GLY B 158 4097 4229 4047 -395 746 -340 N
ATOM 1519 CA GLY B 158 7.754 -68.262 -61.250 1.00 34.69 C
ANISOU 1519 CA GLY B 158 4434 4407 4340 -644 875 -355 C
ATOM 1520 C GLY B 158 8.177 -69.341 -60.268 1.00 39.59 C
ANISOU 1520 C GLY B 158 5071 4911 5060 -575 933 -340 C
ATOM 1521 O GLY B 158 7.650 -70.458 -60.277 1.00 40.37 O
ANISOU 1521 O GLY B 158 5191 5023 5124 -730 1000 -284 O
ATOM 1522 N LEU B 159 9.130 -69.003 -59.407 1.00 32.14 N
ANISOU 1522 N LEU B 159 4119 3852 4240 -347 897 -384 N
ATOM 1523 CA LEU B 159 9.626 -69.934 -58.403 1.00 36.27 C
ANISOU 1523 CA LEU B 159 4652 4259 4870 -258 940 -367 C
ATOM 1524 CB LEU B 159 10.875 -69.386 -57.715 1.00 25.56 C
ANISOU 1524 CB LEU B 159 3297 2750 3666 -31 894 -435 C
ATOM 1525 CG LEU B 159 12.218 -70.011 -58.082 1.00 45.33 C
ANISOU 1525 CG LEU B 159 5876 4982 6367 -84 999 -542 C
ATOM 1526 CD2 LEU B 159 13.321 -68.998 -57.832 1.00 24.84 C
ANISOU 1526 CD2 LEU B 159 3267 2285 3886 99 921 -606 C
ATOM 1527 CD1 LEU B 159 12.248 -70.468 -59.532 1.00 33.73 C
ANISOU 1527 CD1 LEU B 159 4485 3436 4895 -347 1116 -617 C
ATOM 1528 C LEU B 159 8.558 -70.248 -57.353 1.00 41.54 C
ANISOU 1528 C LEU B 159 5239 5126 5417 -176 891 -219 C
ATOM 1529 O LEU B 159 8.406 -71.387 -56.903 1.00 42.78 O
ANISOU 1529 O LEU B 159 5408 5248 5598 -238 952 -165 O
ATOM 1530 N ALA B 160 7.827 -69.220 -56.947 1.00 36.79 N
ANISOU 1530 N ALA B 160 4557 4736 4687 -26 781 -150 N
ATOM 1531 CA ALA B 160 6.806 -69.365 -55.918 1.00 26.97 C
ANISOU 1531 CA ALA B 160 3223 3708 3315 85 733 -2 C
ATOM 1532 CB ALA B 160 6.332 -68.008 -55.444 1.00 32.89 C
ANISOU 1532 CB ALA B 160 3904 4641 3951 315 611 37 C
ATOM 1533 C ALA B 160 5.633 -70.179 -56.448 1.00 48.40 C
ANISOU 1533 C ALA B 160 5909 6572 5908 -157 785 106 C
ATOM 1534 O ALA B 160 5.121 -71.084 -55.787 1.00 28.64 O
ANISOU 1534 O ALA B 160 3373 4137 3372 -184 811 213 O
ATOM 1535 N TRP B 161 5.197 -69.834 -57.650 1.00 27.98 N
ANISOU 1535 N TRP B 161 3337 4042 3251 -340 792 86 N
ATOM 1536 CA TRP B 161 4.117 -70.555 -58.299 1.00 33.96 C
ANISOU 1536 CA TRP B 161 4079 4932 3893 -601 829 185 C
ATOM 1537 CB TRP B 161 3.675 -69.847 -59.572 1.00 28.89 C
ANISOU 1537 CB TRP B 161 3442 4372 3163 -757 808 162 C
ATOM 1538 CG TRP B 161 2.635 -68.829 -59.259 1.00 35.12 C
ANISOU 1538 CG TRP B 161 4103 5443 3797 -617 707 283 C
ATOM 1539 CD1 TRP B 161 2.806 -67.485 -59.104 1.00 28.21 C
ANISOU 1539 CD1 TRP B 161 3193 4620 2905 -397 621 247 C
ATOM 1540 NE1 TRP B 161 1.612 -66.889 -58.772 1.00 60.28 N
ANISOU 1540 NE1 TRP B 161 7133 8966 6806 -300 551 394 N
ATOM 1541 CE2 TRP B 161 0.644 -67.856 -58.693 1.00 45.91 C
ANISOU 1541 CE2 TRP B 161 5252 7294 4896 -464 589 540 C
ATOM 1542 CD2 TRP B 161 1.258 -69.094 -58.977 1.00 44.34 C
ANISOU 1542 CD2 TRP B 161 5158 6884 4807 -669 681 473 C
ATOM 1543 CE3 TRP B 161 0.477 -70.258 -58.960 1.00 31.05 C
ANISOU 1543 CE3 TRP B 161 3450 5286 3062 -875 723 600 C
ATOM 1544 CZ3 TRP B 161 -0.870 -70.153 -58.657 1.00 57.74 C
ANISOU 1544 CZ3 TRP B 161 6689 8972 6278 -874 674 798 C
ATOM 1545 CH2 TRP B 161 -1.454 -68.902 -58.377 1.00 56.94 C
ANISOU 1545 CH2 TRP B 161 6473 9089 6071 -654 594 865 C
ATOM 1546 CZ2 TRP B 161 -0.717 -67.748 -58.393 1.00 45.93 C
ANISOU 1546 CZ2 TRP B 161 5117 7603 4733 -446 550 733 C
ATOM 1547 C TRP B 161 4.474 -72.012 -58.559 1.00 37.56 C
ANISOU 1547 C TRP B 161 4632 5201 4437 -816 936 156 C
ATOM 1548 O TRP B 161 3.636 -72.905 -58.428 1.00 31.88 O
ANISOU 1548 O TRP B 161 3891 4581 3642 -963 954 276 O
ATOM 1549 N SER B 162 5.733 -72.238 -58.914 1.00 46.87 N
ANISOU 1549 N SER B 162 5921 6110 5779 -827 1004 1 N
ATOM 1550 CA SER B 162 6.244 -73.578 -59.175 1.00 36.68 C
ANISOU 1550 CA SER B 162 4743 4602 4591 -999 1114 -50 C
ATOM 1551 C SER B 162 6.380 -74.406 -57.889 1.00 36.66 C
ANISOU 1551 C SER B 162 4714 4561 4655 -877 1122 24 C
ATOM 1552 O SER B 162 6.220 -75.633 -57.888 1.00 40.62 O
ANISOU 1552 O SER B 162 5274 4981 5178 -1038 1185 61 O
ATOM 1553 CB SER B 162 7.588 -73.494 -59.892 1.00 37.53 C
ANISOU 1553 CB SER B 162 4960 4445 4856 -1012 1191 -230 C
ATOM 1554 OG SER B 162 8.282 -74.718 -59.823 1.00 51.15 O
ANISOU 1554 OG SER B 162 6784 5939 6710 -1086 1297 -283 O
ATOM 1555 N TYR B 163 6.690 -73.729 -56.793 1.00 29.49 N
ANISOU 1555 N TYR B 163 3725 3702 3776 -595 1052 47 N
ATOM 1556 CA TYR B 163 6.818 -74.380 -55.503 1.00 29.78 C
ANISOU 1556 CA TYR B 163 3727 3723 3864 -457 1046 124 C
ATOM 1557 CB TYR B 163 7.460 -73.443 -54.498 1.00 37.41 C
ANISOU 1557 CB TYR B 163 4639 4691 4882 -143 967 100 C
ATOM 1558 CG TYR B 163 7.878 -74.119 -53.226 1.00 29.13 C
ANISOU 1558 CG TYR B 163 3575 3574 3917 1 968 152 C
ATOM 1559 CD1 TYR B 163 8.658 -75.280 -53.259 1.00 29.55 C
ANISOU 1559 CD1 TYR B 163 3712 3388 4129 -96 1060 107 C
ATOM 1560 CE1 TYR B 163 9.052 -75.909 -52.099 1.00 29.83 C
ANISOU 1560 CE1 TYR B 163 3731 3357 4246 31 1056 162 C
ATOM 1561 CZ TYR B 163 8.672 -75.369 -50.880 1.00 59.91 C
ANISOU 1561 CZ TYR B 163 7445 7348 7971 257 960 261 C
ATOM 1562 OH TYR B 163 9.077 -76.005 -49.732 1.00 49.72 O
ANISOU 1562 OH TYR B 163 6140 5992 6757 376 954 319 O
ATOM 1563 CE2 TYR B 163 7.900 -74.206 -50.819 1.00 29.30 C
ANISOU 1563 CE2 TYR B 163 3493 3709 3929 367 874 299 C
ATOM 1564 CD2 TYR B 163 7.512 -73.596 -51.990 1.00 29.02 C
ANISOU 1564 CD2 TYR B 163 3471 3732 3824 240 878 247 C
ATOM 1565 C TYR B 163 5.448 -74.798 -54.988 1.00 44.33 C
ANISOU 1565 C TYR B 163 5479 5820 5546 -512 1010 311 C
ATOM 1566 O TYR B 163 5.297 -75.824 -54.320 1.00 44.16 O
ANISOU 1566 O TYR B 163 5455 5776 5548 -546 1036 396 O
ATOM 1567 N TYR B 164 4.448 -73.982 -55.290 1.00 30.68 N
ANISOU 1567 N TYR B 164 3665 4338 3653 -518 946 385 N
ATOM 1568 CA TYR B 164 3.095 -74.292 -54.900 1.00 48.01 C
ANISOU 1568 CA TYR B 164 5754 6802 5686 -576 912 578 C
ATOM 1569 CB TYR B 164 2.203 -73.063 -55.002 1.00 45.20 C
ANISOU 1569 CB TYR B 164 5286 6720 5169 -472 831 649 C
ATOM 1570 CG TYR B 164 0.746 -73.407 -54.918 1.00 32.61 C
ANISOU 1570 CG TYR B 164 3577 5411 3402 -590 808 855 C
ATOM 1571 CD1 TYR B 164 0.229 -74.030 -53.785 1.00 37.39 C
ANISOU 1571 CD1 TYR B 164 4098 6149 3961 -511 801 1012 C
ATOM 1572 CE1 TYR B 164 -1.103 -74.363 -53.700 1.00 37.07 C
ANISOU 1572 CE1 TYR B 164 3939 6383 3765 -625 780 1219 C
ATOM 1573 CZ TYR B 164 -1.944 -74.070 -54.758 1.00 49.56 C
ANISOU 1573 CZ TYR B 164 5486 8108 5236 -822 761 1273 C
ATOM 1574 OH TYR B 164 -3.277 -74.397 -54.671 1.00 61.70 O
ANISOU 1574 OH TYR B 164 6891 9931 6621 -941 734 1497 O
ATOM 1575 CE2 TYR B 164 -1.455 -73.449 -55.901 1.00 44.78 C
ANISOU 1575 CE2 TYR B 164 4970 7371 4672 -905 765 1114 C
ATOM 1576 CD2 TYR B 164 -0.112 -73.128 -55.972 1.00 34.26 C
ANISOU 1576 CD2 TYR B 164 3756 5765 3495 -788 792 907 C
ATOM 1577 C TYR B 164 2.521 -75.445 -55.732 1.00 54.50 C
ANISOU 1577 C TYR B 164 6635 7597 6475 -919 969 631 C
ATOM 1578 O TYR B 164 1.954 -76.396 -55.195 1.00 56.97 O
ANISOU 1578 O TYR B 164 6917 7974 6754 -1003 976 765 O
ATOM 1579 N ILE B 165 2.685 -75.363 -57.046 1.00 57.40 N
ANISOU 1579 N ILE B 165 7095 7864 6851 -1123 1005 526 N
ATOM 1580 CA ILE B 165 2.143 -76.365 -57.959 1.00 44.53 C
ANISOU 1580 CA ILE B 165 5546 6200 5175 -1463 1049 560 C

ATOM 1581 CB ILE B 165 2.130 -75.866 -59.428 1.00 33.68 C
ANISOU 1581 CB ILE B 165 4246 4795 3757 -1651 1063 458 C
ATOM 1582 CG1 ILE B 165 1.361 -74.551 -59.560 1.00 36.68 C
ANISOU 1582 CG1 ILE B 165 4490 5446 4000 -1550 974 530 C
ATOM 1583 CD1 ILE B 165 -0.100 -74.644 -59.088 1.00 38.43 C
ANISOU 1583 CD1 ILE B 165 4561 5989 4052 -1588 906 763 C
ATOM 1584 CG2 ILE B 165 1.545 -76.924 -60.351 1.00 35.04 C
ANISOU 1584 CG2 ILE B 165 4518 4928 3867 -2011 1099 494 C
ATOM 1585 C ILE B 165 2.932 -77.670 -57.892 1.00 49.39 C
ANISOU 1585 C ILE B 165 6302 6530 5936 -1568 1137 488 C
ATOM 1586 O ILE B 165 2.366 -78.759 -58.002 1.00 63.30 O
ANISOU 1586 O ILE B 165 8107 8285 7660 -1787 1154 577 O
ATOM 1587 N GLY B 166 4.240 -77.569 -57.736 1.00 45.47 N
ANISOU 1587 N GLY B 166 5876 5793 5606 -1412 1189 333 N
ATOM 1588 CA GLY B 166 5.113 -78.712 -57.832 1.00 40.49 C
ANISOU 1588 CA GLY B 166 5395 4862 5128 -1509 1287 235 C
ATOM 1589 C GLY B 166 5.567 -79.380 -56.570 1.00 50.71 C
ANISOU 1589 C GLY B 166 6666 6068 6533 -1347 1295 286 C
ATOM 1590 O GLY B 166 6.226 -80.367 -56.617 1.00 53.81 O
ANISOU 1590 O GLY B 166 7177 6204 7066 -1401 1376 214 O
ATOM 1591 N TYR B 167 5.229 -78.815 -55.437 1.00 49.00 N
ANISOU 1591 N TYR B 167 6301 6062 6254 -1143 1212 413 N
ATOM 1592 CA TYR B 167 5.491 -79.458 -54.180 1.00 43.43 C
ANISOU 1592 CA TYR B 167 5566 5301 5635 -995 1209 481 C
ATOM 1593 CB TYR B 167 6.755 -78.908 -53.568 1.00 33.03 C
ANISOU 1593 CB TYR B 167 4253 3822 4473 -731 1215 361 C
ATOM 1594 CG TYR B 167 7.127 -79.517 -52.263 1.00 49.16 C
ANISOU 1594 CG TYR B 167 6261 5816 6603 -571 1202 437 C
ATOM 1595 CD1 TYR B 167 7.430 -80.839 -52.161 1.00 40.45 C
ANISOU 1595 CD1 TYR B 167 5246 4514 5609 -694 1270 450 C
ATOM 1596 CE1 TYR B 167 7.777 -81.386 -50.966 1.00 36.31 C
ANISOU 1596 CE1 TYR B 167 4686 3945 5165 -555 1255 527 C
ATOM 1597 CZ TYR B 167 7.827 -80.621 -49.875 1.00 39.10 C
ANISOU 1597 CZ TYR B 167 4921 4456 5479 -290 1171 588 C
ATOM 1598 OH TYR B 167 8.176 -81.142 -48.687 1.00 45.50 O
ANISOU 1598 OH TYR B 167 5700 5226 6363 -157 1152 669 O
ATOM 1599 CE2 TYR B 167 7.531 -79.306 -49.944 1.00 32.94 C
ANISOU 1599 CE2 TYR B 167 4064 3867 4584 -157 1104 568 C
ATOM 1600 CD2 TYR B 167 7.189 -78.756 -51.134 1.00 32.64 C
ANISOU 1600 CD2 TYR B 167 4056 3871 4476 -297 1119 496 C
ATOM 1601 C TYR B 167 4.329 -79.357 -53.204 1.00 48.10 C
ANISOU 1601 C TYR B 167 6003 6192 6081 -904 1126 685 C
ATOM 1602 O TYR B 167 3.822 -80.344 -52.760 1.00 55.34 O
ANISOU 1602 O TYR B 167 6907 7143 6975 -1005 1127 817 O
ATOM 1603 N LEU B 168 3.946 -78.152 -52.833 1.00 42.29 N
ANISOU 1603 N LEU B 168 5151 5676 5241 -711 1053 716 N
ATOM 1604 CA LEU B 168 3.056 -77.956 -51.722 1.00 42.28 C
ANISOU 1604 CA LEU B 168 5000 5958 5107 -559 983 898 C
ATOM 1605 CB LEU B 168 2.952 -76.480 -51.413 1.00 33.21 C
ANISOU 1605 CB LEU B 168 3762 4984 3874 -297 912 879 C
ATOM 1606 CG LEU B 168 4.163 -75.971 -50.672 1.00 35.57 C
ANISOU 1606 CG LEU B 168 4093 5120 4302 -25 894 761 C
ATOM 1607 CD1 LEU B 168 4.005 -74.554 -50.241 1.00 37.53 C
ANISOU 1607 CD1 LEU B 168 4264 5551 4446 234 809 759 C
ATOM 1608 CD2 LEU B 168 4.462 -76.820 -49.480 1.00 34.97 C
ANISOU 1608 CD2 LEU B 168 4002 4993 4291 66 901 842 C
ATOM 1609 C LEU B 168 1.672 -78.546 -51.914 1.00 53.61 C
ANISOU 1609 C LEU B 168 6364 7620 6387 -778 968 1090 C
ATOM 1610 O LEU B 168 1.157 -79.205 -51.059 1.00 36.39 O
ANISOU 1610 O LEU B 168 4109 5556 4162 -762 951 1252 O
ATOM 1611 N ARG B 169 1.100 -78.342 -53.076 1.00 50.76 N
ANISOU 1611 N ARG B 169 6019 7326 5940 -990 969 1084 N
ATOM 1612 CA ARG B 169 -0.270 -78.792 -53.279 1.00 60.81 C
ANISOU 1612 CA ARG B 169 7208 8842 7055 -1200 938 1282 C
ATOM 1613 CB ARG B 169 -0.957 -78.010 -54.392 1.00 51.65 C
ANISOU 1613 CB ARG B 169 6019 7832 5774 -1325 909 1281 C
ATOM 1614 CG ARG B 169 -0.830 -78.591 -55.776 1.00 54.22 C
ANISOU 1614 CG ARG B 169 6497 7975 6131 -1654 952 1185 C
ATOM 1615 CD ARG B 169 -1.611 -77.701 -56.714 1.00 60.70 C
ANISOU 1615 CD ARG B 169 7257 8994 6813 -1746 908 1215 C
ATOM 1616 NE ARG B 169 -1.643 -78.152 -58.097 1.00 74.02 N
ANISOU 1616 NE ARG B 169 9082 10549 8492 -2073 936 1138 N
ATOM 1617 CZ ARG B 169 -2.516 -77.696 -58.988 1.00 70.95 C
ANISOU 1617 CZ ARG B 169 8653 10322 7983 -2209 878 1188 C
ATOM 1618 NH1 ARG B 169 -3.412 -76.797 -58.611 1.00 71.31 N
ANISOU 1618 NH1 ARG B 169 8517 10667 7909 -2054 801 1323 N
ATOM 1619 NH2 ARG B 169 -2.502 -78.136 -60.241 1.00 62.31 N
ANISOU 1619 NH2 ARG B 169 7707 9053 6913 -2413 866 1069 N
ATOM 1620 C ARG B 169 -0.345 -80.302 -53.518 1.00 66.92 C
ANISOU 1620 C ARG B 169 8085 9460 7882 -1486 977 1330 C
ATOM 1621 O ARG B 169 -1.426 -80.881 -53.657 1.00 71.65 O
ANISOU 1621 O ARG B 169 8630 10230 8366 -1697 945 1507 O
ATOM 1622 N LEU B 170 0.820 -80.935 -53.548 1.00 66.93 N
ANISOU 1622 N LEU B 170 8235 9134 8061 -1488 1042 1179 N
ATOM 1623 CA LEU B 170 0.913 -82.372 -53.725 1.00 74.46 C
ANISOU 1623 CA LEU B 170 9313 9892 9087 -1728 1083 1200 C
ATOM 1624 CB LEU B 170 1.978 -82.698 -54.774 1.00 80.00 C
ANISOU 1624 CB LEU B 170 10220 10248 9930 -1846 1169 973 C
ATOM 1625 CG LEU B 170 1.810 -81.921 -56.083 1.00 86.52 C
ANISOU 1625 CG LEU B 170 11086 11107 10680 -1967 1174 871 C
ATOM 1626 CD1 LEU B 170 3.155 -81.663 -56.726 1.00 84.69 C
ANISOU 1626 CD1 LEU B 170 10993 10585 10602 -1901 1258 630 C
ATOM 1627 CD2 LEU B 170 0.892 -82.658 -57.052 1.00 86.63 C
ANISOU 1627 CD2 LEU B 170 11177 11156 10583 -2332 1163 944 C
ATOM 1628 C LEU B 170 1.250 -83.025 -52.387 1.00 65.89 C
ANISOU 1628 C LEU B 170 8189 8760 8085 -1573 1082 1282 C
ATOM 1629 O LEU B 170 0.874 -84.167 -52.118 1.00 67.30 O
ANISOU 1629 O LEU B 170 8396 8905 8268 -1740 1079 1401 O
ATOM 1630 N ILE B 171 1.943 -82.270 -51.544 1.00 56.51 N
ANISOU 1630 N ILE B 171 6938 7574 6958 -1258 1074 1224 N
ATOM 1631 CA ILE B 171 2.448 -82.770 -50.275 1.00 57.34 C
ANISOU 1631 CA ILE B 171 7017 7613 7156 -1083 1072 1276 C
ATOM 1632 CB ILE B 171 3.904 -82.277 -50.027 1.00 60.02 C
ANISOU 1632 CB ILE B 171 7421 7715 7670 -847 1106 1085 C
ATOM 1633 CG1 ILE B 171 4.906 -83.417 -50.235 1.00 58.39 C
ANISOU 1633 CG1 ILE B 171 7372 7154 7660 -951 1184 987 C
ATOM 1634 CD1 ILE B 171 5.310 -84.128 -48.938 1.00 54.50 C
ANISOU 1634 CD1 ILE B 171 6850 6595 7261 -817 1174 1075 C
ATOM 1635 CG2 ILE B 171 4.057 -81.657 -48.630 1.00 55.88 C
ANISOU 1635 CG2 ILE B 171 6774 7332 7127 -528 1048 1152 C
ATOM 1636 C ILE B 171 1.529 -82.406 -49.098 1.00 54.34 C
ANISOU 1636 C ILE B 171 6449 7570 6628 -916 1000 1483 C
ATOM 1637 O ILE B 171 1.309 -83.212 -48.187 1.00 62.23 O
ANISOU 1637 O ILE B 171 7406 8607 7633 -913 987 1625 O
ATOM 1638 N LEU B 172 0.985 -81.194 -49.124 1.00 40.73 N
ANISOU 1638 N LEU B 172 4614 6093 4769 -775 956 1503 N
ATOM 1639 CA LEU B 172 0.141 -80.713 -48.030 1.00 49.61 C
ANISOU 1639 CA LEU B 172 5562 7547 5741 -579 899 1685 C
ATOM 1640 CB LEU B 172 -0.139 -79.212 -48.149 1.00 48.51 C
ANISOU 1640 CB LEU B 172 5340 7603 5487 -373 860 1644 C
ATOM 1641 CG LEU B 172 1.020 -78.271 -47.828 1.00 41.26 C
ANISOU 1641 CG LEU B 172 4478 6529 4668 -95 851 1456 C
ATOM 1642 CD1 LEU B 172 0.544 -76.843 -47.895 1.00 39.83 C
ANISOU 1642 CD1 LEU B 172 4214 6569 4351 95 800 1448 C
ATOM 1643 CD2 LEU B 172 1.584 -78.564 -46.447 1.00 48.72 C
ANISOU 1643 CD2 LEU B 172 5407 7428 5674 122 838 1491 C
ATOM 1644 C LEU B 172 -1.170 -81.477 -47.787 1.00 63.57 C
ANISOU 1644 C LEU B 172 7220 9565 7369 -760 875 1939 C
ATOM 1645 O LEU B 172 -1.561 -81.651 -46.625 1.00 68.56 O
ANISOU 1645 O LEU B 172 7739 10374 7937 -620 850 2098 O
ATOM 1646 N PRO B 173 -1.871 -81.903 -48.864 1.00 58.72 N
ANISOU 1646 N PRO B 173 6633 8980 6700 -1070 876 1987 N
ATOM 1647 CA PRO B 173 -3.172 -82.549 -48.642 1.00 64.63 C
ANISOU 1647 CA PRO B 173 7259 9991 7309 -849 839 2250 C
ATOM 1648 CB PRO B 173 -3.577 -83.004 -50.042 1.00 57.76 C
ANISOU 1648 CB PRO B 173 6485 9044 6420 -1611 841 2230 C
ATOM 1649 CG PRO B 173 -2.985 -81.972 -50.927 1.00 58.83 C
ANISOU 1649 CG PRO B 173 6693 9073 6589 -1535 864 2012 C
ATOM 1650 CD PRO B 173 -1.650 -81.652 -50.301 1.00 46.16 C
ANISOU 1650 CD PRO B 173 5160 7240 5139 -1258 901 1829 C
ATOM 1651 C PRO B 173 -3.153 -83.747 -47.692 1.00 64.28 C
ANISOU 1651 C PRO B 173 7210 9898 7313 -1295 837 2386 C
ATOM 1652 O PRO B 173 -4.082 -83.891 -46.896 1.00 65.21 O
ANISOU 1652 O PRO B 173 7167 10307 7304 -1261 801 2619 O
ATOM 1653 N GLU B 174 -2.124 -84.586 -47.774 1.00 62.33 N
ANISOU 1653 N GLU B 174 7133 9300 7250 -1620 876 2253 N
ATOM 1654 CA GLU B 174 -2.043 -85.763 -46.914 1.00 51.04 C
ANISOU 1654 CA GLU B 174 5714 7794 5885 -1420 873 2377 C
ATOM 1655 CB GLU B 174 -1.623 -86.998 -47.708 1.00 52.82 C
ANISOU 1655 CB GLU B 174 6138 7689 6243 -1725 904 2303 C
ATOM 1656 CG GLU B 174 -2.767 -87.699 -48.405 1.00 75.76 C
ANISOU 1656 CG GLU B 174 9040 10710 9034 -2079 862 2467 C
ATOM 1657 CD GLU B 174 -3.715 -88.372 -47.427 1.00 99.46 C
ANISOU 1657 CD GLU B 174 11912 13921 11955 -2084 785 2694 C
ATOM 1658 OE1 GLU B 174 -4.920 -88.043 -47.447 1.00107.31 O
ANISOU 1658 OE1 GLU B 174 12772 15198 12804 -2075 702 2784 O
ATOM 1659 OE2 GLU B 174 -3.253 -89.229 -46.643 1.00109.14 O
ANISOU 1659 OE2 GLU B 174 13172 15018 13278 -2084 799 2766 O
ATOM 1660 C GLU B 174 -1.098 -85.588 -45.730 1.00 49.22 C
ANISOU 1660 C GLU B 174 5473 7471 5756 -1110 886 2318 C
ATOM 1661 O GLU B 174 -0.711 -86.567 -45.100 1.00 52.18 O
ANISOU 1661 O GLU B 174 5895 7699 6233 -1140 892 2369 O
ATOM 1662 N LEU B 175 -0.721 -84.351 -45.428 1.00 42.59 N
ANISOU 1662 N LEU B 175 4580 6710 4891 -817 883 2215 N
ATOM 1663 CA LEU B 175 0.287 -84.119 -44.400 1.00 51.79 C
ANISOU 1663 CA LEU B 175 5759 7759 6160 -532 887 2136 C
ATOM 1664 CB LEU B 175 0.852 -82.698 -44.468 1.00 56.18 C
ANISOU 1664 CB LEU B 175 6312 8324 6711 -267 879 1966 C
ATOM 1665 CG LEU B 175 2.121 -82.507 -43.635 1.00 51.60 C
ANISOU 1665 CG LEU B 175 5787 7543 6274 -16 879 1845 C
ATOM 1666 CD1 LEU B 175 3.278 -83.296 -44.236 1.00 48.68 C
ANISOU 1666 CD1 LEU B 175 5585 6780 6132 -151 935 1687 C
ATOM 1667 CD2 LEU B 175 2.483 -81.036 -43.519 1.00 43.28 C
ANISOU 1667 CD2 LEU B 175 4711 6557 5176 257 846 1721 C
ATOM 1668 C LEU B 175 -0.233 -84.397 -42.993 1.00 49.48 C
ANISOU 1668 C LEU B 175 5329 7694 5776 -392 849 2349 C
ATOM 1669 O LEU B 175 0.381 -85.137 -42.221 1.00 60.46 O
ANISOU 1669 O LEU B 175 6759 8934 7279 -349 853 2370 O
ATOM 1670 N GLN B 176 -1.368 -83.794 -42.669 1.00 62.04 N
ANISOU 1670 N GLN B 176 7513 8513 7545 -1054 817 2513 N

ATOM 1671 CA GLN B 176 -1.961 -83.906 -41.344 1.00 55.13 C
ANISOU 1671 CA GLN B 176 5733 9047 6165 -159 788 2723 C
ATOM 1672 CB GLN B 176 -3.194 -83.018 -41.244 1.00 61.77 C
ANISOU 1672 CB GLN B 176 6399 10298 6775 -60 767 2870 C
ATOM 1673 CG GLN B 176 -3.112 -82.000 -40.142 1.00 76.66 C
ANISOU 1673 CG GLN B 176 8203 12368 8558 323 752 2870 C
ATOM 1674 CD GLN B 176 -3.742 -80.680 -40.531 1.00 92.34 C
ANISOU 1674 CD GLN B 176 10108 14589 10387 472 743 2848 C
ATOM 1675 OE1 GLN B 176 -4.062 -80.451 -41.700 1.00 96.95 O
ANISOU 1675 OE1 GLN B 176 10710 15160 10966 295 748 2799 O
ATOM 1676 NE2 GLN B 176 -3.923 -79.800 -39.552 1.00 96.28 N
ANISOU 1676 NE2 GLN B 176 10526 15302 10755 803 729 2883 N
ATOM 1677 C GLN B 176 -2.328 -85.347 -41.010 1.00 59.33 C
ANISOU 1677 C GLN B 176 6256 9558 6730 -392 782 2911 C
ATOM 1678 O GLN B 176 -2.211 -85.784 -39.862 1.00 46.35 O
ANISOU 1678 O GLN B 176 4562 7959 5089 -276 768 3023 O
ATOM 1679 N ALA B 177 -2.772 -86.078 -42.025 1.00 56.68 N
ANISOU 1679 N ALA B 177 5975 9148 6414 -727 786 2947 N
ATOM 1680 CA ALA B 177 -3.102 -87.485 -41.870 1.00 58.53 C
ANISOU 1680 CA ALA B 177 6229 9321 6689 -988 770 3113 C
ATOM 1681 CB ALA B 177 -3.701 -88.031 -43.148 1.00 48.93 C
ANISOU 1681 CB ALA B 177 5080 8053 5459 -1354 763 3136 C
ATOM 1682 C ALA B 177 -1.851 -88.269 -41.505 1.00 63.19 C
ANISOU 1682 C ALA B 177 6972 9540 7496 -964 794 2991 C
ATOM 1683 O ALA B 177 -1.878 -89.170 -40.660 1.00 71.04 O
ANISOU 1683 O ALA B 177 7944 10525 8523 -994 774 3138 O
ATOM 1684 N ARG B 178 -0.748 -87.934 -42.163 1.00 58.22 N
ANISOU 1684 N ARG B 178 6495 8608 7017 -911 837 2728 N
ATOM 1685 CA ARG B 178 0.502 -88.655 -41.972 1.00 56.34 C
ANISOU 1685 CA ARG B 178 6407 7999 7001 -893 868 2600 C
ATOM 1686 CB ARG B 178 1.488 -88.318 -43.081 1.00 55.24 C
ANISOU 1686 CB ARG B 178 6432 7553 7004 -915 925 2326 C
ATOM 1687 CG ARG B 178 1.178 -89.005 -44.389 1.00 59.72 C
ANISOU 1687 CG ARG B 178 7127 7972 7591 -1254 951 2286 C
ATOM 1688 CD ARG B 178 2.037 -88.439 -45.499 1.00 62.22 C
ANISOU 1688 CD ARG B 178 7578 8054 8007 -1246 1011 2022 C
ATOM 1689 NE ARG B 178 3.460 -88.642 -45.250 1.00 70.66 N
ANISOU 1689 NE ARG B 178 8757 8800 9290 -1097 1062 1857 N
ATOM 1690 CZ ARG B 178 4.393 -87.702 -45.385 1.00 74.13 C
ANISOU 1690 CZ ARG B 178 9216 9145 9807 -886 1090 1673 C
ATOM 1691 NH1 ARG B 178 4.050 -86.480 -45.767 1.00 62.98 N
ANISOU 1691 NH1 ARG B 178 7731 7924 8273 -795 1070 1620 N
ATOM 1692 NH2 ARG B 178 5.668 -87.982 -45.140 1.00 80.72 N
ANISOU 1692 NH2 ARG B 178 10138 9690 10841 -767 1133 1549 N
ATOM 1693 C ARG B 178 1.114 -88.352 -40.617 1.00 63.40 C
ANISOU 1693 C ARG B 178 7235 8925 7927 -582 851 2618 C
ATOM 1694 O ARG B 178 1.718 -89.219 -39.978 1.00 68.21 O
ANISOU 1694 O ARG B 178 7897 9353 8668 -579 852 2649 O
ATOM 1695 N ILE B 179 0.953 -87.111 -40.182 1.00 55.37 N
ANISOU 1695 N ILE B 179 6112 8139 6787 -322 832 2598 N
ATOM 1696 CA ILE B 179 1.448 -86.687 -38.887 1.00 52.15 C
ANISOU 1696 CA ILE B 179 5645 7794 6375 -17 805 2616 C
ATOM 1697 CB ILE B 179 1.314 -85.176 -38.715 1.00 54.36 C
ANISOU 1697 CB ILE B 179 5851 8283 6519 254 786 2542 C
ATOM 1698 CG1 ILE B 179 2.300 -84.469 -39.642 1.00 58.58 C
ANISOU 1698 CG1 ILE B 179 6512 8563 7184 295 810 2276 C
ATOM 1699 CD1 ILE B 179 2.559 -83.029 -39.294 1.00 51.49 C
ANISOU 1699 CD1 ILE B 179 5582 7776 6207 598 777 2172 C
ATOM 1700 CG2 ILE B 179 1.532 -84.786 -37.266 1.00 43.34 C
ANISOU 1700 CG2 ILE B 179 4383 7022 5062 554 746 2609 C
ATOM 1701 C ILE B 179 0.721 -87.398 -37.752 1.00 60.84 C
ANISOU 1701 C ILE B 179 6625 9113 7377 -20 771 2877 C
ATOM 1702 O ILE B 179 1.346 -87.886 -36.803 1.00 59.33 O
ANISOU 1702 O ILE B 179 6449 8818 7275 83 757 2912 O
ATOM 1703 N ARG B 180 -0.587 -87.455 -37.813 1.00 65.85 N
ANISOU 1703 N ARG B 180 7132 10058 7827 -144 756 3073 N
ATOM 1704 CA ARG B 180 -1.335 -88.132 -36.792 1.00 73.03 C
ANISOU 1704 CA ARG B 180 7909 11214 8626 -153 725 3344 C
ATOM 1705 CB ARG B 180 -2.821 -87.834 -36.887 1.00 83.96 C
ANISOU 1705 CB ARG B 180 9119 13006 9776 -228 712 3553 C
ATOM 1706 CG ARG B 180 -3.552 -88.462 -38.043 1.00 93.72 C
ANISOU 1706 CG ARG B 180 10384 14215 11011 -588 711 3604 C
ATOM 1707 CD ARG B 180 -5.020 -88.080 -37.976 1.00 98.78 C
ANISOU 1707 CD ARG B 180 10854 15197 11481 -594 635 3681 C
ATOM 1708 NE ARG B 180 -5.282 -86.739 -38.466 1.00103.55 N
ANISOU 1708 NE ARG B 180 11399 15966 11978 -407 648 3578 N
ATOM 1709 CZ ARG B 180 -5.854 -86.490 -39.635 1.00107.42 C
ANISOU 1709 CZ ARG B 180 11896 16484 12436 -553 628 3506 C
ATOM 1710 NH1 ARG B 180 -6.050 -85.239 -40.031 1.00111.09 N
ANISOU 1710 NH1 ARG B 180 12431 16823 12954 -885 593 3519 N
ATOM 1711 NH2 ARG B 180 -6.221 -87.509 -40.406 1.00101.12 N
ANISOU 1711 NH2 ARG B 180 11043 15828 11548 -365 636 3417 N
ATOM 1712 C ARG B 180 -1.045 -89.600 -36.777 1.00 72.29 C
ANISOU 1712 C ARG B 180 7903 10879 8687 -402 719 3421 C
ATOM 1713 O ARG B 180 -1.005 -90.205 -35.743 1.00 70.11 O
ANISOU 1713 O ARG B 180 7577 10644 8417 -349 695 3569 O
ATOM 1714 N THR B 181 -0.871 -90.171 -37.948 1.00 69.60 N
ANISOU 1714 N THR B 181 7703 10273 8469 -666 742 3313 N
ATOM 1715 CA THR B 181 -0.544 -91.586 -38.062 1.00 60.87 C
ANISOU 1715 CA THR B 181 6716 8891 7521 -907 738 3357 C
ATOM 1716 CB THR B 181 -0.437 -92.000 -39.525 1.00 56.51 C
ANISOU 1716 CB THR B 181 6328 8085 7059 -1188 768 3218 C
ATOM 1717 OG1 THR B 181 -1.530 -91.439 -40.257 1.00 63.53 O
ANISOU 1717 OG1 THR B 181 7132 9239 7769 -1308 754 3281 O
ATOM 1718 CG2 THR B 181 -0.465 -93.506 -39.661 1.00 53.47 C
ANISOU 1718 CG2 THR B 181 6054 7481 6782 -1476 751 3316 C
ATOM 1719 C THR B 181 0.778 -91.857 -37.363 1.00 60.09 C
ANISOU 1719 C THR B 181 6708 8509 7614 -728 753 3243 C
ATOM 1720 O THR B 181 0.945 -92.857 -36.666 1.00 69.84 O
ANISOU 1720 O THR B 181 7956 9652 8928 -785 730 3367 O
ATOM 1721 N TYR B 182 1.720 -90.946 -37.554 1.00 59.94 N
ANISOU 1721 N TYR B 182 6747 8355 7673 -514 785 3014 N
ATOM 1722 CA TYR B 182 3.000 -91.015 -36.877 1.00 59.17 C
ANISOU 1722 CA TYR B 182 6716 8017 7749 -317 792 2906 C
ATOM 1723 CB TYR B 182 3.946 -89.962 -37.446 1.00 63.09 C
ANISOU 1723 CB TYR B 182 7287 8360 8327 -145 826 2643 C
ATOM 1724 CG TYR B 182 5.285 -89.953 -36.769 1.00 59.41 C
ANISOU 1724 CG TYR B 182 6876 7657 8039 60 825 2539 C
ATOM 1725 CD2 TYR B 182 6.331 -90.736 -37.253 1.00 66.67 C
ANISOU 1725 CD2 TYR B 182 7944 8191 9199 -33 873 2417 C
ATOM 1726 CE2 TYR B 182 7.562 -90.739 -36.631 1.00 53.00 C
ANISOU 1726 CE2 TYR B 182 6250 6251 7638 153 870 2339 C
ATOM 1727 CZ TYR B 182 7.751 -89.956 -35.506 1.00 51.54 C
ANISOU 1727 CZ TYR B 182 5968 6239 7377 422 809 2379 C
ATOM 1728 OH TYR B 182 8.969 -89.949 -34.874 1.00 56.88 O
ANISOU 1728 OH TYR B 182 6677 6715 8219 596 793 2313 O
ATOM 1729 CE1 TYR B 182 6.726 -89.173 -35.006 1.00 58.48 C
ANISOU 1729 CE1 TYR B 182 6719 7492 8010 522 763 2487 C
ATOM 1730 CD1 TYR B 182 5.506 -89.174 -35.638 1.00 49.54 C
ANISOU 1730 CD1 TYR B 182 5537 6570 6716 347 776 2568 C
ATOM 1731 C TYR B 182 2.814 -90.809 -35.372 1.00 62.27 C
ANISOU 1731 C TYR B 182 6971 8652 8039 -89 741 3070 C
ATOM 1732 O TYR B 182 3.416 -91.509 -34.552 1.00 65.18 O
ANISOU 1732 O TYR B 182 7361 8882 8521 -42 723 3128 O
ATOM 1733 N ASN B 183 1.978 -89.836 -35.022 1.00 63.75 N
ANISOU 1733 N ASN B 183 7018 9199 8004 57 719 3146 N
ATOM 1734 CA ASN B 183 1.655 -89.529 -33.630 1.00 59.44 C
ANISOU 1734 CA ASN B 183 6339 8929 7315 284 678 3305 C
ATOM 1735 CB ASN B 183 0.732 -88.315 -33.549 1.00 62.04 C
ANISOU 1735 CB ASN B 183 6539 9634 7400 446 673 3344 C
ATOM 1736 CG ASN B 183 1.486 -87.005 -33.558 1.00 62.65 C
ANISOU 1736 CG ASN B 183 6665 9657 7483 722 670 3123 C
ATOM 1737 OD1 ASN B 183 2.706 -86.974 -33.385 1.00 62.90 O
ANISOU 1737 OD1 ASN B 183 6804 9409 7687 825 663 2968 O
ATOM 1738 ND2 ASN B 183 0.760 -85.907 -33.750 1.00 61.78 N
ANISOU 1738 ND2 ASN B 183 6474 9816 7184 845 671 3116 N
ATOM 1739 C ASN B 183 0.997 -90.675 -32.877 1.00 56.75 C
ANISOU 1739 C ASN B 183 5919 8712 6933 143 650 3574 C
ATOM 1740 O ASN B 183 1.208 -90.846 -31.675 1.00 60.03 O
ANISOU 1740 O ASN B 183 6281 9199 7328 298 619 3680 O
ATOM 1741 N GLN B 184 0.152 -91.398 -33.578 1.00 59.61 N
ANISOU 1741 N GLN B 184 6272 9106 7271 -159 654 3693 N
ATOM 1742 CA GLN B 184 -0.516 -92.551 -33.047 1.00 68.99 C
ANISOU 1742 CA GLN B 184 7382 10418 8413 -332 618 3966 C
ATOM 1743 CB GLN B 184 -1.605 -93.021 -33.993 1.00 82.55 C
ANISOU 1743 CB GLN B 184 9066 12255 10044 -651 611 4097 C
ATOM 1744 CG GLN B 184 -2.840 -92.143 -34.049 1.00 94.76 C
ANISOU 1744 CG GLN B 184 10450 14197 11358 -582 602 4154 C
ATOM 1745 CD GLN B 184 -3.620 -92.416 -35.311 1.00111.99 C
ANISOU 1745 CD GLN B 184 12066 16255 13230 -1045 611 4097 C
ATOM 1746 OE1 GLN B 184 -3.508 -93.492 -35.884 1.00118.95 O
ANISOU 1746 OE1 GLN B 184 13670 16998 14529 -1153 555 4105 O
ATOM 1747 NE2 GLN B 184 -4.391 -91.441 -35.766 1.00116.17 N
ANISOU 1747 NE2 GLN B 184 13094 17136 13909 -807 564 4056 N
ATOM 1748 C GLN B 184 0.387 -93.705 -32.714 1.00 59.54 C
ANISOU 1748 C GLN B 184 6312 8866 7442 -434 607 3956 C
ATOM 1749 O GLN B 184 0.184 -94.354 -31.723 1.00 59.88 O
ANISOU 1749 O GLN B 184 6291 8988 7473 -440 569 4156 O
ATOM 1750 N HIS B 185 1.423 -93.911 -33.512 1.00 73.31 N
ANISOU 1750 N HIS B 185 7831 10418 9606 -826 2814 1752 N
ATOM 1751 C HIS B 185 2.578 -95.731 -32.338 1.00 85.65 C
ANISOU 1751 C HIS B 185 9529 11590 11424 -909 2458 1760 C
ATOM 1752 O HIS B 185 2.990 -95.013 -31.467 1.00 69.94 O
ANISOU 1752 O HIS B 185 7860 9395 9321 -717 2189 1713 O
ATOM 1753 CA HIS B 185 2.090 -95.186 -33.646 1.00 76.96 C
ANISOU 1753 CA HIS B 185 8123 10728 10391 -1025 2719 1721 C
ATOM 1754 CB HIS B 185 3.269 -95.078 -34.603 1.00 68.76 C
ANISOU 1754 CB HIS B 185 6809 9502 9814 -1233 2580 1525 C
ATOM 1755 CG HIS B 185 3.783 -96.399 -35.083 1.00 76.80 C
ANISOU 1755 CG HIS B 185 7554 10435 11193 -1483 2578 1493 C
ATOM 1756 ND1 HIS B 185 4.688 -97.151 -34.375 1.00 73.05 N
ANISOU 1756 ND1 HIS B 185 7172 9659 10925 -1491 2282 1437 N
ATOM 1757 CE1 HIS B 185 4.944 -98.260 -35.036 1.00 66.97 C
ANISOU 1757 CE1 HIS B 185 6101 8879 10465 -1733 2360 1418 C
ATOM 1758 NE2 HIS B 185 4.240 -98.256 -36.146 1.00 72.19 N
ANISOU 1758 NE2 HIS B 185 6484 9827 11118 -1886 2698 1462 N
ATOM 1759 CD2 HIS B 185 3.504 -97.105 -36.198 1.00 79.32 C
ANISOU 1759 CD2 HIS B 185 7511 10925 11699 -1731 2834 1511 C
ATOM 1760 N TYR B 186 2.568 -97.042 -32.213 1.00 86.34 N
ANISOU 1760 N TYR B 186 9525 11705 11576 -1030 2538 1848 N

ATOM 1761 CA TYR B 186 2.961 -97.669 -30.972 1.00 89.54 C
ANISOU 1761 CA TYR B 186 10224 11898 11899 -938 2311 1906 C
ATOM 1762 CB TYR B 186 2.702 -99.168 -31.000 1.00 87.32 C
ANISOU 1762 CB TYR B 186 9777 11695 11705 -1107 2463 2011 C
ATOM 1763 CG TYR B 186 3.574-100.021 -31.883 1.00 79.14 C
ANISOU 1763 CG TYR B 186 8387 10502 11180 -1367 2359 1889 C
ATOM 1764 CD1 TYR B 186 4.815-100.416 -31.491 1.00 72.30 C
ANISOU 1764 CD1 TYR B 186 7613 9272 10584 -1382 1980 1792 C
ATOM 1765 CE1 TYR B 186 5.584-101.220 -32.293 1.00 74.95 C
ANISOU 1765 CE1 TYR B 186 7615 9457 11408 -1620 1893 1667 C
ATOM 1766 CZ TYR B 186 5.108-101.650 -33.485 1.00 73.04 C
ANISOU 1766 CZ TYR B 186 6953 9432 11368 -1856 2198 1646 C
ATOM 1767 OH TYR B 186 5.842-102.452 -34.297 1.00 66.80 O
ANISOU 1767 OH TYR B 186 5828 8488 11065 -2104 2131 1516 O
ATOM 1768 CE2 TYR B 186 3.870-101.288 -33.884 1.00 72.22 C
ANISOU 1768 CE2 TYR B 186 6764 9689 10988 -1847 2565 1750 C
ATOM 1769 CD2 TYR B 186 3.106-100.491 -33.077 1.00 80.13 C
ANISOU 1769 CD2 TYR B 186 8087 10835 11523 -1601 2640 1868 C
ATOM 1770 C TYR B 186 4.382 -97.411 -30.588 1.00 96.22 C
ANISOU 1770 C TYR B 186 11152 12355 13051 -931 1883 1739 C
ATOM 1771 O TYR B 186 4.669 -97.153 -29.444 1.00 73.39 O
ANISOU 1771 O TYR B 186 8635 9249 9998 -743 1606 1744 O
ATOM 1772 O ASN B 187 8.035 -95.640 -30.296 1.00113.96 O
ANISOU 1772 O ASN B 187 13116 13919 16262 -1049 1187 1129 O
ATOM 1773 N ASN B 187 5.267 -97.474 -31.568 1.00101.84 N
ANISOU 1773 N ASN B 187 11515 12968 14212 -1141 1830 1581 N
ATOM 1774 CA ASN B 187 6.697 -97.312 -31.354 1.00108.32 C
ANISOU 1774 CA ASN B 187 12356 13410 15389 -1160 1436 1398 C
ATOM 1775 C ASN B 187 7.021 -95.908 -30.920 1.00108.58 C
ANISOU 1775 C ASN B 187 12608 13355 15292 -970 1277 1307 C
ATOM 1776 CB ASN B 187 7.482 -97.724 -32.587 1.00105.16 C
ANISOU 1776 CB ASN B 187 11515 12922 15517 -1449 1449 1239 C
ATOM 1777 CG ASN B 187 8.374 -98.917 -32.329 1.00105.41 C
ANISOU 1777 CG ASN B 187 11532 12592 15926 -1522 1102 1132 C
ATOM 1778 OD1 ASN B 187 8.919 -99.059 -31.244 1.00107.70 O
ANISOU 1778 OD1 ASN B 187 12145 12625 16153 -1344 761 1111 O
ATOM 1779 ND2 ASN B 187 8.543 -99.776 -33.335 1.00102.24 N
ANISOU 1779 ND2 ASN B 187 10757 12164 15927 -1787 1183 1060 N
ATOM 1780 O ASN B 188 4.913 -92.779 -29.418 1.00107.10 O
ANISOU 1780 O ASN B 188 12717 13368 14609 -625 1374 1249 O
ATOM 1781 N ASN B 188 6.137 -95.003 -31.270 1.00106.51 N
ANISOU 1781 N ASN B 188 12732 13163 14575 -723 1273 1435 N
ATOM 1782 CA ASN B 188 6.395 -93.613 -31.063 1.00108.75 C
ANISOU 1782 CA ASN B 188 13360 13280 14681 -488 1021 1375 C
ATOM 1783 C ASN B 188 6.018 -93.219 -29.684 1.00111.68 C
ANISOU 1783 C ASN B 188 13640 13759 15034 -450 1121 1280 C
ATOM 1784 CB ASN B 188 5.613 -92.794 -32.056 1.00132.65 C
ANISOU 1784 CB ASN B 188 16555 15887 17959 -453 556 1260 C
ATOM 1785 CG ASN B 188 6.375 -92.563 -33.324 1.00131.08 C
ANISOU 1785 CG ASN B 188 15988 15475 18340 -682 407 1060 C
ATOM 1786 OD1 ASN B 188 7.111 -91.620 -33.412 1.00129.45 O
ANISOU 1786 OD1 ASN B 188 15749 15035 18401 -765 182 1022 O
ATOM 1787 ND2 ASN B 188 6.201 -93.422 -34.304 1.00131.47 N
ANISOU 1787 ND2 ASN B 188 15765 15597 18590 -791 534 930 N
ATOM 1788 O LEU B 189 6.333 -90.882 -27.862 1.00132.56 O
ANISOU 1788 O LEU B 189 17206 16594 16568 227 1145 1452 O
ATOM 1789 N LEU B 189 7.025 -93.249 -28.837 1.00120.16 N
ANISOU 1789 N LEU B 189 15034 14733 15888 -222 945 1246 N
ATOM 1790 CA LEU B 189 6.879 -93.144 -27.412 1.00123.95 C
ANISOU 1790 CA LEU B 189 15968 15037 16091 3 693 1310 C
ATOM 1791 C LEU B 189 6.162 -91.852 -27.137 1.00130.79 C
ANISOU 1791 C LEU B 189 17116 16137 16440 217 901 1451 C
ATOM 1792 CB LEU B 189 8.261 -93.088 -26.777 1.00115.83 C
ANISOU 1792 CB LEU B 189 15091 13633 15287 85 257 1127 C
ATOM 1793 CG LEU B 189 9.465 -92.799 -27.677 1.00104.58 C
ANISOU 1793 CG LEU B 189 13395 11923 14417 -116 11 955 C
ATOM 1794 CD1 LEU B 189 9.234 -91.662 -28.654 1.00 98.03 C
ANISOU 1794 CD1 LEU B 189 12193 11097 13956 -284 89 772 C
ATOM 1795 CD2 LEU B 189 10.704 -92.560 -26.835 1.00100.47 C
ANISOU 1795 CD2 LEU B 189 13155 11001 14018 -3 -467 870 C
ATOM 1796 N LEU B 190 5.364 -91.839 -26.081 1.00132.03 N
ANISOU 1796 N LEU B 190 17671 16230 16266 384 809 1567 N
ATOM 1797 CA LEU B 190 4.355 -90.823 -25.900 1.00133.05 C
ANISOU 1797 CA LEU B 190 18111 16521 15919 606 959 1667 C
ATOM 1798 CB LEU B 190 3.666 -90.980 -24.560 1.00129.40 C
ANISOU 1798 CB LEU B 190 18091 15972 15104 747 876 1800 C
ATOM 1799 CG LEU B 190 3.474 -92.408 -24.081 1.00126.80 C
ANISOU 1799 CG LEU B 190 17929 15941 14307 857 1246 1969 C
ATOM 1800 CD1 LEU B 190 4.498 -92.755 -23.006 1.00122.80 C
ANISOU 1800 CD1 LEU B 190 17113 15761 13786 825 1598 1968 C
ATOM 1801 CD2 LEU B 190 2.042 -92.603 -23.587 1.00124.67 C
ANISOU 1801 CD2 LEU B 190 17676 15748 13944 757 1406 2115 C
ATOM 1802 C LEU B 190 5.044 -89.489 -25.941 1.00139.48 C
ANISOU 1802 C LEU B 190 19043 17179 16774 740 731 1520 C
ATOM 1803 O LEU B 190 4.454 -88.485 -26.336 1.00141.79 O
ANISOU 1803 O LEU B 190 19434 17632 16807 880 882 1539 O
ATOM 1804 N ARG B 191 6.310 -89.477 -25.562 1.00137.25 N
ANISOU 1804 N ARG B 191 18728 16575 16844 688 368 1364 N
ATOM 1805 CA ARG B 191 7.045 -88.249 -25.599 1.00131.45 C
ANISOU 1805 CA ARG B 191 18049 15658 16238 778 131 1196 C
ATOM 1806 CB ARG B 191 8.484 -88.488 -25.176 1.00129.64 C
ANISOU 1806 CB ARG B 191 17870 15025 16363 746 -318 1046 C
ATOM 1807 CG ARG B 191 8.663 -88.557 -23.677 1.00133.40 C
ANISOU 1807 CG ARG B 191 18845 15262 16580 961 -640 1085 C
ATOM 1808 CD ARG B 191 7.557 -89.380 -23.032 1.00135.60 C
ANISOU 1808 CD ARG B 191 19362 15666 16494 1003 -489 1297 C
ATOM 1809 NE ARG B 191 7.279 -88.980 -21.661 1.00135.46 N
ANISOU 1809 NE ARG B 191 19859 15592 16020 1249 -590 1378 N
ATOM 1810 CZ ARG B 191 6.552 -89.697 -20.822 1.00131.20 C
ANISOU 1810 CZ ARG B 191 19611 15154 15083 1321 -446 1556 C
ATOM 1811 NH1 ARG B 191 6.343 -89.261 -19.587 1.00133.13 N
ANISOU 1811 NH1 ARG B 191 20334 15328 14921 1536 -539 1612 N
ATOM 1812 NH2 ARG B 191 6.041 -90.849 -21.222 1.00123.52 N
ANISOU 1812 NH2 ARG B 191 18461 14352 14120 1172 -199 1674 N
ATOM 1813 C ARG B 191 7.010 -87.715 -27.000 1.00122.20 C
ANISOU 1813 C ARG B 191 16487 14652 15291 643 341 1099 C
ATOM 1814 O ARG B 191 7.106 -88.454 -27.969 1.00118.48 O
ANISOU 1814 O ARG B 191 15643 14297 15075 418 525 1093 O
ATOM 1815 N GLY B 192 6.829 -86.411 -27.089 1.00116.92 N
ANISOU 1815 N GLY B 192 15922 13990 14513 779 313 1025 N
ATOM 1816 CA GLY B 192 6.946 -85.727 -28.351 1.00114.99 C
ANISOU 1816 CA GLY B 192 15367 13833 14491 665 440 906 C
ATOM 1817 C GLY B 192 5.923 -85.769 -29.453 1.00110.83 C
ANISOU 1817 C GLY B 192 15532 13662 13915 524 857 1004 C
ATOM 1818 O GLY B 192 6.217 -86.221 -30.557 1.00111.63 O
ANISOU 1818 O GLY B 192 14285 13798 14330 282 960 965 O
ATOM 1819 N ALA B 193 4.705 -85.344 -29.145 1.00102.03 N
ANISOU 1819 N ALA B 193 13548 12805 12415 673 1094 1124 N
ATOM 1820 CA ALA B 193 3.734 -85.141 -30.195 1.00 96.07 C
ANISOU 1820 CA ALA B 193 12512 12381 11607 565 1469 1202 C
ATOM 1821 CB ALA B 193 2.379 -84.863 -29.592 1.00 73.06 C
ANISOU 1821 CB ALA B 193 9795 9725 8240 746 1711 1375 C
ATOM 1822 C ALA B 193 4.118 -84.024 -31.150 1.00 89.86 C
ANISOU 1822 C ALA B 193 11563 11602 10978 518 1482 1068 C
ATOM 1823 O ALA B 193 4.195 -82.886 -30.754 1.00 92.05 O
ANISOU 1823 O ALA B 193 12054 11837 11085 704 1392 1025 O
ATOM 1824 N VAL B 194 4.332 -84.369 -32.412 1.00 75.71 N
ANISOU 1824 N VAL B 194 9404 9856 9505 265 1596 999 N
ATOM 1825 CA VAL B 194 4.730 -83.404 -33.410 1.00 69.96 C
ANISOU 1825 CA VAL B 194 8530 9098 8952 189 1596 857 C
ATOM 1826 CB VAL B 194 5.381 -84.066 -34.659 1.00 79.58 C
ANISOU 1826 CB VAL B 194 9371 10256 10611 -130 1642 742 C
ATOM 1827 CG1 VAL B 194 6.018 -85.383 -34.302 1.00 77.25 C
ANISOU 1827 CG1 VAL B 194 9006 9803 10543 -247 1517 738 C
ATOM 1828 CG2 VAL B 194 4.423 -84.256 -35.809 1.00 64.73 C
ANISOU 1828 CG2 VAL B 194 7221 8685 8689 -286 1990 829 C
ATOM 1829 C VAL B 194 3.598 -82.463 -33.758 1.00 73.60 C
ANISOU 1829 C VAL B 194 8998 9847 9120 288 1851 946 C
ANISOU 1829 C VAL B 194 8998 9847 9120 288 1851 946 C
ATOM 1830 O VAL B 194 2.460 -82.850 -33.750 1.00 76.48 O
ANISOU 1830 O VAL B 194 9314 10481 9265 306 2108 1105 O
ATOM 1831 N SER B 195 3.927 -81.228 -34.077 1.00 67.11 N
ANISOU 1831 N SER B 195 8238 8956 8303 357 1772 837 N
ATOM 1832 CA SER B 195 2.920 -80.254 -34.464 1.00 68.83 C
ANISOU 1832 CA SER B 195 8478 9410 8263 463 1971 903 C
ATOM 1833 CB SER B 195 3.498 -78.845 -34.429 1.00 69.50 C
ANISOU 1833 CB SER B 195 8724 9339 8342 587 1796 770 C
ATOM 1834 OG SER B 195 3.980 -78.570 -33.132 1.00 75.38 O
ANISOU 1834 OG SER B 195 9792 9884 8964 802 1543 745 O
ATOM 1835 C SER B 195 2.359 -80.582 -35.835 1.00 67.58 C
ANISOU 1835 C SER B 195 7980 9472 8225 233 2242 936 C
ATOM 1836 O SER B 195 2.993 -81.280 -36.625 1.00 69.16 O
ANISOU 1836 O SER B 195 7932 9597 8750 -22 2247 859 O
ATOM 1837 N GLN B 196 1.173 -80.061 -36.119 1.00 73.42 N
ANISOU 1837 N GLN B 196 8712 10477 8709 323 2462 1044 N
ATOM 1838 CA GLN B 196 0.407 -80.502 -37.276 1.00 79.39 C
ANISOU 1838 CA GLN B 196 9169 11476 9518 131 2733 1114 C
ATOM 1839 CB GLN B 196 -1.081 -80.536 -36.925 1.00 80.62 C
ANISOU 1839 CB GLN B 196 9371 11924 9337 289 2964 1292 C
ATOM 1840 CG GLN B 196 -1.388 -81.324 -35.658 1.00 92.59 C
ANISOU 1840 CG GLN B 196 11064 13445 10672 427 2957 1397 C
ATOM 1841 CD GLN B 196 -1.864 -82.739 -35.945 1.00 96.38 C
ANISOU 1841 CD GLN B 196 11319 14075 11228 251 3152 1500 C
ATOM 1842 OE1 GLN B 196 -2.392 -83.019 -37.023 1.00 95.20 O
ANISOU 1842 OE1 GLN B 196 10893 14110 11168 81 3353 1533 O
ATOM 1843 NE2 GLN B 196 -1.680 -83.638 -34.980 1.00 96.65 N
ANISOU 1843 NE2 GLN B 196 11480 14024 11220 290 3085 1552 N
ATOM 1844 C GLN B 196 0.633 -79.679 -38.550 1.00 82.00 C
ANISOU 1844 C GLN B 196 9349 11809 9999 -13 2770 1011 C
ATOM 1845 O GLN B 196 0.001 -79.940 -39.570 1.00 85.40 O
ANISOU 1845 O GLN B 196 9550 12434 10465 -174 2981 1063 O
ATOM 1846 N ARG B 197 1.525 -78.693 -38.496 1.00 70.77 N
ANISOU 1846 N ARG B 197 8064 10167 8659 41 2565 865 N
ATOM 1847 CA ARG B 197 1.804 -77.872 -39.672 1.00 65.26 C
ANISOU 1847 CA ARG B 197 7256 9444 8095 -100 2592 758 C
ATOM 1848 CB ARG B 197 1.687 -76.378 -39.353 1.00 62.00 C
ANISOU 1848 CB ARG B 197 7083 8995 7477 132 2495 722 C
ATOM 1849 CG ARG B 197 1.138 -76.053 -37.982 1.00 67.41 C
ANISOU 1849 CG ARG B 197 8047 9721 7844 453 2433 817 C
ATOM 1850 CD ARG B 197 -0.095 -75.161 -38.082 1.00 71.93 C
ANISOU 1850 CD ARG B 197 8688 10526 8116 629 2585 920 C

ATOM 1851 NE ARG B 197 0.103 -74.009 -38.956 1.00 65.71 N
ANISOU 1851 NE ARG B 197 7890 9699 7377 591 2559 826 N
ATOM 1852 CZ ARG B 197 -0.814 -73.070 -39.175 1.00 76.21 C
ANISOU 1852 CZ ARG B 197 9278 11189 8490 731 2653 886 C
ATOM 1853 NH1 ARG B 197 -0.556 -72.052 -39.991 1.00 79.34 N
ANISOU 1853 NH1 ARG B 197 9676 11526 8941 681 2613 796 N
ATOM 1854 NH2 ARG B 197 -1.993 -73.148 -38.573 1.00 79.11 N
ANISOU 1854 NH2 ARG B 197 9701 11766 8589 918 2788 1031 N
ATOM 1855 C ARG B 197 3.182 -78.158 -40.259 1.00 70.72 C
ANISOU 1855 C ARG B 197 7815 9873 9183 -347 2463 571 C
ATOM 1856 O ARG B 197 4.055 -78.713 -39.589 1.00 71.06 O
ANISOU 1856 O ARG B 197 7902 9707 9391 -350 2284 501 O
ATOM 1857 N LEU B 198 3.369 -77.769 -41.516 1.00 59.90 N
ANISOU 1857 N LEU B 198 8054 8945 5763 -704 156 1396 N
ATOM 1858 CA LEU B 198 4.670 -77.840 -42.169 1.00 66.08 C
ANISOU 1858 CA LEU B 198 8764 9710 6634 -607 66 1263 C
ATOM 1859 CB LEU B 198 4.522 -78.011 -43.678 1.00 40.58 C
ANISOU 1859 CB LEU B 198 5472 6400 3547 -603 108 1100 C
ATOM 1860 CG LEU B 198 5.517 -78.918 -44.409 1.00 54.88 C
ANISOU 1860 CG LEU B 198 7251 8063 5540 -502 39 1021 C
ATOM 1861 CD1 LEU B 198 5.577 -78.543 -45.884 1.00 48.83 C
ANISOU 1861 CD1 LEU B 198 6444 7286 4824 -500 109 816 C
ATOM 1862 CD2 LEU B 198 6.913 -78.891 -43.790 1.00 45.42 C
ANISOU 1862 CD2 LEU B 198 6001 6902 4354 -390 -57 1055 C
ATOM 1863 C LEU B 198 5.402 -76.538 -41.906 1.00 62.97 C
ANISOU 1863 C LEU B 198 8343 9493 6090 -595 73 1176 C
ATOM 1864 O LEU B 198 4.926 -75.466 -42.283 1.00 57.55 O
ANISOU 1864 O LEU B 198 7645 8908 5315 -644 189 1084 O
ATOM 1865 N TYR B 199 6.562 -76.621 -41.271 1.00 58.59 N
ANISOU 1865 N TYR B 199 7775 8972 5515 -534 -55 1213 N
ATOM 1866 CA TYR B 199 7.344 -75.427 -41.028 1.00 56.04 C
ANISOU 1866 CA TYR B 199 7422 8807 5062 -543 -71 1125 C
ATOM 1867 CB TYR B 199 7.931 -75.430 -39.626 1.00 68.63 C
ANISOU 1867 CB TYR B 199 9089 10476 6510 -560 -209 1265 C
ATOM 1868 CG TYR B 199 6.870 -75.257 -38.573 1.00 78.54 C
ANISOU 1868 CG TYR B 199 10516 11765 7560 -653 -132 1390 C
ATOM 1869 CD1 TYR B 199 6.082 -76.333 -38.170 1.00 79.03 C
ANISOU 1869 CD1 TYR B 199 10649 11710 7668 -654 -122 1556 C
ATOM 1870 CE1 TYR B 199 5.100 -76.179 -37.216 1.00 80.21 C
ANISOU 1870 CE1 TYR B 199 10952 11882 7640 -733 -22 1682 C
ATOM 1871 CZ TYR B 199 4.890 -74.933 -36.655 1.00 83.73 C
ANISOU 1871 CZ TYR B 199 11501 12461 7851 -808 80 1632 C
ATOM 1872 OH TYR B 199 3.911 -74.780 -35.702 1.00 91.29 O
ANISOU 1872 OH TYR B 199 12627 13425 8633 -876 216 1759 O
ATOM 1873 CE2 TYR B 199 5.653 -73.845 -37.045 1.00 80.33 C
ANISOU 1873 CE2 TYR B 199 11015 12139 7368 -815 67 1458 C
ATOM 1874 CD2 TYR B 199 6.633 -74.012 -38.003 1.00 79.60 C
ANISOU 1874 CD2 TYR B 199 10750 12031 7462 -740 -43 1343 C
ATOM 1875 C TYR B 199 8.408 -75.269 -42.094 1.00 49.32 C
ANISOU 1875 C TYR B 199 6428 7946 4364 -460 -94 969 C
ATOM 1876 O TYR B 199 9.326 -76.075 -42.204 1.00 41.86 O
ANISOU 1876 O TYR B 199 5407 6920 3577 -366 -202 1003 O
ATOM 1877 N ILE B 200 8.245 -74.232 -42.901 1.00 39.04 N
ANISOU 1877 N ILE B 200 5091 6717 3026 -488 27 811 N
ATOM 1878 CA ILE B 200 9.087 -74.019 -44.055 1.00 50.96 C
ANISOU 1878 CA ILE B 200 6480 8209 4673 -415 53 655 C
ATOM 1879 CB ILE B 200 8.240 -73.709 -45.275 1.00 45.61 C
ANISOU 1879 CB ILE B 200 5809 7504 4015 -439 201 533 C
ATOM 1880 CG1 ILE B 200 7.323 -74.891 -45.562 1.00 47.06 C
ANISOU 1880 CG1 ILE B 200 6052 7542 4286 -451 198 601 C
ATOM 1881 CD1 ILE B 200 6.407 -74.669 -46.736 1.00 45.30 C
ANISOU 1881 CD1 ILE B 200 5840 7299 4071 -499 305 504 C
ATOM 1882 CG2 ILE B 200 9.124 -73.414 -46.475 1.00 36.49 C
ANISOU 1882 CG2 ILE B 200 4558 6335 2972 -365 251 369 C
ATOM 1883 C ILE B 200 10.073 -72.896 -43.788 1.00 57.28 C
ANISOU 1883 C ILE B 200 7215 9149 5401 -427 27 583 C
ATOM 1884 O ILE B 200 9.686 -71.747 -43.573 1.00 48.74 O
ANISOU 1884 O ILE B 200 6184 8177 4157 -509 113 529 O
ATOM 1885 N LEU B 201 11.351 -73.247 -43.784 1.00 39.60 N
ANISOU 1885 N LEU B 201 4857 6894 3296 -347 -87 591 N
ATOM 1886 CA LEU B 201 12.382 -72.276 -43.481 1.00 58.20 C
ANISOU 1886 CA LEU B 201 7126 9378 5611 -373 -144 540 C
ATOM 1887 CB LEU B 201 13.637 -72.957 -42.942 1.00 54.35 C
ANISOU 1887 CB LEU B 201 6512 8879 5260 -300 -339 656 C
ATOM 1888 CG LEU B 201 13.450 -73.647 -41.594 1.00 57.73 C
ANISOU 1888 CG LEU B 201 7034 9315 5585 -332 -509 859 C
ATOM 1889 CD1 LEU B 201 14.664 -74.489 -41.268 1.00 46.05 C
ANISOU 1889 CD1 LEU B 201 5401 7800 4295 -228 -698 997 C
ATOM 1890 CD2 LEU B 201 13.226 -72.613 -40.509 1.00 64.44 C
ANISOU 1890 CD2 LEU B 201 8011 10323 6151 -484 -558 871 C
ATOM 1891 C LEU B 201 12.697 -71.443 -44.714 1.00 50.57 C
ANISOU 1891 C LEU B 201 6071 8428 4714 -350 4 355 C
ATOM 1892 O LEU B 201 12.817 -71.967 -45.821 1.00 38.34 O
ANISOU 1892 O LEU B 201 4466 6772 3328 -257 84 285 O
ATOM 1893 N LEU B 202 12.809 -70.137 -44.510 1.00 52.60 N
ANISOU 1893 N LEU B 202 6341 8810 4836 -439 53 275 N
ATOM 1894 CA LEU B 202 13.062 -69.214 -45.600 1.00 51.98 C
ANISOU 1894 CA LEU B 202 6192 8755 4802 -428 207 112 C
ATOM 1895 CB LEU B 202 11.796 -68.437 -45.944 1.00 52.06 C
ANISOU 1895 CB LEU B 202 6328 8791 4661 -492 383 52 C
ATOM 1896 CG LEU B 202 10.672 -69.242 -46.577 1.00 45.95 C
ANISOU 1896 CG LEU B 202 5620 7922 3918 -457 448 80 C
ATOM 1897 CD1 LEU B 202 9.365 -68.509 -46.408 1.00 51.03 C
ANISOU 1897 CD1 LEU B 202 6375 8615 4400 -538 573 96 C
ATOM 1898 CD2 LEU B 202 10.965 -69.457 -48.043 1.00 45.46 C
ANISOU 1898 CD2 LEU B 202 5487 7786 4000 -373 537 -35 C
ATOM 1899 C LEU B 202 14.173 -68.245 -45.249 1.00 44.28 C
ANISOU 1899 C LEU B 202 5121 7885 3819 -481 153 62 C
ATOM 1900 O LEU B 202 13.905 -67.084 -44.915 1.00 43.72 O
ANISOU 1900 O LEU B 202 5128 7900 3584 -590 221 1 O
ATOM 1901 N PRO B 203 15.423 -68.725 -45.304 1.00 44.72 N
ANISOU 1901 N PRO B 203 5002 7924 4066 -410 35 97 N
ATOM 1902 CA PRO B 203 16.555 -67.809 -45.150 1.00 45.86 C
ANISOU 1902 CA PRO B 203 5011 8163 4250 -466 -16 46 C
ATOM 1903 CB PRO B 203 17.771 -68.736 -45.162 1.00 41.96 C
ANISOU 1903 CB PRO B 203 4306 7626 4011 -354 -161 146 C
ATOM 1904 CG PRO B 203 17.289 -69.992 -45.866 1.00 47.92 C
ANISOU 1904 CG PRO B 203 5091 8223 4893 -206 -83 176 C
ATOM 1905 CD PRO B 203 15.853 -70.123 -45.458 1.00 42.28 C
ANISOU 1905 CD PRO B 203 4605 7502 3960 -276 -53 198 C
ATOM 1906 C PRO B 203 16.616 -66.851 -46.334 1.00 46.13 C
ANISOU 1906 C PRO B 203 5004 8195 4328 -456 205 -122 C
ATOM 1907 O PRO B 203 16.713 -67.282 -47.486 1.00 39.94 O
ANISOU 1907 O PRO B 203 4158 7319 4027 -336 332 -178 O
ATOM 1908 N LEU B 204 16.553 -65.557 -46.049 1.00 51.09 N
ANISOU 1908 N LEU B 204 5689 8913 4809 -585 261 -202 N
ATOM 1909 CA LEU B 204 16.578 -64.553 -47.097 1.00 51.59 C
ANISOU 1909 CA LEU B 204 5728 8975 4900 -582 477 -346 C
ATOM 1910 CB LEU B 204 16.164 -63.192 -46.558 1.00 58.39 C
ANISOU 1910 CB LEU B 204 6720 9912 5553 -735 551 -413 C
ATOM 1911 CG LEU B 204 14.708 -63.113 -46.138 1.00 59.56 C
ANISOU 1911 CG LEU B 204 7087 10053 5489 -772 629 -381 C
ATOM 1912 CD1 LEU B 204 14.376 -61.695 -45.750 1.00 66.56 C
ANISOU 1912 CD1 LEU B 204 8102 10987 6201 -901 757 -460 C
ATOM 1913 CD2 LEU B 204 13.812 -63.580 -47.279 1.00 53.69 C
ANISOU 1913 CD2 LEU B 204 6363 9236 4799 -657 780 -393 C
ATOM 1914 C LEU B 204 17.940 -64.449 -47.774 1.00 55.69 C
ANISOU 1914 C LEU B 204 6018 9484 5658 -522 489 -390 C
ATOM 1915 O LEU B 204 18.037 -64.001 -48.917 1.00 57.20 O
ANISOU 1915 O LEU B 204 6169 9638 5927 -465 687 -492 O
ATOM 1916 N ASP B 205 18.995 -64.850 -47.071 1.00 57.66 N
ANISOU 1916 N ASP B 205 6112 9770 6028 -534 282 -297 N
ATOM 1917 CA ASP B 205 20.325 -64.859 -47.668 1.00 41.42 C
ANISOU 1917 CA ASP B 205 3799 7697 4242 -463 293 -306 C
ATOM 1918 CB ASP B 205 21.419 -64.855 -46.599 1.00 43.92 C
ANISOU 1918 CB ASP B 205 3946 8106 4636 -551 24 -194 C
ATOM 1919 CG ASP B 205 21.443 -66.130 -45.773 1.00 81.55 C
ANISOU 1919 CG ASP B 205 8698 12857 9429 -490 -203 -15 C
ATOM 1920 OD1 ASP B 205 20.459 -66.904 -45.816 1.00 78.72 O
ANISOU 1920 OD1 ASP B 205 8505 12424 8980 -418 -160 13 O
ATOM 1921 OD2 ASP B 205 22.453 -66.346 -45.071 1.00 85.58 O
ANISOU 1921 OD2 ASP B 205 9024 13432 10059 -520 -433 109 O
ATOM 1922 C ASP B 205 20.463 -66.065 -48.604 1.00 48.66 C
ANISOU 1922 C ASP B 205 4640 8481 5368 -260 381 -276 C
ATOM 1923 O ASP B 205 21.492 -66.250 -49.266 1.00 60.16 O
ANISOU 1923 O ASP B 205 5892 9889 7076 -158 446 -277 O
ATOM 1924 N CYS B 206 19.412 -66.885 -48.627 1.00 53.14 N
ANISOU 1924 N CYS B 206 5382 8978 5832 -208 392 -248 N
ATOM 1925 CA CYS B 206 19.302 -68.069 -49.484 1.00 48.49 C
ANISOU 1925 CA CYS B 206 4795 8239 5390 -41 483 -239 C
ATOM 1926 CB CYS B 206 19.382 -67.688 -50.966 1.00 45.91 C
ANISOU 1926 CB CYS B 206 4505 7850 5091 -26 747 -386 C
ATOM 1927 SG CYS B 206 18.035 -66.634 -51.515 1.00 53.11 S
ANISOU 1927 SG CYS B 206 5603 8807 5770 -67 912 -514 S
ATOM 1928 C CYS B 206 20.320 -69.155 -49.161 1.00 42.93 C
ANISOU 1928 C CYS B 206 3906 7469 4937 78 350 -100 C
ATOM 1929 O CYS B 206 20.613 -70.004 -49.998 1.00 48.50 O
ANISOU 1929 O CYS B 206 4568 8030 5829 233 469 -109 O
ATOM 1930 N GLY B 207 20.871 -69.117 -47.953 1.00 53.82 N
ANISOU 1930 N GLY B 207 5182 8948 6319 5 109 32 N
ATOM 1931 CA GLY B 207 21.794 -70.145 -47.505 1.00 51.71 C
ANISOU 1931 CA GLY B 207 4726 8633 6288 116 -50 206 C
ATOM 1932 C GLY B 207 21.070 -71.383 -46.996 1.00 60.15 C
ANISOU 1932 C GLY B 207 5936 9603 7316 232 -296 390 C
ATOM 1933 O GLY B 207 20.353 -71.342 -45.993 1.00 55.02 O
ANISOU 1933 O GLY B 207 5436 9013 6457 190 -296 390 O
ATOM 1934 N VAL B 208 21.263 -72.495 -47.694 1.00 62.08 N
ANISOU 1934 N VAL B 208 6143 9677 7768 354 -39 354 N
ATOM 1935 CA VAL B 208 20.581 -73.740 -47.369 1.00 61.34 C
ANISOU 1935 CA VAL B 208 6189 9458 7661 418 -94 455 C
ATOM 1936 CB VAL B 208 19.648 -74.156 -48.508 1.00 55.52 C
ANISOU 1936 CB VAL B 208 5650 8564 6881 466 138 304 C
ATOM 1937 CG1 VAL B 208 18.960 -75.468 -48.172 1.00 60.75 C
ANISOU 1937 CG1 VAL B 208 6453 9080 7550 516 82 408 C
ATOM 1938 CG2 VAL B 208 18.634 -73.060 -48.787 1.00 44.02 C
ANISOU 1938 CG2 VAL B 208 4360 7216 5148 314 224 149 C
ATOM 1939 C VAL B 208 21.569 -74.877 -47.136 1.00 71.47 C
ANISOU 1939 C VAL B 208 7282 10627 9246 590 -178 641 C
ATOM 1940 O VAL B 208 22.240 -75.307 -48.079 1.00 73.14 O
ANISOU 1940 O VAL B 208 7379 10697 9714 750 -1 604 O

ATOM 1941 N PRO B 209 21.674 -75.369 -45.892 1.00 76.75 N
ANISOU 1941 N PRO B 209 7921 11351 9890 566 -434 850 N
ATOM 1942 CA PRO B 209 22.599 -76.484 -45.683 1.00 74.40 C
ANISOU 1942 CA PRO B 209 7432 10936 9902 748 -510 1055 C
ATOM 1943 CB PRO B 209 22.866 -76.460 -44.173 1.00 67.01 C
ANISOU 1943 CB PRO B 209 6433 10164 8865 653 -849 1279 C
ATOM 1944 CG PRO B 209 22.309 -75.152 -43.677 1.00 67.57 C
ANISOU 1944 CG PRO B 209 6637 10444 8594 417 -926 1159 C
ATOM 1945 CD PRO B 209 21.194 -74.813 -44.622 1.00 75.22 C
ANISOU 1945 CD PRO B 209 7831 11340 9410 381 -662 924 C
ATOM 1946 C PRO B 209 22.011 -77.839 -46.067 1.00 81.19 C
ANISOU 1946 C PRO B 209 8446 11551 10853 884 -388 1083 C
ATOM 1947 O PRO B 209 20.804 -78.063 -45.959 1.00 74.82 O
ANISOU 1947 O PRO B 209 7894 10707 9828 799 -368 1027 O
ATOM 1948 N ASP B 210 22.886 -78.736 -46.506 1.00 98.88 N
ANISOU 1948 N ASP B 210 10522 13614 13433 1093 -300 1177 N
ATOM 1949 CA ASP B 210 22.538 -80.125 -46.751 1.00105.98 C
ANISOU 1949 CA ASP B 210 11545 14254 14468 1237 -198 1238 C
ATOM 1950 CB ASP B 210 23.759 -80.852 -47.304 1.00116.33 C
ANISOU 1950 CB ASP B 210 12625 15383 16190 1482 -62 1333 C
ATOM 1951 CG ASP B 210 25.039 -80.065 -47.091 1.00113.98 C
ANISOU 1951 CG ASP B 210 11981 15260 16066 1504 -160 1426 C
ATOM 1952 OD1 ASP B 210 25.440 -79.884 -45.919 1.00113.95 O
ANISOU 1952 OD1 ASP B 210 11825 15434 16039 1440 -465 1637 O
ATOM 1953 OD2 ASP B 210 25.635 -79.618 -48.094 1.00107.48 O
ANISOU 1953 OD2 ASP B 210 11045 14398 15394 1573 64 1290 O
ATOM 1954 C ASP B 210 22.112 -80.772 -45.445 1.00103.09 C
ANISOU 1954 C ASP B 210 11251 13918 14002 1194 -451 1465 C
ATOM 1955 O ASP B 210 21.257 -81.657 -45.418 1.00102.62 O
ANISOU 1955 O ASP B 210 11402 13697 13893 1206 -404 1479 O
ATOM 1956 N ASN B 211 22.723 -80.330 -44.354 1.00101.38 N
ANISOU 1956 N ASN B 211 10862 13907 13751 1134 -724 1649 N
ATOM 1957 CA ASN B 211 22.332 -80.813 -43.041 1.00 96.37 C
ANISOU 1957 CA ASN B 211 10314 13331 12970 1074 -978 1871 C
ATOM 1958 CB ASN B 211 23.459 -81.586 -42.374 1.00103.55 C
ANISOU 1958 CB ASN B 211 10969 14213 14163 1233 -1163 2181 C
ATOM 1959 CG ASN B 211 23.017 -82.950 -41.924 1.00104.56 C
ANISOU 1959 CG ASN B 211 11226 14144 14360 1342 -1184 2370 C
ATOM 1960 OD1 ASN B 211 22.190 -83.079 -41.028 1.00106.42 O
ANISOU 1960 OD1 ASN B 211 11661 14442 14333 1220 -1328 2451 O
ATOM 1961 ND2 ASN B 211 23.534 -83.984 -42.577 1.00103.81 N
ANISOU 1961 ND2 ASN B 211 11035 13788 14620 1574 -1010 2436 N
ATOM 1962 C ASN B 211 21.826 -79.711 -42.131 1.00 85.61 C
ANISOU 1962 C ASN B 211 9058 12235 11236 832 -1171 1841 C
ATOM 1963 O ASN B 211 22.604 -78.920 -41.598 1.00 82.44 O
ANISOU 1963 O ASN B 211 8484 12033 10805 754 -1357 1900 O
ATOM 1964 N LEU B 212 20.508 -79.666 -41.967 1.00 78.49 N
ANISOU 1964 N LEU B 212 8443 11324 10056 709 -1116 1749 N
ATOM 1965 CA LEU B 212 19.887 -78.660 -41.125 1.00 76.93 C
ANISOU 1965 CA LEU B 212 8390 11344 9495 490 -1243 1711 C
ATOM 1966 CB LEU B 212 18.364 -78.700 -41.257 1.00 75.74 C
ANISOU 1966 CB LEU B 212 8532 11134 9113 393 -1096 1593 C
ATOM 1967 CG LEU B 212 17.512 -78.064 -40.154 1.00 72.30 C
ANISOU 1967 CG LEU B 212 8299 10862 8311 200 -1206 1626 C
ATOM 1968 CD1 LEU B 212 17.952 -76.639 -39.810 1.00 76.19 C
ANISOU 1968 CD1 LEU B 212 8744 11581 8622 52 -1291 1534 C
ATOM 1969 CD2 LEU B 212 16.058 -78.062 -40.593 1.00 57.26 C
ANISOU 1969 CD2 LEU B 212 6619 8877 6260 131 -1005 1494 C
ATOM 1970 C LEU B 212 20.290 -78.872 -39.679 1.00 87.24 C
ANISOU 1970 C LEU B 212 9668 12776 10703 443 -1553 1976 C
ATOM 1971 O LEU B 212 20.689 -77.926 -38.996 1.00 88.34 O
ANISOU 1971 O LEU B 212 9767 13128 10668 299 -1732 1987 O
ATOM 1972 N SER B 213 20.194 -80.116 -39.219 1.00 95.53 N
ANISOU 1972 N SER B 213 10752 13688 11857 556 -1620 2192 N
ATOM 1973 CA SER B 213 20.435 -80.437 -37.814 1.00 99.86 C
ANISOU 1973 CA SER B 213 11318 14343 12280 514 -1915 2469 C
ATOM 1974 CB SER B 213 20.388 -81.949 -37.578 1.00 98.55 C
ANISOU 1974 CB SER B 213 11165 13968 12312 689 -1928 2705 C
ATOM 1975 OG SER B 213 20.275 -82.654 -38.802 1.00 98.47 O
ANISOU 1975 OG SER B 213 11126 13704 12585 849 -1657 2587 O
ATOM 1976 C SER B 213 21.757 -79.856 -37.325 1.00106.65 C
ANISOU 1976 C SER B 213 11918 15398 13208 488 -2173 2586 C
ATOM 1977 O SER B 213 21.910 -79.529 -36.151 1.00111.35 O
ANISOU 1977 O SER B 213 12565 16174 13569 355 -2444 2732 O
ATOM 1978 N MET B 214 22.699 -79.699 -38.247 1.00111.66 N
ANISOU 1978 N MET B 214 12279 15992 14153 604 -2083 2516 N
ATOM 1979 CA MET B 214 24.029 -79.195 -37.930 1.00116.13 C
ANISOU 1979 CA MET B 214 12541 16724 14859 590 -2312 2634 C
ATOM 1980 CB MET B 214 25.026 -79.653 -38.995 1.00118.92 C
ANISOU 1980 CB MET B 214 12578 16926 15679 820 -2152 2648 C
ATOM 1981 CG MET B 214 25.832 -80.881 -38.605 1.00124.68 C
ANISOU 1981 CG MET B 214 13093 17546 16732 1034 -2289 2984 C
ATOM 1982 SD MET B 214 24.996 -81.995 -37.456 1.00203.20 S
ANISOU 1982 SD MET B 214 23302 27421 26484 1045 -2447 3233 S
ATOM 1983 CE MET B 214 23.737 -82.718 -38.496 1.00102.87 C
ANISOU 1983 CE MET B 214 10881 14410 13793 1136 -2041 3008 C
ATOM 1984 C MET B 214 24.070 -77.679 -37.801 1.00111.16 C
ANISOU 1984 C MET B 214 11941 16320 13975 353 -2371 2439 C
ATOM 1985 O MET B 214 24.795 -77.143 -36.960 1.00109.07 O
ANISOU 1985 O MET B 214 11562 16255 13626 226 -2666 2559 O
ATOM 1986 N ALA B 215 23.291 -76.996 -38.638 1.00108.50 N
ANISOU 1986 N ALA B 215 11763 15945 13517 289 -2097 2145 N
ATOM 1987 CA ALA B 215 23.247 -75.533 -38.640 1.00106.46 C
ANISOU 1987 CA ALA B 215 11553 15863 13033 78 -2095 1939 C
ATOM 1988 CB ALA B 215 22.180 -75.030 -39.599 1.00 99.85 C
ANISOU 1988 CB ALA B 215 10919 14943 12077 50 -1765 1655 C
ATOM 1989 C ALA B 215 23.010 -74.983 -37.239 1.00113.63 C
ANISOU 1989 C ALA B 215 12643 16967 13564 -146 -2368 2022 C
ATOM 1990 O ALA B 215 23.570 -73.954 -36.859 1.00119.67 O
ANISOU 1990 O ALA B 215 13349 17907 14215 -320 -2518 1971 O
ATOM 1991 N ASP B 216 22.187 -75.684 -36.470 1.00109.50 N
ANISOU 1991 N ASP B 216 12357 16404 12846 -150 -2423 2149 N
ATOM 1992 CA ASP B 216 21.976 -75.336 -35.075 1.00100.68 C
ANISOU 1992 CA ASP B 216 11443 15452 11360 -345 -2677 2259 C
ATOM 1993 CB ASP B 216 20.602 -74.698 -34.886 1.00 86.77 C
ANISOU 1993 CB ASP B 216 10044 13696 9229 -491 -2485 2074 C
ATOM 1994 CG ASP B 216 20.473 -73.963 -33.562 1.00 85.74 C
ANISOU 1994 CG ASP B 216 10145 13749 8685 -729 -2696 2112 C
ATOM 1995 OD1 ASP B 216 21.070 -74.404 -32.555 1.00 81.84 O
ANISOU 1995 OD1 ASP B 216 9628 13346 8122 -762 -3010 2351 O
ATOM 1996 OD2 ASP B 216 19.773 -72.930 -33.537 1.00 86.19 O
ANISOU 1996 OD2 ASP B 216 10418 13852 8477 -884 -2541 1904 O
ATOM 1997 C ASP B 216 22.099 -76.578 -34.206 1.00103.64 C
ANISOU 1997 C ASP B 216 11826 15787 11767 -245 -2889 2578 C
ATOM 1998 O ASP B 216 21.372 -77.552 -34.423 1.00112.65 O
ANISOU 1998 O ASP B 216 13072 16750 12979 -109 -2734 2634 O
ATOM 1999 N PRO B 217 23.005 -76.550 -33.217 1.00102.82 N
ANISOU 1999 N PRO B 217 11614 15844 11607 -322 -3252 2797 N
ATOM 2000 CA PRO B 217 23.112 -77.683 -32.297 1.00105.41 C
ANISOU 2000 CA PRO B 217 11969 16150 11933 -236 -3474 3127 C
ATOM 2001 CB PRO B 217 24.246 -77.266 -31.358 1.00108.70 C
ANISOU 2001 CB PRO B 217 12232 16797 12272 -374 -3896 3313 C
ATOM 2002 CG PRO B 217 24.243 -75.769 -31.418 1.00106.06 C
ANISOU 2002 CG PRO B 217 11982 16616 11699 -620 -3878 3036 C
ATOM 2003 CD PRO B 217 23.918 -75.460 -32.848 1.00101.90 C
ANISOU 2003 CD PRO B 217 11371 15944 11405 -514 -3488 2757 C
ATOM 2004 C PRO B 217 21.824 -77.866 -31.501 1.00102.07 C
ANISOU 2004 C PRO B 217 11957 15705 11119 -332 -3412 3140 C
ATOM 2005 O PRO B 217 21.486 -78.987 -31.116 1.00101.06 O
ANISOU 2005 O PRO B 217 11904 15463 11032 -209 -3431 3355 O
ATOM 2006 N ASN B 218 21.111 -76.768 -31.265 1.00101.95 N
ANISOU 2006 N ASN B 218 12205 15788 10744 -544 -3317 2917 N
ATOM 2007 CA ASN B 218 19.824 -76.817 -30.578 1.00103.23 C
ANISOU 2007 CA ASN B 218 12756 15922 10543 -636 -3198 2906 C
ATOM 2008 CB ASN B 218 19.442 -75.444 -30.025 1.00 99.42 C
ANISOU 2008 CB ASN B 218 12534 15599 9644 -898 -3189 2711 C
ATOM 2009 CG ASN B 218 20.028 -75.176 -28.658 1.00 99.11 C
ANISOU 2009 CG ASN B 218 12622 15644 9390 -1032 -3442 2779 C
ATOM 2010 OD1 ASN B 218 20.559 -76.076 -28.006 1.00 96.31 O
ANISOU 2010 OD1 ASN B 218 12200 15274 9121 -946 -3655 3022 O
ATOM 2011 ND2 ASN B 218 19.919 -73.932 -28.206 1.00 97.11 N
ANISOU 2011 ND2 ASN B 218 12567 15457 8871 -1234 -3393 2550 N
ATOM 2012 C ASN B 218 18.698 -77.336 -31.468 1.00 99.24 C
ANISOU 2012 C ASN B 218 12333 15202 10171 -505 -2830 2785 C
ATOM 2013 O ASN B 218 17.532 -77.322 -31.078 1.00 99.62 O
ANISOU 2013 O ASN B 218 12673 15211 9968 -574 -2674 2754 O
ATOM 2014 N ILE B 219 19.045 -77.773 -32.671 1.00 91.90 N
ANISOU 2014 N ILE B 219 11149 14132 9636 -325 -2687 2718 N
ATOM 2015 CA ILE B 219 18.074 -78.369 -33.572 1.00 84.84 C
ANISOU 2015 CA ILE B 219 10319 13027 8889 -208 -2374 2613 C
ATOM 2016 CB ILE B 219 17.821 -77.503 -34.803 1.00 80.55 C
ANISOU 2016 CB ILE B 219 9718 12462 8424 -227 -2117 2301 C
ATOM 2017 CG1 ILE B 219 17.124 -76.210 -34.395 1.00 82.56 C
ANISOU 2017 CG1 ILE B 219 10199 12859 8310 -441 -2046 2128 C
ATOM 2018 CD1 ILE B 219 16.530 -75.441 -35.549 1.00 80.61 C
ANISOU 2018 CD1 ILE B 219 9956 12569 8105 -455 -1754 1848 C
ATOM 2019 CG2 ILE B 219 16.970 -78.258 -35.816 1.00 73.92 C
ANISOU 2019 CG2 ILE B 219 8912 11401 7775 -100 -1840 2216 C
ATOM 2020 C ILE B 219 18.564 -79.726 -34.018 1.00 91.93 C
ANISOU 2020 C ILE B 219 11024 13737 10167 23 -2383 2788 C
ATOM 2021 O ILE B 219 19.578 -79.835 -34.703 1.00 99.18 O
ANISOU 2021 O ILE B 219 11661 14626 11396 145 -2409 2783 O
ATOM 2022 N ARG B 220 17.847 -80.767 -33.621 1.00 91.03 N
ANISOU 2022 N ARG B 220 11066 13483 10040 86 -2343 2949 N
ATOM 2023 CA ARG B 220 18.286 -82.121 -33.900 1.00 87.09 C
ANISOU 2023 CA ARG B 220 10420 12782 9887 303 -2352 3141 C
ATOM 2024 CB ARG B 220 18.643 -82.844 -32.603 1.00 99.40 C
ANISOU 2024 CB ARG B 220 12018 14386 11365 327 -2628 3493 C
ATOM 2025 CG ARG B 220 20.120 -82.856 -32.282 1.00107.39 C
ANISOU 2025 CG ARG B 220 12740 15515 12548 399 -2921 3686 C
ATOM 2026 CD ARG B 220 20.465 -84.098 -31.477 1.00119.55 C
ANISOU 2026 CD ARG B 220 14254 16972 14199 538 -3107 4064 C
ATOM 2027 NE ARG B 220 21.508 -84.894 -32.118 1.00126.77 N
ANISOU 2027 NE ARG B 220 14839 17741 15588 782 -3113 4200 N
ATOM 2028 CZ ARG B 220 21.759 -86.169 -31.837 1.00129.76 C
ANISOU 2028 CZ ARG B 220 15159 17946 16198 974 -3161 4497 C
ATOM 2029 NH1 ARG B 220 22.732 -86.813 -32.470 1.00129.01 N
ANISOU 2029 NH1 ARG B 220 14757 17707 16552 1206 -3131 4609 N
ATOM 2030 NH2 ARG B 220 21.036 -86.807 -30.927 1.00132.27 N
ANISOU 2030 NH2 ARG B 220 15728 18220 16309 942 -3217 4691 N

ATOM 2031 C ARG B 220 17.238 -82.915 -34.647 1.00 73.27 C
ANISOU 2031 C ARG B 220 8797 10782 8259 378 -2068 3054 C
ATOM 2032 O ARG B 220 16.046 -82.821 -34.362 1.00 72.31 O
ANISOU 2032 O ARG B 220 8920 10648 7906 264 -1954 3002 O
ATOM 2033 N PHE B 221 17.702 -83.706 -35.604 1.00 76.14 N
ANISOU 2033 N PHE B 221 8992 10941 8995 566 -1952 3041 N
ATOM 2034 CA PHE B 221 16.843 -84.614 -36.337 1.00 76.47 C
ANISOU 2034 CA PHE B 221 9151 10719 9186 637 -1710 2973 C
ATOM 2035 CB PHE B 221 17.611 -85.244 -37.489 1.00 71.19 C
ANISOU 2035 CB PHE B 221 8284 9845 8918 838 -1576 2914 C
ATOM 2036 CG PHE B 221 16.893 -86.382 -38.147 1.00 72.78 C
ANISOU 2036 CG PHE B 221 8615 9740 9297 919 -1361 2881 C
ATOM 2037 CD1 PHE B 221 15.934 -86.141 -39.120 1.00 76.27 C
ANISOU 2037 CD1 PHE B 221 9194 10100 9683 829 -1135 2607 C
ATOM 2038 CE1 PHE B 221 15.273 -87.189 -39.737 1.00 76.02 C
ANISOU 2038 CE1 PHE B 221 9293 9785 9807 874 -958 2567 C
ATOM 2039 CZ PHE B 221 15.573 -88.499 -39.379 1.00 76.06 C
ANISOU 2039 CZ PHE B 221 9299 9565 10036 1023 -979 2799 C
ATOM 2040 CE2 PHE B 221 16.531 -88.751 -38.407 1.00 73.04 C
ANISOU 2040 CE2 PHE B 221 8772 9259 9722 1136 -1190 3089 C
ATOM 2041 CD2 PHE B 221 17.184 -87.695 -37.801 1.00 74.16 C
ANISOU 2041 CD2 PHE B 221 8776 9703 9697 1078 -1392 3131 C
ATOM 2042 C PHE B 221 16.310 -85.682 -35.402 1.00 84.19 C
ANISOU 2042 C PHE B 221 10288 11583 10118 661 -1776 3239 C
ATOM 2043 O PHE B 221 17.066 -86.343 -34.683 1.00 98.40 O
ANISOU 2043 O PHE B 221 11997 13370 12022 770 -1965 3519 O
ATOM 2044 N LEU B 222 14.997 -85.853 -35.416 1.00 81.21 N
ANISOU 2044 N LEU B 222 10139 11121 9597 558 -1618 3166 N
ATOM 2045 CA LEU B 222 14.344 -86.789 -34.525 1.00 80.21 C
ANISOU 2045 CA LEU B 222 10186 10885 9403 554 -1648 3407 C
ATOM 2046 CB LEU B 222 13.034 -86.192 -34.028 1.00 74.82 C
ANISOU 2046 CB LEU B 222 9743 10304 8383 354 -1564 3337 C
ATOM 2047 CG LEU B 222 12.665 -86.447 -32.571 1.00 85.34 C
ANISOU 2047 CG LEU B 222 11259 11708 9457 287 -1693 3608 C
ATOM 2048 CD2 LEU B 222 11.926 -87.767 -32.426 1.00 90.23 C
ANISOU 2048 CD2 LEU B 222 11999 12070 10214 341 -1586 3778 C
ATOM 2049 CD1 LEU B 222 11.809 -85.305 -32.083 1.00 83.99 C
ANISOU 2049 CD1 LEU B 222 11266 11733 8912 88 -1634 3490 C
ATOM 2050 C LEU B 222 14.074 -88.082 -35.268 1.00 68.40 C
ANISOU 2050 C LEU B 222 8702 9061 8227 684 -1477 3423 C
ATOM 2051 O LEU B 222 14.440 -89.169 -34.817 1.00 90.57 O
ANISOU 2051 O LEU B 222 11495 11712 11205 816 -1543 3676 O
ATOM 2052 N ASP B 223 13.449 -87.950 -36.428 1.00 66.05 N
ANISOU 2052 N ASP B 223 8437 8652 8007 641 -1258 3151 N
ATOM 2053 CA ASP B 223 12.876 -89.092 -37.104 1.00 68.40 C
ANISOU 2053 CA ASP B 223 8820 8636 8531 693 -1080 3127 C
ATOM 2054 CB ASP B 223 11.741 -89.643 -36.253 1.00 69.52 C
ANISOU 2054 CB ASP B 223 9170 8714 8530 587 -1066 3292 C
ATOM 2055 CG ASP B 223 11.650 -91.139 -36.301 1.00 74.01 C
ANISOU 2055 CG ASP B 223 9800 8957 9364 698 -997 3453 C
ATOM 2056 OD1 ASP B 223 11.716 -91.698 -37.418 1.00 77.66 O
ANISOU 2056 OD1 ASP B 223 10244 9186 10079 764 -844 3295 O
ATOM 2057 OD2 ASP B 223 11.524 -91.749 -35.218 1.00 85.74 O
ANISOU 2057 OD2 ASP B 223 11369 10412 10797 716 -1089 3738 O
ATOM 2058 C ASP B 223 12.328 -88.681 -38.459 1.00 70.87 C
ANISOU 2058 C ASP B 223 9155 8890 8883 621 -880 2795 C
ATOM 2059 O ASP B 223 12.285 -87.497 -38.791 1.00 73.99 O
ANISOU 2059 O ASP B 223 9505 9492 9115 530 -871 2606 O
ATOM 2060 N LYS B 224 11.895 -89.665 -39.235 1.00 70.99 N
ANISOU 2060 N LYS B 224 9252 8616 9106 652 -723 2729 N
ATOM 2061 CA LYS B 224 11.299 -89.410 -40.534 1.00 71.08 C
ANISOU 2061 CA LYS B 224 9316 8551 9141 567 -549 2428 C
ATOM 2062 CB LYS B 224 11.991 -90.243 -41.612 1.00 78.77 C
ANISOU 2062 CB LYS B 224 10257 9247 10425 723 -417 2327 C
ATOM 2063 CG LYS B 224 13.242 -89.615 -42.199 1.00 85.97 C
ANISOU 2063 CG LYS B 224 10977 10252 11434 859 -410 2221 C
ATOM 2064 CD LYS B 224 12.896 -88.333 -42.931 1.00 91.59 C
ANISOU 2064 CD LYS B 224 11677 11171 11951 726 -359 1952 C
ATOM 2065 CE LYS B 224 13.744 -88.137 -44.181 1.00 91.82 C
ANISOU 2065 CE LYS B 224 11616 11127 12146 840 -218 1744 C
ATOM 2066 NZ LYS B 224 13.362 -86.877 -44.907 1.00 78.39 N
ANISOU 2066 NZ LYS B 224 9915 9625 10244 708 -164 1495 N
ATOM 2067 C LYS B 224 9.821 -89.748 -40.489 1.00 66.39 C
ANISOU 2067 C LYS B 224 8904 7870 8451 389 -472 2413 C
ATOM 2068 O LYS B 224 9.417 -90.699 -39.823 1.00 72.47 O
ANISOU 2068 O LYS B 224 9771 8484 9280 390 -484 2614 O
ATOM 2069 N LEU B 225 9.010 -88.961 -41.189 1.00 64.95 N
ANISOU 2069 N LEU B 225 8757 7788 8132 237 -393 2192 N
ATOM 2070 CA LEU B 225 7.598 -89.274 -41.350 1.00 69.97 C
ANISOU 2070 CA LEU B 225 9530 8334 8720 61 -314 2162 C
ATOM 2071 CB LEU B 225 6.863 -88.104 -41.998 1.00 60.51 C
ANISOU 2071 CB LEU B 225 8319 7329 7344 -89 -262 1951 C
ATOM 2072 CG LEU B 225 6.184 -87.069 -41.103 1.00 68.75 C
ANISOU 2072 CG LEU B 225 9360 8637 8126 -203 -296 2031 C
ATOM 2073 CD1 LEU B 225 5.432 -86.076 -41.971 1.00 52.06 C
ANISOU 2073 CD1 LEU B 225 7226 6654 5903 -332 -216 1820 C
ATOM 2074 CD2 LEU B 225 5.239 -87.737 -40.117 1.00 79.39 C
ANISOU 2074 CD2 LEU B 225 10814 9911 9442 -287 -293 2256 C
ATOM 2075 C LEU B 225 7.500 -90.495 -42.247 1.00 90.96 C
ANISOU 2075 C LEU B 225 12279 10654 11628 85 -212 2084 C
ATOM 2076 O LEU B 225 8.450 -90.790 -42.984 1.00 96.21 O
ANISOU 2076 O LEU B 225 12903 11193 12461 226 -164 1981 O
ATOM 2077 N PRO B 226 6.367 -91.216 -42.201 1.00 95.47 N
ANISOU 2077 N PRO B 226 12979 11064 12232 -57 -165 2132 N
ATOM 2078 CA PRO B 226 6.280 -92.330 -43.146 1.00 97.42 C
ANISOU 2078 CA PRO B 226 13337 10976 12702 -60 -66 2020 C
ATOM 2079 CB PRO B 226 4.971 -93.030 -42.757 1.00 97.09 C
ANISOU 2079 CB PRO B 226 13415 10801 12674 -241 -49 2135 C
ATOM 2080 CG PRO B 226 4.172 -91.983 -42.048 1.00 93.34 C
ANISOU 2080 CG PRO B 226 12878 10630 11957 -367 -101 2210 C
ATOM 2081 CD PRO B 226 5.177 -91.119 -41.342 1.00 92.08 C
ANISOU 2081 CD PRO B 226 12604 10719 11663 -216 -184 2285 C
ATOM 2082 C PRO B 226 6.223 -91.820 -44.585 1.00 91.99 C
ANISOU 2082 C PRO B 226 12663 10298 11992 -125 8 1704 C
ATOM 2083 O PRO B 226 5.623 -90.775 -44.853 1.00 83.24 O
ANISOU 2083 O PRO B 226 11509 9421 10696 -252 -12 1594 O
ATOM 2084 N GLN B 227 6.869 -92.550 -45.488 1.00 90.49 N
ANISOU 2084 N GLN B 227 12543 9851 11989 -27 104 1570 N
ATOM 2085 CA GLN B 227 6.978 -92.157 -46.885 1.00 84.23 C
ANISOU 2085 CA GLN B 227 11794 9040 11170 -65 188 1272 C
ATOM 2086 CB GLN B 227 7.701 -93.240 -47.677 1.00 78.72 C
ANISOU 2086 CB GLN B 227 11219 7987 10703 60 327 1169 C
ATOM 2087 CG GLN B 227 9.147 -93.415 -47.305 1.00 80.79 C
ANISOU 2087 CG GLN B 227 11355 8208 11133 341 361 1287 C
ATOM 2088 CD GLN B 227 9.696 -94.739 -47.786 1.00 95.49 C
ANISOU 2088 CD GLN B 227 13353 9661 13269 475 519 1268 C
ATOM 2089 OE1 GLN B 227 9.152 -95.801 -47.471 1.00 96.72 O
ANISOU 2089 OE1 GLN B 227 13646 9565 13536 417 537 1370 O
ATOM 2090 NE2 GLN B 227 10.772 -94.687 -48.560 1.00100.70 N
ANISOU 2090 NE2 GLN B 227 13980 10234 14048 654 656 1138 N
ATOM 2091 C GLN B 227 5.624 -91.905 -47.527 1.00 89.11 C
ANISOU 2091 C GLN B 227 12506 9696 11655 -329 176 1129 C
ATOM 2092 O GLN B 227 4.626 -92.522 -47.157 1.00 88.83 O
ANISOU 2092 O GLN B 227 12549 9557 11646 -482 146 1231 O
ATOM 2093 N GLN B 228 5.596 -90.993 -48.492 1.00 94.73 N
ANISOU 2093 N GLN B 228 13198 10560 12233 -384 195 910 N
ATOM 2094 CA GLN B 228 4.401 -90.798 -49.297 1.00 93.52 C
ANISOU 2094 CA GLN B 228 13132 10429 11970 -627 174 765 C
ATOM 2095 CB GLN B 228 3.826 -89.398 -49.126 1.00 85.12 C
ANISOU 2095 CB GLN B 228 11926 9723 10693 -715 106 773 C
ATOM 2096 CG GLN B 228 2.385 -89.323 -49.573 1.00 78.85 C
ANISOU 2096 CG GLN B 228 11176 8961 9824 -974 53 736 C
ATOM 2097 CD GLN B 228 1.948 -87.920 -49.899 1.00 80.65 C
ANISOU 2097 CD GLN B 228 11286 9498 9858 -1041 24 673 C
ATOM 2098 OE1 GLN B 228 2.002 -87.029 -49.051 1.00 80.98 O
ANISOU 2098 OE1 GLN B 228 11189 9772 9807 -980 14 796 O
ATOM 2099 NE2 GLN B 228 1.521 -87.706 -51.139 1.00 84.72 N
ANISOU 2099 NE2 GLN B 228 11872 10014 10305 -1170 14 481 N
ATOM 2100 C GLN B 228 4.677 -91.064 -50.769 1.00 90.83 C
ANISOU 2100 C GLN B 228 12948 9915 11647 -650 264 487 C
ATOM 2101 O GLN B 228 5.680 -90.609 -51.322 1.00 93.30 O
ANISOU 2101 O GLN B 228 13232 10268 11950 -496 344 360 O
ATOM 2102 N THR B 229 3.774 -91.805 -51.395 1.00 84.09 N
ANISOU 2102 N THR B 229 12268 8866 10816 -855 253 396 N
ATOM 2103 CA THR B 229 3.910 -92.155 -52.796 1.00 81.57 C
ANISOU 2103 CA THR B 229 12154 8357 10481 -917 331 124 C
ATOM 2104 CB THR B 229 3.653 -93.650 -53.020 1.00 89.58 C
ANISOU 2104 CB THR B 229 13402 9191 11442 -1004 382 91 C
ATOM 2105 OG1 THR B 229 4.468 -94.405 -52.119 1.00 93.66 O
ANISOU 2105 OG1 THR B 229 13885 9705 11995 -785 460 270 O
ATOM 2106 CG2 THR B 229 3.988 -94.051 -54.451 1.00 92.26 C
ANISOU 2106 CG2 THR B 229 12998 9361 11742 -1041 497 -207 C
ATOM 2107 C THR B 229 2.949 -91.301 -53.606 1.00 74.13 C
ANISOU 2107 C THR B 229 11214 7625 9327 -1141 237 -7 C
ATOM 2108 O THR B 229 1.940 -90.828 -53.088 1.00 68.42 O
ANISOU 2108 O THR B 229 10366 7098 8533 -1288 117 127 O
ATOM 2109 N ILE B 230 3.284 -91.080 -54.870 1.00 86.55 N
ANISOU 2109 N ILE B 230 12925 9160 10801 -1155 301 -256 N
ATOM 2110 CA ILE B 230 2.616 -90.068 -55.666 1.00 97.11 C
ANISOU 2110 CA ILE B 230 14237 10741 11919 -1313 216 -368 C
ATOM 2111 C ILE B 230 1.945 -90.697 -56.854 1.00103.87 C
ANISOU 2111 C ILE B 230 15254 10742 13469 -1532 253 -577 C
ATOM 2112 O ILE B 230 2.503 -91.586 -57.496 1.00103.69 O
ANISOU 2112 O ILE B 230 15572 10192 13632 -1555 301 -733 O
ATOM 2113 CB ILE B 230 3.614 -89.040 -56.212 1.00101.03 C
ANISOU 2113 CB ILE B 230 14673 11407 12307 -1132 317 -491 C
ATOM 2114 CG1 ILE B 230 4.762 -88.848 -55.229 1.00100.37 C
ANISOU 2114 CG1 ILE B 230 14412 11370 12352 -855 401 -352 C
ATOM 2115 CG2 ILE B 230 2.916 -87.721 -56.492 1.00 99.24 C
ANISOU 2115 CG2 ILE B 230 14313 11518 11875 -1244 217 -490 C
ATOM 2116 CD1 ILE B 230 4.298 -88.390 -53.865 1.00100.15 C
ANISOU 2116 CD1 ILE B 230 14163 11556 12332 -857 289 -96 C
ATOM 2117 N ASP B 231 0.749 -90.222 -57.159 1.00110.22 N
ANISOU 2117 N ASP B 231 15848 11377 14654 -1712 230 -584 N
ATOM 2118 CA ASP B 231 0.047 -90.694 -58.331 1.00119.46 C
ANISOU 2118 CA ASP B 231 17153 11777 16459 -1941 253 -788 C
ATOM 2119 CB ASP B 231 -1.428 -90.904 -58.011 1.00117.13 C
ANISOU 2119 CB ASP B 231 16717 11369 16417 -2170 169 -677 C
ATOM 2120 CG ASP B 231 -2.062 -91.964 -58.879 1.00119.36 C
ANISOU 2120 CG ASP B 231 17153 11000 17197 -2373 220 -824 C
ATOM 2121 OD1 ASP B 231 -1.328 -92.844 -59.377 1.00120.46 O
ANISOU 2121 OD1 ASP B 231 17525 10777 17466 -2299 335 -1000 O
ATOM 2122 OD2 ASP B 231 -3.294 -91.918 -59.067 1.00118.79 O
ANISOU 2122 OD2 ASP B 231 16966 10773 17395 -2606 150 -760 O

ATOM 2121 OD2 ASP B 231 -2.060 -93.142 -58.463 1.00123.34 O
ANISOU 2121 OD2 ASP B 231 18328 13400 15135 -2666 -316 -719 O
ATOM 2122 OD1 ASP B 231 -2.553 -91.624 -59.977 1.00116.74 O
ANISOU 2122 OD1 ASP B 231 17481 12949 13927 -2827 -476 -894 O
ATOM 2123 C ASP B 231 0.180 -89.661 -59.429 1.00124.08 C
ANISOU 2123 C ASP B 231 18139 14215 14791 -2074 -80 -903 C
ATOM 2124 O ASP B 231 0.368 -90.005 -60.598 1.00124.61 O
ANISOU 2124 O ASP B 231 18480 14125 14741 -2157 -44 -1138 O
ATOM 2125 N ARG B 232 0.110 -88.395 -59.020 1.00123.32 N
ANISOU 2125 N ARG B 232 17780 14457 14621 -1985 -111 -777 N
ATOM 2126 CA ARG B 232 -0.134 -87.270 -59.921 1.00120.75 C
ANISOU 2126 CA ARG B 232 17426 14381 14071 -2045 -165 -862 C
ATOM 2127 CB ARG B 232 0.000 -85.937 -59.181 1.00111.88 C
ANISOU 2127 CB ARG B 232 16001 13585 12925 -1887 -143 -697 C
ATOM 2128 CG ARG B 232 -0.742 -85.877 -57.864 1.00106.07 C
ANISOU 2128 CG ARG B 232 15031 12955 12316 -1917 -220 -432 C
ATOM 2129 CD ARG B 232 -2.209 -85.469 -58.008 1.00105.07 C
ANISOU 2129 CD ARG B 232 14786 13004 12131 -2161 -397 -311 C
ATOM 2130 NE ARG B 232 -2.598 -84.446 -57.033 1.00102.74 N
ANISOU 2130 NE ARG B 232 14211 12973 11852 -2086 -388 -91 N
ATOM 2131 CZ ARG B 232 -2.495 -84.563 -55.707 1.00103.39 C
ANISOU 2131 CZ ARG B 232 14166 13057 12060 -1978 -329 88 C
ATOM 2132 NH1 ARG B 232 -2.010 -85.668 -55.153 1.00106.19 N
ANISOU 2132 NH1 ARG B 232 14622 13172 12555 -1922 -285 97 N
ATOM 2133 NH2 ARG B 232 -2.880 -83.564 -54.922 1.00 97.17 N
ANISOU 2133 NH2 ARG B 232 13161 12505 11252 -1924 -304 264 N
ATOM 2134 C ARG B 232 0.720 -87.255 -61.183 1.00123.82 C
ANISOU 2134 C ARG B 232 18068 14661 14315 -1982 -40 -1130 C
ATOM 2135 O ARG B 232 1.802 -87.840 -61.236 1.00127.43 O
ANISOU 2135 O ARG B 232 18660 14895 14864 -1803 145 -1238 O
ATOM 2136 N ALA B 233 0.206 -86.564 -62.193 1.00120.79 N
ANISOU 2136 N ALA B 233 17744 14441 13709 -2128 -136 -1220 N
ATOM 2137 CA ALA B 233 0.765 -86.589 -63.536 1.00116.54 C
ANISOU 2137 CA ALA B 233 17497 13801 12983 -2134 -43 -1479 C
ATOM 2138 CB ALA B 233 -0.140 -85.839 -64.479 1.00107.16 C
ANISOU 2138 CB ALA B 233 16337 12833 11546 -2350 -225 -1507 C
ATOM 2139 C ALA B 233 2.178 -86.031 -63.620 1.00121.46 C
ANISOU 2139 C ALA B 233 18098 14440 13613 -1826 209 -1559 C
ATOM 2140 O ALA B 233 2.563 -85.150 -62.850 1.00114.68 O
ANISOU 2140 O ALA B 233 16960 13791 12823 -1646 255 -1414 O
ATOM 2141 N GLY B 234 2.941 -86.548 -64.579 1.00131.81 N
ANISOU 2141 N GLY B 234 19712 15519 14852 -1777 377 -1794 N
ATOM 2142 CA GLY B 234 4.302 -86.103 -64.805 1.00135.87 C
ANISOU 2142 CA GLY B 234 20222 16017 15387 -1495 639 -1881 C
ATOM 2143 C GLY B 234 5.242 -86.488 -63.680 1.00145.69 C
ANISOU 2143 C GLY B 234 21283 17151 16921 -1239 781 -1761 C
ATOM 2144 O GLY B 234 6.353 -85.964 -63.591 1.00144.33 O
ANISOU 2144 O GLY B 234 20997 17026 16817 -994 965 -1764 O
ATOM 2145 N ILE B 235 4.800 -87.415 -62.832 1.00155.51 N
ANISOU 2145 N ILE B 235 22497 18248 18342 -1301 691 -1644 N
ATOM 2146 CA ILE B 235 5.556 -87.799 -61.636 1.00151.99 C
ANISOU 2146 CA ILE B 235 21860 17721 18167 -1076 779 -1482 C
ATOM 2147 CB ILE B 235 5.568 -86.633 -60.600 1.00138.87 C
ANISOU 2147 CB ILE B 235 19830 16407 16528 -976 694 -1265 C
ATOM 2148 CG1 ILE B 235 6.451 -86.947 -59.398 1.00133.39 C
ANISOU 2148 CG1 ILE B 235 18946 15655 16081 -744 768 -1098 C
ATOM 2149 CD1 ILE B 235 6.095 -86.150 -58.163 1.00130.97 C
ANISOU 2149 CD1 ILE B 235 18341 15632 15789 -731 630 -864 C
ATOM 2150 CG2 ILE B 235 4.155 -86.247 -60.171 1.00138.70 C
ANISOU 2150 CG2 ILE B 235 19690 16594 16418 -1204 457 -1123 C
ATOM 2151 C ILE B 235 5.438 -89.236 -61.087 1.00142.70 C
ANISOU 2151 C ILE B 235 20772 16287 17161 -1179 708 -1404 C
ATOM 2152 O ILE B 235 5.874 -89.548 -59.976 1.00140.03 O
ANISOU 2152 O ILE B 235 20222 16016 16969 -1147 617 -1182 O
ATOM 2153 N LYS B 236 4.812 -90.119 -61.856 1.00134.69 N
ANISOU 2153 N LYS B 236 20092 14965 16120 -1310 759 -1589 N
ATOM 2154 CA LYS B 236 4.291 -91.359 -61.308 1.00125.94 C
ANISOU 2154 CA LYS B 236 19078 13600 15174 -1431 693 -1518 C
ATOM 2155 CB LYS B 236 3.765 -92.287 -62.409 1.00123.68 C
ANISOU 2155 CB LYS B 236 19193 13022 14779 -1680 688 -1754 C
ATOM 2156 CG LYS B 236 4.774 -93.247 -62.975 1.00118.98 C
ANISOU 2156 CG LYS B 236 18898 12028 14280 -1530 968 -1943 C
ATOM 2157 CD LYS B 236 4.067 -94.332 -63.757 1.00112.62 C
ANISOU 2157 CD LYS B 236 18491 10902 13397 -1819 930 -2138 C
ATOM 2158 CE LYS B 236 4.027 -94.031 -65.238 1.00104.95 C
ANISOU 2158 CE LYS B 236 17842 9922 12115 -1963 964 -2425 C
ATOM 2159 NZ LYS B 236 3.192 -95.049 -65.931 1.00104.61 N
ANISOU 2159 NZ LYS B 236 18184 9594 11969 -2301 868 -2607 N
ATOM 2160 C LYS B 236 5.300 -92.055 -60.400 1.00119.11 C
ANISOU 2160 C LYS B 236 18129 12531 14598 -1157 862 -1394 C
ATOM 2161 O LYS B 236 6.496 -92.105 -60.695 1.00119.34 O
ANISOU 2161 O LYS B 236 18197 12439 14707 -913 1088 -1475 O
ATOM 2162 N ASP B 237 4.804 -92.535 -59.266 1.00115.87 N
ANISOU 2162 N ASP B 237 17577 12100 14348 -1191 748 -1174 N
ATOM 2163 CA ASP B 237 5.586 -93.357 -58.351 1.00113.72 C
ANISOU 2163 CA ASP B 237 17244 11612 14352 -966 869 -1023 C
ATOM 2164 CB ASP B 237 5.972 -94.673 -59.022 1.00116.41 C
ANISOU 2164 CB ASP B 237 17924 11493 14814 -954 1059 -1194 C
ATOM 2165 CG ASP B 237 4.978 -95.769 -58.750 1.00117.04 C
ANISOU 2165 CG ASP B 237 18161 11333 14975 -1189 957 -1152 C
ATOM 2166 OD1 ASP B 237 3.867 -95.718 -59.316 1.00117.48 O
ANISOU 2166 OD1 ASP B 237 18343 11438 14856 -1503 793 -1255 O
ATOM 2167 OD2 ASP B 237 5.302 -96.674 -57.953 1.00113.38 O
ANISOU 2167 OD2 ASP B 237 17683 10636 14759 -1063 1033 -999 O
ATOM 2168 C ASP B 237 6.823 -92.692 -57.752 1.00104.16 C
ANISOU 2168 C ASP B 237 15774 10559 13243 -643 975 -901 C
ATOM 2169 O ASP B 237 7.798 -93.371 -57.423 1.00109.02 O
ANISOU 2169 O ASP B 237 16388 10953 14083 -414 1134 -842 O
ATOM 2170 N ARG B 238 6.796 -91.372 -57.609 1.00 85.47 N
ANISOU 2170 N ARG B 238 13183 8566 10726 -627 885 -856 N
ATOM 2171 CA ARG B 238 7.854 -90.710 -56.872 1.00 75.40 C
ANISOU 2171 CA ARG B 238 11637 7464 9546 -364 937 -713 C
ATOM 2172 CB ARG B 238 7.801 -89.201 -57.072 1.00 59.15 C
ANISOU 2172 CB ARG B 238 9408 5782 7285 -383 873 -741 C
ATOM 2173 CG ARG B 238 9.123 -88.509 -56.843 1.00 75.14 C
ANISOU 2173 CG ARG B 238 11230 7928 9391 -122 985 -700 C
ATOM 2174 CD ARG B 238 9.622 -87.841 -58.116 1.00 74.99 C
ANISOU 2174 CD ARG B 238 11301 7949 9243 -87 1134 -927 C
ATOM 2175 NE ARG B 238 9.274 -86.424 -58.164 1.00 71.44 N
ANISOU 2175 NE ARG B 238 10698 7854 8590 -161 1038 -924 N
ATOM 2176 CZ ARG B 238 9.582 -85.605 -59.165 1.00 72.13 C
ANISOU 2176 CZ ARG B 238 10829 8044 8534 -148 1139 -1087 C
ATOM 2177 NH1 ARG B 238 10.257 -86.064 -60.211 1.00 73.10 N
ANISOU 2177 NH1 ARG B 238 11154 7943 8679 -66 1348 -1274 N
ATOM 2178 NH2 ARG B 238 9.218 -84.329 -59.123 1.00 74.26 N
ANISOU 2178 NH2 ARG B 238 10953 8624 8636 -213 1051 -1059 N
ATOM 2179 C ARG B 238 7.633 -91.057 -55.409 1.00 80.76 C
ANISOU 2179 C ARG B 238 12141 8179 10367 -330 815 -430 C
ATOM 2180 O ARG B 238 6.511 -91.365 -55.010 1.00 88.18 O
ANISOU 2180 O ARG B 238 13114 9123 11268 -531 675 -347 O
ATOM 2181 N VAL B 239 8.685 -91.044 -54.603 1.00 61.80 N
ANISOU 2181 N VAL B 239 9553 5796 8130 -83 863 -269 N
ATOM 2182 CA VAL B 239 8.494 -91.237 -53.173 1.00 68.99 C
ANISOU 2182 CA VAL B 239 10301 6784 9129 -54 730 12 C
ATOM 2183 CB VAL B 239 9.048 -92.578 -52.653 1.00 71.55 C
ANISOU 2183 CB VAL B 239 10684 6779 9724 98 811 149 C
ATOM 2184 CG1 VAL B 239 8.890 -92.661 -51.144 1.00 70.00 C
ANISOU 2184 CG1 VAL B 239 10316 6699 9580 133 663 457 C
ATOM 2185 CG2 VAL B 239 8.342 -93.746 -53.324 1.00 66.73 C
ANISOU 2185 CG2 VAL B 239 10371 5819 9166 -59 879 19 C
ATOM 2186 C VAL B 239 9.087 -90.084 -52.385 1.00 64.72 C
ANISOU 2186 C VAL B 239 9482 6579 8531 69 653 148 C
ATOM 2187 O VAL B 239 10.280 -89.810 -52.465 1.00 59.43 O
ANISOU 2187 O VAL B 239 8696 5928 7957 276 742 145 O
ATOM 2188 N TYR B 240 8.230 -89.400 -51.637 1.00 67.75 N
ANISOU 2188 N TYR B 240 8658 6217 8761 -68 496 267 N
ATOM 2189 CA TYR B 240 8.658 -88.287 -50.811 1.00 65.26 C
ANISOU 2189 CA TYR B 240 9220 7215 8360 10 414 391 C
ATOM 2190 CB TYR B 240 7.656 -87.153 -50.891 1.00 52.70 C
ANISOU 2190 CB TYR B 240 7591 5902 6530 -175 334 345 C
ATOM 2191 CG TYR B 240 7.664 -86.410 -52.188 1.00 74.23 C
ANISOU 2191 CG TYR B 240 10365 8702 9136 -222 410 106 C
ATOM 2192 CD2 TYR B 240 8.281 -85.175 -52.299 1.00 61.95 C
ANISOU 2192 CD2 TYR B 240 8667 7384 7486 -145 433 57 C
ATOM 2193 CE2 TYR B 240 8.276 -84.488 -53.489 1.00 58.98 C
ANISOU 2193 CE2 TYR B 240 8343 7073 6994 -185 512 -147 C
ATOM 2194 CZ TYR B 240 7.650 -85.036 -54.593 1.00 73.55 C
ANISOU 2194 CZ TYR B 240 10398 8755 8795 -311 552 -310 C
ATOM 2195 OH TYR B 240 7.640 -84.358 -55.788 1.00 68.54 O
ANISOU 2195 OH TYR B 240 9835 8189 8018 -355 622 -503 O
ATOM 2196 CE1 TYR B 240 7.028 -86.262 -54.504 1.00 82.85 C
ANISOU 2196 CE1 TYR B 240 11725 9696 10060 -406 515 -277 C
ATOM 2197 CD1 TYR B 240 7.046 -86.938 -53.307 1.00 78.22 C
ANISOU 2197 CD1 TYR B 240 11073 9037 9611 -356 455 -69 C
ATOM 2198 C TYR B 240 8.757 -88.702 -49.364 1.00 70.75 C
ANISOU 2198 C TYR B 240 9821 7925 9135 74 311 669 C
ATOM 2199 O TYR B 240 8.005 -89.556 -48.894 1.00 71.35 O
ANISOU 2199 O TYR B 240 9993 7856 9259 -15 271 782 O
ATOM 2200 N SER B 241 9.675 -88.075 -48.649 1.00 73.13 N
ANISOU 2200 N SER B 241 9938 8407 9441 217 259 784 N
ATOM 2201 CA SER B 241 9.734 -88.242 -47.215 1.00 74.30 C
ANISOU 2201 CA SER B 241 10000 8633 9596 255 131 1053 C
ATOM 2202 CB SER B 241 10.872 -89.179 -46.813 1.00 70.03 C
ANISOU 2202 CB SER B 241 9402 7902 9304 474 144 1206 C
ATOM 2203 OG SER B 241 12.097 -88.479 -46.758 1.00 76.28 O
ANISOU 2203 OG SER B 241 10001 8845 10137 627 128 1215 O
ATOM 2204 C SER B 241 9.921 -86.870 -46.586 1.00 69.65 C
ANISOU 2204 C SER B 241 9258 8389 8816 236 34 1094 C
ATOM 2205 O SER B 241 10.463 -85.956 -47.209 1.00 61.40 O
ANISOU 2205 O SER B 241 8128 7480 7720 269 78 945 O
ATOM 2206 N ASN B 242 9.454 -86.732 -45.354 1.00 70.57 N
ANISOU 2206 N ASN B 242 9359 8634 8819 174 -83 1293 N
ATOM 2207 CA ASN B 242 9.621 -85.505 -44.603 1.00 52.13 C
ANISOU 2207 CA ASN B 242 6916 6601 6288 145 -173 1345 C
ATOM 2208 CB ASN B 242 8.276 -84.819 -44.395 1.00 60.04 C
ANISOU 2208 CB ASN B 242 7990 7599 7223 -47 -173 1325 C
ATOM 2209 CG ASN B 242 7.598 -84.466 -45.700 1.00 59.03 C
ANISOU 2209 CG ASN B 242 7909 7604 6916 -148 -62 1098 C
ATOM 2210 OD1 ASN B 242 6.952 -85.311 -46.322 1.00 58.02 O
ANISOU 2210 OD1 ASN B 242 7889 7279 6877 -214 -15 1047 O

ATOM 2211 ND2 ASN B 242 7.762 -83.217 -46.138 1.00 53.49 N
ANISOU 2211 ND2 ASN B 242 7135 7103 6086 -168 -32 962 N
ATOM 2212 C ASN B 242 10.268 -85.802 -43.267 1.00 57.66 C
ANISOU 2212 C ASN B 242 7555 7349 7005 236 -311 1601 C
ATOM 2213 O ASN B 242 10.037 -86.858 -42.681 1.00 55.55 O
ANISOU 2213 O ASN B 242 7361 6918 6829 261 -342 1778 O
ATOM 2214 N SER B 243 11.069 -84.863 -42.781 1.00 55.40 N
ANISOU 2214 N SER B 243 7141 7285 6625 275 -402 1628 N
ATOM 2215 CA SER B 243 11.867 -85.090 -41.589 1.00 57.61 C
ANISOU 2215 CA SER B 243 7346 7628 6916 362 -567 1868 C
ATOM 2216 CB SER B 243 13.307 -84.661 -41.827 1.00 63.12 C
ANISOU 2216 CB SER B 243 7842 8405 7736 496 -620 1842 C
ATOM 2217 OG SER B 243 13.840 -85.318 -42.955 1.00 80.80 O
ANISOU 2217 OG SER B 243 10033 10425 10241 630 -482 1733 O
ATOM 2218 C SER B 243 11.320 -84.377 -40.367 1.00 64.20 C
ANISOU 2218 C SER B 243 8245 8683 7465 232 -676 1988 C
ATOM 2219 O SER B 243 10.816 -83.258 -40.456 1.00 64.72 O
ANISOU 2219 O SER B 243 8335 8926 7328 111 -634 1858 O
ATOM 2220 N ILE B 244 11.450 -85.032 -39.219 1.00 63.60 N
ANISOU 2220 N ILE B 244 8209 8586 7370 265 -803 2245 N
ATOM 2221 CA ILE B 244 10.965 -84.496 -37.958 1.00 70.32 C
ANISOU 2221 CA ILE B 244 9162 9621 7935 149 -899 2383 C
ATOM 2222 CB ILE B 244 10.158 -85.544 -37.200 1.00 69.84 C
ANISOU 2222 CB ILE B 244 9254 9415 7867 127 -893 2598 C
ATOM 2223 CG1 ILE B 244 9.018 -86.055 -38.068 1.00 65.43 C
ANISOU 2223 CG1 ILE B 244 8778 8668 7413 60 -708 2479 C
ATOM 2224 CD1 ILE B 244 8.306 -87.231 -37.472 1.00 61.07 C
ANISOU 2224 CD1 ILE B 244 8355 7926 6923 46 -687 2687 C
ATOM 2225 CG2 ILE B 244 9.621 -84.972 -35.901 1.00 69.56 C
ANISOU 2225 CG2 ILE B 244 9354 9562 7512 6 -958 2737 C
ATOM 2226 C ILE B 244 12.135 -84.060 -37.093 1.00 71.63 C
ANISOU 2226 C ILE B 244 9228 9966 8023 197 -1109 2515 C
ATOM 2227 O ILE B 244 13.123 -84.779 -36.970 1.00 78.15 O
ANISOU 2227 O ILE B 244 9935 10711 9049 343 -1221 2660 O
ATOM 2228 N TYR B 245 12.022 -82.886 -36.487 1.00 68.99 N
ANISOU 2228 N TYR B 245 8942 9867 7403 70 -1165 2472 N
ATOM 2229 CA TYR B 245 13.115 -82.332 -35.708 1.00 72.23 C
ANISOU 2229 CA TYR B 245 9267 10466 7710 73 -1385 2567 C
ATOM 2230 CB TYR B 245 13.679 -81.097 -36.398 1.00 64.00 C
ANISOU 2230 CB TYR B 245 8094 9572 6649 33 -1360 2334 C
ATOM 2231 CG TYR B 245 14.442 -81.406 -37.660 1.00 65.21 C
ANISOU 2231 CG TYR B 245 8040 9603 7134 178 -1284 2215 C
ATOM 2232 CD1 TYR B 245 13.778 -81.569 -38.876 1.00 54.88 C
ANISOU 2232 CD1 TYR B 245 6758 8147 5946 196 -1057 2021 C
ATOM 2233 CE1 TYR B 245 14.472 -81.854 -40.029 1.00 54.85 C
ANISOU 2233 CE1 TYR B 245 6604 8020 6216 326 -965 1905 C
ATOM 2234 CZ TYR B 245 15.857 -81.982 -39.979 1.00 68.45 C
ANISOU 2234 CZ TYR B 245 8113 9761 8133 456 -1084 1995 C
ATOM 2235 OH TYR B 245 16.572 -82.265 -41.122 1.00 56.99 O
ANISOU 2235 OH TYR B 245 6515 8174 6964 599 -956 1886 O
ATOM 2236 CE2 TYR B 245 16.538 -81.824 -38.782 1.00 60.73 C
ANISOU 2236 CE2 TYR B 245 7070 8940 7067 439 -1330 2204 C
ATOM 2237 CD2 TYR B 245 15.829 -81.538 -37.637 1.00 62.09 C
ANISOU 2237 CD2 TYR B 245 7425 9238 6929 294 -1436 2305 C
ATOM 2238 C TYR B 245 12.680 -81.971 -34.301 1.00 83.23 C
ANISOU 2238 C TYR B 245 10854 12009 8759 -58 -1493 2719 C
ATOM 2239 O TYR B 245 11.529 -81.603 -34.075 1.00 91.08 O
ANISOU 2239 O TYR B 245 12031 13023 9552 -176 -1350 2666 O
ATOM 2240 N GLU B 246 13.596 -82.083 -33.348 1.00 81.90 N
ANISOU 2240 N GLU B 246 10650 11947 8522 -37 -1745 2920 N
ATOM 2241 CA GLU B 246 13.318 -81.576 -32.018 1.00 86.01 C
ANISOU 2241 CA GLU B 246 11379 12635 8666 -181 -1862 3037 C
ATOM 2242 CB GLU B 246 13.632 -82.606 -30.927 1.00 96.92 C
ANISOU 2242 CB GLU B 246 12823 13982 10019 -120 -2064 3373 C
ATOM 2243 CG GLU B 246 15.082 -82.672 -30.488 1.00108.60 C
ANISOU 2243 CG GLU B 246 14118 15577 11567 -58 -2379 3537 C
ATOM 2244 CD GLU B 246 15.432 -84.013 -29.872 1.00123.05 C
ANISOU 2244 CD GLU B 246 15927 17289 13536 82 -2530 3876 C
ATOM 2245 OE1 GLU B 246 15.051 -84.262 -28.705 1.00123.49 O
ANISOU 2245 OE1 GLU B 246 16203 17395 13321 13 -2630 4085 O
ATOM 2246 OE2 GLU B 246 16.076 -84.827 -30.566 1.00130.20 O
ANISOU 2246 OE2 GLU B 246 16606 18037 14825 269 -2528 3938 O
ATOM 2247 C GLU B 246 14.092 -80.290 -31.806 1.00 84.01 C
ANISOU 2247 C GLU B 246 11073 12613 8235 -290 -2001 2917 C
ATOM 2248 O GLU B 246 15.216 -80.127 -32.291 1.00 79.50 O
ANISOU 2248 O GLU B 246 10260 12086 7862 -222 -2124 2880 O
ATOM 2249 N LEU B 247 13.462 -79.370 -31.091 1.00 90.72 N
ANISOU 2249 N LEU B 247 12154 13596 8720 -463 -1958 2852 N
ATOM 2250 CA LEU B 247 14.046 -78.076 -30.811 1.00 95.56 C
ANISOU 2250 CA LEU B 247 12776 14414 9120 -603 -2065 2718 C
ATOM 2251 CB LEU B 247 13.072 -76.983 -31.208 1.00 87.34 C
ANISOU 2251 CB LEU B 247 11875 13397 7914 -718 -1790 2466 C
ATOM 2252 CG LEU B 247 12.490 -77.211 -32.592 1.00 81.32 C
ANISOU 2252 CG LEU B 247 10978 12481 7440 -614 -1537 2308 C
ATOM 2253 CD1 LEU B 247 11.454 -76.169 -32.813 1.00 82.23 C
ANISOU 2253 CD1 LEU B 247 11241 12629 7372 -726 -1284 2116 C
ATOM 2254 CD2 LEU B 247 13.584 -77.114 -33.638 1.00 75.08 C
ANISOU 2254 CD2 LEU B 247 9894 11687 6947 -517 -1600 2194 C
ATOM 2255 C LEU B 247 14.319 -77.990 -29.330 1.00 99.21 C
ANISOU 2255 C LEU B 247 13437 15018 9241 -720 -2306 2914 C
ATOM 2256 O LEU B 247 13.601 -78.584 -28.525 1.00101.58 O
ANISOU 2256 O LEU B 247 13950 15240 9404 -719 -2252 3052 O
ATOM 2257 N LEU B 248 15.337 -77.259 -28.929 1.00 97.94 N
ANISOU 2257 N LEU B 248 13204 15014 8995 -808 -2533 2872 N
ATOM 2258 CA LEU B 248 15.681 -77.234 -27.525 1.00102.92 C
ANISOU 2258 CA LEU B 248 13989 15685 9431 -871 -2718 2957 C
ATOM 2259 CB LEU B 248 17.048 -77.859 -27.315 1.00 99.32 C
ANISOU 2259 CB LEU B 248 13268 15289 9182 -786 -3067 3174 C
ATOM 2260 CG LEU B 248 17.505 -78.935 -28.285 1.00 89.53 C
ANISOU 2260 CG LEU B 248 11732 13958 8327 -574 -3135 3398 C
ATOM 2261 CD1 LEU B 248 18.782 -79.583 -27.795 1.00 79.76 C
ANISOU 2261 CD1 LEU B 248 10273 12766 7264 -494 -3462 3619 C
ATOM 2262 CD2 LEU B 248 16.441 -79.989 -28.464 1.00 86.34 C
ANISOU 2262 CD2 LEU B 248 11471 13373 7962 -465 -2956 3547 C
ATOM 2263 C LEU B 248 15.661 -75.850 -26.900 1.00110.24 C
ANISOU 2263 C LEU B 248 15107 16704 10077 -1056 -2680 2719 C
ATOM 2264 O LEU B 248 16.100 -74.882 -27.510 1.00111.08 O
ANISOU 2264 O LEU B 248 15104 16889 10211 -1136 -2663 2524 O
ATOM 2265 N GLU B 249 15.133 -75.757 -25.685 1.00107.55 N
ANISOU 2265 N GLU B 249 15057 16340 9469 -1115 -2653 2742 N
ATOM 2266 CA GLU B 249 15.349 -74.591 -24.850 1.00107.14 C
ANISOU 2266 CA GLU B 249 15188 16371 9148 -1280 -2695 2581 C
ATOM 2267 CB GLU B 249 14.046 -73.874 -24.516 1.00104.50 C
ANISOU 2267 CB GLU B 249 15161 15953 8592 -1335 -2345 2400 C
ATOM 2268 CG GLU B 249 14.199 -72.367 -24.602 1.00112.35 C
ANISOU 2268 CG GLU B 249 16190 16986 9514 -1464 -2220 2115 C
ATOM 2269 CD GLU B 249 12.937 -71.598 -24.308 1.00116.37 C
ANISOU 2269 CD GLU B 249 16973 17393 9850 -1486 -1858 1956 C
ATOM 2270 OE1 GLU B 249 12.294 -71.123 -25.256 1.00114.53 O
ANISOU 2270 OE1 GLU B 249 16688 17090 9737 -1447 -1588 1818 O
ATOM 2271 OE2 GLU B 249 12.599 -71.444 -23.129 1.00118.74 O
ANISOU 2271 OE2 GLU B 249 17527 17685 9903 -1535 -1841 1979 O
ATOM 2272 C GLU B 249 16.060 -75.028 -23.586 1.00112.53 C
ANISOU 2272 C GLU B 249 15940 17113 9703 -1295 -2986 2781 C
ATOM 2273 O GLU B 249 15.608 -75.930 -22.908 1.00121.73 O
ANISOU 2273 O GLU B 249 17245 18207 10801 -1213 -2959 2961 O
ATOM 2274 N ASN B 250 17.176 -74.399 -23.262 1.00109.84 N
ANISOU 2274 N ASN B 250 15489 16903 9341 -1402 -3266 2758 N
ATOM 2275 CA ASN B 250 17.925 -74.807 -22.090 1.00120.61 C
ANISOU 2275 CA ASN B 250 16880 18349 10596 -1432 -3585 2949 C
ATOM 2276 CB ASN B 250 17.037 -74.702 -20.868 1.00129.25 C
ANISOU 2276 CB ASN B 250 18374 19422 11314 -1509 -3484 2933 C
ATOM 2277 CG ASN B 250 16.461 -73.322 -20.696 1.00131.19 C
ANISOU 2277 CG ASN B 250 18854 19662 11329 -1665 -3254 2636 C
ATOM 2278 OD1 ASN B 250 17.194 -72.338 -20.649 1.00136.26 O
ANISOU 2278 OD1 ASN B 250 19487 20399 11888 -1826 -3399 2501 O
ATOM 2279 ND2 ASN B 250 15.145 -73.237 -20.596 1.00125.70 N
ANISOU 2279 ND2 ASN B 250 18357 18845 10557 -1615 -2884 2540 N
ATOM 2280 C ASN B 250 18.472 -76.226 -22.190 1.00117.49 C
ANISOU 2280 C ASN B 250 16252 17930 10458 -1252 -3789 3263 C
ATOM 2281 O ASN B 250 18.643 -76.908 -21.198 1.00115.12 O
ANISOU 2281 O ASN B 250 16056 17641 10045 -1222 -3947 3465 O
ATOM 2282 N GLY B 251 18.753 -76.666 -23.399 1.00114.76 N
ANISOU 2282 N GLY B 251 15594 17546 10465 -1123 -3773 3307 N
ATOM 2283 CA GLY B 251 19.474 -77.898 -23.590 1.00114.27 C
ANISOU 2283 CA GLY B 251 15272 17440 10708 -934 -3950 3602 C
ATOM 2284 C GLY B 251 18.570 -79.078 -23.477 1.00117.08 C
ANISOU 2284 C GLY B 251 15777 17634 11072 -792 -3773 3761 C
ATOM 2285 O GLY B 251 19.023 -80.206 -23.568 1.00120.17 O
ANISOU 2285 O GLY B 251 15997 17967 11693 -626 -3911 4017 O
ATOM 2286 N GLN B 252 17.283 -78.811 -23.313 1.00117.47 N
ANISOU 2286 N GLN B 252 16142 17620 10870 -860 -3490 3617 N
ATOM 2287 CA GLN B 252 16.277 -79.854 -23.204 1.00119.13 C
ANISOU 2287 CA GLN B 252 16504 17669 11089 -748 -3294 3747 C
ATOM 2288 CB GLN B 252 15.707 -79.884 -21.791 1.00131.29 C
ANISOU 2288 CB GLN B 252 18387 19205 12292 -800 -3256 3816 C
ATOM 2289 CG GLN B 252 14.357 -80.573 -21.648 1.00137.67 C
ANISOU 2289 CG GLN B 252 19424 19854 13030 -744 -2935 3850 C
ATOM 2290 CD GLN B 252 14.341 -81.963 -22.230 1.00142.83 C
ANISOU 2290 CD GLN B 252 19942 20349 13976 -568 -2922 4101 C
ATOM 2291 OE1 GLN B 252 15.237 -82.340 -22.975 1.00145.38 O
ANISOU 2291 OE1 GLN B 252 19974 20662 14603 -463 -3103 4226 O
ATOM 2292 NE2 GLN B 252 13.313 -82.731 -21.903 1.00143.70 N
ANISOU 2292 NE2 GLN B 252 20262 20321 14018 -529 -2687 4179 N
ATOM 2293 C GLN B 252 15.171 -79.620 -24.209 1.00108.97 C
ANISOU 2293 C GLN B 252 15261 16285 9856 -749 -2939 3567 C
ATOM 2294 O GLN B 252 14.888 -78.498 -24.572 1.00101.43 O
ANISOU 2294 O GLN B 252 14387 15385 8765 -870 -2790 3308 O
ATOM 2295 N ARG B 253 14.539 -80.701 -24.640 1.00112.48 N
ANISOU 2295 N ARG B 253 15778 18102 8859 -576 -1105 2972 N
ATOM 2296 CA ARG B 253 13.600 -80.650 -25.738 1.00106.03 C
ANISOU 2296 CA ARG B 253 14840 17795 9656 -815 -2896 3702 C
ATOM 2297 CB ARG B 253 14450 16845 8323 -417 -672 3195 C
ATOM 2298 CG ARG B 253 11.713 -82.084 -26.750 1.00104.17 C
ANISOU 2298 CG ARG B 253 14318 16730 8534 -366 -351 3144 C
ATOM 2299 CD ARG B 253 11.300 -83.510 -27.032 1.00106.79 C
ANISOU 2299 CD ARG B 253 14518 16937 9121 -299 -232 3446 C
ATOM 2300 NE ARG B 253 12.413 -84.313 -27.519 1.00109.44 N
ANISOU 2300 NE ARG B 253 14665 17183 9734 -239 -489 3644 N

ATOM 2301 CZ ARG B 253 12.302 -85.576 -27.902 1.00109.01 C
ANISOU 2301 CZ ARG B 253 14495 16976 9947 -174 -435 3903 C
ATOM 2302 NH1 ARG B 253 11.131 -86.170 -27.856 1.00110.67 N
ANISOU 2302 NH1 ARG B 253 14746 17118 10187 -184 -153 3999 N
ATOM 2303 NH2 ARG B 253 13.358 -86.246 -28.328 1.00104.40 N
ANISOU 2303 NH2 ARG B 253 13757 16293 9616 -98 -647 4062 N
ATOM 2304 C ARG B 253 12.501 -79.736 -25.337 1.00101.97 C
ANISOU 2304 C ARG B 253 14578 16686 7481 -543 -481 2660 C
ATOM 2305 O ARG B 253 11.990 -79.831 -24.251 1.00100.27 O
ANISOU 2305 O ARG B 253 14606 16517 6975 -551 -312 2719 O
ATOM 2306 N ALA B 254 12.131 -78.847 -26.237 1.00 98.19 N
ANISOU 2306 N ALA B 254 14040 16165 7102 -544 -373 2403 N
ATOM 2307 CA ALA B 254 11.086 -77.879 -25.945 1.00 89.90 C
ANISOU 2307 CA ALA B 254 13209 15115 5833 -545 -45 2158 C
ATOM 2308 CB ALA B 254 11.694 -76.511 -25.678 1.00 91.63 C
ANISOU 2308 CB ALA B 254 13645 15367 5806 -634 -177 1837 C
ATOM 2309 C ALA B 254 10.088 -77.798 -27.091 1.00 85.63 C
ANISOU 2309 C ALA B 254 12443 14488 5604 -459 231 2110 C
ATOM 2310 O ALA B 254 9.178 -76.971 -27.074 1.00 80.87 O
ANISOU 2310 O ALA B 254 11950 13867 4910 -428 530 1908 O
ATOM 2311 N GLY B 255 10.274 -78.649 -28.095 1.00 90.59 N
ANISOU 2311 N GLY B 255 12757 15052 6612 -407 134 2296 N
ATOM 2312 CA GLY B 255 9.376 -78.691 -29.232 1.00 65.34 C
ANISOU 2312 CA GLY B 255 9327 11770 3731 -325 359 2284 C
ATOM 2313 C GLY B 255 9.712 -79.780 -30.233 1.00 73.76 C
ANISOU 2313 C GLY B 255 10101 12696 5228 -275 217 2489 C
ATOM 2314 O GLY B 255 10.854 -80.232 -30.327 1.00 74.38 O
ANISOU 2314 O GLY B 255 10116 12793 5352 -290 -83 2614 O
ATOM 2315 N THR B 256 8.704 -80.201 -30.988 1.00 73.09 N
ANISOU 2315 N THR B 256 9840 12457 5474 -214 439 2520 N
ATOM 2316 CA THR B 256 8.885 -81.197 -32.031 1.00 67.31 C
ANISOU 2316 CA THR B 256 8869 11542 5165 -175 342 2666 C
ATOM 2317 CB THR B 256 8.457 -82.589 -31.551 1.00 69.95 C
ANISOU 2317 CB THR B 256 9190 11857 5530 -180 425 3012 C
ATOM 2318 OG1 THR B 256 9.159 -82.928 -30.352 1.00 73.64 O
ANISOU 2318 OG1 THR B 256 9836 12484 5660 -211 284 3190 O
ATOM 2319 CG2 THR B 256 8.745 -83.623 -32.618 1.00 58.75 C
ANISOU 2319 CG2 THR B 256 7572 10218 4534 -145 318 3144 C
ATOM 2320 C THR B 256 8.060 -80.807 -33.256 1.00 67.67 C
ANISOU 2320 C THR B 256 8734 11415 5561 -136 497 2483 C
ATOM 2321 O THR B 256 6.867 -80.541 -33.138 1.00 77.30 O
ANISOU 2321 O THR B 256 9947 12642 6780 -128 770 2443 O
ATOM 2322 N CYS B 257 8.685 -80.771 -34.430 1.00 66.39 N
ANISOU 2322 N CYS B 257 8421 11107 5696 -109 329 2387 N
ATOM 2323 CA CYS B 257 7.982 -80.309 -35.623 1.00 70.95 C
ANISOU 2323 CA CYS B 257 8847 11538 6574 -81 440 2207 C
ATOM 2324 CB CYS B 257 7.947 -78.777 -35.656 1.00 76.14 C
ANISOU 2324 CB CYS B 257 9580 12253 7098 -66 488 1909 C
ATOM 2325 SG CYS B 257 9.560 -78.008 -35.989 1.00123.88 S
ANISOU 2325 SG CYS B 257 15664 18308 13097 -83 178 1735 S
ATOM 2326 C CYS B 257 8.569 -80.827 -36.938 1.00 65.27 C
ANISOU 2326 C CYS B 257 7965 10627 6209 -57 276 2206 C
ATOM 2327 O CYS B 257 9.745 -81.184 -37.014 1.00 67.68 O
ANISOU 2327 O CYS B 257 8268 10918 6530 -40 63 2272 O
ATOM 2328 N VAL B 258 7.731 -80.849 -37.972 1.00 53.60 N
ANISOU 2328 N VAL B 258 6351 9008 5008 -55 383 2136 N
ATOM 2329 CA VAL B 258 8.169 -81.139 -39.332 1.00 49.06 C
ANISOU 2329 CA VAL B 258 5656 8244 4741 -38 260 2078 C
ATOM 2330 CB VAL B 258 7.025 -81.674 -40.202 1.00 54.71 C
ANISOU 2330 CB VAL B 258 6248 8814 5724 -80 380 2111 C
ATOM 2331 CG2 VAL B 258 6.482 -82.959 -39.620 1.00 67.44 C
ANISOU 2331 CG2 VAL B 258 7871 10397 7357 -137 461 2378 C
ATOM 2332 CG1 VAL B 258 7.489 -81.886 -41.642 1.00 49.40 C
ANISOU 2332 CG1 VAL B 258 5499 7947 5324 -70 255 2019 C
ATOM 2333 C VAL B 258 8.720 -79.860 -39.949 1.00 53.21 C
ANISOU 2333 C VAL B 258 6173 8777 5269 -4 179 1815 C
ATOM 2334 O VAL B 258 8.020 -78.855 -40.052 1.00 53.18 O
ANISOU 2334 O VAL B 258 6167 8810 5231 3 301 1650 O
ATOM 2335 N LEU B 259 9.975 -79.907 -40.374 1.00 58.54 N
ANISOU 2335 N LEU B 259 6834 9406 6001 23 -13 1792 N
ATOM 2336 CA LEU B 259 10.723 -78.699 -40.658 1.00 53.14 C
ANISOU 2336 CA LEU B 259 6165 8764 5263 34 -111 1579 C
ATOM 2337 CB LEU B 259 11.633 -78.403 -39.470 1.00 53.17 C
ANISOU 2337 CB LEU B 259 6283 8947 4974 5 -241 1618 C
ATOM 2338 CG LEU B 259 12.281 -77.038 -39.290 1.00 62.54 C
ANISOU 2338 CG LEU B 259 7544 10221 5999 -34 -331 1401 C
ATOM 2339 CD1 LEU B 259 11.268 -76.035 -38.779 1.00 59.33 C
ANISOU 2339 CD1 LEU B 259 7267 9869 5405 -52 -137 1232 C
ATOM 2340 CD2 LEU B 259 13.426 -77.176 -38.310 1.00 73.41 C
ANISOU 2340 CD2 LEU B 259 8986 11756 7150 -86 -542 1513 C
ATOM 2341 C LEU B 259 11.571 -78.904 -41.899 1.00 61.07 C
ANISOU 2341 C LEU B 259 7259 9618 6521 73 -235 1541 C
ATOM 2342 O LEU B 259 12.289 -79.897 -41.996 1.00 70.70 O
ANISOU 2342 O LEU B 259 8250 10777 7836 105 -329 1705 O
ATOM 2343 N GLU B 260 11.501 -77.972 -42.846 1.00 58.63 N
ANISOU 2343 N GLU B 260 6717 9242 6319 81 -221 1335 N
ATOM 2344 CA GLU B 260 12.359 -78.051 -44.021 1.00 58.16 C
ANISOU 2344 CA GLU B 260 6578 9052 6470 118 -319 1288 C
ATOM 2345 CB GLU B 260 11.824 -79.078 -45.020 1.00 50.41 C
ANISOU 2345 CB GLU B 260 5546 7884 5724 134 -259 1358 C
ATOM 2346 CG GLU B 260 10.596 -78.650 -45.780 1.00 55.43 C
ANISOU 2346 CG GLU B 260 6155 8455 6452 103 -147 1241 C
ATOM 2347 CD GLU B 260 9.917 -79.823 -46.470 1.00 65.19 C
ANISOU 2347 CD GLU B 260 7369 9533 7869 69 -105 1343 C
ATOM 2348 OE1 GLU B 260 10.023 -80.956 -45.948 1.00 75.25 O
ANISOU 2348 OE1 GLU B 260 8672 10771 9147 61 -106 1523 O
ATOM 2349 OE2 GLU B 260 9.294 -79.609 -47.531 1.00 48.80 O
ANISOU 2349 OE2 GLU B 260 5257 7362 5922 40 -81 1248 O
ATOM 2350 C GLU B 260 12.609 -76.709 -44.704 1.00 54.88 C
ANISOU 2350 C GLU B 260 6152 8624 6077 115 -335 1061 C
ATOM 2351 O GLU B 260 11.821 -75.769 -44.577 1.00 57.42 O
ANISOU 2351 O GLU B 260 6516 8982 6320 98 -237 927 O
ATOM 2352 N TYR B 261 13.730 -76.639 -45.419 1.00 54.81 N
ANISOU 2352 N TYR B 261 6083 8556 6187 142 -443 1037 N
ATOM 2353 CA TYR B 261 14.097 -75.467 -46.197 1.00 49.69 C
ANISOU 2353 CA TYR B 261 5417 7871 5591 134 -461 848 C
ATOM 2354 CB TYR B 261 15.597 -75.452 -46.472 1.00 52.50 C
ANISOU 2354 CB TYR B 261 5696 8233 6018 147 -599 881 C
ATOM 2355 CG TYR B 261 16.446 -74.967 -45.325 1.00 55.29 C
ANISOU 2355 CG TYR B 261 6068 8763 6179 81 -740 905 C
ATOM 2356 CD1 TYR B 261 16.571 -73.605 -45.053 1.00 44.20 C
ANISOU 2356 CD1 TYR B 261 4732 7421 4643 -4 -770 724 C
ATOM 2357 CE1 TYR B 261 17.347 -73.156 -44.004 1.00 48.79 C
ANISOU 2357 CE1 TYR B 261 5353 8159 5024 -101 -923 733 C
ATOM 2358 CZ TYR B 261 18.020 -74.078 -43.213 1.00 62.25 C
ANISOU 2358 CZ TYR B 261 7005 9985 6662 -101 -1060 949 C
ATOM 2359 OH TYR B 261 18.801 -73.647 -42.164 1.00 60.64 O
ANISOU 2359 OH TYR B 261 6842 9959 6241 -219 -1247 972 O
ATOM 2360 CE2 TYR B 261 17.913 -75.438 -43.469 1.00 60.16 C
ANISOU 2360 CE2 TYR B 261 6659 9655 6544 9 -1018 1149 C
ATOM 2361 CD2 TYR B 261 17.131 -75.871 -44.519 1.00 58.55 C
ANISOU 2361 CD2 TYR B 261 6439 9270 6536 93 -853 1114 C
ATOM 2362 C TYR B 261 13.366 -75.457 -47.528 1.00 41.40 C
ANISOU 2362 C TYR B 261 4337 6665 4727 162 -368 770 C
ATOM 2363 O TYR B 261 13.243 -76.491 -48.185 1.00 37.07 O
ANISOU 2363 O TYR B 261 3763 6001 4323 190 -350 859 O
ATOM 2364 N ALA B 262 12.901 -74.283 -47.936 1.00 31.44 N
ANISOU 2364 N ALA B 262 3097 5392 3458 151 -315 606 N
ATOM 2365 CA ALA B 262 12.297 -74.126 -49.247 1.00 28.20 C
ANISOU 2365 CA ALA B 262 2656 4852 3207 172 -259 537 C
ATOM 2366 CB ALA B 262 11.648 -72.769 -49.381 1.00 36.77 C
ANISOU 2366 CB ALA B 262 3768 5948 4256 174 -189 390 C
ATOM 2367 C ALA B 262 13.349 -74.314 -50.329 1.00 45.59 C
ANISOU 2367 C ALA B 262 4826 6949 5546 197 -322 525 C
ATOM 2368 O ALA B 262 14.293 -73.528 -50.435 1.00 50.76 O
ANISOU 2368 O ALA B 262 5470 7625 6192 194 -373 453 O
ATOM 2369 N THR B 263 13.176 -75.356 -51.136 1.00 46.93 N
ANISOU 2369 N THR B 263 4992 6998 5841 215 -305 593 N
ATOM 2370 CA THR B 263 14.098 -75.662 -52.232 1.00 45.40 C
ANISOU 2370 CA THR B 263 4793 6684 5772 257 -320 584 C
ATOM 2371 CB THR B 263 13.665 -76.930 -53.001 1.00 45.13 C
ANISOU 2371 CB THR B 263 4812 6495 5842 260 -281 648 C
ATOM 2372 OG1 THR B 263 12.305 -76.803 -53.422 1.00 51.16 O
ANISOU 2372 OG1 THR B 263 5600 7234 6606 195 -254 603 O
ATOM 2373 CG2 THR B 263 13.804 -78.148 -52.116 1.00 27.84 C
ANISOU 2373 CG2 THR B 263 2624 4305 3648 276 -287 811 C
ATOM 2374 C THR B 263 14.404 -74.528 -53.234 1.00 39.46 C
ANISOU 2374 C THR B 263 4042 5890 5060 260 -310 445 C
ATOM 2375 O THR B 263 15.538 -74.428 -53.704 1.00 41.27 O
ANISOU 2375 O THR B 263 4243 6087 5352 295 -323 442 O
ATOM 2376 N PRO B 264 13.401 -73.689 -53.583 1.00 28.90 N
ANISOU 2376 N PRO B 264 2726 4553 3700 232 -278 352 N
ATOM 2377 CA PRO B 264 13.715 -72.660 -54.584 1.00 29.23 C
ANISOU 2377 CA PRO B 264 2781 4539 3784 240 -267 245 C
ATOM 2378 CB PRO B 264 12.387 -71.930 -54.778 1.00 23.87 C
ANISOU 2378 CB PRO B 264 2124 3870 3087 227 -232 191 C
ATOM 2379 CG PRO B 264 11.347 -72.934 -54.421 1.00 43.54 C
ANISOU 2379 CG PRO B 264 4588 6377 5587 202 -216 259 C
ATOM 2380 CD PRO B 264 11.952 -73.734 -53.302 1.00 39.45 C
ANISOU 2380 CD PRO B 264 4063 5921 5017 203 -239 366 C
ATOM 2381 C PRO B 264 14.782 -71.654 -54.158 1.00 30.34 C
ANISOU 2381 C PRO B 264 2897 4741 3891 232 -298 188 C
ATOM 2382 O PRO B 264 15.325 -70.970 -55.018 1.00 35.93 O
ANISOU 2382 O PRO B 264 3609 5389 4655 236 -285 127 O
ATOM 2383 N LEU B 265 15.051 -71.537 -52.861 1.00 25.26 N
ANISOU 2383 N LEU B 265 2238 4214 3146 204 -342 209 N
ATOM 2384 CA LEU B 265 16.114 -70.660 -52.390 1.00 25.91 C
ANISOU 2384 CA LEU B 265 2300 4359 3186 157 -405 160 C
ATOM 2385 CB LEU B 265 16.068 -70.511 -50.873 1.00 29.44 C
ANISOU 2385 CB LEU B 265 2779 4943 3464 104 -459 168 C
ATOM 2386 CG LEU B 265 14.828 -69.860 -50.275 1.00 42.21 C
ANISOU 2386 CG LEU B 265 4494 6582 4962 98 -377 80 C
ATOM 2387 CD1 LEU B 265 15.017 -69.705 -48.790 1.00 47.27 C
ANISOU 2387 CD1 LEU B 265 5202 7357 5402 36 -427 78 C
ATOM 2388 CD2 LEU B 265 14.544 -68.502 -50.911 1.00 27.69 C
ANISOU 2388 CD2 LEU B 265 2710 4654 3157 96 -314 -66 C
ATOM 2389 C LEU B 265 17.475 -71.206 -52.827 1.00 42.92 C
ANISOU 2389 C LEU B 265 4359 6499 5448 178 -452 247 C
ATOM 2390 O LEU B 265 18.435 -70.457 -53.015 1.00 38.56 O
ANISOU 2390 O LEU B 265 3758 5960 4933 138 -489 213 O

ATOM 2391 N GLN B 266 17.558 -72.526 -52.962 1.00 37.72 N
ANISOU 2391 N GLN B 266 3672 5808 4853 243 -439 370 N
ATOM 2392 CA GLN B 266 18.759 -73.163 -53.484 1.00 40.02 C
ANISOU 2392 CA GLN B 266 3873 6058 5274 304 -437 467 C
ATOM 2393 C GLN B 266 18.989 -72.722 -54.915 1.00 35.27 C
ANISOU 2393 C GLN B 266 3293 5334 4775 330 -347 390 C
ATOM 2394 O GLN B 266 20.116 -72.453 -55.333 1.00 31.24 O
ANISOU 2394 O GLN B 266 2692 4821 4355 347 -337 418 O
ATOM 2395 CB GLN B 266 18.624 -74.676 -53.457 1.00 33.31 C
ANISOU 2395 CB GLN B 266 3035 5144 4479 384 -402 600 C
ATOM 2396 CG GLN B 266 19.182 -75.333 -52.231 1.00 30.58 C
ANISOU 2396 CG GLN B 266 2609 4913 4095 399 -493 758 C
ATOM 2397 CD GLN B 266 18.959 -76.826 -52.252 1.00 48.22 C
ANISOU 2397 CD GLN B 266 4880 7046 6397 484 -439 893 C
ATOM 2398 OE1 GLN B 266 19.738 -77.566 -52.851 1.00 52.55 O
ANISOU 2398 OE1 GLN B 266 5502 7601 6864 452 -438 923 O
ATOM 2399 NE2 GLN B 266 17.907 -77.285 -51.569 1.00 54.98 N
ANISOU 2399 NE2 GLN B 266 5691 7788 7410 594 -371 978 N
ATOM 2400 N THR B 267 17.903 -72.669 -55.671 1.00 28.45 N
ANISOU 2400 N THR B 267 2541 4376 3894 330 -284 310 N
ATOM 2401 CA THR B 267 17.976 -72.242 -57.053 1.00 33.19 C
ANISOU 2401 CA THR B 267 3194 4864 4552 346 -207 240 C
ATOM 2402 CB THR B 267 16.653 -72.474 -57.785 1.00 23.69 C
ANISOU 2402 CB THR B 267 2112 3576 3314 336 -177 189 C
ATOM 2403 OG1 THR B 267 16.428 -73.875 -57.901 1.00 35.41 O
ANISOU 2403 OG1 THR B 267 3646 4986 4823 366 -154 259 O
ATOM 2404 CG2 THR B 267 16.682 -71.856 -59.182 1.00 23.29 C
ANISOU 2404 CG2 THR B 267 2135 3431 3283 338 -118 120 C
ATOM 2405 C THR B 267 18.414 -70.781 -57.144 1.00 33.42 C
ANISOU 2405 C THR B 267 3192 4931 4575 292 -221 160 C
ATOM 2406 O THR B 267 19.252 -70.419 -57.965 1.00 33.85 O
ANISOU 2406 O THR B 267 3220 4937 4705 305 -168 157 O
ATOM 2407 N LEU B 268 17.848 -69.945 -56.284 1.00 39.86 N
ANISOU 2407 N LEU B 268 4022 5820 5301 230 -277 96 N
ATOM 2408 CA LEU B 268 18.213 -68.534 -56.241 1.00 45.74 C
ANISOU 2408 CA LEU B 268 4769 6574 6035 163 -290 9 C
ATOM 2409 CB LEU B 268 17.344 -67.789 -55.237 1.00 37.50 C
ANISOU 2409 CB LEU B 268 3792 5583 4874 118 -318 -72 C
ATOM 2410 CG LEU B 268 15.940 -67.513 -55.733 1.00 35.81 C
ANISOU 2410 CG LEU B 268 3658 5303 4645 165 -248 -117 C
ATOM 2411 CD1 LEU B 268 15.191 -66.758 -54.663 1.00 40.90 C
ANISOU 2411 CD1 LEU B 268 4361 5994 5186 145 -236 -190 C
ATOM 2412 CD2 LEU B 268 15.991 -66.713 -57.035 1.00 31.24 C
ANISOU 2412 CD2 LEU B 268 3118 4613 4141 178 -196 -158 C
ATOM 2413 C LEU B 268 19.674 -68.359 -55.864 1.00 34.11 C
ANISOU 2413 C LEU B 268 4613 4613 4141 113 -350 59 C
ATOM 2414 O LEU B 268 20.355 -67.455 -56.334 1.00 33.73 O
ANISOU 2414 O LEU B 268 3104 5090 4623 60 -336 23 O
ATOM 2415 N PHE B 269 20.148 -69.225 -54.988 1.00 26.46 N
ANISOU 2415 N PHE B 269 2124 4299 3630 121 -424 160 N
ATOM 2416 CA PHE B 269 21.533 -69.164 -54.593 1.00 27.89 C
ANISOU 2416 CA PHE B 269 2153 4570 3874 73 -506 245 C
ATOM 2417 CB PHE B 269 21.799 -70.087 -53.427 1.00 28.96 C
ANISOU 2417 CB PHE B 269 2215 4833 3956 83 -615 370 C
ATOM 2418 CG PHE B 269 23.194 -70.009 -52.931 1.00 40.48 C
ANISOU 2418 CG PHE B 269 3488 6414 5477 24 -736 485 C
ATOM 2419 CD1 PHE B 269 23.563 -69.010 -52.042 1.00 38.58 C
ANISOU 2419 CD1 PHE B 269 3243 6285 5131 -145 -884 426 C
ATOM 2420 CE1 PHE B 269 24.861 -68.911 -51.586 1.00 47.05 C
ANISOU 2420 CE1 PHE B 269 4123 7489 6265 -232 -1031 546 C
ATOM 2421 CZ PHE B 269 25.821 -69.816 -52.039 1.00 49.71 C
ANISOU 2421 CZ PHE B 269 4242 7849 6797 -116 -1003 746 C
ATOM 2422 CE2 PHE B 269 25.463 -70.813 -52.945 1.00 45.06 C
ANISOU 2422 CE2 PHE B 269 3679 7125 6316 80 -818 795 C
ATOM 2423 CD2 PHE B 269 24.158 -70.898 -53.389 1.00 34.56 C
ANISOU 2423 CD2 PHE B 269 2569 5663 4901 132 -698 656 C
ATOM 2424 C PHE B 269 22.430 -69.543 -55.771 1.00 40.31 C
ANISOU 2424 C PHE B 269 3629 6068 5620 153 -405 325 C
ATOM 2425 O PHE B 269 23.424 -68.874 -56.072 1.00 32.89 O
ANISOU 2425 O PHE B 269 2580 5146 4769 97 -409 344 O
ATOM 2426 N ALA B 270 22.062 -70.619 -56.451 1.00 33.97 N
ANISOU 2426 N ALA B 270 2876 5171 4861 278 -300 371 N
ATOM 2427 CA ALA B 270 22.816 -71.085 -57.604 1.00 29.48 C
ANISOU 2427 CA ALA B 270 2263 4508 4431 376 -162 434 C
ATOM 2428 CB ALA B 270 22.225 -72.375 -58.140 1.00 28.83 C
ANISOU 2428 CB ALA B 270 2297 4305 4352 493 -63 459 C
ATOM 2429 C ALA B 270 22.862 -70.028 -58.702 1.00 33.02 C
ANISOU 2429 C ALA B 270 2770 4876 4899 336 -73 339 C
ATOM 2430 O ALA B 270 23.913 -69.779 -59.299 1.00 44.38 O
ANISOU 2430 O ALA B 270 4103 6305 6449 396 -44 396 O
ATOM 2431 N MET B 271 21.721 -69.416 -58.984 1.00 30.23 N
ANISOU 2431 N MET B 271 2576 4468 4442 293 -76 216 N
ATOM 2432 CA MET B 271 21.670 -68.408 -60.028 1.00 37.61 C
ANISOU 2432 CA MET B 271 3584 5320 5385 263 2 144 C
ATOM 2433 CB MET B 271 20.249 -67.895 -60.225 1.00 34.47 C
ANISOU 2433 CB MET B 271 3347 4872 4880 242 -18 42 C
ATOM 2434 CG MET B 271 19.271 -68.970 -60.646 1.00 36.44 C
ANISOU 2434 CG MET B 271 3702 5066 5076 308 4 46 C
ATOM 2435 SD MET B 271 17.587 -68.349 -60.699 1.00 35.84 S
ANISOU 2435 SD MET B 271 3740 4974 4903 279 -46 -32 S
ATOM 2436 CE MET B 271 17.595 -67.547 -62.290 1.00 31.60 C
ANISOU 2436 CE MET B 271 3310 4330 4368 284 33 -57 C
ATOM 2437 C MET B 271 22.630 -67.269 -59.723 1.00 36.85 C
ANISOU 2437 C MET B 271 3373 5279 5351 157 -37 145 C
ATOM 2438 O MET B 271 23.251 -66.704 -60.623 1.00 41.85 O
ANISOU 2438 O MET B 271 3988 5856 6058 145 58 158 O
ATOM 2439 N SER B 272 22.776 -66.938 -58.447 1.00 33.01 N
ANISOU 2439 N SER B 272 2816 4900 4824 65 -179 136 N
ATOM 2440 CA SER B 272 23.716 -65.895 -58.050 1.00 30.97 C
ANISOU 2440 CA SER B 272 2456 4695 4616 -76 -249 132 C
ATOM 2441 CB SER B 272 23.505 -65.507 -56.580 1.00 29.22 C
ANISOU 2441 CB SER B 272 2258 4577 4275 -194 -418 74 C
ATOM 2442 OG SER B 272 23.991 -66.508 -55.705 1.00 31.03 O
ANISOU 2442 OG SER B 272 2350 4942 4500 -172 -520 192 O
ATOM 2443 C SER B 272 25.172 -66.344 -58.274 1.00 35.53 C
ANISOU 2443 C SER B 272 2807 5338 5356 -62 -227 287 C
ATOM 2444 O SER B 272 26.091 -65.521 -58.312 1.00 38.97 O
ANISOU 2444 O SER B 272 3124 5802 5879 -181 -253 314 O
ATOM 2445 N GLN B 273 25.384 -67.652 -58.401 1.00 38.03 N
ANISOU 2445 N GLN B 273 3052 5671 5725 82 -172 399 N
ATOM 2446 CA GLN B 273 26.738 -68.213 -58.476 1.00 36.20 C
ANISOU 2446 CA GLN B 273 2577 5510 5666 134 -139 577 C
ATOM 2447 CB GLN B 273 26.870 -69.427 -57.559 1.00 40.53 C
ANISOU 2447 CB GLN B 273 3030 6151 6218 220 -227 701 C
ATOM 2448 CG GLN B 273 26.559 -69.142 -56.110 1.00 49.91 C
ANISOU 2448 CG GLN B 273 4221 7476 7267 87 -458 672 C
ATOM 2449 CD GLN B 273 27.785 -68.733 -55.316 1.00 67.27 C
ANISOU 2449 CD GLN B 273 6174 9846 9538 -45 -631 793 C
ATOM 2450 OE1 GLN B 273 28.719 -69.519 -55.155 1.00 66.78 O
ANISOU 2450 OE1 GLN B 273 5886 9872 9618 39 -647 994 O
ATOM 2451 NE2 GLN B 273 27.789 -67.498 -54.816 1.00 74.28 N
ANISOU 2451 NE2 GLN B 273 7107 10780 10338 -256 -763 678 N
ATOM 2452 C GLN B 273 27.174 -68.620 -59.877 1.00 34.65 C
ANISOU 2452 C GLN B 273 2379 5198 5588 273 100 632 C
ATOM 2453 O GLN B 273 28.325 -68.989 -60.084 1.00 44.07 O
ANISOU 2453 O GLN B 273 3360 6435 6949 336 177 786 O
ATOM 2454 N TYR B 274 26.254 -68.586 -60.830 1.00 34.70 N
ANISOU 2454 N TYR B 274 2621 5063 5502 325 220 516 N
ATOM 2455 CA TYR B 274 26.584 -68.936 -62.203 1.00 33.36 C
ANISOU 2455 CA TYR B 274 2511 4773 5391 444 454 545 C
ATOM 2456 CB TYR B 274 25.696 -70.069 -62.711 1.00 30.27 C
ANISOU 2456 CB TYR B 274 2334 4262 4903 573 539 496 C
ATOM 2457 CG TYR B 274 25.938 -71.361 -61.993 1.00 50.54 C
ANISOU 2457 CG TYR B 274 4814 6857 7530 682 517 599 C
ATOM 2458 CD1 TYR B 274 27.239 -71.849 -61.819 1.00 57.48 C
ANISOU 2458 CD1 TYR B 274 5455 7791 8593 777 591 771 C
ATOM 2459 CE1 TYR B 274 27.468 -73.038 -61.148 1.00 60.64 C
ANISOU 2459 CE1 TYR B 274 5773 8206 9059 895 571 892 C
ATOM 2460 CZ TYR B 274 26.395 -73.740 -60.629 1.00 63.95 C
ANISOU 2460 CZ TYR B 274 6361 8584 9355 898 479 831 C
ATOM 2461 OH TYR B 274 26.615 -74.933 -59.963 1.00 69.82 O
ANISOU 2461 OH TYR B 274 7037 9324 10167 1016 466 966 O
ATOM 2462 CE2 TYR B 274 25.102 -73.282 -60.782 1.00 47.12 C
ANISOU 2462 CE2 TYR B 274 4449 6408 7046 791 407 660 C
ATOM 2463 CD2 TYR B 274 24.877 -72.095 -61.458 1.00 40.02 C
ANISOU 2463 CD2 TYR B 274 3618 5499 6088 692 423 548 C
ATOM 2464 C TYR B 274 26.472 -67.724 -63.106 1.00 40.80 C
ANISOU 2464 C TYR B 274 3553 5648 6302 358 527 468 C
ATOM 2465 O TYR B 274 25.477 -67.000 -63.062 1.00 35.56 O
ANISOU 2465 O TYR B 274 3049 4949 5515 277 443 347 O
ATOM 2466 N SER B 275 27.510 -67.516 -63.914 1.00 35.66 N
ANISOU 2466 N SER B 275 2796 4977 5775 386 698 559 N
ATOM 2467 CA SER B 275 27.631 -66.352 -64.782 1.00 37.42 C
ANISOU 2467 CA SER B 275 3084 5139 5993 301 788 527 C
ATOM 2468 CB SER B 275 28.962 -66.377 -65.522 1.00 34.81 C
ANISOU 2468 CB SER B 275 2579 4816 5832 351 1002 672 C
ATOM 2469 OG SER B 275 30.033 -66.339 -64.612 1.00 48.21 O
ANISOU 2469 OG SER B 275 3952 6656 7711 289 907 803 O
ATOM 2470 C SER B 275 26.512 -66.314 -65.792 1.00 31.32 C
ANISOU 2470 C SER B 275 2618 4235 5047 347 864 415 C
ATOM 2471 O SER B 275 26.025 -65.250 -66.155 1.00 37.98 O
ANISOU 2471 O SER B 275 3577 5030 5825 257 839 352 O
ATOM 2472 N GLN B 276 26.132 -67.492 -66.266 1.00 38.37 N
ANISOU 2472 N GLN B 276 3646 5064 5870 485 956 402 N
ATOM 2473 CA GLN B 276 25.134 -67.619 -67.315 1.00 36.83 C
ANISOU 2473 CA GLN B 276 3742 5497 5757 1017 311 C
ATOM 2474 CB GLN B 276 25.037 -69.063 -67.771 1.00 40.27 C
ANISOU 2474 CB GLN B 276 4309 5108 5885 655 1136 307 C
ATOM 2475 CG GLN B 276 25.096 -69.221 -69.265 1.00 55.59 C
ANISOU 2475 CG GLN B 276 6480 6927 7715 716 1352 286 C
ATOM 2476 CD GLN B 276 24.170 -70.302 -69.764 1.00 62.07 C
ANISOU 2476 CD GLN B 276 7578 7639 8368 762 1354 195 C
ATOM 2477 OE1 GLN B 276 24.314 -71.473 -69.407 1.00 67.46 O
ANISOU 2477 OE1 GLN B 276 8258 8277 9095 852 1394 205 O
ATOM 2478 NE2 GLN B 276 23.195 -69.913 -70.578 1.00 60.22 N
ANISOU 2478 NE2 GLN B 276 7583 7356 7941 690 1297 115 N
ATOM 2479 C GLN B 276 23.745 -67.115 -66.897 1.00 28.53 C
ANISOU 2479 C GLN B 276 2817 3705 4317 433 815 206 C
ATOM 2480 O GLN B 276 22.935 -66.726 -67.737 1.00 32.88 O
ANISOU 2480 O GLN B 276 3566 4188 4740 416 821 153 O

ATOM 2481 N ALA B 277 23.472 -67.133 -65.599 1.00 27.77 N
ANISOU 2481 N ALA B 277 2603 3697 4253 386 643 190 N
ATOM 2482 CA ALA B 277 22.157 -66.754 -65.094 1.00 35.65 C
ANISOU 2482 CA ALA B 277 3697 4703 5145 331 483 103 C
ATOM 2483 CB ALA B 277 21.918 -67.308 -63.689 1.00 25.90 C
ANISOU 2483 CB ALA B 277 2356 3563 3924 321 343 100 C
ATOM 2484 C ALA B 277 21.988 -65.237 -65.116 1.00 37.93 C
ANISOU 2484 C ALA B 277 3998 4978 5434 236 444 67 C
ATOM 2485 O ALA B 277 20.865 -64.723 -65.039 1.00 34.68 O
ANISOU 2485 O ALA B 277 3692 4543 4943 216 363 8 O
ATOM 2486 N GLY B 278 23.110 -64.528 -65.207 1.00 37.18 N
ANISOU 2486 N GLY B 278 3789 4890 5448 178 508 117 N
ATOM 2487 CA GLY B 278 23.100 -63.077 -65.243 1.00 27.77 C
ANISOU 2487 CA GLY B 278 2621 3654 4277 74 488 90 C
ATOM 2488 C GLY B 278 22.449 -62.525 -63.994 1.00 35.28 C
ANISOU 2488 C GLY B 278 3566 4639 5200 3 328 6 C
ATOM 2489 O GLY B 278 21.693 -61.551 -64.025 1.00 48.27 O
ANISOU 2489 O GLY B 278 5325 6211 6803 -27 302 -52 O
ATOM 2490 N PHE B 279 22.755 -63.163 -62.877 1.00 30.97 N
ANISOU 2490 N PHE B 279 2895 4201 4673 -14 231 8 N
ATOM 2491 CA PHE B 279 22.033 -62.945 -61.647 1.00 37.34 C
ANISOU 2491 CA PHE B 279 3727 5054 5409 -58 96 -74 C
ATOM 2492 CB PHE B 279 21.358 -64.250 -61.279 1.00 41.73 C
ANISOU 2492 CB PHE B 279 4288 5670 5896 40 58 -61 C
ATOM 2493 CG PHE B 279 20.146 -64.096 -60.435 1.00 32.44 C
ANISOU 2493 CG PHE B 279 3194 4512 4619 41 -23 -139 C
ATOM 2494 CD1 PHE B 279 19.054 -63.370 -60.896 1.00 38.73 C
ANISOU 2494 CD1 PHE B 279 4121 5224 5371 69 6 -192 C
ATOM 2495 CE1 PHE B 279 17.906 -63.232 -60.116 1.00 43.92 C
ANISOU 2495 CE1 PHE B 279 4831 5901 5955 91 -37 -246 C
ATOM 2496 CZ PHE B 279 17.853 -63.839 -58.855 1.00 41.75 C
ANISOU 2496 CZ PHE B 279 4504 5732 5626 73 -108 -258 C
ATOM 2497 CE2 PHE B 279 18.951 -64.581 -58.392 1.00 46.69 C
ANISOU 2497 CE2 PHE B 279 5016 6445 6278 35 -158 -202 C
ATOM 2498 CD2 PHE B 279 20.084 -64.700 -59.187 1.00 32.06 C
ANISOU 2498 CD2 PHE B 279 3087 4571 4523 26 -117 -139 C
ATOM 2499 C PHE B 279 22.997 -62.525 -60.556 1.00 41.74 C
ANISOU 2499 C PHE B 279 4148 5694 6017 -195 -7 -73 C
ATOM 2500 O PHE B 279 23.904 -63.282 -60.203 1.00 52.23 O
ANISOU 2500 O PHE B 279 5309 7127 7410 -197 -40 16 O
ATOM 2501 N SER B 280 22.821 -61.316 -60.032 1.00 41.01 N
ANISOU 2501 N SER B 280 4132 5551 5897 -313 -59 -166 N
ATOM 2502 CA SER B 280 23.709 -60.805 -59.004 1.00 30.32 C
ANISOU 2502 CA SER B 280 2687 4267 4566 -486 -182 -185 C
ATOM 2503 CB SER B 280 23.894 -59.300 -59.149 1.00 45.50 C
ANISOU 2503 CB SER B 280 4707 6058 6524 -630 -164 -261 C
ATOM 2504 OG SER B 280 22.746 -58.625 -58.682 1.00 47.58 O
ANISOU 2504 OG SER B 280 5179 6225 6676 -613 -164 -396 O
ATOM 2505 C SER B 280 23.188 -61.107 -57.607 1.00 40.62 C
ANISOU 2505 C SER B 280 4033 5666 5734 -512 -314 -256 C
ATOM 2506 O SER B 280 22.039 -61.528 -57.410 1.00 34.68 O
ANISOU 2506 O SER B 280 3388 4906 4883 -398 -291 -300 O
ATOM 2507 N ARG B 281 24.048 -60.867 -56.629 1.00 38.99 N
ANISOU 2507 N ARG B 281 3740 5556 5518 -677 -457 -257 N
ATOM 2508 CA ARG B 281 23.722 -61.144 -55.245 1.00 50.02 C
ANISOU 2508 CA ARG B 281 5186 7061 6757 -725 -593 -313 C
ATOM 2509 CB ARG B 281 24.964 -60.966 -54.399 1.00 53.59 C
ANISOU 2509 CB ARG B 281 5498 7644 7219 -929 -777 -268 C
ATOM 2510 CG ARG B 281 24.740 -61.191 -52.947 1.00 77.79 C
ANISOU 2510 CG ARG B 281 8635 10834 10089 -1006 -936 -320 C
ATOM 2511 CD ARG B 281 25.802 -60.458 -52.169 1.00 92.12 C
ANISOU 2511 CD ARG B 281 10402 12723 11876 -1278 -1133 -340 C
ATOM 2512 NE ARG B 281 25.752 -60.757 -50.769 1.00101.63 N
ANISOU 2512 NE ARG B 281 11668 14077 12868 -1371 -1312 -366 N
ATOM 2513 CZ ARG B 281 26.155 -61.904 -50.239 1.00108.82 C
ANISOU 2513 CZ ARG B 281 12403 15184 13761 -1319 -1431 -199 C
ATOM 2514 NH1 ARG B 281 26.081 -62.101 -48.916 1.00115.47 N
ANISOU 2514 NH1 ARG B 281 13333 16166 14375 -1418 -1602 -221 N
ATOM 2515 NH2 ARG B 281 26.631 -62.866 -51.011 1.00106.78 N
ANISOU 2515 NH2 ARG B 281 11898 14973 13699 -1162 -1370 -6 N
ATOM 2516 C ARG B 281 22.618 -60.215 -54.741 1.00 54.56 C
ANISOU 2516 C ARG B 281 6015 7523 7192 -744 -557 -491 C
ATOM 2517 O ARG B 281 21.763 -60.603 -53.940 1.00 48.05 O
ANISOU 2517 O ARG B 281 5286 6748 6224 -682 -570 -541 O
ATOM 2518 N GLU B 282 22.659 -58.977 -55.219 1.00 52.67 N
ANISOU 2518 N GLU B 282 5885 7121 7005 -823 -493 -574 N
ATOM 2519 CA GLU B 282 21.651 -57.975 -54.897 1.00 50.47 C
ANISOU 2519 CA GLU B 282 5855 6690 6633 -814 -418 -734 C
ATOM 2520 CB GLU B 282 22.046 -56.610 -55.473 1.00 59.30 C
ANISOU 2520 CB GLU B 282 7069 7615 7848 -932 -361 -793 C
ATOM 2521 CG GLU B 282 23.300 -55.981 -54.852 1.00 66.14 C
ANISOU 2521 CG GLU B 282 7905 8502 8725 -1212 -509 -831 C
ATOM 2522 CD GLU B 282 24.589 -56.761 -55.130 1.00 75.64 C
ANISOU 2522 CD GLU B 282 8808 9882 10049 -1286 -614 -657 C
ATOM 2523 OE1 GLU B 282 25.470 -56.781 -54.242 1.00 83.50 O
ANISOU 2523 OE1 GLU B 282 9716 11004 11006 -1485 -799 -651 O
ATOM 2524 OE2 GLU B 282 24.723 -57.347 -56.230 1.00 71.09 O
ANISOU 2524 OE2 GLU B 282 8088 9319 9604 -1143 -510 -522 O
ATOM 2525 C GLU B 282 20.318 -58.421 -55.475 1.00 42.93 C
ANISOU 2525 C GLU B 282 4952 5690 5669 -581 -283 -712 C
ATOM 2526 O GLU B 282 19.278 -58.366 -54.808 1.00 48.03 O
ANISOU 2526 O GLU B 282 5724 6324 6201 -505 -240 -790 O
ATOM 2527 N ASP B 283 20.357 -58.861 -56.728 1.00 39.35 N
ANISOU 2527 N ASP B 283 4401 5217 5335 -476 -212 -599 N
ATOM 2528 CA ASP B 283 19.184 -59.412 -57.397 1.00 43.06 C
ANISOU 2528 CA ASP B 283 4895 5667 5800 -286 -123 -555 C
ATOM 2529 CB ASP B 283 19.554 -59.987 -58.765 1.00 58.00 C
ANISOU 2529 CB ASP B 283 6691 7553 7793 -218 -72 -434 C
ATOM 2530 CG ASP B 283 19.794 -58.922 -59.810 1.00 68.52 C
ANISOU 2530 CG ASP B 283 8089 8734 9213 -243 14 -424 C
ATOM 2531 OD1 ASP B 283 19.360 -57.772 -59.591 1.00 77.38 O
ANISOU 2531 OD1 ASP B 283 9343 9729 10328 -271 48 -506 O
ATOM 2532 OD2 ASP B 283 20.410 -59.245 -60.851 1.00 67.51 O
ANISOU 2532 OD2 ASP B 283 7892 8603 9155 -227 64 -331 O
ATOM 2533 C ASP B 283 18.577 -60.520 -56.559 1.00 46.48 C
ANISOU 2533 C ASP B 283 5290 6240 6132 -217 -171 -539 C
ATOM 2534 O ASP B 283 17.361 -60.580 -56.356 1.00 51.52 O
ANISOU 2534 O ASP B 283 6000 6863 6714 -113 -116 -565 O
ATOM 2535 N ARG B 284 19.453 -61.391 -56.073 1.00 39.50 N
ANISOU 2535 N ARG B 284 4279 5492 5239 -274 -269 -476 N
ATOM 2536 CA ARG B 284 19.053 -62.591 -55.364 1.00 33.67 C
ANISOU 2536 CA ARG B 284 3490 4883 4420 -212 -317 -425 C
ATOM 2537 CB ARG B 284 20.272 -63.428 -54.987 1.00 28.15 C
ANISOU 2537 CB ARG B 284 2630 4315 3750 -271 -426 -322 C
ATOM 2538 CG ARG B 284 19.912 -64.691 -54.250 1.00 27.84 C
ANISOU 2538 CG ARG B 284 2548 4395 3635 -205 -473 -247 C
ATOM 2539 CD ARG B 284 21.133 -65.407 -53.748 1.00 28.92 C
ANISOU 2539 CD ARG B 284 2523 4662 3804 -256 -591 -127 C
ATOM 2540 NE ARG B 284 21.669 -64.773 -52.553 1.00 33.95 N
ANISOU 2540 NE ARG B 284 3179 5395 4327 -418 -734 -176 N
ATOM 2541 CZ ARG B 284 22.957 -64.737 -52.232 1.00 41.87 C
ANISOU 2541 CZ ARG B 284 4031 6497 5379 -534 -868 -96 C
ATOM 2542 NH1 ARG B 284 23.338 -64.132 -51.113 1.00 40.81 N
ANISOU 2542 NH1 ARG B 284 3948 6452 5106 -711 -1022 -155 N
ATOM 2543 NH2 ARG B 284 23.860 -65.305 -53.030 1.00 36.38 N
ANISOU 2543 NH2 ARG B 284 3139 5814 4869 -477 -845 47 N
ATOM 2544 C ARG B 284 18.241 -62.282 -54.115 1.00 38.55 C
ANISOU 2544 C ARG B 284 4231 5533 4882 -227 -326 -520 C
ATOM 2545 O ARG B 284 17.240 -62.947 -53.833 1.00 43.50 O
ANISOU 2545 O ARG B 284 4873 6204 5452 -128 -285 -495 O
ATOM 2546 N LEU B 285 18.674 -61.282 -53.356 1.00 33.79 N
ANISOU 2546 N LEU B 285 3726 4907 4205 -362 -371 -631 N
ATOM 2547 CA LEU B 285 17.985 -60.910 -52.124 1.00 34.65 C
ANISOU 2547 CA LEU B 285 3996 5033 4135 -384 -356 -743 C
ATOM 2548 CB LEU B 285 18.823 -59.925 -51.299 1.00 36.43 C
ANISOU 2548 CB LEU B 285 4339 5240 4264 -587 -449 -866 C
ATOM 2549 CG LEU B 285 18.129 -59.286 -50.088 1.00 48.66 C
ANISOU 2549 CG LEU B 285 6128 6758 5601 -620 -398 -1025 C
ATOM 2550 CD1 LEU B 285 17.621 -60.344 -49.105 1.00 42.16 C
ANISOU 2550 CD1 LEU B 285 5294 6110 4614 -562 -421 -969 C
ATOM 2551 CD2 LEU B 285 19.065 -58.307 -49.385 1.00 37.47 C
ANISOU 2551 CD2 LEU B 285 4853 5303 4081 -863 -515 -1160 C
ATOM 2552 C LEU B 285 16.598 -60.319 -52.403 1.00 39.78 C
ANISOU 2552 C LEU B 285 4769 5554 4791 -242 -182 -807 C
ATOM 2553 O LEU B 285 15.622 -60.620 -51.710 1.00 45.18 O
ANISOU 2553 O LEU B 285 5508 6285 5374 -158 -113 -821 O
ATOM 2554 N GLU B 286 16.510 -59.470 -53.418 1.00 38.57 N
ANISOU 2554 N GLU B 286 4647 5243 4766 -209 -104 -826 N
ATOM 2555 CA GLU B 286 15.245 -58.823 -53.738 1.00 36.15 C
ANISOU 2555 CA GLU B 286 4434 4809 4491 -63 53 -857 C
ATOM 2556 CB GLU B 286 15.451 -57.655 -54.716 1.00 33.14 C
ANISOU 2556 CB GLU B 286 4120 4235 4237 -68 114 -882 C
ATOM 2557 CG GLU B 286 14.712 -57.756 -56.037 1.00 55.45 C
ANISOU 2557 CG GLU B 286 6870 7007 7191 84 180 -764 C
ATOM 2558 CD GLU B 286 15.366 -56.918 -57.124 1.00 85.14 C
ANISOU 2558 CD GLU B 286 10659 10623 11067 37 195 -742 C
ATOM 2559 OE1 GLU B 286 15.889 -55.828 -56.803 1.00 89.53 O
ANISOU 2559 OE1 GLU B 286 11345 11044 11628 -66 220 -843 O
ATOM 2560 OE2 GLU B 286 15.380 -57.361 -58.294 1.00 98.84 O
ANISOU 2560 OE2 GLU B 286 12304 12375 12878 89 183 -625 O
ATOM 2561 C GLU B 286 14.256 -59.870 -54.268 1.00 39.59 C
ANISOU 2561 C GLU B 286 5061 5327 4975 91 85 -727 C
ATOM 2562 O GLU B 286 13.061 -59.818 -53.980 1.00 34.72 O
ANISOU 2562 O GLU B 286 4148 4705 4338 210 188 -723 O
ATOM 2563 N GLN B 287 14.776 -60.843 -55.012 1.00 44.75 N
ANISOU 2563 N GLN B 287 5654 6054 5694 80 1 -618 N
ATOM 2564 CA GLN B 287 13.964 -61.939 -55.535 1.00 41.43 C
ANISOU 2564 CA GLN B 287 4732 5702 5309 182 4 -503 C
ATOM 2565 CB GLN B 287 14.714 -62.720 -56.617 1.00 40.76 C
ANISOU 2565 CB GLN B 287 4555 5628 5304 163 -58 -414 C
ATOM 2566 CG GLN B 287 14.775 -62.028 -57.972 1.00 29.92 C
ANISOU 2566 CG GLN B 287 3211 4134 4024 189 -16 -395 C
ATOM 2567 CD GLN B 287 13.396 -61.570 -58.451 1.00 31.93 C
ANISOU 2567 CD GLN B 287 3497 4330 4305 299 46 -367 C
ATOM 2568 OE1 GLN B 287 12.576 -62.378 -58.900 1.00 39.66 O
ANISOU 2568 OE1 GLN B 287 4418 5358 5291 355 25 -286 O
ATOM 2569 NE2 GLN B 287 13.131 -60.272 -58.333 1.00 27.71 N
ANISOU 2569 NE2 GLN B 287 3051 3684 3794 325 120 -426 N
ATOM 2570 C GLN B 287 13.545 -62.899 -54.427 1.00 39.65 C
ANISOU 2570 C GLN B 287 4473 5613 4981 188 -16 -478 C

ATOM 2571 O GLN B 287 12.519 -63.563 -54.519 1.00 41.19 O
ANISOU 2571 O GLN B 287 4612 5850 5188 268 19 -404 O
ATOM 2572 N ALA B 288 14.355 -62.991 -53.381 1.00 33.95 N
ANISOU 2572 N ALA B 288 3781 4967 4153 90 -83 -523 N
ATOM 2573 CA ALA B 288 14.047 -63.891 -52.279 1.00 36.31 C
ANISOU 2573 CA ALA B 288 4064 5399 4332 89 -105 -483 C
ATOM 2574 CB ALA B 288 15.283 -64.149 -51.418 1.00 31.44 C
ANISOU 2574 CB ALA B 288 3445 4882 3618 -37 -237 -488 C
ATOM 2575 C ALA B 288 12.908 -63.316 -51.436 1.00 39.30 C
ANISOU 2575 C ALA B 288 4551 5770 4610 150 25 -553 C
ATOM 2576 O ALA B 288 12.043 -64.044 -50.945 1.00 45.30 O
ANISOU 2576 O ALA B 288 5274 6612 5325 210 77 -485 O
ATOM 2577 O LYS B 289 9.476 -61.562 -50.849 1.00 39.69 O
ANISOU 2577 O LYS B 289 4734 5668 4677 487 508 -625 O
ATOM 2578 N LYS B 289 12.924 -62.001 -51.261 1.00 41.72 N
ANISOU 2578 N LYS B 289 4998 5966 4889 135 96 -686 N
ATOM 2579 CA LYS B 289 11.853 -61.317 -50.557 1.00 42.18 C
ANISOU 2579 CA LYS B 289 5178 5978 4870 223 265 -761 C
ATOM 2580 C LYS B 289 10.570 -61.385 -51.379 1.00 34.77 C
ANISOU 2580 C LYS B 289 4130 4999 4083 387 381 -663 C
ATOM 2581 CB LYS B 289 12.231 -59.865 -50.288 1.00 43.09 C
ANISOU 2581 CB LYS B 289 5495 5939 4937 169 323 -933 C
ATOM 2582 CG LYS B 289 13.396 -59.703 -49.335 1.00 36.93 C
ANISOU 2582 CG LYS B 289 4839 5210 3982 -25 194 -1039 C
ATOM 2583 CD LYS B 289 13.807 -58.250 -49.216 1.00 38.40 C
ANISOU 2583 CD LYS B 289 5238 5211 4141 -111 237 -1214 C
ATOM 2584 CE LYS B 289 14.775 -58.046 -48.066 1.00 42.13 C
ANISOU 2584 CE LYS B 289 5866 5745 4395 -328 103 -1334 C
ATOM 2585 NZ LYS B 289 15.258 -56.640 -48.000 1.00 48.68 N
ANISOU 2585 NZ LYS B 289 6918 6373 5204 -455 124 -1514 N
ATOM 2586 N LEU B 290 10.716 -61.248 -52.689 1.00 35.65 N
ANISOU 2586 N LEU B 290 4161 5033 4351 408 331 -606 N
ATOM 2587 CA LEU B 290 9.582 -61.303 -53.598 1.00 33.78 C
ANISOU 2587 CA LEU B 290 3811 4771 4254 539 391 -494 C
ATOM 2588 CB LEU B 290 9.995 -60.865 -55.003 1.00 27.96 C
ANISOU 2588 CB LEU B 290 3054 3927 3641 535 329 -462 C
ATOM 2589 CG LEU B 290 8.893 -60.718 -56.051 1.00 39.48 C
ANISOU 2589 CG LEU B 290 4415 5352 5232 655 360 -340 C
ATOM 2590 CD1 LEU B 290 7.794 -59.783 -55.558 1.00 29.63 C
ANISOU 2590 CD1 LEU B 290 3192 4042 4023 803 532 -345 C
ATOM 2591 CD2 LEU B 290 9.483 -60.197 -57.344 1.00 39.77 C
ANISOU 2591 CD2 LEU B 290 4482 5282 5345 633 301 -320 C
ATOM 2592 C LEU B 290 9.002 -62.717 -53.631 1.00 36.63 C
ANISOU 2592 C LEU B 290 4019 5274 4627 544 336 -359 C
ATOM 2593 O LEU B 290 7.807 -62.918 -53.846 1.00 36.44 O
ANISOU 2593 O LEU B 290 3888 5280 4676 636 398 -260 O
ATOM 2594 N PHE B 291 9.870 -63.698 -53.433 1.00 33.79 N
ANISOU 2594 N PHE B 291 3639 4994 4207 441 217 -342 N
ATOM 2595 CA PHE B 291 9.461 -65.087 -53.417 1.00 35.66 C
ANISOU 2595 CA PHE B 291 3763 5334 4453 428 165 -222 C
ATOM 2596 CB PHE B 291 10.687 -65.996 -53.407 1.00 38.41 C
ANISOU 2596 CB PHE B 291 4106 5720 4765 333 38 -205 C
ATOM 2597 CG PHE B 291 10.380 -67.418 -53.073 1.00 33.19 C
ANISOU 2597 CG PHE B 291 3373 5146 4090 314 2 -92 C
ATOM 2598 CD1 PHE B 291 9.874 -68.273 -54.041 1.00 31.66 C
ANISOU 2598 CD1 PHE B 291 3106 4926 3997 316 -36 0 C
ATOM 2599 CE1 PHE B 291 9.585 -69.598 -53.739 1.00 24.91 C
ANISOU 2599 CE1 PHE B 291 2204 4122 3139 283 -65 103 C
ATOM 2600 CZ PHE B 291 9.794 -70.071 -52.441 1.00 29.79 C
ANISOU 2600 CZ PHE B 291 2839 4830 3651 264 -50 133 C
ATOM 2601 CE2 PHE B 291 10.294 -69.212 -51.461 1.00 28.65 C
ANISOU 2601 CE2 PHE B 291 2767 4734 3382 265 -21 46 C
ATOM 2602 CD2 PHE B 291 10.579 -67.899 -51.783 1.00 30.67 C
ANISOU 2602 CD2 PHE B 291 3082 4928 3645 282 3 -76 C
ATOM 2603 C PHE B 291 8.598 -65.352 -52.188 1.00 34.67 C
ANISOU 2603 C PHE B 291 3632 5304 4238 464 270 -197 C
ATOM 2604 O PHE B 291 7.539 -65.978 -52.274 1.00 40.53 O
ANISOU 2604 O PHE B 291 4260 6100 5040 504 308 -84 O
ATOM 2605 N CYS B 292 9.067 -64.875 -51.039 1.00 28.81 N
ANISOU 2605 N CYS B 292 3018 4585 3343 435 314 -298 N
ATOM 2606 CA CYS B 292 8.345 -65.044 -49.784 1.00 37.29 C
ANISOU 2606 CA CYS B 292 4130 5750 4290 468 439 -289 C
ATOM 2607 CB CYS B 292 9.150 -64.507 -48.597 1.00 37.22 C
ANISOU 2607 CB CYS B 292 4314 5761 4067 394 442 -424 C
ATOM 2608 SG CYS B 292 10.529 -65.576 -48.103 1.00 57.95 S
ANISOU 2608 SG CYS B 292 6935 8504 6579 245 224 -375 S
ATOM 2609 C CYS B 292 6.973 -64.377 -49.820 1.00 41.57 C
ANISOU 2609 C CYS B 292 4632 6255 4909 609 633 -268 C
ATOM 2610 O CYS B 292 5.978 -64.929 -49.347 1.00 51.19 O
ANISOU 2610 O CYS B 292 5759 7561 6129 660 737 -164 O
ATOM 2611 N ARG B 293 6.932 -63.176 -50.379 1.00 34.57 N
ANISOU 2611 N ARG B 293 3802 5234 4099 675 691 -349 N
ATOM 2612 CA ARG B 293 5.693 -62.428 -50.480 1.00 43.87 C
ANISOU 2612 CA ARG B 293 4932 6359 5379 838 883 -314 C
ATOM 2613 CB ARG B 293 5.943 -61.038 -51.024 1.00 33.54 C
ANISOU 2613 CB ARG B 293 3737 4869 4135 899 935 -419 C
ATOM 2614 CG ARG B 293 4.782 -60.115 -50.788 1.00 56.13 C
ANISOU 2614 CG ARG B 293 6601 7653 7072 1093 1180 -405 C
ATOM 2615 CD ARG B 293 5.002 -58.831 -51.517 1.00 64.41 C
ANISOU 2615 CD ARG B 293 7748 8502 8222 1160 1215 -472 C
ATOM 2616 NE ARG B 293 4.456 -58.852 -52.864 1.00 88.04 N
ANISOU 2616 NE ARG B 293 10543 11483 11425 1232 1135 -304 N
ATOM 2617 CZ ARG B 293 4.550 -57.840 -53.718 1.00 99.42 C
ANISOU 2617 CZ ARG B 293 12033 12762 12981 1300 1144 -306 C
ATOM 2618 NH1 ARG B 293 4.020 -57.937 -54.929 1.00 95.00 N
ANISOU 2618 NH1 ARG B 293 11294 12218 12582 1356 1050 -133 N
ATOM 2619 NH2 ARG B 293 5.179 -56.728 -53.356 1.00110.97 N
ANISOU 2619 NH2 ARG B 293 13735 14041 14386 1297 1239 -475 N
ATOM 2620 C ARG B 293 4.682 -63.129 -51.383 1.00 55.14 C
ANISOU 2620 C ARG B 293 6110 7849 6990 889 844 -119 C
ATOM 2621 O ARG B 293 3.496 -63.269 -51.048 1.00 33.81 O
ANISOU 2621 O ARG B 293 3282 5215 4350 987 984 -10 O
ATOM 2622 N THR B 294 5.159 -63.554 -52.546 1.00 35.91 N
ANISOU 2622 N THR B 294 3610 5393 4642 813 655 -72 N
ATOM 2623 CA THR B 294 4.299 -64.206 -53.517 1.00 33.96 C
ANISOU 2623 CA THR B 294 3163 5196 4545 820 574 96 C
ATOM 2624 CB THR B 294 5.002 -64.397 -54.856 1.00 34.59 C
ANISOU 2624 CB THR B 294 3252 5213 4676 740 387 100 C
ATOM 2625 OG1 THR B 294 5.428 -63.126 -55.348 1.00 42.60 O
ANISOU 2625 OG1 THR B 294 4370 6098 5720 801 420 17 O
ATOM 2626 CG2 THR B 294 4.058 -65.035 -55.861 1.00 36.75 C
ANISOU 2626 CG2 THR B 294 3353 5538 5074 723 286 263 C
ATOM 2627 C THR B 294 3.757 -65.532 -52.980 1.00 41.59 C
ANISOU 2627 C THR B 294 4011 6298 5492 754 557 210 C
ATOM 2628 O THR B 294 2.570 -65.842 -53.122 1.00 43.13 O
ANISOU 2628 O THR B 294 4024 6564 5800 792 597 357 O
ATOM 2629 N LEU B 295 4.625 -66.300 -52.336 1.00 34.03 N
ANISOU 2629 N LEU B 295 3147 5380 4403 652 498 160 N
ATOM 2630 CA LEU B 295 4.220 -67.570 -51.755 1.00 31.60 C
ANISOU 2630 CA LEU B 295 2758 5181 4069 584 490 272 C
ATOM 2631 CB LEU B 295 5.423 -68.324 -51.191 1.00 36.27 C
ANISOU 2631 CB LEU B 295 3470 5789 4522 484 397 221 C
ATOM 2632 CG LEU B 295 5.126 -69.743 -50.718 1.00 42.93 C
ANISOU 2632 CG LEU B 295 4247 6713 5350 407 370 354 C
ATOM 2633 CD1 LEU B 295 4.521 -70.570 -51.840 1.00 38.47 C
ANISOU 2633 CD1 LEU B 295 3551 6120 4945 344 265 469 C
ATOM 2634 CD2 LEU B 295 6.399 -70.394 -50.217 1.00 39.81 C
ANISOU 2634 CD2 LEU B 295 3966 6325 4834 336 272 324 C
ATOM 2635 C LEU B 295 3.156 -67.374 -50.668 1.00 38.30 C
ANISOU 2635 C LEU B 295 3548 6116 4890 671 701 330 C
ATOM 2636 O LEU B 295 2.194 -68.138 -50.572 1.00 41.36 O
ANISOU 2636 O LEU B 295 3772 6588 5356 733 484 484 O
ATOM 2637 N GLU B 296 3.335 -66.338 -49.855 1.00 43.48 N
ANISOU 2637 N GLU B 296 4347 6742 5432 758 856 204 N
ATOM 2638 CA GLU B 296 2.371 -66.014 -48.810 1.00 40.89 C
ANISOU 2638 CA GLU B 296 4003 6476 5057 867 1105 237 C
ATOM 2639 CB GLU B 296 2.831 -64.813 -47.997 1.00 56.06 C
ANISOU 2639 CB GLU B 296 6167 8320 6815 940 1256 46 C
ATOM 2640 CG GLU B 296 3.488 -65.183 -46.695 1.00 74.55 C
ANISOU 2640 CG GLU B 296 8700 10735 8890 855 1277 -34 C
ATOM 2641 CD GLU B 296 3.062 -64.281 -45.560 1.00 88.96 C
ANISOU 2641 CD GLU B 296 10707 12542 10552 963 1552 -142 C
ATOM 2642 OE1 GLU B 296 3.334 -63.067 -45.641 1.00 94.34 O
ANISOU 2642 OE1 GLU B 296 11550 13082 11213 1024 1623 -303 O
ATOM 2643 OE2 GLU B 296 2.444 -64.784 -44.598 1.00 94.25 O
ANISOU 2643 OE2 GLU B 296 11373 13325 11112 987 1712 -66 O
ATOM 2644 C GLU B 296 0.987 -65.739 -49.385 1.00 45.46 C
ANISOU 2644 C GLU B 296 4346 7072 5855 987 1212 388 C
ATOM 2645 O GLU B 296 -0.016 -66.282 -48.907 1.00 46.46 O
ANISOU 2645 O GLU B 296 4312 7308 6033 1013 1335 538 O
ATOM 2646 N ASP B 297 0.937 -64.887 -50.407 1.00 44.94 N
ANISOU 2646 N ASP B 297 4246 6903 5925 1059 1164 369 N
ATOM 2647 CA ASP B 297 -0.320 -64.536 -51.066 1.00 43.98 C
ANISOU 2647 CA ASP B 297 3882 6801 6027 1180 1230 536 C
ATOM 2648 CB ASP B 297 -0.100 -63.544 -52.206 1.00 55.26 C
ANISOU 2648 CB ASP B 297 5333 8099 7565 1249 1147 501 C
ATOM 2649 CG ASP B 297 0.364 -62.195 -51.730 1.00 55.60 C
ANISOU 2649 CG ASP B 297 5603 7991 7530 1377 1322 323 C
ATOM 2650 OD1 ASP B 297 0.296 -61.941 -50.512 1.00 59.05 O
ANISOU 2650 OD1 ASP B 297 6168 8432 7838 1437 1536 235 O
ATOM 2651 OD2 ASP B 297 0.795 -61.395 -52.587 1.00 65.99 O
ANISOU 2651 OD2 ASP B 297 6990 9177 8906 1406 1247 273 O
ATOM 2652 C ASP B 297 -1.041 -65.762 -51.612 1.00 38.33 C
ANISOU 2652 C ASP B 297 2914 6210 5440 1064 1083 740 C
ATOM 2653 O ASP B 297 -2.264 -65.860 -51.532 1.00 42.92 O
ANISOU 2653 O ASP B 297 3255 6885 6169 1132 1188 920 O
ATOM 2654 N ILE B 298 -0.278 -66.691 -52.176 1.00 35.77 N
ANISOU 2654 N ILE B 298 2645 5879 5068 884 845 717 N
ATOM 2655 CA ILE B 298 -0.846 -67.912 -52.735 1.00 40.37 C
ANISOU 2655 CA ILE B 298 3045 6542 5751 737 685 881 C
ATOM 2656 CB ILE B 298 0.202 -68.768 -53.461 1.00 46.53 C
ANISOU 2656 CB ILE B 298 3961 7257 6463 566 446 809 C
ATOM 2657 CG1 ILE B 298 0.770 -68.028 -54.658 1.00 36.57 C
ANISOU 2657 CG1 ILE B 298 2779 5889 5225 589 320 727 C
ATOM 2658 CD1 ILE B 298 1.810 -68.840 -55.397 1.00 41.99 C
ANISOU 2658 CD1 ILE B 298 3605 6504 5844 444 127 657 C
ATOM 2659 CG2 ILE B 298 -0.414 -70.075 -53.955 1.00 54.61 C
ANISOU 2659 CG2 ILE B 298 4841 8335 7574 397 297 961 C
ATOM 2660 C ILE B 298 -1.461 -68.766 -51.642 1.00 40.22 C
ANISOU 2660 C ILE B 298 2935 6641 5708 696 814 990 C

ATOM 2661 O ILE B 298 -2.615 -69.194 -51.738 1.00 53.46 O
ANISOU 2661 O ILE B 298 4363 8414 7535 672 837 1181 O
ATOM 2662 N LEU B 299 -0.684 -69.014 -50.596 1.00 38.66 N
ANISOU 2662 N LEU B 299 2930 6441 5319 678 892 883 N
ATOM 2663 CA LEU B 299 -1.113 -69.917 -49.538 1.00 46.92 C
ANISOU 2663 CA LEU B 299 3929 7592 6306 624 1004 989 C
ATOM 2664 CB LEU B 299 0.058 -70.313 -48.638 1.00 40.37 C
ANISOU 2664 CB LEU B 299 3349 6748 5241 568 992 869 C
ATOM 2665 CG LEU B 299 1.242 -71.008 -49.298 1.00 47.07 C
ANISOU 2665 CG LEU B 299 4317 7514 6054 439 743 802 C
ATOM 2666 CD1 LEU B 299 2.249 -71.378 -48.227 1.00 34.26 C
ANISOU 2666 CD1 LEU B 299 2889 5913 4214 406 751 735 C
ATOM 2667 CD2 LEU B 299 0.786 -72.245 -50.063 1.00 56.46 C
ANISOU 2667 CD2 LEU B 299 5367 8698 7387 294 593 949 C
ATOM 2668 C LEU B 299 -2.200 -69.268 -48.702 1.00 53.70 C
ANISOU 2668 C LEU B 299 4669 8535 7199 782 1299 1069 C
ATOM 2669 O LEU B 299 -2.954 -69.947 -48.008 1.00 57.94 O
ANISOU 2669 O LEU B 299 5079 9180 7755 752 1424 1220 O
ATOM 2670 N ALA B 300 -2.267 -67.946 -48.767 1.00 63.18 N
ANISOU 2670 N ALA B 300 5919 9672 8414 958 1429 972 N
ATOM 2671 CA ALA B 300 -3.282 -67.204 -48.040 1.00 59.85 C
ANISOU 2671 CA ALA B 300 5401 9299 8039 1150 1747 1037 C
ATOM 2672 CB ALA B 300 -3.050 -65.706 -48.178 1.00 60.38 C
ANISOU 2672 CB ALA B 300 5611 9233 8097 1337 1868 881 C
ATOM 2673 C ALA B 300 -4.695 -67.582 -48.493 1.00 57.08 C
ANISOU 2673 C ALA B 300 4669 9062 7957 1165 1780 1306 C
ATOM 2674 O ALA B 300 -5.610 -67.662 -47.677 1.00 66.06 O
ANISOU 2674 O ALA B 300 5712 10267 9119 1226 2000 1412 O
ATOM 2675 N ASP B 301 -4.886 -67.815 -49.788 1.00 65.21 N
ANISOU 2675 N ASP B 301 5528 10083 9166 1075 1521 1398 N
ATOM 2676 CA ASP B 301 -6.214 -68.201 -50.283 1.00 67.76 C
ANISOU 2676 CA ASP B 301 5586 10456 9703 1011 1440 1610 C
ATOM 2677 CB ASP B 301 -6.868 -67.074 -51.115 1.00 81.90 C
ANISOU 2677 CB ASP B 301 7289 12176 11655 1153 1416 1647 C
ATOM 2678 CG ASP B 301 -5.877 -66.324 -52.000 1.00 89.10 C
ANISOU 2678 CG ASP B 301 8343 12981 12531 1204 1283 1505 C
ATOM 2679 OD2 ASP B 301 -5.328 -65.298 -51.536 1.00 88.15 O
ANISOU 2679 OD2 ASP B 301 8401 12769 12323 1381 1473 1352 O
ATOM 2680 OD1 ASP B 301 -5.663 -66.743 -53.161 1.00 90.10 O
ANISOU 2680 OD1 ASP B 301 8421 13104 12710 1060 995 1542 O
ATOM 2681 C ASP B 301 -6.288 -69.545 -51.025 1.00 56.04 C
ANISOU 2681 C ASP B 301 3986 9021 8286 745 1149 1724 C
ATOM 2682 O ASP B 301 -7.196 -69.770 -51.820 1.00 56.45 O
ANISOU 2682 O ASP B 301 3860 9089 8499 659 991 1865 O
ATOM 2683 N ALA B 302 -5.345 -70.439 -50.748 1.00 57.46 N
ANISOU 2683 N ALA B 302 4278 9220 8334 611 1081 1668 N
ATOM 2684 CA ALA B 302 -5.311 -71.733 -51.428 1.00 56.84 C
ANISOU 2684 CA ALA B 302 4155 9138 8303 351 814 1745 C
ATOM 2685 CB ALA B 302 -3.879 -72.149 -51.719 1.00 45.83 C
ANISOU 2685 CB ALA B 302 3079 7607 6728 257 640 1543 C
ATOM 2686 C ALA B 302 -6.028 -72.827 -50.645 1.00 71.42 C
ANISOU 2686 C ALA B 302 5889 11064 10181 221 894 1908 C
ATOM 2687 O ALA B 302 -5.816 -72.955 -49.431 1.00 74.27 O
ANISOU 2687 O ALA B 302 6326 11478 10417 283 1119 1901 O
ATOM 2688 N PRO B 303 -6.855 -73.631 -51.336 1.00 72.68 N
ANISOU 2688 N PRO B 303 5904 11225 10487 28 703 2047 N
ATOM 2689 CA PRO B 303 -7.617 -74.701 -50.690 1.00 74.37 C
ANISOU 2689 CA PRO B 303 6012 11491 10754 -118 758 2211 C
ATOM 2690 CB PRO B 303 -8.429 -75.305 -51.839 1.00 73.83 C
ANISOU 2690 CB PRO B 303 5805 11401 10846 -328 484 2322 C
ATOM 2691 CG PRO B 303 -7.663 -74.932 -53.083 1.00 71.49 C
ANISOU 2691 CG PRO B 303 5624 11023 10516 -351 247 2187 C
ATOM 2692 CD PRO B 303 -7.105 -73.574 -52.781 1.00 66.21 C
ANISOU 2692 CD PRO B 303 5031 10355 9771 -75 420 2058 C
ATOM 2693 C PRO B 303 -6.731 -75.775 -50.063 1.00 73.91 C
ANISOU 2693 C PRO B 303 6098 11416 10568 -251 769 2197 C
ATOM 2694 O PRO B 303 -7.024 -76.250 -48.963 1.00 77.94 O
ANISOU 2694 O PRO B 303 6599 11982 11032 -255 960 2290 O
ATOM 2695 N GLU B 304 -5.661 -76.151 -50.754 1.00 69.48 N
ANISOU 2695 N GLU B 304 5728 10742 9929 -347 561 2066 N
ATOM 2696 CA GLU B 304 -4.767 -77.200 -50.281 1.00 68.27 C
ANISOU 2696 CA GLU B 304 5821 10486 9634 -454 525 2008 C
ATOM 2697 CB GLU B 304 -3.688 -77.501 -51.328 1.00 73.82 C
ANISOU 2697 CB GLU B 304 6759 11016 10274 -531 277 1836 C
ATOM 2698 CG GLU B 304 -4.210 -78.117 -52.613 1.00 87.50 C
ANISOU 2698 CG GLU B 304 8408 12687 12152 -748 29 1895 C
ATOM 2699 CD GLU B 304 -4.517 -77.086 -53.689 1.00 96.38 C
ANISOU 2699 CD GLU B 304 9428 13848 13345 -684 -86 1853 C
ATOM 2700 OE1 GLU B 304 -4.824 -77.498 -54.830 1.00 98.39 O
ANISOU 2700 OE1 GLU B 304 9657 14053 13673 -864 -319 1877 O
ATOM 2701 OE2 GLU B 304 -4.445 -75.871 -53.398 1.00 99.97 O
ANISOU 2701 OE2 GLU B 304 9844 14369 13770 -459 53 1798 O
ATOM 2702 C GLU B 304 -4.079 -76.849 -48.966 1.00 72.34 C
ANISOU 2702 C GLU B 304 6514 11032 9939 -286 747 1927 C
ATOM 2703 O GLU B 304 -3.619 -77.731 -48.239 1.00 68.39 O
ANISOU 2703 O GLU B 304 6152 10500 9333 -356 777 1959 O
ATOM 2704 N SER B 305 -4.003 -75.559 -48.660 1.00 81.91 N
ANISOU 2704 N SER B 305 7740 12297 11084 -73 896 1825 N
ATOM 2705 CA SER B 305 -3.018 -75.088 -47.694 1.00 81.25 C
ANISOU 2705 CA SER B 305 7910 12203 10758 60 1021 1672 C
ATOM 2706 CB SER B 305 -1.918 -74.309 -48.420 1.00 90.03 C
ANISOU 2706 CB SER B 305 9204 13206 11798 132 876 1450 C
ATOM 2707 OG SER B 305 -2.281 -72.947 -48.558 1.00 95.84 O
ANISOU 2707 OG SER B 305 9881 13966 12568 304 994 1381 O
ATOM 2708 C SER B 305 -3.557 -74.213 -46.568 1.00 68.97 C
ANISOU 2708 C SER B 305 6326 10763 9115 240 1333 1685 C
ATOM 2709 O SER B 305 -2.983 -73.166 -46.268 1.00 60.24 O
ANISOU 2709 O SER B 305 5386 9633 7868 391 1416 1510 O
ATOM 2710 N GLN B 306 -4.645 -74.633 -45.936 1.00 61.47 N
ANISOU 2710 N GLN B 306 5182 9929 8245 220 1520 1888 N
ATOM 2711 CA GLN B 306 -5.167 -73.874 -44.810 1.00 71.71 C
ANISOU 2711 CA GLN B 306 6477 11330 9440 401 1862 1904 C
ATOM 2712 CB GLN B 306 -6.651 -73.553 -44.986 1.00 79.97 C
ANISOU 2712 CB GLN B 306 7229 12429 10725 462 1993 2060 C
ATOM 2713 CG GLN B 306 -6.918 -72.103 -45.367 1.00 82.70 C
ANISOU 2713 CG GLN B 306 7564 12723 11135 676 2073 1941 C
ATOM 2714 CD GLN B 306 -7.004 -71.895 -46.871 1.00 84.65 C
ANISOU 2714 CD GLN B 306 7669 12905 11589 625 1793 1943 C
ATOM 2715 OE1 GLN B 306 -7.975 -72.313 -47.504 1.00 89.64 O
ANISOU 2715 OE1 GLN B 306 8084 13547 12428 524 1664 2096 O
ATOM 2716 NE2 GLN B 306 -5.986 -71.250 -47.452 1.00 66.88 N
ANISOU 2716 NE2 GLN B 306 5553 10590 9267 685 1690 1774 N
ATOM 2717 C GLN B 306 -4.918 -74.564 -43.471 1.00 77.44 C
ANISOU 2717 C GLN B 306 7367 12119 9938 361 2015 1958 C
ATOM 2718 O GLN B 306 -5.391 -75.679 -43.241 1.00 68.72 O
ANISOU 2718 O GLN B 306 6149 11059 8904 213 2014 2157 O
ATOM 2719 N ASN B 307 -4.164 -73.880 -42.608 1.00 85.87 N
ANISOU 2719 N ASN B 307 8718 13183 10724 480 2133 1782 N
ATOM 2720 CA ASN B 307 -3.852 -74.336 -41.251 1.00 89.27 C
ANISOU 2720 CA ASN B 307 9355 13690 10870 463 2282 1814 C
ATOM 2721 CB ASN B 307 -5.124 -74.653 -40.455 1.00 97.75 C
ANISOU 2721 CB ASN B 307 10244 14899 11997 490 2602 2043 C
ATOM 2722 CG ASN B 307 -5.812 -73.412 -39.938 1.00109.38 C
ANISOU 2722 CG ASN B 307 11753 16370 13437 700 2886 1936 C
ATOM 2723 OD1 ASN B 307 -5.588 -72.993 -38.803 1.00113.80 O
ANISOU 2723 OD1 ASN B 307 12569 16962 13708 785 3096 1839 O
ATOM 2724 ND2 ASN B 307 -6.647 -72.805 -40.776 1.00112.34 N
ANISOU 2724 ND2 ASN B 307 11900 16687 14098 776 2872 1944 N
ATOM 2725 C ASN B 307 -2.870 -75.502 -41.150 1.00 91.34 C
ANISOU 2725 C ASN B 307 9769 13907 11029 293 2040 1845 C
ATOM 2726 O ASN B 307 -2.672 -76.062 -40.072 1.00 99.67 O
ANISOU 2726 O ASN B 307 10967 15032 11872 259 2134 1926 O
ATOM 2727 N ASN B 308 -2.248 -75.871 -42.261 1.00 85.11 N
ANISOU 2727 N ASN B 308 8959 12997 10380 200 1741 1790 N
ATOM 2728 CA ASN B 308 -1.301 -76.979 -42.251 1.00 75.53 C
ANISOU 2728 CA ASN B 308 7882 11716 9100 67 1527 1827 C
ATOM 2729 CB ASN B 308 -1.801 -78.114 -43.143 1.00 75.11 C
ANISOU 2729 CB ASN B 308 7645 11583 9312 -98 1383 1987 C
ATOM 2730 CG ASN B 308 -2.246 -77.625 -44.508 1.00 73.38 C
ANISOU 2730 CG ASN B 308 7246 11300 9333 -106 1263 1923 C
ATOM 2731 OD1 ASN B 308 -2.113 -76.441 -44.824 1.00 84.42 O
ANISOU 2731 OD1 ASN B 308 8657 12703 10714 28 1285 1766 O
ATOM 2732 ND2 ASN B 308 -2.776 -78.531 -45.326 1.00 64.61 N
ANISOU 2732 ND2 ASN B 308 5984 10124 8439 -272 1127 2049 N
ATOM 2733 C ASN B 308 0.105 -76.575 -42.679 1.00 70.87 C
ANISOU 2733 C ASN B 308 7487 11032 8408 94 1308 1619 C
ATOM 2734 O ASN B 308 0.948 -77.427 -42.962 1.00 67.49 O
ANISOU 2734 O ASN B 308 7137 10521 7986 8 1112 1642 O
ATOM 2735 N CYS B 309 0.362 -75.275 -42.722 1.00 65.83 N
ANISOU 2735 N CYS B 309 6925 10399 7689 216 1357 1426 N
ATOM 2736 CA CYS B 309 1.624 -74.785 -43.246 1.00 66.74 C
ANISOU 2736 CA CYS B 309 7186 10425 7746 229 1155 1236 C
ATOM 2737 CB CYS B 309 1.482 -74.528 -44.745 1.00 65.90 C
ANISOU 2737 CB CYS B 309 6938 10208 7892 221 1017 1181 C
ATOM 2738 SG CYS B 309 3.012 -74.649 -45.686 1.00 83.51 S
ANISOU 2738 SG CYS B 309 9288 12305 10135 176 734 1046 S
ATOM 2739 C CYS B 309 2.053 -73.505 -42.537 1.00 72.59 C
ANISOU 2739 C CYS B 309 8114 11205 8261 334 1261 1048 C
ATOM 2740 O CYS B 309 1.223 -72.648 -42.247 1.00 89.26 O
ANISOU 2740 O CYS B 309 10198 13353 10365 439 1484 1009 O
ATOM 2741 N ARG B 310 3.346 -73.374 -42.262 1.00 64.25 N
ANISOU 2741 N ARG B 310 7248 10135 7030 303 1105 935 N
ATOM 2742 CA ARG B 310 3.873 -72.173 -41.621 1.00 65.46 C
ANISOU 2742 CA ARG B 310 7609 10307 6954 358 1163 738 C
ATOM 2743 CB ARG B 310 4.147 -72.420 -40.136 1.00 71.32 C
ANISOU 2743 CB ARG B 310 8553 11178 7369 325 1235 773 C
ATOM 2744 CG ARG B 310 3.201 -71.715 -39.172 1.00 76.79 C
ANISOU 2744 CG ARG B 310 9347 11941 7889 416 1555 735 C
ATOM 2745 CD ARG B 310 3.302 -70.200 -39.288 1.00 85.28 C
ANISOU 2745 CD ARG B 310 10560 12934 8909 502 1644 486 C
ATOM 2746 NE ARG B 310 2.225 -69.649 -40.104 1.00 98.75 N
ANISOU 2746 NE ARG B 310 12068 14564 10890 628 1813 493 N
ATOM 2747 CZ ARG B 310 1.021 -69.330 -39.637 1.00 98.10 C
ANISOU 2747 CZ ARG B 310 11932 14522 10820 751 2135 549 C
ATOM 2748 NH1 ARG B 310 0.101 -68.839 -40.457 1.00100.92 N
ANISOU 2748 NH1 ARG B 310 12070 14816 11457 870 2254 584 N
ATOM 2749 NH2 ARG B 310 0.736 -69.504 -38.352 1.00 93.93 N
ANISOU 2749 NH2 ARG B 310 11564 14104 10023 761 2343 586 N
ATOM 2750 C ARG B 310 5.157 -71.710 -42.296 1.00 56.07 C
ANISOU 2750 C ARG B 310 6493 9031 5780 322 928 585 C

ATOM 2751 O ARG B 310 6.097 -72.485 -42.452 1.00 46.80 O
ANISOU 2751 O ARG B 310 5322 7851 4609 244 723 644 O
ATOM 2752 N LEU B 311 5.201 -70.440 -42.681 1.00 55.08 N
ANISOU 2752 N LEU B 311 6423 8829 5675 385 974 403 N
ATOM 2753 CA LEU B 311 6.395 -69.888 -43.306 1.00 47.77 C
ANISOU 2753 CA LEU B 311 5563 7821 4768 342 775 260 C
ATOM 2754 CB LEU B 311 6.038 -68.967 -44.469 1.00 41.67 C
ANISOU 2754 CB LEU B 311 4706 6920 4208 417 807 165 C
ATOM 2755 CG LEU B 311 5.259 -69.562 -45.632 1.00 47.31 C
ANISOU 2755 CG LEU B 311 5188 7590 5198 441 785 296 C
ATOM 2756 CD1 LEU B 311 5.151 -68.525 -46.734 1.00 39.47 C
ANISOU 2756 CD1 LEU B 311 4153 6478 4365 507 780 196 C
ATOM 2757 CD2 LEU B 311 5.937 -70.826 -46.136 1.00 56.26 C
ANISOU 2757 CD2 LEU B 311 6254 8717 6406 343 581 404 C
ATOM 2758 C LEU B 311 7.222 -69.107 -42.310 1.00 49.00 C
ANISOU 2758 C LEU B 311 5965 8014 4637 295 755 105 C
ATOM 2759 O LEU B 311 6.756 -68.125 -41.731 1.00 53.93 O
ANISOU 2759 O LEU B 311 6738 8624 5128 351 941 -24 O
ATOM 2760 N ILE B 312 8.460 -69.539 -42.127 1.00 50.10 N
ANISOU 2760 N ILE B 312 6151 8196 4687 190 527 120 N
ATOM 2761 CA ILE B 312 9.385 -68.840 -41.260 1.00 56.88 C
ANISOU 2761 CA ILE B 312 7229 9103 5279 102 440 -17 C
ATOM 2762 CB ILE B 312 9.977 -69.777 -40.214 1.00 57.55 C
ANISOU 2762 CB ILE B 312 7378 9346 5143 14 312 121 C
ATOM 2763 CG1 ILE B 312 8.854 -70.395 -39.383 1.00 58.06 C
ANISOU 2763 CG1 ILE B 312 7470 9499 5091 69 525 249 C
ATOM 2764 CD1 ILE B 312 9.348 -71.173 -38.184 1.00 66.92 C
ANISOU 2764 CD1 ILE B 312 8708 10783 5936 -14 429 383 C
ATOM 2765 CG2 ILE B 312 10.946 -69.028 -39.314 1.00 62.34 C
ANISOU 2765 CG2 ILE B 312 8215 10021 5453 -109 183 -18 C
ATOM 2766 C ILE B 312 10.488 -68.203 -42.094 1.00 58.72 C
ANISOU 2766 C ILE B 312 7442 9245 5626 42 251 -132 C
ATOM 2767 O ILE B 312 11.409 -68.883 -42.548 1.00 58.08 O
ANISOU 2767 O ILE B 312 7241 9181 5645 -11 47 -37 O
ATOM 2768 N ALA B 313 10.368 -66.897 -42.314 1.00 49.35 N
ANISOU 2768 N ALA B 313 6367 7946 4437 60 341 -327 N
ATOM 2769 CA ALA B 313 11.343 -66.146 -43.085 1.00 56.06 C
ANISOU 2769 CA ALA B 313 7212 8694 5393 -6 193 -442 C
ATOM 2770 CB ALA B 313 10.643 -65.213 -44.061 1.00 52.60 C
ANISOU 2770 CB ALA B 313 6745 8087 5154 102 346 -539 C
ATOM 2771 C ALA B 313 12.248 -65.352 -42.150 1.00 61.09 C
ANISOU 2771 C ALA B 313 8081 9365 5764 -156 88 -596 C
ATOM 2772 O ALA B 313 11.772 -64.751 -41.185 1.00 68.71 O
ANISOU 2772 O ALA B 313 9278 10337 6491 -161 231 -716 O
ATOM 2773 N TYR B 314 13.550 -65.334 -42.429 1.00 47.83 N
ANISOU 2773 N TYR B 314 6346 7705 4122 -285 -157 -593 N
ATOM 2774 CA TYR B 314 14.497 -64.704 -41.515 1.00 44.44 C
ANISOU 2774 CA TYR B 314 6111 7336 3437 -471 -314 -711 C
ATOM 2775 CB TYR B 314 14.834 -65.652 -40.365 1.00 52.33 C
ANISOU 2775 CB TYR B 314 7144 8547 4191 -546 -448 -571 C
ATOM 2776 CG TYR B 314 15.399 -66.985 -40.809 1.00 54.74 C
ANISOU 2776 CG TYR B 314 7175 8948 4676 -514 -610 -319 C
ATOM 2777 CD1 TYR B 314 14.552 -68.036 -41.168 1.00 45.98 C
ANISOU 2777 CD1 TYR B 314 5924 7835 3711 -361 -480 -157 C
ATOM 2778 CE1 TYR B 314 15.057 -69.256 -41.575 1.00 51.00 C
ANISOU 2778 CE1 TYR B 314 6348 8520 4510 -326 -605 61 C
ATOM 2779 CZ TYR B 314 16.431 -69.438 -41.630 1.00 53.70 C
ANISOU 2779 CZ TYR B 314 6586 8930 4888 -417 -852 138 C
ATOM 2780 OH TYR B 314 16.939 -70.650 -42.029 1.00 57.45 O
ANISOU 2780 OH TYR B 314 6860 9432 5538 -353 -944 359 O
ATOM 2781 CE2 TYR B 314 17.299 -68.412 -41.274 1.00 49.58 C
ANISOU 2781 CE2 TYR B 314 6160 8442 4235 -576 -1000 1 C
ATOM 2782 CD2 TYR B 314 16.779 -67.196 -40.869 1.00 50.19 C
ANISOU 2782 CD2 TYR B 314 6479 8455 4135 -636 -886 -235 C
ATOM 2783 C TYR B 314 15.790 -64.197 -42.149 1.00 53.73 C
ANISOU 2783 C TYR B 314 7207 8468 4741 -608 -532 -753 C
ATOM 2784 O TYR B 314 16.194 -64.631 -43.229 1.00 57.40 O
ANISOU 2784 O TYR B 314 7435 8897 5476 -559 -595 -643 O
ATOM 2785 N GLN B 315 16.430 -63.265 -41.449 1.00 63.40 N
ANISOU 2785 N GLN B 315 8643 9690 5755 -793 -636 -916 N
ATOM 2786 CA GLN B 315 17.754 -62.769 -41.784 1.00 58.19 C
ANISOU 2786 CA GLN B 315 7915 9023 5170 -978 -872 -945 C
ATOM 2787 CB GLN B 315 17.682 -61.320 -42.249 1.00 63.88 C
ANISOU 2787 CB GLN B 315 8803 9520 5950 -1030 -768 -1173 C
ATOM 2788 CG GLN B 315 17.232 -61.139 -43.684 1.00 76.11 C
ANISOU 2788 CG GLN B 315 10187 10898 7834 -859 -611 -1148 C
ATOM 2789 CD GLN B 315 16.845 -59.703 -43.998 1.00 78.59 C
ANISOU 2789 CD GLN B 315 10712 10970 8179 -863 -446 -1363 C
ATOM 2790 OE1 GLN B 315 16.212 -59.028 -43.182 1.00 79.14 O
ANISOU 2790 OE1 GLN B 315 11067 10965 8038 -863 -301 -1531 O
ATOM 2791 NE2 GLN B 315 17.233 -59.226 -45.179 1.00 72.97 N
ANISOU 2791 NE2 GLN B 315 9876 10124 7726 -858 -453 -1355 N
ATOM 2792 C GLN B 315 18.601 -62.846 -40.517 1.00 76.95 C
ANISOU 2792 C GLN B 315 10416 11586 7237 -1200 -1119 -940 C
ATOM 2793 O GLN B 315 18.141 -62.471 -39.446 1.00 89.39 O
ANISOU 2793 O GLN B 315 12286 13186 8493 -1260 -1055 -1070 O
ATOM 2794 N GLU B 316 19.829 -63.340 -40.641 1.00 91.32 N
ANISOU 2794 N GLU B 316 12012 13541 9145 -1317 -1396 -780 N
ATOM 2795 CA GLU B 316 20.745 -63.371 -39.512 1.00103.82 C
ANISOU 2795 CA GLU B 316 13675 15319 10452 -1552 -1684 -747 C
ATOM 2796 CB GLU B 316 21.678 -64.576 -39.595 1.00104.60 C
ANISOU 2796 CB GLU B 316 13440 15618 10684 -1540 -1918 -441 C
ATOM 2797 CG GLU B 316 20.938 -65.885 -39.352 1.00107.98 C
ANISOU 2797 CG GLU B 316 13801 16131 11094 -1329 -1806 -248 C
ATOM 2798 CD GLU B 316 21.616 -67.105 -39.941 1.00108.58 C
ANISOU 2798 CD GLU B 316 13521 16292 11443 -1215 -1916 46 C
ATOM 2799 OE1 GLU B 316 21.908 -67.099 -41.155 1.00110.89 O
ANISOU 2799 OE1 GLU B 316 13604 16465 12064 -1130 -1858 71 O
ATOM 2800 OE2 GLU B 316 21.844 -68.076 -39.186 1.00107.84 O
ANISOU 2800 OE2 GLU B 316 13373 16374 11226 -1202 -2045 257 O
ATOM 2801 C GLU B 316 21.498 -62.044 -39.454 1.00106.74 C
ANISOU 2801 C GLU B 316 14194 15602 10762 -1812 -1819 -953 C
ATOM 2802 O GLU B 316 21.997 -61.573 -40.481 1.00 93.77 O
ANISOU 2802 O GLU B 316 12385 13837 9404 -1831 -1827 -967 O
ATOM 2803 N PRO B 317 21.567 -61.425 -38.261 1.00122.71 N
ANISOU 2803 N PRO B 317 16548 17673 12402 -2024 -1916 -1118 N
ATOM 2804 CA PRO B 317 21.948 -60.013 -38.191 1.00132.63 C
ANISOU 2804 CA PRO B 317 18048 18767 13576 -2260 -1962 -1380 C
ATOM 2805 CB PRO B 317 21.568 -59.613 -36.766 1.00135.12 C
ANISOU 2805 CB PRO B 317 18755 19068 13515 -2318 -1917 -1530 C
ATOM 2806 CG PRO B 317 21.634 -60.870 -35.987 1.00134.36 C
ANISOU 2806 CG PRO B 317 18545 19228 13276 -2251 -2038 -1289 C
ATOM 2807 CD PRO B 317 21.250 -61.978 -36.937 1.00127.50 C
ANISOU 2807 CD PRO B 317 17354 18461 12629 -2051 -1964 -1076 C
ATOM 2808 C PRO B 317 23.423 -59.711 -38.449 1.00136.31 C
ANISOU 2808 C PRO B 317 18280 19257 14254 -2455 -2252 -1283 C
ATOM 2809 O PRO B 317 24.275 -60.600 -38.460 1.00137.99 O
ANISOU 2809 O PRO B 317 18171 19659 14602 -2449 -2462 -1018 O
ATOM 2810 N ALA B 318 23.698 -58.425 -38.644 1.00134.68 N
ANISOU 2810 N ALA B 318 18244 18839 14088 -2615 -2233 -1496 N
ATOM 2811 CA ALA B 318 25.045 -57.927 -38.868 1.00134.75 C
ANISOU 2811 CA ALA B 318 18067 18844 14287 -2827 -2473 -1435 C
ATOM 2812 CB ALA B 318 24.989 -56.513 -39.418 1.00130.58 C
ANISOU 2812 CB ALA B 318 17740 18024 13849 -2946 -2352 -1682 C
ATOM 2813 C ALA B 318 25.845 -57.962 -37.571 1.00142.07 C
ANISOU 2813 C ALA B 318 19063 19921 14997 -3003 -2729 -1385 C
ATOM 2814 O ALA B 318 27.007 -58.367 -37.557 1.00141.03 O
ANISOU 2814 O ALA B 318 18626 19946 15012 -3096 -2977 -1173 O
ATOM 2815 N ASP B 319 25.212 -57.527 -36.485 1.00148.14 N
ANISOU 2815 N ASP B 319 20234 20636 15417 -3041 -2650 -1580 N
ATOM 2816 CA ASP B 319 25.834 -57.534 -35.164 1.00154.39 C
ANISOU 2816 CA ASP B 319 21149 21569 15944 -3215 -2879 -1558 C
ATOM 2817 CB ASP B 319 24.908 -56.862 -34.135 1.00155.73 C
ANISOU 2817 CB ASP B 319 21823 21614 15735 -3226 -2698 -1831 C
ATOM 2818 CG ASP B 319 25.460 -56.892 -32.705 1.00156.17 C
ANISOU 2818 CG ASP B 319 22047 21824 15468 -3409 -2927 -1821 C
ATOM 2819 OD2 ASP B 319 24.720 -56.475 -31.790 1.00154.31 O
ANISOU 2819 OD2 ASP B 319 22214 21512 14904 -3402 -2775 -2019 O
ATOM 2820 OD1 ASP B 319 26.617 -57.306 -32.482 1.00157.72 O
ANISOU 2820 OD1 ASP B 319 21981 22212 15735 -3553 -3243 -1617 O
ATOM 2821 C ASP B 319 26.207 -58.955 -34.734 1.00158.08 C
ANISOU 2821 C ASP B 319 21342 22330 16393 -3121 -3053 -1246 C
ATOM 2822 O ASP B 319 27.335 -59.199 -34.309 1.00158.92 O
ANISOU 2822 O ASP B 319 21258 22595 16530 -3265 -3338 -1080 O
ATOM 2823 N ASP B 320 25.280 -59.899 -34.853 1.00162.03 N
ANISOU 2823 N ASP B 320 21812 22895 16857 -2878 -2880 -1152 N
ATOM 2824 CA ASP B 320 25.534 -61.216 -34.276 1.00165.55 C
ANISOU 2824 CA ASP B 320 22067 23590 17246 -2785 -3022 -867 C
ATOM 2825 CB ASP B 320 24.931 -61.301 -32.866 1.00166.08 C
ANISOU 2825 CB ASP B 320 22495 23724 16883 -2800 -2989 -950 C
ATOM 2826 CG ASP B 320 23.511 -60.766 -32.801 1.00159.31 C
ANISOU 2826 CG ASP B 320 22006 22693 15833 -2684 -2638 -1210 C
ATOM 2827 OD1 ASP B 320 23.335 -59.533 -32.894 1.00160.32 O
ANISOU 2827 OD1 ASP B 320 22385 22609 15921 -2786 -2530 -1486 O
ATOM 2828 OD2 ASP B 320 22.572 -61.577 -32.650 1.00151.47 O
ANISOU 2828 OD2 ASP B 320 21046 21765 14740 -2484 -2455 -1130 O
ATOM 2829 C ASP B 320 25.139 -62.449 -35.096 1.00160.85 C
ANISOU 2829 C ASP B 320 21342 22330 16393 -3121 -3053 -1246 C
ATOM 2830 O ASP B 320 24.187 -62.435 -35.871 1.00153.36 O
ANISOU 2830 O ASP B 320 20252 22015 15001 -2672 -718 O
ATOM 2831 N SER B 321 25.906 -63.518 -34.914 1.00160.92 N
ANISOU 2831 N SER B 321 20877 23269 16997 -2477 -3108 -329 N
ATOM 2832 CA SER B 321 25.512 -64.834 -35.387 1.00151.93 C
ANISOU 2832 CA SER B 321 19501 22211 16013 -2229 -3015 -86 C
ATOM 2833 CB SER B 321 26.713 -65.606 -35.929 1.00146.23 C
ANISOU 2833 CB SER B 321 18341 21583 15637 -2176 -3187 212 C
ATOM 2834 OG SER B 321 27.142 -65.068 -37.169 1.00139.13 O
ANISOU 2834 OG SER B 321 17238 20565 15059 -2188 -3145 166 O
ATOM 2835 C SER B 321 24.888 -65.553 -34.201 1.00151.24 C
ANISOU 2835 C SER B 321 19618 22246 15599 -2165 -2993 -13 C
ANISOU 2835 C SER B 321 19618 22246 15599 -2165 -2993 -13 C
ATOM 2836 O SER B 321 24.579 -66.745 -34.263 1.00149.88 O
ANISOU 2836 O SER B 321 19295 22158 15493 -1979 -2940 214 O
ATOM 2837 N SER B 322 24.703 -64.796 -33.120 1.00148.53 N
ANISOU 2837 N SER B 322 19634 23797 14003 -2453 -2696 -1897 N
ATOM 2838 CA SER B 322 24.074 -65.282 -31.896 1.00139.82 C
ANISOU 2838 CA SER B 322 18789 20897 13441 -2284 -2975 -183 C
ATOM 2839 CB SER B 322 24.248 -64.263 -30.769 1.00136.69 C
ANISOU 2839 CB SER B 322 18759 20839 12339 -2609 -3061 -412 C
ATOM 2840 OG SER B 322 23.663 -64.732 -29.567 1.00135.33 O
ANISOU 2840 OG SER B 322 18841 20418 12161 -2461 -3009 -380 O

ATOM 2841 C SER B 322 22.594 -65.528 -32.130 1.00131.96 C
ANISOU 2841 C SER B 322 17957 19828 12355 -2092 -2633 -263 C
ATOM 2842 O SER B 322 21.897 -66.087 -31.280 1.00124.96 O
ANISOU 2842 O SER B 322 17249 19021 11209 -2011 -2529 -207 O
ATOM 2843 N PHE B 323 22.124 -65.067 -33.282 1.00131.11 N
ANISOU 2843 N PHE B 323 17787 19571 12458 -2026 -2453 -394 N
ATOM 2844 CA PHE B 323 20.783 -65.336 -33.756 1.00125.36 C
ANISOU 2844 CA PHE B 323 17128 18784 11719 -1837 -2131 -441 C
ATOM 2845 CB PHE B 323 20.672 -64.887 -35.206 1.00115.89 C
ANISOU 2845 CB PHE B 323 15754 17449 10831 -1794 -2031 -533 C
ATOM 2846 CG PHE B 323 19.483 -65.432 -35.919 1.00103.25 C
ANISOU 2846 CG PHE B 323 14067 15762 9402 -1530 -1712 -493 C
ATOM 2847 CD2 PHE B 323 18.332 -64.680 -36.026 1.00 98.48 C
ANISOU 2847 CD2 PHE B 323 13693 14968 8757 -1426 -1379 -722 C
ATOM 2848 CE2 PHE B 323 17.246 -65.176 -36.682 1.00 91.99 C
ANISOU 2848 CE2 PHE B 323 12749 14045 8158 -1171 -1092 -659 C
ATOM 2849 CZ PHE B 323 17.285 -66.447 -37.242 1.00 89.11 C
ANISOU 2849 CZ PHE B 323 12068 13746 8044 -1030 -1128 -389 C
ATOM 2850 CE1 PHE B 323 18.427 -67.206 -37.140 1.00 90.71 C
ANISOU 2850 CE1 PHE B 323 12070 14108 8286 -1114 -1429 -174 C
ATOM 2851 CD1 PHE B 323 19.516 -66.698 -36.490 1.00 96.20 C
ANISOU 2851 CD1 PHE B 323 12848 14925 8778 -1352 -1719 -213 C
ATOM 2852 C PHE B 323 20.493 -66.827 -33.655 1.00118.50 C
ANISOU 2852 C PHE B 323 16065 18067 10893 -1665 -2116 -131 C
ATOM 2853 O PHE B 323 21.286 -67.654 -34.106 1.00114.91 O
ANISOU 2853 O PHE B 323 15277 17687 10698 -1619 -2294 120 O
ATOM 2854 N SER B 324 19.344 -67.169 -33.084 1.00109.51 N
ANISOU 2854 N SER B 324 15132 16955 9522 -1558 -1876 -141 N
ATOM 2855 CA SER B 324 18.992 -68.567 -32.937 1.00103.68 C
ANISOU 2855 CA SER B 324 14236 16340 8817 -1404 -1840 156 C
ATOM 2856 CB SER B 324 18.778 -68.928 -31.470 1.00106.53 C
ANISOU 2856 CB SER B 324 14848 16804 8823 -1428 -1842 222 C
ATOM 2857 OG SER B 324 19.087 -70.292 -31.240 1.00107.49 O
ANISOU 2857 OG SER B 324 14763 17046 9034 -1339 -1960 562 O
ATOM 2858 C SER B 324 17.758 -68.907 -33.752 1.00 97.37 C
ANISOU 2858 C SER B 324 13358 15440 8196 -1195 -1505 155 C
ATOM 2859 O SER B 324 16.683 -68.338 -33.549 1.00 89.22 O
ANISOU 2859 O SER B 324 12553 14306 7040 -1133 -1208 -35 O
ATOM 2860 N LEU B 325 17.936 -69.831 -34.689 1.00 92.59 N
ANISOU 2860 N LEU B 325 12414 14792 7974 -1050 -1523 364 N
ATOM 2861 CA LEU B 325 16.844 -70.345 -35.487 1.00 77.71 C
ANISOU 2861 CA LEU B 325 10408 12755 6362 -833 -1227 400 C
ATOM 2862 CB LEU B 325 17.380 -71.355 -36.490 1.00 67.08 C
ANISOU 2862 CB LEU B 325 8717 11366 5403 -723 -1323 625 C
ATOM 2863 CG LEU B 325 16.495 -71.622 -37.698 1.00 58.36 C
ANISOU 2863 CG LEU B 325 7468 10063 4644 -547 -1077 602 C
ATOM 2864 CD1 LEU B 325 16.414 -70.353 -38.494 1.00 59.41 C
ANISOU 2864 CD1 LEU B 325 7634 10047 4894 -569 -999 337 C
ATOM 2865 CD2 LEU B 325 17.079 -72.746 -38.530 1.00 52.74 C
ANISOU 2865 CD2 LEU B 325 6476 9311 4253 -449 -1172 830 C
ATOM 2866 C LEU B 325 15.881 -71.044 -34.550 1.00 78.74 C
ANISOU 2866 C LEU B 325 10687 12974 6257 -767 -1051 517 C
ATOM 2867 O LEU B 325 14.665 -70.868 -34.639 1.00 80.00 O
ANISOU 2867 O LEU B 325 10929 13037 6432 -659 -742 426 O
ATOM 2868 N SER B 326 16.454 -71.842 -33.651 1.00 79.29 N
ANISOU 2868 N SER B 326 10773 13235 6119 -832 -1251 743 N
ATOM 2869 CA SER B 326 15.705 -72.604 -32.657 1.00 82.66 C
ANISOU 2869 CA SER B 326 11344 13772 6291 -790 -1118 903 C
ATOM 2870 CB SER B 326 16.638 -73.137 -31.575 1.00 82.97 C
ANISOU 2870 CB SER B 326 11446 14000 6080 -901 -1408 1102 C
ATOM 2871 OG SER B 326 17.338 -74.275 -32.027 1.00 84.18 O
ANISOU 2871 OG SER B 326 11301 14158 6527 -820 -1580 1394 O
ATOM 2872 C SER B 326 14.607 -71.785 -32.006 1.00 89.06 C
ANISOU 2872 C SER B 326 12468 14558 6812 -795 -821 678 C
ATOM 2873 O SER B 326 13.459 -72.218 -31.932 1.00 91.15 O
ANISOU 2873 O SER B 326 12744 14781 7108 -668 -527 737 O
ATOM 2874 N GLN B 327 14.968 -70.598 -31.533 1.00 94.43 N
ANISOU 2874 N GLN B 327 13405 15257 7219 -945 -889 422 N
ATOM 2875 CA GLN B 327 14.006 -69.728 -30.870 1.00100.82 C
ANISOU 2875 CA GLN B 327 14554 16022 7729 -942 -589 185 C
ATOM 2876 CB GLN B 327 14.705 -68.571 -30.154 1.00100.96 C
ANISOU 2876 CB GLN B 327 14876 16005 7480 -1115 -741 -70 C
ATOM 2877 CG GLN B 327 15.542 -69.003 -28.964 1.00 93.11 C
ANISOU 2877 CG GLN B 327 13988 15136 6254 -1218 -1017 65 C
ATOM 2878 CD GLN B 327 14.704 -69.601 -27.846 1.00 92.22 C
ANISOU 2878 CD GLN B 327 14083 15104 5853 -1132 -806 179 C
ATOM 2879 OE1 GLN B 327 14.798 -70.796 -27.554 1.00 94.63 O
ANISOU 2879 OE1 GLN B 327 14252 15521 6182 -1086 -889 478 O
ATOM 2880 NE2 GLN B 327 13.886 -68.770 -27.207 1.00 94.87 N
ANISOU 2880 NE2 GLN B 327 14748 15369 5928 -1097 -516 -53 N
ATOM 2881 C GLN B 327 12.977 -69.201 -31.857 1.00 96.35 C
ANISOU 2881 C GLN B 327 13891 15230 7487 -768 -256 28 C
ATOM 2882 O GLN B 327 11.796 -69.087 -31.530 1.00 99.40 O
ANISOU 2882 O GLN B 327 14400 15577 7790 -652 90 -18 O
ATOM 2883 N GLU B 328 13.424 -68.883 -33.067 1.00 88.48 N
ANISOU 2883 N GLU B 328 12664 14094 6862 -746 -359 -35 N
ATOM 2884 CA GLU B 328 12.514 -68.406 -34.097 1.00 90.78 C
ANISOU 2884 CA GLU B 328 12838 14180 7475 -585 -88 -153 C
ATOM 2885 CB GLU B 328 13.255 -68.096 -35.383 1.00 98.28 C
ANISOU 2885 CB GLU B 328 13555 15004 8785 -596 -262 -200 C
ATOM 2886 CG GLU B 328 12.697 -66.895 -36.085 1.00108.87 C
ANISOU 2886 CG GLU B 328 14955 16138 10272 -527 -56 -445 C
ATOM 2887 CD GLU B 328 13.614 -65.709 -35.959 1.00117.73 C
ANISOU 2887 CD GLU B 328 16269 17203 11260 -702 -218 -676 C
ATOM 2888 OE1 GLU B 328 13.467 -64.924 -34.994 1.00123.80 O
ANISOU 2888 OE1 GLU B 328 17383 17974 11682 -788 -134 -864 O
ATOM 2889 OE2 GLU B 328 14.484 -65.578 -36.826 1.00117.61 O
ANISOU 2889 OE2 GLU B 328 16069 17136 11482 -760 -421 -667 O
ATOM 2890 C GLU B 328 11.466 -69.457 -34.393 1.00 94.75 C
ANISOU 2890 C GLU B 328 13139 14679 8182 -414 124 61 C
ATOM 2891 O GLU B 328 10.273 -69.160 -34.489 1.00104.29 O
ANISOU 2891 O GLU B 328 14372 15807 9448 -285 445 -1 O
ATOM 2892 N VAL B 329 11.922 -70.692 -34.547 1.00 87.98 N
ANISOU 2892 N VAL B 329 12074 13904 7450 -415 -57 323 N
ATOM 2893 CA VAL B 329 11.021 -71.789 -34.843 1.00 76.45 C
ANISOU 2893 CA VAL B 329 10427 12428 6194 -289 108 539 C
ATOM 2894 CB VAL B 329 11.776 -73.066 -35.218 1.00 63.80 C
ANISOU 2894 CB VAL B 329 8603 10858 4780 -296 -128 800 C
ATOM 2895 CG1 VAL B 329 10.790 -74.173 -35.534 1.00 55.84 C
ANISOU 2895 CG1 VAL B 329 7434 9800 3982 -192 50 1004 C
ATOM 2896 CG2 VAL B 329 12.669 -72.807 -36.413 1.00 53.65 C
ANISOU 2896 CG2 VAL B 329 7130 9460 3794 -301 -320 732 C
ATOM 2897 C VAL B 329 10.123 -72.062 -33.654 1.00 77.23 C
ANISOU 2897 C VAL B 329 10716 12641 5989 -270 339 614 C
ATOM 2898 O VAL B 329 8.917 -72.254 -33.806 1.00 81.90 O
ANISOU 2898 O VAL B 329 11236 13182 6700 -158 627 659 O
ATOM 2899 N LEU B 330 10.720 -72.072 -32.467 1.00 85.03 N
ANISOU 2899 N LEU B 330 11940 13791 6576 -387 210 640 N
ATOM 2900 CA LEU B 330 9.979 -72.305 -31.232 1.00 87.54 C
ANISOU 2900 CA LEU B 330 12487 14236 6537 -383 426 712 C
ATOM 2901 CB LEU B 330 10.918 -72.294 -30.031 1.00 86.76 C
ANISOU 2901 CB LEU B 330 12655 14329 5981 -548 185 740 C
ATOM 2902 CG LEU B 330 11.548 -73.642 -29.702 1.00 86.00 C
ANISOU 2902 CG LEU B 330 12431 14371 5876 -583 -58 1083 C
ATOM 2903 CD1 LEU B 330 12.777 -73.452 -28.833 1.00 89.09 C
ANISOU 2903 CD1 LEU B 330 12998 14849 6001 -733 -401 1072 C
ATOM 2904 CD2 LEU B 330 10.523 -74.525 -29.009 1.00 82.24 C
ANISOU 2904 CD2 LEU B 330 12003 13964 5282 -509 208 1303 C
ATOM 2905 C LEU B 330 8.916 -71.244 -31.044 1.00 83.28 C
ANISOU 2905 C LEU B 330 12128 13614 5899 -303 794 476 C
ATOM 2906 O LEU B 330 7.772 -71.545 -30.702 1.00 69.29 O
ANISOU 2906 O LEU B 330 10360 11860 4109 -199 1116 565 O
ATOM 2907 N ARG B 331 9.323 -69.998 -31.256 1.00 89.37 N
ANISOU 2907 N ARG B 331 13049 14292 6618 -350 752 188 N
ATOM 2908 CA ARG B 331 8.427 -68.857 -31.161 1.00 99.06 C
ANISOU 2908 CA ARG B 331 14462 15399 7778 -256 1098 -59 C
ATOM 2909 CB ARG B 331 9.116 -67.599 -31.675 1.00101.32 C
ANISOU 2909 CB ARG B 331 14854 15538 8105 -326 969 -348 C
ATOM 2910 CG ARG B 331 8.181 -66.445 -31.847 1.00100.55 C
ANISOU 2910 CG ARG B 331 14892 15262 8051 -189 1331 -581 C
ATOM 2911 CD ARG B 331 8.909 -65.180 -32.265 1.00102.02 C
ANISOU 2911 CD ARG B 331 15229 15284 8249 -280 1203 -866 C
ATOM 2912 NE ARG B 331 8.630 -64.744 -33.637 1.00100.43 N
ANISOU 2912 NE ARG B 331 14763 14893 8504 -153 1255 -906 N
ATOM 2913 CZ ARG B 331 7.418 -64.585 -34.172 1.00100.26 C
ANISOU 2913 CZ ARG B 331 14591 14765 8738 65 1582 -876 C
ATOM 2914 NH1 ARG B 331 6.315 -64.840 -33.479 1.00105.24 N
ANISOU 2914 NH1 ARG B 331 15280 15458 9249 197 1919 -801 N
ATOM 2915 NH2 ARG B 331 7.307 -64.168 -35.426 1.00 96.48 N
ANISOU 2915 NH2 ARG B 331 13888 14127 8643 152 1569 -904 N
ATOM 2916 C ARG B 331 7.147 -69.115 -31.945 1.00 98.93 C
ANISOU 2916 C ARG B 331 14170 15281 8140 -56 1405 36 C
ATOM 2917 O ARG B 331 6.054 -69.081 -31.383 1.00 99.18 O
ANISOU 2917 O ARG B 331 14280 15336 8067 53 1759 64 O
ATOM 2918 N HIS B 332 7.291 -69.397 -33.238 1.00 96.73 N
ANISOU 2918 N HIS B 332 13562 14899 8292 -15 1265 100 N
ATOM 2919 CA HIS B 332 6.155 -69.778 -34.076 1.00 90.75 C
ANISOU 2919 CA HIS B 332 12508 14064 7909 138 1479 223 C
ATOM 2920 CB HIS B 332 6.599 -70.048 -35.513 1.00 80.89 C
ANISOU 2920 CB HIS B 332 10961 12703 7070 138 1249 262 C
ATOM 2921 CG HIS B 332 7.070 -68.842 -36.254 1.00 82.31 C
ANISOU 2921 CG HIS B 332 11183 12737 7355 141 1178 18 C
ATOM 2922 ND1 HIS B 332 8.304 -68.271 -36.036 1.00 93.69 N
ANISOU 2922 ND1 HIS B 332 12801 14178 8618 6 936 -133 N
ATOM 2923 CE1 HIS B 332 8.453 -67.233 -36.838 1.00 90.28 C
ANISOU 2923 CE1 HIS B 332 12366 13587 8349 32 936 -322 C
ATOM 2924 NE2 HIS B 332 7.363 -67.112 -37.572 1.00 78.63 N
ANISOU 2924 NE2 HIS B 332 10717 12015 7143 191 1161 -291 N
ATOM 2925 CD2 HIS B 332 6.484 -68.109 -37.226 1.00 76.20 C
ANISOU 2925 CD2 HIS B 332 10287 11810 6855 254 1308 -80 C
ATOM 2926 C HIS B 332 5.508 -71.052 -33.563 1.00 93.35 C
ANISOU 2926 C HIS B 332 12730 14519 8220 153 1585 509 C
ATOM 2927 O HIS B 332 4.306 -71.252 -33.702 1.00 95.85 O
ANISOU 2927 O HIS B 332 12899 14821 8699 264 1866 608 O
ATOM 2928 N LEU B 333 6.321 -71.936 -33.000 1.00 97.34 N
ANISOU 2928 N LEU B 333 13290 15146 8550 37 1350 663 N
ATOM 2929 CA LEU B 333 5.851 -73.270 -32.662 1.00 92.43 C
ANISOU 2929 CA LEU B 333 12544 14613 7963 38 1403 965 C
ATOM 2930 CB LEU B 333 7.021 -74.184 -32.310 1.00 86.42 C
ANISOU 2930 CB LEU B 333 11808 13945 7081 -78 1066 1134 C

ATOM 2931 CG LEU B 333 7.060 -75.490 -33.095 1.00 79.82 C
ANISOU 2931 CG LEU B 333 10685 13047 6598 -69 941 1385 C
ATOM 2932 CD1 LEU B 333 8.087 -76.405 -32.494 1.00 75.19 C
ANISOU 2932 CD1 LEU B 333 10155 12564 5851 -151 675 1589 C
ATOM 2933 CD2 LEU B 333 5.701 -76.139 -33.059 1.00 77.71 C
ANISOU 2933 CD2 LEU B 333 10289 12768 6470 -10 1236 1557 C
ATOM 2934 C LEU B 333 4.846 -73.249 -31.521 1.00 93.42 C
ANISOU 2934 C LEU B 333 12842 14845 7807 85 1755 1022 C
ATOM 2935 O LEU B 333 3.900 -74.035 -31.499 1.00 96.59 O
ANISOU 2935 O LEU B 333 13077 15270 8351 134 1953 1235 O
ATOM 2936 N ARG B 334 5.057 -72.344 -30.575 1.00 94.55 N
ANISOU 2936 N ARG B 334 13332 15050 7545 59 1841 829 N
ATOM 2937 CA ARG B 334 4.224 -72.275 -29.384 1.00 99.20 C
ANISOU 2937 CA ARG B 334 14150 15748 7795 102 2190 864 C
ATOM 2938 CB ARG B 334 5.045 -71.778 -28.201 1.00100.52 C
ANISOU 2938 CB ARG B 334 14750 16013 7428 -23 2078 721 C
ATOM 2939 CG ARG B 334 6.370 -72.466 -28.025 1.00100.08 C
ANISOU 2939 CG ARG B 334 14710 16058 7257 -185 1622 845 C
ATOM 2940 CD ARG B 334 7.260 -71.668 -27.100 1.00 96.93 C
ANISOU 2940 CD ARG B 334 14713 15656 6460 -304 1440 631 C
ATOM 2941 NE ARG B 334 8.211 -72.527 -26.405 1.00 93.55 N
ANISOU 2941 NE ARG B 334 14344 15333 5867 -417 1097 832 N
ATOM 2942 CZ ARG B 334 9.371 -72.112 -25.911 1.00 90.12 C
ANISOU 2942 CZ ARG B 334 14093 14932 5216 -538 760 725 C
ATOM 2943 NH1 ARG B 334 9.731 -70.843 -26.044 1.00 92.11 N
ANISOU 2943 NH1 ARG B 334 14500 15107 5389 -581 715 408 N
ATOM 2944 NH2 ARG B 334 10.173 -72.966 -25.290 1.00 87.05 N
ANISOU 2944 NH2 ARG B 334 13710 14647 4718 -616 463 943 N
ATOM 2945 C ARG B 334 3.051 -71.329 -29.574 1.00105.20 C
ANISOU 2945 C ARG B 334 14899 16407 8666 270 2606 711 C
ATOM 2946 O ARG B 334 2.972 -70.311 -28.891 1.00106.41 O
ANISOU 2946 O ARG B 334 15366 16513 8551 275 2774 471 O
ATOM 2947 N GLN B 335 2.151 -71.656 -30.499 1.00110.13 N
ANISOU 2947 N GLN B 335 15156 16954 9735 377 2740 839 N
ATOM 2948 CA GLN B 335 0.966 -70.834 -30.755 1.00117.76 C
ANISOU 2948 CA GLN B 335 16035 17825 10885 551 3122 746 C
ATOM 2949 CB GLN B 335 1.361 -69.420 -31.188 1.00120.81 C
ANISOU 2949 CB GLN B 335 16579 18065 11257 612 3111 422 C
ATOM 2950 CG GLN B 335 2.490 -69.384 -32.185 1.00120.50 C
ANISOU 2950 CG GLN B 335 16437 17937 11411 503 2674 339 C
ATOM 2951 CD GLN B 335 3.390 -68.182 -32.004 1.00124.25 C
ANISOU 2951 CD GLN B 335 17237 18322 11651 445 2558 23 C
ATOM 2952 OE1 GLN B 335 3.520 -67.352 -32.902 1.00120.49 O
ANISOU 2952 OE1 GLN B 335 16690 17685 11405 495 2512 -138 O
ATOM 2953 NE2 GLN B 335 4.030 -68.088 -30.840 1.00126.10 N
ANISOU 2953 NE2 GLN B 335 17837 18660 11416 321 2496 -60 N
ATOM 2954 C GLN B 335 0.043 -71.446 -31.797 1.00114.50 C
ANISOU 2954 C GLN B 335 15167 17378 10959 630 3193 961 C
ATOM 2955 O GLN B 335 -1.171 -71.477 -31.614 1.00115.60 O
ANISOU 2955 O GLN B 335 15158 17485 11278 704 3477 1044 O
TER 2956 GLN B 335
HETATM 2957 OAD DRG D 1 13.814 -74.811 -57.156 1.00 41.47 O
HETATM 2958 CAQ DRG D 1 13.450 -75.957 -56.917 1.00 45.68 C
HETATM 2959 CAS DRG D 1 14.342 -76.902 -56.447 1.00 42.75 C
HETATM 2960 CAJ DRG D 1 15.671 -76.550 -56.238 1.00 42.35 C
HETATM 2961 CAH DRG D 1 16.562 -77.506 -55.749 1.00 49.36 C
HETATM 2962 CAN DRG D 1 16.123 -78.806 -55.462 1.00 48.99 C
HETATM 2963 CAA DRG D 1 17.016 -79.758 -54.970 1.00 26.42 C
HETATM 2964 CAO DRG D 1 14.786 -79.154 -55.664 1.00 51.59 C
HETATM 2965 CAB DRG D 1 14.292 -80.436 -55.390 1.00 28.74 C
HETATM 2966 CAT DRG D 1 13.929 -78.201 -56.179 1.00 49.39 C
HETATM 2967 OAL DRG D 1 12.621 -78.571 -56.317 1.00 46.58 O
HETATM 2968 CAU DRG D 1 11.725 -77.635 -56.724 1.00 40.76 C
HETATM 2969 CAR DRG D 1 12.132 -76.337 -57.038 1.00 46.46 C
HETATM 2970 CAI DRG D 1 11.168 -75.414 -57.440 1.00 47.74 C
HETATM 2971 CAF DRG D 1 9.841 -75.826 -57.549 1.00 48.69 C
HETATM 2972 CAG DRG D 1 9.444 -77.132 -57.259 1.00 36.91 C
HETATM 2973 CAP DRG D 1 10.407 -78.046 -56.856 1.00 38.74 C
HETATM 2974 CAK DRG D 1 10.054 -79.341 -56.541 1.00 42.21 C
HETATM 2975 CAM DRG D 1 10.081 -79.604 -55.033 1.00 54.65 C
HETATM 2976 OAE DRG D 1 10.594 -78.735 -54.276 1.00 48.95 O
HETATM 2977 OAC DRG D 1 9.595 -80.706 -54.692 1.00 41.30 O
HETATM 2979 O HOH S 1 2.217 -85.573 -47.183 1.00 50.78 O
HETATM 2980 O HOH S 2 -3.594 -65.733 -64.471 1.00 36.73 O
HETATM 2981 O HOH S 3 24.930 -64.725 -61.859 1.00 40.78 O
HETATM 2982 O HOH S 4 1.176 -71.805 -74.402 1.00 34.49 O
HETATM 2983 O HOH S 5 11.022 -83.611 -62.726 1.00 42.43 O
HETATM 2984 O HOH S 6 4.883 -80.212 -37.724 1.00 46.39 O
HETATM 2985 O HOH S 7 25.621 -92.276 -66.048 1.00 45.02 O
HETATM 2986 O HOH S 8 10.194 -83.572 -65.584 1.00 47.90 O
HETATM 2987 O HOH S 9 19.849 -63.512 -50.865 1.00 51.16 O
HETATM 2988 O HOH S 10 16.036 -66.137 -69.887 1.00 35.95 O
HETATM 2989 O HOH S 11 7.939 -62.990 -66.847 1.00 41.65 O
HETATM 2990 O HOH S 12 13.158 -79.013 -80.095 1.00 44.90 O
HETATM 2991 O HOH S 13 20.377 -68.249 -68.348 1.00 42.43 O
HETATM 2992 O HOH S 14 16.858 -56.224 -46.295 1.00 56.08 O
HETATM 2994 O HOH S 16 7.586 -92.781 -64.034 1.00 61.96 O
HETATM 2995 O HOH S 17 19.381 -83.199 -40.815 1.00 55.77 O
HETATM 2997 O HOH S 19 15.164 -97.419 -79.818 1.00 54.74 O
HETATM 2998 O HOH S 20 10.123-101.470 -79.963 1.00 56.73 O
HETATM 2999 O HOH S 21 4.593 -92.925 -86.083 1.00 55.37 O
HETATM 3000 O HOH S 22 7.192-104.777 -84.427 1.00 53.62 O
HETATM 3001 O HOH S 23 24.377 -66.599 -48.416 1.00 59.98 O
HETATM 3002 O HOH S 24 1.900 -83.547 -75.937 1.00 42.46 O
HETATM 3003 O HOH S 25 -3.652 -60.328 -73.024 1.00 60.61 O
HETATM 3004 O HOH S 26 26.176 -95.792 -60.275 1.00 56.47 O
HETATM 3006 O HOH S 28 19.316 -67.824 -72.914 1.00 50.53 O
HETATM 3008 O HOH S 30 -7.004 -64.935 -74.273 1.00 62.07 O
HETATM 3009 O HOH S 31 31.241 -83.404 -68.030 1.00 65.30 O
HETATM 3010 O HOH S 32 -4.763 -63.171 -65.860 1.00 52.40 O
HETATM 3011 O HOH S 33 21.227 -63.566 -42.503 1.00 61.42 O
HETATM 3012 O HOH S 34 24.930 -58.511 -50.005 1.00 66.31 O
HETATM 3013 O HOH S 35 14.612 -64.157 -69.006 1.00 41.03 O
HETATM 3014 O HOH S 36 -6.479 -67.372 -58.316 1.00 51.27 O
HETATM 3015 O HOH S 37 9.493 -65.519 -76.010 1.00 32.12 O
HETATM 3016 O HOH S 38 9.375 -89.110 -64.986 1.00 52.41 O
HETATM 3017 O HOH S 39 9.158-100.778 -90.878 1.00 65.90 O
HETATM 3018 O HOH S 40 28.647 -92.308 -65.349 1.00 69.87 O
HETATM 3019 O HOH S 41 15.091-104.360 -71.265 1.00 52.22 O
HETATM 3020 O HOH S 42 2.782 -68.546 -42.680 1.00 57.16 O
HETATM 3021 O HOH S 43 -3.943 -83.815 -83.396 1.00 70.15 O
HETATM 3022 O HOH S 44 -1.599 -90.833 -42.798 1.00 64.86 O
HETATM 3023 O HOH S 45 19.552 -84.988 -42.859 1.00 75.26 O
HETATM 3024 O HOH S 46 20.052 -87.144 -34.562 1.00 69.51 O
HETATM 3026 O HOH S 47 12.863 -82.710 -57.870 1.00 30.00 O
HETATM 3027 O HOH S 48 8.400 -82.027 -55.979 1.00 30.00 O
HETATM 3028 O HOH S 49 10.621 -79.597 -52.004 1.00 30.00 O
HETATM 3029 O HOH S 50 11.112 -77.252 -49.600 1.00 30.00 O
HETATM 3030 O HOH S 51 12.196 -95.589 -62.162 1.00 30.00 O
HETATM 3031 O HOH S 52 3.183 -85.455 -66.846 1.00 30.00 O
HETATM 3032 O HOH S 53 10.175 -63.155 -74.823 1.00 30.00 O
HETATM 3034 O HOH S 55 0.703 -90.850 -62.879 1.00 30.00 O
END

Table 8. DMXAA-hSTING$^{S162A/Q266I}$ complex

REMARK 3
REMARK 3 REFINEMENT.
REMARK 3 PROGRAM : PHENIX (phenix.refine: 1.8.2_1309)
REMARK 3 AUTHORS : Adams,Afonine,Burnley,Chen,Davis,Echols,Gildea,
REMARK 3 : Gopal,Gros,Grosse-Kunstleve,Headd,Hung,Immormino,
REMARK 3 : Ioerger,McCoy,McKee,Moriarty,Pai,Read,Richardson,
REMARK 3 : Richardson,Romo,Sacchettini,Sauter,Smith,Storoni,
REMARK 3 : Terwilliger,Zwart
REMARK 3
REMARK 3 REFINEMENT TARGET : ML
REMARK 3
REMARK 3 DATA USED IN REFINEMENT.
REMARK 3 RESOLUTION RANGE HIGH (ANGSTROMS) : 2.420
REMARK 3 RESOLUTION RANGE LOW (ANGSTROMS) : 128.132
REMARK 3 MIN(FOBS/SIGMA_FOBS) : 1.37
REMARK 3 COMPLETENESS FOR RANGE (%) : 99.92
REMARK 3 NUMBER OF REFLECTIONS : 17687
REMARK 3 NUMBER OF REFLECTIONS (NON-ANOMALOUS) : 17687
REMARK 3
REMARK 3 FIT TO DATA USED IN REFINEMENT.
REMARK 3 R VALUE (WORKING + TEST SET) : 0.1849
REMARK 3 R VALUE (WORKING SET) : 0.1826
REMARK 3 FREE R VALUE : 0.2288
REMARK 3 FREE R VALUE TEST SET SIZE (%) : 5.09
REMARK 3 FREE R VALUE TEST SET COUNT : 900
REMARK 3
REMARK 3 FIT TO DATA USED IN REFINEMENT (IN BINS).
REMARK 3 BIN RESOLUTION RANGE COMPL. NWORK NFREE RWORK
RFREE
REMARK 3 1 128.3118 - 4.3975 1.00 2916 153 0.1666 0.2093
REMARK 3 2 4.3975 - 3.4904 1.00 2807 157 0.1516 0.1892
REMARK 3 3 3.4904 - 3.0491 1.00 2768 152 0.1784 0.2393
REMARK 3 4 3.0491 - 2.7703 1.00 2762 163 0.2125 0.2572
REMARK 3 5 2.7703 - 2.5717 1.00 2785 124 0.2508 0.2956
REMARK 3 6 2.5717 - 2.4201 1.00 2749 151 0.3209 0.3813
REMARK 3
REMARK 3 BULK SOLVENT MODELLING.
REMARK 3 METHOD USED : FLAT BULK SOLVENT MODEL
REMARK 3 SOLVENT RADIUS : 1.11
REMARK 3 SHRINKAGE RADIUS : 0.90
REMARK 3 GRID STEP FACTOR : 4.00
REMARK 3
REMARK 3 ERROR ESTIMATES.
REMARK 3 COORDINATE ERROR (MAXIMUM-LIKELIHOOD BASED) : 0.36
REMARK 3 PHASE ERROR (DEGREES, MAXIMUM-LIKELIHOOD BASED) :
23.15
REMARK 3
REMARK 3 STRUCTURE FACTORS CALCULATION ALGORITHM : FFT
REMARK 3
REMARK 3 DEVIATIONS FROM IDEAL VALUES.
REMARK 3 RMSD MAX COUNT
REMARK 3 BOND : 0.014 0.122 3030
REMARK 3 ANGLE : 1.613 32.388 4116
REMARK 3 CHIRALITY : 0.094 0.461 444
REMARK 3 PLANARITY : 0.006 0.049 542
REMARK 3 DIHEDRAL : 19.567 88.200 1134
REMARK 3 MIN NONBONDED DISTANCE : 1.815
REMARK 3
REMARK 3 MOLPROBITY STATISTICS.
REMARK 3 ALL-ATOM CLASHSCORE : 7.69
REMARK 3 RAMACHANDRAN PLOT:
REMARK 3 OUTLIERS : 0.00 %
REMARK 3 ALLOWED : 2.50 %
REMARK 3 FAVORED : 97.50 %
REMARK 3 ROTAMER OUTLIERS : 11.78 %
REMARK 3 CBETA DEVIATIONS : 1
REMARK 3
REMARK 3 ATOMIC DISPLACEMENT PARAMETERS.
REMARK 3 WILSON B : 51.93
REMARK 3 RMS(B_ISO_OR_EQUIVALENT_BONDED) : 5.80
REMARK 3 ATOMS NUMBER OF ATOMS
REMARK 3 ISO. ANISO.
REMARK 3 ALL : 3043 2920
REMARK 3 ALL (NO H) : 3043 2920
REMARK 3 SOLVENT : 71 0
REMARK 3 NON-SOLVENT : 2972 2920
REMARK 3 HYDROGENS : 0 0
REMARK 3
REMARK 3 TLS DETAILS.
REMARK 3 NUMBER OF TLS GROUPS: 12
REMARK 3 ORIGIN: CENTER OF MASS
REMARK 3 TLS GROUP : 1
REMARK 3 SELECTION: chain 'A' and (resid 154 through 185)
REMARK 3 ORIGIN FOR THE GROUP (A): 172.7210 47.3865 -5.8660
REMARK 3 T TENSOR
REMARK 3 T11: 0.2534 T22: 0.3103
REMARK 3 T33: 0.2519 T12: 0.0735
REMARK 3 T13: 0.0755 T23: 0.0818
REMARK 3 L TENSOR
REMARK 3 L11: 5.9722 L22: 1.3349
REMARK 3 L33: 1.7568 L12: -1.1178
REMARK 3 L13: -0.3822 L23: 0.2016
REMARK 3 S TENSOR
REMARK 3 S11: 0.2128 S12: 0.9436 S13: -0.0733
REMARK 3 S21: -0.3067 S22: -0.3874 S23: -0.1726
REMARK 3 S31: -0.0468 S32: 0.1617 S33: 0.1883
REMARK 3 TLS GROUP : 2
REMARK 3 SELECTION: chain 'A' and (resid 186 through 197)
REMARK 3 ORIGIN FOR THE GROUP (A): 190.7984 42.0205 -3.5854
REMARK 3 T TENSOR
REMARK 3 T11: 0.3433 T22: 0.7278
REMARK 3 T33: 0.9942 T12: 0.0625
REMARK 3 T13: 0.0145 T23: -0.1884
REMARK 3 L TENSOR
REMARK 3 L11: 0.6328 L22: 1.4550
REMARK 3 L33: 1.9966 L12: 0.9561
REMARK 3 L13: -1.1238 L23: -1.7024
REMARK 3 S TENSOR
REMARK 3 S11: 0.2236 S12: 2.5099 S13: 0.4877
REMARK 3 S21: 0.3243 S22: 0.4937 S23: -0.6010
REMARK 3 S31: 0.4014 S32: 0.9611 S33: -0.3780
REMARK 3 TLS GROUP : 3
REMARK 3 SELECTION: chain 'A' and (resid 198 through 211)
REMARK 3 ORIGIN FOR THE GROUP (A): 170.7088 39.7653 7.4402
REMARK 3 T TENSOR
REMARK 3 T11: 0.2740 T22: 0.4544
REMARK 3 T33: 0.4040 T12: 0.0404
REMARK 3 T13: -0.0470 T23: 0.0714
REMARK 3 L TENSOR
REMARK 3 L11: 5.7895 L22: 3.3168
REMARK 3 L33: 4.0196 L12: 1.5375
REMARK 3 L13: -1.1285 L23: -0.3983
REMARK 3 S TENSOR
REMARK 3 S11: 0.2141 S12: -1.2485 S13: -0.3878
REMARK 3 S21: 0.4935 S22: 0.0116 S23: -0.0676
REMARK 3 S31: 0.0221 S32: 0.3522 S33: -0.0548
REMARK 3 TLS GROUP : 4
REMARK 3 SELECTION: chain 'A' and (resid 212 through 224)
REMARK 3 ORIGIN FOR THE GROUP (A): 183.4756 40.9208 10.1738
REMARK 3 T TENSOR
REMARK 3 T11: 0.4807 T22: 0.3883
REMARK 3 T33: 0.4005 T12: -0.0833
REMARK 3 T13: 0.0009 T23: -0.0042
REMARK 3 L TENSOR
REMARK 3 L11: 1.4467 L22: 7.9564
REMARK 3 L33: 2.3372 L12: 0.3458
REMARK 3 L13: 0.8944 L23: -3.1919
REMARK 3 S TENSOR
REMARK 3 S11: -0.2837 S12: -0.0988 S13: 0.1904
REMARK 3 S21: 0.6346 S22: 0.1878 S23: -0.8066
REMARK 3 S31: -0.6748 S32: 0.1563 S33: -0.0333
REMARK 3 TLS GROUP : 5
REMARK 3 SELECTION: chain 'A' and (resid 225 through 280)
REMARK 3 ORIGIN FOR THE GROUP (A): 172.8424 46.4350 4.7085
REMARK 3 T TENSOR
REMARK 3 T11: 0.2443 T22: 0.2704
REMARK 3 T33: 0.3434 T12: -0.0185
REMARK 3 T13: -0.0020 T23: 0.0299
REMARK 3 L TENSOR
REMARK 3 L11: 2.4041 L22: 1.1461
REMARK 3 L33: 1.2070 L12: -1.6704
REMARK 3 L13: -0.6579 L23: 0.4071
REMARK 3 S TENSOR
REMARK 3 S11: -0.0871 S12: 0.2281 S13: 0.3173
REMARK 3 S21: -0.0231 S22: -0.0117 S23: -0.3709
REMARK 3 S31: -0.0217 S32: 0.0440 S33: 0.0348
REMARK 3 TLS GROUP : 6
REMARK 3 SELECTION: chain 'A' and (resid 281 through 300)
REMARK 3 ORIGIN FOR THE GROUP (A): 158.8087 37.1274 2.4555
REMARK 3 T TENSOR
REMARK 3 T11: 0.3605 T22: 0.3488
REMARK 3 T33: 0.2887 T12: -0.0224
REMARK 3 T13: -0.0733 T23: -0.0596
REMARK 3 L TENSOR
REMARK 3 L11: 4.6775 L22: 2.9261
REMARK 3 L33: 2.9523 L12: 0.9648
REMARK 3 L13: -3.4362 L23: -1.5127
REMARK 3 S TENSOR
REMARK 3 S11: -0.3680 S12: 0.2443 S13: -0.4711
REMARK 3 S21: 0.1364 S22: -0.0570 S23: -0.3094
REMARK 3 S31: 0.9835 S32: -0.6684 S33: 0.3625
REMARK 3 TLS GROUP : 7
REMARK 3 SELECTION: chain 'A' and (resid 301 through 314)
REMARK 3 ORIGIN FOR THE GROUP (A): 170.2562 38.6578 -7.1494
REMARK 3 T TENSOR
REMARK 3 T11: 0.5190 T22: 0.6208

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REMARK   3    T33:  0.4400 T12:  0.0640
REMARK   3    T13: -0.0926 T23: -0.0604
REMARK   3   L TENSOR
REMARK   3    L11:  5.8148 L22:  3.1473
REMARK   3    L33:  7.2083 L12: -0.5064
REMARK   3    L13:  0.3236 L23: -1.4244
REMARK   3   S TENSOR
REMARK   3    S11:  0.5128 S12:  1.6665 S13: -0.3026
REMARK   3    S21: -0.7158 S22:  0.0837 S23:  0.1667
REMARK   3    S31:  0.4492 S32: -0.0973 S33: -0.3437
REMARK   3  TLS GROUP : 8
REMARK   3   SELECTION: chain 'A' and (resid  315  through  324 )
REMARK   3   ORIGIN FOR THE GROUP (A): 170.6276 27.3415 14.5534
REMARK   3   T TENSOR
REMARK   3    T11:  1.2692 T22:  0.6924
REMARK   3    T33:  1.1103 T12: -0.0744
REMARK   3    T13:  0.1042 T23:  0.2604
REMARK   3   L TENSOR
REMARK   3    L11:  7.5278 L22:  1.6870
REMARK   3    L33:  9.8141 L12: -3.5637
REMARK   3    L13: -3.7198 L23:  1.7498
REMARK   3   S TENSOR
REMARK   3    S11:  0.0458 S12: -2.0270 S13: -1.4329
REMARK   3    S21:  1.3370 S22: -0.0239 S23:  1.7906
REMARK   3    S31:  2.4361 S32:  0.3927 S33: -0.1444
REMARK   3  TLS GROUP : 9
REMARK   3   SELECTION: chain 'A' and (resid  325  through  335 )
REMARK   3   ORIGIN FOR THE GROUP (A): 178.5034 29.5117  2.0047
REMARK   3   T TENSOR
REMARK   3    T11:  0.4443 T22:  0.4647
REMARK   3    T33:  0.6744 T12: -0.0140
REMARK   3    T13: -0.0648 T23: -0.0400
REMARK   3   L TENSOR
REMARK   3    L11:  9.0488 L22:  3.3618
REMARK   3    L33:  3.4168 L12: -5.0452
REMARK   3    L13:  2.0494 L23: -2.3999
REMARK   3   S TENSOR
REMARK   3    S11:  0.2304 S12:  0.9520 S13: -0.9120
REMARK   3    S21: -0.7421 S22: -0.4966 S23:  1.9928
REMARK   3    S31:  1.4968 S32: -0.7976 S33: -0.1278
REMARK   3  TLS GROUP : 10
REMARK   3   SELECTION: chain 'B' and (resid  154  through  224 )
REMARK   3   ORIGIN FOR THE GROUP (A): 164.5783 68.6137  5.2563
REMARK   3   T TENSOR
REMARK   3    T11:  0.3109 T22:  0.2744
REMARK   3    T33:  0.2894 T12: -0.0050
REMARK   3    T13: -0.0342 T23: -0.0250
REMARK   3   L TENSOR
REMARK   3    L11:  1.1815 L22:  5.4982
REMARK   3    L33:  1.2885 L12:  1.2374
REMARK   3    L13: -0.9898 L23: -2.2745
REMARK   3   S TENSOR
REMARK   3    S11:  0.1075 S12: -0.0459 S13:  0.1579
REMARK   3    S21:  0.2770 S22: -0.1307 S23: -0.1873
REMARK   3    S31: -0.2585 S32:  0.1217 S33:  0.0429
REMARK   3  TLS GROUP : 11
REMARK   3   SELECTION: chain 'B' and (resid  225  through  300 )
REMARK   3   ORIGIN FOR THE GROUP (A): 159.7422 61.6690  0.7515
REMARK   3   T TENSOR
REMARK   3    T11:  0.2675 T22:  0.3443
REMARK   3    T33:  0.2681 T12:  0.0012
REMARK   3    T13: -0.0309 T23:  0.0041
REMARK   3   L TENSOR
REMARK   3    L11:  1.5753 L22:  4.4695
REMARK   3    L33:  0.9759 L12:  0.3661
REMARK   3    L13: -0.3170 L23: -0.1073
REMARK   3   S TENSOR
REMARK   3    S11:  0.0602 S12: -0.2372 S13:  0.0459
REMARK   3    S21:  0.2045 S22: -0.0996 S23: -0.3266
REMARK   3    S31:  0.0274 S32: -0.0058 S33:  0.0686
REMARK   3  TLS GROUP : 12
REMARK   3   SELECTION: chain 'B' and (resid  301  through  335 )
REMARK   3   ORIGIN FOR THE GROUP (A): 153.1948 71.0160  3.2560
REMARK   3   T TENSOR
REMARK   3    T11:  0.3016 T22:  0.2782
REMARK   3    T33:  0.3329 T12:  0.0023
REMARK   3    T13: -0.0231 T23: -0.0370
REMARK   3   L TENSOR
REMARK   3    L11:  3.5463 L22:  6.1072
REMARK   3    L33:  2.9035 L12:  0.1756
REMARK   3    L13: -0.6982 L23: -1.5250
REMARK   3   S TENSOR
REMARK   3    S11: -0.0905 S12: -0.1850 S13:  0.2165
REMARK   3    S21:  0.2176 S22:  0.0114 S23:  0.3911
REMARK   3    S31: -0.4021 S32: -0.2621 S33:  0.0931
REMARK   3
CRYST1 147.954 147.954  36.122 90.00 90.00 120.00 P 6
SCALE1      0.006759  0.003902  0.000000        0.00000
SCALE2      0.000000  0.007804  0.000000        0.00000
SCALE3      0.000000  0.000000  0.027684        0.00000
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ATOM      1  N   SER A 154     149.794  43.875   0.944  1.00 53.87           N
ANISOU    1  N   SER A 154     5844   6672   7950    -33     79  -1372       N
ATOM      2  CA  SER A 154     150.705  43.059   1.743  1.00 52.37           C
ANISOU    2  CA  SER A 154     5691   6277   7929   -137    192  -1196       C
ATOM      3  CB  SER A 154     151.126  41.817   0.973  1.00 55.15           C
ANISOU    3  CB  SER A 154     5970   6490   8496   -178    196  -1360       C
ATOM      4  OG  SER A 154     152.145  41.132   1.673  1.00 59.93           O
ANISOU    4  OG  SER A 154     6624   6898   9249   -245    301  -1157       O
ATOM      5  C   SER A 154     151.949  43.871   2.055  1.00 51.68           C
ANISOU    5  C   SER A 154     5794   6199   7644    -71    204   -980       C
ATOM      6  O   SER A 154     152.510  44.522   1.157  1.00 47.64           O
ANISOU    6  O   SER A 154     5377   5774   6951     40    133  -1015       O
ATOM      7  N   VAL A 155     152.406  43.846   3.308  1.00 48.39           N
ANISOU    7  N   VAL A 155     5417   5714   7255   -135    295   -752       N
ATOM      8  CA  VAL A 155     153.546  44.697   3.647  1.00 43.68           C
ANISOU    8  CA  VAL A 155     4976   5143   6476    -79    293   -583       C
ATOM      9  CB  VAL A 155     153.717  44.980   5.193  1.00 39.56           C
ANISOU    9  CB  VAL A 155     4466   4651   5915   -126    368   -376       C
ATOM     10  CG2 VAL A 155     154.740  44.043   5.841  1.00 38.37           C
ANISOU   10  CG2 VAL A 155     4315   4390   5872   -189    457   -186       C
ATOM     11  CG1 VAL A 155     152.386  44.893   5.884  1.00 36.13           C
ANISOU   11  CG1 VAL A 155     3904   4291   5535   -173    406   -403       C
ATOM     12  C   VAL A 155     154.828  44.185   2.989  1.00 38.14           C
ANISOU   12  C   VAL A 155     4342   4347   5801    -60    297   -559       C
ATOM     13  O   VAL A 155     155.671  44.973   2.577  1.00 36.68           O
ANISOU   13  O   VAL A 155     4270   4211   5455     16    259   -509       O
ATOM     14  N   ALA A 156     154.974  42.865   2.888  1.00 33.51           N
ANISOU   14  N   ALA A 156     3672   3616   5444   -127    351   -593       N
ATOM     15  CA  ALA A 156     156.171  42.292   2.276  1.00 37.55           C
ANISOU   15  CA  ALA A 156     4229   4036   6003    -99    361   -593       C
ATOM     16  CB  ALA A 156     156.183  40.810   2.404  1.00 40.72           C
ANISOU   16  CB  ALA A 156     4514   4232   6727   -180    435   -621       C
ATOM     17  C   ALA A 156     156.284  42.665   0.802  1.00 37.36           C
ANISOU   17  C   ALA A 156     4232   4129   5833     10    269   -797       C
ATOM     18  O   ALA A 156     157.343  43.033   0.317  1.00 41.01           O
ANISOU   18  O   ALA A 156     4786   4633   6161     81    258   -738       O
ATOM     19  N   HIS A 157     155.194  42.518   0.085  1.00 33.78           N
ANISOU   19  N   HIS A 157     3678   3753   5403     26    208  -1032       N
ATOM     20  CA  HIS A 157     155.146  42.901  -1.309  1.00 34.99           C
ANISOU   20  CA  HIS A 157     3829   4094   5373    151    114  -1223       C
ATOM     21  CB  HIS A 157     153.685  42.840  -1.739  1.00 40.24           C
ANISOU   21  CB  HIS A 157     4357   4871   6063    155     42  -1459       C
ATOM     22  CG  HIS A 157     153.477  43.052  -3.196  1.00 44.01           C
ANISOU   22  CG  HIS A 157     4783   5591   6347    295    -63  -1688       C
ATOM     23  ND1 HIS A 157     153.921  42.155  -4.136  1.00 41.61           N
ANISOU   23  ND1 HIS A 157     4403   5312   6094    330    -83  -1922       N
ATOM     24  CE1 HIS A 157     153.587  42.593  -5.347  1.00 44.82           C
ANISOU   24  CE1 HIS A 157     4757   6023   6250    479   -185  -2094       C
ATOM     25  NE2 HIS A 157     152.970  43.752  -5.214  1.00 46.42           N
ANISOU   25  NE2 HIS A 157     5007   6366   6264    543   -226  -1945       N
ATOM     26  CD2 HIS A 157     152.900  44.078  -3.875  1.00 45.40           C
ANISOU   26  CD2 HIS A 157     4962   6024   6265    428   -152  -1709       C
ATOM     27  C   HIS A 157     155.713  44.334  -1.492  1.00 42.87           C
ANISOU   27  C   HIS A 157     4970   5236   6082    259     83  -1039       C
ATOM     28  O   HIS A 157     156.633  44.602  -2.313  1.00 35.34           O
ANISOU   28  O   HIS A 157     4076   4369   4982    353     71  -1010       O
ATOM     29  N   GLY A 158     155.176  45.257  -0.697  1.00 35.52           N
ANISOU   29  N   GLY A 158     4082   4322   5094    245     80   -911       N
ATOM     30  CA  GLY A 158     155.554  46.652  -0.813  1.00 35.14           C
ANISOU   30  CA  GLY A 158     4143   4360   4848    337     53   -755       C
ATOM     31  C   GLY A 158     157.011  46.873  -0.399  1.00 36.27           C
ANISOU   31  C   GLY A 158     4396   4409   4978    314    110   -555       C
ATOM     32  O   GLY A 158     157.714  47.705  -0.954  1.00 39.18           O
ANISOU   32  O   GLY A 158     4835   4836   5217    395     97   -449       O
ATOM     33  N   LEU A 159     157.477  46.116   0.587  1.00 30.24           N
ANISOU   33  N   LEU A 159     3628   3506   4356    207    178   -485       N
ATOM     34  CA  LEU A 159     158.833  46.303   1.112  1.00 26.40           C
ANISOU   34  CA  LEU A 159     3222   2952   3857    183    224   -302       C
ATOM     35  CB  LEU A 159     158.998  45.511   2.409  1.00 32.92           C
ANISOU   35  CB  LEU A 159     4012   3671   4823     77    293   -208       C
ATOM     36  CG  LEU A 159     159.098  46.193   3.779  1.00 34.21           C
ANISOU   36  CG  LEU A 159     4202   3856   4939     32    312    -67       C
ATOM     37  CD2 LEU A 159     158.598  45.229   4.850  1.00 31.07           C
ANISOU   37  CD2 LEU A 159     3714   3423   4669    -49    380    -7       C
ATOM     38  CD1 LEU A 159     158.333  47.454   3.849  1.00 31.46           C
ANISOU   38  CD1 LEU A 159     3878   3590   4485     73    258   -120       C
ATOM     39  C   LEU A 159     159.844  45.791   0.077  1.00 27.87           C
ANISOU   39  C   LEU A 159     3419   3149   4023    237    235   -324       C
ATOM     40  O   LEU A 159     160.921  46.347  -0.093  1.00 31.32           O
ANISOU   40  O   LEU A 159     3922   3602   4378    269    195   -195       O
ATOM     41  N   ALA A 160     159.510  44.686  -0.591  1.00 23.62           N
ANISOU   41  N   ALA A 160     2796   2599   3578    244    233   -507       N
ATOM     42  CA  ALA A 160     160.416  44.064  -1.572  1.00 25.96           C
ANISOU   42  CA  ALA A 160     3077   2922   3863    308    246   -582       C
ATOM     43  CB  ALA A 160     159.885  42.732  -2.032  1.00 24.05           C
ANISOU   43  CB  ALA A 160     2715   2620   3805    291    244   -837       C
ATOM     44  C   ALA A 160     160.610  45.022  -2.760  1.00 28.93           C
ANISOU   44  C   ALA A 160     3487   3516   3989    441    199   -581       C
ATOM     45  O   ALA A 160     161.749  45.312  -3.172  1.00 31.42           O
ANISOU   45  O   ALA A 160     3848   3881   4210    492    231   -463       O
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ATOM 46 N TRP A 161 159.499 45.546 -3.256 1.00 20.34 N
ANISOU 46 N TRP A 161 2366 2566 2797 499 132 -679 N
ATOM 47 CA TRP A 161 159.517 46.595 -4.293 1.00 30.15 C
ANISOU 47 CA TRP A 161 3629 4030 3796 642 91 -613 C
ATOM 48 CB TRP A 161 158.093 46.980 -4.788 1.00 28.13 C
ANISOU 48 CB TRP A 161 3304 3937 3447 716 6 -746 C
ATOM 49 CG TRP A 161 157.609 45.937 -5.725 1.00 31.55 C
ANISOU 49 CG TRP A 161 3606 4520 3861 767 -43 -1056 C
ATOM 50 CD1 TRP A 161 156.851 44.827 -5.427 1.00 29.05 C
ANISOU 50 CD1 TRP A 161 3186 4101 3751 671 -60 -1312 C
ATOM 51 NE1 TRP A 161 156.689 44.070 -6.561 1.00 36.95 N
ANISOU 51 NE1 TRP A 161 4060 5285 4693 754 -112 -1609 N
ATOM 52 CE2 TRP A 161 157.352 44.658 -7.600 1.00 32.48 C
ANISOU 52 CE2 TRP A 161 3517 4983 3840 916 -124 -1532 C
ATOM 53 CD2 TRP A 161 157.965 45.830 -7.110 1.00 32.64 C
ANISOU 53 CD2 TRP A 161 3682 4940 3779 921 -72 -1160 C
ATOM 54 CE3 TRP A 161 158.691 46.639 -7.987 1.00 37.14 C
ANISOU 54 CE3 TRP A 161 4287 5733 4093 1069 -56 -972 C
ATOM 55 CZ3 TRP A 161 158.834 46.226 -9.347 1.00 37.87 C
ANISOU 55 CZ3 TRP A 161 4268 6160 3959 1226 -90 -1155 C
ATOM 56 CH2 TRP A 161 158.217 45.058 -9.810 1.00 33.52 C
ANISOU 56 CH2 TRP A 161 3573 5700 3463 1229 -155 -1569 C
ATOM 57 CZ2 TRP A 161 157.469 44.268 -8.964 1.00 36.44 C
ANISOU 57 CZ2 TRP A 161 3904 5803 4137 1068 -173 -1766 C
ATOM 58 C TRP A 161 160.280 47.820 -3.842 1.00 30.40 C
ANISOU 58 C TRP A 161 3766 4004 3779 639 127 -324 C
ATOM 59 O TRP A 161 161.075 48.391 -4.592 1.00 29.27 O
ANISOU 59 O TRP A 161 3647 3970 3504 726 150 -185 O
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ANISOU 60 N ALA A 162 2923 2951 3008 538 137 -241 N
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ANISOU 61 CA ALA A 162 2820 2692 2825 522 162 -21 C
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ANISOU 62 CB ALA A 162 2339 2066 2425 434 152 -8 C
ATOM 63 C ALA A 162 162.289 49.105 -2.025 1.00 25.44 C
ANISOU 63 C ALA A 162 3292 3080 3294 483 225 97 C
ATOM 64 O ALA A 162 163.126 49.951 -2.332 1.00 31.86 O
ANISOU 64 O ALA A 162 4137 3903 4065 514 251 267 O
ATOM 65 N TYR A 163 162.657 47.900 -1.634 1.00 26.08 N
ANISOU 65 N TYR A 163 3346 3095 3466 420 255 19 N
ATOM 66 CA TYR A 163 164.076 47.618 -1.441 1.00 27.22 C
ANISOU 66 CA TYR A 163 3506 3188 3647 388 311 133 C
ATOM 67 CB TYR A 163 164.215 46.291 -0.698 1.00 24.76 C
ANISOU 67 CB TYR A 163 3157 2764 3486 315 342 67 C
ATOM 68 CG TYR A 163 165.644 45.909 -0.383 1.00 24.16 C
ANISOU 68 CG TYR A 163 3082 2637 3460 292 395 187 C
ATOM 69 CD1 TYR A 163 166.475 46.777 0.322 1.00 22.18 C
ANISOU 69 CD1 TYR A 163 2866 2370 3191 246 403 356 C
ATOM 70 CE1 TYR A 163 167.780 46.432 0.631 1.00 25.57 C
ANISOU 70 CE1 TYR A 163 3276 2777 3663 228 444 461 C
ATOM 71 CZ TYR A 163 168.266 45.202 0.210 1.00 33.88 C
ANISOU 71 CZ TYR A 163 4283 3808 4783 269 486 409 C
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ANISOU 72 OH TYR A 163 4745 4286 5325 268 527 517 O
ATOM 73 CE2 TYR A 163 167.457 44.331 -0.517 1.00 31.48 C
ANISOU 73 CE2 TYR A 163 3946 3495 4520 317 482 225 C
ATOM 74 CD2 TYR A 163 166.160 44.687 -0.798 1.00 28.59 C
ANISOU 74 CD2 TYR A 163 3592 3168 4105 322 434 110 C
ATOM 75 C TYR A 163 164.768 47.551 -2.814 1.00 32.43 C
ANISOU 75 C TYR A 163 4144 3997 4181 499 335 140 C
ATOM 76 O TYR A 163 165.939 47.881 -2.965 1.00 40.06 O
ANISOU 76 O TYR A 163 5122 4975 5123 506 381 288 O
ATOM 77 N TYR A 164 164.026 47.114 -3.828 1.00 30.44 N
ANISOU 77 N TYR A 164 3839 3890 3837 592 302 -32 N
ATOM 78 CA TYR A 164 164.548 47.078 -5.207 1.00 31.03 C
ANISOU 78 CA TYR A 164 3869 4186 3733 726 320 -48 C
ATOM 79 CB TYR A 164 163.669 46.203 -6.080 1.00 25.75 C
ANISOU 79 CB TYR A 164 3111 3672 3001 809 268 -341 C
ATOM 80 CG TYR A 164 163.938 46.379 -7.528 1.00 33.74 C
ANISOU 80 CG TYR A 164 4060 5002 3758 979 270 -368 C
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ANISOU 81 CD1 TYR A 164 5381 6448 5047 1036 336 -349 C
ATOM 82 CE1 TYR A 164 165.383 46.121 -9.427 1.00 51.28 C
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ANISOU 84 OH TYR A 164 8281 10597 7361 1528 295 -401 O
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ATOM 87 C TYR A 164 164.629 48.474 -5.831 1.00 32.16 C
ANISOU 87 C TYR A 164 4038 4468 3715 814 325 174 C
ATOM 88 O TYR A 164 165.632 48.876 -6.382 1.00 39.33 O
ANISOU 88 O TYR A 164 4939 5467 4538 866 385 344 O
ATOM 89 N ILE A 165 163.575 49.229 -5.672 1.00 24.47 N
ANISOU 89 N ILE A 165 3081 3487 2728 826 271 195 N
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ANISOU 109 CE2 TYR A 167 3441 3190 3763 302 566 824 C
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ANISOU 127 CZ ARG A 169 6169 7689 5197 1475 355 1036 C
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ANISOU 133 CA LEU A 170 6173 6856 5869 868 755 1507 C
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ANISOU 134 CB LEU A 170 6550 6867 6427 734 708 1567 C
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ANISOU 135 CG LEU A 170 7430 7669 7237 780 624 1479 C

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ATOM 137 CD2 LEU A 170 168.233 54.157 -7.595 1.00 61.54 C
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ANISOU 138 C LEU A 170 6325 7032 6135 801 824 1540 C
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ATOM 151 CG LEU A 172 172.259 45.226 -7.375 1.00 48.68 C
ANISOU 151 CG LEU A 172 5874 6801 5822 957 753 335 C
ATOM 152 CD1 LEU A 172 171.335 44.085 -7.733 1.00 51.07 C
ANISOU 152 CD1 LEU A 172 6139 7113 6151 1017 699 -13 C
ATOM 153 CD2 LEU A 172 173.490 44.698 -6.612 1.00 42.38 C
ANISOU 153 CD2 LEU A 172 5054 5849 5199 893 803 409 C
ATOM 154 C LEU A 172 174.415 47.406 -9.765 1.00 51.61 C
ANISOU 154 C LEU A 172 6082 7828 5701 1177 990 960 C
ATOM 155 O LEU A 172 175.421 46.807 -10.142 1.00 57.40 O
ANISOU 155 O LEU A 172 6731 8684 6397 1238 1062 924 O
ATOM 156 N PRO A 173 173.819 48.353 -10.518 1.00 50.56 N
ANISOU 156 N PRO A 173 5942 7881 5385 1256 998 1123 N
ATOM 157 CA PRO A 173 174.427 48.673 -11.822 1.00 57.61 C
ANISOU 157 CA PRO A 173 6718 9161 6009 1420 1105 1291 C
ATOM 158 CB PRO A 173 173.648 49.907 -12.277 1.00 57.66 C
ANISOU 158 CB PRO A 173 6741 9236 5930 1459 1081 1534 C
ATOM 159 CG PRO A 173 172.249 49.662 -11.693 1.00 55.73 C
ANISOU 159 CG PRO A 173 6596 8840 5739 1424 960 1305 C
ATOM 160 CD PRO A 173 172.509 49.013 -10.349 1.00 52.05 C
ANISOU 160 CD PRO A 173 6207 7997 5572 1240 913 1138 C
ATOM 161 C PRO A 173 175.928 48.981 -11.773 1.00 59.73 C
ANISOU 161 C PRO A 173 6920 9399 6375 1361 1202 1522 C
ATOM 162 O PRO A 173 176.638 48.581 -12.685 1.00 61.49 O
ANISOU 162 O PRO A 173 7041 9870 6451 1470 1235 1483 O
ATOM 163 N GLU A 174 176.411 49.662 -10.738 1.00 56.89 N
ANISOU 163 N GLU A 174 6606 8720 6288 1178 1205 1708 N
ATOM 164 CA GLU A 174 177.823 50.037 -10.719 1.00 54.95 C
ANISOU 164 CA GLU A 174 6278 8426 6174 1107 1253 1877 C
ATOM 165 CB GLU A 174 178.022 51.509 -10.342 1.00 57.70 C
ANISOU 165 CB GLU A 174 6626 8541 6756 969 1227 2109 C
ATOM 166 CG GLU A 174 177.490 52.511 -11.355 1.00 67.68 C
ANISOU 166 CG GLU A 174 7846 9937 7930 1062 1234 2282 C
ATOM 167 CD GLU A 174 178.155 52.387 -12.725 1.00 80.62 C
ANISOU 167 CD GLU A 174 9352 11927 9351 1225 1306 2387 C
ATOM 168 OE1 GLU A 174 179.293 51.839 -12.802 1.00 84.29 O
ANISOU 168 OE1 GLU A 174 9751 12469 9807 1223 1357 2372 O
ATOM 169 OE2 GLU A 174 177.522 52.844 -13.714 1.00 83.96 O
ANISOU 169 OE2 GLU A 174 9728 12564 9610 1361 1309 2485 O
ATOM 170 C GLU A 174 178.634 49.172 -9.779 1.00 48.63 C
ANISOU 170 C GLU A 174 5472 7486 5521 1023 1279 1768 C
ATOM 171 O GLU A 174 179.766 49.496 -9.461 1.00 51.76 O
ANISOU 171 O GLU A 174 5808 7792 6067 933 1297 1887 O
ATOM 172 N LEU A 175 178.077 48.067 -9.327 1.00 45.45 N
ANISOU 172 N LEU A 175 5120 7024 5125 1047 1236 1495 N
ATOM 173 CA LEU A 175 178.783 47.309 -8.305 1.00 47.79 C
ANISOU 173 CA LEU A 175 5414 7115 5629 957 1211 1394 C
ATOM 174 CB LEU A 175 177.864 46.317 -7.610 1.00 44.51 C
ANISOU 174 CB LEU A 175 5086 6510 5314 938 1104 1111 C
ATOM 175 CG LEU A 175 178.599 45.713 -6.426 1.00 46.88 C
ANISOU 175 CG LEU A 175 5378 6598 5836 844 1083 1096 C
ATOM 176 CD1 LEU A 175 178.824 46.798 -5.403 1.00 43.61 C
ANISOU 176 CD1 LEU A 175 4996 6023 5553 675 1051 1302 C
ATOM 177 CD2 LEU A 175 177.785 44.579 -5.867 1.00 48.55 C
ANISOU 177 CD2 LEU A 175 5645 6641 6161 849 1008 853 C
ATOM 178 C LEU A 175 180.048 46.608 -8.827 1.00 56.12 C
ANISOU 178 C LEU A 175 6337 8351 6634 1052 1309 1376 C
ATOM 179 O LEU A 175 181.137 46.765 -8.251 1.00 54.98 O
ANISOU 179 O LEU A 175 6131 8128 6630 967 1347 1515 O
ATOM 180 N GLN A 176 179.914 45.859 -9.921 1.00 57.81 N
ANISOU 180 N GLN A 176 6490 8828 6645 1234 1345 1188 N
ATOM 181 CA GLN A 176 181.055 45.127 -10.476 1.00 59.62 C
ANISOU 181 CA GLN A 176 6588 9245 6820 1347 1432 1122 C
ATOM 182 CB GLN A 176 180.661 44.404 -11.748 1.00 69.15 C
ANISOU 182 CB GLN A 176 7752 10731 7793 1529 1414 845 C
ATOM 183 CG GLN A 176 179.248 43.921 -11.722 1.00 84.31 C
ANISOU 183 CG GLN A 176 9737 12605 9692 1578 1337 572 C
ATOM 184 CD GLN A 176 179.136 42.455 -12.086 1.00 97.37 C
ANISOU 184 CD GLN A 176 11337 14269 11391 1690 1298 145 C
ATOM 185 OE1 GLN A 176 178.572 42.101 -13.129 1.00102.93 O
ANISOU 185 OE1 GLN A 176 12011 15190 11909 1790 1240 -100 O
ATOM 186 NE2 GLN A 176 179.685 41.586 -11.232 1.00100.03 N
ANISOU 186 NE2 GLN A 176 11658 14345 12006 1659 1311 56 N
ATOM 187 C GLN A 176 182.234 46.050 -10.777 1.00 58.38 C
ANISOU 187 C GLN A 176 6366 9163 6651 1281 1475 1420 C
ATOM 188 O GLN A 176 183.389 45.691 -10.557 1.00 62.58 O
ANISOU 188 O GLN A 176 6817 9683 7276 1266 1514 1443 O
ATOM 189 N ALA A 177 181.931 47.239 -11.283 1.00 53.99 N
ANISOU 189 N ALA A 177 5833 8667 6014 1250 1461 1640 N
ATOM 190 CA ALA A 177 182.965 48.208 -11.613 1.00 51.61 C
ANISOU 190 CA ALA A 177 5452 8398 5759 1194 1497 1914 C
ATOM 191 CB ALA A 177 182.385 49.410 -12.334 1.00 41.97 C
ANISOU 191 CB ALA A 177 4237 7246 4464 1212 1482 2120 C
ATOM 192 C ALA A 177 183.647 48.632 -10.331 1.00 54.09 C
ANISOU 192 C ALA A 177 5772 8412 6369 1002 1474 2017 C
ATOM 193 O ALA A 177 184.864 48.741 -10.281 1.00 59.93 O
ANISOU 193 O ALA A 177 6414 9165 7190 962 1511 2111 O
ATOM 194 N ARG A 178 182.867 48.847 -9.275 1.00 48.28 N
ANISOU 194 N ARG A 178 5139 7421 5784 885 1403 1977 N
ATOM 195 CA ARG A 178 183.472 49.247 -8.018 1.00 47.16 C
ANISOU 195 CA ARG A 178 4994 7025 5902 708 1352 2026 C
ATOM 196 CB ARG A 178 182.410 49.647 -7.008 1.00 42.63 C
ANISOU 196 CB ARG A 178 4540 6207 5451 594 1258 1970 C
ATOM 197 CG ARG A 178 181.715 50.932 -7.412 1.00 37.36 C
ANISOU 197 CG ARG A 178 3913 5483 4798 562 1227 2079 C
ATOM 198 CD ARG A 178 180.454 51.157 -6.528 1.00 42.44 C
ANISOU 198 CD ARG A 178 4686 5923 5518 485 1135 1976 C
ATOM 199 NE ARG A 178 180.816 51.341 -5.120 1.00 40.41 N
ANISOU 199 NE ARG A 178 4434 5452 5468 327 1058 1911 N
ATOM 200 CZ ARG A 178 180.109 50.884 -4.094 1.00 44.12 C
ANISOU 200 CZ ARG A 178 4987 5796 5981 276 986 1778 C
ATOM 201 NH1 ARG A 178 178.997 50.213 -4.326 1.00 44.59 N
ANISOU 201 NH1 ARG A 178 5136 5887 5920 359 990 1701 N
ATOM 202 NH2 ARG A 178 180.519 51.082 -2.842 1.00 45.29 N
ANISOU 202 NH2 ARG A 178 5114 5811 6282 150 915 1726 N
ATOM 203 C ARG A 178 184.386 48.174 -7.464 1.00 47.72 C
ANISOU 203 C ARG A 178 6097 6016 6032 721 1377 1934 C
ATOM 204 O ARG A 178 185.439 48.475 -6.911 1.00 47.05 O
ANISOU 204 O ARG A 178 4831 6954 6090 626 1364 2010 O
ATOM 205 N ILE A 179 183.958 46.926 -7.634 1.00 48.20 N
ANISOU 205 N ILE A 179 5066 7251 5995 852 1412 1750 N
ATOM 206 CA ILE A 179 184.694 45.760 -7.193 1.00 48.50 C
ANISOU 206 CA ILE A 179 5025 7286 6115 910 1439 1634 C
ATOM 207 CB ILE A 179 183.815 44.516 -7.290 1.00 51.23 C
ANISOU 207 CB ILE A 179 5430 7600 6437 1037 1413 1356 C
ATOM 208 CG1 ILE A 179 182.643 44.624 -6.342 1.00 60.80 C
ANISOU 208 CG1 ILE A 179 6794 8553 7754 925 1289 1294 C
ATOM 209 CD1 ILE A 179 183.063 44.561 -4.944 1.00 62.50 C
ANISOU 209 CD1 ILE A 179 7012 8566 8169 802 1223 1362 C
ATOM 210 CG2 ILE A 179 184.581 43.302 -6.871 1.00 50.72 C
ANISOU 210 CG2 ILE A 179 5289 7472 6509 1109 1417 1232 C
ATOM 211 C ILE A 179 185.942 45.532 -8.055 1.00 51.38 C
ANISOU 211 C ILE A 179 5265 7862 6394 999 1508 1661 C
ATOM 212 O ILE A 179 187.017 45.249 -7.538 1.00 50.58 O
ANISOU 212 O ILE A 179 5076 7729 6412 969 1513 1697 O
ATOM 213 N ARG A 180 185.771 45.628 -9.372 1.00 52.67 N
ANISOU 213 N ARG A 180 5415 8263 6336 1117 1554 1639 N
ATOM 214 CA ARG A 180 186.860 45.449 -10.326 1.00 60.20 C
ANISOU 214 CA ARG A 180 6249 9461 7169 1214 1647 1662 C
ATOM 215 CB ARG A 180 186.346 45.651 -11.753 1.00 69.09 C
ANISOU 215 CB ARG A 180 7373 10861 8017 1345 1651 1638 C
ATOM 216 CG ARG A 180 186.513 44.452 -12.661 1.00 77.82 C
ANISOU 216 CG ARG A 180 8412 12202 8954 1535 1683 1356 C
ATOM 217 CD ARG A 180 185.184 44.024 -13.309 1.00 83.31 C
ANISOU 217 CD ARG A 180 9174 13008 9474 1649 1632 1109 C
ATOM 218 NE ARG A 180 185.152 44.261 -14.760 1.00 90.87 N
ANISOU 218 NE ARG A 180 10069 14328 10130 1783 1647 1114 N
ATOM 219 CZ ARG A 180 185.845 43.559 -15.666 1.00 93.66 C
ANISOU 219 CZ ARG A 180 10312 14935 10339 1920 1685 951 C
ATOM 220 NH1 ARG A 180 186.643 42.567 -15.276 1.00 95.47 N
ANISOU 220 NH1 ARG A 180 10486 15066 10723 1941 1717 765 N
ATOM 221 NH2 ARG A 180 185.745 43.846 -16.965 1.00 89.93 N
ANISOU 221 NH2 ARG A 180 9774 14822 9574 2048 1687 980 N
ATOM 222 C ARG A 180 187.936 46.479 -10.019 1.00 63.20 C
ANISOU 222 C ARG A 180 6557 9780 7675 1073 1633 1926 C
ATOM 223 O ARG A 180 189.132 46.195 -10.045 1.00 69.21 O
ANISOU 223 O ARG A 180 7206 10615 8477 1086 1676 1953 O
ATOM 224 N THR A 181 187.481 47.680 -9.701 1.00 59.04 N
ANISOU 224 N THR A 181 6091 9106 7237 939 1587 2092 N
ATOM 225 CA THR A 181 188.355 48.787 -9.363 1.00 60.45 C
ANISOU 225 CA THR A 181 6199 9182 7588 793 1581 2295 C

ATOM 226 CB THR A 181 187.535 50.065 -9.221 1.00 64.03 C
ANISOU 226 CB THR A 181 6728 9467 8132 687 1529 2411 C
ATOM 227 OG1 THR A 181 186.779 50.270 -10.422 1.00 71.50 O
ANISOU 227 OG1 THR A 181 7702 10595 8870 818 1566 2464 O
ATOM 228 CG2 THR A 181 188.428 51.265 -8.975 1.00 61.76 C
ANISOU 228 CG2 THR A 181 6348 9066 8053 544 1535 2591 C
ATOM 229 C THR A 181 189.083 48.538 -8.055 1.00 62.27 C
ANISOU 229 C THR A 181 6388 9240 8029 674 1530 2252 C
ATOM 230 O THR A 181 190.294 48.767 -7.940 1.00 66.40 O
ANISOU 230 O THR A 181 6790 9797 8643 621 1557 2337 O
ATOM 231 N TYR A 182 188.333 48.077 -7.059 1.00 55.44 N
ANISOU 231 N TYR A 182 5614 8211 7238 635 1456 2126 N
ATOM 232 CA TYR A 182 188.908 47.788 -5.762 1.00 51.41 C
ANISOU 232 CA TYR A 182 5059 7572 6903 542 1393 2088 C
ATOM 233 CB TYR A 182 187.862 47.251 -4.783 1.00 51.61 C
ANISOU 233 CB TYR A 182 5190 7441 6976 525 1319 1968 C
ATOM 234 CG TYR A 182 188.451 47.077 -3.412 1.00 52.63 C
ANISOU 234 CG TYR A 182 5257 7477 7263 433 1241 1958 C
ATOM 235 CD1 TYR A 182 188.452 48.120 -2.501 1.00 53.21 C
ANISOU 235 CD1 TYR A 182 5330 7426 7460 261 1149 1987 C
ATOM 236 CE1 TYR A 182 189.013 47.969 -1.256 1.00 56.47 C
ANISOU 236 CE1 TYR A 182 5658 7819 7981 189 1072 1967 C
ATOM 237 CZ TYR A 182 189.597 46.759 -0.915 1.00 56.67 C
ANISOU 237 CZ TYR A 182 5603 7929 7999 300 1084 1952 C
ATOM 238 OH TYR A 182 190.184 46.565 0.322 1.00 52.52 O
ANISOU 238 OH TYR A 182 4972 7430 7554 255 1000 1954 O
ATOM 239 CE2 TYR A 182 189.606 45.720 -1.821 1.00 56.74 C
ANISOU 239 CE2 TYR A 182 5620 8013 7925 474 1178 1925 C
ATOM 240 CD2 TYR A 182 189.034 45.885 -3.048 1.00 53.18 C
ANISOU 240 CD2 TYR A 182 5248 7600 7358 534 1256 1910 C
ATOM 241 C TYR A 182 190.007 46.765 -5.923 1.00 54.62 C
ANISOU 241 C TYR A 182 5343 8122 7286 649 1450 2048 C
ATOM 242 O TYR A 182 191.080 46.876 -5.325 1.00 59.92 O
ANISOU 242 O TYR A 182 5904 8790 8074 581 1430 2099 O
ATOM 243 N ASN A 183 189.732 45.772 -6.756 1.00 53.60 N
ANISOU 243 N ASN A 183 5225 8130 7011 825 1517 1930 N
ATOM 244 CA ASN A 183 190.646 44.665 -6.942 1.00 53.00 C
ANISOU 244 CA ASN A 183 5041 8167 6928 955 1567 1837 C
ATOM 245 CB ASN A 183 189.962 43.542 -7.698 1.00 46.46 C
ANISOU 245 CB ASN A 183 4252 7418 5981 1144 1609 1614 C
ATOM 246 CG ASN A 183 189.160 42.670 -6.801 1.00 50.13 C
ANISOU 246 CG ASN A 183 4785 7677 6584 1174 1552 1475 C
ATOM 247 OD1 ASN A 183 189.393 42.643 -5.596 1.00 53.02 O
ANISOU 247 OD1 ASN A 183 5139 7887 7119 1088 1490 1552 O
ATOM 248 ND2 ASN A 183 188.191 41.952 -7.363 1.00 51.38 N
ANISOU 248 ND2 ASN A 183 5007 7837 6680 1298 1563 1261 N
ATOM 249 C ASN A 183 191.914 45.059 -7.666 1.00 63.84 C
ANISOU 249 C ASN A 183 6282 9724 8248 962 1636 1948 C
ATOM 250 O ASN A 183 192.806 44.238 -7.830 1.00 63.31 O
ANISOU 250 O ASN A 183 6112 9762 8183 1063 1678 1878 O
ATOM 251 N GLN A 184 191.971 46.306 -8.135 1.00 71.57 N
ANISOU 251 N GLN A 184 7260 10734 9199 865 1651 2122 N
ATOM 252 CA GLN A 184 193.142 46.814 -8.846 1.00 72.56 C
ANISOU 252 CA GLN A 184 7251 11024 9295 860 1727 2264 C
ATOM 253 CB GLN A 184 192.741 47.603 -10.082 1.00 77.47 C
ANISOU 253 CB GLN A 184 7892 11786 9758 900 1786 2392 C
ATOM 254 CG GLN A 184 193.816 47.645 -11.115 1.00 89.42 C
ANISOU 254 CG GLN A 184 9261 13555 11159 981 1891 2493 C
ATOM 255 CD GLN A 184 193.420 46.872 -12.347 1.00 99.01 C
ANISOU 255 CD GLN A 184 10484 15045 12089 1191 1950 2367 C
ATOM 256 OE1 GLN A 184 192.223 46.698 -12.617 1.00102.65 O
ANISOU 256 OE1 GLN A 184 11061 15509 12431 1255 1914 2264 O
ATOM 257 NE2 GLN A 184 194.414 46.390 -13.103 1.00 99.98 N
ANISOU 257 NE2 GLN A 184 10475 15416 12098 1303 2036 2350 N
ATOM 258 C GLN A 184 193.943 47.718 -7.928 1.00 67.85 C
ANISOU 258 C GLN A 184 6574 10285 8919 671 1680 2393 C
ATOM 259 O GLN A 184 195.121 47.500 -7.705 1.00 69.36 O
ANISOU 259 O GLN A 184 6629 10544 9179 659 1702 2412 O
ATOM 260 N HIS A 185 193.283 48.724 -7.375 1.00 66.88 N
ANISOU 260 N HIS A 185 6528 9967 8915 524 1611 2452 N
ATOM 261 C HIS A 185 194.528 49.038 -5.239 1.00 64.41 C
ANISOU 261 C HIS A 185 6065 9470 8938 291 1483 2416 C
ATOM 262 O HIS A 185 195.565 49.466 -4.741 1.00 67.11 O
ANISOU 262 O HIS A 185 6265 9815 9418 184 1469 2454 O
ATOM 263 CA HIS A 185 193.957 49.672 -6.502 1.00 70.84 C
ANISOU 263 CA HIS A 185 6946 10328 9642 335 1561 2524 C
ATOM 264 CB HIS A 185 193.009 50.815 -6.111 1.00 82.67 C
ANISOU 264 CB HIS A 185 8545 11610 11256 201 1496 2554 C
ATOM 265 CG HIS A 185 192.687 51.749 -7.236 1.00 96.48 C
ANISOU 265 CG HIS A 185 10310 13384 12963 219 1568 2716 C
ATOM 266 ND1 HIS A 185 192.488 51.319 -8.528 1.00101.42 N
ANISOU 266 ND1 HIS A 185 10949 14227 13360 391 1655 2775 N
ATOM 267 CE1 HIS A 185 192.224 52.366 -9.301 1.00102.33 C
ANISOU 267 CE1 HIS A 185 11057 14338 13485 382 1701 2952 C
ATOM 268 NE2 HIS A 185 192.244 53.449 -8.556 1.00101.32 N
ANISOU 268 NE2 HIS A 185 10917 13968 13612 208 1653 2998 N
ATOM 269 CD2 HIS A 185 192.534 53.099 -7.254 1.00100.08 C
ANISOU 269 CD2 HIS A 185 10756 13684 13587 98 1566 2837 C
ATOM 270 N TYR A 186 193.843 48.028 -4.714 1.00 79.81 N
ANISOU 270 N TYR A 186 5238 11580 13504 -283 1014 164 N
ATOM 271 CA TYR A 186 194.184 47.498 -3.400 1.00 73.48 C
ANISOU 271 CA TYR A 186 4687 10033 13197 -165 822 -213 C
ATOM 272 CB TYR A 186 193.062 47.795 -2.398 1.00 77.23 C
ANISOU 272 CB TYR A 186 5654 9664 14026 -251 895 43 C
ATOM 273 CG TYR A 186 192.903 49.276 -2.113 1.00 81.99 C
ANISOU 273 CG TYR A 186 6419 9992 14742 -506 1140 661 C
ATOM 274 CD2 TYR A 186 193.624 49.886 -1.085 1.00 84.01 C
ANISOU 274 CD2 TYR A 186 6857 9699 15363 -618 1114 688 C
ATOM 275 CE2 TYR A 186 193.500 51.241 -0.835 1.00 86.12 C
ANISOU 275 CE2 TYR A 186 7398 9728 15594 -794 1307 1190 C
ATOM 276 CZ TYR A 186 192.643 52.014 -1.619 1.00 86.21 C
ANISOU 276 CZ TYR A 186 7482 10044 15231 -824 1494 1621 C
ATOM 277 OH TYR A 186 192.524 53.368 -1.358 1.00 84.17 O
ANISOU 277 OH TYR A 186 7514 9580 14886 -899 1618 1983 O
ATOM 278 CE1 TYR A 186 191.921 51.429 -2.658 1.00 83.80 C
ANISOU 278 CE1 TYR A 186 6972 10268 14602 -754 1509 1606 C
ATOM 279 CD1 TYR A 186 192.059 50.068 -2.896 1.00 82.09 C
ANISOU 279 CD1 TYR A 186 6492 10303 14396 -614 1348 1155 C
ATOM 280 C TYR A 186 194.509 46.016 -3.430 1.00 69.53 C
ANISOU 280 C TYR A 186 4176 9656 12587 126 552 -909 C
ATOM 281 O TYR A 186 194.486 45.341 -2.411 1.00 66.10 O
ANISOU 281 O TYR A 186 4217 8603 12293 267 325 -1275 O
ATOM 282 N ASN A 187 194.823 45.520 -4.620 1.00 72.65 N
ANISOU 282 N ASN A 187 4243 10828 12532 213 562 -1032 N
ATOM 283 CA ASN A 187 195.232 44.135 -4.798 1.00 77.73 C
ANISOU 283 CA ASN A 187 4922 11652 12961 487 344 -1668 C
ATOM 284 CB ASN A 187 195.418 43.856 -6.294 1.00 87.96 C
ANISOU 284 CB ASN A 187 5909 13749 13763 493 452 -1583 C
ATOM 285 CG ASN A 187 196.187 42.568 -6.572 1.00 94.75 C
ANISOU 285 CG ASN A 187 6785 14838 14379 753 277 -2204 C
ATOM 286 OD1 ASN A 187 197.261 42.592 -7.184 1.00 97.40 O
ANISOU 286 OD1 ASN A 187 6883 15567 14558 788 301 -2227 O
ATOM 287 ND2 ASN A 187 195.640 41.436 -6.121 1.00 95.95 N
ANISOU 287 ND2 ASN A 187 7236 14712 14508 943 108 -2701 N
ATOM 288 C ASN A 187 196.514 43.803 -4.015 1.00 80.60 C
ANISOU 288 C ASN A 187 5348 11774 13501 641 123 -2079 C
ATOM 289 O ASN A 187 196.698 42.687 -3.528 1.00 82.25 O
ANISOU 289 O ASN A 187 5795 11742 13712 884 -104 -2629 O
ATOM 290 N ASN A 188 197.413 44.773 -3.902 1.00 80.08 N
ANISOU 290 N ASN A 188 5079 11784 13562 495 188 -1791 N
ATOM 291 CA ASN A 188 198.638 44.572 -3.128 1.00 79.06 C
ANISOU 291 CA ASN A 188 4978 11438 13623 598 -20 -2108 C
ATOM 292 CB ASN A 188 199.709 45.602 -3.515 1.00 78.83 C
ANISOU 292 CB ASN A 188 4593 11802 13557 427 94 -1736 C
ATOM 293 CG ASN A 188 200.261 45.380 -4.932 1.00 80.94 C
ANISOU 293 CG ASN A 188 4510 12853 13389 494 205 -1650 C
ATOM 294 OD1 ASN A 188 200.393 44.234 -5.403 1.00 79.45 O
ANISOU 294 OD1 ASN A 188 4346 12882 12960 718 123 -2058 O
ATOM 295 ND2 ASN A 188 200.567 46.486 -5.627 1.00 78.94 N
ANISOU 295 ND2 ASN A 188 3965 12955 13072 295 400 -1108 N
ATOM 296 C ASN A 188 198.390 44.571 -1.616 1.00 75.93 C
ANISOU 296 C ASN A 188 4994 10146 13711 598 -202 -2272 C
ATOM 297 O ASN A 188 199.138 43.971 -0.851 1.00 77.52 O
ANISOU 297 O ASN A 188 5366 10058 14029 753 -450 -2664 O
ATOM 298 N LEU A 189 197.328 45.250 -1.202 1.00 74.42 N
ANISOU 298 N LEU A 189 5136 9474 13665 401 -64 -1872 N
ATOM 299 CA LEU A 189 196.952 45.339 0.207 1.00 74.28 C
ANISOU 299 CA LEU A 189 5746 8524 13955 348 -191 -1883 C
ATOM 300 CB LEU A 189 196.158 46.618 0.468 1.00 69.37 C
ANISOU 300 CB LEU A 189 5297 7534 13528 46 74 -1256 C
ATOM 301 CG LEU A 189 195.568 46.750 1.872 1.00 63.47 C
ANISOU 301 CG LEU A 189 5245 5791 13081 -25 -1 -1218 C
ATOM 302 CD1 LEU A 189 196.680 46.688 2.959 1.00 53.27 C
ANISOU 302 CD1 LEU A 189 4159 4074 12006 -34 -257 -1501 C
ATOM 303 CD2 LEU A 189 194.732 48.034 1.970 1.00 58.82 C
ANISOU 303 CD2 LEU A 189 4789 4900 12658 -308 329 -555 C
ATOM 304 C LEU A 189 196.096 44.158 0.631 1.00 76.72 C
ANISOU 304 C LEU A 189 6522 8430 14196 568 -362 -2271 C
ATOM 305 O LEU A 189 196.207 43.651 1.741 1.00 79.34 O
ANISOU 305 O LEU A 189 7311 8127 14709 666 -591 -2577 O
ATOM 306 N LEU A 190 195.217 43.744 -0.263 1.00 76.74 N
ANISOU 306 N LEU A 190 6415 8811 13931 627 -248 -2239 N
ATOM 307 CA LEU A 190 194.313 42.650 0.012 1.00 76.66 C
ANISOU 307 CA LEU A 190 6826 8482 13820 810 -387 -2568 C
ATOM 308 CB LEU A 190 193.137 42.728 -0.948 1.00 80.46 C
ANISOU 308 CB LEU A 190 7177 9332 14060 725 -176 -2256 C
ATOM 309 CG LEU A 190 191.986 41.783 -0.659 1.00 82.98 C
ANISOU 309 CG LEU A 190 7956 9288 14285 847 -284 -2468 C
ATOM 310 CD1 LEU A 190 191.358 42.118 0.703 1.00 80.85 C
ANISOU 310 CD1 LEU A 190 8294 8079 14348 769 -331 -2301 C
ATOM 311 CD2 LEU A 190 190.992 41.956 -1.763 1.00 85.13 C
ANISOU 311 CD2 LEU A 190 7981 10074 14290 724 -69 -2106 C
ATOM 312 C LEU A 190 195.005 41.297 -0.138 1.00 74.98 C
ANISOU 312 C LEU A 190 6627 8577 13402 1120 -627 -3234 C
ATOM 313 O LEU A 190 194.738 40.373 0.622 1.00 74.17 O
ANISOU 313 O LEU A 190 6997 8019 13164 1161 -849 -3456 O
ATOM 314 N ARG A 191 195.893 41.202 -1.126 1.00 76.78 N
ANISOU 314 N ARG A 191 6248 9499 13424 1184 -573 -3339 N
ATOM 315 CA ARG A 191 196.549 39.949 -1.515 1.00 74.92 C
ANISOU 315 CA ARG A 191 5957 9609 12902 1448 -727 -3886 C

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ATOM   316 CB  ARG A 191    197.569 39.520 -0.480  1.00 71.91           C
ANISOU 316 CB  ARG A 191     5850  8826 12647  1524  -986 -4165       C
ATOM   317 CG  ARG A 191    198.486 40.631 -0.111  1.00 78.51           C
ANISOU 317 CG  ARG A 191     6381  9627 13824  1414  -950 -3928       C
ATOM   318 CD  ARG A 191    199.356 40.258  1.053  1.00 80.75           C
ANISOU 318 CD  ARG A 191     6969  9448 14265  1451 -1224 -4163       C
ATOM   319 NE  ARG A 191    200.745 40.162  0.640  1.00 87.19           N
ANISOU 319 NE  ARG A 191     7359 10759 15012  1558 -1251 -4304       N
ATOM   320 CZ  ARG A 191    201.755 40.020  1.484  1.00 88.94           C
ANISOU 320 CZ  ARG A 191     7648 10740 15406  1590 -1461 -4459       C
ATOM   321 NH1 ARG A 191    201.500 39.963  2.784  1.00 90.54           N
ANISOU 321 NH1 ARG A 191     8331 10278 15791  1458 -1671 -4424       N
ATOM   322 NH2 ARG A 191    203.003 39.951  1.029  1.00 84.26           N
ANISOU 322 NH2 ARG A 191     6663 10638 14716  1680 -1453 -4521       N
ATOM   323 C   ARG A 191    195.516 38.865 -1.735  1.00 70.49           C
ANISOU 323 C   ARG A 191     5753  8982 12048  1539  -787 -4121       C
ATOM   324 O   ARG A 191    195.642 37.738 -1.267  1.00 71.89           O
ANISOU 324 O   ARG A 191     6330  8961 12024  1595 -1020 -4386       O
ATOM   325 N   GLY A 192    194.491 39.230 -2.469  1.00 68.29           N
ANISOU 325 N   GLY A 192     5287  8968 11693  1452  -586 -3857       N
ATOM   326 CA  GLY A 192    193.364 38.359 -2.702  1.00 72.34           C
ANISOU 326 CA  GLY A 192     6099  9421 11966  1513  -619 -4025       C
ATOM   327 C   GLY A 192    192.430 39.101 -3.633  1.00 76.79           C
ANISOU 327 C   GLY A 192     6411 10403 12364  1255  -367 -3474       C
ATOM   328 O   GLY A 192    192.726 40.211 -4.076  1.00 85.31           O
ANISOU 328 O   GLY A 192     7094 11804 13514  1062  -173 -3015       O
ATOM   329 N   ALA A 193    191.308 38.481 -3.949  1.00 73.37           N
ANISOU 329 N   ALA A 193     6194  9984 11698  1244  -370 -3506       N
ATOM   330 CA  ALA A 193    190.294 39.132 -4.751  1.00 72.20           C
ANISOU 330 CA  ALA A 193     5846 10187 11401   991  -150 -2951       C
ATOM   331 CB  ALA A 193    190.137 38.448 -6.105  1.00 58.81           C
ANISOU 331 CB  ALA A 193     3848  9290  9208   987  -90 -3113       C
ATOM   332 C   ALA A 193    189.017 39.038 -3.952  1.00 65.68           C
ANISOU 332 C   ALA A 193     5540  8690 10726   943  -202 -2784       C
ATOM   333 O   ALA A 193    188.763 38.029 -3.286  1.00 63.96           O
ANISOU 333 O   ALA A 193     5778  8021 10504  1123  -415 -3233       O
ATOM   334 N   VAL A 194    188.220 40.096 -3.985  1.00 62.09           N
ANISOU 334 N   VAL A 194     5025  8148 10418   709     2 -2128       N
ATOM   335 CA  VAL A 194    186.891 39.982 -3.456  1.00 57.00           C
ANISOU 335 CA  VAL A 194     4807  6994  9855   654    -8 -1911       C
ATOM   336 CB  VAL A 194    186.368 41.310 -2.911  1.00 59.54           C
ANISOU 336 CB  VAL A 194     5193  6884 10545   462   206 -1233       C
ATOM   337 CG1 VAL A 194    187.485 42.059 -2.217  1.00 59.14           C
ANISOU 337 CG1 VAL A 194     5115  6529 10826   469   216 -1239       C
ATOM   338 CG2 VAL A 194    185.821 42.137 -4.004  1.00 64.87           C
ANISOU 338 CG2 VAL A 194     5405  8175 11066   229   484  -608       C
ATOM   339 C   VAL A 194    186.023 39.448 -4.584  1.00 55.58           C
ANISOU 339 C   VAL A 194     4451  7423  9244   563    43 -1831       C
ATOM   340 O   VAL A 194    186.301 39.681 -5.759  1.00 63.32           O
ANISOU 340 O   VAL A 194     4931  9181  9948   454   179 -1686       O
ATOM   341 N   SER A 195    184.991 38.706 -4.217  1.00 52.74           N
ANISOU 341 N   SER A 195     4513  6711  8815   600   -77 -1939       N
ATOM   342 CA  SER A 195    184.047 38.165 -5.178  1.00 60.35           C
ANISOU 342 CA  SER A 195     5379  8184  9368   481   -53 -1843       C
ATOM   343 CB  SER A 195    183.164 37.144 -4.484  1.00 62.44           C
ANISOU 343 CB  SER A 195     6212  7910  9601   586  -259 -2144       C
ATOM   344 OG  SER A 195    183.932 36.434 -3.539  1.00 67.30           O
ANISOU 344 OG  SER A 195     7191  8001 10379   852  -480 -2771       O
ATOM   345 C   SER A 195    183.190 39.283 -5.743  1.00 66.73           C
ANISOU 345 C   SER A 195     5879  9268 10208   204   215 -1025       C
ATOM   346 O   SER A 195    183.070 40.365 -5.138  1.00 61.40           O
ANISOU 346 O   SER A 195     5229  8181  9920   132   371  -547       O
ATOM   347 N   GLN A 196    182.552 39.019 -6.879  1.00 72.27           N
ANISOU 347 N   GLN A 196     6313 10644 10502    38   275  -847       N
ATOM   348 CA  GLN A 196    181.906 40.109 -7.599  1.00 76.29           C
ANISOU 348 CA  GLN A 196     6417 11564 11006  -229   544   -58       C
ATOM   349 CB  GLN A 196    182.222 40.042 -9.090  1.00 83.04           C
ANISOU 349 CB  GLN A 196     6726 13420 11408  -377   631   -29       C
ATOM   350 CG  GLN A 196    182.975 41.256 -9.590  1.00 91.02           C
ANISOU 350 CG  GLN A 196     7214 14819 12550  -479   868   371       C
ATOM   351 CD  GLN A 196    184.056 40.876 -10.575  1.00103.44           C
ANISOU 351 CD  GLN A 196     8405 17117 13781  -446   850   -34       C
ATOM   352 OE1 GLN A 196    185.199 41.357 -10.500  1.00107.61           O
ANISOU 352 OE1 GLN A 196     8825 17586 14476  -351   884  -142       O
ATOM   353 NE2 GLN A 196    183.708 39.992 -11.508  1.00108.52           N
ANISOU 353 NE2 GLN A 196     8991 18307 13935  -519   778  -254       N
ATOM   354 C   GLN A 196    180.406 40.274 -7.380  1.00 73.93           C
ANISOU 354 C   GLN A 196     6326 10996 10769  -369   605   471       C
ATOM   355 O   GLN A 196    179.790 41.210 -7.909  1.00 82.14           O
ANISOU 355 O   GLN A 196     7040 12330 11840  -582   844  1186       O
ATOM   356 N   ARG A 197    179.806 39.378 -6.615  1.00 59.52           N
ANISOU 356 N   ARG A 197     5026  8624  8965  -248   400   149       N
ATOM   357 CA  ARG A 197    178.393 39.518 -6.371  1.00 57.55           C
ANISOU 357 CA  ARG A 197     4975  8106  8788  -370   456   659       C
ATOM   358 CB  ARG A 197    177.712 38.156 -6.390  1.00 57.63           C
ANISOU 358 CB  ARG A 197     5335  8092  8471  -334   203   229       C
ATOM   359 CG  ARG A 197    177.949 37.357 -7.667  1.00 59.69           C
ANISOU 359 CG  ARG A 197     5308  9217  8156  -436   121   -96       C
ATOM   360 CD  ARG A 197    176.651 37.022 -8.377  1.00 63.39           C
ANISOU 360 CD  ARG A 197     5724 10086  8277  -684   116   272       C
ATOM   361 NE  ARG A 197    176.188 35.645 -8.150  1.00 71.00           N
ANISOU 361 NE  ARG A 197     7146 10864  8967  -617  -151  -274       N
ATOM   362 CZ  ARG A 197    175.052 35.130 -8.644  1.00 72.31           C
ANISOU 362 CZ  ARG A 197     7367 11307  8801  -828  -216   -64       C
ATOM   363 NH1 ARG A 197    174.716 33.867 -8.389  1.00 68.80           N
ANISOU 363 NH1 ARG A 197     7368 10660  8114  -760  -460  -605       N
ATOM   364 NH2 ARG A 197    174.251 35.877 -9.399  1.00 70.80           N
ANISOU 364 NH2 ARG A 197     6781 11604  8514 -1116  -38   700       N
ATOM   365 C   ARG A 197    178.149 40.262 -5.055  1.00 57.06           C
ANISOU 365 C   ARG A 197     5271  7129  9277  -283   547   948       C
ATOM   366 O   ARG A 197    179.034 40.414 -4.239  1.00 51.66           O
ANISOU 366 O   ARG A 197     4783  5969  8879  -120   496   628       O
ATOM   367 N   LEU A 198    176.949 40.771 -4.870  1.00 44.55           N
ANISOU 367 N   LEU A 198     4735  5178  7014   151   -71  -712       N
ATOM   368 CA  LEU A 198    176.587 41.332 -3.586  1.00 45.83           C
ANISOU 368 CA  LEU A 198     4882  5420  7110   176  -155  -605       C
ATOM   369 CB  LEU A 198    175.699 42.538 -3.785  1.00 38.51           C
ANISOU 369 CB  LEU A 198     4112  4443  6076    65  -125  -587       C
ATOM   370 CG  LEU A 198    175.448 43.567 -2.687  1.00 44.18           C
ANISOU 370 CG  LEU A 198     4847  5228  6712    36  -134  -576       C
ATOM   371 CD1 LEU A 198    173.938 43.767 -2.548  1.00 44.36           C
ANISOU 371 CD1 LEU A 198     4983  5141  6729    75  -145  -445       C
ATOM   372 CD2 LEU A 198    176.073 43.239 -1.352  1.00 45.55           C
ANISOU 372 CD2 LEU A 198     4874  5584  6847    94  -209  -571       C
ATOM   373 C   LEU A 198    175.808 40.253 -2.877  1.00 44.85           C
ANISOU 373 C   LEU A 198     4749  5232  7062   311  -244  -436       C
ATOM   374 O   LEU A 198    174.880 39.666 -3.429  1.00 44.45           O
ANISOU 374 O   LEU A 198     4794  5034  7061   314  -245  -381       O
ATOM   375 N   TYR A 199    176.203 39.969 -1.655  1.00 43.41           N
ANISOU 375 N   TYR A 199     4441  5179  6876   400  -325  -342       N
ATOM   376 CA  TYR A 199    175.521 38.928 -0.919  1.00 38.79           C
ANISOU 376 CA  TYR A 199     3844  4538  6357   517  -403  -138       C
ATOM   377 CB  TYR A 199    176.528 37.970 -0.310  1.00 35.56           C
ANISOU 377 CB  TYR A 199     3248  4195  6067   664  -473   -39       C
ATOM   378 CG  TYR A 199    177.166 37.157 -1.381  1.00 40.62           C
ANISOU 378 CG  TYR A 199     3845  4664  6924   733  -395  -146       C
ATOM   379 CD1 TYR A 199    178.279 37.642 -2.082  1.00 43.95           C
ANISOU 379 CD1 TYR A 199     4175  5169  7355   691  -315  -350       C
ATOM   380 CE1 TYR A 199    178.870 36.881 -3.070  1.00 48.80           C
ANISOU 380 CE1 TYR A 199     4741  5639  8161   755  -204  -481       C
ATOM   381 CZ  TYR A 199    178.318 35.643 -3.386  1.00 51.40           C
ANISOU 381 CZ  TYR A 199     5139  5703  8688   851  -176  -430       C
ATOM   382 OH  TYR A 199    178.883 34.872 -4.366  1.00 55.33           O
ANISOU 382 OH  TYR A 199     5603  6034  9385   909   -34  -609       O
ATOM   383 CE2 TYR A 199    177.211 35.157 -2.718  1.00 47.17           C
ANISOU 383 CE2 TYR A 199     4702  5060  8160   874  -268  -219       C
ATOM   384 CD2 TYR A 199    176.641 35.920 -1.726  1.00 42.53           C
ANISOU 384 CD2 TYR A 199     4141  4652  7366   818  -375   -69       C
ATOM   385 C   TYR A 199    174.597 39.508  0.122  1.00 30.77           C
ANISOU 385 C   TYR A 199     2883  3622  5185   483  -440   -31       C
ATOM   386 O   TYR A 199    175.015 40.266  0.988  1.00 30.62           O
ANISOU 386 O   TYR A 199     2812  3803  5017   441  -462   -68       O
ATOM   387 N   ILE A 200    173.336 39.143  0.014  1.00 33.04           N
ANISOU 387 N   ILE A 200     3266  3782  5506   485  -434    80       N
ATOM   388 CA  ILE A 200    172.293 39.746  0.829  1.00 36.10           C
ANISOU 388 CA  ILE A 200     3703  4248  5766   453  -423   157       C
ATOM   389 CB  ILE A 200    171.144 40.278 -0.028  1.00 37.90           C
ANISOU 389 CB  ILE A 200     4040  4340  6019   391  -364   131       C
ATOM   390 CG1 ILE A 200    171.669 41.270 -1.047  1.00 38.94           C
ANISOU 390 CG1 ILE A 200     4231  4429  6135   314  -308   -44       C
ATOM   391 CD1 ILE A 200    170.590 41.839 -1.914  1.00 38.68           C
ANISOU 391 CD1 ILE A 200     4287  4289  6120   265  -277   -17       C
ATOM   392 CG2 ILE A 200    170.174 41.006  0.835  1.00 39.79           C
ANISOU 392 CG2 ILE A 200     4297  4661  6160   387  -319   183       C
ATOM   393 C   ILE A 200    171.765 38.689  1.763  1.00 32.03           C
ANISOU 393 C   ILE A 200     3142  3758  5271   524  -482   390       C
ATOM   394 O   ILE A 200    171.202 37.675  1.335  1.00 32.54           O
ANISOU 394 O   ILE A 200     3229  3647  5488   548  -434   502       O
ATOM   395 N   LEU A 201    171.992 38.915  3.046  1.00 32.87           N
ANISOU 395 N   LEU A 201     3187  4093  5210   534  -516   463       N
ATOM   396 CA  LEU A 201    171.582 37.971  4.068  1.00 30.50           C
ANISOU 396 CA  LEU A 201     2839  3869  4880   586  -572   727       C
ATOM   397 CB  LEU A 201    172.417 38.160  5.313  1.00 31.52           C
ANISOU 397 CB  LEU A 201     2867  4313  4794   590  -650   785       C
ATOM   398 CG  LEU A 201    173.909 37.941  5.129  1.00 33.16           C
ANISOU 398 CG  LEU A 201     2947  4585  5066   651  -745   746       C
ATOM   399 CD1 LEU A 201    174.678 38.668  6.253  1.00 33.71           C
ANISOU 399 CD1 LEU A 201     2919  5043  4847   577  -819   698       C
ATOM   400 CD2 LEU A 201    174.152 36.442  5.181  1.00 30.89           C
ANISOU 400 CD2 LEU A 201     2581  4164  4993   801  -829  1028       C
ATOM   401 C   LEU A 201    170.129 38.235  4.404  1.00 33.91           C
ANISOU 401 C   LEU A 201     3303  4303  5245   531  -491   790       C
ATOM   402 O   LEU A 201    169.746 39.370  4.652  1.00 30.78           O
ANISOU 402 O   LEU A 201     2976  4008  4710   475  -406   645       O
ATOM   403 N   LEU A 202    169.316 37.187  4.389  1.00 36.73           N
ANISOU 403 N   LEU A 202     3698  4530  5729   545  -499   999       N
ATOM   404 CA  LEU A 202    167.921 37.287  4.777  1.00 33.21           C
ANISOU 404 CA  LEU A 202     3267  4116  5236   490  -420  1094       C
ATOM   405 CB  LEU A 202    167.015 37.006  3.599  1.00 35.24           C
ANISOU 405 CB  LEU A 202     3560  4133  5696   448  -398  1070       C
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ATOM 406 CG LEU A 202 167.102 38.050 2.513 1.00 47.00 C
ANISOU 406 CG LEU A 202 5099 5555 7205 430 -370 833 C
ATOM 407 CD1 LEU A 202 167.223 37.393 1.176 1.00 51.53 C
ANISOU 407 CD1 LEU A 202 5713 5909 7956 395 -420 778 C
ATOM 408 CD2 LEU A 202 165.825 38.840 2.588 1.00 52.64 C
ANISOU 408 CD2 LEU A 202 5792 6321 7886 404 -284 835 C
ATOM 409 C LEU A 202 167.602 36.300 5.880 1.00 36.93 C
ANISOU 409 C LEU A 202 3691 4686 5653 493 -445 1395 C
ATOM 410 O LEU A 202 167.137 35.191 5.608 1.00 40.92 O
ANISOU 410 O LEU A 202 4201 4998 6351 484 -467 1577 O
ATOM 411 N PRO A 203 167.870 36.687 7.129 1.00 39.37 N
ANISOU 411 N PRO A 203 3965 5302 5693 482 -440 1449 N
ATOM 412 CA PRO A 203 167.459 35.800 8.224 1.00 37.69 C
ANISOU 412 CA PRO A 203 3713 5225 5380 461 -454 1777 C
ATOM 413 CB PRO A 203 168.193 36.363 9.440 1.00 39.77 C
ANISOU 413 CB PRO A 203 3938 5881 5291 439 -490 1770 C
ATOM 414 CG PRO A 203 168.535 37.822 9.072 1.00 41.48 C
ANISOU 414 CG PRO A 203 4189 6156 5414 409 -422 1369 C
ATOM 415 CD PRO A 203 168.699 37.823 7.574 1.00 39.28 C
ANISOU 415 CD PRO A 203 3947 5527 5450 464 -438 1225 C
ATOM 416 C PRO A 203 165.948 35.914 8.391 1.00 37.63 C
ANISOU 416 C PRO A 203 3708 5229 5361 378 -309 1823 C
ATOM 417 O PRO A 203 165.424 37.009 8.560 1.00 38.75 O
ANISOU 417 O PRO A 203 3851 5505 5367 347 -186 1620 O
ATOM 418 N LEU A 204 165.244 34.793 8.321 1.00 39.73 N
ANISOU 418 N LEU A 204 3961 5334 5799 342 -311 2081 N
ATOM 419 CA LEU A 204 163.787 34.823 8.405 1.00 47.52 C
ANISOU 419 CA LEU A 204 4908 6338 6807 248 -177 2137 C
ATOM 420 CB LEU A 204 163.211 33.497 7.921 1.00 54.03 C
ANISOU 420 CB LEU A 204 5731 6883 7916 182 -211 2366 C
ATOM 421 CG LEU A 204 163.504 33.260 6.450 1.00 50.88 C
ANISOU 421 CG LEU A 204 5383 6149 7802 202 -290 2185 C
ATOM 422 CD1 LEU A 204 162.843 31.990 6.023 1.00 49.99 C
ANISOU 422 CD1 LEU A 204 5276 5762 7958 92 -300 2361 C
ATOM 423 CD2 LEU A 204 163.016 34.457 5.631 1.00 47.99 C
ANISOU 423 CD2 LEU A 204 5000 5817 7419 200 -242 1895 C
ATOM 424 C LEU A 204 163.243 35.138 9.808 1.00 49.90 C
ANISOU 424 C LEU A 204 5162 7004 6794 186 -51 2251 C
ATOM 425 O LEU A 204 162.093 35.559 9.955 1.00 54.08 O
ANISOU 425 O LEU A 204 5629 7621 7298 130 106 2208 O
ATOM 426 N ASP A 205 164.033 34.893 10.845 1.00 47.20 N
ANISOU 426 N ASP A 205 4830 6900 6205 190 -115 2411 N
ATOM 427 CA ASP A 205 163.648 35.354 12.183 1.00 53.52 C
ANISOU 427 CA ASP A 205 5600 8115 6621 106 13 2455 C
ATOM 428 CB ASP A 205 164.446 34.644 13.280 1.00 57.82 C
ANISOU 428 CB ASP A 205 6143 8915 6909 83 -112 2778 C
ATOM 429 CG ASP A 205 165.951 34.809 13.113 1.00 76.39 C
ANISOU 429 CG ASP A 205 8506 11284 9233 180 -311 2691 C
ATOM 430 OD1 ASP A 205 166.470 34.591 11.983 1.00 84.11 O
ANISOU 430 OD1 ASP A 205 9499 11912 10546 284 -406 2596 O
ATOM 431 OD2 ASP A 205 166.613 35.163 14.114 1.00 82.62 O
ANISOU 431 OD2 ASP A 205 9275 12468 9648 135 -367 2708 O
ATOM 432 C ASP A 205 163.814 36.895 12.282 1.00 52.25 C
ANISOU 432 C ASP A 205 5458 8131 6265 119 123 2031 C
ATOM 433 O ASP A 205 163.511 37.510 13.320 1.00 57.47 O
ANISOU 433 O ASP A 205 6108 9134 6596 43 271 1945 O
ATOM 434 N CYS A 206 164.307 37.500 11.199 1.00 42.26 N
ANISOU 434 N CYS A 206 4230 6622 5205 201 67 1765 N
ATOM 435 CA CYS A 206 164.399 38.963 11.064 1.00 51.67 C
ANISOU 435 CA CYS A 206 5455 7861 6318 215 183 1371 C
ATOM 436 CB CYS A 206 163.012 39.628 11.122 1.00 54.26 C
ANISOU 436 CB CYS A 206 5734 8195 6689 212 422 1257 C
ATOM 437 SG CYS A 206 161.955 39.293 9.713 1.00 49.38 S
ANISOU 437 SG CYS A 206 5050 7214 6499 272 413 1338 S
ATOM 438 C CYS A 206 165.307 39.643 12.088 1.00 56.73 C
ANISOU 438 C CYS A 206 6128 8841 6588 150 181 1205 C
ATOM 439 O CYS A 206 165.205 40.854 12.268 1.00 62.15 O
ANISOU 439 O CYS A 206 6850 9595 7170 124 335 872 O
ATOM 440 N GLY A 207 166.157 38.872 12.772 1.00 51.40 N
ANISOU 440 N GLY A 207 5432 8377 5720 116 11 1440 N
ATOM 441 CA GLY A 207 167.140 39.431 13.684 1.00 46.91 C
ANISOU 441 CA GLY A 207 4867 8176 4780 27 -48 1301 C
ATOM 442 C GLY A 207 168.324 40.024 12.926 1.00 51.15 C
ANISOU 442 C GLY A 207 5417 8578 5439 63 -170 1051 C
ATOM 443 O GLY A 207 169.102 39.307 12.282 1.00 54.48 O
ANISOU 443 O GLY A 207 5796 8833 6072 153 -356 1212 O
ATOM 444 N VAL A 208 168.450 41.348 12.975 1.00 52.62 N
ANISOU 444 N VAL A 208 5661 8813 5520 -12 -39 643 N
ATOM 445 CA VAL A 208 169.529 42.026 12.263 1.00 52.80 C
ANISOU 445 CA VAL A 208 5697 8709 5655 -17 -122 389 C
ATOM 446 CB VAL A 208 169.020 43.031 11.218 1.00 46.33 C
ANISOU 446 CB VAL A 208 4963 7519 5120 29 47 103 C
ATOM 447 CG1 VAL A 208 170.214 43.707 10.534 1.00 42.09 C
ANISOU 447 CG1 VAL A 208 4442 6876 4673 -10 -33 -130 C
ATOM 448 CG2 VAL A 208 168.145 42.334 10.214 1.00 38.22 C
ANISOU 448 CG2 VAL A 208 3930 6161 4433 167 51 320 C
ATOM 449 C VAL A 208 170.377 42.757 13.267 1.00 55.06 C
ANISOU 449 C VAL A 208 5975 9389 5555 -191 -147 158 C
ATOM 450 O VAL A 208 169.904 43.690 13.888 1.00 64.15 O
ANISOU 450 O VAL A 208 7199 10669 6507 -305 52 -130 O
ATOM 451 N PRO A 209 171.621 42.301 13.457 1.00 54.01 N
ANISOU 451 N PRO A 209 5738 9464 5318 -218 -389 281 N
ATOM 452 CA PRO A 209 172.518 42.844 14.487 1.00 56.06 C
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ATOM 453 CB PRO A 209 173.649 41.819 14.541 1.00 55.46 C
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ANISOU 454 CG PRO A 209 5714 9816 5625 -134 -806 574 C
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ANISOU 455 CD PRO A 209 5312 8931 5285 -57 -590 571 C
ATOM 456 C PRO A 209 173.040 44.178 13.988 1.00 61.24 C
ANISOU 456 C PRO A 209 6669 10705 5894 -534 -374 -367 C
ATOM 457 O PRO A 209 173.034 44.443 12.771 1.00 55.77 O
ANISOU 457 O PRO A 209 6020 9588 5583 -430 -320 -453 O
ATOM 458 N ASP A 210 173.484 45.016 14.914 1.00 70.14 N
ANISOU 458 N ASP A 210 7811 12191 6649 -772 -343 -675 N
ATOM 459 CA ASP A 210 174.008 46.331 14.557 1.00 78.15 C
ANISOU 459 CA ASP A 210 8898 13070 7727 -930 -231 -1146 C
ATOM 460 CB ASP A 210 174.034 47.249 15.772 1.00 90.37 C
ANISOU 460 CB ASP A 210 10514 14993 8830 -1215 -106 -1532 C
ATOM 461 CG ASP A 210 172.642 47.548 16.281 1.00100.89 C
ANISOU 461 CG ASP A 210 11987 16263 10084 -1187 196 -1644 C
ATOM 462 OD1 ASP A 210 171.727 46.740 15.984 1.00102.43 O
ANISOU 462 OD1 ASP A 210 12172 16289 10458 -967 227 -1303 O
ATOM 463 OD2 ASP A 210 172.461 48.590 16.954 1.00106.91 O
ANISOU 463 OD2 ASP A 210 12862 17133 10626 -1390 418 -2089 O
ATOM 464 C ASP A 210 175.362 46.251 13.879 1.00 77.18 C
ANISOU 464 C ASP A 210 8639 12930 7755 -948 -448 -1129 C
ATOM 465 O ASP A 210 175.708 47.099 13.064 1.00 75.95 O
ANISOU 465 O ASP A 210 8543 12480 7836 -999 -354 -1401 O
ATOM 466 N ASN A 211 176.119 45.218 14.213 1.00 81.47 N
ANISOU 466 N ASN A 211 8987 13786 8179 -897 -728 -785 N
ATOM 467 CA ASN A 211 177.344 44.923 13.496 1.00 83.47 C
ANISOU 467 CA ASN A 211 9064 14011 8641 -848 -927 -701 C
ATOM 468 CB ASN A 211 178.584 45.347 14.280 1.00 91.00 C
ANISOU 468 CB ASN A 211 9846 15472 9259 -1104 -1112 -862 C
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ANISOU 470 OD1 ASN A 211 10595 15678 10197 -1365 -876 -1547 O
ATOM 471 ND2 ASN A 211 178.588 47.591 15.182 1.00102.97 N
ANISOU 471 ND2 ASN A 211 11579 17186 10360 -1638 -836 -1712 N
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ANISOU 473 O ASN A 211 8763 14182 8628 -517 -1278 132 O
ATOM 474 N LEU A 212 177.401 43.289 11.755 1.00 72.02 N
ANISOU 474 N LEU A 212 7401 12303 7636 -663 -1255 -255 N
ATOM 475 CA LEU A 212 177.526 41.982 11.148 1.00 74.96 C
ANISOU 475 CA LEU A 212 7657 12657 8144 -475 -1475 -255 C
ATOM 476 CB LEU A 212 177.577 42.153 9.634 1.00 71.49 C
ANISOU 476 CB LEU A 212 7201 12295 7643 -645 -1645 -374 C
ATOM 477 CG LEU A 212 178.036 40.968 8.797 1.00 61.88 C
ANISOU 477 CG LEU A 212 6010 11249 6230 -1099 -1215 -215 C
ATOM 478 CD1 LEU A 212 177.249 39.743 9.142 1.00 53.11 C
ANISOU 478 CD1 LEU A 212 6348 7348 6741 6091 -265 692 511 C
ATOM 479 CD2 LEU A 212 177.860 41.330 7.323 1.00 60.95 C
ANISOU 479 CD2 LEU A 212 8393 7597 7167 -569 638 458 C
ATOM 480 C LEU A 212 178.790 41.298 11.653 1.00 81.24 C
ANISOU 480 C LEU A 212 11438 10032 9397 -91 480 176 C
ATOM 481 O LEU A 212 178.814 40.085 11.934 1.00 79.10 O
ANISOU 481 O LEU A 212 11031 9883 9138 -72 490 208 O
ATOM 482 N SER A 213 179.831 42.115 11.795 1.00 87.74 N
ANISOU 482 N SER A 213 12393 10713 10230 -212 289 44 N
ATOM 483 CA SER A 213 181.140 41.687 12.276 1.00 89.64 C
ANISOU 483 CA SER A 213 12600 10918 10542 -346 57 -52 C
ATOM 484 CB SER A 213 182.083 42.890 12.295 1.00 90.28 C
ANISOU 484 CB SER A 213 12825 10797 10681 -494 -174 -134 C
ATOM 485 OG SER A 213 181.653 43.879 11.370 1.00 87.46 O
ANISOU 485 OG SER A 213 12471 10404 10356 -533 -68 -104 O
ATOM 486 C SER A 213 181.078 41.053 13.668 1.00 90.15 C
ANISOU 486 C SER A 213 12866 10962 10427 -195 -20 -78 C
ATOM 487 O SER A 213 182.059 40.476 14.132 1.00 87.69 O
ANISOU 487 O SER A 213 12496 10627 10196 -300 -234 -120 O
ATOM 488 N MET A 214 179.927 41.178 14.329 1.00 93.51 N
ANISOU 488 N MET A 214 13525 11376 10628 54 167 -28 N
ATOM 489 CA MET A 214 179.741 40.689 15.697 1.00 92.02 C
ANISOU 489 CA MET A 214 13617 11143 10202 226 150 -40 C
ATOM 490 CB MET A 214 179.187 41.789 16.605 1.00 95.79 C
ANISOU 490 CB MET A 214 14618 11400 10377 444 230 -87 C
ATOM 491 CG MET A 214 180.076 43.026 16.691 1.00 99.58 C
ANISOU 491 CG MET A 214 15390 11628 10818 305 -63 -231 C
ATOM 492 SD MET A 214 181.803 42.652 17.092 1.00123.79 S
ANISOU 492 SD MET A 214 18432 14595 14007 1 -581 -321 S
ATOM 493 CE MET A 214 182.529 44.294 17.009 1.00 90.59 C
ANISOU 493 CE MET A 214 14539 10078 9804 -152 -891 -420 C
ATOM 494 C MET A 214 178.832 39.472 15.766 1.00 87.07 C
ANISOU 494 C MET A 214 12782 10718 9582 363 382 108 C
ATOM 495 O MET A 214 178.939 38.675 16.686 1.00 89.43 O
ANISOU 495 O MET A 214 13183 11037 9760 428 331 114 O

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ATOM   496  N  ALA A 215    177.942  39.328  14.791  1.00 84.78           N
ANISOU 496  N  ALA A 215    12213 10558  9442   385   596   248       N
ATOM   497  CA ALA A 215    176.979  38.214  14.764  1.00 84.02           C
ANISOU 497  CA ALA A 215    11894 10629  9400   492   780   438       C
ATOM   498  CB ALA A 215    175.975  38.393  13.614  1.00 80.60           C
ANISOU 498  CB ALA A 215    11211 10261  9151   482   937   617       C
ATOM   499  C  ALA A 215    177.609  36.817  14.689  1.00 82.11           C
ANISOU 499  C  ALA A 215    11416 10521  9260   355   638   427       C
ATOM   500  O  ALA A 215    177.112  35.868  15.286  1.00 84.87           O
ANISOU 500  O  ALA A 215    11725 10956  9566   464   708   538       O
ATOM   501  N  ASP A 216    178.667  36.681  13.901  1.00 73.77           N
ANISOU 501  N  ASP A 216    10191  9473  8366   127   468   315       N
ATOM   502  CA ASP A 216    179.448  35.465  13.908  1.00 60.81           C
ANISOU 502  CA ASP A 216    8357  7906  6841    17   339   284       C
ATOM   503  CB ASP A 216    179.281  34.700  12.597  1.00 59.38           C
ANISOU 503  CB ASP A 216    7890  7832  6839  -104   416   350       C
ATOM   504  CG ASP A 216    180.061  33.362  12.571  1.00 63.17           C
ANISOU 504  CG ASP A 216    8183  8365  7453  -188   323   318       C
ATOM   505  OD1 ASP A 216    181.121  33.247  13.216  1.00 69.78           O
ANISOU 505  OD1 ASP A 216    9024  9140  8349  -229   163   226       O
ATOM   506  OD2 ASP A 216    179.627  32.414  11.877  1.00 59.47           O
ANISOU 506  OD2 ASP A 216    7571  7973  7052  -220   387   400       O
ATOM   507  C  ASP A 216    180.867  35.936  14.078  1.00 57.66           C
ANISOU 507  C  ASP A 216    8002  7383  6523  -132   111   133       C
ATOM   508  O  ASP A 216    181.282  36.881  13.413  1.00 62.08           O
ANISOU 508  O  ASP A 216    8560  7866  7160  -239    91    76       O
ATOM   509  N  PRO A 217    181.613  35.304  14.997  1.00 53.53           N
ANISOU 509  N  PRO A 217    7511  6822  6006  -149   -90    97       N
ATOM   510  CA PRO A 217    183.036  35.658  15.131  1.00 50.42           C
ANISOU 510  CA PRO A 217    7084  6285  5787  -322  -364    12       C
ATOM   511  CB PRO A 217    183.479  34.878  16.382  1.00 47.90           C
ANISOU 511  CB PRO A 217    6871  5915  5413  -301  -604    21       C
ATOM   512  CG PRO A 217    182.443  33.740  16.509  1.00 46.76           C
ANISOU 512  CG PRO A 217    6658  5950  5158  -150  -395   112       C
ATOM   513  CD PRO A 217    181.157  34.389  16.062  1.00 45.32           C
ANISOU 513  CD PRO A 217    6576  5833  4812  -14  -103   161       C
ATOM   514  C  PRO A 217    183.900  35.287  13.899  1.00 48.46           C
ANISOU 514  C  PRO A 217    6447  6077  5888  -493  -313    14       C
ATOM   515  O  PRO A 217    185.002  35.798  13.727  1.00 56.63           O
ANISOU 515  O  PRO A 217    7385  6990  7142  -641  -467    -9       O
ATOM   516  N  ASN A 218    183.411  34.401  13.046  1.00 42.40           N
ANISOU 516  N  ASN A 218    5482  5452  5176  -473   -91    60       N
ATOM   517  CA ASN A 218    184.142  34.033  11.828  1.00 41.56           C
ANISOU 517  CA ASN A 218    5102  5355  5333  -600    35    54       C
ATOM   518  CB ASN A 218    183.901  32.563  11.492  1.00 38.76           C
ANISOU 518  CB ASN A 218    4598  5100  5031  -559   149    93       C
ATOM   519  CG ASN A 218    184.624  31.638  12.434  1.00 43.16           C
ANISOU 519  CG ASN A 218    5037  5628  5732  -541   -37   104       C
ATOM   520  OD1 ASN A 218    185.804  31.820  12.727  1.00 48.51           O
ANISOU 520  OD1 ASN A 218    5584  6193  6656  -626  -194    97       O
ATOM   521  ND2 ASN A 218    183.899  30.684  12.973  1.00 41.31           N
ANISOU 521  ND2 ASN A 218    4844  5482  5369  -441   -56   152       N
ATOM   522  C  ASN A 218    183.845  34.920  10.606  1.00 41.71           C
ANISOU 522  C  ASN A 218    5151  5370  5328  -671   222    48       C
ATOM   523  O  ASN A 218    184.177  34.577  9.470  1.00 38.32           O
ANISOU 523  O  ASN A 218    4586  4950  5023  -753   401    52       O
ATOM   524  N  ILE A 219    183.198  36.047  10.848  1.00 40.26           N
ANISOU 524  N  ILE A 219    5182  5152  4964  -630   191    43       N
ATOM   525  CA ILE A 219    182.997  37.058  9.819  1.00 38.43           C
ANISOU 525  CA ILE A 219    4994  4886  4721  -712   307    46       C
ATOM   526  CB ILE A 219    181.509  37.271  9.523  1.00 37.87           C
ANISOU 526  CB ILE A 219    5059  4880  4450  -613   426   122       C
ATOM   527  CG1 ILE A 219    180.874  36.011  8.972  1.00 37.84           C
ANISOU 527  CG1 ILE A 219    4953  4985  4437  -599   532   202       C
ATOM   528  CD1 ILE A 219    179.336  36.066  8.988  1.00 38.26           C
ANISOU 528  CD1 ILE A 219    5085  5088  4364  -488   584   349       C
ATOM   529  CG2 ILE A 219    181.298  38.356  8.513  1.00 36.09           C
ANISOU 529  CG2 ILE A 219    4896  4598  4219  -710   499   139       C
ATOM   530  C  ILE A 219    183.581  38.359  10.344  1.00 42.50           C
ANISOU 530  C  ILE A 219    5640  5255  5254  -761   127    -4       C
ATOM   531  O  ILE A 219    183.030  38.942  11.266  1.00 47.93           O
ANISOU 531  O  ILE A 219    6577  5886  5748  -646    26   -24       O
ATOM   532  N  ARG A 220    184.711  38.784  9.784  1.00 40.51           N
ANISOU 532  N  ARG A 220    5236  4918  5240  -927    94    -8       N
ATOM   533  CA ARG A 220    185.372  40.016  10.182  1.00 44.61           C
ANISOU 533  CA ARG A 220    5856  5267  5828  -1019  -128   -27       C
ATOM   534  CB ARG A 220    186.836  39.782  10.523  1.00 48.60           C
ANISOU 534  CB ARG A 220    6130  5663  6672  -1155  -332    15       C
ATOM   535  CG ARG A 220    187.091  39.039  11.809  1.00 60.63           C
ANISOU 535  CG ARG A 220    7698  7151  8186  -1094  -587     7       C
ATOM   536  CD ARG A 220    188.144  37.951  11.572  1.00 67.16           C
ANISOU 536  CD ARG A 220    8126  7994  9399  -1165  -560    87       C
ATOM   537  NE ARG A 220    189.254  37.955  12.525  1.00 67.76           N
ANISOU 537  NE ARG A 220    8113  7891  9742  -1274  -959   162       N
ATOM   538  CZ ARG A 220    190.536  37.896  12.175  1.00 69.11           C
ANISOU 538  CZ ARG A 220    7901  7952 10405  -1424  -1021   299       C
ATOM   539  NH1 ARG A 220    191.476  37.899  13.116  1.00 77.92           N
ANISOU 539  NH1 ARG A 220    8940  8878 11790  -1541  -1461   405       N
ATOM   540  NH2 ARG A 220    190.882  37.833  10.890  1.00 62.23           N
ANISOU 540  NH2 ARG A 220    6738  7139  9768  -1458  -642   355       N
ATOM   541  C  ARG A 220    185.329  41.014  9.041  1.00 45.06           C
ANISOU 541  C  ARG A 220    5911  5291  5920  -1130     6    -3       C
ATOM   542  O  ARG A 220    185.486  40.658  7.863  1.00 43.25           O
ANISOU 542  O  ARG A 220    5513  5129  5791  -1208   247    37       O
ATOM   543  N  PHE A 221    185.121  42.266  9.419  1.00 42.21           N
ANISOU 543  N  PHE A 221    5787 4799  5450  -1133  -154   -31       N
ATOM   544  CA PHE A 221    185.214  43.379  8.503  1.00 46.16           C
ANISOU 544  CA PHE A 221    6304 5228  6006  -1259  -103    -1       C
ATOM   545  CB PHE A 221    184.749  44.649  9.228  1.00 45.92           C
ANISOU 545  CB PHE A 221    6620 5034  5794  -1196  -305   -52       C
ATOM   546  CG PHE A 221    185.047  45.921  8.479  1.00 43.47           C
ANISOU 546  CG PHE A 221    6337 4600  5578  -1350  -347   -17       C
ATOM   547  CD1 PHE A 221    184.170  46.385  7.498  1.00 42.22           C
ANISOU 547  CD1 PHE A 221    6225 4496  5321  -1341  -142    19       C
ATOM   548  CE1 PHE A 221    184.422  47.574  6.794  1.00 40.98           C
ANISOU 548  CE1 PHE A 221    6107 4220  5244  -1492  -189    62       C
ATOM   549  CZ  PHE A 221    185.581  48.284  7.061  1.00 41.93           C
ANISOU 549  CZ  PHE A 221    6195 4168  5569  -1658  -438    80       C
ATOM   550  CE2 PHE A 221    186.483  47.814  8.048  1.00 41.87           C
ANISOU 550  CE2 PHE A 221    6122 4093  5695  -1681  -673    64       C
ATOM   551  CD2 PHE A 221    186.208  46.638  8.734  1.00 40.72           C
ANISOU 551  CD2 PHE A 221    5957 4066  5446  -1527  -624    11       C
ATOM   552  C  PHE A 221    186.683  43.510  8.052  1.00 48.57           C
ANISOU 552  C  PHE A 221    6331 5449  6675  -1469  -159    72       C
ATOM   553  O  PHE A 221    187.612  43.426  8.868  1.00 39.77           O
ANISOU 553  O  PHE A 221    5130 4223  5757  -1528  -422    95       O
ATOM   554  N  LEU A 222    186.918  43.717  6.761  1.00 47.04           N
ANISOU 554  N  LEU A 222    5994 5285  6594  -1589    83   139       N
ATOM   555  CA LEU A 222    188.281  44.066  6.388  1.00 52.68           C
ANISOU 555  CA LEU A 222    6443 5889  7686  -1775    56   252       C
ATOM   556  CB LEU A 222    189.024  42.912  5.705  1.00 56.36           C
ANISOU 556  CB LEU A 222    6584 6432  8398  -1792   365   326       C
ATOM   557  CG LEU A 222    188.340  42.119  4.620  1.00 59.61           C
ANISOU 557  CG LEU A 222    7065 6986  8599  -1725   760   291       C
ATOM   558  CD1 LEU A 222    187.983  43.055  3.503  1.00 71.12           C
ANISOU 558  CD1 LEU A 222    8681 8418  9923  -1833   915   326       C
ATOM   559  CD2 LEU A 222    189.299  41.098  4.120  1.00 56.17           C
ANISOU 559  CD2 LEU A 222    6343 6555  8445  -1728  1048   363       C
ATOM   560  C  LEU A 222    188.458  45.419  5.691  1.00 52.54           C
ANISOU 560  C  LEU A 222    6483 5758  7721  -1930    37   317       C
ATOM   561  O  LEU A 222    189.480  46.096  5.877  1.00 56.19           O
ANISOU 561  O  LEU A 222    6800 6062  8486  -2086  -167   421       O
ATOM   562  N  ASP A 223    187.452  45.836  4.940  1.00 48.10           N
ANISOU 562  N  ASP A 223    6131 5256  6890  -1902   201   282       N
ATOM   563  CA ASP A 223    187.563  47.109  4.245  1.00 45.52           C
ANISOU 563  CA ASP A 223    5875 4820  6600  -2053   179   350       C
ATOM   564  CB ASP A 223    188.658  47.023  3.167  1.00 49.29           C
ANISOU 564  CB ASP A 223    6070 5285  7373  -2227   443   500       C
ATOM   565  CG ASP A 223    189.242  48.385  2.833  1.00 61.44           C
ANISOU 565  CG ASP A 223    7587 6660  9096  -2421   307   618       C
ATOM   566  OD1 ASP A 223    188.687  49.357  3.372  1.00 66.54           O
ANISOU 566  OD1 ASP A 223    8481 7205  9595  -2411     8   555       O
ATOM   567  OD2 ASP A 223    190.216  48.487  2.044  1.00 66.63           O
ANISOU 567  OD2 ASP A 223    7994 7276 10044  -2570   517   784       O
ATOM   568  C  ASP A 223    186.257  47.593  3.627  1.00 40.46           C
ANISOU 568  C  ASP A 223    5504 4222  5646  -2001   274   315       C
ATOM   569  O  ASP A 223    185.325  46.834  3.459  1.00 43.19           O
ANISOU 569  O  ASP A 223    5932 4694  5783  -1878   415   275       O
ATOM   570  N  LYS A 224    186.214  48.854  3.237  1.00 47.58           N
ANISOU 570  N  LYS A 224    6522 5001  6556  -2114   176   363       N
ATOM   571  CA LYS A 224    185.067  49.374  2.507  1.00 50.53           C
ANISOU 571  CA LYS A 224    7456 5733  7047  -2098   254   376       C
ATOM   572  CB LYS A 224    184.726  50.788  2.972  1.00 58.17           C
ANISOU 572  CB LYS A 224    8288 6175  7638  -2091  -11   360       C
ATOM   573  CG LYS A 224    184.207  50.835  4.397  1.00 66.42           C
ANISOU 573  CG LYS A 224    9518 7158  8561  -1867  -212   240       C
ATOM   574  CD LYS A 224    182.890  51.563  4.482  1.00 70.47           C
ANISOU 574  CD LYS A 224    10286 7602  8888  -1710  -223   230       C
ATOM   575  CE LYS A 224    182.288  51.446  5.875  1.00 74.74           C
ANISOU 575  CE LYS A 224    11042 8085  9270  -1438  -304   123       C
ATOM   576  NZ LYS A 224    181.414  50.237  6.022  1.00 78.08           N
ANISOU 576  NZ LYS A 224    11380 8702  9585  -1256   -94   137       N
ATOM   577  C  LYS A 224    185.374  49.394  1.029  1.00 56.63           C
ANISOU 577  C  LYS A 224    7834 6186  7498  -2286   512   486       C
ATOM   578  O  LYS A 224    186.522  49.525  0.633  1.00 64.42           O
ANISOU 578  O  LYS A 224    8638 7127  8711  -2436   606   571       O
ATOM   579  N  LEU A 225    184.337  49.269  0.215  1.00 49.72           N
ANISOU 579  N  LEU A 225    7010 5552  6331  -2255   1010       N
ATOM   580  CA LEU A 225    184.433  49.552 -1.223  1.00 52.36           C
ANISOU 580  CA LEU A 225    7522 5889  6487  -2414   1222       C
ATOM   581  CB LEU A 225    183.189  49.046 -1.950  1.00 47.89           C
ANISOU 581  CB LEU A 225    7104 5694  5403  -2255   1262       C
ATOM   582  CG LEU A 225    183.139  47.597 -2.374  1.00 41.47           C
ANISOU 582  CG LEU A 225    6651 5189  5189  -2117   1212       C
ATOM   583  CD1 LEU A 225    181.944  47.427 -3.271  1.00 39.36           C
ANISOU 583  CD1 LEU A 225    6503 5284  5441  -2003   1262       C
ATOM   584  CD2 LEU A 225    184.417  47.246 -3.091  1.00 44.24           C
ANISOU 584  CD2 LEU A 225    7044 5488  6552  -2284   1606       C
ATOM   585  C  LEU A 225    184.547  51.046 -1.496  1.00 53.26           C
ANISOU 585  C  LEU A 225    7514 5753  6974  -2553   1353       C
ANISOU 585  C  LEU A 225    5114 6175  8946   -382   788  1353       C
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ATOM 586 O LEU A 225 184.123 51.853 -0.680 1.00 57.16 O
ANISOU 586 O LEU A 225 5606 6540 9573 -434 694 1274 O
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ATOM 592 C PRO A 226 183.647 53.319 -3.157 1.00 63.26 C
ANISOU 592 C PRO A 226 6352 7307 10376 -338 1068 1752 C
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ANISOU 593 O PRO A 226 5754 6746 9329 -252 1057 1744 O
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ANISOU 594 N GLN A 227 6948 7759 11246 -395 1065 1775 N
ATOM 595 CA GLN A 227 182.078 55.090 -2.654 1.00 65.90 C
ANISOU 595 CA GLN A 227 6768 7447 10825 -358 1023 1776 C
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ANISOU 596 CB GLN A 227 6764 7274 11216 -449 973 1730 C
ATOM 597 CG GLN A 227 182.686 56.144 -0.471 1.00 67.98 C
ANISOU 597 CG GLN A 227 6891 7384 11554 -543 781 1478 C
ATOM 598 CD GLN A 227 183.030 57.434 0.215 1.00 73.56 C
ANISOU 598 CD GLN A 227 7475 7838 12635 -635 747 1424 C
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ATOM 615 OG1 THR A 229 179.230 60.581 -4.521 1.00 74.09 O
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ATOM 616 CG2 THR A 229 177.203 61.616 -5.278 1.00 74.79 C
ANISOU 616 CG2 THR A 229 8179 8161 12077 64 1618 2716 C
ATOM 617 C THR A 229 176.099 59.099 -5.947 1.00 65.14 C
ANISOU 617 C THR A 229 7140 7527 10084 218 1452 2525 C
ATOM 618 O THR A 229 176.119 58.778 -7.138 1.00 59.32 O
ANISOU 618 O THR A 229 6410 6974 9156 362 1594 2684 O
ATOM 619 N GLY A 230 174.981 59.419 -5.289 1.00 68.21 N
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ATOM 620 CA GLY A 230 173.667 59.369 -5.907 1.00 68.15 C
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ATOM 621 C GLY A 230 173.418 60.605 -6.758 1.00 73.08 C
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ATOM 622 O GLY A 230 173.611 61.736 -6.312 1.00 68.15 O
ANISOU 622 O GLY A 230 7693 7793 10407 451 1571 2787 O
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ATOM 624 CA ASP A 231 172.624 61.482 -8.893 1.00 92.32 C
ANISOU 624 CA ASP A 231 10845 11342 12890 888 1852 3137 C
ATOM 625 CB ASP A 231 173.674 61.689 -9.993 1.00103.54 C
ANISOU 625 CB ASP A 231 12176 12771 14392 989 2065 3342 C
ATOM 626 CG ASP A 231 173.926 60.426 -10.831 1.00109.80 C
ANISOU 626 CG ASP A 231 12963 13854 14902 1086 2080 3331 C
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ANISOU 627 OD1 ASP A 231 13153 14155 14841 1028 1912 3123 O
ATOM 628 OD2 ASP A 231 174.587 60.549 -11.895 1.00112.19 O
ANISOU 628 OD2 ASP A 231 13210 14225 15192 1227 2227 3464 O
ATOM 629 C ASP A 231 171.245 61.192 -9.492 1.00 88.71 C
ANISOU 629 C ASP A 231 10494 11187 12026 1081 1808 3106 C
ATOM 630 O ASP A 231 171.078 61.085 -10.704 1.00 91.37 O
ANISOU 630 O ASP A 231 10840 11747 12131 1296 1947 3265 O
ATOM 631 N ARG A 232 170.259 61.057 -8.616 1.00 80.13 N
ANISOU 631 N ARG A 232 9479 10116 10852 1012 1610 2888 N
ATOM 632 CA ARG A 232 168.967 60.531 -8.988 1.00 72.26 C
ANISOU 632 CA ARG A 232 8561 9413 9483 1149 1521 2779 C
ATOM 633 CB ARG A 232 169.026 59.020 -8.882 1.00 72.82 C
ANISOU 633 CB ARG A 232 8624 9666 9380 1077 1383 2546 C
ATOM 634 CG ARG A 232 168.592 58.275 -10.091 1.00 78.81 C
ANISOU 634 CG ARG A 232 9389 10761 9795 1274 1427 2550 C
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ANISOU 635 CD ARG A 232 9607 11108 9913 1165 1278 2290 C
ATOM 636 NE ARG A 232 167.968 55.961 -10.769 1.00 86.47 N
ANISOU 636 NE ARG A 232 10356 12186 10314 1335 1264 2201 N
ATOM 637 CZ ARG A 232 166.650 55.912 -10.940 1.00 87.60 C
ANISOU 637 CZ ARG A 232 10540 12523 10223 1438 1184 2087 C
ATOM 638 NH1 ARG A 232 165.855 56.672 -10.203 1.00 88.15 N
ANISOU 638 NH1 ARG A 232 10657 12485 10350 1396 1119 2068 N
ATOM 639 NH2 ARG A 232 166.127 55.105 -11.856 1.00 89.07 N
ANISOU 639 NH2 ARG A 232 10709 13016 10117 1591 1164 1978 N
ATOM 640 C ARG A 232 167.988 61.035 -7.954 1.00 67.72 C
ANISOU 640 C ARG A 232 8052 8738 8939 1077 1371 2642 C
ATOM 641 O ARG A 232 168.386 61.408 -6.845 1.00 68.33 O
ANISOU 641 O ARG A 232 8114 8557 9293 899 1291 2563 O
ATOM 642 N ALA A 233 166.705 61.003 -8.287 1.00 57.64 N
ANISOU 642 N ALA A 233 6842 7684 7374 1221 1323 2593 N
ATOM 643 CA ALA A 233 165.688 61.414 -7.331 1.00 54.38 C
ANISOU 643 CA ALA A 233 6493 7208 6960 1168 1178 2458 C
ATOM 644 CB ALA A 233 164.323 61.289 -7.936 1.00 57.37 C
ANISOU 644 CB ALA A 233 6925 7881 6991 1355 1147 2417 C
ATOM 645 C ALA A 233 165.750 60.628 -6.021 1.00 56.23 C
ANISOU 645 C ALA A 233 6727 7352 7284 947 973 2189 C
ATOM 646 O ALA A 233 165.770 59.393 -6.013 1.00 62.51 O
ANISOU 646 O ALA A 233 7509 8296 7944 895 890 2026 O
ATOM 647 N GLY A 234 165.764 61.363 -4.907 1.00 50.91 N
ANISOU 647 N GLY A 234 6070 6433 6841 831 897 2144 N
ATOM 648 CA GLY A 234 165.740 60.794 -3.579 1.00 43.85 C
ANISOU 648 CA GLY A 234 5183 5450 6026 658 708 1906 C
ATOM 649 C GLY A 234 167.116 60.476 -2.997 1.00 53.59 C
ANISOU 649 C GLY A 234 6346 6495 7522 496 691 1863 C
ATOM 650 O GLY A 234 167.269 60.272 -1.770 1.00 52.04 O
ANISOU 650 O GLY A 234 6149 6176 7448 366 546 1690 O
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ANISOU 651 N ILE A 235 5696 5900 7018 517 839 2015 N
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ANISOU 652 CA ILE A 235 5340 5456 7000 372 831 1977 C
ATOM 653 CB ILE A 235 169.916 58.718 -3.667 1.00 47.15 C
ANISOU 653 CB ILE A 235 5359 5669 6885 347 807 1885 C
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ATOM 655 CD1 ILE A 235 170.676 57.243 -5.602 1.00 47.21 C
ANISOU 655 CD1 ILE A 235 5316 6007 6615 482 982 2002 C
ATOM 656 CG2 ILE A 235 169.078 57.733 -2.869 1.00 43.74 C
ANISOU 656 CG2 ILE A 235 4992 5356 6270 298 627 1645 C
ATOM 657 C ILE A 235 170.521 61.124 -3.894 1.00 49.60 C
ANISOU 657 C ILE A 235 5605 5611 7629 377 1014 2201 C
ATOM 658 O ILE A 235 171.722 60.844 -3.844 1.00 49.59 O
ANISOU 658 O ILE A 235 5513 5514 7814 286 1051 2209 O
ATOM 659 N LYS A 236 170.064 62.251 -4.432 1.00 49.16 N
ANISOU 659 N LYS A 236 5575 5499 7606 491 1141 2389 N
ATOM 660 CA LYS A 236 170.982 63.228 -5.001 1.00 57.34 C
ANISOU 660 CA LYS A 236 6529 6333 8923 509 1349 2630 C
ATOM 661 CB LYS A 236 170.238 64.454 -5.521 1.00 60.71 C
ANISOU 661 CB LYS A 236 7010 6708 9348 659 1484 2833 C
ATOM 662 CG LYS A 236 170.823 64.993 -6.790 1.00 69.34 C
ANISOU 662 CG LYS A 236 8055 7786 10505 795 1762 3150 C
ATOM 663 CD LYS A 236 169.883 64.721 -7.950 1.00 80.28 C
ANISOU 663 CD LYS A 236 9522 9502 11480 1042 1840 3264 C
ATOM 664 CE LYS A 236 170.597 64.863 -9.296 1.00 87.79 C
ANISOU 664 CE LYS A 236 10402 10539 12399 1190 2051 3435 C
ATOM 665 NZ LYS A 236 169.649 64.836 -10.453 1.00 90.14 N
ANISOU 665 NZ LYS A 236 10765 11165 12321 1463 2126 3525 N
ATOM 666 C LYS A 236 172.033 63.657 -3.966 1.00 61.62 C
ANISOU 666 C LYS A 236 6971 6568 9874 313 1292 2535 C
ATOM 667 O LYS A 236 171.682 64.100 -2.859 1.00 60.83 O
ANISOU 667 O LYS A 236 6892 6323 9897 229 1141 2373 O
ATOM 668 N ASP A 237 173.309 63.507 -4.339 1.00 62.20 N
ANISOU 668 N ASP A 237 6930 6558 10146 254 1408 2625 N
ATOM 669 CA ASP A 237 174.464 63.799 -3.476 1.00 65.66 C
ANISOU 669 CA ASP A 237 7240 6732 10976 73 1361 2523 C
ATOM 670 CB ASP A 237 174.521 65.290 -3.125 1.00 74.50 C
ANISOU 670 CB ASP A 237 8316 7559 12433 41 1419 2594 C
ATOM 671 CG ASP A 237 174.971 66.159 -4.307 1.00 84.88 C
ANISOU 671 CG ASP A 237 9574 8854 13822 157 1665 2794 C
ATOM 672 OD2 ASP A 237 174.134 66.965 -4.794 1.00 86.07 O
ANISOU 672 OD2 ASP A 237 9801 9019 13883 289 1760 2924 O
ATOM 673 OD1 ASP A 237 176.149 66.022 -4.740 1.00 88.75 O
ANISOU 673 OD1 ASP A 237 9946 9320 14456 125 1762 2836 O
ATOM 674 C ASP A 237 174.579 62.945 -2.203 1.00 64.36 C
ANISOU 674 C ASP A 237 7076 6593 10786 -58 1103 2208 C
ATOM 675 O ASP A 237 175.279 63.313 -1.264 1.00 62.37 O
ANISOU 675 O ASP A 237 6731 6131 10835 -189 1014 2071 O

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ATOM   676 N  ARG A 238    173.883 61.812 -2.180 1.00 63.93        N
ANISOU 676 N  ARG A 238     7118  6796 10376   -12   988  2092     N
ATOM   677 CA ARG A 238    173.946 60.878 -1.062 1.00 57.81        C
ANISOU 677 CA ARG A 238     6356  6070  9539  -107   773  1824     C
ATOM   678 CB ARG A 238    172.667 60.056 -0.996 1.00 51.32        C
ANISOU 678 CB ARG A 238     5669  5486  8344   -33   667  1722     C
ATOM   679 CG ARG A 238    172.590 59.093  0.175 1.00 46.30        C
ANISOU 679 CG ARG A 238     5063  4901  7629  -109   466  1470     C
ATOM   680 CD ARG A 238    171.246 59.283  0.800 1.00 51.91        C
ANISOU 680 CD ARG A 238     5881  5661  8184   -68   348  1370     C
ATOM   681 NE ARG A 238    170.476 58.060  0.876 1.00 54.99        N
ANISOU 681 NE ARG A 238     6351  6267  8275   -40   273  1257     N
ATOM   682 CZ ARG A 238    169.219 58.003  1.289 1.00 49.90        C
ANISOU 682 CZ ARG A 238     5796  5711  7453     3   185  1173     C
ATOM   683 NH1 ARG A 238    168.585 59.125  1.653 1.00 43.26        N
ANISOU 683 NH1 ARG A 238     4985  4769  6682    33   156  1195     N
ATOM   684 NH2 ARG A 238    168.618 56.818  1.334 1.00 48.41        N
ANISOU 684 NH2 ARG A 238     5660  5701  7031    14   134  1068     N
ATOM   685 C  ARG A 238    175.135 59.943 -1.256 1.00 58.98        C
ANISOU 685 C  ARG A 238     6417  6268  9726  -165   798  1802     C
ATOM   686 O  ARG A 238    175.433 59.523 -2.379 1.00 61.86        O
ANISOU 686 O  ARG A 238     6768  6760  9976   -95   946  1959     O
ATOM   687 N  VAL A 239    175.821 59.603 -0.169 1.00 54.77        N
ANISOU 687 N  VAL A 239     5823  5647  9340  -274   654  1606     N
ATOM   688 CA VAL A 239    176.994 58.750 -0.305 1.00 53.85        C
ANISOU 688 CA VAL A 239     5617  5573  9269  -324   675  1581     C
ATOM   689 CB VAL A 239    178.221 59.402  0.292 1.00 50.09        C
ANISOU 689 CB VAL A 239     4980  4867  9184  -435   664  1528     C
ATOM   690 CG1 VAL A 239    179.400 58.444  0.191 1.00 44.19        C
ANISOU 690 CG1 VAL A 239     4143  4189  8458  -476   675  1491     C
ATOM   691 CG2 VAL A 239    178.503 60.719 -0.469 1.00 44.58        C
ANISOU 691 CG2 VAL A 239     4201  3980  8759  -434   862  1753     C
ATOM   692 C  VAL A 239    176.792 57.349  0.252 1.00 53.32        C
ANISOU 692 C  VAL A 239     5623  5685  8953  -325   531  1397     C
ATOM   693 O  VAL A 239    176.536 57.199  1.441 1.00 53.63        O
ANISOU 693 O  VAL A 239     5691  5690  8996  -361   359  1202     O
ATOM   694 N  TYR A 240    176.852 56.347 -0.640 1.00 53.62        N
ANISOU 694 N  TYR A 240     5692  5912  8770  -268   611  1465     N
ATOM   695 CA TYR A 240    176.723 54.920 -0.286 1.00 46.69        C
ANISOU 695 CA TYR A 240     4879  5195  7666  -264   512  1313     C
ATOM   696 CB TYR A 240    175.832 54.173 -1.290 1.00 41.59        C
ANISOU 696 CB TYR A 240     4329  4770  6702  -166   576  1371     C
ATOM   697 CG TYR A 240    174.355 54.473 -1.144 1.00 40.56        C
ANISOU 697 CG TYR A 240     4306  4698  6407  -117   519  1335     C
ATOM   698 CD1 TYR A 240    173.611 53.854 -0.149 1.00 30.59        C
ANISOU 698 CD1 TYR A 240     3123  3472  5029  -143   370  1149     C
ATOM   699 CE1 TYR A 240    172.277 54.121  0.008 1.00 34.17        C
ANISOU 699 CE1 TYR A 240     3661  3981  5340  -100   320  1114     C
ATOM   700 CZ TYR A 240    171.670 55.064 -0.817 1.00 41.88        C
ANISOU 700 CZ TYR A 240     4650  4979  6284   -24   409  1261     C
ATOM   701 OH TYR A 240    170.345 55.362 -0.649 1.00 44.82        O
ANISOU 701 OH TYR A 240     5102  5415  6515    25   355  1222     O
ATOM   702 CE2 TYR A 240    172.378 55.713 -1.819 1.00 41.64        C
ANISOU 702 CE2 TYR A 240     4552  4911  6359    17   564  1457     C
ATOM   703 CD2 TYR A 240    173.718 55.417 -1.973 1.00 40.00        C
ANISOU 703 CD2 TYR A 240     4253  4642  6303   -34   622  1496     C
ATOM   704 C  TYR A 240    178.084 54.239 -0.291 1.00 54.08        C
ANISOU 704 C  TYR A 240     5717  6128  8702  -309   534  1291     C
ATOM   705 O  TYR A 240    178.884 54.421 -1.215 1.00 62.56        O
ANISOU 705 O  TYR A 240     6706  7196  9866  -296   682  1448     O
ATOM   706 N  SER A 241    178.368 53.463  0.736 1.00 54.06        N
ANISOU 706 N  SER A 241     5724  6134  8681  -346   397  1106     N
ATOM   707 CA SER A 241    179.548 52.619  0.685 1.00 61.88        C
ANISOU 707 CA SER A 241     6641  7163  9707  -365   415  1078     C
ATOM   708 CB SER A 241    180.555 53.018  1.766 1.00 71.91        C
ANISOU 708 CB SER A 241     7794  8287 11243  -436   315   955     C
ATOM   709 OG SER A 241    179.905 53.208  3.013 1.00 77.21        O
ANISOU 709 OG SER A 241     8523  8911 11903  -440   150   786     O
ATOM   710 C  SER A 241    179.078 51.196  0.898 1.00 56.59        C
ANISOU 710 C  SER A 241     6083  6651  8767  -324   355   966     C
ATOM   711 O  SER A 241    177.921 50.973  1.230 1.00 56.74        O
ANISOU 711 O  SER A 241     6214  6723  8622  -299   290   898     O
ATOM   712 N  ASN A 242    179.984 50.242  0.731 1.00 50.25        N
ANISOU 712 N  ASN A 242     5244  5913  7935  -318   381   946     N
ATOM   713 CA ASN A 242    179.691 48.856  1.008 1.00 43.74        C
ANISOU 713 CA ASN A 242     4515  5207  6897  -283   335   836     C
ATOM   714 CB ASN A 242    179.417 48.103 -0.283 1.00 49.20        C
ANISOU 714 CB ASN A 242     5252  6050  7392  -226   451   921     C
ATOM   715 CG ASN A 242    178.136 48.561 -0.964 1.00 54.41        C
ANISOU 715 CG ASN A 242     5982  6773  7919  -187   489   984     C
ATOM   716 OD1 ASN A 242    177.139 47.668 -1.017 1.00 45.05        O
ANISOU 716 OD1 ASN A 242     6981  7763  9058  -181   548  1111     O
ATOM   717 ND2 ASN A 242    178.876 48.243  1.690 1.00 46.66        N
ANISOU 717 ND2 ASN A 242     4820  5555  7353  -296   286   748     N
ATOM   718 C  ASN A 242    180.015 48.646  1.470 1.00 55.03        C
ANISOU 718 C  ASN A 242     5752  6563  8596  -323   330   802     O
ATOM   719 O  ASN A 242    179.620 47.248  2.514 1.00 42.16        O
ANISOU 719 O  ASN A 242     4335  5031  6655  -266   205   615     N
ATOM   720 N  SER A 243    181.688 46.703  3.310 1.00 38.08        N
ANISOU 720 N  SER A 243     3762  4501  6205  -253   145   522     C
ATOM   721 CA SER A 243    181.245 46.539  4.759 1.00 44.38        C
ANISOU 721 CA SER A 243     4623  5270  6969  -220     7   371     C
ATOM   722 CB SER A 243    181.128 47.785  5.403 1.00 53.30        O
ANISOU 722 OG SER A 243     5693  6294  8263  -251   -83   331     O
ATOM   723 OG SER A 243    182.126 45.371  2.747 1.00 36.00        C
ANISOU 723 C  SER A 243     3535  4346  5798  -209   222   535     C
ATOM   724 C  SER A 243    181.309 44.574  2.285 1.00 32.42        O
ANISOU 725 O  SER A 243     3189  3969  5158  -182   267   537     O
ATOM   725 O  SER A 243    183.428 45.119  2.827 1.00 35.98        N
ANISOU 726 N  ILE A 244     3432  4345  5892  -201   230   527     N
ATOM   726 N  ILE A 244    183.976 43.836  2.440 1.00 35.60        C
ANISOU 727 CA ILE A 244     3415  4392  5720  -148   292   526     C
ATOM   727 CA ILE A 244    185.205 44.028  1.575 1.00 37.60        C
ANISOU 728 CB ILE A 244     3532  4667  6087  -159   382   627     C
ATOM   728 CB ILE A 244    184.847 44.936  0.409 1.00 36.47        C
ANISOU 729 CG1 ILE A 244     3352  4518  5988  -193   485   782     C
ATOM   729 CG1 ILE A 244    186.053 45.305 -0.425 1.00 40.22        C
ANISOU 730 CD1 ILE A 244     3678  4997  6605  -201   593   909     C
ATOM   730 CD1 ILE A 244    185.686 42.713  1.009 1.00 31.42        C
ANISOU 731 CG2 ILE A 244     2789  3992  5155  -95   456   636     C
ATOM   731 CG2 ILE A 244    184.293 43.056  3.696 1.00 36.97        C
ANISOU 732 C  ILE A 244     3626  4567  5853  -90   199   390     C
ATOM   732 C  ILE A 244    184.788 43.619  4.662 1.00 46.78        O
ANISOU 733 O  ILE A 244     4794  5756  7225  -87   98   312     O
ATOM   733 O  ILE A 244    183.975 41.772  3.688 1.00 31.91        N
ANISOU 734 N  TYR A 245     3102  3987  5036   -33   237   358     N
ATOM   734 N  TYR A 245    184.223 40.912  4.837 1.00 33.02        C
ANISOU 735 CA TYR A 245     3298  4134  5115    50   178   255     C
ATOM   735 CA TYR A 245    182.900 40.422  5.432 1.00 32.35        C
ANISOU 736 CB TYR A 245     3363  4031  4898    75   163   204     C
ATOM   736 CB TYR A 245    182.085 41.533  6.035 1.00 33.04        C
ANISOU 737 CG TYR A 245     3449  4059  5044    39    73   179     C
ATOM   737 CG TYR A 245    181.179 42.267  5.257 1.00 36.26        C
ANISOU 738 CD1 TYR A 245     3867  4453  5457   -38   101   241     C
ATOM   738 CD1 TYR A 245    180.451 43.321  5.807 1.00 40.76        C
ANISOU 739 CE1 TYR A 245     4436  4965  6083   -65    19   219     C
ATOM   739 CE1 TYR A 245    180.627 43.627  7.159 1.00 40.60        C
ANISOU 740 CZ TYR A 245     4406  4908  6114   -13   -99   124     C
ATOM   740 CZ TYR A 245    179.933 44.650  7.744 1.00 43.41        O
ANISOU 741 OH TYR A 245     4762  5209  6524   -28   -187    90     O
ATOM   741 OH TYR A 245    181.514 42.910  7.944 1.00 40.21        C
ANISOU 742 CE2 TYR A 245     4342  4886  6050    75   -133    56     C
ATOM   742 CE2 TYR A 245    182.244 41.872  7.372 1.00 36.38        C
ANISOU 743 CD2 TYR A 245     3858  4453  5510    98   -44    89     C
ATOM   743 CD2 TYR A 245    185.116 39.708  4.535 1.00 41.92        C
ANISOU 744 C  TYR A 245     4432  5326  6170   116   249   259     C
ATOM   744 C  TYR A 245    185.195 39.211  3.410 1.00 41.03        O
ANISOU 745 O  TYR A 245     4330  5262  5996   104   350   324     O
ATOM   745 O  TYR A 245    185.779 39.249  5.587 1.00 43.49        N
ANISOU 746 N  GLU A 246     4625  5534  6365   205   189   181     N
ATOM   746 N  GLU A 246    186.558 38.040  5.574 1.00 32.25        C
ANISOU 747 CA GLU A 246     3229  4166  4857   295   246   172     C
ATOM   747 CA GLU A 246    187.702 38.267  6.524 1.00 41.94        C
ANISOU 748 CB GLU A 246     4349  5420  6166   371   152   101     C
ATOM   748 CB GLU A 246    188.957 37.513  6.238 1.00 52.80        C
ANISOU 749 CG GLU A 246     5667  6869  7527   441   200   111     C
ATOM   749 CG GLU A 246    190.093 37.923  7.205 1.00 61.18        C
ANISOU 750 CD GLU A 246     6588  7970  8688   515    85    17     C
ATOM   750 CD GLU A 246    191.279 37.631  6.885 1.00 61.76        O
ANISOU 751 OE1 GLU A 246     6559  8109  8799   550   111    24     O
ATOM   751 OE1 GLU A 246    189.779 38.536  8.276 1.00 61.68        O
ANISOU 752 OE2 GLU A 246     6638  8009  8788   546   -35   -75     O
ATOM   752 OE2 GLU A 246    185.664 36.943  6.146 1.00 37.40        C
ANISOU 753 C  GLU A 246     4052  4800  5358   366   281   135     C
ATOM   753 C  GLU A 246    184.950 37.161  7.120 1.00 40.60        O
ANISOU 754 O  GLU A 246     4516  5167  5744   395   219    88     O
ATOM   754 O  GLU A 246    185.674 35.762  5.542 1.00 36.83        N
ANISOU 755 N  LEU A 247     4058  4747  5188   397   390   157     N
ATOM   755 N  LEU A 247    185.000 34.614  6.123 1.00 31.28        C
ANISOU 756 CA LEU A 247     3505  4005  4376   471   448   124     C
ATOM   756 CA LEU A 247    184.104 33.961  5.097 1.00 34.20        C
ANISOU 757 CB LEU A 247     3954  4354  4686   405   552   136     C
ATOM   757 CB LEU A 247    183.099 34.920  4.470 1.00 38.29        C
ANISOU 758 CG LEU A 247     4448  4867  5232   287   524   150     C
ATOM   758 CG LEU A 247    182.364 34.190  3.395 1.00 44.84        C
ANISOU 759 CD1 LEU A 247     5336  5707  5996   245   618   135     C
ATOM   759 CD1 LEU A 247    182.117 35.418  5.501 1.00 38.58        C
ANISOU 760 CD2 LEU A 247     4536  4846  5276   280   459   120     C
ATOM   760 CD2 LEU A 247    186.032 33.610  6.615 1.00 40.39        C
ANISOU 761 C  LEU A 247     4677  5190  5480   609   482   112     C
ATOM   761 C  LEU A 247    186.896 33.175  5.847 1.00 44.71        O
ANISOU 762 O  LEU A 247     5179  5786  6023   620   535   137     O
ATOM   762 O  LEU A 247    185.934 33.235  7.889 1.00 38.75        N
ANISOU 763 N  LEU A 248     4538  4963  5223   731   458   79     N
ATOM   763 N  LEU A 248    186.919 32.339  8.478 1.00 39.41        C
ANISOU 764 CA LEU A 248     4641  5088  5246   893   487   72     C
ATOM   765 CB LEU A 248    187.325 32.784  9.885 1.00 36.66        C
ANISOU 765 CB LEU A 248     4256  4786  4886  1031   372   21     C
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ATOM 766 CG LEU A 248 187.850 34.205 10.062 1.00 40.38 C
ANISOU 766 CG LEU A 248 4560 5308 5476 974 216 -36 C
ATOM 767 CD1 LEU A 248 188.338 34.337 11.509 1.00 44.76 C
ANISOU 767 CD1 LEU A 248 5087 5930 5989 1159 106 -116 C
ATOM 768 CD2 LEU A 248 188.994 34.498 9.096 1.00 34.68 C
ANISOU 768 CD2 LEU A 248 3690 4638 4847 903 214 -22 C
ATOM 769 C LEU A 248 186.421 30.915 8.537 1.00 41.46 C
ANISOU 769 C LEU A 248 5058 5280 5415 966 633 96 C
ATOM 770 O LEU A 248 185.251 30.658 8.804 1.00 43.27 O
ANISOU 770 O LEU A 248 5389 5425 5626 940 684 100 O
ATOM 771 N GLU A 249 187.344 29.995 8.314 1.00 43.16 N
ANISOU 771 N GLU A 249 5285 5526 5587 1060 704 110 N
ATOM 772 CA GLU A 249 187.132 28.586 8.557 1.00 41.96 C
ANISOU 772 CA GLU A 249 5277 5303 5364 1167 847 132 C
ATOM 773 CB GLU A 249 187.012 27.831 7.242 1.00 43.73 C
ANISOU 773 CB GLU A 249 5531 5486 5598 1078 958 133 C
ATOM 774 CG GLU A 249 186.039 26.692 7.244 1.00 53.18 C
ANISOU 774 CG GLU A 249 6872 6545 6786 1082 1106 130 C
ATOM 775 CD GLU A 249 185.737 26.187 5.822 1.00 67.77 C
ANISOU 775 CD GLU A 249 8723 8365 8661 965 1179 89 C
ATOM 776 OE1 GLU A 249 186.693 25.916 5.054 1.00 75.01 O
ANISOU 776 OE1 GLU A 249 9591 9355 9556 990 1190 90 O
ATOM 777 OE2 GLU A 249 184.541 26.070 5.466 1.00 73.89 O
ANISOU 777 OE2 GLU A 249 9541 9058 9476 858 1222 48 O
ATOM 778 C GLU A 249 188.389 28.180 9.300 1.00 43.37 C
ANISOU 778 C GLU A 249 5433 5565 5479 1364 831 138 C
ATOM 779 O GLU A 249 189.525 28.431 8.849 1.00 38.87 O
ANISOU 779 O GLU A 249 4748 5093 4926 1371 779 126 O
ATOM 780 N ASN A 250 188.190 27.571 10.456 1.00 45.70 N
ANISOU 780 N ASN A 250 5834 5830 5701 1536 880 159 N
ATOM 781 CA ASN A 250 189.312 27.116 11.258 1.00 49.49 C
ANISOU 781 CA ASN A 250 6306 6404 6094 1762 870 164 C
ATOM 782 CB ASN A 250 189.997 25.907 10.597 1.00 53.24 C
ANISOU 782 CB ASN A 250 6834 6862 6534 1824 1004 199 C
ATOM 783 CG ASN A 250 189.070 24.727 10.465 1.00 53.56 C
ANISOU 783 CG ASN A 250 7045 6735 6571 1826 1194 248 C
ATOM 784 OD1 ASN A 250 188.628 24.143 11.475 1.00 54.11 O
ANISOU 784 OD1 ASN A 250 7232 6738 6588 1977 1283 299 O
ATOM 785 ND2 ASN A 250 188.730 24.385 9.211 1.00 51.11 N
ANISOU 785 ND2 ASN A 250 6744 6352 6324 1662 1264 231 N
ATOM 786 C ASN A 250 190.345 28.218 11.522 1.00 45.83 C
ANISOU 786 C ASN A 250 5661 6095 5658 1783 686 96 C
ATOM 787 O ASN A 250 191.540 27.967 11.503 1.00 48.32 O
ANISOU 787 O ASN A 250 5905 6512 5943 1889 665 79 O
ATOM 788 N GLY A 251 189.880 29.441 11.735 1.00 48.08 N
ANISOU 788 N GLY A 251 5864 6390 6015 1677 555 48 N
ATOM 789 CA GLY A 251 190.762 30.549 12.083 1.00 47.56 C
ANISOU 789 CA GLY A 251 5616 6444 6010 1688 378 -38 C
ATOM 790 C GLY A 251 191.492 31.197 10.910 1.00 50.43 C
ANISOU 790 C GLY A 251 5820 6840 6503 1516 338 -49 C
ATOM 791 O GLY A 251 192.290 32.111 11.094 1.00 50.50 O
ANISOU 791 O GLY A 251 5655 6929 6602 1504 207 -122 O
ATOM 792 N GLN A 252 191.228 30.730 9.690 1.00 45.66 N
ANISOU 792 N GLN A 252 5263 6173 5914 1390 456 19 N
ATOM 793 CA GLN A 252 191.912 31.268 8.526 1.00 41.57 C
ANISOU 793 CA GLN A 252 4603 5694 5499 1253 445 34 C
ATOM 794 CB GLN A 252 192.767 30.180 7.880 1.00 44.63 C
ANISOU 794 CB GLN A 252 5012 6126 5821 1329 552 74 C
ATOM 795 CG GLN A 252 193.831 29.564 8.817 1.00 43.77 C
ANISOU 795 CG GLN A 252 4887 6116 5629 1552 529 37 C
ATOM 796 CD GLN A 252 195.008 30.531 9.158 1.00 52.64 C
ANISOU 796 CD GLN A 252 5788 7363 6849 1573 383 -39 C
ATOM 797 OE1 GLN A 252 195.194 31.575 8.510 1.00 53.74 O
ANISOU 797 OE1 GLN A 252 5778 7503 7139 1408 328 -44 O
ATOM 798 NE2 GLN A 252 195.808 30.163 10.172 1.00 48.08 N
ANISOU 798 NE2 GLN A 252 5184 6891 6192 1784 328 -101 N
ATOM 799 C GLN A 252 190.919 31.829 7.537 1.00 40.28 C
ANISOU 799 C GLN A 252 4454 5450 5402 1053 476 76 C
ATOM 800 O GLN A 252 189.766 31.424 7.518 1.00 45.76 O
ANISOU 800 O GLN A 252 5284 6058 6044 1021 539 93 O
ATOM 801 N ARG A 253 191.352 32.784 6.725 1.00 46.55 N
ANISOU 801 N ARG A 253 5099 6274 6315 927 437 94 N
ATOM 802 CA ARG A 253 190.474 33.328 5.698 1.00 44.28 C
ANISOU 802 CA ARG A 253 4820 5932 6073 764 475 147 C
ATOM 803 CB ARG A 253 191.109 34.528 5.016 1.00 43.48 C
ANISOU 803 CB ARG A 253 4534 5863 6123 655 433 181 C
ATOM 804 CG ARG A 253 190.319 35.032 3.815 1.00 49.44 C
ANISOU 804 CG ARG A 253 5297 6587 6901 521 494 257 C
ATOM 805 CD ARG A 253 190.975 36.289 3.228 1.00 50.67 C
ANISOU 805 CD ARG A 253 5267 6758 7227 429 474 315 C
ATOM 806 NE ARG A 253 191.429 37.164 4.302 1.00 54.86 N
ANISOU 806 NE ARG A 253 5685 7264 7897 428 348 239 N
ATOM 807 CZ ARG A 253 192.291 38.167 4.160 1.00 60.69 C
ANISOU 807 CZ ARG A 253 6232 8002 8827 368 314 250 C
ATOM 808 NH1 ARG A 253 192.812 38.434 2.963 1.00 59.91 N
ANISOU 808 NH1 ARG A 253 6038 7928 8798 309 414 363 N
ATOM 809 NH2 ARG A 253 192.624 38.891 5.231 1.00 62.31 N
ANISOU 809 NH2 ARG A 253 6336 8182 9158 375 184 142 N
ATOM 810 C ARG A 253 190.103 32.254 4.658 1.00 44.13 C
ANISOU 810 C ARG A 253 4910 5900 5956 755 612 191 C
ATOM 811 O ARG A 253 190.954 31.576 4.122 1.00 47.33 O
ANISOU 811 O ARG A 253 5295 6363 6324 813 675 212 O
ATOM 812 N ALA A 254 188.816 32.095 4.409 1.00 47.77 N
ANISOU 812 N ALA A 254 5482 6292 6378 688 652 189 N
ATOM 813 CA ALA A 254 188.299 31.058 3.532 1.00 45.10 C
ANISOU 813 CA ALA A 254 5246 5930 5959 681 768 190 C
ATOM 814 CB ALA A 254 187.364 30.145 4.344 1.00 33.43 C
ANISOU 814 CB ALA A 254 3926 4352 4423 732 817 147 C
ATOM 815 C ALA A 254 187.549 31.685 2.333 1.00 48.17 C
ANISOU 815 C ALA A 254 5603 6335 6365 554 782 215 C
ATOM 816 O ALA A 254 187.140 30.987 1.427 1.00 51.69 O
ANISOU 816 O ALA A 254 6102 6787 6748 543 862 198 O
ATOM 817 N GLY A 255 187.352 32.999 2.359 1.00 48.58 N
ANISOU 817 N GLY A 255 5567 6393 6499 471 705 246 N
ATOM 818 CA GLY A 255 186.634 33.712 1.312 1.00 49.97 C
ANISOU 818 CA GLY A 255 5712 6592 6684 375 719 285 C
ATOM 819 C GLY A 255 186.546 35.188 1.666 1.00 50.63 C
ANISOU 819 C GLY A 255 5701 6653 6882 303 631 322 C
ATOM 820 O GLY A 255 186.704 35.562 2.835 1.00 48.70 O
ANISOU 820 O GLY A 255 5443 6364 6697 320 547 284 O
ATOM 821 N THR A 256 186.315 36.017 0.652 1.00 54.30 N
ANISOU 821 N THR A 256 6101 7155 7377 238 654 394 N
ATOM 822 CA THR A 256 186.234 37.472 0.809 1.00 54.70 C
ANISOU 822 CA THR A 256 6058 7170 7557 165 594 445 C
ATOM 823 CB THR A 256 187.467 38.169 0.261 1.00 54.57 C
ANISOU 823 CB THR A 256 5882 7189 7665 155 622 537 C
ATOM 824 OG1 THR A 256 188.616 37.712 0.968 1.00 66.88 O
ANISOU 824 OG1 THR A 256 7387 8756 9267 211 591 492 O
ATOM 825 CG2 THR A 256 187.349 39.658 0.452 1.00 52.31 C
ANISOU 825 CG2 THR A 256 5497 6835 7542 75 573 584 C
ATOM 826 C THR A 256 185.066 38.009 0.009 1.00 53.41 C
ANISOU 826 C THR A 256 5928 7017 7348 112 620 483 C
ATOM 827 O THR A 256 184.992 37.781 -1.194 1.00 64.56 O
ANISOU 827 O THR A 256 7336 8511 8683 130 702 534 O
ATOM 828 N CYS A 257 184.163 38.746 0.636 1.00 42.89 N
ANISOU 828 N CYS A 257 4625 5619 6052 62 551 458 N
ATOM 829 CA CYS A 257 182.978 39.162 -0.107 1.00 39.87 C
ANISOU 829 CA CYS A 257 5262 5604 27 575 484 C
ATOM 830 CB CYS A 257 181.972 38.013 -0.185 1.00 39.45 C
ANISOU 830 CB CYS A 257 4355 5230 5405 47 600 387 C
ATOM 831 SG CYS A 257 181.117 37.740 1.371 1.00 62.74 S
ANISOU 831 SG CYS A 257 7405 8075 8359 35 523 285 S
ATOM 832 C CYS A 257 182.291 40.402 0.442 1.00 38.97 C
ANISOU 832 C CYS A 257 4153 5076 5575 -30 502 498 C
ATOM 833 O CYS A 257 182.448 40.760 1.626 1.00 37.05 O
ANISOU 833 O CYS A 257 3901 4755 5420 -42 414 447 O
ATOM 834 N VAL A 258 181.507 41.034 -0.437 1.00 31.20 N
ANISOU 834 N VAL A 258 3169 4132 4552 -49 538 560 N
ATOM 835 CA VAL A 258 180.677 42.160 -0.057 1.00 35.87 C
ANISOU 835 CA VAL A 258 3764 4664 5201 -93 480 576 C
ATOM 836 CB VAL A 258 180.384 43.074 -1.239 1.00 36.20 C
ANISOU 836 CB VAL A 258 3757 4758 5238 -89 550 702 C
ATOM 837 CG2 VAL A 258 181.690 43.414 -1.993 1.00 28.11 C
ANISOU 837 CG2 VAL A 258 2615 3752 4313 -71 636 831 C
ATOM 838 CG1 VAL A 258 179.678 44.330 -0.731 1.00 31.65 C
ANISOU 838 CG1 VAL A 258 3178 4097 4751 -132 490 725 C
ATOM 839 C VAL A 258 179.369 41.626 0.515 1.00 40.20 C
ANISOU 839 C VAL A 258 4430 5207 5639 -98 434 468 C
ATOM 840 O VAL A 258 178.633 40.909 -0.159 1.00 43.05 O
ANISOU 840 O VAL A 258 4847 5643 5865 -80 481 429 O
ATOM 841 N LEU A 259 179.064 42.002 1.752 1.00 39.97 N
ANISOU 841 N LEU A 259 4427 5091 5670 -117 343 411 N
ATOM 842 CA LEU A 259 178.033 41.324 2.510 1.00 37.53 C
ANISOU 842 CA LEU A 259 4223 4763 5271 -109 311 313 C
ATOM 843 CB LEU A 259 178.705 40.391 3.520 1.00 42.73 C
ANISOU 843 CB LEU A 259 4915 5383 5937 -62 294 249 C
ATOM 844 CG LEU A 259 178.007 39.173 4.108 1.00 47.75 C
ANISOU 844 CG LEU A 259 5661 6002 6479 -30 323 169 C
ATOM 845 CD1 LEU A 259 177.508 38.258 3.004 1.00 46.75 C
ANISOU 845 CD1 LEU A 259 5568 5932 6262 -45 418 146 C
ATOM 846 CD2 LEU A 259 179.000 38.433 5.026 1.00 47.44 C
ANISOU 846 CD2 LEU A 259 5635 5934 6457 46 317 142 C
ATOM 847 C LEU A 259 177.171 42.333 3.240 1.00 34.99 C
ANISOU 847 C LEU A 259 3919 4387 4989 -133 229 301 C
ATOM 848 O LEU A 259 177.681 43.233 3.906 1.00 39.40 O
ANISOU 848 O LEU A 259 4422 4880 5668 -139 157 312 O
ATOM 849 N GLU A 260 175.859 42.196 3.121 1.00 34.03 N
ANISOU 849 N GLU A 260 3865 4292 4772 -145 235 266 N
ATOM 850 CA GLU A 260 174.989 42.988 3.969 1.00 39.69 C
ANISOU 850 CA GLU A 260 4612 4960 5508 -154 155 243 C
ATOM 851 CB GLU A 260 174.808 44.407 3.425 1.00 38.71 C
ANISOU 851 CB GLU A 260 4431 4831 5446 -179 136 324 C
ATOM 852 CG GLU A 260 174.310 44.497 2.018 1.00 48.57 C
ANISOU 852 CG GLU A 260 5669 6178 6608 -180 214 384 C
ATOM 853 CD GLU A 260 174.415 45.932 1.484 1.00 61.93 C
ANISOU 853 CD GLU A 260 7298 7849 8384 -184 220 500 C
ATOM 854 OE1 GLU A 260 175.548 46.477 1.417 1.00 67.69 O
ANISOU 854 OE1 GLU A 260 7947 8517 9255 -195 234 572 O
ATOM 855 OE2 GLU A 260 173.359 46.526 1.172 1.00 63.44 O
ANISOU 855 OE2 GLU A 260 7516 8078 8512 -173 216 520 O

ATOM 856 C GLU A 260 173.645 42.340 4.222 1.00 40.15 C
ANISOU 856 C GLU A 260 4756 5040 5459 -155 168 172 C
ATOM 857 O GLU A 260 173.217 41.467 3.481 1.00 39.26 O
ANISOU 857 O GLU A 260 4666 4987 5265 -163 240 138 O
ATOM 858 N TYR A 261 172.996 42.793 5.294 1.00 40.09 N
ANISOU 858 N TYR A 261 4786 4983 5462 -142 97 141 N
ATOM 859 CA TYR A 261 171.683 42.317 5.673 1.00 36.80 C
ANISOU 859 CA TYR A 261 4440 4576 4965 -143 110 83 C
ATOM 860 CB TYR A 261 171.457 42.542 7.161 1.00 35.89 C
ANISOU 860 CB TYR A 261 4368 4398 4870 -92 39 56 C
ATOM 861 CG TYR A 261 172.019 41.474 8.084 1.00 38.36 C
ANISOU 861 CG TYR A 261 4726 4673 5178 -27 68 26 C
ATOM 862 CD1 TYR A 261 171.315 40.294 8.316 1.00 41.21 C
ANISOU 862 CD1 TYR A 261 5153 5021 5482 -16 159 -6 C
ATOM 863 CE1 TYR A 261 171.805 39.335 9.180 1.00 46.64 C
ANISOU 863 CE1 TYR A 261 5891 5667 6165 64 205 -11 C
ATOM 864 CZ TYR A 261 173.016 39.552 9.817 1.00 42.02 C
ANISOU 864 CZ TYR A 261 5282 5074 5609 143 143 1 C
ATOM 865 OH TYR A 261 173.484 38.600 10.654 1.00 41.83 O
ANISOU 865 OH TYR A 261 5310 5026 5559 247 192 2 O
ATOM 866 CE2 TYR A 261 173.740 40.705 9.623 1.00 40.80 C
ANISOU 866 CE2 TYR A 261 5047 4936 5519 124 39 9 C
ATOM 867 CD2 TYR A 261 173.236 41.666 8.750 1.00 39.10 C
ANISOU 867 CD2 TYR A 261 4788 4739 5330 34 10 30 C
ATOM 868 C TYR A 261 170.649 43.104 4.883 1.00 31.16 C
ANISOU 868 C TYR A 261 3710 3924 4205 -175 103 100 C
ATOM 869 O TYR A 261 170.844 44.260 4.587 1.00 34.20 O
ANISOU 869 O TYR A 261 4052 4306 4635 -179 63 164 O
ATOM 870 N ALA A 262 169.548 42.477 4.538 1.00 34.81 N
ANISOU 870 N ALA A 262 4201 4439 4585 -193 148 40 N
ATOM 871 CA ALA A 262 168.494 43.186 3.815 1.00 33.08 C
ANISOU 871 CA ALA A 262 3964 4302 4302 -205 136 43 C
ATOM 872 CB ALA A 262 167.532 42.203 3.166 1.00 23.66 C
ANISOU 872 CB ALA A 262 2772 3190 3027 -227 198 -56 C
ATOM 873 C ALA A 262 167.759 44.053 4.814 1.00 34.49 C
ANISOU 873 C ALA A 262 4173 4437 4494 -191 59 49 C
ATOM 874 O ALA A 262 167.095 43.543 5.702 1.00 34.14 O
ANISOU 874 O ALA A 262 4175 4362 4436 -186 58 -6 O
ATOM 875 N THR A 263 167.867 45.366 4.659 1.00 38.05 N
ANISOU 875 N THR A 263 4598 4882 4979 -178 5 120 N
ATOM 876 CA THR A 263 167.260 46.294 5.601 1.00 32.91 C
ANISOU 876 CA THR A 263 3973 4182 4348 -156 -77 122 C
ATOM 877 CB THR A 263 167.618 47.734 5.239 1.00 37.37 C
ANISOU 877 CB THR A 263 4498 4716 4984 -147 -117 209 C
ATOM 878 OG1 THR A 263 167.194 48.014 3.900 1.00 42.95 O
ANISOU 878 OG1 THR A 263 5178 5523 5619 -142 -57 262 O
ATOM 879 CG2 THR A 263 169.134 47.951 5.400 1.00 22.85 C
ANISOU 879 CG2 THR A 263 2610 2789 3283 -156 -128 249 C
ATOM 880 C THR A 263 165.749 46.164 5.867 1.00 30.46 C
ANISOU 880 C THR A 263 3701 3928 3945 -151 -82 65 C
ATOM 881 O THR A 263 165.315 46.464 6.981 1.00 36.89 O
ANISOU 881 O THR A 263 4553 4695 4769 -121 -139 46 O
ATOM 882 N PRO A 264 164.949 45.745 4.866 1.00 28.89 N
ANISOU 882 N PRO A 264 3482 3838 3656 -169 -27 29 N
ATOM 883 CA PRO A 264 163.520 45.660 5.212 1.00 34.23 C
ANISOU 883 CA PRO A 264 4178 4564 4264 -168 -37 -35 C
ATOM 884 CB PRO A 264 162.861 45.134 3.925 1.00 35.89 C
ANISOU 884 CB PRO A 264 4341 4910 4385 -185 20 -99 C
ATOM 885 CG PRO A 264 163.749 45.669 2.806 1.00 36.87 C
ANISOU 885 CG PRO A 264 4429 5080 4501 -159 33 -17 C
ATOM 886 CD PRO A 264 165.171 45.668 3.398 1.00 30.68 C
ANISOU 886 CD PRO A 264 3660 4165 3832 -170 27 50 C
ATOM 887 C PRO A 264 163.207 44.704 6.364 1.00 31.81 C
ANISOU 887 C PRO A 264 3914 4191 3981 -175 -13 -94 C
ATOM 888 O PRO A 264 162.135 44.797 6.950 1.00 31.84 O
ANISOU 888 O PRO A 264 3937 4210 3952 -164 -26 -125 O
ATOM 889 N LEU A 265 164.110 43.774 6.640 1.00 29.12 N
ANISOU 889 N LEU A 265 3587 3784 3692 -184 34 -100 N
ATOM 890 CA LEU A 265 163.946 42.824 7.753 1.00 35.90 C
ANISOU 890 CA LEU A 265 4494 4570 4576 -166 81 -129 C
ATOM 891 CB LEU A 265 165.011 41.719 7.742 1.00 30.23 C
ANISOU 891 CB LEU A 265 3786 3794 3905 -169 151 -132 C
ATOM 892 CG LEU A 265 164.866 40.883 6.471 1.00 38.08 C
ANISOU 892 CG LEU A 265 4737 4843 4887 -234 229 -198 C
ATOM 893 CD1 LEU A 265 165.784 39.725 6.463 1.00 38.86 C
ANISOU 893 CD1 LEU A 265 4853 4881 5032 -234 308 -209 C
ATOM 894 CD2 LEU A 265 163.427 40.375 6.259 1.00 32.74 C
ANISOU 894 CD2 LEU A 265 4040 4209 4192 -280 281 -291 C
ATOM 895 C LEU A 265 163.961 43.576 9.080 1.00 38.25 C
ANISOU 895 C LEU A 265 4835 4814 4882 -91 1 -88 C
ATOM 896 O LEU A 265 163.263 43.212 10.020 1.00 37.89 O
ANISOU 896 O LEU A 265 4829 4747 4821 -53 26 -100 O
ATOM 897 N ILE A 266 164.758 44.641 9.139 1.00 33.90 N
ANISOU 897 N ILE A 266 4271 4244 4366 -65 -91 -43 N
ATOM 898 CA ILE A 266 164.762 45.544 10.278 1.00 26.69 C
ANISOU 898 CA ILE A 266 3384 3292 3466 11 -191 -31 C
ATOM 899 CB ILE A 266 165.798 46.639 10.089 1.00 22.47 C
ANISOU 899 CB ILE A 266 2808 2718 3012 14 -278 -1 C
ATOM 900 CG1 ILE A 266 167.182 45.998 9.981 1.00 22.54 C
ANISOU 900 CG1 ILE A 266 2792 2690 3083 9 -251 4 C
ATOM 901 CD1 ILE A 266 168.361 47.078 9.639 1.00 31.49 C
ANISOU 901 CD1 ILE A 266 3854 3773 4336 -8 -320 35 C
ATOM 902 CG2 ILE A 266 165.769 47.638 11.250 1.00 20.19 C
ANISOU 902 CG2 ILE A 266 2535 2386 2751 94 -397 -19 C
ATOM 903 C ILE A 266 163.384 46.137 10.480 1.00 30.65 C
ANISOU 903 C ILE A 266 3901 3839 3904 24 -219 -41 C
ATOM 904 O ILE A 266 162.851 46.191 11.590 1.00 28.64 O
ANISOU 904 O ILE A 266 3689 3574 3621 95 -246 -51 O
ATOM 905 N THR A 267 162.756 46.513 9.375 1.00 28.23 N
ANISOU 905 N THR A 267 3561 3602 3564 -32 -204 -39 N
ATOM 906 CA THR A 267 161.402 47.027 9.469 1.00 26.25 C
ANISOU 906 CA THR A 267 3317 3412 3244 -17 -226 -54 C
ATOM 907 CB THR A 267 160.988 47.658 8.144 1.00 30.07 C
ANISOU 907 CB THR A 267 3756 3983 3684 -50 -224 -40 C
ATOM 908 OG1 THR A 267 161.706 48.877 8.008 1.00 25.90 O
ANISOU 908 OG1 THR A 267 3223 3407 3211 -25 -292 27 O
ATOM 909 CG2 THR A 267 159.452 47.977 8.086 1.00 19.90 C
ANISOU 909 CG2 THR A 267 2463 2791 2305 -35 -232 -74 C
ATOM 910 C THR A 267 160.372 45.964 9.957 1.00 33.02 C
ANISOU 910 C THR A 267 4189 4294 4061 -23 -146 -105 C
ATOM 911 O THR A 267 159.531 46.218 10.853 1.00 30.10 O
ANISOU 911 O THR A 267 3848 3931 3657 30 -168 -106 O
ATOM 912 N LEU A 268 160.452 44.772 9.376 1.00 28.90 N
ANISOU 912 N LEU A 268 3644 3779 3557 -85 -46 -145 N
ATOM 913 CA LEU A 268 159.563 43.660 9.790 1.00 32.30 C
ANISOU 913 CA LEU A 268 4075 4202 3995 -106 56 -195 C
ATOM 914 CB LEU A 268 159.798 42.366 8.988 1.00 31.99 C
ANISOU 914 CB LEU A 268 3999 4151 4003 -185 165 -257 C
ATOM 915 CG LEU A 268 159.392 42.437 7.515 1.00 37.02 C
ANISOU 915 CG LEU A 268 4561 4901 4603 -249 161 -333 C
ATOM 916 CD1 LEU A 268 159.681 41.124 6.818 1.00 34.64 C
ANISOU 916 CD1 LEU A 268 4223 4582 4355 -313 260 -415 C
ATOM 917 CD2 LEU A 268 157.894 42.754 7.420 1.00 37.29 C
ANISOU 917 CD2 LEU A 268 4551 5029 4588 -260 151 -394 C
ATOM 918 C LEU A 268 159.691 43.376 11.278 1.00 29.78 C
ANISOU 918 C LEU A 268 3820 3803 3693 -21 73 -149 C
ATOM 919 O LEU A 268 158.726 43.099 11.978 1.00 28.79 O
ANISOU 919 O LEU A 268 3706 3677 3554 6 123 -151 O
ATOM 920 N PHE A 269 160.915 43.438 11.766 1.00 25.98 N
ANISOU 920 N PHE A 269 3374 3260 3236 36 36 -106 N
ATOM 921 CA PHE A 269 161.125 43.152 13.142 1.00 30.76 C
ANISOU 921 CA PHE A 269 4038 3813 3835 149 48 -67 C
ATOM 922 CB PHE A 269 162.602 42.968 13.398 1.00 33.35 C
ANISOU 922 CB PHE A 269 4385 4092 4195 198 21 -46 C
ATOM 923 CG PHE A 269 162.886 42.549 14.782 1.00 26.90 C
ANISOU 923 CG PHE A 269 3627 3242 3353 343 41 -9 C
ATOM 924 CD1 PHE A 269 162.894 41.194 15.098 1.00 31.54 C
ANISOU 924 CD1 PHE A 269 4247 3778 3958 368 195 20 C
ATOM 925 CE1 PHE A 269 163.131 40.753 16.394 1.00 35.98 C
ANISOU 925 CE1 PHE A 269 4871 4321 4479 533 236 74 C
ATOM 926 CZ PHE A 269 163.311 41.709 17.417 1.00 37.65 C
ANISOU 926 CZ PHE A 269 5104 4581 4621 681 101 76 C
ATOM 927 CE2 PHE A 269 163.310 43.100 17.106 1.00 32.32 C
ANISOU 927 CE2 PHE A 269 4389 3948 3944 641 -68 23 C
ATOM 928 CD2 PHE A 269 163.085 43.504 15.782 1.00 30.78 C
ANISOU 928 CD2 PHE A 269 4115 3754 3800 470 -86 -7 C
ATOM 929 C PHE A 269 160.548 44.271 14.027 1.00 29.15 C
ANISOU 929 C PHE A 269 3859 3642 3573 243 -58 -51 C
ATOM 930 O PHE A 269 159.909 44.026 15.025 1.00 32.93 O
ANISOU 930 O PHE A 269 4375 4122 4015 329 -19 -27 O
ATOM 931 N ALA A 270 160.741 45.504 13.619 1.00 31.66 N
ANISOU 931 N ALA A 270 4155 3986 3887 230 -181 -60 N
ATOM 932 CA ALA A 270 160.251 46.629 14.389 1.00 28.71 C
ANISOU 932 CA ALA A 270 3804 3635 3469 319 -291 -58 C
ATOM 933 CB ALA A 270 160.836 47.898 13.852 1.00 23.93 C
ANISOU 933 CB ALA A 270 3170 3016 2905 296 -410 -64 C
ATOM 934 C ALA A 270 158.733 46.671 14.388 1.00 35.95 C
ANISOU 934 C ALA A 270 4718 4616 4325 309 -250 -62 C
ATOM 935 O ALA A 270 158.126 46.956 15.404 1.00 41.09 O
ANISOU 935 O ALA A 270 5404 5286 4922 411 -277 -50 O
ATOM 936 N MET A 271 158.110 46.361 13.254 1.00 31.54 N
ANISOU 936 N MET A 271 4111 4106 3768 196 -186 -88 N
ATOM 937 CA MET A 271 156.656 46.290 13.221 1.00 31.16 C
ANISOU 937 CA MET A 271 4040 4129 3672 181 -141 -110 C
ATOM 938 CB MET A 271 156.115 46.067 11.805 1.00 26.65 C
ANISOU 938 CB MET A 271 3395 3632 3097 66 -99 -168 C
ATOM 939 CG MET A 271 156.346 47.253 10.865 1.00 23.58 C
ANISOU 939 CG MET A 271 2988 3297 2673 58 -198 -158 C
ATOM 940 SD MET A 271 155.811 46.796 9.201 1.00 31.04 S
ANISOU 940 SD MET A 271 3845 4361 3589 -37 -140 -234 S
ATOM 941 CE MET A 271 154.013 46.892 9.317 1.00 41.06 C
ANISOU 941 CE MET A 271 5747 4787 -29 -127 -298 C
ATOM 942 C MET A 271 156.104 45.222 14.167 1.00 34.55 C
ANISOU 942 C MET A 271 4488 4528 4112 219 -21 -95 C
ATOM 943 O MET A 271 155.030 45.385 14.715 1.00 33.73 O
ANISOU 943 O MET A 271 4382 4467 3966 263 -4 -88 O
ATOM 944 N SER A 272 156.817 44.114 14.342 1.00 27.46 N
ANISOU 944 N SER A 272 3605 3554 3275 209 77 -80 N
ATOM 945 CA SER A 272 156.346 43.102 15.289 1.00 24.33 C
ANISOU 945 CA SER A 272 3232 3109 2901 264 216 -39 C

ATOM 946 CB SER A 272 157.043 41.741 15.077 1.00 36.15 C
ANISOU 946 CB SER A 272 4733 4516 4488 216 353 -35 C
ATOM 947 OG SER A 272 158.449 41.812 15.317 1.00 39.69 O
ANISOU 947 OG SER A 272 5229 4924 4929 281 293 -4 O
ATOM 948 C SER A 272 156.526 43.620 16.758 1.00 36.59 C
ANISOU 948 C SER A 272 4860 4663 4381 451 157 31 C
ATOM 949 O SER A 272 155.879 43.155 17.678 1.00 35.78 O
ANISOU 949 O SER A 272 4781 4554 4260 538 254 85 O
ATOM 950 N GLN A 273 157.385 44.601 16.983 1.00 31.67 N
ANISOU 950 N GLN A 273 4265 4051 3718 521 1 25 N
ATOM 951 CA GLN A 273 157.627 45.035 18.368 1.00 36.43 C
ANISOU 951 CA GLN A 273 4928 4666 4248 714 -67 61 C
ATOM 952 CB GLN A 273 159.098 45.361 18.605 1.00 36.99 C
ANISOU 952 CB GLN A 273 5016 4707 4332 779 -177 39 C
ATOM 953 CG GLN A 273 159.969 44.191 18.358 1.00 43.09 C
ANISOU 953 CG GLN A 273 5793 5420 5160 746 -67 60 C
ATOM 954 CD GLN A 273 159.540 42.969 19.197 1.00 58.66 C
ANISOU 954 CD GLN A 273 7809 7368 7110 842 111 139 C
ATOM 955 OE1 GLN A 273 159.407 43.050 20.436 1.00 67.33 O
ANISOU 955 OE1 GLN A 273 8957 8502 8125 1034 106 184 O
ATOM 956 NE2 GLN A 273 159.304 41.831 18.516 1.00 57.30 N
ANISOU 956 NE2 GLN A 273 7616 7135 7019 719 277 154 N
ATOM 957 C GLN A 273 156.765 46.223 18.753 1.00 37.67 C
ANISOU 957 C GLN A 273 5089 4892 4331 779 -179 46 C
ATOM 958 O GLN A 273 156.557 46.513 19.928 1.00 40.34 O
ANISOU 958 O GLN A 273 5471 5264 4592 950 -216 71 O
ATOM 959 N TYR A 274 156.257 46.918 17.752 1.00 35.08 N
ANISOU 959 N TYR A 274 4716 4596 4016 660 -233 5 N
ATOM 960 CA TYR A 274 155.437 48.096 18.013 1.00 32.17 C
ANISOU 960 CA TYR A 274 4353 4290 3580 718 -340 -9 C
ATOM 961 CB TYR A 274 155.803 49.260 17.106 1.00 32.83 C
ANISOU 961 CB TYR A 274 4412 4370 3692 647 -467 -49 C
ATOM 962 CG TYR A 274 157.145 49.841 17.408 1.00 41.09 C
ANISOU 962 CG TYR A 274 5474 5349 4790 698 -583 -73 C
ATOM 963 CD1 TYR A 274 157.416 50.373 18.654 1.00 50.76 C
ANISOU 963 CD1 TYR A 274 6738 6571 5978 862 -685 -95 C
ATOM 964 CE1 TYR A 274 158.663 50.890 18.937 1.00 58.15 C
ANISOU 964 CE1 TYR A 274 7667 7448 6979 907 -800 -146 C
ATOM 965 CZ TYR A 274 159.647 50.901 17.945 1.00 58.66 C
ANISOU 965 CZ TYR A 274 7687 7449 7154 778 -799 -153 C
ATOM 966 OH TYR A 274 160.897 51.410 18.179 1.00 66.21 O
ANISOU 966 OH TYR A 274 8616 8342 8199 807 -905 -209 O
ATOM 967 CE2 TYR A 274 159.404 50.371 16.711 1.00 50.67 C
ANISOU 967 CE2 TYR A 274 6647 6442 6164 626 -691 -112 C
ATOM 968 CD2 TYR A 274 158.161 49.841 16.448 1.00 46.70 C
ANISOU 968 CD2 TYR A 274 6150 6005 5591 590 -590 -82 C
ATOM 969 C TYR A 274 153.948 47.857 17.901 1.00 35.66 C
ANISOU 969 C TYR A 274 4765 4800 3983 686 -251 2 C
ATOM 970 O TYR A 274 153.467 47.357 16.889 1.00 40.53 O
ANISOU 970 O TYR A 274 5323 5434 4641 547 -170 -24 O
ATOM 971 N SER A 275 153.232 48.267 18.945 1.00 36.12 N
ANISOU 971 N SER A 275 4857 4908 3960 827 -276 30 N
ATOM 972 CA SER A 275 151.783 48.098 19.044 1.00 35.13 C
ANISOU 972 CA SER A 275 4699 4855 3795 822 -192 47 C
ATOM 973 CB SER A 275 151.234 48.754 20.311 1.00 28.33 C
ANISOU 973 CB SER A 275 3888 4050 2826 1016 -251 82 C
ATOM 974 OG SER A 275 151.848 48.110 21.389 1.00 37.34 O
ANISOU 974 OG SER A 275 5082 5156 3952 1155 -196 138 O
ATOM 975 C SER A 275 151.114 48.696 17.857 1.00 32.61 C
ANISOU 975 C SER A 275 4320 4597 3475 699 -237 -10 C
ATOM 976 O SER A 275 150.280 48.091 17.215 1.00 36.34 O
ANISOU 976 O SER A 275 4722 5110 3976 594 -136 -35 O
ATOM 977 N GLN A 276 151.492 49.924 17.581 1.00 29.32 N
ANISOU 977 N GLN A 276 3926 4187 3027 724 -390 -34 N
ATOM 978 CA GLN A 276 150.796 50.692 16.587 1.00 28.30 C
ANISOU 978 CA GLN A 276 3754 4131 2867 659 -439 -67 C
ATOM 979 CB GLN A 276 151.389 52.080 16.563 1.00 37.83 C
ANISOU 979 CB GLN A 276 5006 5306 4064 719 -596 -71 C
ATOM 980 CG GLN A 276 150.394 53.099 16.181 1.00 53.00 C
ANISOU 980 CG GLN A 276 6916 7311 5910 746 -656 -79 C
ATOM 981 CD GLN A 276 151.000 54.455 16.087 1.00 69.55 C
ANISOU 981 CD GLN A 276 9053 9347 8027 797 -790 -78 C
ATOM 982 OE1 GLN A 276 152.136 54.678 16.529 1.00 78.92 O
ANISOU 982 OE1 GLN A 276 10270 10427 9289 825 -853 -85 O
ATOM 983 NE2 GLN A 276 150.250 55.390 15.509 1.00 74.27 N
ANISOU 983 NE2 GLN A 276 9643 10006 8569 814 -831 -73 N
ATOM 984 C GLN A 276 150.868 50.103 15.181 1.00 24.09 C
ANISOU 984 C GLN A 276 3151 3616 2388 499 -371 -107 C
ATOM 985 O GLN A 276 150.202 50.585 14.298 1.00 30.13 O
ANISOU 985 O GLN A 276 3870 4468 3110 459 -393 -138 O
ATOM 986 N ALA A 277 151.723 49.114 14.967 1.00 21.60 N
ANISOU 986 N ALA A 277 2828 3226 2153 429 -295 -109 N
ATOM 987 CA ALA A 277 151.927 48.533 13.630 1.00 32.33 C
ANISOU 987 CA ALA A 277 4123 4603 3560 292 -239 -157 C
ATOM 988 CB ALA A 277 153.382 47.964 13.450 1.00 20.34 C
ANISOU 988 CB ALA A 277 2627 2979 2121 252 -220 -142 C
ATOM 989 C ALA A 277 150.891 47.465 13.330 1.00 36.29 C
ANISOU 989 C ALA A 277 4544 5158 4087 212 -215 -215 C
ATOM 990 O ALA A 277 150.624 47.169 12.175 1.00 38.84 O
ANISOU 990 O ALA A 277 4792 5546 4421 118 -85 -290 O
ATOM 991 N GLY A 278 150.312 46.884 14.382 1.00 39.41 N
ANISOU 991 N GLY A 278 4947 5527 4500 258 -25 -186 N
ATOM 992 CA GLY A 278 149.262 45.883 14.252 1.00 31.13 C
ANISOU 992 CA GLY A 278 3810 4507 3512 181 114 -239 C
ATOM 993 C GLY A 278 149.798 44.622 13.610 1.00 36.70 C
ANISOU 993 C GLY A 278 4470 5135 4337 60 226 -291 C
ATOM 994 O GLY A 278 149.200 44.068 12.713 1.00 45.21 O
ANISOU 994 O GLY A 278 5447 6263 5468 -49 281 -398 O
ATOM 995 N PHE A 279 150.975 44.186 14.040 1.00 38.94 N
ANISOU 995 N PHE A 279 4828 5305 4663 89 251 -229 N
ATOM 996 CA PHE A 279 151.720 43.184 13.303 1.00 37.78 C
ANISOU 996 CA PHE A 279 4654 5087 4613 -13 326 -277 C
ATOM 997 CB PHE A 279 152.834 43.907 12.581 1.00 35.12 C
ANISOU 997 CB PHE A 279 4352 4766 4225 -13 198 -274 C
ATOM 998 CG PHE A 279 153.454 43.136 11.477 1.00 33.62 C
ANISOU 998 CG PHE A 279 4117 4556 4100 -118 244 -344 C
ATOM 999 CD1 PHE A 279 152.778 42.996 10.266 1.00 37.69 C
ANISOU 999 CD1 PHE A 279 4533 5174 4612 -206 247 -463 C
ATOM 1000 CE1 PHE A 279 153.347 42.325 9.223 1.00 40.78 C
ANISOU 1000 CE1 PHE A 279 4881 5565 5048 -284 277 -539 C
ATOM 1001 CZ PHE A 279 154.652 41.759 9.371 1.00 42.69 C
ANISOU 1001 CZ PHE A 279 5184 5692 5346 -283 313 -486 C
ATOM 1002 CE2 PHE A 279 155.344 41.901 10.576 1.00 37.69 C
ANISOU 1002 CE2 PHE A 279 4646 4957 4716 -198 310 -366 C
ATOM 1003 CD2 PHE A 279 154.726 42.591 11.625 1.00 32.19 C
ANISOU 1003 CD2 PHE A 279 3989 4273 3969 -111 273 -301 C
ATOM 1004 C PHE A 279 152.320 42.197 14.297 1.00 40.89 C
ANISOU 1004 C PHE A 279 5109 5345 5082 36 452 -195 C
ATOM 1005 O PHE A 279 153.166 42.568 15.105 1.00 41.72 O
ANISOU 1005 O PHE A 279 5304 5411 5136 153 396 -108 O
ATOM 1006 N SER A 280 151.873 40.945 14.236 1.00 42.12 N
ANISOU 1006 N SER A 280 5209 5430 5365 -43 624 -228 N
ATOM 1007 CA SER A 280 152.262 39.931 15.212 1.00 41.57 C
ANISOU 1007 CA SER A 280 5195 5225 5376 19 781 -132 C
ATOM 1008 CB SER A 280 151.094 38.987 15.460 1.00 37.73 C
ANISOU 1008 CB SER A 280 4629 4685 5022 -41 974 -148 C
ATOM 1009 OG SER A 280 150.820 38.248 14.299 1.00 41.29 O
ANISOU 1009 OG SER A 280 4972 5117 5601 -212 1031 -296 O
ATOM 1010 C SER A 280 153.498 39.144 14.767 1.00 45.95 C
ANISOU 1010 C SER A 280 5779 5684 5995 -22 821 -141 C
ATOM 1011 O SER A 280 153.826 39.131 13.578 1.00 53.79 O
ANISOU 1011 O SER A 280 6723 6710 7006 -130 764 -244 O
ATOM 1012 N ARG A 281 154.180 38.492 15.712 1.00 48.13 N
ANISOU 1012 N ARG A 281 7352 6684 4251 -506 -879 -110 N
ATOM 1013 CA ARG A 281 155.290 37.584 15.387 1.00 53.77 C
ANISOU 1013 CA ARG A 281 8116 7253 5060 -402 -978 47 C
ATOM 1014 CB ARG A 281 155.775 36.829 16.618 1.00 57.87 C
ANISOU 1014 CB ARG A 281 8844 7743 5400 -366 -1017 267 C
ATOM 1015 CG ARG A 281 156.665 37.647 17.525 1.00 69.29 C
ANISOU 1015 CG ARG A 281 10296 9357 6674 -304 -1248 311 C
ATOM 1016 CD ARG A 281 156.647 37.091 18.947 1.00 83.15 C
ANISOU 1016 CD ARG A 281 12259 11195 8138 -334 -1251 501 C
ATOM 1017 NE ARG A 281 157.986 36.822 19.473 1.00 93.63 N
ANISOU 1017 NE ARG A 281 13586 12601 9386 -211 -1480 754 N
ATOM 1018 CZ ARG A 281 158.239 36.038 20.520 1.00 99.97 C
ANISOU 1018 CZ ARG A 281 14533 13474 9977 -180 -1500 1040 C
ATOM 1019 NH1 ARG A 281 159.491 35.851 20.932 1.00100.22 N
ANISOU 1019 NH1 ARG A 281 14505 13628 9945 -60 -1731 1311 N
ATOM 1020 NH2 ARG A 281 157.238 35.433 21.149 1.00103.35 N
ANISOU 1020 NH2 ARG A 281 15143 13865 10261 -261 -1284 1085 N
ATOM 1021 C ARG A 281 154.949 36.572 14.295 1.00 57.29 C
ANISOU 1021 C ARG A 281 8542 7546 5678 -460 -822 35 C
ATOM 1022 O ARG A 281 155.793 36.263 13.448 1.00 60.48 O
ANISOU 1022 O ARG A 281 8893 7836 6251 -372 -872 70 O
ATOM 1023 N GLU A 282 153.718 36.066 14.299 1.00 53.65 N
ANISOU 1023 N GLU A 282 8126 7084 5175 -630 -617 -31 N
ATOM 1024 CA GLU A 282 153.291 35.134 13.243 1.00 52.18 C
ANISOU 1024 CA GLU A 282 7919 6822 5084 -707 -466 -106 C
ATOM 1025 CB GLU A 282 151.995 34.397 13.607 1.00 51.84 C
ANISOU 1025 CB GLU A 282 7965 6723 5008 -971 -215 -139 C
ATOM 1026 CG GLU A 282 152.118 33.493 14.838 1.00 62.24 C
ANISOU 1026 CG GLU A 282 9540 7874 6233 -941 -107 54 C
ATOM 1027 CD GLU A 282 152.274 34.257 16.187 1.00 84.70 C
ANISOU 1027 CD GLU A 282 12459 10858 8865 -832 -238 159 C
ATOM 1028 OE1 GLU A 282 12482 10620 8613 -730 -254 380 O
ATOM 1029 OE2 GLU A 282 151.768 35.410 16.298 1.00 82.54 O
ANISOU 1029 OE2 GLU A 282 12064 10782 8517 -855 -301 31 O
ATOM 1030 C GLU A 282 153.152 35.851 11.895 1.00 50.50 C
ANISOU 1030 C GLU A 282 7965 7217 5526 -786 -507 -263 C
ATOM 1031 O GLU A 282 153.541 35.315 10.845 1.00 50.57 O
ANISOU 1031 O GLU A 282 7438 6625 5149 -814 -470 -312 O
ATOM 1032 N ASP A 283 152.594 37.063 11.924 1.00 55.20 N
ANISOU 1032 N ASP A 283 7875 7528 5572 -774 -566 -333 N
ATOM 1033 CA ASP A 283 152.600 37.919 10.745 1.00 57.32 C
ANISOU 1033 CA ASP A 283 7882 7954 5943 -737 -635 -418 C
ATOM 1034 CB ASP A 283 152.065 39.332 11.067 1.00 67.20 C
ANISOU 1034 CB ASP A 283 8958 9398 7179 -672 -650 -437 C
ATOM 1035 CG ASP A 283 150.570 39.364 11.372 1.00 75.62 C
ANISOU 1035 CG ASP A 283 9953 10610 8168 -831 -477 -455 C

ATOM 1036 OD1 ASP A 283 149.878 38.396 11.010 1.00 84.12 O
ANISOU 1036 OD1 ASP A 283 11043 11704 9214 -1019 -376 -483 O
ATOM 1037 OD2 ASP A 283 150.093 40.372 11.964 1.00 73.39 O
ANISOU 1037 OD2 ASP A 283 9596 10415 7872 -778 -418 -446 O
ATOM 1038 C ASP A 283 154.045 38.044 10.207 1.00 53.01 C
ANISOU 1038 C ASP A 283 7330 7289 5524 -556 -786 -380 C
ATOM 1039 O ASP A 283 154.296 38.018 8.992 1.00 52.20 O
ANISOU 1039 O ASP A 283 7103 7209 5520 -554 -795 -434 O
ATOM 1040 N ARG A 284 154.992 38.179 11.128 1.00 46.40 N
ANISOU 1040 N ARG A 284 6617 6346 4667 -414 -904 -277 N
ATOM 1041 CA ARG A 284 156.377 38.486 10.779 1.00 42.64 C
ANISOU 1041 CA ARG A 284 6095 5785 4321 -230 -1064 -217 C
ATOM 1042 CB ARG A 284 157.195 38.798 12.027 1.00 39.49 C
ANISOU 1042 CB ARG A 284 5795 5374 3836 -128 -1216 -106 C
ATOM 1043 CG ARG A 284 158.564 39.326 11.680 1.00 34.59 C
ANISOU 1043 CG ARG A 284 5068 4714 3361 44 -1397 -54 C
ATOM 1044 CD ARG A 284 159.388 39.590 12.890 1.00 33.51 C
ANISOU 1044 CD ARG A 284 4999 4626 3107 100 -1572 54 C
ATOM 1045 NE ARG A 284 159.851 38.361 13.510 1.00 33.84 N
ANISOU 1045 NE ARG A 284 5205 4564 3090 132 -1578 284 N
ATOM 1046 CZ ARG A 284 160.102 38.219 14.803 1.00 34.87 C
ANISOU 1046 CZ ARG A 284 5449 4792 3007 120 -1678 422 C
ATOM 1047 NH1 ARG A 284 160.532 37.043 15.255 1.00 37.78 N
ANISOU 1047 NH1 ARG A 284 5936 5060 3357 186 -1652 693 N
ATOM 1048 NH2 ARG A 284 159.928 39.245 15.633 1.00 36.36 N
ANISOU 1048 NH2 ARG A 284 5632 5180 3002 39 -1778 299 N
ATOM 1049 C ARG A 284 157.102 37.385 9.979 1.00 45.63 C
ANISOU 1049 C ARG A 284 6545 5957 4837 -202 -1011 -157 C
ATOM 1050 O ARG A 284 157.802 37.665 8.990 1.00 42.08 O
ANISOU 1050 O ARG A 284 5976 5475 4536 -106 -1062 -179 O
ATOM 1051 N LEU A 285 156.960 36.136 10.411 1.00 42.10 N
ANISOU 1051 N LEU A 285 6298 5340 4358 -277 -871 -74 N
ATOM 1052 CA LEU A 285 157.719 35.072 9.754 1.00 46.17 C
ANISOU 1052 CA LEU A 285 6906 5597 5038 -238 -756 -3 C
ATOM 1053 CB LEU A 285 157.795 33.806 10.618 1.00 50.99 C
ANISOU 1053 CB LEU A 285 7748 5985 5641 -247 -596 180 C
ATOM 1054 CG LEU A 285 158.369 32.580 9.888 1.00 61.78 C
ANISOU 1054 CG LEU A 285 9233 7024 7218 -238 -357 236 C
ATOM 1055 CD1 LEU A 285 159.839 32.795 9.394 1.00 48.71 C
ANISOU 1055 CD1 LEU A 285 7493 5251 5763 5 -468 378 C
ATOM 1056 CD2 LEU A 285 158.239 31.309 10.736 1.00 64.56 C
ANISOU 1056 CD2 LEU A 285 9807 7136 7587 -256 -122 428 C
ATOM 1057 C LEU A 285 157.115 34.763 8.376 1.00 47.74 C
ANISOU 1057 C LEU A 285 7044 5806 5287 -415 -597 -211 C
ATOM 1058 O LEU A 285 157.793 34.379 7.428 1.00 49.85 O
ANISOU 1058 O LEU A 285 7316 5926 5698 -381 -526 -234 O
ATOM 1059 N GLU A 286 155.810 34.925 8.294 1.00 45.36 N
ANISOU 1059 N GLU A 286 6681 5704 4849 -623 -533 -358 N
ATOM 1060 CA GLU A 286 155.094 34.682 7.071 1.00 41.70 C
ANISOU 1060 CA GLU A 286 6126 5353 4365 -844 -415 -554 C
ATOM 1061 CB GLU A 286 153.598 34.746 7.361 1.00 48.17 C
ANISOU 1061 CB GLU A 286 6875 6399 5027 -1072 -348 -646 C
ATOM 1062 CG GLU A 286 152.737 34.232 6.258 1.00 67.13 C
ANISOU 1062 CG GLU A 286 9195 8947 7364 -1377 -213 -843 C
ATOM 1063 CD GLU A 286 151.441 35.023 6.117 1.00 84.13 C
ANISOU 1063 CD GLU A 286 11081 11501 9385 -1509 -271 -886 C
ATOM 1064 OE1 GLU A 286 150.558 34.589 5.327 1.00 91.17 O
ANISOU 1064 OE1 GLU A 286 11868 12593 10179 -1808 -179 -1033 O
ATOM 1065 OE2 GLU A 286 151.319 36.074 6.798 1.00 88.67 O
ANISOU 1065 OE2 GLU A 286 11543 12192 9955 -1325 -391 -768 O
ATOM 1066 C GLU A 286 155.509 35.754 6.060 1.00 40.93 C
ANISOU 1066 C GLU A 286 5794 5444 4312 -727 -568 -597 C
ATOM 1067 O GLU A 286 155.829 35.437 4.916 1.00 45.09 O
ANISOU 1067 O GLU A 286 6300 5943 4890 -785 -501 -690 O
ATOM 1068 N GLN A 287 155.546 37.018 6.506 1.00 39.93 N
ANISOU 1068 N GLN A 287 5508 5488 4176 -563 -744 -529 N
ATOM 1069 CA GLN A 287 155.860 38.147 5.630 1.00 38.77 C
ANISOU 1069 CA GLN A 287 5120 5516 4096 -432 -857 -542 C
ATOM 1070 CB GLN A 287 155.527 39.501 6.267 1.00 37.77 C
ANISOU 1070 CB GLN A 287 4828 5565 3958 -313 -956 -492 C
ATOM 1071 CG GLN A 287 154.045 39.809 6.392 1.00 31.08 C
ANISOU 1071 CG GLN A 287 3848 4973 2988 -470 -871 -526 C
ATOM 1072 CD GLN A 287 153.346 39.856 5.058 1.00 37.26 C
ANISOU 1072 CD GLN A 287 4403 6027 3727 -597 -827 -574 C
ATOM 1073 OE1 GLN A 287 153.662 40.693 4.207 1.00 42.82 O
ANISOU 1073 OE1 GLN A 287 4897 6867 4504 -464 -882 -534 O
ATOM 1074 NE2 GLN A 287 152.360 38.981 4.866 1.00 37.40 N
ANISOU 1074 NE2 GLN A 287 4444 6156 3612 -869 -723 -654 N
ATOM 1075 C GLN A 287 157.320 38.126 5.255 1.00 37.62 C
ANISOU 1075 C GLN A 287 5015 5157 4120 -231 -924 -475 C
ATOM 1076 O GLN A 287 157.673 38.564 4.185 1.00 40.38 O
ANISOU 1076 O GLN A 287 5223 5580 4539 -169 -944 -506 O
ATOM 1077 N ALA A 288 158.180 37.615 6.127 1.00 33.83 N
ANISOU 1077 N ALA A 288 4713 4432 3710 -121 -954 -353 N
ATOM 1078 CA ALA A 288 159.603 37.491 5.767 1.00 33.35 C
ANISOU 1078 CA ALA A 288 4670 4160 3841 75 -1001 -251 C
ATOM 1079 CB ALA A 288 160.451 37.154 6.975 1.00 27.03 C
ANISOU 1079 CB ALA A 288 3994 3191 3084 210 -1086 -53 C
ATOM 1080 C ALA A 288 159.819 36.450 4.656 1.00 32.71 C
ANISOU 1080 C ALA A 288 4688 3902 3839 -13 -798 -319 C

ATOM 1081 O ALA A 288 160.631 36.638 3.742 1.00 27.78 O
ANISOU 1081 O ALA A 288 3995 3207 3353 100 -794 -317 O
ATOM 1082 N LYS A 289 159.081 35.345 4.716 1.00 32.97 N
ANISOU 1082 N LYS A 289 4890 3848 3787 -234 -597 -398 N
ATOM 1083 CA LYS A 289 159.212 34.371 3.642 1.00 40.64 C
ANISOU 1083 CA LYS A 289 5978 4645 4820 -374 -354 -522 C
ATOM 1084 CB LYS A 289 158.454 33.095 3.962 1.00 45.73 C
ANISOU 1084 CB LYS A 289 6839 5133 5404 -627 -97 -603 C
ATOM 1085 CG LYS A 289 158.947 32.367 5.166 1.00 53.34 C
ANISOU 1085 CG LYS A 289 7985 5805 6478 -491 -25 -372 C
ATOM 1086 CD LYS A 289 158.071 31.172 5.411 1.00 60.77 C
ANISOU 1086 CD LYS A 289 9125 6593 7372 -756 268 -468 C
ATOM 1087 CE LYS A 289 158.309 30.557 6.764 1.00 65.86 C
ANISOU 1087 CE LYS A 289 9923 7024 8076 -620 328 -200 C
ATOM 1088 NZ LYS A 289 157.026 29.967 7.298 1.00 70.20 N
ANISOU 1088 NZ LYS A 289 10577 7607 8489 -883 492 -303 N
ATOM 1089 C LYS A 289 158.682 34.962 2.330 1.00 40.56 C
ANISOU 1089 C LYS A 289 5787 4930 4695 -511 -375 -716 C
ATOM 1090 O LYS A 289 159.265 34.771 1.260 1.00 44.17 O
ANISOU 1090 O LYS A 289 6256 5306 5222 -507 -277 -786 O
ATOM 1091 N LEU A 290 157.558 35.664 2.439 1.00 38.93 N
ANISOU 1091 N LEU A 290 5407 5077 4307 -627 -486 -777 N
ATOM 1092 CA LEU A 290 156.888 36.273 1.290 1.00 39.99 C
ANISOU 1092 CA LEU A 290 5315 5581 4299 -756 -523 -898 C
ATOM 1093 CB LEU A 290 155.508 36.775 1.676 1.00 39.79 C
ANISOU 1093 CB LEU A 290 5115 5904 4098 -901 -590 -911 C
ATOM 1094 CG LEU A 290 154.759 37.524 0.588 1.00 42.28 C
ANISOU 1094 CG LEU A 290 5128 6671 4265 -997 -651 -948 C
ATOM 1095 CD1 LEU A 290 154.625 36.633 -0.667 1.00 39.70 C
ANISOU 1095 CD1 LEU A 290 4859 6431 3794 -1293 -515 -1150 C
ATOM 1096 CD2 LEU A 290 153.386 37.905 1.160 1.00 43.89 C
ANISOU 1096 CD2 LEU A 290 5161 7174 4343 -1123 -681 -911 C
ATOM 1097 C LEU A 290 157.712 37.413 0.702 1.00 37.64 C
ANISOU 1097 C LEU A 290 4824 5366 4113 -484 -668 -799 C
ATOM 1098 O LEU A 290 157.747 37.599 -0.502 1.00 35.35 O
ANISOU 1098 O LEU A 290 4423 5243 3765 -533 -641 -869 O
ATOM 1099 N PHE A 291 158.423 38.143 1.559 1.00 35.96 N
ANISOU 1099 N PHE A 291 4578 5032 4054 -211 -809 -640 N
ATOM 1100 CA PHE A 291 159.389 39.144 1.098 1.00 37.04 C
ANISOU 1100 CA PHE A 291 4557 5163 4353 54 -916 -547 C
ATOM 1101 CB PHE A 291 160.013 39.834 2.301 1.00 32.88 C
ANISOU 1101 CB PHE A 291 4018 4518 3958 266 -1066 -414 C
ATOM 1102 CG PHE A 291 161.158 40.752 1.971 1.00 28.86 C
ANISOU 1102 CG PHE A 291 3369 3939 3659 522 -1161 -326 C
ATOM 1103 CD1 PHE A 291 160.921 42.039 1.508 1.00 24.80 C
ANISOU 1103 CD1 PHE A 291 2606 3638 3180 622 -1203 -314 C
ATOM 1104 CE1 PHE A 291 161.969 42.936 1.260 1.00 23.28 C
ANISOU 1104 CE1 PHE A 291 2354 3315 3177 746 -1112 -198 C
ATOM 1105 CZ PHE A 291 163.272 42.524 1.414 1.00 22.73 C
ANISOU 1105 CZ PHE A 291 2382 3002 3252 836 -1122 -137 C
ATOM 1106 CE2 PHE A 291 163.533 41.205 1.875 1.00 34.84 C
ANISOU 1106 CE2 PHE A 291 4074 4349 4813 891 -1272 -145 C
ATOM 1107 CD2 PHE A 291 162.461 40.339 2.155 1.00 33.79 C
ANISOU 1107 CD2 PHE A 291 4091 4279 4468 671 -1187 -227 C
ATOM 1108 C PHE A 291 160.504 38.516 0.252 1.00 41.72 C
ANISOU 1108 C PHE A 291 5261 5503 5086 123 -813 -554 C
ATOM 1109 O PHE A 291 160.838 38.979 -0.834 1.00 41.53 O
ANISOU 1109 O PHE A 291 5111 5575 5093 191 -800 -570 O
ATOM 1110 N CYS A 292 161.076 37.435 0.758 1.00 40.86 N
ANISOU 1110 N CYS A 292 5389 5061 5074 117 -707 -519 N
ATOM 1111 CA CYS A 292 162.187 36.798 0.075 1.00 38.37 C
ANISOU 1111 CA CYS A 292 5190 4798 4592 -210 -492 -492 C
ATOM 1112 CB CYS A 292 162.805 35.730 0.999 1.00 35.67 C
ANISOU 1112 CB CYS A 292 5070 3732 4751 269 -452 -353 C
ATOM 1113 SG CYS A 292 163.858 34.524 0.122 1.00 82.68 S
ANISOU 1113 SG CYS A 292 11230 9247 10939 305 -112 -340 S
ATOM 1114 C CYS A 292 161.763 36.235 -1.325 1.00 42.76 C
ANISOU 1114 C CYS A 292 5804 5077 5365 -28 -346 -709 C
ATOM 1115 O CYS A 292 162.497 36.368 -2.328 1.00 38.32 O
ANISOU 1115 O CYS A 292 5216 4451 4892 62 -270 -723 O
ATOM 1116 N ARG A 293 160.577 35.625 -1.385 1.00 39.54 N
ANISOU 1116 N ARG A 293 5469 4827 4727 -353 -246 -887 N
ATOM 1117 CA ARG A 293 160.037 35.102 -2.651 1.00 41.86 C
ANISOU 1117 CA ARG A 293 5805 5275 4823 -660 -65 -1132 C
ATOM 1118 CB ARG A 293 158.742 34.334 -2.412 1.00 46.88 C
ANISOU 1118 CB ARG A 293 6526 6051 5237 -1041 36 -1316 C
ATOM 1119 CG ARG A 293 158.936 32.883 -2.086 1.00 57.16 C
ANISOU 1119 CG ARG A 293 8157 6916 6647 -1199 350 -1410 C
ATOM 1120 CD ARG A 293 157.589 32.204 -1.812 1.00 69.42 C
ANISOU 1120 CD ARG A 293 9767 8621 7990 -1591 449 -1599 C
ATOM 1121 NE ARG A 293 157.159 32.366 -0.415 1.00 74.96 N
ANISOU 1121 NE ARG A 293 10447 9300 8734 -1478 320 -1424 N
ATOM 1122 CZ ARG A 293 155.900 32.564 -0.023 1.00 76.60 C
ANISOU 1122 CZ ARG A 293 10531 9825 8749 -1679 228 -1479 C
ATOM 1123 NH1 ARG A 293 155.613 32.696 1.277 1.00 73.04 N
ANISOU 1123 NH1 ARG A 293 10094 9312 8345 -1557 142 -1315 N
ATOM 1124 NH2 ARG A 293 154.930 32.629 -0.932 1.00 81.62 N
ANISOU 1124 NH2 ARG A 293 11018 10862 9133 -2009 224 -1684 N
ATOM 1125 C ARG A 293 159.755 36.221 -3.653 1.00 42.39 C
ANISOU 1125 C ARG A 293 5589 5780 4736 -632 -220 -1140 C

ATOM 1126 O ARG A 293 159.984 36.088 -4.872 1.00 43.46 O
ANISOU 1126 O ARG A 293 5733 5998 4781 -728 -105 -1259 O
ATOM 1127 N THR A 294 159.227 37.325 -3.135 1.00 41.28 N
ANISOU 1127 N THR A 294 5199 5925 4561 -503 -451 -1003 N
ATOM 1128 CA THR A 294 158.891 38.445 -3.990 1.00 42.47 C
ANISOU 1128 CA THR A 294 5046 6493 4597 -438 -572 -944 C
ATOM 1129 CB THR A 294 158.109 39.480 -3.247 1.00 42.63 C
ANISOU 1129 CB THR A 294 4824 6772 4600 -338 -743 -801 C
ATOM 1130 OG1 THR A 294 156.937 38.857 -2.729 1.00 48.86 O
ANISOU 1130 OG1 THR A 294 5661 7698 5206 -626 -714 -900 O
ATOM 1131 CG2 THR A 294 157.673 40.560 -4.187 1.00 42.71 C
ANISOU 1131 CG2 THR A 294 4502 7222 4505 -270 -815 -697 C
ATOM 1132 C THR A 294 160.166 39.058 -4.560 1.00 38.76 C
ANISOU 1132 C THR A 294 4527 5860 4342 -129 -582 -830 C
ATOM 1133 O THR A 294 160.291 39.314 -5.757 1.00 38.60 O
ANISOU 1133 O THR A 294 4408 6036 4223 -144 -537 -857 O
ATOM 1134 N LEU A 295 161.136 39.248 -3.695 1.00 32.38 N
ANISOU 1134 N LEU A 295 3785 4702 3817 136 -636 -698 N
ATOM 1135 CA LEU A 295 162.383 39.869 -4.115 1.00 36.47 C
ANISOU 1135 CA LEU A 295 4231 5047 4580 434 -653 -575 C
ATOM 1136 CB LEU A 295 163.274 40.117 -2.914 1.00 29.51 C
ANISOU 1136 CB LEU A 295 3380 3860 3972 673 -764 -424 C
ATOM 1137 CG LEU A 295 164.565 40.869 -3.137 1.00 33.60 C
ANISOU 1137 CG LEU A 295 3782 4208 4778 979 -813 -281 C
ATOM 1138 CD1 LEU A 295 164.236 42.207 -3.772 1.00 32.42 C
ANISOU 1138 CD1 LEU A 295 3369 4356 4592 1057 -852 -226 C
ATOM 1139 CD2 LEU A 295 165.267 41.056 -1.771 1.00 32.89 C
ANISOU 1139 CD2 LEU A 295 3720 3916 4863 1096 -930 -143 C
ATOM 1140 C LEU A 295 163.120 38.994 -5.134 1.00 44.47 C
ANISOU 1140 C LEU A 295 5428 5844 5625 379 -435 -671 C
ATOM 1141 O LEU A 295 163.733 39.514 -6.072 1.00 41.63 O
ANISOU 1141 O LEU A 295 4967 5518 5331 524 -400 -626 O
ATOM 1142 N GLU A 296 163.063 37.667 -4.927 1.00 42.51 N
ANISOU 1142 N GLU A 296 5458 5346 5348 174 -249 -798 N
ATOM 1143 CA GLU A 296 163.575 36.697 -5.901 1.00 47.34 C
ANISOU 1143 CA GLU A 296 6289 5732 5967 49 41 -943 C
ATOM 1144 CB GLU A 296 163.294 35.255 -5.462 1.00 56.37 C
ANISOU 1144 CB GLU A 296 7736 6586 7096 -203 283 -1085 C
ATOM 1145 CG GLU A 296 164.530 34.494 -5.052 1.00 73.53 C
ANISOU 1145 CG GLU A 296 10109 8203 9628 4 484 -944 C
ATOM 1146 CD GLU A 296 164.996 33.465 -6.098 1.00 92.45 C
ANISOU 1146 CD GLU A 296 12761 10298 12067 -149 897 -1123 C
ATOM 1147 OE1 GLU A 296 164.130 32.766 -6.685 1.00 99.22 O
ANISOU 1147 OE1 GLU A 296 13769 11273 12658 -546 1094 -1423 O
ATOM 1148 OE2 GLU A 296 166.229 33.353 -6.326 1.00 97.34 O
ANISOU 1148 OE2 GLU A 296 13429 10562 12994 111 1043 -972 O
ATOM 1149 C GLU A 296 162.976 36.919 -7.297 1.00 46.31 C
ANISOU 1149 C GLU A 296 6070 6000 5523 -168 96 -1116 C
ATOM 1150 O GLU A 296 163.712 36.994 -8.284 1.00 48.13 O
ANISOU 1150 O GLU A 296 6325 6162 5801 -86 225 -1130 O
ATOM 1151 N ASP A 297 161.640 36.990 -7.369 1.00 47.82 N
ANISOU 1151 N ASP A 297 6154 6628 5386 -454 3 -1231 N
ATOM 1152 CA ASP A 297 160.923 37.217 -8.638 1.00 50.39 C
ANISOU 1152 CA ASP A 297 6344 7454 5350 -698 9 -1363 C
ATOM 1153 CB ASP A 297 159.400 37.170 -8.459 1.00 50.69 C
ANISOU 1153 CB ASP A 297 6241 7960 5060 -1026 -107 -1453 C
ATOM 1154 CG ASP A 297 158.896 35.804 -8.014 1.00 73.14 C
ANISOU 1154 CG ASP A 297 9369 10592 7828 -1394 81 -1705 C
ATOM 1155 OD1 ASP A 297 159.731 34.867 -7.957 1.00 84.86 O
ANISOU 1155 OD1 ASP A 297 11169 11568 9506 -1397 338 -1809 O
ATOM 1156 OD2 ASP A 297 157.669 35.675 -7.726 1.00 76.13 O
ANISOU 1156 OD2 ASP A 297 9644 11300 7981 -1670 0 -1779 O
ATOM 1157 C ASP A 297 161.314 38.537 -9.304 1.00 48.34 C
ANISOU 1157 C ASP A 297 5792 7451 5123 -397 -134 -1150 C
ATOM 1158 O ASP A 297 161.571 38.602 -10.511 1.00 52.73 O
ANISOU 1158 O ASP A 297 6333 8175 5528 -447 -36 -1207 O
ATOM 1159 N ILE A 298 161.387 39.589 -8.505 1.00 39.96 N
ANISOU 1159 N ILE A 298 4514 6401 4268 -87 -336 -910 N
ATOM 1160 CA ILE A 298 161.789 40.874 -9.045 1.00 40.43 C
ANISOU 1160 CA ILE A 298 4297 6639 4424 220 -427 -694 C
ATOM 1161 CB ILE A 298 161.742 41.994 -7.997 1.00 39.09 C
ANISOU 1161 CB ILE A 298 3913 6447 4493 504 -606 -476 C
ATOM 1162 CG1 ILE A 298 160.319 42.281 -7.556 1.00 34.56 C
ANISOU 1162 CG1 ILE A 298 3161 6268 3701 338 -716 -453 C
ATOM 1163 CD1 ILE A 298 160.329 43.195 -6.333 1.00 33.00 C
ANISOU 1163 CD1 ILE A 298 2913 5849 3776 549 -784 -284 C
ATOM 1164 CG2 ILE A 298 162.329 43.278 -8.543 1.00 39.22 C
ANISOU 1164 CG2 ILE A 298 3675 6540 4688 837 -632 -261 C
ATOM 1165 C ILE A 298 163.187 40.777 -9.625 1.00 43.20 C
ANISOU 1165 C ILE A 298 4776 6627 5011 430 -282 -672 C
ATOM 1166 O ILE A 298 163.429 41.230 -10.741 1.00 49.83 O
ANISOU 1166 O ILE A 298 5504 7665 5762 497 -225 -625 O
ATOM 1167 N LEU A 299 164.095 40.162 -8.875 1.00 40.86 N
ANISOU 1167 N LEU A 299 4700 5815 5011 537 -212 -679 N
ATOM 1168 CA LEU A 299 165.474 40.075 -9.302 1.00 43.31 C
ANISOU 1168 CA LEU A 299 5104 5745 5607 766 -68 -614 C
ATOM 1169 CB LEU A 299 166.409 39.644 -8.171 1.00 40.43 C
ANISOU 1169 CB LEU A 299 4873 4880 5608 946 -69 -513 C
ATOM 1170 CG LEU A 299 166.555 40.632 -7.013 1.00 44.72 C
ANISOU 1170 CG LEU A 299 5211 5427 6354 1178 -331 -324 C
ATOM 1171 CD1 LEU A 299 167.690 40.208 -6.110 1.00 45.51 C
ANISOU 1171 CD1 LEU A 299 5412 5086 6794 1360 -334 -192 C
ATOM 1172 CD2 LEU A 299 166.741 42.051 -7.471 1.00 38.90 C
ANISOU 1172 CD2 LEU A 299 4201 4897 5683 1358 -412 -170 C
ATOM 1173 C LEU A 299 165.630 39.150 -10.498 1.00 47.60 C
ANISOU 1173 C LEU A 299 5870 6246 5968 544 214 -817 C
ATOM 1174 O LEU A 299 166.419 39.435 -11.383 1.00 49.81 O
ANISOU 1174 O LEU A 299 6133 6457 6337 699 333 -767 O
ATOM 1175 N ALA A 300 164.895 38.043 -10.519 1.00 47.91 N
ANISOU 1175 N ALA A 300 6130 6312 5762 166 348 -1062 N
ATOM 1176 CA ALA A 300 165.064 37.060 -11.585 1.00 52.71 C
ANISOU 1176 CA ALA A 300 7001 6825 6201 -101 673 -1314 C
ATOM 1177 CB ALA A 300 164.106 35.902 -11.410 1.00 55.88 C
ANISOU 1177 CB ALA A 300 7623 7263 6344 -556 809 -1603 C
ATOM 1178 C ALA A 300 164.880 37.687 -12.962 1.00 59.63 C
ANISOU 1178 C ALA A 300 7729 8154 6772 -161 674 -1347 C
ATOM 1179 O ALA A 300 165.459 37.225 -13.942 1.00 69.93 O
ANISOU 1179 O ALA A 300 9218 9327 8026 -238 945 -1481 O
ATOM 1180 N ASP A 301 164.082 38.749 -13.032 1.00 78.43 N
ANISOU 1180 N ASP A 301 9138 13383 7279 506 -2196 -37 N
ATOM 1181 CA ASP A 301 163.776 39.365 -14.309 1.00 76.60 C
ANISOU 1181 CA ASP A 301 8775 13780 6549 654 -2224 189 C
ATOM 1182 CB ASP A 301 162.311 39.135 -14.652 1.00 88.45 C
ANISOU 1182 CB ASP A 301 10032 15637 7939 495 -2594 323 C
ATOM 1183 CG ASP A 301 162.090 38.887 -16.139 1.00 99.91 C
ANISOU 1183 CG ASP A 301 11442 17750 8770 522 -2856 168 C
ATOM 1184 OD1 ASP A 301 162.875 38.115 -16.750 1.00103.81 O
ANISOU 1184 OD1 ASP A 301 12173 18269 9002 520 -2927 -352 O
ATOM 1185 OD2 ASP A 301 161.137 39.482 -16.693 1.00103.61 O
ANISOU 1185 OD2 ASP A 301 11693 18551 9124 557 -2898 557 O
ATOM 1186 C ASP A 301 164.069 40.859 -14.355 1.00 71.91 C
ANISOU 1186 C ASP A 301 8109 13279 5936 902 -1831 755 C
ATOM 1187 O ASP A 301 163.419 41.594 -15.088 1.00 78.03 O
ANISOU 1187 O ASP A 301 8712 14502 6435 1028 -1848 1154 O
ATOM 1188 N ALA A 302 165.038 41.321 -13.577 1.00 66.10 N
ANISOU 1188 N ALA A 302 7508 12114 5493 964 -1491 806 N
ATOM 1189 CA ALA A 302 165.325 42.759 -13.536 1.00 66.66 C
ANISOU 1189 CA ALA A 302 7557 12167 5605 1146 -1124 1338 C
ATOM 1190 CB ALA A 302 165.374 43.291 -12.090 1.00 55.52 C
ANISOU 1190 CB ALA A 302 6205 10156 4734 1113 -901 1512 C
ATOM 1191 C ALA A 302 166.625 43.070 -14.231 1.00 70.80 C
ANISOU 1191 C ALA A 302 8188 12861 5850 1248 -879 1291 C
ATOM 1192 O ALA A 302 167.625 42.392 -13.972 1.00 74.53 O
ANISOU 1192 O ALA A 302 8783 13150 6385 1193 -834 878 O
ATOM 1193 N PRO A 303 166.634 44.132 -15.069 1.00 71.39 N
ANISOU 1193 N PRO A 303 8201 13288 5636 1407 -700 1761 N
ATOM 1194 CA PRO A 303 167.805 44.523 -15.875 1.00 69.71 C
ANISOU 1194 CA PRO A 303 8039 13353 5093 1491 -448 1817 C
ATOM 1195 CB PRO A 303 167.345 45.822 -16.560 1.00 71.25 C
ANISOU 1195 CB PRO A 303 8156 13829 5086 1648 -295 2496 C
ATOM 1196 CG PRO A 303 165.861 45.739 -16.581 1.00 71.68 C
ANISOU 1196 CG PRO A 303 8070 14021 5145 1697 -587 2651 C
ATOM 1197 CD PRO A 303 165.493 45.044 -15.291 1.00 70.35 C
ANISOU 1197 CD PRO A 303 7928 13327 5475 1535 -721 2318 C
ATOM 1198 C PRO A 303 169.083 44.777 -15.055 1.00 67.25 C
ANISOU 1198 C PRO A 303 7842 12600 5111 1410 -138 1739 C
ATOM 1199 O PRO A 303 170.195 44.509 -15.517 1.00 65.10 O
ANISOU 1199 O PRO A 303 7583 12539 4613 1427 -6 1529 O
ATOM 1200 N GLU A 304 168.935 45.280 -13.836 1.00 70.91 N
ANISOU 1200 N GLU A 304 8368 12494 6082 1329 -25 1896 N
ATOM 1201 CA GLU A 304 170.113 45.624 -13.039 1.00 74.00 C
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ATOM 1202 CB GLU A 304 169.828 46.825 -12.130 1.00 75.99 C
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ATOM 1203 CG GLU A 304 169.240 48.018 -12.858 1.00 79.46 C
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ATOM 1204 CD GLU A 304 167.710 48.036 -12.830 1.00 83.04 C
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ANISOU 1205 OE1 GLU A 304 10717 14081 8879 1651 482 3577 O
ATOM 1206 OE2 GLU A 304 167.099 46.993 -12.501 1.00 79.39 O
ANISOU 1206 OE2 GLU A 304 9454 12942 7769 1440 90 2694 O
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ATOM 1208 O GLU A 304 171.841 44.433 -11.856 1.00 67.78 O
ANISOU 1208 O GLU A 304 8133 11318 6305 1054 294 1152 O
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ANISOU 1209 N SER A 305 8097 11353 6257 1096 -185 995 N
ATOM 1210 CA SER A 305 170.188 42.474 -10.938 1.00 71.97 C
ANISOU 1210 CA SER A 305 8719 11517 7108 996 -299 569 C
ATOM 1211 CB SER A 305 169.003 42.234 -10.016 1.00 79.79 C
ANISOU 1211 CB SER A 305 9711 12186 8418 903 -485 612 C
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ANISOU 1212 OG SER A 305 10539 13421 9109 912 -765 599 O
ATOM 1213 C SER A 305 170.575 41.152 -11.553 1.00 71.29 C
ANISOU 1213 C SER A 305 8667 11648 6772 1045 -510 49 C
ATOM 1214 O SER A 305 170.432 40.095 -10.917 1.00 67.98 O
ANISOU 1214 O SER A 305 8330 10936 6565 974 -724 -309 O
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ANISOU 1215 N GLN A 306 8395 11927 6081 1178 -452 13 N

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ATOM 1219 CD GLN A 306 168.741 38.993 -15.019 1.00 91.37 C
ANISOU 1219 CD GLN A 306 11211 15496 8010 1169 -1387 -705 C
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ANISOU 1220 OE1 GLN A 306 11053 15185 8277 1104 -1243 -254 O
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ATOM 1231 O ASN A 307 176.548 38.716 -11.142 1.00 71.83 O
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ANISOU 1236 OD1 ASN A 308 6362 9039 4861 989 140 139 O
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ANISOU 1237 ND2 ASN A 308 8515 11883 6821 995 596 596 N
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ANISOU 1239 O ASN A 308 5892 7634 5193 775 213 -241 O
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ANISOU 1240 N CYS A 309 5184 6749 4238 923 -240 -695 N
ATOM 1241 CA CYS A 309 173.419 39.797 -6.488 1.00 44.26 C
ANISOU 1241 CA CYS A 309 5475 6528 4815 771 -329 -583 C
ATOM 1242 CB CYS A 309 172.133 40.566 -6.713 1.00 48.09 C
ANISOU 1242 CB CYS A 309 5948 7047 5277 706 -337 -246 C
ATOM 1243 SG CYS A 309 171.250 40.861 -5.210 1.00 94.69 S
ANISOU 1243 SG CYS A 309 11906 12496 11578 564 -358 -51 S
ATOM 1244 C CYS A 309 173.094 38.377 -6.118 1.00 46.10 C
ANISOU 1244 C CYS A 309 5816 6531 5171 787 -620 -933 C
ATOM 1245 O CYS A 309 172.869 37.543 -6.983 1.00 47.55 O
ANISOU 1245 O CYS A 309 6050 6873 5145 876 -803 -1201 O
ATOM 1246 N ARG A 310 173.060 38.088 -4.825 1.00 37.20 N
ANISOU 1246 N ARG A 310 4746 5016 4373 690 -672 -934 N
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ATOM 1249 CG ARG A 310 173.741 34.397 -4.368 1.00 68.20 C
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ATOM 1256 O ARG A 310 172.563 37.443 -2.165 1.00 42.68 O
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ATOM 1257 N LEU A 311 170.944 36.124 -2.980 1.00 49.64 N
ANISOU 1257 N LEU A 311 6524 5835 6503 381 -1219 -1020 N
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ANISOU 1258 CA LEU A 311 5868 4925 6116 212 -1251 -795 C
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ANISOU 1259 CB LEU A 311 4954 4208 5270 65 -1393 -623 C
ATOM 1260 CG LEU A 311 168.190 37.285 -2.987 1.00 43.55 C
ANISOU 1260 CG LEU A 311 5524 5275 5749 139 -1251 -402 C
ATOM 1261 CD1 LEU A 311 166.665 37.238 -3.148 1.00 43.00 C
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ANISOU 1262 CD2 LEU A 311 4612 4360 4909 225 -924 -149 C
ATOM 1263 C LEU A 311 170.442 34.929 -0.897 1.00 43.86 C
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ATOM 1264 O LEU A 311 170.256 33.767 -1.315 1.00 37.66 O
ANISOU 1264 O LEU A 311 5252 3566 5489 145 -1682 -1213 O
ATOM 1265 N ILE A 312 170.839 35.201 0.336 1.00 37.83 N
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ANISOU 1266 CA ILE A 312 5937 3877 6528 126 -1465 -916 C
ATOM 1267 CB ILE A 312 172.530 34.254 1.828 1.00 48.67 C
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ATOM 1268 CG1 ILE A 312 173.509 34.573 0.700 1.00 52.31 C
ANISOU 1268 CG1 ILE A 312 7056 5312 7506 482 -1236 -1203 C
ATOM 1269 CD1 ILE A 312 174.946 34.652 1.145 1.00 54.27 C
ANISOU 1269 CD1 ILE A 312 7241 5620 7759 636 -1130 -1283 C
ATOM 1270 CG2 ILE A 312 172.941 33.002 2.567 1.00 45.06 C
ANISOU 1270 CG2 ILE A 312 6335 3799 6986 339 -1534 -1105 C
ATOM 1271 C ILE A 312 170.066 34.093 2.394 1.00 34.28 C
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ANISOU 1272 O ILE A 312 5142 2987 6018 -92 -1322 -441 O
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ATOM 1274 CA ALA A 313 167.946 33.153 3.187 1.00 40.07 C
ANISOU 1274 CA ALA A 313 5495 3158 6571 -476 -1748 -305 C
ATOM 1275 CB ALA A 313 166.599 32.963 2.504 1.00 36.67 C
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ANISOU 1277 O ALA A 313 6712 3617 7676 -475 -2048 -556 O
ATOM 1278 N TYR A 314 167.988 32.060 5.328 1.00 45.45 N
ANISOU 1278 N TYR A 314 6282 3360 7630 -610 -1796 -51 N
ATOM 1279 CA TYR A 314 168.285 30.983 6.261 1.00 47.66 C
ANISOU 1279 CA TYR A 314 6647 3625 7835 -612 -1836 13 C
ATOM 1280 CB TYR A 314 169.755 30.980 6.672 1.00 40.06 C
ANISOU 1280 CB TYR A 314 5761 2650 6809 -368 -1746 -126 C
ATOM 1281 CG TYR A 314 170.206 32.304 7.203 1.00 36.63 C
ANISOU 1281 CG TYR A 314 5247 2377 6292 -290 -1530 -61 C
ATOM 1282 CD1 TYR A 314 170.550 33.345 6.335 1.00 32.71 C
ANISOU 1282 CD1 TYR A 314 4711 1987 5729 -201 -1435 -202 C
ATOM 1283 CE1 TYR A 314 170.970 34.590 6.849 1.00 34.97 C
ANISOU 1283 CE1 TYR A 314 4954 2379 5953 -155 -1229 -140 C
ATOM 1284 CZ TYR A 314 171.022 34.767 8.242 1.00 36.24 C
ANISOU 1284 CZ TYR A 314 5122 2551 6098 -194 -1139 28 C
ATOM 1285 OH TYR A 314 171.443 35.969 8.763 1.00 43.14 O
ANISOU 1285 OH TYR A 314 5986 3525 6882 -168 -943 45 O
ATOM 1286 CE2 TYR A 314 170.695 33.737 9.100 1.00 28.94 C
ANISOU 1286 CE2 TYR A 314 4227 1547 5222 -263 -1245 165 C
ATOM 1287 CD2 TYR A 314 170.300 32.523 8.589 1.00 35.45 C
ANISOU 1287 CD2 TYR A 314 5084 2255 6128 -314 -1429 136 C
ATOM 1288 C TYR A 314 167.415 31.118 7.484 1.00 46.93 C
ANISOU 1288 C TYR A 314 6455 3581 7795 -780 -1758 363 C
ATOM 1289 O TYR A 314 167.003 32.212 7.843 1.00 50.49 O
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ATOM 1299 N GLU A 316 167.457 30.132 11.509 1.00 80.87 N
ANISOU 1299 N GLU A 316 10823 6621 13281 -1734 948 991 N
ATOM 1300 CA GLU A 316 168.211 29.620 12.635 1.00 88.80 C
ANISOU 1300 CA GLU A 316 12265 7785 13689 -1626 1087 1399 C
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ATOM 1302 CG GLU A 316 169.971 31.293 13.482 1.00 92.92 C
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ATOM 1303 CD GLU A 316 170.120 32.722 13.990 1.00 94.83 C
ANISOU 1303 CD GLU A 316 12575 10300 13158 -1201 1393 655 C
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ANISOU 1304 OE1 GLU A 316 12906 11124 12812 -1159 1597 701 O
ATOM 1305 OE2 GLU A 316 169.708 33.650 13.253 1.00 93.08 O
ANISOU 1305 OE2 GLU A 316 12032 9995 13340 -1260 1428 283 O

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ANISOU 1307 O GLU A 316 14121 9455 16037 -2452 1838 1847 O
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ANISOU 1308 N PRO A 317 15956 9825 16699 -1874 1288 2226 N
ATOM 1309 CA PRO A 317 167.211 26.354 14.219 1.00125.33 C
ANISOU 1309 CA PRO A 317 17979 11174 18466 -2222 1743 2748 C
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ATOM 1312 CD PRO A 317 168.969 26.714 12.569 1.00109.55 C
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ATOM 1323 CG ASP A 319 167.491 22.611 17.219 1.00175.99 C
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ATOM 1324 OD1 ASP A 319 168.713 22.851 17.129 1.00174.11 O
ANISOU 1324 OD1 ASP A 319 26418 16579 23159 -1362 2666 5038 O
ATOM 1325 OD2 ASP A 319 166.853 22.120 16.267 1.00176.59 O
ANISOU 1325 OD2 ASP A 319 26437 15833 24826 -2471 2804 4754 O
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ATOM 1327 O ASP A 319 168.931 23.928 20.726 1.00174.27 O
ANISOU 1327 O ASP A 319 26214 18751 21249 -883 3772 5871 O
ATOM 1328 N ASP A 320 169.492 24.551 18.635 1.00159.54 N
ANISOU 1328 N ASP A 320 24000 16563 20054 -895 2802 4880 N
ATOM 1329 CA ASP A 320 170.930 24.506 18.886 1.00153.95 C
ANISOU 1329 CA ASP A 320 23562 16464 18468 -98 2506 4968 C
ATOM 1330 CB ASP A 320 171.624 23.423 18.025 1.00152.48 C
ANISOU 1330 CB ASP A 320 23981 15572 18384 326 2132 5172 C
ATOM 1331 CG ASP A 320 171.911 23.883 16.582 1.00143.02 C
ANISOU 1331 CG ASP A 320 22484 14190 17669 285 1511 4509 C
ATOM 1332 OD2 ASP A 320 171.357 23.301 15.624 1.00142.07 O
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ATOM 1333 OD1 ASP A 320 172.719 24.809 16.391 1.00136.60 O
ANISOU 1333 OD1 ASP A 320 21301 14145 16457 565 1174 4062 O
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ATOM 1347 O SER A 322 176.824 25.979 14.440 1.00105.30 O
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ATOM 1348 N PHE A 323 174.606 26.410 14.615 1.00 98.66 N
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ATOM 1349 CA PHE A 323 174.464 27.016 13.283 1.00 85.21 C
ANISOU 1349 CA PHE A 323 13767 8303 10304 949 -239 2382 C
ATOM 1350 CB PHE A 323 173.048 27.578 13.075 1.00 79.09 C
ANISOU 1350 CB PHE A 323 12605 7142 10303 278 44 2161 C
ATOM 1351 CG PHE A 323 172.947 28.556 11.936 1.00 70.29 C
ANISOU 1351 CG PHE A 323 11023 6043 9641 184 -205 1599 C
ATOM 1352 CD1 PHE A 323 172.712 28.110 10.641 1.00 67.70 C
ANISOU 1352 CD1 PHE A 323 10726 5123 9873 246 -568 1471 C
ATOM 1353 CE1 PHE A 323 172.631 29.006 9.570 1.00 59.38 C
ANISOU 1353 CE1 PHE A 323 9249 4136 9175 265 -772 1009 C
ATOM 1354 CZ PHE A 323 172.771 30.375 9.798 1.00 62.30 C
ANISOU 1354 CZ PHE A 323 9216 5056 9400 178 -560 686 C
ATOM 1355 CE2 PHE A 323 173.011 30.842 11.096 1.00 65.39 C
ANISOU 1355 CE2 PHE A 323 9582 5985 9278 45 -196 744 C
ATOM 1356 CD2 PHE A 323 173.095 29.925 12.158 1.00 68.69 C
ANISOU 1356 CD2 PHE A 323 10368 6443 9288 68 -44 1193 C
ATOM 1357 C PHE A 323 175.533 28.080 12.976 1.00 75.85 C
ANISOU 1357 C PHE A 323 12197 7910 8711 1201 -509 1891 C
ATOM 1358 O PHE A 323 175.892 28.894 13.833 1.00 73.30 O
ANISOU 1358 O PHE A 323 11597 8366 7887 1150 -290 1703 O
ATOM 1359 N SER A 324 176.028 28.060 11.741 1.00 70.66 N
ANISOU 1359 N SER A 324 11514 7051 8282 1449 -962 1660 N
ATOM 1360 CA SER A 324 177.138 28.903 11.332 1.00 63.86 C
ANISOU 1360 CA SER A 324 10344 6870 7051 1710 -1221 1250 C
ATOM 1361 CB SER A 324 178.307 28.020 10.908 1.00 67.94 C
ANISOU 1361 CB SER A 324 11211 7520 7081 2386 -1677 1442 C
ATOM 1362 OG SER A 324 179.476 28.775 10.702 1.00 72.60 O
ANISOU 1362 OG SER A 324 11475 8924 7184 2630 -1883 1072 O
ATOM 1363 C SER A 324 176.702 29.772 10.168 1.00 60.64 C
ANISOU 1363 C SER A 324 9548 6175 7317 1472 -1319 819 C
ATOM 1364 O SER A 324 176.383 29.270 9.103 1.00 54.58 O
ANISOU 1364 O SER A 324 8884 4817 7038 1580 -1605 840 O
ATOM 1365 N LEU A 325 176.675 31.081 10.386 1.00 47.50 N
ANISOU 1365 N LEU A 325 3856 5727 8465 -131 1773 752 N
ATOM 1366 CA LEU A 325 176.357 32.031 9.330 1.00 49.10 C
ANISOU 1366 CA LEU A 325 3824 6036 8795 -152 1371 587 C
ATOM 1367 CB LEU A 325 176.217 33.446 9.899 1.00 50.45 C
ANISOU 1367 CB LEU A 325 3969 6512 8688 154 1205 504 C
ATOM 1368 CG LEU A 325 175.763 34.480 8.860 1.00 54.85 C
ANISOU 1368 CG LEU A 325 4345 7186 9311 146 785 376 C
ATOM 1369 CD1 LEU A 325 174.428 34.067 8.216 1.00 54.33 C
ANISOU 1369 CD1 LEU A 325 3916 7128 9599 -180 656 342 C
ATOM 1370 CD2 LEU A 325 175.639 35.875 9.469 1.00 57.04 C
ANISOU 1370 CD2 LEU A 325 4649 7699 9323 412 650 272 C
ATOM 1371 C LEU A 325 177.473 32.018 8.315 1.00 49.16 C
ANISOU 1371 C LEU A 325 4096 5920 8661 -76 1201 539 C
ATOM 1372 O LEU A 325 177.245 32.088 7.104 1.00 49.87 O
ANISOU 1372 O LEU A 325 4180 5993 8776 -195 793 400 O
ATOM 1373 N SER A 326 178.687 31.945 8.849 1.00 49.02 N
ANISOU 1373 N SER A 326 4459 5872 8294 188 1432 643 N
ATOM 1374 CA SER A 326 179.910 31.837 8.080 1.00 47.68 C
ANISOU 1374 CA SER A 326 4747 5620 7748 339 1270 655 C
ATOM 1375 CB SER A 326 181.041 31.517 9.038 1.00 52.27 C
ANISOU 1375 CB SER A 326 5679 6160 8021 574 1650 806 C
ATOM 1376 OG SER A 326 182.081 32.433 8.862 1.00 60.63 O
ANISOU 1376 OG SER A 326 6958 7328 8750 794 1356 843 O
ATOM 1377 C SER A 326 179.842 30.714 7.057 1.00 48.45 C
ANISOU 1377 C SER A 326 5127 5489 7794 100 1092 534 C
ATOM 1378 O SER A 326 180.204 30.879 5.895 1.00 52.63 O
ANISOU 1378 O SER A 326 5806 6079 8112 194 739 460 O
ATOM 1379 N GLN A 327 179.424 29.544 7.524 1.00 49.29 N
ANISOU 1379 N GLN A 327 5301 5332 8094 -163 1336 530 N
ATOM 1380 CA GLN A 327 179.339 28.352 6.683 1.00 50.98 C
ANISOU 1380 CA GLN A 327 5798 5224 8349 -393 1137 352 C
ATOM 1381 CB GLN A 327 179.073 27.129 7.544 1.00 49.95 C
ANISOU 1381 CB GLN A 327 5721 4746 8513 -646 1512 471 C
ATOM 1382 CG GLN A 327 180.305 26.696 8.310 1.00 47.82 C
ANISOU 1382 CG GLN A 327 5890 4418 7863 -391 1940 683 C
ATOM 1383 CD GLN A 327 181.397 26.178 7.395 1.00 50.32 C
ANISOU 1383 CD GLN A 327 6788 4593 7737 -211 1740 546 C
ATOM 1384 OE1 GLN A 327 181.153 25.323 6.529 1.00 59.71 O
ANISOU 1384 OE1 GLN A 327 8164 5483 9038 -381 1435 297 O
ATOM 1385 NE2 GLN A 327 182.602 26.725 7.547 1.00 44.62 N
ANISOU 1385 NE2 GLN A 327 6334 4104 6517 168 1868 693 N
ATOM 1386 C GLN A 327 178.247 28.488 5.651 1.00 51.53 C
ANISOU 1386 C GLN A 327 5553 5313 8713 -627 652 96 C
ATOM 1387 O GLN A 327 178.397 28.076 4.500 1.00 54.83 O
ANISOU 1387 O GLN A 327 6211 5654 8968 -611 259 -152 O
ATOM 1388 N GLU A 328 177.145 29.078 6.081 1.00 55.32 N
ANISOU 1388 N GLU A 328 5484 5941 9594 -794 675 147 N
ATOM 1389 CA GLU A 328 176.029 29.364 5.194 1.00 60.12 C
ANISOU 1389 CA GLU A 328 5706 6634 10502 -1004 227 -65 C
ATOM 1390 CB GLU A 328 174.877 30.025 5.956 1.00 65.13 C
ANISOU 1390 CB GLU A 328 5718 7465 11563 -1141 381 80 C
ATOM 1391 CG GLU A 328 173.598 30.128 5.148 1.00 77.21 C
ANISOU 1391 CG GLU A 328 6803 9046 13487 -1426 -46 -110 C
ATOM 1392 CD GLU A 328 172.939 28.778 4.916 1.00 92.31 C
ANISOU 1392 CD GLU A 328 8683 10537 15856 -1872 -186 -240 C
ATOM 1393 OE1 GLU A 328 172.781 28.381 3.737 1.00 96.59 O
ANISOU 1393 OE1 GLU A 328 9345 10956 16399 -1973 -703 -588 O
ATOM 1394 OE2 GLU A 328 172.578 28.118 5.921 1.00100.14 O
ANISOU 1394 OE2 GLU A 328 9568 11350 17131 -2050 200 18 O
ATOM 1395 C GLU A 328 176.491 30.265 4.051 1.00 52.40 C
ANISOU 1395 C GLU A 328 4813 5959 9137 -701 -176 -176 C

ATOM 1396 O GLU A 328 176.229 30.006 2.885 1.00 62.88 O
ANISOU 1396 O GLU A 328 6186 7300 10406 -736 -619 -431 O
ATOM 1397 N VAL A 329 177.205 31.318 4.376 1.00 43.86 N
ANISOU 1397 N VAL A 329 3734 5127 7803 -369 -40 32 N
ATOM 1398 CA VAL A 329 177.678 32.222 3.329 1.00 44.46 C
ANISOU 1398 CA VAL A 329 3817 5492 7583 -66 -385 60 C
ATOM 1399 CB VAL A 329 178.251 33.510 3.940 1.00 41.13 C
ANISOU 1399 CB VAL A 329 3243 5257 7129 225 -239 327 C
ATOM 1400 CG1 VAL A 329 178.903 34.399 2.878 1.00 40.20 C
ANISOU 1400 CG1 VAL A 329 3114 5396 6763 549 -556 495 C
ATOM 1401 CG2 VAL A 329 177.118 34.256 4.615 1.00 38.47 C
ANISOU 1401 CG2 VAL A 329 2370 5015 7233 104 -195 307 C
ATOM 1402 C VAL A 329 178.664 31.523 2.396 1.00 44.09 C
ANISOU 1402 C VAL A 329 4284 5414 7053 136 -544 -3 C
ATOM 1403 O VAL A 329 178.602 31.652 1.176 1.00 45.57 O
ANISOU 1403 O VAL A 329 4469 5817 7029 287 -939 -112 O
ATOM 1404 N LEU A 330 179.560 30.749 2.986 1.00 41.98 N
ANISOU 1404 N LEU A 330 4453 4920 6576 185 -226 69 N
ATOM 1405 CA LEU A 330 180.551 30.025 2.206 1.00 39.11 C
ANISOU 1405 CA LEU A 330 4609 4532 5721 428 -331 18 C
ATOM 1406 CB LEU A 330 181.568 29.369 3.131 1.00 39.36 C
ANISOU 1406 CB LEU A 330 5059 4332 5565 495 112 181 C
ATOM 1407 CG LEU A 330 182.552 30.327 3.780 1.00 43.39 C
ANISOU 1407 CG LEU A 330 5555 5036 5894 776 365 547 C
ATOM 1408 CD1 LEU A 330 183.276 29.646 4.980 1.00 44.13 C
ANISOU 1408 CD1 LEU A 330 5966 4901 5902 776 848 673 C
ATOM 1409 CD2 LEU A 330 183.560 30.791 2.726 1.00 37.18 C
ANISOU 1409 CD2 LEU A 330 4938 4549 4640 1187 141 746 C
ATOM 1410 C LEU A 330 179.923 28.976 1.294 1.00 45.41 C
ANISOU 1410 C LEU A 330 5542 5158 6555 272 -700 -398 C
ATOM 1411 O LEU A 330 180.461 28.656 0.225 1.00 44.05 O
ANISOU 1411 O LEU A 330 5679 5130 5929 579 -988 -536 O
ATOM 1412 N ARG A 331 178.806 28.413 1.740 1.00 43.86 N
ANISOU 1412 N ARG A 331 5103 4655 6908 -174 -703 -592 N
ATOM 1413 CA ARG A 331 178.094 27.424 0.946 1.00 50.07 C
ANISOU 1413 CA ARG A 331 5945 5189 7890 -384 -1128 -1031 C
ATOM 1414 CB ARG A 331 176.869 26.912 1.698 1.00 55.85 C
ANISOU 1414 CB ARG A 331 6289 5554 9378 -931 -1041 -1082 C
ATOM 1415 CG ARG A 331 176.263 25.621 1.161 1.00 63.99 C
ANISOU 1415 CG ARG A 331 7417 6109 10788 -1233 -1435 -1508 C
ATOM 1416 CD ARG A 331 174.723 25.600 1.377 1.00104.65 C
ANISOU 1416 CD ARG A 331 11926 11117 16720 -1742 -1597 -1561 C
ATOM 1417 NE ARG A 331 174.344 26.087 2.704 1.00102.73 N
ANISOU 1417 NE ARG A 331 11283 10943 16807 -1927 -1033 -1085 N
ATOM 1418 CZ ARG A 331 173.970 25.311 3.715 1.00106.52 C
ANISOU 1418 CZ ARG A 331 11610 11039 17824 -2268 -673 -843 C
ATOM 1419 NH1 ARG A 331 173.884 23.996 3.547 1.00113.86 N
ANISOU 1419 NH1 ARG A 331 12731 11387 19143 -2540 -848 -1027 N
ATOM 1420 NH2 ARG A 331 173.668 25.855 4.890 1.00103.69 N
ANISOU 1420 NH2 ARG A 331 10882 10887 17629 -2298 -155 -405 N
ATOM 1421 C ARG A 331 177.676 28.051 -0.379 1.00 53.80 C
ANISOU 1421 C ARG A 331 6218 6073 8151 -175 -1671 -1246 C
ATOM 1422 O ARG A 331 177.869 27.476 -1.443 1.00 60.61 O
ANISOU 1422 O ARG A 331 7366 6973 8691 45 -2082 -1588 O
ATOM 1423 N HIS A 332 177.108 29.252 -0.305 1.00 51.62 N
ANISOU 1423 N HIS A 332 5445 6134 8035 -189 -1676 -1046 N
ATOM 1424 CA HIS A 332 176.729 29.995 -1.501 1.00 54.98 C
ANISOU 1424 CA HIS A 332 5619 7018 8254 51 -2133 -1145 C
ATOM 1425 CB HIS A 332 175.819 31.179 -1.134 1.00 53.62 C
ANISOU 1425 CB HIS A 332 4825 7066 8481 -107 -2089 -941 C
ATOM 1426 CG HIS A 332 174.473 30.767 -0.661 1.00 60.75 C
ANISOU 1426 CG HIS A 332 5343 7712 10028 -618 -2136 -1138 C
ATOM 1427 ND1 HIS A 332 174.263 30.160 0.578 1.00 62.39 N
ANISOU 1427 ND1 HIS A 332 5535 7520 10649 -967 -1728 -1037 N
ATOM 1428 CE1 HIS A 332 172.994 29.878 0.719 1.00 68.23 C
ANISOU 1428 CE1 HIS A 332 5841 8126 11958 -1374 -1863 -1164 C
ATOM 1429 NE2 HIS A 332 172.343 30.257 -0.382 1.00 65.54 N
ANISOU 1429 NE2 HIS A 332 5248 8062 11593 -1326 -2374 -1405 N
ATOM 1430 CD2 HIS A 332 173.253 30.802 -1.252 1.00 60.87 C
ANISOU 1430 CD2 HIS A 332 4939 7820 10368 -837 -2540 -1391 C
ATOM 1431 C HIS A 332 177.951 30.493 -2.263 1.00 53.44 C
ANISOU 1431 C HIS A 332 5707 7231 7365 636 -2172 -912 C
ATOM 1432 O HIS A 332 178.017 30.405 -3.486 1.00 57.61 O
ANISOU 1432 O HIS A 332 6320 8084 7486 972 -2580 -1097 O
ATOM 1433 N LEU A 333 178.901 31.045 -1.529 1.00 48.63 N
ANISOU 1433 N LEU A 333 5199 6643 6634 788 -1757 -479 N
ATOM 1434 CA LEU A 333 180.111 31.573 -2.134 1.00 60.37 C
ANISOU 1434 CA LEU A 333 6877 8502 7559 1316 -1744 -125 C
ATOM 1435 CB LEU A 333 181.116 32.001 -1.070 1.00 58.85 C
ANISOU 1435 CB LEU A 333 6795 8181 7383 1368 -1281 297 C
ATOM 1436 CG LEU A 333 181.275 33.510 -0.922 1.00 64.22 C
ANISOU 1436 CG LEU A 333 7041 9112 8249 1515 -1250 740 C
ATOM 1437 CD1 LEU A 333 182.617 33.828 -0.281 1.00 64.06 C
ANISOU 1437 CD1 LEU A 333 7333 8883 8124 1507 -866 1003 C
ATOM 1438 CD2 LEU A 333 181.168 34.209 -2.264 1.00 66.79 C
ANISOU 1438 CD2 LEU A 333 7275 9654 8448 1576 -1472 812 C
ATOM 1439 C LEU A 333 180.789 30.609 -3.097 1.00 69.76 C
ANISOU 1439 C LEU A 333 8563 9799 8144 1681 -1954 -338 C
ATOM 1440 O LEU A 333 181.145 30.986 -4.206 1.00 75.74 O
ANISOU 1440 O LEU A 333 9301 11052 8424 2158 -2209 -212 O
ATOM 1441 N ARG A 334 180.960 29.365 -2.673 1.00 73.05 N
ANISOU 1441 N ARG A 334 9408 9770 8576 1503 -1846 -642 N
ATOM 1442 CA ARG A 334 181.733 28.398 -3.435 1.00 75.97 C
ANISOU 1442 CA ARG A 334 10320 10181 8364 1898 -2009 -864 C
ATOM 1443 CB ARG A 334 182.038 27.177 -2.573 1.00 74.03 C
ANISOU 1443 CB ARG A 334 10510 9329 8288 1632 -1740 -1052 C
ATOM 1444 CG ARG A 334 183.164 27.415 -1.606 1.00 69.26 C
ANISOU 1444 CG ARG A 334 10095 8676 7544 1716 -1187 -555 C
ATOM 1445 CD ARG A 334 182.987 26.586 -0.365 1.00 72.23 C
ANISOU 1445 CD ARG A 334 10611 8461 8373 1269 -828 -629 C
ATOM 1446 NE ARG A 334 184.094 26.758 0.571 1.00 73.01 N
ANISOU 1446 NE ARG A 334 10908 8547 8285 1394 -319 -195 N
ATOM 1447 CZ ARG A 334 184.043 26.420 1.858 1.00 73.65 C
ANISOU 1447 CZ ARG A 334 10993 8274 8717 1083 105 -82 C
ATOM 1448 NH1 ARG A 334 182.924 25.900 2.353 1.00 78.15 N
ANISOU 1448 NH1 ARG A 334 11344 8474 9874 617 107 -302 N
ATOM 1449 NH2 ARG A 334 185.100 26.605 2.649 1.00 65.04 N
ANISOU 1449 NH2 ARG A 334 10085 7233 7395 1260 521 283 N
ATOM 1450 C ARG A 334 181.047 27.948 -4.711 1.00 86.29 C
ANISOU 1450 C ARG A 334 11630 11684 9473 2084 -2617 -1395 C
ATOM 1451 O ARG A 334 180.798 26.752 -4.857 1.00 91.93 O
ANISOU 1451 O ARG A 334 12665 12003 10261 1969 -2851 -1926 O
ATOM 1452 N GLN A 335 180.747 28.912 -5.600 1.00 87.58 N
ANISOU 1452 N GLN A 335 11417 12438 9423 2384 -2886 -1246 N
ATOM 1453 CA GLN A 335 180.170 28.742 -6.954 1.00 87.87 C
ANISOU 1453 CA GLN A 335 11383 12860 9144 2706 -3459 -1670 C
ATOM 1454 CB GLN A 335 179.095 27.665 -7.022 1.00 90.28 C
ANISOU 1454 CB GLN A 335 11747 12685 9872 2310 -3914 -2446 C
ATOM 1455 CG GLN A 335 177.881 28.007 -6.206 1.00 88.26 C
ANISOU 1455 CG GLN A 335 10979 12076 10480 1596 -3838 -2450 C
ATOM 1456 CD GLN A 335 177.590 26.982 -5.121 1.00 91.28 C
ANISOU 1456 CD GLN A 335 11521 11658 11502 995 -3630 -2652 C
ATOM 1457 OE1 GLN A 335 176.433 26.764 -4.768 1.00 96.56 O
ANISOU 1457 OE1 GLN A 335 11834 11989 12866 456 -3773 -2872 O
ATOM 1458 NE2 GLN A 335 178.632 26.343 -4.595 1.00 90.37 N
ANISOU 1458 NE2 GLN A 335 11906 11258 11170 1100 -3279 -2525 N
ATOM 1459 C GLN A 335 179.538 30.052 -7.398 1.00 83.01 C
ANISOU 1459 C GLN A 335 10183 12615 8741 2623 -3360 -1298 C
ATOM 1460 O GLN A 335 180.012 30.697 -8.325 1.00 82.36 O
ANISOU 1460 O GLN A 335 10049 12888 8354 2898 -3109 -926 O
TER 1461 GLN A 335
ATOM 1461 N SER B 154 148.849 45.994 3.869 1.00 61.24 N
ANISOU 1461 N SER B 154 7667 7421 8180 -452 -1039 158 N
ATOM 1462 CA SER B 154 148.821 46.818 2.655 1.00 62.18 C
ANISOU 1462 CA SER B 154 7904 7529 8192 -597 -1236 209 C
ATOM 1463 CB SER B 154 147.769 47.936 2.754 1.00 63.13 C
ANISOU 1463 CB SER B 154 7769 7644 8574 -584 -1380 415 C
ATOM 1464 OG SER B 154 148.239 48.999 3.570 1.00 57.09 O
ANISOU 1464 OG SER B 154 6881 6936 7874 -386 -1183 383 O
ATOM 1465 C SER B 154 150.192 47.452 2.385 1.00 54.84 C
ANISOU 1465 C SER B 154 7135 6654 7046 -528 -1086 66 C
ATOM 1466 O SER B 154 151.064 47.518 3.277 1.00 47.88 O
ANISOU 1466 O SER B 154 6204 5830 6158 -355 -859 -33 O
ATOM 1467 N VAL B 155 150.353 47.963 1.158 1.00 43.13 N
ANISOU 1467 N VAL B 155 5842 5145 5400 -675 -1231 78 N
ATOM 1468 CA VAL B 155 151.638 48.468 0.734 1.00 32.52 C
ANISOU 1468 CA VAL B 155 4671 3826 3857 -631 -1084 -44 C
ATOM 1469 CB VAL B 155 151.657 48.752 -0.776 1.00 43.29 C
ANISOU 1469 CB VAL B 155 6320 5124 5005 -841 -1255 -26 C
ATOM 1470 CG1 VAL B 155 152.878 49.611 -1.148 1.00 38.57 C
ANISOU 1470 CG1 VAL B 155 5836 4552 4268 -766 -1095 -113 C
ATOM 1471 CG2 VAL B 155 151.663 47.430 -1.548 1.00 46.08 C
ANISOU 1471 CG2 VAL B 155 6997 5361 5151 -1027 -1278 -96 C
ATOM 1472 C VAL B 155 151.991 49.711 1.508 1.00 31.39 C
ANISOU 1472 C VAL B 155 4323 3769 3837 -453 -984 -30 C
ATOM 1473 O VAL B 155 153.060 49.824 2.066 1.00 38.82 O
ANISOU 1473 O VAL B 155 5261 4752 4736 -322 -782 -131 O
ATOM 1474 N ALA B 156 151.078 50.666 1.529 1.00 35.88 N
ANISOU 1474 N ALA B 156 4718 4345 4572 -459 -1130 115 N
ATOM 1475 CA ALA B 156 151.347 51.956 2.147 1.00 32.65 C
ANISOU 1475 CA ALA B 156 4157 3986 4264 -313 -1030 131 C
ATOM 1476 CB ALA B 156 150.141 52.858 1.981 1.00 34.00 C
ANISOU 1476 CB ALA B 156 4142 4123 4654 -345 -1194 330 C
ATOM 1477 C ALA B 156 151.690 51.793 3.637 1.00 32.13 C
ANISOU 1477 C ALA B 156 3964 3956 4288 -132 -809 61 C
ATOM 1478 O ALA B 156 152.512 52.502 4.215 1.00 34.92 O
ANISOU 1478 O ALA B 156 4308 4350 4608 -25 -673 -6 O
ATOM 1479 N HIS B 157 151.045 50.848 4.264 1.00 32.63 N
ANISOU 1479 N HIS B 157 3946 3994 4458 -115 -789 88 N
ATOM 1480 CA HIS B 157 151.190 50.694 5.704 1.00 35.60 C
ANISOU 1480 CA HIS B 157 4224 4387 4916 39 -597 47 C
ATOM 1481 CB HIS B 157 150.170 49.654 6.196 1.00 34.17 C
ANISOU 1481 CB HIS B 157 3939 4155 4890 35 -605 117 C
ATOM 1482 CG HIS B 157 150.342 49.250 7.607 1.00 34.58 C
ANISOU 1482 CG HIS B 157 3943 4212 4983 172 -406 69 C
ATOM 1483 ND1 HIS B 157 150.119 50.116 8.665 1.00 34.37 N
ANISOU 1483 ND1 HIS B 157 3843 4160 5056 291 -260 100 N
ATOM 1484 CE1 HIS B 157 150.339 49.496 9.808 1.00 33.86 C
ANISOU 1484 CE1 HIS B 157 3802 4094 4971 374 -110 49 C
ATOM 1485 NE2 HIS B 157 150.709 48.246 9.541 1.00 34.91 N

ANISOU 1485 NE2 HIS B 157 3983 4258 5021 327 -151 -6 N
ATOM 1486 CD2 HIS B 157 150.721 48.067 8.179 1.00 32.57 C
ANISOU 1486 CD2 HIS B 157 3733 3970 4672 202 -318 -2 C
ATOM 1487 C HIS B 157 152.632 50.271 6.002 1.00 31.36 C
ANISOU 1487 C HIS B 157 3813 3904 4198 88 -465 -100 C
ATOM 1488 O HIS B 157 153.313 50.874 6.822 1.00 31.54 O
ANISOU 1488 O HIS B 157 3821 3962 4201 182 -355 -143 O
ATOM 1489 N GLY B 158 153.102 49.242 5.307 1.00 30.84 N
ANISOU 1489 N GLY B 158 3880 3826 4011 11 -477 -161 N
ATOM 1490 CA GLY B 158 154.491 48.812 5.431 1.00 25.71 C
ANISOU 1490 CA GLY B 158 3323 3200 3245 57 -337 -258 C
ATOM 1491 C GLY B 158 155.493 49.890 5.044 1.00 33.08 C
ANISOU 1491 C GLY B 158 4304 4164 4103 73 -310 -286 C
ATOM 1492 O GLY B 158 156.557 50.009 5.651 1.00 32.77 O
ANISOU 1492 O GLY B 158 4240 4156 4054 148 -206 -317 O
ATOM 1493 N LEU B 159 155.145 50.720 4.053 1.00 22.02 N
ANISOU 1493 N LEU B 159 2957 2747 2661 -6 -423 -254 N
ATOM 1494 CA LEU B 159 156.053 51.753 3.543 1.00 27.46 C
ANISOU 1494 CA LEU B 159 3702 3454 3279 0 -397 -275 C
ATOM 1495 CB LEU B 159 155.536 52.317 2.210 1.00 32.75 C
ANISOU 1495 CB LEU B 159 4484 4087 3874 -124 -540 -231 C
ATOM 1496 CG LEU B 159 155.790 51.492 0.964 1.00 37.07 C
ANISOU 1496 CG LEU B 159 5282 4555 4246 -255 -542 -271 C
ATOM 1497 CD1 LEU B 159 155.476 52.380 -0.212 1.00 39.69 C
ANISOU 1497 CD1 LEU B 159 5738 4860 4484 -373 -690 -217 C
ATOM 1498 CD2 LEU B 159 157.241 51.052 0.950 1.00 35.04 C
ANISOU 1498 CD2 LEU B 159 5116 4271 3925 -190 -312 -356 C
ATOM 1499 C LEU B 159 156.232 52.902 4.545 1.00 28.73 C
ANISOU 1499 C LEU B 159 3729 3664 3524 98 -368 -259 C
ATOM 1500 O LEU B 159 157.314 53.468 4.701 1.00 26.38 O
ANISOU 1500 O LEU B 159 3441 3389 3194 136 -302 -289 O
ATOM 1501 N ALA B 160 155.137 53.283 5.194 1.00 21.13 N
ANISOU 1501 N ALA B 160 2655 2696 2679 129 -410 -199 N
ATOM 1502 CA ALA B 160 155.194 54.351 6.170 1.00 23.35 C
ANISOU 1502 CA ALA B 160 2869 2985 3020 208 -348 -192 C
ATOM 1503 CB ALA B 160 153.799 54.727 6.623 1.00 25.38 C
ANISOU 1503 CB ALA B 160 3017 3186 3439 239 -350 -99 C
ATOM 1504 C ALA B 160 156.069 53.899 7.347 1.00 22.52 C
ANISOU 1504 C ALA B 160 2778 2907 2873 267 -248 -250 C
ATOM 1505 O ALA B 160 156.904 54.651 7.860 1.00 32.99 O
ANISOU 1505 O ALA B 160 4130 4249 4157 286 -219 -275 O
ATOM 1506 N TRP B 161 155.866 52.670 7.785 1.00 25.95 N
ANISOU 1506 N TRP B 161 3199 3341 3322 281 -217 -257 N
ATOM 1507 CA TRP B 161 156.726 52.080 8.818 1.00 27.65 C
ANISOU 1507 CA TRP B 161 3425 3581 3501 321 -151 -284 C
ATOM 1508 CB TRP B 161 156.168 50.735 9.275 1.00 25.21 C
ANISOU 1508 CB TRP B 161 3088 3258 3234 341 -113 -275 C
ATOM 1509 CG TRP B 161 155.099 50.971 10.320 1.00 25.58 C
ANISOU 1509 CG TRP B 161 3105 3264 3352 390 -62 -244 C
ATOM 1510 CD1 TRP B 161 153.734 50.969 10.138 1.00 25.33 C
ANISOU 1510 CD1 TRP B 161 3002 3176 3446 396 -62 -186 C
ATOM 1511 NE1 TRP B 161 153.103 51.248 11.331 1.00 29.84 N
ANISOU 1511 NE1 TRP B 161 3572 3686 4078 463 57 -158 N
ATOM 1512 CE2 TRP B 161 154.048 51.454 12.306 1.00 29.97 C
ANISOU 1512 CE2 TRP B 161 3701 3724 3962 479 107 -210 C
ATOM 1513 CD2 TRP B 161 155.321 51.312 11.700 1.00 24.86 C
ANISOU 1513 CD2 TRP B 161 3072 3156 3216 431 12 -250 C
ATOM 1514 CE3 TRP B 161 156.469 51.472 12.490 1.00 25.57 C
ANISOU 1514 CE3 TRP B 161 3240 3276 3197 416 -1 -268 C
ATOM 1515 CZ3 TRP B 161 156.314 51.796 13.869 1.00 22.68 C
ANISOU 1515 CZ3 TRP B 161 2992 2860 2764 426 64 -267 C
ATOM 1516 CH2 TRP B 161 155.027 51.953 14.433 1.00 30.80 C
ANISOU 1516 CH2 TRP B 161 4052 3796 3856 479 201 -254 C
ATOM 1517 CZ2 TRP B 161 153.889 51.804 13.672 1.00 33.70 C
ANISOU 1517 CZ2 TRP B 161 4285 4130 4388 517 233 -214 C
ATOM 1518 C TRP B 161 158.190 51.971 8.422 1.00 27.74 C
ANISOU 1518 C TRP B 161 3460 3620 3460 304 -143 -300 C
ATOM 1519 O TRP B 161 159.089 52.336 9.197 1.00 29.74 O
ANISOU 1519 O TRP B 161 3709 3894 3699 313 -145 -287 O
ATOM 1520 N ALA B 162 158.426 51.509 7.195 1.00 25.01 N
ANISOU 1520 N ALA B 162 3155 3254 3093 265 -132 -312 N
ATOM 1521 CA ALA B 162 159.794 51.407 6.677 1.00 20.92 C
ANISOU 1521 CA ALA B 162 2656 2725 2566 262 -66 -307 C
ATOM 1522 CB ALA B 162 159.830 50.798 5.319 1.00 20.66 C
ANISOU 1522 CB ALA B 162 2738 2630 2484 213 -5 -332 C
ATOM 1523 C ALA B 162 160.427 52.777 6.612 1.00 27.98 C
ANISOU 1523 C ALA B 162 3538 3639 3454 256 -105 -295 C
ATOM 1524 O ALA B 162 161.627 52.937 6.808 1.00 31.83 O
ANISOU 1524 O ALA B 162 3980 4127 3987 266 -75 -255 O
ATOM 1525 N TYR B 163 159.629 53.778 6.273 1.00 23.24 N
ANISOU 1525 N TYR B 163 2963 3042 2824 234 -172 -308 N
ATOM 1526 CA TYR B 163 160.180 55.110 6.096 1.00 26.46 C
ANISOU 1526 CA TYR B 163 3372 3458 3225 224 -198 -301 C
ATOM 1527 CB TYR B 163 159.166 55.998 5.385 1.00 25.88 C
ANISOU 1527 CB TYR B 163 3328 3370 3136 198 -258 -297 C
ATOM 1528 CG TYR B 163 159.670 57.379 5.079 1.00 21.09 C
ANISOU 1528 CG TYR B 163 2729 2760 2523 188 -273 -290 C
ATOM 1529 CD1 TYR B 163 160.847 57.573 4.328 1.00 30.99 C
ANISOU 1529 CD1 TYR B 163 4013 4005 3758 171 -231 -288 C
ATOM 1530 CE1 TYR B 163 161.308 58.858 4.012 1.00 28.67 C
ANISOU 1530 CE1 TYR B 163 3722 3703 3469 160 -243 -276 C
ATOM 1531 CZ TYR B 163 160.538 59.947 4.428 1.00 28.27 C
ANISOU 1531 CZ TYR B 163 3656 3650 3436 166 -292 -272 C
ATOM 1532 OH TYR B 163 160.932 61.233 4.197 1.00 32.54 O
ANISOU 1532 OH TYR B 163 4203 4173 3986 155 -297 -262 O
ATOM 1533 CE2 TYR B 163 159.369 59.768 5.159 1.00 26.60 C
ANISOU 1533 CE2 TYR B 163 3421 3432 3255 190 -306 -268 C
ATOM 1534 CD2 TYR B 163 158.941 58.478 5.462 1.00 23.25 C
ANISOU 1534 CD2 TYR B 163 2983 3020 2832 201 -300 -275 C
ATOM 1535 C TYR B 163 160.524 55.701 7.473 1.00 26.39 C
ANISOU 1535 C TYR B 163 3330 3468 3230 239 -226 -291 C
ATOM 1536 O TYR B 163 161.564 56.336 7.670 1.00 27.97 O
ANISOU 1536 O TYR B 163 3516 3671 3439 219 -248 -268 O
ATOM 1537 N TYR B 164 159.631 55.504 8.431 1.00 24.02 N
ANISOU 1537 N TYR B 164 3039 3162 2927 261 -225 -301 N
ATOM 1538 CA TYR B 164 159.949 55.867 9.817 1.00 27.38 C
ANISOU 1538 CA TYR B 164 3508 3581 3316 251 -239 -297 C
ATOM 1539 CB TYR B 164 158.769 55.592 10.693 1.00 29.36 C
ANISOU 1539 CB TYR B 164 3799 3793 3562 286 -181 -310 C
ATOM 1540 CG TYR B 164 159.099 55.663 12.137 1.00 32.24 C
ANISOU 1540 CG TYR B 164 4272 4133 3844 259 -183 -310 C
ATOM 1541 CD1 TYR B 164 159.400 56.875 12.738 1.00 33.93 C
ANISOU 1541 CD1 TYR B 164 4616 4299 3977 205 -197 -328 C
ATOM 1542 CE1 TYR B 164 159.642 56.950 14.062 1.00 38.24 C
ANISOU 1542 CE1 TYR B 164 5328 4799 4403 147 -211 -331 C
ATOM 1543 CZ TYR B 164 159.608 55.786 14.815 1.00 46.86 C
ANISOU 1543 CZ TYR B 164 6433 5906 5467 153 -215 -303 C
ATOM 1544 OH TYR B 164 159.859 55.831 16.160 1.00 49.68 O
ANISOU 1544 OH TYR B 164 6996 6208 5672 73 -247 -295 O
ATOM 1545 CE2 TYR B 164 159.306 54.564 14.242 1.00 49.26 C
ANISOU 1545 CE2 TYR B 164 6574 6264 5879 226 -188 -281 C
ATOM 1546 CD2 TYR B 164 159.047 54.520 12.911 1.00 42.81 C
ANISOU 1546 CD2 TYR B 164 5617 5481 5169 272 -171 -291 C
ATOM 1547 C TYR B 164 161.165 55.126 10.389 1.00 29.31 C
ANISOU 1547 C TYR B 164 3719 3852 3566 227 -281 -250 C
ATOM 1548 O TYR B 164 162.105 55.714 10.929 1.00 33.26 O
ANISOU 1548 O TYR B 164 4238 4352 4048 171 -358 -213 O
ATOM 1549 N ILE B 165 161.181 53.815 10.188 1.00 26.46 N
ANISOU 1549 N ILE B 165 3298 3503 3251 259 -239 -230 N
ATOM 1550 CA ILE B 165 162.238 52.991 10.770 1.00 27.93 C
ANISOU 1550 CA ILE B 165 3421 3702 3490 249 -265 -150 C
ATOM 1551 CB ILE B 165 161.769 51.537 10.947 1.00 26.50 C
ANISOU 1551 CB ILE B 165 3209 3518 3340 296 -195 -146 C
ATOM 1552 CG1 ILE B 165 160.927 51.476 12.211 1.00 33.14 C
ANISOU 1552 CG1 ILE B 165 4130 4357 4103 297 -217 -165 C
ATOM 1553 CD1 ILE B 165 159.788 50.636 12.060 1.00 45.03 C
ANISOU 1553 CD1 ILE B 165 5633 5850 5628 347 -135 -205 C
ATOM 1554 CG2 ILE B 165 163.010 50.516 11.068 1.00 24.02 C
ANISOU 1554 CG2 ILE B 165 2781 3196 3149 305 -176 -31 C
ATOM 1555 C ILE B 165 163.618 53.101 10.073 1.00 37.62 C
ANISOU 1555 C ILE B 165 4551 4919 4824 234 -263 -71 C
ATOM 1556 O ILE B 165 164.691 53.081 10.724 1.00 34.98 O
ANISOU 1556 O ILE B 165 4144 4585 4564 193 -346 40 O
ATOM 1557 N GLY B 166 163.568 53.186 8.756 1.00 33.98 N
ANISOU 1557 N GLY B 166 4096 4433 4383 257 -169 -110 N
ATOM 1558 CA GLY B 166 164.730 53.257 7.924 1.00 25.09 C
ANISOU 1558 CA GLY B 166 2902 3262 3371 264 -87 -40 C
ATOM 1559 C GLY B 166 165.231 54.604 7.548 1.00 32.79 C
ANISOU 1559 C GLY B 166 3875 4234 4349 226 -141 -29 C
ATOM 1560 O GLY B 166 166.191 54.688 6.863 1.00 39.19 O
ANISOU 1560 O GLY B 166 4617 4995 5279 234 -64 46 O
ATOM 1561 N TYR B 167 164.555 55.654 7.950 1.00 31.76 N
ANISOU 1561 N TYR B 167 3820 4138 4109 191 -247 -93 N
ATOM 1562 CA TYR B 167 165.041 56.984 7.697 1.00 32.07 C
ANISOU 1562 CA TYR B 167 3865 4167 4154 151 -295 -84 C
ATOM 1563 CB TYR B 167 164.531 57.492 6.353 1.00 32.26 C
ANISOU 1563 CB TYR B 167 3955 4172 4129 175 -212 -150 C
ATOM 1564 CG TYR B 167 165.023 58.833 6.000 1.00 26.29 C
ANISOU 1564 CG TYR B 167 3203 3400 3385 142 -244 -139 C
ATOM 1565 CD1 TYR B 167 166.335 59.037 5.772 1.00 30.21 C
ANISOU 1565 CD1 TYR B 167 3606 3863 4011 126 -225 -44 C
ATOM 1566 CE1 TYR B 167 166.806 60.255 5.439 1.00 32.16 C
ANISOU 1566 CE1 TYR B 167 3848 4088 4282 93 -252 -28 C
ATOM 1567 CZ TYR B 167 165.970 61.277 5.350 1.00 33.93 C
ANISOU 1567 CZ TYR B 167 4172 4325 4395 80 -292 -110 C
ATOM 1568 OH TYR B 167 166.490 62.468 5.035 1.00 47.66 O
ANISOU 1568 OH TYR B 167 5905 6035 6169 48 -309 -89 O
ATOM 1569 CE2 TYR B 167 164.647 61.115 5.576 1.00 27.99 C
ANISOU 1569 CE2 TYR B 167 3502 3599 3535 103 -300 -189 C
ATOM 1570 CD2 TYR B 167 164.182 59.889 5.906 1.00 27.51 C
ANISOU 1570 CD2 TYR B 167 3436 3560 3457 132 -281 -201 C
ATOM 1571 C TYR B 167 164.835 57.996 8.800 1.00 31.73 C
ANISOU 1571 C TYR B 167 3897 4135 4025 88 -424 -109 C
ATOM 1572 O TYR B 167 165.748 58.565 9.274 1.00 31.83 O
ANISOU 1572 O TYR B 167 3882 4135 4075 14 -530 -37 O
ATOM 1573 N LEU B 168 163.593 58.279 9.099 1.00 33.53 N
ANISOU 1573 N LEU B 168 4230 4363 4148 106 -405 -196 N
ATOM 1574 CA LEU B 168 163.237 59.338 10.000 1.00 31.15 C
ANISOU 1574 CA LEU B 168 4053 4028 3755 54 -453 -235 C
ATOM 1575 CB LEU B 168 161.748 59.556 9.976 1.00 28.01 C

ANISOU 1575 CB LEU B 168 3731 3599 3314 110 -358 -304 C
ATOM 1576 CG LEU B 168 161.126 60.100 8.709 1.00 35.64 C
ANISOU 1576 CG LEU B 168 4648 4563 4331 154 -308 -316 C
ATOM 1577 CD1 LEU B 168 159.656 60.278 8.928 1.00 34.19 C
ANISOU 1577 CD1 LEU B 168 4489 4333 4168 204 -232 -330 C
ATOM 1578 CD2 LEU B 168 161.747 61.393 8.265 1.00 22.45 C
ANISOU 1578 CD2 LEU B 168 2992 2872 2668 116 -333 -311 C
ATOM 1579 C LEU B 168 163.689 59.166 11.419 1.00 32.58 C
ANISOU 1579 C LEU B 168 4312 4195 3871 -29 -558 -197 C
ATOM 1580 O LEU B 168 164.153 60.077 12.005 1.00 31.87 O
ANISOU 1580 O LEU B 168 4322 4066 3721 -127 -650 -188 O
ATOM 1581 N ARG B 169 163.557 57.978 11.971 1.00 33.20 N
ANISOU 1581 N ARG B 169 4371 4297 3947 -7 -557 -171 N
ATOM 1582 CA ARG B 169 164.013 57.765 13.358 1.00 33.77 C
ANISOU 1582 CA ARG B 169 4548 4351 3933 -106 -681 -119 C
ATOM 1583 CB ARG B 169 163.517 56.418 13.905 1.00 32.35 C
ANISOU 1583 CB ARG B 169 4355 4192 3744 -54 -638 -105 C
ATOM 1584 CG ARG B 169 164.574 55.351 13.997 1.00 37.97 C
ANISOU 1584 CG ARG B 169 4905 4943 4580 -70 -729 32 C
ATOM 1585 CD ARG B 169 164.009 54.013 13.670 1.00 39.72 C
ANISOU 1585 CD ARG B 169 5033 5190 4869 40 -602 21 C
ATOM 1586 NE ARG B 169 163.623 53.254 14.840 1.00 44.18 N
ANISOU 1586 NE ARG B 169 5686 5748 5351 24 -627 41 N
ATOM 1587 CZ ARG B 169 163.968 51.991 15.069 1.00 43.78 C
ANISOU 1587 CZ ARG B 169 5524 5717 5392 53 -630 133 C
ATOM 1588 NH1 ARG B 169 163.550 51.416 16.181 1.00 45.14 N
ANISOU 1588 NH1 ARG B 169 5807 5879 5465 32 -653 147 N
ATOM 1589 NH2 ARG B 169 164.726 51.312 14.206 1.00 41.98 N
ANISOU 1589 NH2 ARG B 169 5094 5500 5357 104 -582 216 N
ATOM 1590 C ARG B 169 165.552 57.931 13.477 1.00 30.97 C
ANISOU 1590 C ARG B 169 4095 4005 3667 -214 -864 20 C
ATOM 1591 O ARG B 169 166.093 58.143 14.550 1.00 35.97 O
ANISOU 1591 O ARG B 169 4839 4611 4217 -350 -1035 86 O
ATOM 1592 N LEU B 170 166.248 57.851 12.343 1.00 35.89 N
ANISOU 1592 N LEU B 170 4520 4650 4467 -162 -825 79 N
ATOM 1593 CA LEU B 170 167.713 57.934 12.278 1.00 35.74 C
ANISOU 1593 CA LEU B 170 4340 4620 4619 -238 -956 248 C
ATOM 1594 CB LEU B 170 168.262 57.022 11.166 1.00 41.55 C
ANISOU 1594 CB LEU B 170 4850 5358 5581 -124 -806 330 C
ATOM 1595 CG LEU B 170 167.827 55.555 11.118 1.00 39.07 C
ANISOU 1595 CG LEU B 170 4485 5059 5300 -27 -682 329 C
ATOM 1596 CD1 LEU B 170 168.341 54.916 9.833 1.00 39.17 C
ANISOU 1596 CD1 LEU B 170 4350 5029 5502 74 -477 379 C
ATOM 1597 CD2 LEU B 170 168.301 54.765 12.340 1.00 33.70 C
ANISOU 1597 CD2 LEU B 170 3755 4387 4663 -92 -833 470 C
ATOM 1598 C LEU B 170 168.218 59.328 11.995 1.00 39.25 C
ANISOU 1598 C LEU B 170 4815 5031 5067 -317 -1027 248 C
ATOM 1599 O LEU B 170 169.376 59.648 12.270 1.00 49.62 O
ANISOU 1599 O LEU B 170 6034 6319 6501 -428 -1196 400 O
ATOM 1600 N ILE B 171 167.383 60.167 11.409 1.00 39.73 N
ANISOU 1600 N ILE B 171 4984 5082 5028 -266 -909 102 N
ATOM 1601 CA ILE B 171 167.885 61.456 10.974 1.00 34.91 C
ANISOU 1601 CA ILE B 171 4382 4436 4446 -323 -947 104 C
ATOM 1602 CB ILE B 171 167.608 61.715 9.462 1.00 47.78 C
ANISOU 1602 CB ILE B 171 5930 6073 6150 -201 -762 50 C
ATOM 1603 CG1 ILE B 171 168.561 62.769 8.913 1.00 55.82 C
ANISOU 1603 CG1 ILE B 171 6879 7053 7279 -253 -800 115 C
ATOM 1604 CD1 ILE B 171 169.188 62.401 7.583 1.00 59.72 C
ANISOU 1604 CD1 ILE B 171 7204 7534 7952 -162 -652 186 C
ATOM 1605 CG2 ILE B 171 166.206 62.235 9.240 1.00 47.62 C
ANISOU 1605 CG2 ILE B 171 6058 6050 5984 -141 -655 -99 C
ATOM 1606 C ILE B 171 167.321 62.568 11.839 1.00 37.31 C
ANISOU 1606 C ILE B 171 4942 4685 4547 -423 -1006 4 C
ATOM 1607 O ILE B 171 167.951 63.620 12.026 1.00 41.72 O
ANISOU 1607 O ILE B 171 5561 5194 5097 -541 -1118 31 O
ATOM 1608 N LEU B 172 166.119 62.347 12.357 1.00 41.71 N
ANISOU 1608 N LEU B 172 5663 5231 4954 -376 -907 -107 N
ATOM 1609 CA LEU B 172 165.449 63.361 13.177 1.00 48.20 C
ANISOU 1609 CA LEU B 172 6765 5960 5590 -448 -878 -208 C
ATOM 1610 CB LEU B 172 163.966 63.054 13.385 1.00 43.37 C
ANISOU 1610 CB LEU B 172 6257 5320 4901 -334 -677 -310 C
ATOM 1611 CG LEU B 172 163.153 63.228 12.097 1.00 46.31 C
ANISOU 1611 CG LEU B 172 6481 5721 5394 -184 -517 -347 C
ATOM 1612 CD1 LEU B 172 161.677 63.092 12.391 1.00 44.18 C
ANISOU 1612 CD1 LEU B 172 6294 5394 5097 -91 -337 -406 C
ATOM 1613 CD2 LEU B 172 163.417 64.574 11.405 1.00 51.32 C
ANISOU 1613 CD2 LEU B 172 7117 6317 6066 -204 -504 -360 C
ATOM 1614 C LEU B 172 166.115 63.755 14.510 1.00 54.45 C
ANISOU 1614 C LEU B 172 7786 6678 6224 -657 -1075 -170 C
ATOM 1615 O LEU B 172 166.154 64.945 14.825 1.00 60.35 O
ANISOU 1615 O LEU B 172 8737 7329 6863 -762 -1089 -224 O
ATOM 1616 N PRO B 173 166.629 62.784 15.291 1.00 58.69 N
ANISOU 1616 N PRO B 173 8314 7246 6741 -735 -1235 -71 N
ATOM 1617 CA PRO B 173 167.090 63.174 16.639 1.00 60.84 C
ANISOU 1617 CA PRO B 173 8880 7430 6807 -967 -1444 -37 C
ATOM 1618 CB PRO B 173 167.629 61.869 17.245 1.00 56.11 C
ANISOU 1618 CB PRO B 173 8177 6892 6248 -1014 -1618 111 C
ATOM 1619 CG PRO B 173 167.082 60.755 16.381 1.00 57.75 C
ANISOU 1619 CG PRO B 173 8111 7198 6632 -777 -1416 96 C
ATOM 1620 CD PRO B 173 166.935 61.370 15.001 1.00 61.16 C
ANISOU 1620 CD PRO B 173 8370 7656 7213 -645 -1255 34 C
ATOM 1621 C PRO B 173 168.217 64.189 16.568 1.00 66.54 C
ANISOU 1621 C PRO B 173 9599 8110 7571 -1144 -1660 47 C
ATOM 1622 O PRO B 173 168.258 65.132 17.352 1.00 72.82 O
ANISOU 1622 O PRO B 173 10725 8788 8156 -1328 -1746 -5 O
ATOM 1623 N GLU B 174 169.113 64.009 15.609 1.00 65.05 N
ANISOU 1623 N GLU B 174 9057 7997 7660 -1091 -1725 178 N
ATOM 1624 CA GLU B 174 170.276 64.873 15.501 1.00 66.84 C
ANISOU 1624 CA GLU B 174 9220 8184 7991 -1255 -1940 298 C
ATOM 1625 CB GLU B 174 171.468 64.072 14.993 1.00 75.01 C
ANISOU 1625 CB GLU B 174 9857 9285 9359 -1235 -2072 538 C
ATOM 1626 CG GLU B 174 172.751 64.422 15.709 1.00 88.99 C
ANISOU 1626 CG GLU B 174 11603 11000 11208 -1502 -2446 761 C
ATOM 1627 CD GLU B 174 172.638 64.256 17.232 1.00100.41 C
ANISOU 1627 CD GLU B 174 13517 12522 12492 -1733 -2700 779 C
ATOM 1628 OE1 GLU B 174 172.530 65.285 17.946 1.00104.06 O
ANISOU 1628 OE1 GLU B 174 14213 12749 12574 -1909 -2771 691 O
ATOM 1629 OE2 GLU B 174 172.657 63.095 17.714 1.00107.22 O
ANISOU 1629 OE2 GLU B 174 14178 13305 13254 -1715 -2765 881 O
ATOM 1630 C GLU B 174 170.036 66.088 14.599 1.00 61.60 C
ANISOU 1630 C GLU B 174 8565 7484 7357 -1188 -1777 185 C
ATOM 1631 O GLU B 174 170.914 66.931 14.407 1.00 64.70 O
ANISOU 1631 O GLU B 174 8908 7834 7843 -1310 -1919 266 O
ATOM 1632 N LEU B 175 168.843 66.170 14.036 1.00 59.61 N
ANISOU 1632 N LEU B 175 8358 7244 7046 -1000 -1489 18 N
ATOM 1633 CA LEU B 175 168.555 67.194 13.045 1.00 56.22 C
ANISOU 1633 CA LEU B 175 7891 6793 6677 -911 -1325 -63 C
ATOM 1634 CB LEU B 175 167.190 66.954 12.427 1.00 57.22 C
ANISOU 1634 CB LEU B 175 8012 6948 6783 -702 -1048 -190 C
ATOM 1635 CG LEU B 175 166.707 68.024 11.455 1.00 59.28 C
ANISOU 1635 CG LEU B 175 8255 7175 7093 -612 -882 -261 C
ATOM 1636 CD1 LEU B 175 167.372 67.844 10.092 1.00 57.54 C
ANISOU 1636 CD1 LEU B 175 7748 7035 7081 -523 -870 -177 C
ATOM 1637 CD2 LEU B 175 165.184 67.991 11.338 1.00 55.19 C
ANISOU 1637 CD2 LEU B 175 7818 6633 6518 -469 -652 -365 C
ATOM 1638 C LEU B 175 168.533 68.527 13.726 1.00 58.36 C
ANISOU 1638 C LEU B 175 8472 6930 6773 -1078 -1373 -138 C
ATOM 1639 O LEU B 175 169.133 69.489 13.259 1.00 59.43 O
ANISOU 1639 O LEU B 175 8563 7027 6989 -1138 -1421 -111 O
ATOM 1640 N GLN B 176 167.832 68.586 14.849 1.00 60.35 N
ANISOU 1640 N GLN B 176 9064 7090 6776 -1157 -1337 -234 N
ATOM 1641 CA GLN B 176 167.639 69.857 15.508 1.00 64.55 C
ANISOU 1641 CA GLN B 176 9966 7453 7107 -1308 -1306 -334 C
ATOM 1642 CB GLN B 176 166.600 69.769 16.618 1.00 72.10 C
ANISOU 1642 CB GLN B 176 11314 8284 7798 -1333 -1142 -457 C
ATOM 1643 CG GLN B 176 165.680 70.980 16.636 1.00 79.14 C
ANISOU 1643 CG GLN B 176 12468 9002 8599 -1290 -842 -602 C
ATOM 1644 CD GLN B 176 164.204 70.608 16.718 1.00 79.33 C
ANISOU 1644 CD GLN B 176 12547 8977 8619 -1084 -494 -687 C
ATOM 1645 OE1 GLN B 176 163.733 70.126 17.755 1.00 82.90 O
ANISOU 1645 OE1 GLN B 176 13273 9342 8884 -1131 -424 -728 O
ATOM 1646 NE2 GLN B 176 163.467 70.826 15.622 1.00 75.00 N
ANISOU 1646 NE2 GLN B 176 11735 8473 8288 -863 -284 -693 N
ATOM 1647 C GLN B 176 168.960 70.417 16.020 1.00 66.67 C
ANISOU 1647 C GLN B 176 10322 7667 7341 -1587 -1641 -226 C
ATOM 1648 O GLN B 176 169.160 71.624 16.012 1.00 71.77 O
ANISOU 1648 O GLN B 176 11136 8201 7933 -1697 -1643 -274 O
ATOM 1649 N ALA B 177 169.879 69.549 16.434 1.00 58.25 N
ANISOU 1649 N ALA B 177 9122 6673 6336 -1706 -1935 -58 N
ATOM 1650 CA ALA B 177 171.208 70.031 16.810 1.00 53.97 C
ANISOU 1650 CA ALA B 177 8584 6085 5837 -1980 -2300 104 C
ATOM 1651 CB ALA B 177 172.028 68.944 17.441 1.00 48.14 C
ANISOU 1651 CB ALA B 177 7694 5413 5182 -2072 -2568 325 C
ATOM 1652 C ALA B 177 171.932 70.602 15.588 1.00 51.40 C
ANISOU 1652 C ALA B 177 7903 5805 5822 -1902 -2290 190 C
ATOM 1653 O ALA B 177 172.542 71.672 15.645 1.00 55.18 O
ANISOU 1653 O ALA B 177 8477 6189 6299 -2078 -2428 217 O
ATOM 1654 N ARG B 178 171.858 69.886 14.473 1.00 47.23 N
ANISOU 1654 N ARG B 178 6991 5404 5548 -1646 -2116 231 N
ATOM 1655 CA ARG B 178 172.541 70.342 13.254 1.00 50.99 C
ANISOU 1655 CA ARG B 178 7149 5910 6315 -1557 -2064 318 C
ATOM 1656 CB ARG B 178 172.388 69.324 12.127 1.00 53.34 C
ANISOU 1656 CB ARG B 178 7107 6328 6834 -1289 -1851 355 C
ATOM 1657 CG ARG B 178 173.271 68.113 12.223 1.00 57.18 C
ANISOU 1657 CG ARG B 178 7312 6871 7543 -1296 -1994 573 C
ATOM 1658 CD ARG B 178 172.670 66.985 11.375 1.00 56.47 C
ANISOU 1658 CD ARG B 178 7048 6872 7534 -1037 -1725 528 C
ATOM 1659 NE ARG B 178 172.934 67.111 9.938 1.00 58.22 N
ANISOU 1659 NE ARG B 178 7104 7104 7971 -873 -1500 552 N
ATOM 1660 CZ ARG B 178 172.117 66.678 8.973 1.00 59.84 C
ANISOU 1660 CZ ARG B 178 7231 7357 8147 -671 -1241 435 C
ATOM 1661 NH1 ARG B 178 170.962 66.103 9.293 1.00 60.03 N
ANISOU 1661 NH1 ARG B 178 7405 7429 7974 -599 -1159 295 N
ATOM 1662 NH2 ARG B 178 172.454 66.817 7.689 1.00 56.18 N
ANISOU 1662 NH2 ARG B 178 6616 6881 7850 -555 -1058 469 N
ATOM 1663 C ARG B 178 172.078 71.720 12.745 1.00 51.79 C
ANISOU 1663 C ARG B 178 7401 5933 6345 -1528 -1889 168 C
ATOM 1664 O ARG B 178 172.868 72.494 12.178 1.00 53.43 O
ANISOU 1664 O ARG B 178 7472 6105 6722 -1580 -1949 250 O
ATOM 1665 N ILE B 179 170.791 72.014 12.916 1.00 47.96 N

ANISOU 1665 N ILE B 179 7173 5408 5643 -1433 -1653 -32 N
ATOM 1666 CA ILE B 179 170.261 73.280 12.429 1.00 51.34 C
ANISOU 1666 CA ILE B 179 7726 5749 6033 -1385 -1457 -155 C
ATOM 1667 CB ILE B 179 168.746 73.208 12.200 1.00 49.51 C
ANISOU 1667 CB ILE B 179 7591 5513 5706 -1178 -1137 -309 C
ATOM 1668 CG1 ILE B 179 168.443 72.253 11.047 1.00 45.65 C
ANISOU 1668 CG1 ILE B 179 6765 5178 5401 -943 -1018 -265 C
ATOM 1669 CD1 ILE B 179 166.948 71.995 10.853 1.00 44.85 C
ANISOU 1669 CD1 ILE B 179 6718 5080 5241 -760 -762 -371 C
ATOM 1670 CG2 ILE B 179 168.166 74.586 11.903 1.00 45.73 C
ANISOU 1670 CG2 ILE B 179 7273 4909 5192 -1151 -936 -413 C
ATOM 1671 C ILE B 179 170.665 74.442 13.365 1.00 60.56 C
ANISOU 1671 C ILE B 179 9242 6746 7022 -1657 -1608 -191 C
ATOM 1672 O ILE B 179 171.000 75.563 12.906 1.00 58.94 O
ANISOU 1672 O ILE B 179 9041 6468 6884 -1702 -1587 -199 O
ATOM 1673 N ARG B 180 170.686 74.164 14.669 1.00 66.48 N
ANISOU 1673 N ARG B 180 10304 7422 7535 -1858 -1771 -205 N
ATOM 1674 CA ARG B 180 171.163 75.166 15.637 1.00 69.06 C
ANISOU 1674 CA ARG B 180 11026 7567 7647 -2172 -1961 -228 C
ATOM 1675 CB ARG B 180 170.896 74.746 17.062 1.00 75.44 C
ANISOU 1675 CB ARG B 180 12178 8320 8168 -2281 -1995 -234 C
ATOM 1676 CG ARG B 180 169.562 74.122 17.178 1.00 82.90 C
ANISOU 1676 CG ARG B 180 13252 9258 8989 -2104 -1706 -391 C
ATOM 1677 CD ARG B 180 168.622 74.866 18.089 1.00 91.41 C
ANISOU 1677 CD ARG B 180 14795 10145 9790 -2119 -1413 -532 C
ATOM 1678 NE ARG B 180 169.129 74.968 19.456 1.00100.91 N
ANISOU 1678 NE ARG B 180 16315 11264 10761 -2343 -1573 -441 N
ATOM 1679 CZ ARG B 180 169.443 73.937 20.246 1.00103.16 C
ANISOU 1679 CZ ARG B 180 16615 11608 10973 -2421 -1766 -325 C
ATOM 1680 NH1 ARG B 180 169.887 74.169 21.481 1.00106.20 N
ANISOU 1680 NH1 ARG B 180 17341 11878 11131 -2650 -1909 -236 N
ATOM 1681 NH2 ARG B 180 169.322 72.682 19.815 1.00 98.28 N
ANISOU 1681 NH2 ARG B 180 15690 11149 10501 -2284 -1818 -288 N
ATOM 1682 C ARG B 180 172.637 75.428 15.462 1.00 60.80 C
ANISOU 1682 C ARG B 180 9743 6551 6807 -2339 -2292 -15 C
ATOM 1683 O ARG B 180 173.079 76.566 15.548 1.00 57.56 O
ANISOU 1683 O ARG B 180 9460 6038 6372 -2462 -2329 -10 O
ATOM 1684 N THR B 181 173.391 74.373 15.189 1.00 57.39 N
ANISOU 1684 N THR B 181 8938 6255 6611 -2315 -2492 181 N
ATOM 1685 CA THR B 181 174.795 74.556 14.870 1.00 59.91 C
ANISOU 1685 CA THR B 181 8944 6598 7222 -2411 -2738 428 C
ATOM 1686 CB THR B 181 175.523 73.230 14.599 1.00 66.32 C
ANISOU 1686 CB THR B 181 9331 7539 8330 -2337 -2878 662 C
ATOM 1687 OG1 THR B 181 175.603 72.481 15.816 1.00 73.88 O
ANISOU 1687 OG1 THR B 181 10457 8499 9114 -2430 -3025 745 O
ATOM 1688 CG2 THR B 181 176.947 73.498 14.086 1.00 62.18 C
ANISOU 1688 CG2 THR B 181 8440 7006 8180 -2390 -3049 935 C
ATOM 1689 C THR B 181 174.908 75.477 13.669 1.00 52.36 C
ANISOU 1689 C THR B 181 7812 5615 6469 -2333 -2603 386 C
ATOM 1690 O THR B 181 175.606 76.470 13.708 1.00 57.02 O
ANISOU 1690 O THR B 181 8440 6117 7108 -2479 -2720 449 O
ATOM 1691 N TYR B 182 174.187 75.161 12.606 1.00 51.70 N
ANISOU 1691 N TYR B 182 7527 5630 6486 -2013 -2259 296 N
ATOM 1692 CA TYR B 182 174.224 75.977 11.396 1.00 50.09 C
ANISOU 1692 CA TYR B 182 7150 5422 6460 -1864 -2051 272 C
ATOM 1693 CB TYR B 182 173.351 75.356 10.309 1.00 46.79 C
ANISOU 1693 CB TYR B 182 6547 5122 6109 -1538 -1719 192 C
ATOM 1694 CG TYR B 182 173.556 75.997 8.969 1.00 50.20 C
ANISOU 1694 CG TYR B 182 6769 5562 6744 -1392 -1539 215 C
ATOM 1695 CD1 TYR B 182 172.789 77.099 8.588 1.00 53.00 C
ANISOU 1695 CD1 TYR B 182 7291 5850 6996 -1329 -1341 69 C
ATOM 1696 CE1 TYR B 182 172.979 77.721 7.373 1.00 54.48 C
ANISOU 1696 CE1 TYR B 182 7308 6040 7353 -1209 -1189 100 C
ATOM 1697 CZ TYR B 182 173.945 77.240 6.508 1.00 55.96 C
ANISOU 1697 CZ TYR B 182 7175 6281 7808 -1145 -1200 268 C
ATOM 1698 OH TYR B 182 174.075 77.899 5.296 1.00 58.47 O
ANISOU 1698 OH TYR B 182 7372 6583 8261 -1027 -1022 289 O
ATOM 1699 CE2 TYR B 182 174.740 76.135 6.863 1.00 51.93 C
ANISOU 1699 CE2 TYR B 182 6479 5818 7433 -1194 -1362 422 C
ATOM 1700 CD2 TYR B 182 174.536 75.527 8.093 1.00 51.75 C
ANISOU 1700 CD2 TYR B 182 6608 5807 7246 -1320 -1547 399 C
ATOM 1701 C TYR B 182 173.771 77.415 11.657 1.00 52.92 C
ANISOU 1701 C TYR B 182 7853 5631 6624 -1967 -1967 111 C
ATOM 1702 O TYR B 182 174.367 78.359 11.136 1.00 51.49 O
ANISOU 1702 O TYR B 182 7590 5389 6586 -2020 -1987 160 O
ATOM 1703 N ASN B 183 172.724 77.574 12.468 1.00 54.55 N
ANISOU 1703 N ASN B 183 8447 5758 6521 -1992 -1844 -73 N
ATOM 1704 CA ASN B 183 172.195 78.906 12.788 1.00 57.74 C
ANISOU 1704 CA ASN B 183 9221 5981 6736 -2078 -1698 -233 C
ATOM 1705 CB ASN B 183 170.885 78.824 13.580 1.00 55.14 C
ANISOU 1705 CB ASN B 183 9274 5559 6116 -2032 -1460 -418 C
ATOM 1706 CG ASN B 183 169.674 78.672 12.674 1.00 56.88 C
ANISOU 1706 CG ASN B 183 9328 5849 6436 -1697 -1085 -499 C
ATOM 1707 OD1 ASN B 183 169.761 78.933 11.458 1.00 57.99 O
ANISOU 1707 OD1 ASN B 183 9159 6072 6802 -1532 -990 -449 O
ATOM 1708 ND2 ASN B 183 168.535 78.247 13.251 1.00 50.75 N
ANISOU 1708 ND2 ASN B 183 8757 5027 5497 -1607 -877 -606 N
ATOM 1709 C ASN B 183 173.179 79.783 13.522 1.00 65.45 C
ANISOU 1709 C ASN B 183 10428 6806 7635 -2424 -1996 -178 C
ATOM 1710 O ASN B 183 173.167 81.008 13.404 1.00 65.84 O
ANISOU 1710 O ASN B 183 10654 6715 7649 -2497 -1907 -253 O
ATOM 1711 N GLN B 184 174.032 79.142 14.299 1.00 73.30 N
ANISOU 1711 N GLN B 184 11379 7858 8612 -2580 -2307 -12 N
ATOM 1712 CA GLN B 184 174.948 79.884 15.138 1.00 82.13 C
ANISOU 1712 CA GLN B 184 12671 8898 9636 -2810 -2535 101 C
ATOM 1713 CB GLN B 184 175.150 79.186 16.482 1.00 91.25 C
ANISOU 1713 CB GLN B 184 14043 10061 10565 -2947 -2729 196 C
ATOM 1714 CG GLN B 184 174.084 79.545 17.531 1.00101.96 C
ANISOU 1714 CG GLN B 184 15942 11286 11513 -2986 -2506 1 C
ATOM 1715 CD GLN B 184 172.658 79.754 16.965 1.00106.22 C
ANISOU 1715 CD GLN B 184 16583 11780 11998 -2761 -2074 -251 C
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ANISOU 1716 OE1 GLN B 184 16971 12068 12436 -2702 -1879 -359 O
ATOM 1717 NE2 GLN B 184 171.761 78.821 17.278 1.00105.45 N
ANISOU 1717 NE2 GLN B 184 16554 11721 11792 -2635 -1920 -328 N
ATOM 1718 C GLN B 184 176.256 80.101 14.418 1.00 80.15 C
ANISOU 1718 C GLN B 184 12019 8692 9741 -2864 -2761 324 C
ATOM 1719 O GLN B 184 176.783 81.207 14.375 1.00 82.41 O
ANISOU 1719 O GLN B 184 12376 8884 10051 -2981 -2817 348 O
ATOM 1720 N HIS B 185 176.786 79.066 13.828 1.00 75.86 N
ANISOU 1720 N HIS B 185 11044 8282 9496 -2762 -2859 497 N
ATOM 1721 CA HIS B 185 178.049 79.195 13.178 1.00 74.68 C
ANISOU 1721 CA HIS B 185 10473 8162 9739 -2777 -3022 748 C
ATOM 1722 CB HIS B 185 178.551 77.841 12.772 1.00 77.52 C
ANISOU 1722 CB HIS B 185 10412 8651 10392 -2650 -3082 950 C
ATOM 1723 CG HIS B 185 179.149 77.080 13.899 1.00 88.03 C
ANISOU 1723 CG HIS B 185 11789 9999 11660 -2778 -3359 1147 C
ATOM 1724 ND1 HIS B 185 179.135 77.551 15.190 1.00 93.29 N
ANISOU 1724 ND1 HIS B 185 12851 10573 12022 -3002 -3550 1147 N
ATOM 1725 CE1 HIS B 185 179.719 76.676 15.980 1.00 97.67 C
ANISOU 1725 CE1 HIS B 185 13359 11147 12602 -3089 -3788 1370 C
ATOM 1726 NE2 HIS B 185 180.104 75.650 15.246 1.00 97.08 N
ANISOU 1726 NE2 HIS B 185 12864 11175 12849 -2910 -3731 1501 N
ATOM 1727 CD2 HIS B 185 179.769 75.883 13.940 1.00 90.14 C
ANISOU 1727 CD2 HIS B 185 11758 10345 12146 -2712 -3458 1366 C
ATOM 1728 C HIS B 185 178.042 80.071 11.976 1.00 72.41 C
ANISOU 1728 C HIS B 185 10028 7824 9659 -2694 -2837 688 C
ATOM 1729 O HIS B 185 179.011 80.716 11.674 1.00 80.31 O
ANISOU 1729 O HIS B 185 10906 8768 10839 -2781 -2944 820 O
ATOM 1730 N TYR B 186 176.943 80.076 11.274 1.00 72.02 N
ANISOU 1730 N TYR B 186 9985 7808 9570 -2478 -2519 501 N
ATOM 1731 CA TYR B 186 176.873 80.634 9.954 1.00 71.52 C
ANISOU 1731 CA TYR B 186 9724 7758 9693 -2262 -2234 471 C
ATOM 1732 CB TYR B 186 176.359 79.551 9.030 1.00 75.47 C
ANISOU 1732 CB TYR B 186 9949 8416 10312 -1926 -1955 465 C
ATOM 1733 CG TYR B 186 177.374 78.926 8.142 1.00 84.72 C
ANISOU 1733 CG TYR B 186 10677 9649 11864 -1849 -1995 710 C
ATOM 1734 CD2 TYR B 186 177.670 79.485 6.930 1.00 88.16 C
ANISOU 1734 CD2 TYR B 186 10885 10073 12540 -1701 -1792 772 C
ATOM 1735 CE2 TYR B 186 178.587 78.916 6.089 1.00 92.39 C
ANISOU 1735 CE2 TYR B 186 11040 10625 13438 -1615 -1759 1001 C
ATOM 1736 CZ TYR B 186 179.205 77.766 6.452 1.00 96.59 C
ANISOU 1736 CZ TYR B 186 11380 11191 14130 -1673 -1939 1188 C
ATOM 1737 OH TYR B 186 180.111 77.224 5.594 1.00102.22 O
ANISOU 1737 OH TYR B 186 11706 11885 15248 -1572 -1849 1436 O
ATOM 1738 CE1 TYR B 186 178.928 77.178 7.648 1.00 93.23 C
ANISOU 1738 CE1 TYR B 186 11154 10796 13473 -1827 -2182 1141 C
ATOM 1739 CD1 TYR B 186 178.007 77.756 8.488 1.00 89.24 C
ANISOU 1739 CD1 TYR B 186 11064 10271 12572 -1917 -2205 895 C
ATOM 1740 C TYR B 186 175.902 81.785 9.931 1.00 64.14 C
ANISOU 1740 C TYR B 186 9138 6710 8523 -2247 -2010 241 C
ATOM 1741 O TYR B 186 175.281 82.029 8.942 1.00 61.93 O
ANISOU 1741 O TYR B 186 8761 6463 8307 -2009 -1705 164 O
ATOM 1742 N ASN B 187 175.763 82.478 11.039 1.00 62.32 N
ANISOU 1742 N ASN B 187 9334 6328 8017 -2511 -2154 143 N
ATOM 1743 CA ASN B 187 174.815 83.559 11.123 1.00 67.81 C
ANISOU 1743 CA ASN B 187 10402 6871 8490 -2510 -1905 -71 C
ATOM 1744 CB ASN B 187 174.679 83.976 12.561 1.00 78.04 C
ANISOU 1744 CB ASN B 187 12167 8034 9453 -2770 -2046 -140 C
ATOM 1745 CG ASN B 187 173.505 84.876 12.787 1.00 84.41 C
ANISOU 1745 CG ASN B 187 13399 8677 9997 -2718 -1697 -373 C
ATOM 1746 OD1 ASN B 187 172.619 85.002 11.948 1.00 86.04 O
ANISOU 1746 OD1 ASN B 187 13577 8858 10257 -2505 -1379 -490 O
ATOM 1747 ND2 ASN B 187 173.493 85.519 13.926 1.00 85.00 N
ANISOU 1747 ND2 ASN B 187 13857 8637 9801 -2892 -1729 -413 N
ATOM 1748 C ASN B 187 175.186 84.759 10.276 1.00 68.04 C
ANISOU 1748 C ASN B 187 10310 6831 8711 -2465 -1781 -54 C
ATOM 1749 O ASN B 187 174.344 85.483 9.799 1.00 64.82 O
ANISOU 1749 O ASN B 187 9985 6379 8266 -2283 -1448 -188 O
ATOM 1750 N ASN B 188 176.469 84.958 10.090 1.00 69.05 N
ANISOU 1750 N ASN B 188 10230 6938 9067 -2638 -2054 133 N
ATOM 1751 CA ASN B 188 176.944 86.043 9.271 1.00 71.48 C
ANISOU 1751 CA ASN B 188 10403 7177 9579 -2606 -1951 170 C
ATOM 1752 CB ASN B 188 178.460 86.061 9.288 1.00 76.31 C
ANISOU 1752 CB ASN B 188 10765 7759 10470 -2829 -2302 419 C
ATOM 1753 CG ASN B 188 179.009 86.591 10.567 1.00 83.08 C
ANISOU 1753 CG ASN B 188 11918 8568 11082 -3066 -2548 430 C
ATOM 1754 OD1 ASN B 188 178.295 87.161 11.355 1.00 89.66 O
ANISOU 1754 OD1 ASN B 188 13199 9292 11574 -3143 -2440 232 O
ATOM 1755 ND2 ASN B 188 180.276 86.390 10.786 1.00 82.66 N

ANISOU 1755 ND2 ASN B 188 11627 8574 11206 -3179 -2865 685 N
ATOM 1756 C ASN B 188 176.470 85.965 7.843 1.00 66.95 C
ANISOU 1756 C ASN B 188 9517 6728 9194 -2239 -1602 166 C
ATOM 1757 O ASN B 188 176.148 86.962 7.261 1.00 67.49 O
ANISOU 1757 O ASN B 188 9636 6725 9283 -2144 -1375 90 O
ATOM 1758 N LEU B 189 176.465 84.771 7.285 1.00 61.56 N
ANISOU 1758 N LEU B 189 8531 6217 8640 -2049 -1569 257 N
ATOM 1759 CA LEU B 189 176.128 84.548 5.895 1.00 62.09 C
ANISOU 1759 CA LEU B 189 8331 6393 8866 -1742 -1282 276 C
ATOM 1760 CB LEU B 189 176.511 83.127 5.495 1.00 61.64 C
ANISOU 1760 CB LEU B 189 7971 6485 8965 -1617 -1313 410 C
ATOM 1761 CG LEU B 189 177.470 82.897 4.332 1.00 62.17 C
ANISOU 1761 CG LEU B 189 7663 6583 9376 -1500 -1236 606 C
ATOM 1762 CD1 LEU B 189 177.618 81.404 4.133 1.00 62.87 C
ANISOU 1762 CD1 LEU B 189 7543 6788 9555 -1378 -1219 701 C
ATOM 1763 CD2 LEU B 189 176.984 83.562 3.060 1.00 57.30 C
ANISOU 1763 CD2 LEU B 189 7021 5966 8785 -1294 -929 547 C
ATOM 1764 C LEU B 189 174.634 84.678 5.739 1.00 62.94 C
ANISOU 1764 C LEU B 189 8642 6519 8754 -1557 -1001 82 C
ATOM 1765 O LEU B 189 174.133 85.388 4.861 1.00 61.02 O
ANISOU 1765 O LEU B 189 8375 6256 8552 -1405 -768 42 O
ATOM 1766 N LEU B 190 173.946 83.959 6.618 1.00 62.94 N
ANISOU 1766 N LEU B 190 8826 6548 8542 -1578 -1035 -11 N
ATOM 1767 CA LEU B 190 172.509 83.727 6.555 1.00 63.15 C
ANISOU 1767 CA LEU B 190 8984 6606 8406 -1390 -786 -151 C
ATOM 1768 CB LEU B 190 172.129 82.742 7.643 1.00 67.75 C
ANISOU 1768 CB LEU B 190 9723 7219 8798 -1457 -889 -206 C
ATOM 1769 CG LEU B 190 171.276 81.566 7.219 1.00 74.45 C
ANISOU 1769 CG LEU B 190 10432 8218 9636 -1232 -759 -221 C
ATOM 1770 CD1 LEU B 190 171.050 80.704 8.472 1.00 77.34 C
ANISOU 1770 CD1 LEU B 190 10987 8588 9811 -1340 -886 -269 C
ATOM 1771 CD2 LEU B 190 169.958 82.026 6.591 1.00 73.51 C
ANISOU 1771 CD2 LEU B 190 10355 8081 9496 -1027 -459 -304 C
ATOM 1772 C LEU B 190 171.660 84.976 6.744 1.00 61.83 C
ANISOU 1772 C LEU B 190 9091 6274 8126 -1388 -573 -282 C
ATOM 1773 O LEU B 190 170.708 85.197 6.003 1.00 56.91 O
ANISOU 1773 O LEU B 190 8414 5670 7538 -1180 -324 -312 O
ATOM 1774 N ARG B 191 172.014 85.788 7.738 1.00 68.47 N
ANISOU 1774 N ARG B 191 10238 6938 8839 -1634 -674 -342 N
ATOM 1775 CA ARG B 191 171.209 86.949 8.119 1.00 74.22 C
ANISOU 1775 CA ARG B 191 11298 7462 9441 -1655 -435 -477 C
ATOM 1776 CB ARG B 191 171.350 88.090 7.109 1.00 74.04 C
ANISOU 1776 CB ARG B 191 11145 7383 9603 -1573 -288 -438 C
ATOM 1777 CG ARG B 191 172.740 88.712 7.108 1.00 75.92 C
ANISOU 1777 CG ARG B 191 11337 7563 9945 -1796 -533 -353 C
ATOM 1778 CD ARG B 191 172.757 90.056 6.420 1.00 79.96 C
ANISOU 1778 CD ARG B 191 11847 7953 10581 -1758 -355 -353 C
ATOM 1779 NE ARG B 191 173.104 91.147 7.335 1.00 89.29 N
ANISOU 1779 NE ARG B 191 13402 8892 11634 -2034 -411 -436 N
ATOM 1780 CZ ARG B 191 172.425 92.291 7.463 1.00 88.21 C
ANISOU 1780 CZ ARG B 191 13536 8548 11431 -2024 -136 -546 C
ATOM 1781 NH1 ARG B 191 171.333 92.505 6.733 1.00 88.25 N
ANISOU 1781 NH1 ARG B 191 13440 8569 11521 -1741 203 -560 N
ATOM 1782 NH2 ARG B 191 172.842 93.220 8.326 1.00 84.38 N
ANISOU 1782 NH2 ARG B 191 13431 7823 10804 -2310 -204 -626 N
ATOM 1783 C ARG B 191 169.759 86.529 8.274 1.00 73.97 C
ANISOU 1783 C ARG B 191 11365 7431 9311 -1460 -161 -567 C
ATOM 1784 O ARG B 191 168.854 87.141 7.717 1.00 77.21 O
ANISOU 1784 O ARG B 191 11758 7781 9798 -1283 125 -588 O
ATOM 1785 N GLY B 192 169.569 85.445 9.018 1.00 70.73 N
ANISOU 1785 N GLY B 192 11027 7088 8760 -1493 -263 -592 N
ATOM 1786 CA GLY B 192 168.259 84.914 9.309 1.00 71.86 C
ANISOU 1786 CA GLY B 192 11261 7224 8820 -1331 -28 -662 C
ATOM 1787 C GLY B 192 168.454 83.629 10.075 1.00 76.87 C
ANISOU 1787 C GLY B 192 11927 7962 9319 -1408 -230 -660 C
ATOM 1788 O GLY B 192 169.567 83.326 10.507 1.00 85.87 O
ANISOU 1788 O GLY B 192 13070 9139 10418 -1612 -542 -607 O
ATOM 1789 N ALA B 193 167.375 82.875 10.251 1.00 70.09 N
ANISOU 1789 N ALA B 193 11074 7140 8417 -1249 -60 -697 N
ATOM 1790 CA ALA B 193 167.443 81.577 10.900 1.00 57.93 C
ANISOU 1790 CA ALA B 193 9539 5708 6765 -1288 -220 -690 C
ATOM 1791 CB ALA B 193 166.814 81.629 12.279 1.00 54.00 C
ANISOU 1791 CB ALA B 193 9495 5018 6006 -1404 -98 -811 C
ATOM 1792 C ALA B 193 166.671 80.625 10.035 1.00 57.55 C
ANISOU 1792 C ALA B 193 9166 5837 6863 -1025 -113 -636 C
ATOM 1793 O ALA B 193 165.511 80.879 9.707 1.00 59.23 O
ANISOU 1793 O ALA B 193 9366 5996 7142 -851 158 -655 O
ATOM 1794 N VAL B 194 167.298 79.523 9.650 1.00 53.72 N
ANISOU 1794 N VAL B 194 8418 5546 6447 -1004 -323 -551 N
ATOM 1795 CA VAL B 194 166.524 78.480 9.037 1.00 50.37 C
ANISOU 1795 CA VAL B 194 7770 5266 6101 -797 -237 -519 C
ATOM 1796 CB VAL B 194 167.408 77.467 8.283 1.00 47.68 C
ANISOU 1796 CB VAL B 194 7119 5115 5880 -765 -427 -412 C
ATOM 1797 CG1 VAL B 194 168.853 77.887 8.368 1.00 50.34 C
ANISOU 1797 CG1 VAL B 194 7418 5435 6273 -941 -644 -342 C
ATOM 1798 CG2 VAL B 194 167.199 76.065 8.777 1.00 39.36 C
ANISOU 1798 CG2 VAL B 194 6031 4160 4764 -739 -498 -407 C
ATOM 1799 C VAL B 194 165.680 77.874 10.160 1.00 46.53 C
ANISOU 1799 C VAL B 194 7511 4717 5452 -806 -151 -595 C
ATOM 1800 O VAL B 194 166.131 77.793 11.296 1.00 48.60 O
ANISOU 1800 O VAL B 194 8028 4902 5535 -992 -272 -639 O
ATOM 1801 N SER B 195 164.443 77.521 9.840 1.00 42.07 N
ANISOU 1801 N SER B 195 6867 4165 4952 -617 57 -597 N
ATOM 1802 CA SER B 195 163.552 76.840 10.766 1.00 52.48 C
ANISOU 1802 CA SER B 195 8347 5429 6166 -586 176 -647 C
ATOM 1803 CB SER B 195 162.170 76.712 10.131 1.00 60.75 C
ANISOU 1803 CB SER B 195 9230 6474 7379 -367 412 -601 C
ATOM 1804 OG SER B 195 161.732 78.018 9.787 1.00 69.72 O
ANISOU 1804 OG SER B 195 10413 7460 8618 -321 614 -592 O
ATOM 1805 C SER B 195 164.064 75.484 11.234 1.00 51.84 C
ANISOU 1805 C SER B 195 8215 5485 5996 -645 -39 -630 C
ATOM 1806 O SER B 195 164.925 74.879 10.602 1.00 42.86 O
ANISOU 1806 O SER B 195 6838 4509 4939 -651 -243 -557 O
ATOM 1807 N GLN B 196 163.480 74.987 12.316 1.00 64.16 N
ANISOU 1807 N GLN B 196 10002 6966 7410 -672 44 -687 N
ATOM 1808 CA GLN B 196 164.055 73.855 13.039 1.00 72.80 C
ANISOU 1808 CA GLN B 196 11130 8149 8381 -774 -170 -672 C
ATOM 1809 CB GLN B 196 163.972 74.078 14.546 1.00 80.99 C
ANISOU 1809 CB GLN B 196 12621 9001 9149 -951 -138 -757 C
ATOM 1810 CG GLN B 196 165.316 74.343 15.193 1.00 95.59 C
ANISOU 1810 CG GLN B 196 14648 10827 10844 -1229 -457 -736 C
ATOM 1811 CD GLN B 196 165.674 75.830 15.239 1.00108.14 C
ANISOU 1811 CD GLN B 196 16464 12247 12378 -1367 -425 -787 C
ATOM 1812 OE1 GLN B 196 166.392 76.280 16.142 1.00110.78 O
ANISOU 1812 OE1 GLN B 196 17129 12459 12502 -1637 -608 -808 O
ATOM 1813 NE2 GLN B 196 165.174 76.600 14.260 1.00112.63 N
ANISOU 1813 NE2 GLN B 196 16864 12799 13132 -1199 -207 -796 N
ATOM 1814 C GLN B 196 163.509 72.463 12.711 1.00 70.84 C
ANISOU 1814 C GLN B 196 10643 8054 8219 -618 -163 -628 C
ATOM 1815 O GLN B 196 163.999 71.467 13.245 1.00 76.13 O
ANISOU 1815 O GLN B 196 11308 8803 8813 -687 -334 -601 O
ATOM 1816 N ARG B 197 162.508 72.374 11.852 1.00 59.95 N
ANISOU 1816 N ARG B 197 9069 6708 7002 -424 16 -605 N
ATOM 1817 CA ARG B 197 161.961 71.056 11.539 1.00 49.55 C
ANISOU 1817 CA ARG B 197 7550 5520 5758 -301 10 -563 C
ATOM 1818 CB ARG B 197 160.438 71.021 11.711 1.00 53.83 C
ANISOU 1818 CB ARG B 197 8120 5962 6373 -163 275 -566 C
ATOM 1819 CG ARG B 197 159.874 72.262 12.354 1.00 64.15 C
ANISOU 1819 CG ARG B 197 9690 7037 7647 -180 523 -615 C
ATOM 1820 CD ARG B 197 158.752 72.003 13.355 1.00 68.99 C
ANISOU 1820 CD ARG B 197 10495 7485 8232 -122 790 -639 C
ATOM 1821 NE ARG B 197 158.929 72.811 14.570 1.00 80.52 N
ANISOU 1821 NE ARG B 197 12398 8719 9478 -259 934 -738 N
ATOM 1822 CZ ARG B 197 158.862 74.147 14.633 1.00 86.32 C
ANISOU 1822 CZ ARG B 197 13318 9265 10213 -292 1114 -773 C
ATOM 1823 NH1 ARG B 197 159.057 74.768 15.793 1.00 91.37 N
ANISOU 1823 NH1 ARG B 197 14425 9682 10610 -447 1239 -877 N
ATOM 1824 NH2 ARG B 197 158.606 74.869 13.548 1.00 84.76 N
ANISOU 1824 NH2 ARG B 197 12879 9169 10244 -184 1169 -702 N
ATOM 1825 C ARG B 197 162.345 70.607 10.146 1.00 44.78 C
ANISOU 1825 C ARG B 197 6627 5082 5304 -221 -102 -489 C
ATOM 1826 O ARG B 197 162.632 71.413 9.264 1.00 48.26 O
ANISOU 1826 O ARG B 197 6980 5527 5829 -207 -104 -462 O
ATOM 1827 N LEU B 198 162.348 69.301 9.930 1.00 41.67 N
ANISOU 1827 N LEU B 198 6087 4812 4935 -172 -178 -456 N
ATOM 1828 CA LEU B 198 162.463 68.791 8.575 1.00 41.75 C
ANISOU 1828 CA LEU B 198 5858 4942 5063 -90 -223 -396 C
ATOM 1829 CB LEU B 198 162.963 67.366 8.608 1.00 37.38 C
ANISOU 1829 CB LEU B 198 5205 4496 4502 -90 -326 -369 C
ATOM 1830 CG LEU B 198 163.005 66.664 7.259 1.00 41.71 C
ANISOU 1830 CG LEU B 198 5576 5136 5137 -15 -332 -322 C
ATOM 1831 CD1 LEU B 198 164.036 67.316 6.311 1.00 38.71 C
ANISOU 1831 CD1 LEU B 198 5126 4766 4818 -41 -365 -280 C
ATOM 1832 CD2 LEU B 198 163.310 65.171 7.472 1.00 36.17 C
ANISOU 1832 CD2 LEU B 198 4807 4505 4430 -5 -380 -303 C
ATOM 1833 C LEU B 198 161.090 68.855 7.879 1.00 44.48 C
ANISOU 1833 C LEU B 198 6124 5271 5505 32 -94 -368 C
ATOM 1834 O LEU B 198 160.102 68.354 8.425 1.00 50.79 O
ANISOU 1834 O LEU B 198 6949 6034 6314 84 -7 -371 O
ATOM 1835 N TYR B 199 161.014 69.517 6.720 1.00 36.43 N
ANISOU 1835 N TYR B 199 5009 4262 4570 67 -87 -320 N
ATOM 1836 CA TYR B 199 159.753 69.591 5.955 1.00 34.46 C
ANISOU 1836 CA TYR B 199 4660 3998 4435 156 -23 -246 C
ATOM 1837 CB TYR B 199 159.447 71.013 5.497 1.00 33.63 C
ANISOU 1837 CB TYR B 199 4555 3801 4420 175 59 -201 C
ATOM 1838 CG TYR B 199 159.161 71.921 6.666 1.00 42.42 C
ANISOU 1838 CG TYR B 199 5828 4757 5532 167 225 -249 C
ATOM 1839 CD1 TYR B 199 160.206 72.425 7.464 1.00 43.64 C
ANISOU 1839 CD1 TYR B 199 6160 4867 5555 63 206 -343 C
ATOM 1840 CE1 TYR B 199 159.948 73.236 8.544 1.00 44.58 C
ANISOU 1840 CE1 TYR B 199 6501 4813 5625 27 367 -401 C
ATOM 1841 CZ TYR B 199 158.620 73.567 8.857 1.00 46.43 C
ANISOU 1841 CZ TYR B 199 6761 4902 5979 126 606 -359 C
ATOM 1842 OH TYR B 199 158.344 74.384 9.954 1.00 48.34 O
ANISOU 1842 OH TYR B 199 7277 4928 6164 92 833 -423 O
ATOM 1843 CE2 TYR B 199 157.570 73.054 8.093 1.00 44.08 C
ANISOU 1843 CE2 TYR B 199 6228 4652 5867 245 625 -238 C
ATOM 1844 CD2 TYR B 199 157.852 72.235 7.010 1.00 42.22 C
ANISOU 1844 CD2 TYR B 199 5796 4604 5642 250 409 -188 C
ATOM 1845 C TYR B 199 159.683 68.588 4.799 1.00 32.02 C

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ANISOU 1845  C   TYR B 199     4230   3801   4137    173   -129   -195       C
ATOM   1846  O   TYR B 199      160.528  68.569   3.904  1.00 32.01           O
ANISOU 1846  O   TYR B 199     4207   3856   4101    144   -196   -188       O
ATOM   1847  N   ILE B 200      158.669  67.735   4.847  1.00 26.37           N
ANISOU 1847  N   ILE B 200     3458   3096   3465    213   -129   -156       N
ATOM   1848  CA  ILE B 200      158.608  66.578   3.969  1.00 28.90           C
ANISOU 1848  CA  ILE B 200     3723   3504   3753    201   -232   -129       C
ATOM   1849  CB  ILE B 200      158.457  65.306   4.803  1.00 33.30           C
ANISOU 1849  CB  ILE B 200     4284   4092   4276    211   -228   -172       C
ATOM   1850  CG1 ILE B 200      159.714  65.132   5.652  1.00 39.48           C
ANISOU 1850  CG1 ILE B 200     5136   4897   4968    177   -225   -253       C
ATOM   1851  CD1 ILE B 200      159.619  64.067   6.703  1.00 41.48           C
ANISOU 1851  CD1 ILE B 200     5411   5165   5183    183   -215   -287       C
ATOM   1852  CG2 ILE B 200      158.231  64.093   3.926  1.00 23.10           C
ANISOU 1852  CG2 ILE B 200     2958   2862   2955    191   -314   -145       C
ATOM   1853  C   ILE B 200      157.476  66.717   2.973  1.00 27.65           C
ANISOU 1853  C   ILE B 200     3487   3329   3690    207   -290     -8       C
ATOM   1854  O   ILE B 200      156.283  66.619   3.324  1.00 30.64           O
ANISOU 1854  O   ILE B 200     3788   3656   4199    245   -264     70       O
ATOM   1855  N   LEU B 201      157.861  66.984   1.731  1.00 26.69           N
ANISOU 1855  N   LEU B 201     3388   3236   3516    163   -369     28       N
ATOM   1856  CA  LEU B 201      156.897  67.079   0.648  1.00 31.08           C
ANISOU 1856  CA  LEU B 201     3902   3780   4129    127   -484    164       C
ATOM   1857  CB  LEU B 201      157.549  67.681  -0.591  1.00 36.06           C
ANISOU 1857  CB  LEU B 201     4614   4420   4667     74   -536    188       C
ATOM   1858  CG  LEU B 201      157.997  69.132  -0.381  1.00 38.64           C
ANISOU 1858  CG  LEU B 201     4920   4699   5061    115   -440    185       C
ATOM   1859  CD1 LEU B 201      158.874  69.532  -1.545  1.00 35.08           C
ANISOU 1859  CD1 LEU B 201     4567   4263   4501     66   -465    187       C
ATOM   1860  CD2 LEU B 201      156.817  70.089  -0.262  1.00 36.75           C
ANISOU 1860  CD2 LEU B 201     4564   4380   5021    156   -427    325       C
ATOM   1861  C   LEU B 201      156.247  65.727   0.329  1.00 28.35           C
ANISOU 1861  C   LEU B 201     3556   3466   3749     78   -596    197       C
ATOM   1862  O   LEU B 201      156.924  64.757   0.084  1.00 27.03           O
ANISOU 1862  O   LEU B 201     3487   3345   3437     41   -607    112       O
ATOM   1863  N   LEU B 202      154.919  65.672   0.349  1.00 29.08           N
ANISOU 1863  N   LEU B 202     3529   3517   4003     78   -668    337       N
ATOM   1864  CA  LEU B 202      154.187  64.475  -0.015  1.00 26.99           C
ANISOU 1864  CA  LEU B 202     3257   3269   3729      7   -810    396       C
ATOM   1865  CB  LEU B 202      153.418  63.988   1.195  1.00 34.82           C
ANISOU 1865  CB  LEU B 202     4120   4227   4884     85   -719    410       C
ATOM   1866  CG  LEU B 202      154.268  63.364   2.288  1.00 46.17           C
ANISOU 1866  CG  LEU B 202     5630   5702   6212    145   -570    230       C
ATOM   1867  CD1 LEU B 202      153.869  63.865   3.636  1.00 52.42           C
ANISOU 1867  CD1 LEU B 202     6355   6420   7143    248   -387    224       C
ATOM   1868  CD2 LEU B 202      153.984  61.910   2.241  1.00 55.81           C
ANISOU 1868  CD2 LEU B 202     6866   6956   7383    100   -645    214       C
ATOM   1869  C   LEU B 202      153.201  64.765  -1.098  1.00 30.78           C
ANISOU 1869  C   LEU B 202     3686   3714   4295    -90  -1018    600       C
ATOM   1870  O   LEU B 202      151.997  64.856  -0.816  1.00 39.87           O
ANISOU 1870  O   LEU B 202     4651   4807   5689    -73  -1069    770       O
ATOM   1871  N   PRO B 203      153.683  64.929  -2.337  1.00 32.30           N
ANISOU 1871  N   PRO B 203     4041   3925   4306   -197  -1139    609       N
ATOM   1872  CA  PRO B 203      152.747  65.054  -3.474  1.00 38.44           C
ANISOU 1872  CA  PRO B 203     4820   4668   5117   -340  -1404    822       C
ATOM   1873  CB  PRO B 203      153.656  65.256  -4.682  1.00 29.90           C
ANISOU 1873  CB  PRO B 203     4006   3599   3757   -442  -1451    763       C
ATOM   1874  CG  PRO B 203      154.925  64.593  -4.286  1.00 37.83           C
ANISOU 1874  CG  PRO B 203     5154   4641   4578   -382  -1241    524       C
ATOM   1875  CD  PRO B 203      155.083  64.880  -2.788  1.00 32.85           C
ANISOU 1875  CD  PRO B 203     4320   4032   4132   -211  -1045    444       C
ATOM   1876  C   PRO B 203      151.942  63.772  -3.656  1.00 37.98           C
ANISOU 1876  C   PRO B 203     4778   4604   5046   -457  -1588    886       C
ATOM   1877  O   PRO B 203      152.504  62.697  -3.851  1.00 42.09           O
ANISOU 1877  O   PRO B 203     5500   5151   5340   -519  -1576    740       O
ATOM   1878  N   LEU B 204      150.622  63.898  -3.587  1.00 34.80           N
ANISOU 1878  N   LEU B 204     4153   4150   4918   -487  -1747   1123       N
ATOM   1879  CA  LEU B 204      149.722  62.761  -3.715  1.00 38.40           C
ANISOU 1879  CA  LEU B 204     4581   4587   5422   -609  -1950   1226       C
ATOM   1880  CB  LEU B 204      148.303  63.181  -3.370  1.00 40.15           C
ANISOU 1880  CB  LEU B 204     4457   4730   6068   -584  -2052   1524       C
ATOM   1881  CG  LEU B 204      148.316  63.585  -1.899  1.00 45.77           C
ANISOU 1881  CG  LEU B 204     4969   5414   7008   -341  -1700   1446       C
ATOM   1882  CD1 LEU B 204      146.967  64.050  -1.469  1.00 51.30           C
ANISOU 1882  CD1 LEU B 204     5325   5997   8169   -278  -1700   1742       C
ATOM   1883  CD2 LEU B 204      148.817  62.433  -0.980  1.00 31.72           C
ANISOU 1883  CD2 LEU B 204     3283   3682   5087   -275  -1528   1208       C
ATOM   1884  C   LEU B 204      149.752  62.085  -5.095  1.00 48.36           C
ANISOU 1884  C   LEU B 204     6138   5844   6391   -863  -2241   1256       C
ATOM   1885  O   LEU B 204      149.519  60.882  -5.196  1.00 55.98           O
ANISOU 1885  O   LEU B 204     7217   6802   7251   -975  -2344   1218       O
ATOM   1886  N   ASP B 205      150.025  62.843  -6.152  1.00 43.11           N
ANISOU 1886  N   ASP B 205     5631   5168   5582   -966  -2365   1323       N
ATOM   1887  CA  ASP B 205      150.189  62.255  -7.499  1.00 49.50           C
ANISOU 1887  CA  ASP B 205     6822   5946   6039  -1225  -2603   1325       C
ATOM   1888  CB  ASP B 205      150.185  63.320  -8.638  1.00 39.30           C
ANISOU 1888  CB  ASP B 205     5650   4624   4657  -1345  -2786   1484       C
ATOM   1889  CG  ASP B 205      151.448  64.235  -8.631  1.00 62.09           C
ANISOU 1889  CG  ASP B 205     8626   7541   7424  -1187  -2483   1305       C
ATOM   1890  OD2 ASP B 205      151.412  65.278  -9.333  1.00 69.87           O
ANISOU 1890  OD2 ASP B 205     9630   8506   8412  -1231  -2583   1443       O
ATOM   1891  OD1 ASP B 205      152.471  63.935  -7.962  1.00 55.03           O
ANISOU 1891  OD1 ASP B 205     7775   6685   6449  -1032  -2167   1052       O
ATOM   1892  C   ASP B 205      151.460  61.361  -7.557  1.00 54.03           C
ANISOU 1892  C   ASP B 205     7732   6535   6264  -1209  -2361   1014       C
ATOM   1893  O   ASP B 205      151.650  60.588  -8.496  1.00 54.35           O
ANISOU 1893  O   ASP B 205     8141   6520   5992  -1410  -2472    964       O
ATOM   1894  N   CYS B 206      152.313  61.466  -6.535  1.00 55.64           N
ANISOU 1894  N   CYS B 206     7815   6792   6535   -979  -2027    823       N
ATOM   1895  CA  CYS B 206      153.575  60.706  -6.452  1.00 56.34           C
ANISOU 1895  CA  CYS B 206     8137   6884   6385   -929  -1767    570       C
ATOM   1896  CB  CYS B 206      153.349  59.202  -6.616  1.00 58.58           C
ANISOU 1896  CB  CYS B 206     8611   7126  6518  -1057  -1827    507       C
ATOM   1897  SG  CYS B 206      152.425  58.494  -5.309  1.00 44.15           S
ANISOU 1897  SG  CYS B 206     6452   5339  4982   -963  -1849    548       S
ATOM   1898  C   CYS B 206      154.666  61.153  -7.426  1.00 55.92           C
ANISOU 1898  C   CYS B 206     8383   6792   6073   -970  -1652    484       C
ATOM   1899  O   CYS B 206      155.628  60.420  -7.658  1.00 63.05           O
ANISOU 1899  O   CYS B 206     9530   7654   6773   -972  -1451    320       O
ATOM   1900  N   GLY B 207      154.531  62.346  -7.986  1.00 47.28           N
ANISOU 1900  N   GLY B 207     7262   5693   5008   -994  -1749    608       N
ATOM   1901  CA  GLY B 207      155.577  62.887  -8.832  1.00 45.91           C
ANISOU 1901  CA  GLY B 207     7346   5478   4621  -1009  -1609    536       C
ATOM   1902  C   GLY B 207      156.695  63.517  -8.020  1.00 49.99           C
ANISOU 1902  C   GLY B 207     7780   6033   5183  -1047  -1300    406       C
ATOM   1903  O   GLY B 207      156.581  64.643  -7.536  1.00 59.06           O
ANISOU 1903  O   GLY B 207     8594   7230   6617  -1290  -1470    470       O
ATOM   1904  N   VAL B 208      157.791  62.784  -7.884  1.00 44.26           N
ANISOU 1904  N   VAL B 208     7102   5288   4427  -729  -1047   237       N
ATOM   1905  CA  VAL B 208      159.029  63.311  -7.332  1.00 39.76           C
ANISOU 1905  CA  VAL B 208     6420   4737   3952  -562  -778   138       C
ATOM   1906  CB  VAL B 208      159.672  62.269  -6.450  1.00 36.82           C
ANISOU 1906  CB  VAL B 208     5982   4377  3632  -468  -592    14       C
ATOM   1907  CG1 VAL B 208      160.931  62.832  -5.831  1.00 27.01           C
ANISOU 1907  CG1 VAL B 208     4593   3150  2521  -322  -369   -46       C
ATOM   1908  CG2 VAL B 208      158.642  61.789  -5.395  1.00 30.42           C
ANISOU 1908  CG2 VAL B 208     5945   3641  2973  -439  -733    38       C
ATOM   1909  C   VAL B 208      160.031  63.656  -8.425  1.00 49.15           C
ANISOU 1909  C   VAL B 208     7882   7852   4915  -1010  -1652    484       C
ATOM   1910  O   VAL B 208      160.427  62.779  -9.188  1.00 57.69           O
ANISOU 1910  O   VAL B 208     9278   6813  5827  -690  -507    53       O
ATOM   1911  N   PRO B 209      160.445  64.930  -8.509  1.00 54.29           N
ANISOU 1911  N   PRO B 209     8432   6498  5698  -535  -573   152       N
ATOM   1912  CA  PRO B 209      161.442  65.311  -9.523  1.00 54.08           C
ANISOU 1912  CA  PRO B 209     8652   6371  5526  -557  -387   136       C
ATOM   1913  CB  PRO B 209      161.362  66.845  -9.557  1.00 49.15           C
ANISOU 1913  CB  PRO B 209     7864   5784  5024  -511  -458   226       C
ATOM   1914  CG  PRO B 209      160.147  67.211  -8.711  1.00 56.32           C
ANISOU 1914  CG  PRO B 209     8484   6791  6122  -488  -692   307       C
ATOM   1915  CD  PRO B 209      159.987  66.089  -7.725  1.00 56.05           C
ANISOU 1915  CD  PRO B 209     8339   6801  6155  -442  -669   223       C
ATOM   1916  C   PRO B 209      162.847  64.879  -9.086  1.00 57.93           C
ANISOU 1916  C   PRO B 209     9099   6815  6099  -431   -62    31       C
ATOM   1917  O   PRO B 209      163.077  64.561  -7.909  1.00 51.36           O
ANISOU 1917  O   PRO B 209     8009   6053  5455  -324   -22   -15       O
ATOM   1918  N   ASP B 210      163.784  64.893 -10.026  1.00 64.29           N
ANISOU 1918  N   ASP B 210     9757   7649  7023  -1018  -1644   1291  -118       O
ATOM   1919  CA  ASP B 210      165.180  64.634  -9.711  1.00 69.95           C
ANISOU 1919  CA  ASP B 210     9757   8135  8135   -323   499   -28       C
ATOM   1920  CB  ASP B 210      165.980  64.408 -10.993  1.00 80.39           C
ANISOU 1920  CB  ASP B 210     9260   8791  9369   792   -31       C
ATOM   1921  CG  ASP B 210      165.926  62.971 -11.457  1.00 93.92           C
ANISOU 1921  CG  ASP B 210     14530  10845  10309   -448   937   -97       C
ATOM   1922  OD1 ASP B 210      164.825  62.489 -11.813  1.00 99.26           O
ANISOU 1922  OD1 ASP B 210     15417  11540  10755   -600   702   -111       O
ATOM   1923  OD2 ASP B 210      166.995  62.325 -11.447  1.00100.19           O
ANISOU 1923  OD2 ASP B 210     15355  11508  11205   -361  1291   -118       O
ATOM   1924  C   ASP B 210      165.759  65.801  -8.941  1.00 67.48           C
ANISOU 1924  C   ASP B 210     10145   7899   7596   -205   501    8       C
ANISOU 1924  C   ASP B 210     8432   6498   5698   -535   -573   152       N
ATOM   1925  O   ASP B 210      166.547  65.626  -8.017  1.00 65.35           O
ANISOU 1925  O   ASP B 210     9635   7650   7543   -103   607   -4       O
ATOM   1926  N   ASN B 211      165.346  66.997  -9.339  1.00 69.44           N
ANISOU 1926  N   ASN B 211     8677   7817   7617   -236   367   67       N
ATOM   1927  CA  ASN B 211      165.870  68.231  -8.792  1.00 69.04           C
ANISOU 1927  CA  ASN B 211     10084   8169   7977   -149   377   100       C
ATOM   1928  CB  ASN B 211      166.590  68.999  -9.894  1.00 79.65           C
ANISOU 1928  CB  ASN B 211     11598   9400   9264   -159   545   150       C
ATOM   1929  CG  ASN B 211      167.768  69.792  -9.378  1.00 88.10           C
ANISOU 1929  CG  ASN B 211     12430  10451  10591   -58   694   175       C
ATOM   1930  OD1 ASN B 211      167.611  70.743  -8.598  1.00 89.43           O
ANISOU 1930  OD1 ASN B 211     12365  10704  10911   -25   557   188       O
ATOM   1931  ND2 ASN B 211      168.967  69.404  -9.814  1.00 91.26           N
ANISOU 1931  ND2 ASN B 211     12899 10718 11058   -14   991   193       N
ATOM   1932  C   ASN B 211      164.751  69.092  -8.182  1.00 60.90           C
ANISOU 1932  C   ASN B 211     8691   6793   7194   -236   -219   -260       C
ATOM   1933  O   ASN B 211      163.932  69.709  -8.888  1.00 54.95           O
ANISOU 1933  O   ASN B 211     8215   6501  6163   -224   -36   209       O
ATOM   1934  N   LEU B 212      164.726  69.119  -6.857  1.00 57.88           N
ANISOU 1934  N   LEU B 212     8233   6949  6808   -87   61   99       N
ATOM   1935  CA  LEU B 212      163.735  69.890  -6.125  1.00 58.26           C
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ANISOU 1935 CA LEU B 212     8115  7069  6951   -73   -114   127       C
ATOM  1936  CB  LEU B 212     163.974 69.758 -4.625  1.00 51.05           C
ANISOU 1936 CB LEU B 212     6999  6207  6192    -9   -107    65       C
ATOM  1937  CG  LEU B 212     162.782 69.985 -3.688  1.00 52.03           C
ANISOU 1937 CG LEU B 212     7002  6379  6388     7   -235    72       C
ATOM  1938  CD1 LEU B 212     163.220 69.677 -2.288  1.00 58.44           C
ANISOU 1938 CD1 LEU B 212     7699  7217  7287    46   -203    -2       C
ATOM  1939  CD2 LEU B 212     162.184 71.368 -3.720  1.00 42.24           C
ANISOU 1939 CD2 LEU B 212     5700  5114  5236    20   -277   141       C
ATOM  1940  C   LEU B 212     163.708 71.380 -6.538  1.00 62.91           C
ANISOU 1940 C   LEU B 212     8674  7632  7596   -67   -129   198       C
ATOM  1941  O   LEU B 212     162.639 71.928 -6.818  1.00 67.47           O
ANISOU 1941 O   LEU B 212     9243  8221  8173   -97   -270   282       O
ATOM  1942  N   SER B 213     164.873 72.021 -6.568  1.00 61.43           N
ANISOU 1942 N   SER B 213     8453  7401  7488   -30    15   186       N
ATOM  1943  CA  SER B 213     164.987 73.452 -6.897  1.00 66.12           C
ANISOU 1943 CA  SER B 213     9012  7960  8150   -19    25   245       C
ATOM  1944  CB  SER B 213     166.458 73.869 -6.925  1.00 67.57           C
ANISOU 1944 CB  SER B 213     9155  8082  8434    13   199   233       C
ATOM  1945  OG  SER B 213     167.259 72.882 -6.295  1.00 70.73           O
ANISOU 1945 OG  SER B 213     9492  8486  8896    34   277   182       O
ATOM  1946  C   SER B 213     164.322 73.872 -8.219  1.00 67.75           C
ANISOU 1946 C   SER B 213     9389  8133  8219   -80   -44   345       C
ATOM  1947  O   SER B 213     163.975 75.039 -8.391  1.00 59.99           O
ANISOU 1947 O   SER B 213     8350  7136  7307   -72   -90   419       O
ATOM  1948  N   MET B 214     164.142 72.925 -9.143  1.00 74.01           N
ANISOU 1948 N   MET B 214     10411  8900  8808  -154   -57   355       N
ATOM  1949  CA  MET B 214     163.585 73.233 -10.470  1.00 77.45           C
ANISOU 1949 CA  MET B 214     11076  9290  9063  -253  -152   461       C
ATOM  1950  CB  MET B 214     164.104 72.251 -11.518  1.00 81.35           C
ANISOU 1950 CB  MET B 214     11911  9694  9305  -334   -29   427       C
ATOM  1951  CG  MET B 214     165.618 72.193 -11.593  1.00 83.59           C
ANISOU 1951 CG  MET B 214     12223  9890  9647  -254   290   361       C
ATOM  1952  SD  MET B 214     166.339 73.817 -11.900  1.00135.11           S
ANISOU 1952 SD  MET B 214     18655 16370 16312  -194   397   430       S
ATOM  1953  CE  MET B 214     168.085 73.411 -11.919  1.00 97.04           C
ANISOU 1953 CE  MET B 214     13832 11427 11612  -109   771   383       C
ATOM  1954  C   MET B 214     162.066 73.227 -10.487  1.00 74.60           C
ANISOU 1954 C   MET B 214     10671  8980  8694  -324   -430   569       C
ATOM  1955  O   MET B 214     161.434 73.816 -11.384  1.00 73.18           O
ANISOU 1955 O   MET B 214     10592  8774  8440  -408   -578   709       O
ATOM  1956  N   ALA B 215     161.497 72.552 -9.487  1.00 72.41           N
ANISOU 1956 N   ALA B 215     10233  8768  8513  -294   -502   525       N
ATOM  1957  CA  ALA B 215     160.044 72.372 -9.370  1.00 73.76           C
ANISOU 1957 CA  ALA B 215     10316  8973  8734  -351   -747   643       C
ATOM  1958  CB  ALA B 215     159.700 71.484 -8.177  1.00 71.88           C
ANISOU 1958 CB  ALA B 215     9921  8792  8599  -296   -746   559       C
ATOM  1959  C   ALA B 215     159.271 73.683 -9.275  1.00 73.99           C
ANISOU 1959 C   ALA B 215     10152  8995  8967  -317   -842   799       C
ATOM  1960  O   ALA B 215     158.138 73.792 -9.758  1.00 78.31           O
ANISOU 1960 O   ALA B 215     10673  9533  9547  -400  -1065   982       O
ATOM  1961  N   ASP B 216     159.889 74.671 -8.636  1.00 67.69           N
ANISOU 1961 N   ASP B 216     9211  8184  8324  -204   -673   745       N
ATOM  1962  CA  ASP B 216     159.248 75.954 -8.413  1.00 60.18           C
ANISOU 1962 CA  ASP B 216     8077  7199  7592  -151   -695   875       C
ATOM  1963  CB  ASP B 216     158.592 75.920 -7.024  1.00 59.93           C
ANISOU 1963 CB  ASP B 216     7823  7170  7778   -61   -649   849       C
ATOM  1964  CG  ASP B 216     157.637 77.075 -6.777  1.00 59.77           C
ANISOU 1964 CG  ASP B 216     7611  7077  8021    -4   -649  1020       C
ATOM  1965  OD1 ASP B 216     157.812 78.144 -7.382  1.00 63.91           O
ANISOU 1965 OD1 ASP B 216     8141  7556  8588     0   -628  1108       O
ATOM  1966  OD2 ASP B 216     156.719 76.902 -5.945  1.00 63.19           O
ANISOU 1966 OD2 ASP B 216     7886  7484  8638    47   -640  1072       O
ATOM  1967  C   ASP B 216     160.287 77.086 -8.551  1.00 47.10           C
ANISOU 1967 C   ASP B 216     6434  5498  5963   -96   -524   829       C
ATOM  1968  O   ASP B 216     161.370 77.038 -7.968  1.00 43.08           O
ANISOU 1968 O   ASP B 216     5925  4992  5451   -46   -360   675       O
ATOM  1969  N   PRO B 217     159.965 78.120 -9.327  1.00 45.65           N
ANISOU 1969 N   PRO B 217     6251  5268  5827   -116   -576   984       N
ATOM  1970  CA  PRO B 217     160.890 79.264 -9.380  1.00 44.12           C
ANISOU 1970 CA  PRO B 217     6049  5024  5693   -59   -406   946       C
ATOM  1971  CB  PRO B 217     160.237 80.217 -10.388 1.00 42.96           C
ANISOU 1971 CB  PRO B 217     5910  4828  5584   -99   -517  1163       C
ATOM  1972  CG  PRO B 217     159.288 79.394 -11.181 1.00 41.49           C
ANISOU 1972 CG  PRO B 217     5826  4671  5267   -220   -770  1306       C
ATOM  1973  CD  PRO B 217     158.805 78.294 -10.213 1.00 43.97           C
ANISOU 1973 CD  PRO B 217     6044  5039  5624   -202   -806  1219       C
ATOM  1974  C   PRO B 217     161.010 79.973 -8.021  1.00 46.42           C
ANISOU 1974 C   PRO B 217     6153  5283  6203    42   -261   861       C
ATOM  1975  O   PRO B 217     161.979 80.678 -7.764  1.00 47.99           O
ANISOU 1975 O   PRO B 217     6350  5443  6440    75   -116   777       O
ATOM  1976  N   ASN B 218     160.014 79.807 -7.163  1.00 45.31           N
ANISOU 1976 N   ASN B 218     5874  5137  6205    80   -293   892       N
ATOM  1977  CA  ASN B 218     160.065 80.422 -5.846  1.00 39.22           C
ANISOU 1977 CA  ASN B 218     4999  4304  5598   157   -131   803       C
ATOM  1978  CB  ASN B 218     158.674 80.872 -5.445  1.00 33.16           C
ANISOU 1978 CB  ASN B 218     4078  3459  5061   211   -125   958       C
ATOM  1979  CG  ASN B 218     158.178 82.005 -6.303  1.00 39.55           C
ANISOU 1979 CG  ASN B 218     4818  4197  6013   221   -146  1168       C
ATOM  1980  OD1 ASN B 218     158.922 82.942 -6.585  1.00 42.84           O
ANISOU 1980 OD1 ASN B 218     5283  4571  6423   230   -52  1139       O
ATOM  1981  ND2 ASN B 218     156.926 81.935 -6.728  1.00 39.75           N
ANISOU 1981 ND2 ASN B 218     4714  4199  6188   215   -281  1401       N
ATOM  1982  C   ASN B 218     160.686 79.571 -4.754  1.00 36.46           C
ANISOU 1982 C   ASN B 218     4682  3996  5173   159   -74   609       C
ATOM  1983  O   ASN B 218     160.653 79.921 -3.590  1.00 37.89           O
ANISOU 1983 O   ASN B 218     4832  4119  5445   195    37   529       O
ATOM  1984  N   ILE B 219     161.244 78.438 -5.117  1.00 38.14           N
ANISOU 1984 N   ILE B 219     4980  4295  5217   113   -143   541       N
ATOM  1985  CA  ILE B 219     162.016 77.683 -4.143  1.00 42.83           C
ANISOU 1985 CA  ILE B 219     5590  4924  5758   112   -93   381       C
ATOM  1986  CB  ILE B 219     161.518 76.263 -3.956  1.00 46.97           C
ANISOU 1986 CB  ILE B 219     6124  5520  6201    97   -180   356       C
ATOM  1987  CG1 ILE B 219     160.057 76.277 -3.544  1.00 48.18           C
ANISOU 1987 CG1 ILE B 219     6182  5649  6475   128   -227   449       C
ATOM  1988  CD1 ILE B 219     159.515 74.913 -3.197  1.00 48.92           C
ANISOU 1988 CD1 ILE B 219     6268  5803  6516   116   -305   423       C
ATOM  1989  CG2 ILE B 219     162.368 75.544 -2.897  1.00 43.26           C
ANISOU 1989 CG2 ILE B 219     5660  5082  5697    96   -131   211       C
ATOM  1990  C   ILE B 219     163.446 77.654 -4.636  1.00 48.06           C
ANISOU 1990 C   ILE B 219     6321  5595  6344    83    -39   324       C
ATOM  1991  O   ILE B 219     163.725 77.265 -5.764  1.00 49.93           O
ANISOU 1991 O   ILE B 219     6651  5848  6473    56   -54   367       O
ATOM  1992  N   ARG B 220     164.365 78.114 -3.807  1.00 52.69           N
ANISOU 1992 N   ARG B 220     6877  6147  6994    79    33   242       N
ATOM  1993  CA  ARG B 220     165.726 78.279 -4.286  1.00 47.28           C
ANISOU 1993 CA  ARG B 220     6209  5443  6313    57    97   233       C
ATOM  1994  CB  ARG B 220     166.006 79.752 -4.493  1.00 51.25           C
ANISOU 1994 CB  ARG B 220     6695  5865  6912    57   159   272       C
ATOM  1995  CG  ARG B 220     165.644 80.201 -5.896  1.00 60.94           C
ANISOU 1995 CG  ARG B 220     7981  7077  8097    74   172   384       C
ATOM  1996  CD  ARG B 220     165.094 81.593 -5.909  1.00 63.66           C
ANISOU 1996 CD  ARG B 220     8288  7349  8550    96   200   449       C
ATOM  1997  NE  ARG B 220     165.875 82.496 -5.067  1.00 68.52           N
ANISOU 1997 NE  ARG B 220     8866  7891  9277    78   277   381       N
ATOM  1998  CZ  ARG B 220     166.240 83.725 -5.426  1.00 65.63           C
ANISOU 1998 CZ  ARG B 220     8495  7443  8999    79   352   425       C
ATOM  1999  NH1 ARG B 220     166.947 84.494 -4.596  1.00 62.09           N
ANISOU 1999 NH1 ARG B 220     8035  6916  8640    35   400   358       N
ATOM  2000  NH2 ARG B 220     165.890 84.176 -6.622  1.00 64.54           N
ANISOU 2000 NH2 ARG B 220     8381  7294  8848   107   364   545       N
ATOM  2001  C   ARG B 220     166.731 77.653 -3.352  1.00 42.62           C
ANISOU 2001 C   ARG B 220     5572  4868  5755    26    97   156       C
ATOM  2002  O   ARG B 220     166.598 77.752 -2.138  1.00 43.73           O
ANISOU 2002 O   ARG B 220     5692  5000  5925     1    56    94       O
ATOM  2003  N   PHE B 221     167.727 76.988 -3.925  1.00 43.65           N
ANISOU 2003 N   PHE B 221     5701  5001  5883    22   152   177       N
ATOM  2004  CA  PHE B 221     168.744 76.344 -3.119  1.00 45.53           C
ANISOU 2004 CA  PHE B 221     5855  5243  6202    -8   141   155       C
ATOM  2005  CB  PHE B 221     169.642 75.480 -3.987  1.00 44.56           C
ANISOU 2005 CB  PHE B 221     5732  5098  6102    17   262   211       C
ATOM  2006  CG  PHE B 221     170.776 74.846 -3.229  1.00 46.85           C
ANISOU 2006  CG  PHE B 221     5885  5373  6543    -9   258   242       C
ATOM  2007  CD1 PHE B 221     170.551 73.735 -2.405  1.00 46.88           C
ANISOU 2007 CD1 PHE B 221     5859  5437  6515   -16   180   204       C
ATOM  2008  CE1 PHE B 221     171.603 73.129 -1.701  1.00 45.40           C
ANISOU 2008 CE1 PHE B 221     5527  5232  6491   -48   154   269       C
ATOM  2009  CZ  PHE B 221     172.915 73.654 -1.830  1.00 48.53           C
ANISOU 2009 CZ  PHE B 221     5784  5542  7115   -76   201   390       C
ATOM  2010  CE2 PHE B 221     173.137 74.777 -2.647  1.00 51.22           C
ANISOU 2010 CE2 PHE B 221     6153  5817  7491   -66   291   417       C
ATOM  2011  CD2 PHE B 221     172.064 75.365 -3.329  1.00 47.63           C
ANISOU 2011 CD2 PHE B 221     5865  5389  6843   -31   321   336       C
ATOM  2012  C   PHE B 221     169.589 77.393 -2.412  1.00 44.95           C
ANISOU 2012 C   PHE B 221     5707  5106  6265   -69   113   164       C
ATOM  2013  O   PHE B 221     170.036 78.350 -3.036  1.00 55.86           O
ANISOU 2013 O   PHE B 221     7081  6425  7718   -69   179   213       O
ATOM  2014  N   LEU B 222     169.826 77.168 -1.136  1.00 41.12           N
ANISOU 2014 N   LEU B 222     5191  4627  5804   -137    3   122       N
ATOM  2015  CA  LEU B 222     170.728 77.974 -0.349  1.00 45.43           C
ANISOU 2015 CA  LEU B 222     5694  5101  6465   -242   -71   142       C
ATOM  2016  CB  LEU B 222     170.058 78.402  0.938  1.00 39.34           C
ANISOU 2016 CB  LEU B 222     5038  4306  5603   -325   -175   49       C
ATOM  2017  CG  LEU B 222     169.010 79.472  0.926  1.00 40.36           C
ANISOU 2017 CG  LEU B 222     5289  4380  5667   -292   -93   -11       C
ATOM  2018  CD1 LEU B 222     168.805 79.969  2.326  1.00 43.40           C
ANISOU 2018 CD1 LEU B 222     5829  4684  5977   -400   -149   -98       C
ATOM  2019  CD2 LEU B 222     169.416 80.600  0.022  1.00 46.26           C
ANISOU 2019 CD2 LEU B 222     6003  5061  6514   -283   -15   46       C
ATOM  2020  C   LEU B 222     171.989 77.233  0.018  1.00 46.04           C
ANISOU 2020 C   LEU B 222     5630  5176  6688   -293   -293   232       C
ATOM  2021  O   LEU B 222     173.043 77.639 -0.337  1.00 51.56           O
ANISOU 2021 O   LEU B 222     6214  5811  7569   -323   -102   336       O
ATOM  2022  N   ASP B 223     171.874 76.153  0.761  1.00 46.95           N
ANISOU 2022 N   ASP B 223     5735  5353  6749   -297   -199   210       N
ATOM  2023  CA  ASP B 223     173.032 75.531  1.354  1.00 48.82           C
ANISOU 2023 CA  ASP B 223     5834  5578  7139   -309   -377   311       C
ATOM  2024  CB  ASP B 223     173.372 76.297  2.620  1.00 57.59           C
ANISOU 2024 CB  ASP B 223     6998  6649  6236   -548   -511   302       C
ATOM  2025  CG  ASP B 223     174.817 76.277  2.951  1.00 61.92           C
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ANISOU 2025 CG ASP B 223 7369 7143 9014 -663 -662 465 C
ATOM 2026 OD1 ASP B 223 175.629 76.531 2.085 1.00 68.73 O
ANISOU 2026 OD1 ASP B 223 8054 8015 10048 -570 -549 580 O
ATOM 2027 OD2 ASP B 223 175.142 76.020 4.098 1.00 57.53 O
ANISOU 2027 OD2 ASP B 223 6856 6530 8474 -847 -877 495 O
ATOM 2028 C ASP B 223 172.799 74.100 1.721 1.00 44.61 C
ANISOU 2028 C ASP B 223 5272 5116 6561 -348 -343 308 C
ATOM 2029 O ASP B 223 171.696 73.657 1.810 1.00 47.55 O
ANISOU 2029 O ASP B 223 5767 5551 6750 -305 -340 196 O
ATOM 2030 N LYS B 224 173.870 73.387 1.981 1.00 44.55 N
ANISOU 2030 N LYS B 224 5084 5086 6756 -374 -375 452 N
ATOM 2031 CA LYS B 224 173.763 72.106 2.610 1.00 42.31 C
ANISOU 2031 CA LYS B 224 4757 4857 6464 -380 -452 474 C
ATOM 2032 CB LYS B 224 174.841 71.190 2.144 1.00 42.88 C
ANISOU 2032 CB LYS B 224 4608 4880 6806 -327 -342 656 C
ATOM 2033 CG LYS B 224 174.779 70.883 0.680 1.00 51.87 C
ANISOU 2033 CG LYS B 224 5780 5985 7944 -172 -37 641 C
ATOM 2034 CD LYS B 224 173.568 70.056 0.328 1.00 59.96 C
ANISOU 2034 CD LYS B 224 6957 7084 8742 -90 42 510 C
ATOM 2035 CE LYS B 224 173.700 69.459 -1.053 1.00 63.11 C
ANISOU 2035 CE LYS B 224 7452 7423 9102 23 329 500 C
ATOM 2036 NZ LYS B 224 172.989 68.165 -1.136 1.00 68.23 N
ANISOU 2036 NZ LYS B 224 8238 8127 9560 73 381 400 N
ATOM 2037 C LYS B 224 173.898 72.265 4.073 1.00 40.20 C
ANISOU 2037 C LYS B 224 4532 4594 6147 -548 -727 478 C
ATOM 2038 O LYS B 224 174.599 73.096 4.536 1.00 50.06 O
ANISOU 2038 O LYS B 224 5757 5778 7486 -691 -883 550 O
ATOM 2039 N LEU B 225 173.183 71.463 4.812 1.00 51.00 N
ANISOU 2039 N LEU B 225 4907 5974 8497 -493 -1634 -269 N
ATOM 2040 CA LEU B 225 173.382 71.348 6.244 1.00 53.84 C
ANISOU 2040 CA LEU B 225 5354 6368 8734 -568 -1987 -311 C
ATOM 2041 CB LEU B 225 172.225 70.559 6.856 1.00 54.51 C
ANISOU 2041 CB LEU B 225 5702 6611 8398 -539 -2008 -305 C
ATOM 2042 CG LEU B 225 171.188 71.199 7.768 1.00 49.85 C
ANISOU 2042 CG LEU B 225 5394 6107 7439 -590 -2050 -426 C
ATOM 2043 CD1 LEU B 225 170.575 70.104 8.617 1.00 46.67 C
ANISOU 2043 CD1 LEU B 225 5190 5820 6723 -580 -2161 -382 C
ATOM 2044 CD2 LEU B 225 171.837 72.236 8.638 1.00 51.88 C
ANISOU 2044 CD2 LEU B 225 5664 6283 7765 -701 -2292 -535 C
ATOM 2045 C LEU B 225 174.654 70.538 6.402 1.00 55.85 C
ANISOU 2045 C LEU B 225 5374 6536 9312 -570 -2190 -211 C
ATOM 2046 O LEU B 225 174.841 69.545 5.703 1.00 58.87 O
ANISOU 2046 O LEU B 225 5645 6911 9813 -489 -2055 -102 O
ATOM 2047 N PRO B 226 175.533 70.947 7.313 1.00 59.12 N
ANISOU 2047 N PRO B 226 5708 6874 9882 -663 -2521 -249 N
ATOM 2048 CA PRO B 226 176.680 70.093 7.620 1.00 64.45 C
ANISOU 2048 CA PRO B 226 6161 7467 10861 -661 -2772 -144 C
ATOM 2049 CB PRO B 226 177.338 70.819 8.777 1.00 65.22 C
ANISOU 2049 CB PRO B 226 6322 7508 10951 -761 -3089 -215 C
ATOM 2050 CG PRO B 226 177.080 72.266 8.450 1.00 65.45 C
ANISOU 2050 CG PRO B 226 6350 7493 11027 -832 -2971 -355 C
ATOM 2051 CD PRO B 226 175.653 72.272 7.941 1.00 64.64 C
ANISOU 2051 CD PRO B 226 6470 7523 10570 -772 -2667 -388 C
ATOM 2052 C PRO B 226 176.213 68.701 8.025 1.00 73.83 C
ANISOU 2052 C PRO B 226 7487 8763 11803 -597 -2850 -44 C
ATOM 2053 O PRO B 226 175.205 68.550 8.719 1.00 71.31 O
ANISOU 2053 O PRO B 226 7470 8576 11050 -610 -2896 -83 O
ATOM 2054 N GLN B 227 176.946 67.691 7.573 1.00 86.84 N
ANISOU 2054 N GLN B 227 8920 10340 13737 -525 -2829 85 N
ATOM 2055 CA GLN B 227 176.398 66.344 7.502 1.00 98.10 C
ANISOU 2055 CA GLN B 227 10439 11850 14984 -442 -2772 187 C
ATOM 2056 CB GLN B 227 177.110 65.522 6.428 1.00100.05 C
ANISOU 2056 CB GLN B 227 10408 11987 15619 -348 -2564 296 C
ATOM 2057 CG GLN B 227 176.401 65.576 5.098 1.00 99.95 C
ANISOU 2057 CG GLN B 227 10442 12005 15530 -281 -2111 276 C
ATOM 2058 CD GLN B 227 177.341 65.775 3.929 1.00100.74 C
ANISOU 2058 CD GLN B 227 10252 11941 16082 -246 -1858 304 C
ATOM 2059 OE1 GLN B 227 178.484 65.299 3.944 1.00 97.83 O
ANISOU 2059 OE1 GLN B 227 9632 11434 16104 -227 -1945 379 O
ATOM 2060 NE2 GLN B 227 176.865 66.499 2.903 1.00101.26 N
ANISOU 2060 NE2 GLN B 227 10379 12009 16087 -235 -1520 247 N
ATOM 2061 C GLN B 227 176.332 65.560 8.798 1.00106.25 C
ANISOU 2061 C GLN B 227 11666 12941 15761 -461 -3093 242 C
ATOM 2062 O GLN B 227 176.810 65.989 9.863 1.00102.24 O
ANISOU 2062 O GLN B 227 11261 12407 15178 -532 -3353 208 O
ATOM 2063 N GLN B 228 175.705 64.398 8.662 1.00115.69 N
ANISOU 2063 N GLN B 228 12948 14213 16798 -391 -3022 330 N
ATOM 2064 CA GLN B 228 175.504 63.462 9.747 1.00127.55 C
ANISOU 2064 CA GLN B 228 14661 15770 18032 -393 -3250 407 C
ATOM 2065 CB GLN B 228 174.077 63.571 10.282 1.00127.77 C
ANISOU 2065 CB GLN B 228 15042 15959 17546 -428 -3203 340 C
ATOM 2066 CG GLN B 228 173.657 62.396 11.146 1.00128.19 C
ANISOU 2066 CG GLN B 228 15312 16074 17319 -416 -3359 444 C
ATOM 2067 CD GLN B 228 172.176 62.401 11.481 1.00125.37 C
ANISOU 2067 CD GLN B 228 15292 15860 16482 -434 -3172 379 C
ATOM 2068 OE1 GLN B 228 171.473 63.405 11.292 1.00124.27 O
ANISOU 2068 OE1 GLN B 228 15248 15777 16193 -467 -2990 245 O
ATOM 2069 NE2 GLN B 228 171.690 61.271 11.978 1.00124.63 N
ANISOU 2069 NE2 GLN B 228 15371 15814 16168 -411 -3207 480 N
ATOM 2070 C GLN B 228 175.761 62.054 9.213 1.00133.27 C
ANISOU 2070 C GLN B 228 15252 16449 18937 -290 -3158 553 C
ATOM 2071 O GLN B 228 175.194 61.638 8.192 1.00130.89 O
ANISOU 2071 O GLN B 228 14910 16176 18644 -220 -2851 565 O
ATOM 2072 N THR B 229 176.629 61.324 9.899 1.00138.46 N
ANISOU 2072 N THR B 229 15882 17020 19708 -277 -3362 649 N
ATOM 2073 CA THR B 229 176.977 59.983 9.465 1.00140.17 C
ANISOU 2073 CA THR B 229 15967 17164 20126 -182 -3288 784 C
ATOM 2074 CB THR B 229 178.503 59.788 9.416 1.00143.45 C
ANISOU 2074 CB THR B 229 16118 17387 21000 -161 -3374 845 C
ATOM 2075 OG1 THR B 229 179.113 60.946 8.829 1.00143.52 O
ANISOU 2075 OG1 THR B 229 15933 17317 21280 -194 -3271 754 O
ATOM 2076 CG2 THR B 229 178.856 58.561 8.596 1.00142.57 C
ANISOU 2076 CG2 THR B 229 15823 17177 21171 -56 -3188 954 C
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ANISOU 2080 CA GLY B 230 15788 16632 18648 -100 -3354 1020 C
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ANISOU 2082 O GLY B 230 15470 16329 19124 -18 -3550 1214 O
ATOM 2083 N ASP B 231 175.293 55.722 12.560 1.00131.82 N
ANISOU 2083 N ASP B 231 15646 16147 17956 -129 -3763 1187 N
ATOM 2084 CA ASP B 231 176.062 54.885 13.470 1.00131.82 C
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ATOM 2085 CB ASP B 231 176.667 55.764 14.550 1.00135.01 C
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ANISOU 2087 OD1 ASP B 231 16901 16767 17588 -342 -4290 1132 O
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ANISOU 2090 O ASP B 231 16024 15929 17230 -169 -4243 1449 O
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ATOM 2094 CG ARG B 232 171.068 52.349 15.015 1.00107.31 C
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ANISOU 2124 CE LYS B 236 10138 11128 16500 212 -3864 1684 C
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ANISOU 2125 NZ LYS B 236 10037 11117 17247 273 -3788 1755 N
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ANISOU 2127 O LYS B 236 11042 12283 16679 341 -2602 1392 O
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ANISOU 2128 N ASP B 237 12195 13434 17510 187 -2960 1279 N
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ANISOU 2131 CG ASP B 237 14248 15618 20953 171 -3121 1314 C
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ANISOU 2132 OD2 ASP B 237 14671 15965 21463 203 -3276 1427 O
ATOM 2133 OD1 ASP B 237 181.325 55.941 8.484 1.00136.94 O
ANISOU 2133 OD1 ASP B 237 14669 16047 21315 92 -3276 1240 O
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ANISOU 2146 O ARG B 238 6093 7559 11050 79 -2460 911 O
ATOM 2147 N VAL B 239 176.254 58.496 4.073 1.00 58.88 N
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ANISOU 2161 OH TYR B 240 5661 6531 7575 56 -1652 737 O
ATOM 2162 CE2 TYR B 240 171.072 58.162 6.706 1.00 55.45 C
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ANISOU 2181 CA SER B 243 4359 5246 6897 -238 -745 -195 C
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ANISOU 2186 N ILE B 244 4132 4877 6523 -327 -811 -369 N
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ATOM 2188 C ILE B 244 167.889 75.046 1.743 1.00 40.59 C
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ANISOU 2189 O ILE B 244 4578 5142 7092 -295 -444 -402 O
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ANISOU 2190 CB ILE B 244 4294 4883 6621 -454 -992 -569 C
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ATOM 2193 CD1 ILE B 244 171.019 75.023 5.608 1.00 38.69 C
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ATOM 2196 CB TYR B 245 164.967 75.430 0.008 1.00 38.34 C
ANISOU 2196 CB TYR B 245 4204 4597 5767 -132 -203 -412 C
ATOM 2197 CG TYR B 245 165.463 74.217 -0.717 1.00 32.77 C
ANISOU 2197 CG TYR B 245 3449 3915 5088 -103 -162 -308 C
ATOM 2198 CD2 TYR B 245 165.500 72.970 -0.090 1.00 35.12 C
ANISOU 2198 CD2 TYR B 245 3744 4308 5291 -109 -268 -292 C
ATOM 2199 CE2 TYR B 245 165.967 71.841 -0.766 1.00 34.82 C
ANISOU 2199 CE2 TYR B 245 3659 4273 5297 -79 -217 -202 C
ATOM 2200 CZ TYR B 245 166.407 71.972 -2.080 1.00 36.42 C
ANISOU 2200 CZ TYR B 245 3834 4383 5621 -46 -44 -134 C
ATOM 2201 OH TYR B 245 166.871 70.866 -2.769 1.00 40.88 O
ANISOU 2201 OH TYR B 245 4370 4935 6228 -16 36 -58 O
ATOM 2202 CE1 TYR B 245 166.377 73.206 -2.714 1.00 28.49 C
ANISOU 2202 CE1 TYR B 245 2850 3287 4689 -43 65 -141 C
ATOM 2203 CD1 TYR B 245 165.898 74.311 -2.033 1.00 33.37 C
ANISOU 2203 CD1 TYR B 245 3498 3902 5280 -69 -1 -224 C
ATOM 2204 C TYR B 245 165.482 77.549 1.173 1.00 31.68 C
ANISOU 2204 C TYR B 245 3347 3607 5082 -235 -292 -587 C
ATOM 2205 O TYR B 245 164.971 77.651 2.288 1.00 35.07 O

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ANISOU 2205  O   TYR B 245     3863   4092   5368   -267   -388   -687      O
ATOM   2206  N   GLU B 246      165.515  78.554   0.315  1.00 35.99           N
ANISOU 2206  N   GLU B 246     3875   4037   5761   -214   -160   -565      N
ATOM   2207  CA  GLU B 246      164.744  79.774   0.607  1.00 41.36           C
ANISOU 2207  CA  GLU B 246     4633   4663   6421   -209   -120   -654      C
ATOM   2208  CB  GLU B 246      165.515  81.054   0.322  1.00 43.01           C
ANISOU 2208  CB  GLU B 246     4780   4698   6863   -253    -70   -678      C
ATOM   2209  CG  GLU B 246      165.638  81.402  -1.140  1.00 49.08           C
ANISOU 2209  CG  GLU B 246     5530   5370   7748   -198    108   -552      C
ATOM   2210  CD  GLU B 246      166.307  82.788  -1.373  1.00 60.08           C
ANISOU 2210  CD  GLU B 246     6875   6573   9381   -246    179   -577      C
ATOM   2211  OE1 GLU B 246      166.835  82.981  -2.509  1.00 58.32           O
ANISOU 2211  OE1 GLU B 246     6620   6247   9290   -228    327   -465      O
ATOM   2212  OE2 GLU B 246      166.300  83.649  -0.422  1.00 56.19           O
ANISOU 2212  OE2 GLU B 246     6391   6025   8935   -305     99   -710      O
ATOM   2213  C   GLU B 246      163.443  79.760  -0.163  1.00 39.95           C
ANISOU 2213  C   GLU B 246     4534   4522   6124   -110     -2   -595      C
ATOM   2214  O   GLU B 246      163.366  79.249  -1.283  1.00 37.53           O
ANISOU 2214  O   GLU B 246     4226   4225   5808    -54     79   -477      O
ATOM   2215  N   LEU B 247      162.400  80.259   0.478  1.00 38.14           N
ANISOU 2215  N   LEU B 247     4379   4311   5802    -91      1   -684      N
ATOM   2216  CA  LEU B 247      161.105  80.334  -0.153  1.00 36.98           C
ANISOU 2216  CA  LEU B 247     4279   4184   5586      2     87   -636      C
ATOM   2217  CB  LEU B 247      160.091  79.730   0.780  1.00 42.06           C
ANISOU 2217  CB  LEU B 247     4974   4945   6063     11     55   -707      C
ATOM   2218  CG  LEU B 247      160.582  78.331   1.108  1.00 51.57           C
ANISOU 2218  CG  LEU B 247     6170   6272   7151    -25    -33   -673      C
ATOM   2219  CD1 LEU B 247      159.903  77.902   2.373  1.00 54.10           C
ANISOU 2219  CD1 LEU B 247     6563   6682   7310    -53    -69   -769      C
ATOM   2220  CD2 LEU B 247      160.296  77.328  -0.017  1.00 49.84           C
ANISOU 2220  CD2 LEU B 247     5933   6114   6889     37     -2   -539      C
ATOM   2221  C   LEU B 247      160.733  81.770  -0.454  1.00 37.47           C
ANISOU 2221  C   LEU B 247     4357   4104   5778     33    170   -662      C
ATOM   2222  O   LEU B 247      160.689  82.604   0.443  1.00 39.46           O
ANISOU 2222  O   LEU B 247     4628   4294   6070     -7    164   -789      O
ATOM   2223  N   LEU B 248      160.473  82.055  -1.721  1.00 39.20           N
ANISOU 2223  N   LEU B 248     4583   4258   6052    103    244   -540      N
ATOM   2224  CA  LEU B 248      160.137  83.411  -2.142  1.00 41.84           C
ANISOU 2224  CA  LEU B 248     4936   4438   6522    142    319   -534      C
ATOM   2225  CB  LEU B 248      160.729  83.731  -3.508  1.00 41.93           C
ANISOU 2225  CB  LEU B 248     4967   4345   6621    165    394   -389      C
ATOM   2226  CG  LEU B 248      162.239  83.724  -3.686  1.00 46.82           C
ANISOU 2226  CG  LEU B 248     5536   4901   7353     82    428   -370      C
ATOM   2227  CD1 LEU B 248      162.543  84.079  -5.155  1.00 47.73           C
ANISOU 2227  CD1 LEU B 248     5711   4898   7526    120    551   -213      C
ATOM   2228  CD2 LEU B 248      162.924  84.694  -2.725  1.00 44.14           C
ANISOU 2228  CD2 LEU B 248     5138   4459   7174     -3    408   -503      C
ATOM   2229  C   LEU B 248      158.635  83.643  -2.205  1.00 46.97           C
ANISOU 2229  C   LEU B 248     5611   5097   7139    235    336   -533      C
ATOM   2230  O   LEU B 248      157.875  82.784  -2.609  1.00 43.36           O
ANISOU 2230  O   LEU B 248     5160   4739   6575    289    304   -465      O
ATOM   2231  N   GLU B 249      158.224  84.844  -1.829  1.00 52.36           N
ANISOU 2231  N   GLU B 249     6294   5656   7943    253    386   -609      N
ATOM   2232  CA  GLU B 249      156.854  85.271  -1.950  1.00 49.95           C
ANISOU 2232  CA  GLU B 249     5984   5314   7682    351    416   -601      C
ATOM   2233  CB  GLU B 249      156.177  85.167  -0.597  1.00 49.67           C
ANISOU 2233  CB  GLU B 249     5939   5334   7600    332    440   -765      C
ATOM   2234  CG  GLU B 249      154.720  85.515  -0.629  1.00 56.49           C
ANISOU 2234  CG  GLU B 249     6761   6154   8547    434    492   -768      C
ATOM   2235  CD  GLU B 249      154.034  85.296   0.718  1.00 67.69           C
ANISOU 2235  CD  GLU B 249     8183   7627   9909    411    562   -931      C
ATOM   2236  OE1 GLU B 249      154.429  85.999   1.693  1.00 70.85           O
ANISOU 2236  OE1 GLU B 249     8641   7955 10323    347    622  -1084      O
ATOM   2237  OE2 GLU B 249      153.121  84.415   0.778  1.00 70.22           O
ANISOU 2237  OE2 GLU B 249     8460   8051 10168    449    560   -905      O
ATOM   2238  C   GLU B 249      156.871  86.723  -2.424  1.00 49.85           C
ANISOU 2238  C   GLU B 249     5981   5098 7860    388    482   -577      C
ATOM   2239  O   GLU B 249      157.385  87.628  -1.724  1.00 46.80           O
ANISOU 2239  O   GLU B 249     5600   4605 7579    331    530   -695      O
ATOM   2240  N   ASN B 250      156.310  86.934  -3.615  1.00 49.08           N
ANISOU 2240  N   ASN B 250     5902   4939 7806    481    471   -420      N
ATOM   2241  CA  ASN B 250      156.260  88.262  -4.220  1.00 37.16           C
ANISOU 2241  CA  ASN B 250     4418   3227 6475    530    525   -358      C
ATOM   2242  CB  ASN B 250      155.487  89.199  -3.283  1.00 38.40           C
ANISOU 2242  CB  ASN B 250     4526   3283 6781    563    585   -499      C
ATOM   2243  CG  ASN B 250      154.974  90.449  -3.967  1.00 40.02           C
ANISOU 2243  CG  ASN B 250     4780   3280 7164    657    659   -826      C
ATOM   2244  OD1 ASN B 250      154.598  90.441  -5.140  1.00 48.59           O
ANISOU 2244  OD1 ASN B 250     5860   4328 8276    736    561   -229      O
ATOM   2245  ND2 ASN B 250      154.957  91.543  -3.221  1.00 46.00           N
ANISOU 2245  ND2 ASN B 250     5480   3888 8110    646    714   -544      N
ATOM   2246  C   ASN B 250      157.700  88.759  -4.484  1.00 37.55           C
ANISOU 2246  C   ASN B 250     4504   3178 6583    443    583   -341      C
ATOM   2247  O   ASN B 250      158.046  89.920  -4.256  1.00 38.85           O
ANISOU 2247  O   ASN B 250     4669   3177 6916    420    652   -394      O
ATOM   2248  N   GLY B 251      158.556  87.844  -4.917  1.00 36.55           N
ANISOU 2248  N   GLY B 251     4397   3148 6341    388    566   -276      N
ATOM   2249  CA  GLY B 251      159.947  88.154  -5.173  1.00 41.22           C
ANISOU 2249  CA  GLY B 251     4993   3652 7016    301    634   -257      C
ATOM   2250  C   GLY B 251      160.868  88.269  -3.951  1.00 43.44           C
ANISOU 2250  C   GLY B 251     5196   3940 7369    184    621   -430      C
ATOM   2251  O   GLY B 251      162.065  88.457  -4.108  1.00 47.51           O
ANISOU 2251  O   GLY B 251     5679   4381 7990    104    663   -419      O
ATOM   2252  N   GLN B 252      160.328  88.146  -2.741  1.00 42.77           N
ANISOU 2252  N   GLN B 252     5088   3934 7231    169    562   -587      N
ATOM   2253  CA  GLN B 252      161.084  88.429  -1.516  1.00 37.73           C
ANISOU 2253  CA  GLN B 252     4416   3277 6643     55    523   -763      C
ATOM   2254  CB  GLN B 252      160.363  89.482  -0.674  1.00 39.00           C
ANISOU 2254  CB  GLN B 252     4608   3333 6876     67    560   -911      C
ATOM   2255  CG  GLN B 252      159.794  90.602  -1.506  1.00 40.00           C
ANISOU 2255  CG  GLN B 252     4752   3280 7164    157    659   -826      C
ATOM   2256  CD  GLN B 252      160.864  91.318  -2.310  1.00 47.39           C
ANISOU 2256  CD  GLN B 252     5680   4055 8270    112    716   -735      C
ATOM   2257  OE1 GLN B 252      161.969  91.573  -1.815  1.00 44.45           O
ANISOU 2257  OE1 GLN B 252     5271   3629 7991     -5    700   -823      O
ATOM   2258  NE2 GLN B 252      160.550  91.631  -3.563  1.00 50.93           N
ANISOU 2258  NE2 GLN B 252     6168   4418 8765    199    779   -552      N
ATOM   2259  C   GLN B 252      161.233  87.178  -0.693  1.00 49.39           C
ANISOU 2259  C   GLN B 252     5880   4946 7940      6    417   -829      C
ATOM   2260  O   GLN B 252      160.370  86.294  -0.718  1.00 50.14           O
ANISOU 2260  O   GLN B 252     5994   4870 8188     -5    328   -829      O
ATOM   2261  N   ARG B 253      162.320  87.106   0.061  1.00 47.02           N
ANISOU 2261  N   ARG B 253     5546   4644 7676   -109    338   -923      N
ATOM   2262  CA  ARG B 253      162.496  85.981   0.962  1.00 44.93           C
ANISOU 2262  CA  ARG B 253     5285   4546 7241   -161    215   -987      C
ATOM   2263  CB  ARG B 253      163.866  85.977   1.626  1.00 37.47           C
ANISOU 2263  CB  ARG B 253     4286   3568 6383   -289     94  -1062      C
ATOM   2264  CG  ARG B 253      164.058  84.755   2.501  1.00 44.88           C
ANISOU 2264  CG  ARG B 253     5240   4672 7139   -334    -55  -1100      C
ATOM   2265  CD  ARG B 253      165.465  84.726   3.094  1.00 50.42           C
ANISOU 2265  CD  ARG B 253     5866   5330 7959   -458   -215  -1155      C
ATOM   2266  NE  ARG B 253      166.504  84.546   2.081  1.00 48.30           N
ANISOU 2266  NE  ARG B 253     5449   4999 7905   -464   -177  -1023      N
ATOM   2267  CZ  ARG B 253      167.796  84.430   2.356  1.00 48.61           C
ANISOU 2267  CZ  ARG B 253     5366   4984 8118   -559   -300  -1035      C
ATOM   2268  NH1 ARG B 253      168.680  84.295   1.363  1.00 47.84           N
ANISOU 2268  NH1 ARG B 253     5124   4811 8241   -557   -212   -913      N
ATOM   2269  NH2 ARG B 253      168.186  84.448   3.629  1.00 50.29           N
ANISOU 2269  NH2 ARG B 253     5609   5211 8288   -657   -512  -1170      N
ATOM   2270  C   ARG B 253      161.406  85.950   2.031  1.00 36.67           C
ANISOU 2270  C   ARG B 253     4329   3566   6036   -144    208  -1119      C
ATOM   2271  O   ARG B 253      161.225  86.892   2.782  1.00 38.21           O
ANISOU 2271  O   ARG B 253     4581   3663   6275   -179    232  -1261      O
ATOM   2272  N   ALA B 254      160.681  84.850   2.098  1.00 35.42           N
ANISOU 2272  N   ALA B 254     4192   3566   6198   -106    -95  -1076      N
ATOM   2273  CA  ALA B 254      159.596  84.715   3.051  1.00 36.89           C
ANISOU 2273  CA  ALA B 254     4458   3813   5744    -77    226  -1187      C
ATOM   2274  CB  ALA B 254      158.287  84.425   2.310  1.00 34.99           C
ANISOU 2274  CB  ALA B 254     4189   3614   5492     46   318  -1089      C
ATOM   2275  C   ALA B 254      159.893  83.621   4.091  1.00 38.55           C
ANISOU 2275  C   ALA B 254     4729   4168   5749   -152   114  -1245      C
ATOM   2276  O   ALA B 254      159.267  83.553   5.131  1.00 37.96           O
ANISOU 2276  O   ALA B 254     4759   4129   5535   -173   138  -1364      O
ATOM   2277  N   GLY B 255      160.832  82.739   3.789  1.00 42.34           N
ANISOU 2277  N   GLY B 255     5152   4722   6213   -188     3  -1154      N
ATOM   2278  CA  GLY B 255      161.196  81.711   4.739  1.00 45.42           C
ANISOU 2278  CA  GLY B 255     5599   5232   6427   -256   -127  -1190      C
ATOM   2279  C   GLY B 255      162.438  80.963   4.331  1.00 44.27           C
ANISOU 2279  C   GLY B 255     5354   5118   6349   -295   -251  -1094      C
ATOM   2280  O   GLY B 255      162.902  81.067   3.202  1.00 42.72           O
ANISOU 2280  O   GLY B 255     5052   4869   6313   -259   -200  -980      O
ATOM   2281  N   THR B 256      162.958  80.184   5.266  1.00 49.96           N
ANISOU 2281  N   THR B 256     6121   5916   6946   -365   -407  -1123      N
ATOM   2282  CA  THR B 256      164.116  79.328   5.022  1.00 53.43           C
ANISOU 2282  CA  THR B 256     6452   6385   7398   -398   -539  -1128      C
ATOM   2283  CB  THR B 256      165.419  79.985   5.467  1.00 56.96           C
ANISOU 2283  CB  THR B 256     6837   6779   7961   -500   -692  -1092      C
ATOM   2284  OG1 THR B 256      165.682  81.120   4.648  1.00 59.40           O
ANISOU 2284  OG1 THR B 256     7060   6888   8620   -490   -576  -1089      O
ATOM   2285  CG2 THR B 256      166.560  79.022   5.306  1.00 56.15           C
ANISOU 2285  CG2 THR B 256     6603   6644   8089   -527   -832   -992      C
ATOM   2286  C   THR B 256      163.988  78.014   5.774  1.00 44.20           C
ANISOU 2286  C   THR B 256     5356   5353   6086   -412   -651  -1004      C
ATOM   2287  O   THR B 256      163.910  77.996   7.002  1.00 48.12           O
ANISOU 2287  O   THR B 256     5990   5876   6416   -479   -761  -1105      O
ATOM   2288  N   CYS B 257      163.980  76.918   5.046  1.00 42.53           N
ANISOU 2288  N   CYS B 257     5070   5216   5873   -354   -621   -872      N
ATOM   2289  CA  CYS B 257      163.762  75.618   5.683  1.00 45.66           C
ANISOU 2289  CA  CYS B 257     5535   5734   6078   -359   -707   -835      C
ATOM   2290  CB  CYS B 257      162.281  75.280   5.735  1.00 46.98           C
ANISOU 2290  CB  CYS B 257     5806   5985  6060   -302   -564   -844      C
ATOM   2291  SG  CYS B 257      161.616  75.095   4.114  1.00 62.00           S
ANISOU 2291  SG  CYS B 257     7603   7891  8063   -193   -389   -729      S
ATOM   2292  C   CYS B 257      164.484  74.503   4.970  1.00 39.83           C
ANISOU 2292  C   CYS B 257     4672   5025  5439   -330   -745   -698      C
ATOM   2293  O   CYS B 257      164.843  74.628   3.810  1.00 40.80           O
ANISOU 2293  O   CYS B 257     4675   5091  5735   -287   -646   -624      O
ATOM   2294  N   VAL B 258      164.696  73.410   5.687  1.00 39.33           N
ANISOU 2294  N   VAL B 258     4651   5036  5257   -355   -879   -663      N
ATOM   2295  CA  VAL B 258      165.297  72.214   5.114  1.00 40.46           C
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ANISOU 2295 CA VAL B 258 4684 5202 5485 -321 -908 -536 C
ATOM 2296 CB VAL B 258 166.183 71.461 6.139 1.00 48.74 C
ANISOU 2296 CB VAL B 258 5739 6265 6515 -380 -1152 -513 C
ATOM 2297 CG1 VAL B 258 165.498 71.423 7.473 1.00 56.92 C
ANISOU 2297 CG1 VAL B 258 6993 7368 7266 -432 -1243 -592 C
ATOM 2298 CG2 VAL B 258 166.509 70.046 5.658 1.00 42.15 C
ANISOU 2298 CG2 VAL B 258 4820 5463 5732 -330 -1157 -381 C
ATOM 2299 C VAL B 258 164.154 71.340 4.606 1.00 41.64 C
ANISOU 2299 C VAL B 258 4891 5444 5486 -250 -765 -478 C
ATOM 2300 O VAL B 258 163.217 70.998 5.334 1.00 38.18 O
ANISOU 2300 O VAL B 258 4586 5083 4836 -256 -756 -512 O
ATOM 2301 N LEU B 259 164.241 70.992 3.331 1.00 39.75 N
ANISOU 2301 N LEU B 259 4557 5184 5364 -189 -644 -393 N
ATOM 2302 CA LEU B 259 163.125 70.470 2.592 1.00 31.26 C
ANISOU 2302 CA LEU B 259 3526 4168 4185 -125 -505 -352 C
ATOM 2303 CB LEU B 259 162.796 71.496 1.532 1.00 39.05 C
ANISOU 2303 CB LEU B 259 4488 5087 5260 -84 -368 -358 C
ATOM 2304 CG LEU B 259 161.373 71.757 1.120 1.00 41.85 C
ANISOU 2304 CG LEU B 259 4909 5477 5513 -34 -263 -372 C
ATOM 2305 CD1 LEU B 259 160.587 71.925 2.390 1.00 43.90 C
ANISOU 2305 CD1 LEU B 259 5253 5793 5635 -65 -297 -464 C
ATOM 2306 CD2 LEU B 259 161.363 73.041 0.286 1.00 44.12 C
ANISOU 2306 CD2 LEU B 259 5175 5667 5921 -6 -176 -379 C
ATOM 2307 C LEU B 259 163.536 69.195 1.882 1.00 34.91 C
ANISOU 2307 C LEU B 259 3931 4642 4693 -90 -485 -247 C
ATOM 2308 O LEU B 259 164.651 69.104 1.389 1.00 40.66 O
ANISOU 2308 O LEU B 259 4552 5295 5601 -90 -490 -199 O
ATOM 2309 N GLU B 260 162.643 68.211 1.837 1.00 35.80 N
ANISOU 2309 N GLU B 260 4107 4833 4663 -64 -451 -214 N
ATOM 2310 CA GLU B 260 162.806 67.089 0.927 1.00 35.84 C
ANISOU 2310 CA GLU B 260 4079 4835 4703 -24 -392 -127 C
ATOM 2311 CB GLU B 260 163.848 66.112 1.448 1.00 45.20 C
ANISOU 2311 CB GLU B 260 5206 6007 5960 -42 -502 -73 C
ATOM 2312 CG GLU B 260 163.593 65.573 2.820 1.00 59.71 C
ANISOU 2312 CG GLU B 260 7122 7915 7652 -84 -640 -83 C
ATOM 2313 CD GLU B 260 164.648 64.522 3.207 1.00 70.97 C
ANISOU 2313 CD GLU B 260 8484 9310 9171 -90 -767 -4 C
ATOM 2314 OE1 GLU B 260 165.715 64.893 3.758 1.00 74.16 O
ANISOU 2314 OE1 GLU B 260 8815 9660 9702 -123 -912 -5 O
ATOM 2315 OE2 GLU B 260 164.422 63.325 2.909 1.00 75.77 O
ANISOU 2315 OE2 GLU B 260 9103 9935 9750 -60 -727 62 O
ATOM 2316 C GLU B 260 161.505 66.363 0.640 1.00 33.53 C
ANISOU 2316 C GLU B 260 3863 4615 4262 4 -328 -114 C
ATOM 2317 O GLU B 260 160.517 66.557 1.330 1.00 33.91 O
ANISOU 2317 O GLU B 260 3975 4722 4190 -10 -333 -164 O
ATOM 2318 N TYR B 261 161.529 65.552 -0.418 1.00 32.17 N
ANISOU 2318 N TYR B 261 3684 4423 4116 40 -257 -53 N
ATOM 2319 CA TYR B 261 160.434 64.665 -0.821 1.00 25.97 C
ANISOU 2319 CA TYR B 261 2959 3690 3220 58 -216 -34 C
ATOM 2320 CB TYR B 261 160.552 64.370 -2.295 1.00 25.81 C
ANISOU 2320 CB TYR B 261 2956 3613 3237 95 -124 8 C
ATOM 2321 CG TYR B 261 159.986 65.482 -3.154 1.00 31.93 C
ANISOU 2321 CG TYR B 261 3768 4358 4005 120 -72 -10 C
ATOM 2322 CD2 TYR B 261 160.850 66.472 -3.687 1.00 30.01 C
ANISOU 2322 CD2 TYR B 261 3504 4030 3868 130 -15 -3 C
ATOM 2323 CE2 TYR B 261 160.343 67.512 -4.499 1.00 31.76 C
ANISOU 2323 CE2 TYR B 261 3777 4210 4079 156 30 -4 C
ATOM 2324 CZ TYR B 261 158.959 67.570 -4.766 1.00 33.66 C
ANISOU 2324 CZ TYR B 261 4072 4495 4222 178 -5 -13 C
ATOM 2325 OH TYR B 261 158.533 68.599 -5.554 1.00 41.27 O
ANISOU 2325 OH TYR B 261 5084 5403 5193 209 15 2 O
ATOM 2326 CE1 TYR B 261 158.048 66.624 -4.245 1.00 27.71 C
ANISOU 2326 CE1 TYR B 261 3315 3824 3389 166 -62 -28 C
ATOM 2327 CD1 TYR B 261 158.578 65.580 -3.409 1.00 26.38 C
ANISOU 2327 CD1 TYR B 261 3111 3698 3213 134 -84 -28 C
ATOM 2328 C TYR B 261 160.460 63.339 -0.116 1.00 31.67 C
ANISOU 2328 C TYR B 261 3694 4453 3887 38 -270 1 C
ATOM 2329 O TYR B 261 161.529 62.825 0.160 1.00 35.76 O
ANISOU 2329 O TYR B 261 4167 4936 4485 32 -321 42 O
ATOM 2330 N ALA B 262 159.284 62.782 0.171 1.00 35.14 N
ANISOU 2330 N ALA B 262 4186 4954 4211 28 -259 -8 N
ATOM 2331 CA ALA B 262 159.202 61.513 0.882 1.00 36.34 C
ANISOU 2331 CA ALA B 262 4367 5137 4302 5 -297 33 C
ATOM 2332 CB ALA B 262 157.830 61.329 1.449 1.00 32.04 C
ANISOU 2332 CB ALA B 262 3874 4654 3645 -19 -264 3 C
ATOM 2333 C ALA B 262 159.518 60.405 -0.135 1.00 35.00 C
ANISOU 2333 C ALA B 262 4188 4922 4190 31 -255 89 C
ATOM 2334 O ALA B 262 158.768 60.200 -1.081 1.00 29.79 O
ANISOU 2334 O ALA B 262 3554 4257 3508 45 -195 81 O
ATOM 2335 N THR B 263 160.622 59.693 0.056 1.00 29.50 N
ANISOU 2335 N THR B 263 3456 4179 3575 37 -294 144 N
ATOM 2336 CA THR B 263 161.078 58.744 -0.960 1.00 31.40 C
ANISOU 2336 CA THR B 263 3685 4349 3896 67 -224 186 C
ATOM 2337 CB THR B 263 162.460 58.179 -0.619 1.00 29.43 C
ANISOU 2337 CB THR B 263 3397 4029 3796 82 -270 247 C
ATOM 2338 OG1 THR B 263 162.403 57.620 0.698 1.00 32.35 O
ANISOU 2338 OG1 THR B 263 3746 4441 4105 54 -395 285 O
ATOM 2339 CG2 THR B 263 163.512 59.292 -0.666 1.00 24.96 C
ANISOU 2339 CG2 THR B 263 2699 3415 3369 90 -287 233 C
ATOM 2340 C THR B 263 160.106 57.594 -1.275 1.00 33.00 C
ANISOU 2340 C THR B 263 3954 4567 4016 58 -186 196 C
ATOM 2341 O THR B 263 160.106 57.143 -2.415 1.00 26.24 O
ANISOU 2341 O THR B 263 3130 3657 3184 77 -106 194 O
ATOM 2342 N PRO B 264 159.297 57.105 -0.275 1.00 23.79 N
ANISOU 2342 N PRO B 264 2823 3464 2753 22 -233 203 N
ATOM 2343 CA PRO B 264 158.442 55.975 -0.642 1.00 23.99 C
ANISOU 2343 CA PRO B 264 2894 3484 2739 6 -191 214 C
ATOM 2344 CB PRO B 264 157.684 55.660 0.659 1.00 25.99 C
ANISOU 2344 CB PRO B 264 3179 3798 2899 -39 -224 227 C
ATOM 2345 CG PRO B 264 158.747 56.024 1.772 1.00 27.24 C
ANISOU 2345 CG PRO B 264 3333 3961 3056 -39 -316 264 C
ATOM 2346 CD PRO B 264 159.354 57.298 1.195 1.00 25.38 C
ANISOU 2346 CD PRO B 264 3040 3715 2889 -10 -319 216 C
ATOM 2347 C PRO B 264 157.464 56.290 -1.765 1.00 30.10 C
ANISOU 2347 C PRO B 264 3693 4261 3482 7 -143 160 C
ATOM 2348 O PRO B 264 156.970 55.348 -2.383 1.00 32.88 O
ANISOU 2348 O PRO B 264 4083 4582 3827 -6 -118 161 O
ATOM 2349 N LEU B 265 157.168 57.576 -1.991 1.00 27.06 N
ANISOU 2349 N LEU B 265 3293 3906 3084 19 -147 116 N
ATOM 2350 CA LEU B 265 156.313 57.983 -3.108 1.00 32.44 C
ANISOU 2350 CA LEU B 265 4004 4579 3744 27 -136 79 C
ATOM 2351 CB LEU B 265 155.934 59.470 -3.070 1.00 32.33 C
ANISOU 2351 CB LEU B 265 3960 4593 3731 44 -150 43 C
ATOM 2352 CG LEU B 265 155.079 59.748 -1.826 1.00 40.02 C
ANISOU 2352 CG LEU B 265 4888 5632 4686 16 -161 16 C
ATOM 2353 CD1 LEU B 265 154.844 61.219 -1.589 1.00 41.69 C
ANISOU 2353 CD1 LEU B 265 5067 5858 4917 36 -158 -27 C
ATOM 2354 CD2 LEU B 265 153.749 59.027 -1.844 1.00 41.60 C
ANISOU 2354 CD2 LEU B 265 5073 5850 4883 -14 -160 7 C
ATOM 2355 C LEU B 265 156.909 57.563 -4.457 1.00 30.89 C
ANISOU 2355 C LEU B 265 3877 4301 3557 49 -91 89 C
ATOM 2356 O LEU B 265 156.191 57.184 -5.374 1.00 33.58 O
ANISOU 2356 O LEU B 265 4286 4619 3853 38 -101 71 O
ATOM 2357 N ILE B 266 158.232 57.589 -4.545 1.00 31.47 N
ANISOU 2357 N ILE B 266 3938 4321 3697 75 -39 116 N
ATOM 2358 CA ILE B 266 158.966 57.063 -5.694 1.00 26.90 C
ANISOU 2358 CA ILE B 266 3431 3645 3145 96 53 124 C
ATOM 2359 CB ILE B 266 160.440 57.269 -5.485 1.00 30.86 C
ANISOU 2359 CB ILE B 266 3860 4088 3776 120 97 157 C
ATOM 2360 CG1 ILE B 266 160.698 58.764 -5.346 1.00 30.99 C
ANISOU 2360 CG1 ILE B 266 3829 4125 3821 135 102 145 C
ATOM 2361 CD1 ILE B 266 162.201 59.094 -4.964 1.00 28.43 C
ANISOU 2361 CD1 ILE B 266 3392 3738 3674 153 136 175 C
ATOM 2362 CG2 ILE B 266 161.297 56.621 -6.639 1.00 33.73 C
ANISOU 2362 CG2 ILE B 266 4291 4326 4201 150 263 163 C
ATOM 2363 C ILE B 266 158.690 55.582 -5.916 1.00 33.07 C
ANISOU 2363 C ILE B 266 4266 4390 3909 76 70 128 C
ATOM 2364 O ILE B 266 158.493 55.106 -7.031 1.00 37.16 O
ANISOU 2364 O ILE B 266 4899 4846 4373 72 119 103 O
ATOM 2365 N THR B 267 158.619 54.848 -4.826 1.00 24.61 N
ANISOU 2365 N THR B 267 3131 3351 2869 59 23 158 N
ATOM 2366 CA THR B 267 158.275 53.451 -4.939 1.00 24.29 C
ANISOU 2366 CA THR B 267 3136 3269 2824 35 37 165 C
ATOM 2367 CB THR B 267 158.540 52.768 -3.615 1.00 25.03 C
ANISOU 2367 CB THR B 267 3161 3382 2969 26 -5 225 C
ATOM 2368 OG1 THR B 267 159.940 52.872 -3.345 1.00 29.83 O
ANISOU 2368 OG1 THR B 267 3703 3937 3692 70 12 271 O
ATOM 2369 CG2 THR B 267 158.077 51.260 -3.645 1.00 23.99 C
ANISOU 2369 CG2 THR B 267 3076 3198 2843 -4 13 239 C
ATOM 2370 C THR B 267 156.799 53.222 -5.378 1.00 30.28 C
ANISOU 2370 C THR B 267 3954 4060 3493 -12 -13 119 C
ATOM 2371 O THR B 267 156.506 52.350 -6.180 1.00 31.27 O
ANISOU 2371 O THR B 267 4165 4122 3596 -33 8 93 O
ATOM 2372 N LEU B 268 155.858 53.968 -4.807 1.00 26.83 N
ANISOU 2372 N LEU B 268 3461 3710 3022 -32 -81 105 N
ATOM 2373 CA LEU B 268 154.448 53.866 -5.228 1.00 25.13 C
ANISOU 2373 CA LEU B 268 3261 3514 2773 -73 -142 64 C
ATOM 2374 CB LEU B 268 153.548 54.794 -4.419 1.00 26.03 C
ANISOU 2374 CB LEU B 268 3280 3712 2899 -82 -183 53 C
ATOM 2375 CG LEU B 268 153.350 54.415 -2.969 1.00 32.17 C
ANISOU 2375 CG LEU B 268 3995 4535 3694 -110 -154 81 C
ATOM 2376 CD1 LEU B 268 152.591 55.496 -2.201 1.00 32.36 C
ANISOU 2376 CD1 LEU B 268 3945 4625 3725 -112 -153 57 C
ATOM 2377 CD2 LEU B 268 152.574 53.136 -2.952 1.00 39.04 C
ANISOU 2377 CD2 LEU B 268 4869 5373 4592 -164 -149 86 C
ATOM 2378 C LEU B 268 154.272 54.206 -6.691 1.00 29.99 C
ANISOU 2378 C LEU B 268 3982 4082 3332 -65 -169 26 C
ATOM 2379 O LEU B 268 153.493 53.568 -7.412 1.00 33.46 O
ANISOU 2379 O LEU B 268 4487 4485 3743 -104 -224 -7 O
ATOM 2380 N PHE B 269 154.989 55.231 -7.140 1.00 25.77 N
ANISOU 2380 N PHE B 269 3479 3539 2775 -19 -137 31 N
ATOM 2381 CA PHE B 269 154.948 55.551 -8.537 1.00 28.93 C
ANISOU 2381 CA PHE B 269 4022 3880 3091 -11 -147 8 C
ATOM 2382 CB PHE B 269 155.734 56.807 -8.835 1.00 31.31 C
ANISOU 2382 CB PHE B 269 4340 4171 3386 37 -92 27 C
ATOM 2383 CG PHE B 269 155.532 57.301 -10.248 1.00 31.43 C
ANISOU 2383 CG PHE B 269 4530 4127 3286 43 -112 17 C
ATOM 2384 CD2 PHE B 269 156.396 56.888 -11.276 1.00 35.94 C
ANISOU 2384 CD2 PHE B 269 5275 4596 3786 49 11 11 C
ATOM 2385 CE2 PHE B 269 156.214 57.312 -12.604 1.00 32.55 C
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ANISOU 2385 CE2 PHE B 269     5060  4101  3208    47    -1     5       C
ATOM  2386  CZ  PHE B 269     155.095  58.141 -12.926  1.00 32.53           C
ANISOU 2386 CZ  PHE B 269     5080  4136  3143    43   -182    14       C
ATOM  2387  CE1 PHE B 269     154.188  58.523 -11.901  1.00 33.96           C
ANISOU 2387 CE1 PHE B 269     5050  4415  3438    43   -310    18       C
ATOM  2388  CD1 PHE B 269     154.432  58.095 -10.563  1.00 28.26           C
ANISOU 2388 CD1 PHE B 269     4135  3757  2847    40   -255    14       C
ATOM  2389  C   PHE B 269     155.466  54.376  -9.396  1.00 35.93           C
ANISOU 2389 C   PHE B 269     5051  4666  3933   -26    -72   -11       C
ATOM  2390  O   PHE B 269     154.783  53.880 -10.302  1.00 40.51           O
ANISOU 2390 O   PHE B 269     5761  5203  4430   -64   -135   -50       O
ATOM  2391  N   ALA B 270     156.670  53.918  -9.084  1.00 33.88           N
ANISOU 2391 N   ALA B 270     4768  4361  3745     1    57    14       N
ATOM  2392  CA  ALA B 270     157.275  52.816  -9.826  1.00 35.16           C
ANISOU 2392 CA  ALA B 270     5053  4408  3898    -3   167    -7       C
ATOM  2393  CB  ALA B 270     158.713  52.527  -9.343  1.00 27.84           C
ANISOU 2393 CB  ALA B 270     4040  3423  3113    45   309    35       C
ATOM  2394  C   ALA B 270     156.423  51.558  -9.768  1.00 35.07           C
ANISOU 2394 C   ALA B 270     5070  4379  3875   -58   103    -37       C
ATOM  2395  O   ALA B 270     156.322  50.827 -10.746  1.00 31.94           O
ANISOU 2395 O   ALA B 270     4837  3891  3406   -86   134    -87       O
ATOM  2396  N   MET B 271     155.812  51.288  -8.623  1.00 25.27           N
ANISOU 2396 N   MET B 271     3686  3214  2703   -82    25    -10       N
ATOM  2397  CA  MET B 271     154.918  50.132  -8.544  1.00 34.49           C
ANISOU 2397 CA  MET B 271     4868  4357  3881   -144   -30    -35       C
ATOM  2398  CB  MET B 271     154.431  49.875  -7.108  1.00 32.35           C
ANISOU 2398 CB  MET B 271     4438  4159  3693   -165   -66    14       C
ATOM  2399  CG  MET B 271     155.475  49.172  -6.256  1.00 30.03           C
ANISOU 2399 CG  MET B 271     4096  3830  3484   -134    21    78       C
ATOM  2400  SD  MET B 271     155.011  48.980  -4.513  1.00 31.26           S
ANISOU 2400 SD  MET B 271     4124  4068  3685   -159   -15   150       S
ATOM  2401  CE  MET B 271     154.005  47.503  -4.530  1.00 25.78           C
ANISOU 2401 CE  MET B 271     3459  3308  3029   -238   -17   138       C
ATOM  2402  C   MET B 271     153.721  50.217  -9.523  1.00 34.08           C
ANISOU 2402 C   MET B 271     4914  4297  3738   -199   -157   -99       C
ATOM  2403  O   MET B 271     153.232  49.215 -10.058  1.00 34.62           O
ANISOU 2403 O   MET B 271     5072  4293  3789   -255   -191   -147      O
ATOM  2404  N   SER B 272     153.229  51.420  -9.747  1.00 29.67           N
ANISOU 2404 N   SER B 272     4335  3802  3135   -185   -247    -99       N
ATOM  2405  CA  SER B 272     152.139  51.565 -10.699  1.00 33.42           C
ANISOU 2405 CA  SER B 272     4900  4261  3539   -230   -405   -147       C
ATOM  2406  CB  SER B 272     151.354  52.867 -10.458  1.00 26.95           C
ANISOU 2406 CB  SER B 272     3965  3526  2748   -210   -523   -125       C
ATOM  2407  OG  SER B 272     152.160  54.000 -10.707  1.00 33.08           O
ANISOU 2407 OG  SER B 272     4787  4315  3465   -145   -461    -96       O
ATOM  2408  C   SER B 272     152.658  51.478 -12.154  1.00 33.85           C
ANISOU 2408 C   SER B 272     5215  4214  3431   -230   -379   -188       C
ATOM  2409  O   SER B 272     151.867  51.405 -13.065  1.00 38.55           O
ANISOU 2409 O   SER B 272     5940  4773  3936   -277   -526   -232       O
ATOM  2410  N   GLN B 273     153.976  51.535 -12.384  1.00 40.89           N
ANISOU 2410 N   GLN B 273     6191  5055  4291   -179   -194   -174       N
ATOM  2411  CA  GLN B 273     154.547  51.444 -13.757  1.00 37.54           C
ANISOU 2411 CA  GLN B 273     6040  4517  3704   -179   -111   -216       C
ATOM  2412  CB  GLN B 273     155.847  52.222 -13.872  1.00 45.99           C
ANISOU 2412 CB  GLN B 273     7131  5564  4780   -109    82   -175       C
ATOM  2413  CG  GLN B 273     155.701  53.708 -13.695  1.00 59.01           C
ANISOU 2413 CG  GLN B 273     8702  7294  6424   -71    14   -124       C
ATOM  2414  CD  GLN B 273     155.001  54.356 -14.867  1.00 77.94           C
ANISOU 2414 CD  GLN B 273    11312  9667  8635   -92   -117   -138       C
ATOM  2415  OE1 GLN B 273     153.781  54.586 -14.832  1.00 86.19           O
ANISOU 2415 OE1 GLN B 273    12310 10767  9670   -123   -341   -141      O
ATOM  2416  NE2 GLN B 273     155.765  54.641 -15.934  1.00 82.74           N
ANISOU 2416 NE2 GLN B 273    12161 10176  9100   -78    24   -142       N
ATOM  2417  C   GLN B 273     153.873  50.030 -14.141  1.00 35.25           C
ANISOU 2417 C   GLN B 273     5877  4112  3403   -215   -11   -274       C
ATOM  2418  O   GLN B 273     154.896  49.671 -15.320  1.00 36.24           O
ANISOU 2418 O   GLN B 273     6267  4135  3370   -248    11   -338      O
ATOM  2419  N   TYR B 274     155.154  49.204 -13.144  1.00 29.70           N
ANISOU 2419 N   TYR B 274     5007  3414  2863   -209    58   -251       N
ATOM  2420  CA  TYR B 274     155.589  47.856 -13.437  1.00 30.65           C
ANISOU 2420 CA  TYR B 274     5231  3408  3008   -230   179   -299       C
ATOM  2421  CB  TYR B 274     156.706  47.415 -12.519  1.00 30.01           C
ANISOU 2421 CB  TYR B 274     4990  3301  3110   -168   348   -238       C
ATOM  2422  CG  TYR B 274     157.988  48.143 -12.751  1.00 50.31           C
ANISOU 2422 CG  TYR B 274     7566  5838  5711   -92   524   -205       C
ATOM  2423  CD1 TYR B 274     158.656  48.036 -13.953  1.00 57.73           C
ANISOU 2423 CD1 TYR B 274     8730  6646  6560   -81   699   -261       C
ATOM  2424  CE1 TYR B 274     159.841  48.723 -14.155  1.00 68.53           C
ANISOU 2424 CE1 TYR B 274    10082  7969  7989   -15   887   -228       C
ATOM  2425  CZ  TYR B 274     160.364  49.521 -13.131  1.00 64.60           C
ANISOU 2425 CZ  TYR B 274     9334  7562  7648    37   866   -141       C
ATOM  2426  OH  TYR B 274     161.539  50.203 -13.296  1.00 66.25           O
ANISOU 2426 OH  TYR B 274     9499  7718  7957    94  1043   -108       O
ATOM  2427  CE2 TYR B 274     159.711  49.639 -11.940  1.00 57.11           C
ANISOU 2427 CE2 TYR B 274     8191  6749  6761    25   676    -93       C
ATOM  2428  CD2 TYR B 274     158.534  48.950 -11.755  1.00 52.53           C
ANISOU 2428 CD2 TYR B 274     7633  6208  6116   -37   523   -122       C
ATOM  2429  C   TYR B 274     154.487  46.872 -13.310  1.00 31.20           C
ANISOU 2429 C   TYR B 274     5292  3463  3098   -313    38   -343       C
ATOM  2430  O   TYR B 274     153.899  46.767 -12.254  1.00 30.50           O
ANISOU 2430 O   TYR B 274     4999  3458  3132   -328   -46   -298       O
ATOM  2431  N   SER B 275     154.243  46.093 -14.372  1.00 33.54           N
ANISOU 2431 N   SER B 275     5824  3640  3279   -373    29   -437       N
ATOM  2432  CA  SER B 275     153.157  45.126 -14.348  1.00 38.44           C
ANISOU 2432 CA  SER B 275     6444  4228  3933   -467   -120   -492       C
ATOM  2433  CB  SER B 275     152.951  44.504 -15.724  1.00 36.20           C
ANISOU 2433 CB  SER B 275     6478  3806  3471   -538   -152   -611       C
ATOM  2434  OG  SER B 275     154.201  44.078 -16.157  1.00 37.28           O
ANISOU 2434 OG  SER B 275     6766  3821  3575   -487   111   -637       O
ATOM  2435  C   SER B 275     153.362  44.016 -13.319  1.00 34.79           C
ANISOU 2435 C   SER B 275     5820  3732  3665   -469   -25   -458       C
ATOM  2436  O   SER B 275     152.409  43.425 -12.845  1.00 36.81           O
ANISOU 2436 O   SER B 275     5976  3999  4011   -539   -142   -464       O
ATOM  2437  N   GLN B 276     154.606  43.698 -13.003  1.00 34.65           N
ANISOU 2437 N   GLN B 276     5781  3655  3728   -395   188   -417       N
ATOM  2438  CA  GLN B 276     154.853  42.642 -12.032  1.00 40.23           C
ANISOU 2438 CA  GLN B 276     6350  4315  4619   -389   264   -367       C
ATOM  2439  CB  GLN B 276     156.333  42.370 -11.941  1.00 48.12           C
ANISOU 2439 CB  GLN B 276     7347  5223  5715   -296   488   -328       C
ATOM  2440  CG  GLN B 276     156.702  40.981 -12.212  1.00 61.35           C
ANISOU 2440 CG  GLN B 276     9117  6719  7475   -309   618   -373       C
ATOM  2441  CD  GLN B 276     158.029  40.626 -11.568  1.00 74.49           C
ANISOU 2441 CD  GLN B 276    10655  8310  9338   -208   795   -285       C
ATOM  2442  OE1 GLN B 276     158.056  40.060 -10.463  1.00 79.33           O
ANISOU 2442 OE1 GLN B 276    11105  8931 10105   -194   763   -192      O
ATOM  2443  NE2 GLN B 276     159.145  40.960 -12.249  1.00 75.54           N
ANISOU 2443 NE2 GLN B 276    10862  8359  9480   -137   982   -307      N
ATOM  2444  C   GLN B 276     154.351  43.003 -10.628  1.00 37.41           C
ANISOU 2444 C   GLN B 276     5742  4101  4373   -384   169   -264       C
ATOM  2445  O   GLN B 276     154.017  42.123  -9.857  1.00 41.62           O
ANISOU 2445 O   GLN B 276     6185  4607  5021   -418   165   -228      O
ATOM  2446  N   ALA B 277     154.320  44.292 -10.299  1.00 30.82           N
ANISOU 2446 N   ALA B 277     4812  3402  3497   -340   110   -217       N
ATOM  2447  CA  ALA B 277     153.905  44.746  -8.965  1.00 35.75           C
ANISOU 2447 CA  ALA B 277     5228  4154  4202   -339    47   -132       C
ATOM  2448  CB  ALA B 277     154.442  46.179  -8.639  1.00 27.95           C
ANISOU 2448 CB  ALA B 277     4162  3279  3179   -267    48    -84       C
ATOM  2449  C   ALA B 277     152.395  44.701  -8.825  1.00 41.92           C
ANISOU 2449 C   ALA B 277     5949  4985  4994   -426   -102   -162       C
ATOM  2450  O   ALA B 277     151.887  44.808  -7.717  1.00 42.80           O
ANISOU 2450 O   ALA B 277     5907  5173  5184   -440   -123   -103       O
ATOM  2451  N   GLY B 278     151.690  44.553  -9.955  1.00 46.93           N
ANISOU 2451 N   GLY B 278     6711  5567  4554   -488   -205   -255       N
ATOM  2452  CA  GLY B 278     150.237  44.428  -9.979  1.00 47.95           C
ANISOU 2452 CA  GLY B 278     6770  5715  5735   -580   -370   -293       C
ATOM  2453  C   GLY B 278     149.556  45.561  -9.231  1.00 47.85           C
ANISOU 2453 C   GLY B 278     6569  5839  5772   -562   -444   -242       C
ATOM  2454  O   GLY B 278     148.781  45.331  -8.310  1.00 53.63           O
ANISOU 2454 O   GLY B 278     7139  6604  6632   -604   -449   -209       O
ATOM  2455  N   PHE B 279     149.851  46.793  -9.632  1.00 41.02           N
ANISOU 2455 N   PHE B 279     5733  5040  4810   -502   -479   -237       N
ATOM  2456  CA  PHE B 279     149.463  47.965  -8.879  1.00 39.38           C
ANISOU 2456 CA  PHE B 279     5361  4952  4649   -465   -509   -188       C
ATOM  2457  CB  PHE B 279     150.726  48.504  -8.215  1.00 46.38           C
ANISOU 2457 CB  PHE B 279     6233  5887  5500   -378   -365   -125       C
ATOM  2458  CG  PHE B 279     150.494  49.319  -6.991  1.00 47.78           C
ANISOU 2458 CG  PHE B 279     6243  6171  5740   -351   -341    -72       C
ATOM  2459  CD1 PHE B 279     150.135  48.703  -5.814  1.00 46.78           C
ANISOU 2459 CD1 PHE B 279     6011  6060  5701   -386   -282    -31       C
ATOM  2460  CE1 PHE B 279     149.952  49.438  -4.684  1.00 43.88           C
ANISOU 2460 CE1 PHE B 279     5532  5780  5362   -367   -240     9       C
ATOM  2461  CZ  PHE B 279     150.161  50.833  -4.713  1.00 42.99           C
ANISOU 2461 CZ  PHE B 279     5392  5736  5205   -309   -263     5       C
ATOM  2462  CE2 PHE B 279     150.524  51.462  -5.874  1.00 40.56           C
ANISOU 2462 CE2 PHE B 279     5169  5412  4831   -272   -326    -27       C
ATOM  2463  CD2 PHE B 279     150.691  50.703  -7.009  1.00 45.04           C
ANISOU 2463 CD2 PHE B 279     5867  5894  5351   -294   -362    -62       C
ATOM  2464  C   PHE B 279     148.935  48.974  -9.880  1.00 33.96           C
ANISOU 2464 C   PHE B 279     4731  4283  3889   -458   -667   -224       C
ATOM  2465  O   PHE B 279     149.671  49.442 -10.726  1.00 40.84           O
ANISOU 2465 O   PHE B 279     5764  5132  4622   -415   -653   -236       O
ATOM  2466  N   SER B 280     147.658  49.331  -9.789  1.00 39.95           N
ANISOU 2466 N   SER B 280     5354  5071  4754   -499   -813   -235       N
ATOM  2467  CA  SER B 280     147.071  50.286 -10.726  1.00 41.59           C
ANISOU 2467 CA  SER B 280     5605  5284  4915   -490 -1001   -255       C
ATOM  2468  CB  SER B 280     145.569  50.035 -10.831  1.00 45.42           C
ANISOU 2468  CB  SER B 280     5948  5742  5566   -568 -1194   -286       C
ATOM  2469  OG  SER B 280     144.876  50.516 -9.688  1.00 51.97           O
ANISOU 2469 OG  SER B 280     6516  6638  6593   -557 -1142   -248      O
ATOM  2470  C   SER B 280     147.346  51.762 -10.349  1.00 43.47           C
ANISOU 2470 C   SER B 280     5764  5608  5148   -402   -966   -203       C
ATOM  2471  O   SER B 280     147.709  52.075 -9.200  1.00 41.15           O
ANISOU 2471 O   SER B 280     5342  5381  4911   -363   -820   -163       O
ATOM  2472  N   ARG B 281     147.139  52.668 -11.310  1.00 44.16           N
ANISOU 2472 N   ARG B 281     5944  5944  4944   -375 -1112   -205       N
ATOM  2473  CA  ARG B 281     147.216  54.104 -11.034  1.00 50.88           C
ANISOU 2473 CA  ARG B 281     6714  6599  6019   -298 -1104   -159       C
ATOM  2474  CB  ARG B 281     146.887  54.901 -12.279  1.00 60.59           C
ANISOU 2474 CB  ARG B 281     8083  7787  7150   -281 -1299   -153       C
ATOM  2475  CG  ARG B 281     148.088  55.500 -12.931  1.00 76.27           C
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ANISOU 2475 CG ARG B 281 10286 9755 8936 -225 -1199 -129 C
ATOM 2476 CD ARG B 281 147.682 56.665 -13.850 1.00 87.95 C
ANISOU 2476 CD ARG B 281 11861 11210 10347 -189 -1376 -93 C
ATOM 2477 NE ARG B 281 148.470 57.870 -13.566 1.00 94.73 N
ANISOU 2477 NE ARG B 281 12706 12100 11185 -108 -1241 -42 N
ATOM 2478 CZ ARG B 281 148.047 59.120 -13.753 1.00 94.24 C
ANISOU 2478 CZ ARG B 281 12603 12040 11164 -57 -1346 6 C
ATOM 2479 NH1 ARG B 281 148.838 60.155 -13.458 1.00 90.45 N
ANISOU 2479 NH1 ARG B 281 12114 11579 10675 9 -1204 45 N
ATOM 2480 NH2 ARG B 281 146.830 59.330 -14.230 1.00 95.49 N
ANISOU 2480 NH2 ARG B 281 12717 12169 11394 -72 -1602 17 N
ATOM 2481 C ARG B 281 146.240 54.520 -9.933 1.00 51.83 C
ANISOU 2481 C ARG B 281 6557 6775 6359 -297 -1106 -144 C
ATOM 2482 O ARG B 281 146.480 55.457 -9.156 1.00 50.26 O
ANISOU 2482 O ARG B 281 6257 6635 6203 -239 -1004 -115 O
ATOM 2483 N GLU B 282 145.121 53.818 -9.884 1.00 50.97 N
ANISOU 2483 N GLU B 282 6332 6634 6401 -368 -1212 -172 N
ATOM 2484 CA GLU B 282 144.092 54.074 -8.887 1.00 54.35 C
ANISOU 2484 CA GLU B 282 6492 7090 7069 -379 -1184 -165 C
ATOM 2485 CB GLU B 282 142.792 53.366 -9.265 1.00 63.19 C
ANISOU 2485 CB GLU B 282 7495 8141 8373 -465 -1362 -198 C
ATOM 2486 CG GLU B 282 142.103 53.972 -10.469 1.00 75.97 C
ANISOU 2486 CG GLU B 282 9143 9709 10012 -460 -1654 -202 C
ATOM 2487 CD GLU B 282 142.995 54.012 -11.719 1.00 85.87 C
ANISOU 2487 CD GLU B 282 10720 10935 10970 -444 -1751 -206 C
ATOM 2488 OE1 GLU B 282 143.430 52.924 -12.183 1.00 86.63 O
ANISOU 2488 OE1 GLU B 282 10995 10987 10933 -503 -1741 -248 O
ATOM 2489 OE2 GLU B 282 143.273 55.136 -12.212 1.00 89.09 O
ANISOU 2489 OE2 GLU B 282 11211 11356 11284 -371 -1813 -168 O
ATOM 2490 C GLU B 282 144.541 53.615 -7.503 1.00 55.29 C
ANISOU 2490 C GLU B 282 6538 7257 7213 -384 -937 -150 C
ATOM 2491 O GLU B 282 144.324 54.306 -6.501 1.00 54.94 O
ANISOU 2491 O GLU B 282 6353 7261 7261 -352 -820 -134 O
ATOM 2492 N ASP B 283 145.146 52.434 -7.451 1.00 54.67 N
ANISOU 2492 N ASP B 283 6569 7153 7050 -427 -862 -156 N
ATOM 2493 CA ASP B 283 145.719 51.938 -6.209 1.00 60.33 C
ANISOU 2493 CA ASP B 283 7261 7905 7757 -428 -654 -124 C
ATOM 2494 CB ASP B 283 146.422 50.584 -6.415 1.00 70.84 C
ANISOU 2494 CB ASP B 283 8731 9180 9005 -468 -607 -125 C
ATOM 2495 CG ASP B 283 145.449 49.439 -6.718 1.00 79.90 C
ANISOU 2495 CG ASP B 283 9835 10247 10276 -566 -682 -161 C
ATOM 2496 OD1 ASP B 283 144.220 49.644 -6.556 1.00 83.36 O
ANISOU 2496 OD1 ASP B 283 10100 10678 10893 -607 -750 -176 O
ATOM 2497 OD2 ASP B 283 145.937 48.338 -7.113 1.00 81.92 O
ANISOU 2497 OD2 ASP B 283 10221 10434 10471 -601 -667 -177 O
ATOM 2498 C ASP B 283 146.727 52.947 -5.692 1.00 57.39 C
ANISOU 2498 C ASP B 283 6928 7601 7276 -345 -552 -93 C
ATOM 2499 O ASP B 283 146.865 53.163 -4.481 1.00 58.73 O
ANISOU 2499 O ASP B 283 7030 7820 7466 -334 -416 -68 O
ATOM 2500 N ARG B 284 147.418 53.577 -6.635 1.00 49.18 N
ANISOU 2500 N ARG B 284 6013 6557 6116 -294 -620 -96 N
ATOM 2501 CA ARG B 284 148.479 54.495 -6.290 1.00 44.91 C
ANISOU 2501 CA ARG B 284 5514 6063 5487 -223 -532 -70 C
ATOM 2502 CB ARG B 284 149.217 54.966 -7.529 1.00 44.99 C
ANISOU 2502 CB ARG B 284 5684 6038 5372 -183 -590 -72 C
ATOM 2503 CG ARG B 284 150.564 55.583 -7.157 1.00 46.17 C
ANISOU 2503 CG ARG B 284 5878 6213 5453 -124 -470 -43 C
ATOM 2504 CD ARG B 284 151.245 56.118 -8.359 1.00 44.35 C
ANISOU 2504 CD ARG B 284 5800 5935 5116 -87 -490 -41 C
ATOM 2505 NE ARG B 284 150.495 57.197 -8.970 1.00 46.36 N
ANISOU 2505 NE ARG B 284 6051 6190 5375 -66 -611 -41 N
ATOM 2506 CZ ARG B 284 150.525 57.454 -10.266 1.00 52.50 C
ANISOU 2506 CZ ARG B 284 6994 6909 6046 -58 -694 -39 C
ATOM 2507 NH1 ARG B 284 149.839 58.467 -10.753 1.00 58.36 N
ANISOU 2507 NH1 ARG B 284 7729 7644 6801 -33 -822 -23 N
ATOM 2508 NH2 ARG B 284 151.239 56.685 -11.070 1.00 52.19 N
ANISOU 2508 NH2 ARG B 284 7139 6806 5886 -76 -643 -52 N
ATOM 2509 C ARG B 284 148.022 55.720 -5.491 1.00 44.78 C
ANISOU 2509 C ARG B 284 5363 6103 5550 -187 -500 -66 C
ATOM 2510 O ARG B 284 148.691 56.162 -4.521 1.00 32.80 O
ANISOU 2510 O ARG B 284 3832 4631 3998 -159 -386 -50 O
ATOM 2511 N LEU B 285 146.910 56.304 -5.929 1.00 43.40 N
ANISOU 2511 N LEU B 285 5093 5912 5485 -186 -612 -84 N
ATOM 2512 CA LEU B 285 146.419 57.484 -5.247 1.00 44.90 C
ANISOU 2512 CA LEU B 285 5150 6133 5776 -145 -569 -88 C
ATOM 2513 CB LEU B 285 145.348 58.202 -6.056 1.00 45.22 C
ANISOU 2513 CB LEU B 285 5101 6132 5947 -126 -733 -95 C
ATOM 2514 CG LEU B 285 144.798 59.411 -5.304 1.00 53.58 C
ANISOU 2514 CG LEU B 285 6006 7205 7148 -77 -662 -104 C
ATOM 2515 CD1 LEU B 285 145.949 60.394 -4.954 1.00 60.00 C
ANISOU 2515 CD1 LEU B 285 6915 8055 7829 -18 -564 -97 C
ATOM 2516 CD2 LEU B 285 143.698 60.103 -6.110 1.00 58.14 C
ANISOU 2516 CD2 LEU B 285 6468 7723 7898 -49 -844 -98 C
ATOM 2517 C LEU B 285 145.879 57.068 -3.869 1.00 48.22 C
ANISOU 2517 C LEU B 285 5449 6578 6294 -185 -417 -97 C
ATOM 2518 O LEU B 285 146.009 57.783 -2.870 1.00 47.51 O
ANISOU 2518 O LEU B 285 5320 6524 6207 -160 -291 -104 O
ATOM 2519 N GLU B 286 145.268 55.895 -3.843 1.00 44.30 N
ANISOU 2519 N GLU B 286 4913 6051 5870 -255 -423 -100 N
ATOM 2520 CA GLU B 286 144.658 55.358 -2.645 1.00 48.57 C
ANISOU 2520 CA GLU B 286 5353 6593 6507 -306 -267 -100 C
ATOM 2521 CB GLU B 286 143.971 54.044 -3.012 1.00 58.43 C
ANISOU 2521 CB GLU B 286 6562 7783 7855 -387 -319 -102 C
ATOM 2522 CG GLU B 286 143.091 53.422 -1.956 1.00 75.50 C
ANISOU 2522 CG GLU B 286 8600 9921 10167 -454 -159 -99 C
ATOM 2523 CD GLU B 286 142.750 51.955 -2.288 1.00 89.29 C
ANISOU 2523 CD GLU B 286 10349 11601 11976 -541 -198 -94 C
ATOM 2524 OE1 GLU B 286 141.551 51.578 -2.180 1.00 94.04 O
ANISOU 2524 OE1 GLU B 286 10780 12143 12808 -605 -185 -111 O
ATOM 2525 OE2 GLU B 286 143.689 51.196 -2.664 1.00 91.51 O
ANISOU 2525 OE2 GLU B 286 10796 11877 12098 -546 -236 -76 O
ATOM 2526 C GLU B 286 145.764 55.130 -1.611 1.00 42.01 C
ANISOU 2526 C GLU B 286 4645 5810 5506 -300 -121 -70 C
ATOM 2527 O GLU B 286 145.635 55.509 -0.451 1.00 35.30 O
ANISOU 2527 O GLU B 286 3770 4988 4655 -301 26 -72 O
ATOM 2528 N GLN B 287 146.865 54.527 -2.054 1.00 35.94 N
ANISOU 2528 N GLN B 287 4017 5040 4598 -292 -166 -44 N
ATOM 2529 CA GLN B 287 147.975 54.193 -1.175 1.00 34.78 C
ANISOU 2529 CA GLN B 287 3976 4921 4317 -286 -74 -3 C
ATOM 2530 CB GLN B 287 148.926 53.178 -1.830 1.00 38.60 C
ANISOU 2530 CB GLN B 287 4573 5366 4727 -288 -123 26 C
ATOM 2531 CG GLN B 287 148.325 51.791 -2.049 1.00 38.43 C
ANISOU 2531 CG GLN B 287 4546 5282 4773 -356 -125 32 C
ATOM 2532 CD GLN B 287 147.817 51.169 -0.752 1.00 43.76 C
ANISOU 2532 CD GLN B 287 5184 5958 5485 -410 3 68 C
ATOM 2533 OE1 GLN B 287 148.592 50.656 0.065 1.00 50.64 O
ANISOU 2533 OE1 GLN B 287 6140 6832 6270 -409 69 126 O
ATOM 2534 NE2 GLN B 287 146.519 51.241 -0.544 1.00 42.04 N
ANISOU 2534 NE2 GLN B 287 4841 5727 5404 -457 40 40 N
ATOM 2535 C GLN B 287 148.741 55.446 -0.762 1.00 35.15 C
ANISOU 2535 C GLN B 287 4054 5018 4283 -226 -54 -10 C
ATOM 2536 O GLN B 287 149.270 55.517 0.341 1.00 30.91 O
ANISOU 2536 O GLN B 287 3567 4511 3665 -229 25 11 O
ATOM 2537 N ALA B 288 148.812 56.429 -1.651 1.00 34.10 N
ANISOU 2537 N ALA B 288 3907 4884 4165 -176 -137 -36 N
ATOM 2538 CA ALA B 288 149.504 57.667 -1.308 1.00 36.04 C
ANISOU 2538 CA ALA B 288 4174 5163 4358 -125 -117 -47 C
ATOM 2539 CB ALA B 288 149.597 58.631 -2.493 1.00 24.00 C
ANISOU 2539 CB ALA B 288 2650 3615 2852 -73 -212 -60 C
ATOM 2540 C ALA B 288 148.797 58.313 -0.125 1.00 33.10 C
ANISOU 2540 C ALA B 288 3735 4026 -136 -10 -78 C
ATOM 2541 O ALA B 288 149.434 58.799 0.789 1.00 30.08 O
ANISOU 2541 O ALA B 288 3408 4461 3558 -129 49 -84 O
ATOM 2542 N LYS B 289 147.467 58.288 -0.118 1.00 29.63 N
ANISOU 2542 N LYS B 289 3177 4354 3726 -157 21 -103 N
ATOM 2543 CA LYS B 289 146.744 58.952 0.948 1.00 35.47 C
ANISOU 2543 CA LYS B 289 3852 5098 4526 -163 163 -143 C
ATOM 2544 CB LYS B 289 145.281 59.113 0.573 1.00 40.07 C
ANISOU 2544 CB LYS B 289 4255 5633 5335 -166 167 -169 C
ATOM 2545 CG LYS B 289 145.080 60.252 -0.383 1.00 50.62 C
ANISOU 2545 CG LYS B 289 5522 6946 6766 -99 44 -186 C
ATOM 2546 CD LYS B 289 144.069 59.890 -1.445 1.00 60.11 C
ANISOU 2546 CD LYS B 289 6597 8097 8147 -107 -102 -175 C
ATOM 2547 CE LYS B 289 142.666 59.918 -0.936 1.00 66.69 C
ANISOU 2547 CE LYS B 289 7228 8881 9231 -129 -6 -203 C
ATOM 2548 NZ LYS B 289 141.767 59.151 -1.870 1.00 75.65 N
ANISOU 2548 NZ LYS B 289 8245 9963 10536 -168 -171 -187 N
ATOM 2549 C LYS B 289 146.901 58.175 2.237 1.00 36.05 C
ANISOU 2549 C LYS B 289 4010 5189 4497 -220 302 -124 C
ATOM 2550 O LYS B 289 147.015 58.738 3.334 1.00 41.82 O
ANISOU 2550 O LYS B 289 4803 5937 5151 -225 422 -151 O
ATOM 2551 N LEU B 290 146.909 56.867 2.081 1.00 35.90 N
ANISOU 2551 N LEU B 290 4016 5156 4468 -265 283 -76 N
ATOM 2552 CA LEU B 290 147.001 56.964 3.207 1.00 36.96 C
ANISOU 2552 CA LEU B 290 4242 5297 4502 -323 403 -37 C
ATOM 2553 CB LEU B 290 146.723 54.530 2.744 1.00 45.99 C
ANISOU 2553 CB LEU B 290 5368 6394 5713 -372 372 10 C
ATOM 2554 CG LEU B 290 146.826 53.395 3.766 1.00 57.05 C
ANISOU 2554 CG LEU B 290 6872 7775 7029 -434 483 73 C
ATOM 2555 CD1 LEU B 290 145.879 53.645 4.912 1.00 60.61 C
ANISOU 2555 CD1 LEU B 290 7309 8214 7504 -478 693 55 C
ATOM 2556 CD2 LEU B 290 146.450 52.070 3.118 1.00 59.94 C
ANISOU 2556 CD2 LEU B 290 7195 8082 7499 -481 445 105 C
ATOM 2557 C LEU B 290 148.390 56.116 3.855 1.00 36.56 C
ANISOU 2557 C LEU B 290 4357 5280 4255 -305 368 -5 C
ATOM 2558 O LEU B 290 148.536 56.176 5.077 1.00 37.37 O
ANISOU 2558 O LEU B 290 4568 5396 4236 -333 466 3 O
ATOM 2559 N PHE B 291 149.400 56.201 3.011 1.00 25.99 N
ANISOU 2559 N PHE B 291 3039 3949 2888 -261 226 12 N
ATOM 2560 CA PHE B 291 150.774 56.421 3.425 1.00 31.73 C
ANISOU 2560 CA PHE B 291 3874 4698 3484 -238 161 41 C
ATOM 2561 CB PHE B 291 151.700 56.515 2.193 1.00 24.44 C
ANISOU 2561 CB PHE B 291 2930 3759 2597 -187 38 51 C
ATOM 2562 CG PHE B 291 153.135 56.944 2.524 1.00 24.11 C
ANISOU 2562 CG PHE B 291 2951 3726 2484 -159 -30 73 C
ATOM 2563 CD1 PHE B 291 154.040 56.024 3.042 1.00 24.36 C
ANISOU 2563 CD1 PHE B 291 3050 3741 2464 -170 -73 145 C
ATOM 2564 CE1 PHE B 291 155.344 56.404 3.379 1.00 24.68 C
ANISOU 2564 CE1 PHE B 291 3120 3778 2479 -148 -160 169 C
ATOM 2565 CZ PHE B 291 155.758 57.753 3.182 1.00 24.04 C

ANISOU 2565 CZ PHE B 291 3006 3709 2419 -120 -189 112 C
ATOM 2566 CE2 PHE B 291 154.862 58.680 2.659 1.00 23.70 C
ANISOU 2566 CE2 PHE B 291 2912 3681 2411 -107 -131 42 C
ATOM 2567 CD2 PHE B 291 153.551 58.274 2.346 1.00 23.77 C
ANISOU 2567 CD2 PHE B 291 2887 3695 2451 -123 -59 26 C
ATOM 2568 C PHE B 291 150.900 57.702 4.275 1.00 34.71 C
ANISOU 2568 C PHE B 291 4292 5105 3791 -228 203 -14 C
ATOM 2569 O PHE B 291 151.507 57.705 5.356 1.00 32.48 O
ANISOU 2569 O PHE B 291 4132 4838 3371 -251 208 4 O
ATOM 2570 N CYS B 292 150.325 58.795 3.777 1.00 26.71 N
ANISOU 2570 N CYS B 292 3186 4090 2872 -194 221 -80 N
ATOM 2571 CA CYS B 292 150.389 60.068 4.499 1.00 34.60 C
ANISOU 2571 CA CYS B 292 4220 5100 3826 -182 273 -146 C
ATOM 2572 CB CYS B 292 149.831 61.211 3.636 1.00 33.07 C
ANISOU 2572 CB CYS B 292 3904 4884 3777 -129 265 -202 C
ATOM 2573 SG CYS B 292 149.785 62.749 4.555 1.00 67.72 S
ANISOU 2573 SG CYS B 292 8333 9263 8136 -117 358 -295 S
ATOM 2574 C CYS B 292 149.647 59.990 5.870 1.00 31.78 C
ANISOU 2574 C CYS B 292 3941 4742 3391 -236 444 -175 C
ATOM 2575 O CYS B 292 150.101 60.454 6.943 1.00 34.22 O
ANISOU 2575 O CYS B 292 4391 5062 3550 -259 479 -204 O
ATOM 2576 N ARG B 293 148.490 59.385 5.844 1.00 28.30 N
ANISOU 2576 N ARG B 293 3421 4278 3053 -262 557 -170 N
ATOM 2577 CA ARG B 293 147.753 59.292 7.094 1.00 35.43 C
ANISOU 2577 CA ARG B 293 4404 5165 3895 -315 763 -195 C
ATOM 2578 CB ARG B 293 146.328 58.878 6.832 1.00 37.06 C
ANISOU 2578 CB ARG B 293 4449 5326 4308 -335 899 -205 C
ATOM 2579 CG ARG B 293 145.623 59.790 5.892 1.00 49.81 C
ANISOU 2579 CG ARG B 293 5862 6914 6150 -277 867 -260 C
ATOM 2580 CD ARG B 293 144.194 59.402 5.889 1.00 69.65 C
ANISOU 2580 CD ARG B 293 8208 9368 8886 -305 1012 -272 C
ATOM 2581 NE ARG B 293 143.483 59.517 4.609 1.00 79.48 N
ANISOU 2581 NE ARG B 293 9232 10581 10385 -268 881 -273 N
ATOM 2582 CZ ARG B 293 143.041 58.479 3.887 1.00 81.59 C
ANISOU 2582 CZ ARG B 293 9403 10828 10769 -302 790 -228 C
ATOM 2583 NH1 ARG B 293 143.253 57.221 4.286 1.00 77.93 N
ANISOU 2583 NH1 ARG B 293 9033 10370 10207 -368 832 -175 N
ATOM 2584 NH2 ARG B 293 142.382 58.696 2.754 1.00 83.46 N
ANISOU 2584 NH2 ARG B 293 9461 11030 11222 -271 643 -235 N
ATOM 2585 C ARG B 293 148.398 58.374 8.137 1.00 35.22 C
ANISOU 2585 C ARG B 293 4584 5152 3647 -373 774 -128 C
ATOM 2586 O ARG B 293 148.290 58.610 9.351 1.00 38.86 O
ANISOU 2586 O ARG B 293 5208 5606 3951 -415 907 -154 O
ATOM 2587 N THR B 294 149.042 57.311 7.658 1.00 31.72 N
ANISOU 2587 N THR B 294 4148 4715 3189 -375 639 -39 N
ATOM 2588 CA THR B 294 149.717 56.370 8.530 1.00 30.38 C
ANISOU 2588 CA THR B 294 4161 4546 2837 -419 611 47 C
ATOM 2589 CB THR B 294 150.065 55.060 7.827 1.00 39.52 C
ANISOU 2589 CB THR B 294 5272 5683 4062 -417 510 140 C
ATOM 2590 OG1 THR B 294 148.870 54.472 7.313 1.00 34.69 O
ANISOU 2590 OG1 THR B 294 4529 5036 3616 -443 621 133 O
ATOM 2591 CG2 THR B 294 150.724 54.079 8.824 1.00 30.66 C
ANISOU 2591 CG2 THR B 294 4342 4544 2762 -458 481 245 C
ATOM 2592 C THR B 294 150.975 57.019 9.078 1.00 30.35 C
ANISOU 2592 C THR B 294 4297 4571 2666 -405 470 44 C
ATOM 2593 O THR B 294 151.264 56.981 10.288 1.00 31.72 O
ANISOU 2593 O THR B 294 4675 4744 2634 -450 492 62 O
ATOM 2594 N LEU B 295 151.723 57.657 8.193 1.00 30.18 N
ANISOU 2594 N LEU B 295 4174 4564 2730 -348 322 19 N
ATOM 2595 CA LEU B 295 152.927 58.350 8.656 1.00 29.13 C
ANISOU 2595 CA LEU B 295 4137 4445 2485 -339 178 9 C
ATOM 2596 CB LEU B 295 153.655 58.976 7.500 1.00 27.69 C
ANISOU 2596 CB LEU B 295 3812 4264 2446 -277 54 -12 C
ATOM 2597 CG LEU B 295 155.051 59.498 7.803 1.00 33.67 C
ANISOU 2597 CG LEU B 295 4622 5018 3152 -270 -117 -6 C
ATOM 2598 CD1 LEU B 295 155.948 58.394 8.281 1.00 28.37 C
ANISOU 2598 CD1 LEU B 295 4031 4334 2415 -287 -247 103 C
ATOM 2599 CD2 LEU B 295 155.623 60.121 6.518 1.00 26.48 C
ANISOU 2599 CD2 LEU B 295 3555 4093 2415 -210 -183 -25 C
ATOM 2600 C LEU B 295 152.606 59.403 9.755 1.00 34.10 C
ANISOU 2600 C LEU B 295 4905 5080 2973 -374 275 -83 C
ATOM 2601 O LEU B 295 153.287 59.502 10.781 1.00 35.13 O
ANISOU 2601 O LEU B 295 5224 5211 2912 -413 199 -74 O
ATOM 2602 N GLU B 296 151.532 60.154 9.530 1.00 32.69 N
ANISOU 2602 N GLU B 296 4636 4890 2894 -361 442 -172 N
ATOM 2603 CA GLU B 296 151.013 61.107 10.507 1.00 39.87 C
ANISOU 2603 CA GLU B 296 5665 5783 3700 -391 596 -274 C
ATOM 2604 CB GLU B 296 149.653 61.594 10.043 1.00 50.68 C
ANISOU 2604 CB GLU B 296 6867 7122 5266 -363 796 -344 C
ATOM 2605 CG GLU B 296 149.482 63.062 9.967 1.00 64.40 C
ANISOU 2605 CG GLU B 296 8558 8833 7076 -327 845 -458 C
ATOM 2606 CD GLU B 296 148.068 63.435 9.516 1.00 77.16 C
ANISOU 2606 CD GLU B 296 9984 10404 8929 -293 1034 -510 C
ATOM 2607 OE1 GLU B 296 147.348 62.538 8.994 1.00 75.78 O
ANISOU 2607 OE1 GLU B 296 9676 10225 8890 -294 1069 -450 O
ATOM 2608 OE2 GLU B 296 147.687 64.622 9.701 1.00 84.25 O
ANISOU 2608 OE2 GLU B 296 10859 11257 9894 -267 1140 -611 O
ATOM 2609 C GLU B 296 150.834 60.471 11.885 1.00 39.90 C
ANISOU 2609 C GLU B 296 5919 5777 3464 -468 703 -246 C
ATOM 2610 O GLU B 296 151.298 60.992 12.900 1.00 39.99 O
ANISOU 2610 O GLU B 296 6150 5784 3263 -509 683 -290 O
ATOM 2611 N ASP B 297 150.134 59.341 11.915 1.00 41.75 N
ANISOU 2611 N ASP B 297 6136 5999 3727 -494 818 -172 N
ATOM 2612 CA ASP B 297 149.846 58.652 13.167 1.00 45.15 C
ANISOU 2612 CA ASP B 297 6812 6406 3936 -570 955 -128 C
ATOM 2613 CB ASP B 297 148.836 57.546 12.925 1.00 51.05 C
ANISOU 2613 CB ASP B 297 7461 7123 4814 -592 1124 -62 C
ATOM 2614 CG ASP B 297 147.451 58.090 12.581 1.00 71.66 C
ANISOU 2614 CG ASP B 297 9878 9697 7651 -579 1372 -156 C
ATOM 2615 OD1 ASP B 297 147.250 59.332 12.680 1.00 76.91 O
ANISOU 2615 OD1 ASP B 297 10523 10354 8344 -553 1441 -271 O
ATOM 2616 OD2 ASP B 297 146.562 57.270 12.230 1.00 79.94 O
ANISOU 2616 OD2 ASP B 297 10790 10713 8872 -597 1494 -114 O
ATOM 2617 C ASP B 297 151.083 58.100 13.876 1.00 44.80 C
ANISOU 2617 C ASP B 297 6997 6376 3648 -601 736 -34 C
ATOM 2618 O ASP B 297 151.174 58.100 15.104 1.00 49.70 O
ANISOU 2618 O ASP B 297 7904 6980 4001 -665 785 -31 O
ATOM 2619 N ILE B 298 152.029 57.625 13.083 1.00 40.14 N
ANISOU 2619 N ILE B 298 6285 5807 3159 -557 493 45 N
ATOM 2620 CA ILE B 298 153.303 57.172 13.609 1.00 40.93 C
ANISOU 2620 CA ILE B 298 6540 5909 3103 -570 244 139 C
ATOM 2621 CB ILE B 298 154.192 56.546 12.510 1.00 34.52 C
ANISOU 2621 CB ILE B 298 5527 5100 2490 -508 37 223 C
ATOM 2622 CG1 ILE B 298 153.591 55.246 11.988 1.00 33.70 C
ANISOU 2622 CG1 ILE B 298 5333 4971 2501 -504 134 311 C
ATOM 2623 CD1 ILE B 298 154.352 54.689 10.784 1.00 32.05 C
ANISOU 2623 CD1 ILE B 298 4927 4750 2500 -440 -21 368 C
ATOM 2624 CG2 ILE B 298 155.572 56.256 13.043 1.00 35.00 C
ANISOU 2624 CG2 ILE B 298 5705 5147 2446 -512 -236 311 C
ATOM 2625 C ILE B 298 154.040 58.334 14.281 1.00 36.85 C
ANISOU 2625 C ILE B 298 6168 5401 2431 -589 115 55 C
ATOM 2626 O ILE B 298 154.479 58.219 15.425 1.00 38.80 O
ANISOU 2626 O ILE B 298 6689 5635 2419 -647 30 87 O
ATOM 2627 N LEU B 299 154.140 59.450 13.581 1.00 35.84 N
ANISOU 2627 N LEU B 299 5875 5287 2456 -545 99 -51 N
ATOM 2628 CA LEU B 299 154.880 60.620 14.073 1.00 41.44 C
ANISOU 2628 CA LEU B 299 6686 5993 3065 -563 -33 -143 C
ATOM 2629 CB LEU B 299 155.061 61.654 12.978 1.00 34.65 C
ANISOU 2629 CB LEU B 299 5583 5137 2445 -500 -61 -226 C
ATOM 2630 CG LEU B 299 155.920 61.154 11.824 1.00 43.21 C
ANISOU 2630 CG LEU B 299 6447 6228 3743 -439 -237 -136 C
ATOM 2631 CD1 LEU B 299 156.041 62.234 10.744 1.00 41.03 C
ANISOU 2631 CD1 LEU B 299 5966 5945 3679 -383 -234 -214 C
ATOM 2632 CD2 LEU B 299 157.334 60.724 12.298 1.00 35.27 C
ANISOU 2632 CD2 LEU B 299 5520 5209 2670 -459 -519 -50 C
ATOM 2633 C LEU B 299 154.254 61.279 15.270 1.00 50.93 C
ANISOU 2633 C LEU B 299 8152 7174 4025 -630 135 -246 C
ATOM 2634 O LEU B 299 154.951 61.844 16.125 1.00 59.15 O
ANISOU 2634 O LEU B 299 9406 8202 4868 -680 -8 -293 O
ATOM 2635 N ALA B 300 152.929 61.217 15.321 1.00 51.13 N
ANISOU 2635 N ALA B 300 8162 7184 4079 -635 445 -289 N
ATOM 2636 CA ALA B 300 152.209 61.780 16.441 1.00 55.44 C
ANISOU 2636 CA ALA B 300 8960 7693 4411 -697 677 -393 C
ATOM 2637 CB ALA B 300 150.733 61.684 16.212 1.00 58.52 C
ANISOU 2637 CB ALA B 300 9227 8055 4953 -684 1027 -432 C
ATOM 2638 C ALA B 300 152.594 61.111 17.767 1.00 61.76 C
ANISOU 2638 C ALA B 300 10136 8478 4850 -784 618 -323 C
ATOM 2639 O ALA B 300 152.700 61.779 18.799 1.00 64.02 O
ANISOU 2639 O ALA B 300 10716 8735 4875 -847 646 -413 O
ATOM 2640 N ASP B 301 152.798 59.795 17.733 1.00 62.76 N
ANISOU 2640 N ASP B 301 9683 8633 6532 15 1371 1184 N
ATOM 2641 CA ASP B 301 153.134 59.034 18.929 1.00 69.90 C
ANISOU 2641 CA ASP B 301 9789 9618 7151 23 1415 1451 C
ATOM 2642 CB ASP B 301 152.460 57.659 18.901 1.00 86.46 C
ANISOU 2642 CB ASP B 301 11695 11635 9522 21 1696 1695 C
ATOM 2643 CG ASP B 301 150.959 57.748 19.051 1.00100.69 C
ANISOU 2643 CG ASP B 301 13425 13416 11415 67 2106 1640 C
ATOM 2644 OD1 ASP B 301 150.426 58.860 18.823 1.00105.45 O
ANISOU 2644 OD1 ASP B 301 14044 14037 11986 113 2155 1387 O
ATOM 2645 OD2 ASP B 301 150.326 56.716 19.393 1.00104.46 O
ANISOU 2645 OD2 ASP B 301 13815 13847 12030 60 2384 1867 O
ATOM 2646 C ASP B 301 154.621 58.831 19.117 1.00 64.09 C
ANISOU 2646 C ASP B 301 9129 8928 6294 -28 1030 1587 C
ATOM 2647 O ASP B 301 155.050 58.318 20.146 1.00 69.18 O
ANISOU 2647 O ASP B 301 9969 9659 6659 -22 982 1824 O
ATOM 2648 N ALA B 302 155.412 59.198 18.119 1.00 55.81 N
ANISOU 2648 N ALA B 302 7912 7821 5474 -76 760 1470 N
ATOM 2649 CA ALA B 302 156.836 58.878 18.176 1.00 54.16 C
ANISOU 2649 CA ALA B 302 7269 5269 -119 419 1642 C
ATOM 2650 CB ALA B 302 157.418 58.732 16.793 1.00 44.24 C
ANISOU 2650 CB ALA B 302 6119 6250 4442 -146 305 1585 C
ATOM 2651 C ALA B 302 157.602 59.923 18.961 1.00 65.37 C
ANISOU 2651 C ALA B 302 9367 9180 6289 -166 110 1560 C
ATOM 2652 O ALA B 302 157.466 61.126 18.685 1.00 65.07 O
ANISOU 2652 O ALA B 302 9411 9136 6175 -191 49 1275 O
ATOM 2653 N PRO B 303 158.426 59.465 19.928 1.00 71.85 N
ANISOU 2653 N PRO B 303 10331 10103 6865 -187 -111 1818 N
ATOM 2654 CA PRO B 303 159.165 60.356 20.834 1.00 73.88 C
ANISOU 2654 CA PRO B 303 10890 10493 6690 -263 -458 1762 C
ATOM 2655 CB PRO B 303 159.747 59.394 21.882 1.00 74.10 C

ANISOU 2655 CB PRO B 303 11033 10628 6492 -257 -610 2144 C
ATOM 2656 CG PRO B 303 159.909 58.078 21.162 1.00 71.42 C
ANISOU 2656 CG PRO B 303 10323 10168 6645 -191 -482 2412 C
ATOM 2657 CD PRO B 303 158.763 58.041 20.149 1.00 72.76 C
ANISOU 2657 CD PRO B 303 10314 10195 7136 -146 -79 2192 C
ATOM 2658 C PRO B 303 160.286 61.078 20.095 1.00 76.72 C
ANISOU 2658 C PRO B 303 11072 10813 7265 -358 -831 1654 C
ATOM 2659 O PRO B 303 160.534 62.271 20.312 1.00 78.51 O
ANISOU 2659 O PRO B 303 11493 11069 7270 -442 -1035 1420 O
ATOM 2660 N GLU B 304 160.945 60.343 19.205 1.00 79.38 N
ANISOU 2660 N GLU B 304 11042 11062 8056 -343 -885 1824 N
ATOM 2661 CA GLU B 304 162.111 60.830 18.470 1.00 80.85 C
ANISOU 2661 CA GLU B 304 11001 11204 8515 -420 -1194 1799 C
ATOM 2662 CB GLU B 304 162.877 59.646 17.899 1.00 84.06 C
ANISOU 2662 CB GLU B 304 11060 11531 9348 -362 -1203 2102 C
ATOM 2663 CG GLU B 304 161.995 58.747 17.073 1.00 86.41 C
ANISOU 2663 CG GLU B 304 11206 11688 9937 -262 -790 2094 C
ATOM 2664 CD GLU B 304 162.050 57.317 17.550 1.00 92.56 C
ANISOU 2664 CD GLU B 304 11925 12438 10805 -180 -683 2442 C
ATOM 2665 OE1 GLU B 304 161.539 57.024 18.653 1.00 96.31 O
ANISOU 2665 OE1 GLU B 304 12375 12983 11234 -177 -954 2734 O
ATOM 2666 OE2 GLU B 304 162.590 56.479 16.813 1.00 92.84 O
ANISOU 2666 OE2 GLU B 304 11933 12373 10971 -123 -343 2439 O
ATOM 2667 C GLU B 304 161.726 61.732 17.305 1.00 74.78 C
ANISOU 2667 C GLU B 304 10131 10322 7961 -436 -1070 1480 C
ATOM 2668 O GLU B 304 162.526 61.980 16.409 1.00 77.24 O
ANISOU 2668 O GLU B 304 10204 10559 8585 -476 -1202 1469 O
ATOM 2669 N SER B 305 160.494 62.205 17.295 1.00 69.17 N
ANISOU 2669 N SER B 305 9586 9593 7101 -393 -798 1246 N
ATOM 2670 CA SER B 305 160.002 62.964 16.166 1.00 70.29 C
ANISOU 2670 CA SER B 305 9622 9624 7460 -386 -668 985 C
ATOM 2671 CB SER B 305 159.486 62.008 15.111 1.00 77.40 C
ANISOU 2671 CB SER B 305 10258 10423 8729 -314 -403 1045 C
ATOM 2672 OG SER B 305 160.463 61.015 14.850 1.00 85.81 O
ANISOU 2672 OG SER B 305 11114 11456 10035 -313 -499 1299 O
ATOM 2673 C SER B 305 158.893 63.860 16.637 1.00 68.21 C
ANISOU 2673 C SER B 305 9626 9374 6915 -353 -494 736 C
ATOM 2674 O SER B 305 157.799 63.874 16.082 1.00 64.85 O
ANISOU 2674 O SER B 305 9130 8886 6623 -276 -206 620 O
ATOM 2675 N GLN B 306 159.182 64.572 17.715 1.00 71.84 N
ANISOU 2675 N GLN B 306 10401 9912 6982 -410 -674 664 N
ATOM 2676 CA GLN B 306 158.214 65.449 18.341 1.00 77.82 C
ANISOU 2676 CA GLN B 306 11476 10668 7425 -364 -485 424 C
ATOM 2677 CB GLN B 306 158.117 65.144 19.835 1.00 86.72 C
ANISOU 2677 CB GLN B 306 12960 11927 8062 -360 -476 521 C
ATOM 2678 CG GLN B 306 157.449 63.825 20.146 1.00 92.23 C
ANISOU 2678 CG GLN B 306 13578 12682 8785 -262 -177 774 C
ATOM 2679 CD GLN B 306 155.932 63.905 20.013 1.00 94.45 C
ANISOU 2679 CD GLN B 306 13855 12908 9125 -135 300 647 C
ATOM 2680 OE1 GLN B 306 155.318 64.885 20.440 1.00 97.56 O
ANISOU 2680 OE1 GLN B 306 14507 13281 9279 -90 448 410 O
ATOM 2681 NE2 GLN B 306 155.325 62.884 19.410 1.00 90.99 N
ANISOU 2681 NE2 GLN B 306 13112 12427 9033 -79 542 803 N
ATOM 2682 C GLN B 306 158.653 66.889 18.123 1.00 76.96 C
ANISOU 2682 C GLN B 306 11476 10726 7277 -451 -703 159 C
ATOM 2683 O GLN B 306 159.639 67.339 18.709 1.00 75.44 O
ANISOU 2683 O GLN B 306 11467 10320 6875 -583 -1057 152 O
ATOM 2684 N ASN B 307 157.923 67.598 17.263 1.00 74.46 N
ANISOU 2684 N ASN B 307 11091 10035 7167 -385 -512 -42 N
ATOM 2685 CA ASN B 307 158.190 69.008 16.965 1.00 72.89 C
ANISOU 2685 CA ASN B 307 11011 9711 6973 -448 -660 -293 C
ATOM 2686 CB ASN B 307 158.341 69.877 18.227 1.00 80.72 C
ANISOU 2686 CB ASN B 307 12463 10707 7500 -514 -783 -477 C
ATOM 2687 CG ASN B 307 157.015 70.261 18.827 1.00 90.27 C
ANISOU 2687 CG ASN B 307 13942 11882 8474 -359 -390 -656 C
ATOM 2688 OD1 ASN B 307 155.975 70.132 18.173 1.00 90.81 O
ANISOU 2688 OD1 ASN B 307 13808 11898 8797 -210 -58 -666 O
ATOM 2689 ND2 ASN B 307 157.036 70.746 20.078 1.00 94.65 N
ANISOU 2689 ND2 ASN B 307 14960 12460 8542 -393 -421 -797 N
ATOM 2690 C ASN B 307 159.404 69.209 16.093 1.00 62.08 C
ANISOU 2690 C ASN B 307 9402 8289 5896 -578 -973 -227 C
ATOM 2691 O ASN B 307 159.990 70.297 16.080 1.00 66.11 O
ANISOU 2691 O ASN B 307 10031 8707 6381 -689 -1195 -380 O
ATOM 2692 N ASN B 308 159.807 68.173 15.374 1.00 44.89 N
ANISOU 2692 N ASN B 308 6897 6149 4009 -567 -976 0 N
ATOM 2693 CA ASN B 308 160.903 68.398 14.462 1.00 47.01 C
ANISOU 2693 CA ASN B 308 6927 6352 4582 -667 -1196 65 C
ATOM 2694 CB ASN B 308 162.194 67.806 15.006 1.00 48.95 C
ANISOU 2694 CB ASN B 308 7084 6691 4823 -776 -1507 298 C
ATOM 2695 CG ASN B 308 162.049 66.372 15.350 1.00 53.67 C
ANISOU 2695 CG ASN B 308 7584 7392 5416 -689 -1390 544 C
ATOM 2696 OD1 ASN B 308 160.992 65.774 15.085 1.00 63.72 O
ANISOU 2696 OD1 ASN B 308 8831 8656 6722 -564 -1066 533 O
ATOM 2697 ND2 ASN B 308 163.097 65.781 15.938 1.00 52.30 N
ANISOU 2697 ND2 ASN B 308 7335 7307 5231 -756 -1660 787 N
ATOM 2698 C ASN B 308 160.633 67.911 13.053 1.00 44.16 C
ANISOU 2698 C ASN B 308 6266 5923 4590 -588 -997 122 C
ATOM 2699 O ASN B 308 161.558 67.706 12.281 1.00 49.48 O
ANISOU 2699 O ASN B 308 6713 6560 5527 -641 -1103 242 O
ATOM 2700 N CYS B 309 159.367 67.763 12.715 1.00 40.72 N
ANISOU 2700 N CYS B 309 5836 5466 4171 -467 -711 34 N
ATOM 2701 CA CYS B 309 158.996 67.190 11.439 1.00 40.83 C
ANISOU 2701 CA CYS B 309 5608 5425 4479 -408 -546 80 C
ATOM 2702 CB CYS B 309 158.925 65.678 11.579 1.00 38.15 C
ANISOU 2702 CB CYS B 309 5140 5149 4207 -369 -431 279 C
ATOM 2703 SG CYS B 309 158.884 64.918 9.998 1.00 65.78 S
ANISOU 2703 SG CYS B 309 8384 8557 8052 -344 -302 328 S
ATOM 2704 C CYS B 309 157.629 67.719 10.988 1.00 45.94 C
ANISOU 2704 C CYS B 309 6289 6018 5150 -310 -335 -87 C
ATOM 2705 O CYS B 309 156.670 67.745 11.782 1.00 50.04 O
ANISOU 2705 O CYS B 309 6935 6575 5503 -236 -175 -148 O
ATOM 2706 N ARG B 310 157.522 68.120 9.717 1.00 38.07 N
ANISOU 2706 N ARG B 310 5169 4931 4364 -300 -323 -139 N
ATOM 2707 CA ARG B 310 156.211 68.485 9.170 1.00 36.65 C
ANISOU 2707 CA ARG B 310 4963 4706 4257 -202 -158 -246 C
ATOM 2708 CB ARG B 310 156.039 69.998 9.064 1.00 48.13 C
ANISOU 2708 CB ARG B 310 6549 6056 5681 -177 -208 -406 C
ATOM 2709 CG ARG B 310 155.996 70.693 10.428 1.00 62.11 C
ANISOU 2709 CG ARG B 310 8577 7824 7196 -169 -209 -523 C
ATOM 2710 CD ARG B 310 154.646 70.468 11.167 1.00 97.31 C
ANISOU 2710 CD ARG B 310 13090 12327 11556 -34 58 -569 C
ATOM 2711 NE ARG B 310 154.800 70.505 12.627 1.00 97.30 N
ANISOU 2711 NE ARG B 310 13355 12383 11231 -46 84 -615 N
ATOM 2712 CZ ARG B 310 154.973 71.614 13.346 1.00 96.18 C
ANISOU 2712 CZ ARG B 310 13505 12160 10878 -56 37 -792 C
ATOM 2713 NH1 ARG B 310 155.120 71.529 14.667 1.00 92.91 N
ANISOU 2713 NH1 ARG B 310 13372 11814 10114 -79 50 -831 N
ATOM 2714 NH2 ARG B 310 155.003 72.805 12.746 1.00 95.74 N
ANISOU 2714 NH2 ARG B 310 13487 12805 9774 -84 -615 N
ATOM 2715 C ARG B 310 155.939 67.837 7.836 1.00 38.44 C
ANISOU 2715 C ARG B 310 4994 4905 4705 -196 -109 -190 C
ATOM 2716 O ARG B 310 156.730 67.954 6.895 1.00 36.60 O
ANISOU 2716 O ARG B 310 4707 4620 4579 -248 -202 -158 O
ATOM 2717 N LEU B 311 154.804 67.144 7.765 1.00 39.68 N
ANISOU 2717 N LEU B 311 5057 5092 4927 -140 46 -178 N
ATOM 2718 CA LEU B 311 154.355 66.545 6.527 1.00 36.13 C
ANISOU 2718 CA LEU B 311 4458 4611 4660 -152 68 -158 C
ATOM 2719 CB LEU B 311 153.427 65.392 6.822 1.00 37.31 C
ANISOU 2719 CB LEU B 311 4494 4798 4883 -144 217 -100 C
ATOM 2720 CG LEU B 311 154.105 64.293 7.617 1.00 42.09 C
ANISOU 2720 CG LEU B 311 5115 5440 5437 -184 266 29 C
ATOM 2721 CD1 LEU B 311 153.166 63.095 7.677 1.00 44.63 C
ANISOU 2721 CD1 LEU B 311 5311 5758 5890 -197 422 96 C
ATOM 2722 CD2 LEU B 311 155.469 63.915 6.998 1.00 40.38 C
ANISOU 2722 CD2 LEU B 311 4894 5179 5271 -243 158 95 C
ATOM 2723 C LEU B 311 153.604 67.556 5.699 1.00 38.65 C
ANISOU 2723 C LEU B 311 4758 4876 5050 -98 31 -250 C
ATOM 2724 O LEU B 311 152.619 68.101 6.156 1.00 37.25 O
ANISOU 2724 O LEU B 311 4574 4702 4878 -12 112 -304 O
ATOM 2725 N ILE B 312 154.066 67.799 4.475 1.00 33.52 N
ANISOU 2725 N ILE B 312 4104 4172 4460 -137 -73 -249 N
ATOM 2726 CA ILE B 312 153.330 68.667 3.569 1.00 26.20 C
ANISOU 2726 CA ILE B 312 3160 3197 3599 -85 -134 -295 C
ATOM 2727 CB ILE B 312 154.233 69.735 3.030 1.00 31.21 C
ANISOU 2727 CB ILE B 312 3908 3752 4200 -101 -234 -303 C
ATOM 2728 CG1 ILE B 312 155.068 70.297 4.160 1.00 33.66 C
ANISOU 2728 CG1 ILE B 312 4325 4044 4419 -121 -244 -331 C
ATOM 2729 CD1 ILE B 312 155.904 71.457 3.709 1.00 47.36 C
ANISOU 2729 CD1 ILE B 312 6156 5672 6166 -156 -344 -339 C
ATOM 2730 CG2 ILE B 312 153.418 70.824 2.359 1.00 32.87 C
ANISOU 2730 CG2 ILE B 312 4123 3897 4470 -17 -291 -329 C
ATOM 2731 C ILE B 312 152.752 67.849 2.432 1.00 28.24 C
ANISOU 2731 C ILE B 312 3319 3464 3945 -126 -168 -272 C
ATOM 2732 O ILE B 312 153.456 67.463 1.494 1.00 32.26 O
ANISOU 2732 O ILE B 312 3880 3952 4425 -168 -268 -257 O
ATOM 2733 N ALA B 313 151.477 67.527 2.567 1.00 27.73 N
ANISOU 2733 N ALA B 313 3117 3435 3984 -93 -133 -276 N
ATOM 2734 CA ALA B 313 150.755 66.701 1.592 1.00 35.88 C
ANISOU 2734 CA ALA B 313 4045 4475 5115 -162 -206 -267 C
ATOM 2735 CB ALA B 313 149.931 65.616 2.283 1.00 25.02 C
ANISOU 2735 CB ALA B 313 2509 3136 3861 -195 -90 -240 C
ATOM 2736 C ALA B 313 149.856 67.550 0.714 1.00 36.74 C
ANISOU 2736 C ALA B 313 4091 4574 5294 -111 -357 -265 C
ATOM 2737 O ALA B 313 149.158 68.421 1.194 1.00 41.56 O
ANISOU 2737 O ALA B 313 4622 5181 5987 6 -328 -256 O
ATOM 2738 N TYR B 314 149.857 67.292 -0.582 1.00 38.85 N
ANISOU 2738 N TYR B 314 4409 4829 5525 -189 -515 -266 N
ATOM 2739 CA TYR B 314 149.088 68.142 -1.481 1.00 37.70 C
ANISOU 2739 CA TYR B 314 4226 4681 5418 -141 -706 -230 C
ATOM 2740 CB TYR B 314 149.881 69.386 -1.813 1.00 39.04 C
ANISOU 2740 CB TYR B 314 4569 4792 5474 -67 -731 -206 C
ATOM 2741 CG TYR B 314 151.289 69.093 -2.302 1.00 39.16 C
ANISOU 2741 CG TYR B 314 4795 4773 5312 -151 -682 -221 C
ATOM 2742 CD1 TYR B 314 152.357 68.958 -1.402 1.00 29.43 C
ANISOU 2742 CD1 TYR B 314 3610 3521 4051 -161 -523 -239 C
ATOM 2743 CE1 TYR B 314 153.661 68.705 -1.866 1.00 28.38 C
ANISOU 2743 CE1 TYR B 314 3614 3349 3820 -225 -463 -222 C
ATOM 2744 CZ TYR B 314 153.884 68.570 -3.244 1.00 39.66 C
ANISOU 2744 CZ TYR B 314 5179 4753 5138 -274 -516 -205 C
ATOM 2745 OH TYR B 314 155.167 68.344 -3.737 1.00 41.74 O

ANISOU 2745 OH TYR B 314 5568 4965 5324 -318 -398 -176 O
ATOM 2746 CE2 TYR B 314 152.828 68.693 -4.151 1.00 41.72 C
ANISOU 2746 CE2 TYR B 314 5453 5040 5361 -276 -688 -205 C
ATOM 2747 CD2 TYR B 314 151.547 68.950 -3.672 1.00 43.14 C
ANISOU 2747 CD2 TYR B 314 5450 5263 5677 -219 -792 -204 C
ATOM 2748 C TYR B 314 148.744 67.449 -2.765 1.00 38.73 C
ANISOU 2748 C TYR B 314 4390 4826 5501 -265 -902 -239 C
ATOM 2749 O TYR B 314 149.355 66.460 -3.151 1.00 42.85 O
ANISOU 2749 O TYR B 314 5037 5327 5918 -383 -867 -297 O
ATOM 2750 N GLN B 315 147.754 67.992 -3.443 1.00 46.91 N
ANISOU 2750 N GLN B 315 5324 5886 6612 -235 -1117 -180 N
ATOM 2751 CA GLN B 315 147.364 67.467 -4.721 1.00 49.23 C
ANISOU 2751 CA GLN B 315 5686 6202 6819 -366 -1369 -190 C
ATOM 2752 CB GLN B 315 145.935 67.007 -4.643 1.00 56.69 C
ANISOU 2752 CB GLN B 315 6327 7196 8016 -416 -1527 -156 C
ATOM 2753 CG GLN B 315 145.711 65.691 -5.330 1.00 71.15 C
ANISOU 2753 CG GLN B 315 8210 9023 9800 -636 -1671 -246 C
ATOM 2754 CD GLN B 315 144.427 65.031 -4.858 1.00 82.29 C
ANISOU 2754 CD GLN B 315 9261 10462 11543 -713 -1740 -215 C
ATOM 2755 OE1 GLN B 315 143.801 65.489 -3.890 1.00 85.10 O
ANISOU 2755 OE1 GLN B 315 9332 10845 12157 -580 -1603 -124 O
ATOM 2756 NE2 GLN B 315 144.025 63.954 -5.535 1.00 84.05 N
ANISOU 2756 NE2 GLN B 315 9501 10663 11769 -934 -1936 -293 N
ATOM 2757 C GLN B 315 147.509 68.555 -5.759 1.00 51.29 C
ANISOU 2757 C GLN B 315 6111 6454 6924 -304 -1552 -109 C
ATOM 2758 O GLN B 315 146.927 69.625 -5.628 1.00 54.45 O
ANISOU 2758 O GLN B 315 6380 6852 7456 -163 -1624 -3 O
ATOM 2759 N GLU B 316 148.306 68.292 -6.783 1.00 60.87 N
ANISOU 2759 N GLU B 316 7622 7646 7858 -395 -1595 -147 N
ATOM 2760 CA GLU B 316 148.424 69.240 -7.878 1.00 72.31 C
ANISOU 2760 CA GLU B 316 9264 9090 9119 -352 -1768 -46 C
ATOM 2761 CB GLU B 316 149.667 68.980 -8.739 1.00 77.10 C
ANISOU 2761 CB GLU B 316 10238 9652 9403 -425 -1655 -91 C
ATOM 2762 CG GLU B 316 150.990 69.377 -8.090 1.00 80.83 C
ANISOU 2762 CG GLU B 316 10777 10052 9882 -356 -1340 -87 C
ATOM 2763 CD GLU B 316 152.032 69.872 -9.112 1.00 87.76 C
ANISOU 2763 CD GLU B 316 11967 10877 10501 -358 -1261 -21 C
ATOM 2764 OE1 GLU B 316 151.646 70.574 -10.089 1.00 93.02 O
ANISOU 2764 OE1 GLU B 316 12772 11557 11015 -336 -1455 87 O
ATOM 2765 OE2 GLU B 316 153.232 69.548 -8.936 1.00 83.38 O
ANISOU 2765 OE2 GLU B 316 11506 10267 9908 -379 -999 -55 O
ATOM 2766 C GLU B 316 147.168 69.138 -8.715 1.00 72.08 C
ANISOU 2766 C GLU B 316 9146 9133 9108 -413 -2139 12 C
ATOM 2767 O GLU B 316 146.686 68.030 -8.956 1.00 69.46 O
ANISOU 2767 O GLU B 316 8783 8833 8777 -573 -2260 -85 O
ATOM 2768 N PRO B 317 146.610 70.294 -9.124 1.00 78.33 N
ANISOU 2768 N PRO B 317 9879 9936 9946 -290 -2338 182 N
ATOM 2769 CA PRO B 317 145.564 70.191 -10.141 1.00 91.70 C
ANISOU 2769 CA PRO B 317 11536 11709 11598 -368 -2756 265 C
ATOM 2770 CB PRO B 317 145.228 71.651 -10.456 1.00 92.44 C
ANISOU 2770 CB PRO B 317 11585 11783 11756 -178 -2896 492 C
ATOM 2771 CG PRO B 317 145.728 72.429 -9.254 1.00 87.59 C
ANISOU 2771 CG PRO B 317 10859 11068 11355 2 -2538 491 C
ATOM 2772 CD PRO B 317 146.943 71.691 -8.798 1.00 78.80 C
ANISOU 2772 CD PRO B 317 9938 9922 10081 -95 -2222 309 C
ATOM 2773 C PRO B 317 146.212 69.503 -11.335 1.00102.17 C
ANISOU 2773 C PRO B 317 13284 13046 12491 -543 -2845 168 C
ATOM 2774 O PRO B 317 147.330 69.869 -11.706 1.00102.61 O
ANISOU 2774 O PRO B 317 13653 13046 12288 -508 -2648 170 O
ATOM 2775 N ALA B 318 145.536 68.506 -11.896 1.00111.55 N
ANISOU 2775 N ALA B 318 14484 14287 13614 -737 -3115 76 N
ATOM 2776 CA ALA B 318 146.181 67.524 -12.775 1.00118.14 C
ANISOU 2776 CA ALA B 318 15734 15094 14060 -925 -3106 -102 C
ATOM 2777 CB ALA B 318 145.151 66.551 -13.327 1.00120.34 C
ANISOU 2777 CB ALA B 318 15971 15419 14332 -1153 -3490 -198 C
ATOM 2778 C ALA B 318 147.026 68.100 -13.911 1.00123.29 C
ANISOU 2778 C ALA B 318 16852 15734 14257 -898 -3091 -46 C
ATOM 2779 O ALA B 318 148.210 67.760 -14.055 1.00122.79 O
ANISOU 2779 O ALA B 318 17087 15594 13973 -909 -2755 -151 O
ATOM 2780 N ASP B 319 146.415 68.969 -14.711 1.00126.19 N
ANISOU 2780 N ASP B 319 17268 16173 14505 -854 -3442 147 N
ATOM 2781 CA ASP B 319 147.056 69.453 -15.925 1.00127.28 C
ANISOU 2781 CA ASP B 319 17877 16312 14173 -848 -3463 226 C
ATOM 2782 CB ASP B 319 146.210 69.096 -17.139 1.00132.16 C
ANISOU 2782 CB ASP B 319 18610 17014 14589 -965 -3761 217 C
ATOM 2783 CG ASP B 319 147.051 68.702 -18.328 1.00134.08 C
ANISOU 2783 CG ASP B 319 19405 17230 14308 -1050 -3617 114 C
ATOM 2784 OD2 ASP B 319 146.648 69.024 -19.467 1.00139.53 O
ANISOU 2784 OD2 ASP B 319 20286 17990 14737 -1069 -3839 211 O
ATOM 2785 OD1 ASP B 319 148.117 68.078 -18.116 1.00130.25 O
ANISOU 2785 OD1 ASP B 319 19157 16649 13682 -1088 -3264 -56 O
ATOM 2786 C ASP B 319 147.318 70.949 -15.894 1.00126.86 C
ANISOU 2786 C ASP B 319 17793 16235 14174 -633 -3408 492 C
ATOM 2787 O ASP B 319 148.441 71.394 -16.147 1.00126.91 O
ANISOU 2787 O ASP B 319 18077 16168 13975 -570 -3098 532 O
ATOM 2788 N ASP B 320 146.277 71.723 -15.601 1.00127.03 N
ANISOU 2788 N ASP B 320 17460 16297 14508 -519 -3687 685 N
ATOM 2789 CA ASP B 320 146.450 73.142 -15.323 1.00126.24 C
ANISOU 2789 CA ASP B 320 17259 16125 14582 -293 -3583 919 C
ATOM 2790 CB ASP B 320 145.102 73.804 -15.040 1.00128.26 C
ANISOU 2790 CB ASP B 320 17086 16418 15230 -164 -3890 1111 C
ATOM 2791 CG ASP B 320 145.248 75.182 -14.415 1.00127.99 C
ANISOU 2791 CG ASP B 320 16893 16253 15483 87 -3720 1304 C
ATOM 2792 OD2 ASP B 320 144.896 75.327 -13.223 1.00127.99 O
ANISOU 2792 OD2 ASP B 320 16525 16200 15907 196 -3545 1252 O
ATOM 2793 OD1 ASP B 320 145.718 76.114 -15.110 1.00127.48 O
ANISOU 2793 OD1 ASP B 320 17094 16125 15219 172 -3724 1497 O
ATOM 2794 C ASP B 320 147.383 73.272 -14.117 1.00122.69 C
ANISOU 2794 C ASP B 320 16689 15560 14370 -206 -3091 807 C
ATOM 2795 O ASP B 320 147.484 72.360 -13.297 1.00123.82 O
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ATOM 2798 CB SER B 321 150.467 74.386 -13.673 1.00110.55 C
ANISOU 2798 CB SER B 321 15564 13755 12686 -98 -2206 824 C
ATOM 2799 OG SER B 321 150.414 73.420 -14.705 1.00113.85 O
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ATOM 2800 C SER B 321 149.005 75.769 -12.186 1.00106.35 C
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ATOM 2801 O SER B 321 149.957 76.547 -12.100 1.00107.41 O
ANISOU 2801 O SER B 321 14709 13153 12948 212 -2143 1025 O
ATOM 2802 N SER B 322 147.836 75.982 -11.593 1.00100.39 N
ANISOU 2802 N SER B 322 13343 12411 12388 267 -2532 997 N
ATOM 2803 CA SER B 322 147.669 77.044 -10.611 1.00 91.19 C
ANISOU 2803 CA SER B 322 11970 11104 11574 453 -2385 1051 C
ATOM 2804 CB SER B 322 146.218 77.476 -10.555 1.00 91.91 C
ANISOU 2804 CB SER B 322 11748 11214 11959 601 -2643 1198 C
ATOM 2805 OG SER B 322 145.433 76.515 -11.224 1.00 93.78 O
ANISOU 2805 OG SER B 322 11912 11628 12093 474 -2959 1199 O
ATOM 2806 C SER B 322 148.109 76.490 -9.261 1.00 79.29 C
ANISOU 2806 C SER B 322 10326 9580 10221 420 -2083 820 C
ATOM 2807 O SER B 322 147.348 76.472 -8.280 1.00 80.75 O
ANISOU 2807 O SER B 322 10225 9763 10696 509 -2035 763 O
ATOM 2808 N PHE B 323 149.336 75.992 -9.232 1.00 61.95 N
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ATOM 2809 CA PHE B 323 149.869 75.480 -8.011 1.00 53.48 C
ANISOU 2809 CA PHE B 323 7164 6294 6864 256 -1619 519 C
ATOM 2810 CB PHE B 323 150.014 73.980 -8.081 1.00 48.51 C
ANISOU 2810 CB PHE B 323 6545 5789 6097 99 -1599 375 C
ATOM 2811 CG PHE B 323 150.498 73.381 -6.809 1.00 43.27 C
ANISOU 2811 CG PHE B 323 5768 5124 5550 68 -1362 221 C
ATOM 2812 CD1 PHE B 323 149.693 73.412 -5.662 1.00 39.66 C
ANISOU 2812 CD1 PHE B 323 5056 4676 5336 151 -1319 171 C
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ANISOU 2813 CE1 PHE B 323 4878 4572 5287 124 -1105 46 C
ATOM 2814 CZ PHE B 323 151.422 72.265 -4.379 1.00 38.91 C
ANISOU 2814 CZ PHE B 323 5039 4583 5160 14 -965 -13 C
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ATOM 2816 CD2 PHE B 323 151.754 72.798 -6.747 1.00 39.61 C
ANISOU 2816 CD2 PHE B 323 5449 4647 4954 -32 -1171 149 C
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ATOM 2818 O PHE B 323 152.061 76.241 -8.648 1.00 53.18 O
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ATOM 2819 N SER B 324 151.393 76.538 -6.516 1.00 44.10 N
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ATOM 2820 CA SER B 324 152.677 77.023 -6.090 1.00 38.30 C
ANISOU 2820 CA SER B 324 5418 5059 5078 245 -1056 400 C
ATOM 2821 CB SER B 324 152.576 78.457 -5.610 1.00 36.64 C
ANISOU 2821 CB SER B 324 5216 3631 5075 362 -1031 445 C
ATOM 2822 OG SER B 324 153.856 78.910 -5.234 1.00 44.39 O
ANISOU 2822 OG SER B 324 6307 4489 6069 270 -893 416 O
ATOM 2823 C SER B 324 153.148 76.114 -4.969 1.00 36.87 C
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ATOM 2824 O SER B 324 152.519 76.040 -3.916 1.00 39.61 O
ANISOU 2824 O SER B 324 5349 4288 5413 229 -884 132 O
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ANISOU 2825 N LEU B 325 5565 4301 4940 40 -813 213 N
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ANISOU 2826 CA LEU B 325 4786 3664 4494 -31 -694 94 C
ATOM 2827 CB LEU B 325 156.017 73.783 -4.754 1.00 35.34 C
ANISOU 2827 CB LEU B 325 5028 3850 4552 -142 -579 125 C
ATOM 2828 CG LEU B 325 156.580 72.684 -3.860 1.00 38.32 C
ANISOU 2828 CG LEU B 325 5301 4293 4965 -205 -474 42 C
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ANISOU 2829 CD1 LEU B 325 5130 4339 4911 -177 -524 -51 C
ATOM 2830 CD2 LEU B 325 157.607 71.885 -4.660 1.00 37.28 C
ANISOU 2830 CD2 LEU B 325 5243 4165 4756 -278 -335 91 C
ATOM 2831 C LEU B 325 155.277 75.372 -2.980 1.00 34.56 C
ANISOU 2831 C LEU B 325 4825 3624 4682 -18 -640 37 C
ATOM 2832 O LEU B 325 155.180 74.936 -1.833 1.00 35.76 O
ANISOU 2832 O LEU B 325 4895 3826 4868 -21 -596 -69 O
ATOM 2833 N SER B 326 155.790 76.573 -3.264 1.00 32.96 N
ANISOU 2833 N SER B 326 4724 3266 4534 -16 -645 111 N
ATOM 2834 CA SER B 326 156.291 77.462 -2.229 1.00 41.01 C
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ATOM 2835 CB SER B 326 157.049 78.643 -2.834 1.00 46.45 C

ANISOU 2835 CB SER B 326 6574 4645 6429 -79 -620 155 C
ATOM 2836 OG SER B 326 156.592 78.877 -4.139 1.00 53.45 O
ANISOU 2836 OG SER B 326 7526 5524 7258 -13 -654 307 O
ATOM 2837 C SER B 326 155.187 77.993 -1.332 1.00 45.22 C
ANISOU 2837 C SER B 326 6277 4632 6274 97 -635 -68 C
ATOM 2838 O SER B 326 155.412 78.223 -0.145 1.00 50.42 O
ANISOU 2838 O SER B 326 6963 5242 6953 76 -598 -198 O
ATOM 2839 N GLN B 327 154.013 78.240 -1.907 1.00 45.11 N
ANISOU 2839 N GLN B 327 6218 4618 6302 236 -687 -7 N
ATOM 2840 CA GLN B 327 152.844 78.649 -1.132 1.00 40.63 C
ANISOU 2840 CA GLN B 327 5578 4008 5850 396 -654 -86 C
ATOM 2841 CB GLN B 327 151.690 78.985 -2.055 1.00 41.27 C
ANISOU 2841 CB GLN B 327 5573 4084 6026 542 -753 53 C
ATOM 2842 CG GLN B 327 151.829 80.336 -2.738 1.00 45.21 C
ANISOU 2842 CG GLN B 327 6195 4368 6615 612 -803 183 C
ATOM 2843 CD GLN B 327 151.718 81.506 -1.746 1.00 52.86 C
ANISOU 2843 CD GLN B 327 7240 5095 7750 718 -687 77 C
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ANISOU 2844 OE1 GLN B 327 8100 6009 8864 902 -628 46 O
ATOM 2845 NE2 GLN B 327 152.868 82.126 -1.386 1.00 47.83 N
ANISOU 2845 NE2 GLN B 327 6780 4296 7096 595 -641 9 N
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ANISOU 2846 C GLN B 327 5406 4127 5752 387 -579 -200 C
ATOM 2847 O GLN B 327 152.113 77.749 0.960 1.00 41.33 O
ANISOU 2847 O GLN B 327 5558 4226 5921 449 -471 -324 O
ATOM 2848 N GLU B 328 152.418 76.300 -0.720 1.00 40.01 N
ANISOU 2848 N GLU B 328 5290 4273 5640 306 -620 -159 N
ATOM 2849 CA GLU B 328 152.123 75.136 0.126 1.00 41.48 C
ANISOU 2849 CA GLU B 328 5365 4603 5792 276 -539 -241 C
ATOM 2850 CB GLU B 328 152.059 73.822 -0.676 1.00 33.20 C
ANISOU 2850 CB GLU B 328 4236 3699 4679 183 -597 -191 C
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ANISOU 2851 CG GLU B 328 6104 5831 6841 253 -659 -159 C
ATOM 2852 CD GLU B 328 149.628 73.552 0.246 1.00 66.48 C
ANISOU 2852 CD GLU B 328 8121 7993 9146 377 -525 -214 C
ATOM 2853 OE1 GLU B 328 149.577 72.621 1.093 1.00 59.28 O
ANISOU 2853 OE1 GLU B 328 7147 7165 8214 331 -404 -268 O
ATOM 2854 OE2 GLU B 328 148.913 74.600 0.329 1.00 72.15 O
ANISOU 2854 OE2 GLU B 328 8795 8615 10003 530 -515 -188 O
ATOM 2855 C GLU B 328 153.067 74.986 1.327 1.00 43.83 C
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ATOM 2856 O GLU B 328 152.653 74.622 2.439 1.00 50.63 O
ANISOU 2856 O GLU B 328 6581 5811 6845 232 -346 -424 O
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ANISOU 2857 N VAL B 329 4415 3401 4514 81 -491 -317 N
ATOM 2858 CA VAL B 329 155.347 75.116 2.134 1.00 34.31 C
ANISOU 2858 CA VAL B 329 4716 3637 4684 -19 -474 -383 C
ATOM 2859 CB VAL B 329 156.742 75.013 1.524 1.00 35.27 C
ANISOU 2859 CB VAL B 329 4852 3736 4812 -158 -524 -292 C
ATOM 2860 CG1 VAL B 329 157.777 74.992 2.580 1.00 31.60 C
ANISOU 2860 CG1 VAL B 329 4419 3269 4319 -270 -564 -332 C
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ANISOU 2861 CG2 VAL B 329 5142 4251 5170 -186 -485 -208 C
ATOM 2862 C VAL B 329 155.225 76.298 3.091 1.00 42.27 C
ANISOU 2862 C VAL B 329 5864 4501 5698 27 -461 -505 C
ATOM 2863 O VAL B 329 155.322 76.154 4.317 1.00 43.88 O
ANISOU 2863 O VAL B 329 6139 4734 5801 8 -426 -610 O
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ANISOU 2864 N LEU B 330 5540 3936 5408 92 -484 -488 N
ATOM 2865 CA LEU B 330 154.841 78.663 3.340 1.00 41.36 C
ANISOU 2865 CA LEU B 330 5980 4022 5712 145 -451 -621 C
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ANISOU 2866 CB LEU B 330 5423 3180 5244 204 -484 -554 C
ATOM 2867 CG LEU B 330 156.120 80.388 2.011 1.00 35.19 C
ANISOU 2867 CG LEU B 330 5337 2914 5120 22 -584 -485 C
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ANISOU 2868 CD1 LEU B 330 5209 2540 5092 82 -602 -353 C
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ANISOU 2869 CD2 LEU B 330 5267 2559 4852 -104 -626 -651 C
ATOM 2870 C LEU B 330 153.644 78.561 4.295 1.00 44.93 C
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ATOM 2871 O LEU B 330 153.710 78.973 5.446 1.00 45.94 O
ANISOU 2871 O LEU B 330 6732 4557 6166 308 -233 -899 O
ATOM 2872 N ARG B 331 152.543 78.014 3.807 1.00 42.62 N
ANISOU 2872 N ARG B 331 5951 4319 5925 432 -242 -654 N
ATOM 2873 CA ARG B 331 151.358 77.881 4.631 1.00 47.47 C
ANISOU 2873 CA ARG B 331 6507 4961 6567 592 -60 -726 C
ATOM 2874 CB ARG B 331 150.240 77.301 3.782 1.00 49.41 C
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ANISOU 2875 CG ARG B 331 7766 6865 8456 792 119 -606 C
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ANISOU 2876 CD ARG B 331 8873 8370 10061 845 42 -452 C
ATOM 2877 NE ARG B 331 147.486 74.836 4.099 1.00 83.28 N
ANISOU 2877 NE ARG B 331 10134 9980 11530 821 153 -432 N
ATOM 2878 CZ ARG B 331 146.363 74.325 3.594 1.00 94.04 C
ANISOU 2878 CZ ARG B 331 11202 11420 13109 868 125 -319 C
ATOM 2879 NH1 ARG B 331 145.756 74.921 2.573 1.00 98.26 N
ANISOU 2879 NH1 ARG B 331 11599 11903 13833 950 -40 -208 N
ATOM 2880 NH2 ARG B 331 145.842 73.220 4.111 1.00 96.27 N
ANISOU 2880 NH2 ARG B 331 11322 11826 13432 823 244 -298 N
ATOM 2881 C ARG B 331 151.607 77.041 5.916 1.00 56.57 C
ANISOU 2881 C ARG B 331 7732 6246 7517 523 41 -827 C
ATOM 2882 O ARG B 331 151.097 77.338 6.999 1.00 58.75 O
ANISOU 2882 O ARG B 331 8124 6474 7723 621 222 -951 O
ATOM 2883 N HIS B 332 152.408 75.996 5.800 1.00 51.38 N
ANISOU 2883 N HIS B 332 7024 5743 6754 364 -60 -763 N
ATOM 2884 CA HIS B 332 152.699 75.178 6.963 1.00 44.61 C
ANISOU 2884 CA HIS B 332 6235 5010 5706 300 6 -812 C
ATOM 2885 CB HIS B 332 153.231 73.819 6.548 1.00 37.46 C
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ATOM 2886 CG HIS B 332 152.181 72.856 6.152 1.00 45.89 C
ANISOU 2886 CG HIS B 332 6027 5446 5962 244 24 -601 C
ATOM 2887 ND1 HIS B 332 151.504 72.920 4.938 1.00 47.90 N
ANISOU 2887 ND1 HIS B 332 6120 5683 6394 292 -31 -531 N
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ANISOU 2888 CE1 HIS B 332 5424 5276 5968 306 36 -473 C
ATOM 2889 NE2 HIS B 332 150.724 71.216 5.969 1.00 47.12 N
ANISOU 2889 NE2 HIS B 332 5868 5763 6271 284 169 -488 N
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ANISOU 2892 O HIS B 332 8339 6600 6998 217 24 -1049 O
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ANISOU 2893 N LEU B 333 7251 5551 6301 69 -262 -907 N
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ANISOU 2894 CA LEU B 333 8198 6200 6925 -81 -408 -1002 C
ATOM 2895 CB LEU B 333 156.791 77.614 6.901 1.00 62.16 C
ANISOU 2895 CB LEU B 333 8914 6841 7862 -192 -563 -921 C
ATOM 2896 CG LEU B 333 158.168 77.023 6.708 1.00 63.00 C
ANISOU 2896 CG LEU B 333 8918 7033 7985 -385 -733 -799 C
ATOM 2897 CD2 LEU B 333 159.156 77.699 7.618 1.00 54.08 C
ANISOU 2897 CD2 LEU B 333 7963 5806 6779 -558 -916 -901 C
ATOM 2898 CD1 LEU B 333 158.526 77.267 5.279 1.00 66.92 C
ANISOU 2898 CD1 LEU B 333 9282 7461 8684 -404 -746 -655 C
ATOM 2899 C LEU B 333 155.396 78.092 8.848 1.00 66.65 C
ANISOU 2899 C LEU B 333 9808 7356 8159 -5 -316 -1215 C
ATOM 2900 O LEU B 333 156.017 78.405 9.863 1.00 72.53 O
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ATOM 2904 CG ARG B 334 153.828 81.762 7.609 1.00 62.47 C
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ATOM 2908 NH1 ARG B 334 152.742 83.209 3.749 1.00 75.45 N
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ATOM 2911 O ARG B 334 151.916 79.817 10.702 1.00 84.62 O
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ATOM 2912 N GLN B 335 153.767 78.664 11.324 1.00 88.39 N
ANISOU 2912 N GLN B 335 13052 10024 10510 250 122 -1587 N
ATOM 2913 CA GLN B 335 153.413 78.453 12.730 1.00 90.10 C
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ATOM 2915 CG GLN B 335 151.932 76.676 11.682 1.00 84.23 C
ANISOU 2915 CG GLN B 335 12170 9850 9985 493 549 -1384 C
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ANISOU 2916 CD GLN B 335 12230 10073 10579 716 772 -1332 C
ATOM 2917 OE1 GLN B 335 149.777 76.036 10.860 1.00 86.21 O
ANISOU 2917 OE1 GLN B 335 11924 10175 10655 788 906 -1195 O
ATOM 2918 NE2 GLN B 335 150.328 78.215 10.718 1.00 86.38 N
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ATOM 2920 O GLN B 335 155.623 78.484 13.627 1.00 90.66 O
ANISOU 2920 O GLN B 335 13924 10409 10114 -122 -230 -1808 O
TER 2922 GLN B 335
HETATM 2921 OAD DRG C 1 162.991 49.038 5.565 1.00 28.90 O
HETATM 2922 CAQ DRG C 1 163.951 49.693 5.137 1.00 31.88 C
HETATM 2923 CAS DRG C 1 165.012 50.082 5.948 1.00 28.82 C
HETATM 2924 CAJ DRG C 1 165.024 49.798 7.306 1.00 26.98 C
HETATM 2925 CAH DRG C 1 166.130 50.171 8.071 1.00 28.53 C
HETATM 2926 CAN DRG C 1 167.237 50.842 7.499 1.00 31.26 C
HETATM 2927 CAA DRG C 1 168.386 51.246 8.285 1.00 24.52 C
HETATM 2928 CAO DRG C 1 167.200 51.163 6.135 1.00 30.95 C

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HETATM 2929 CAB DRG C  1   168.248  51.869   5.487  1.00 23.50           C
HETATM 2930 CAT DRG C  1   166.056  50.821   5.426  1.00 31.37           C
HETATM 2931 OAL DRG C  1   166.098  51.093   4.116  1.00 29.82           O
HETATM 2932 CAU DRG C  1   165.125  50.661   3.280  1.00 23.20           C
HETATM 2933 CAR DRG C  1   164.030  49.989   3.787  1.00 24.45           C
HETATM 2934 CAI DRG C  1   163.050  49.542   2.893  1.00 23.70           C
HETATM 2935 CAF DRG C  1   163.148  49.831   1.533  1.00 24.90           C
HETATM 2936 CAG DRG C  1   164.257  50.533   1.042  1.00 24.70           C
HETATM 2937 CAP DRG C  1   165.250  50.993   1.925  1.00 29.90           C
HETATM 2938 CAK DRG C  1   166.386  51.724   1.462  1.00 26.20           C
HETATM 2939 CAM DRG C  1   167.789  51.131   1.752  1.00 39.78           C
HETATM 2940 OAE DRG C  1   167.893  49.935   2.148  1.00 40.47           O
HETATM 2941 OAC DRG C  1   168.731  51.931   1.552  1.00 41.66           O
HETATM 2942 OAD DRG C  2   160.821  53.562  -0.957  1.00 29.91           O
HETATM 2943 CAQ DRG C  2   161.917  53.977  -0.557  1.00 27.38           C
HETATM 2944 CAS DRG C  2   162.812  54.579  -1.407  1.00 20.36           C
HETATM 2945 CAJ DRG C  2   162.507  54.745  -2.761  1.00 19.81           C
HETATM 2946 CAH DRG C  2   163.441  55.403  -3.591  1.00 24.49           C
HETATM 2947 CAN DRG C  2   164.687  55.855  -3.089  1.00 28.71           C
HETATM 2948 CAA DRG C  2   165.671  56.485  -3.925  1.00 28.17           C
HETATM 2949 CAO DRG C  2   164.978  55.677  -1.721  1.00 26.46           C
HETATM 2950 CAB DRG C  2   166.188  56.089  -1.114  1.00 18.84           C
HETATM 2951 CAT DRG C  2   164.038  55.032  -0.924  1.00 24.41           C
HETATM 2952 OAL DRG C  2   164.378  54.935   0.369  1.00 27.02           O
HETATM 2953 CAU DRG C  2   163.488  54.378   1.221  1.00 27.07           C
HETATM 2954 CAR DRG C  2   162.274  53.883   0.769  1.00 24.72           C
HETATM 2955 CAI DRG C  2   161.376  53.311   1.662  1.00 23.42           C
HETATM 2956 CAF DRG C  2   161.750  53.230   2.996  1.00 24.17           C
HETATM 2957 CAG DRG C  2   162.974  53.719   3.444  1.00 24.73           C
HETATM 2958 CAP DRG C  2   163.876  54.296   2.556  1.00 29.50           C
HETATM 2959 CAK DRG C  2   165.123  54.798   3.007  1.00 31.35           C
HETATM 2960 CAM DRG C  2   165.455  56.308   2.721  1.00 33.32           C
HETATM 2961 OAE DRG C  2   164.570  57.125   2.437  1.00 34.51           O
HETATM 2962 OAC DRG C  2   166.634  56.666   2.839  1.00 40.95           O
HETATM 2963 O   HOH S  1   168.713  53.789  -0.291  1.00 35.33           O
HETATM 2964 O   HOH S  2   161.892  53.727  16.866  1.00 49.67           O
HETATM 2965 O   HOH S  3   164.969  59.956   2.543  1.00 37.40           O
HETATM 2966 O   HOH S  4   153.816  51.547 -17.356  1.00 35.89           O
HETATM 2967 O   HOH S  5   173.955  67.623   4.394  1.00 44.22           O
HETATM 2968 O   HOH S  6   160.329  36.676  11.944  1.00 55.15           O
HETATM 2969 O   HOH S  7   167.121  68.307   2.491  1.00 43.22           O
HETATM 2970 O   HOH S  8   174.241  45.104   7.023  1.00 39.35           O
HETATM 2971 O   HOH S  9   147.991  51.757   8.039  1.00 42.30           O
HETATM 2972 O   HOH S 10   150.720  42.063   5.341  1.00 55.82           O
HETATM 2973 O   HOH S 11   155.127  75.108  -8.066  1.00 54.25           O
HETATM 2974 O   HOH S 12   154.172  39.544  -3.767  1.00 53.24           O
HETATM 2975 O   HOH S 13   165.300  57.764  -7.952  1.00 41.58           O
HETATM 2976 O   HOH S 14   162.850  89.254  -6.796  1.00 52.78           O
HETATM 2977 O   HOH S 15   154.964  70.741  -7.727  1.00 45.98           O
HETATM 2978 O   HOH S 16   164.131  62.771  -1.020  1.00 51.78           O
HETATM 2979 O   HOH S 17   152.520  70.191  15.623  1.00 58.84           O
HETATM 2980 O   HOH S 18   166.251  62.142   0.998  1.00 47.15           O
HETATM 2982 O   HOH S 20   171.080  57.987  13.953  1.00 45.06           O
HETATM 2983 O   HOH S 21   148.067  47.124  -0.587  1.00 45.29           O
HETATM 2984 O   HOH S 22   143.902  55.932 -14.363  1.00 63.60           O
HETATM 2986 O   HOH S 24   150.530  40.637   7.539  1.00 55.40           O
HETATM 2987 O   HOH S 25   166.897  51.082  11.483  1.00 49.70           O
HETATM 2988 O   HOH S 26   182.591  60.441  -1.208  1.00 53.67           O
HETATM 2989 O   HOH S 27   172.503  46.354   5.924  1.00 51.32           O
HETATM 2991 O   HOH S 29   197.473  47.430  -5.671  1.00 56.88           O
HETATM 2992 O   HOH S 30   154.281  64.868  15.755  1.00 61.97           O
HETATM 2993 O   HOH S 31   194.426  33.302   6.916  1.00 47.03           O
HETATM 2994 O   HOH S 32   163.586  73.804   8.275  1.00 40.52           O
HETATM 2995 O   HOH S 33   181.340  40.097  -2.774  1.00 48.13           O
HETATM 2996 O   HOH S 34   184.998  42.705  12.196  1.00 50.78           O
HETATM 2997 O   HOH S 35   151.669  47.690 -11.983  1.00 33.83           O
HETATM 2998 O   HOH S 36   171.381  82.460  13.092  1.00 72.55           O
HETATM 2999 O   HOH S 37   164.720  55.181  -7.543  1.00 35.15           O
HETATM 3000 O   HOH S 38   152.216  75.299 -11.371  1.00 64.67           O
HETATM 3001 O   HOH S 39   162.728  61.240   2.446  1.00 52.37           O
HETATM 3002 O   HOH S 40   157.809  85.373  -5.397  1.00 49.67           O
HETATM 3003 O   HOH S 41   160.833  54.824 -11.983  1.00 53.47           O
HETATM 3004 O   HOH S 42   172.438  36.666  11.131  1.00 50.31           O
HETATM 3005 O   HOH S 43   143.215  55.825   1.242  1.00 51.98           O
HETATM 3006 O   HOH S 44   178.194  34.813  -9.692  1.00 61.99           O
HETATM 3007 O   HOH S 45   160.209  55.971  -9.794  1.00 51.89           O
HETATM 3009 O   HOH S 47   170.559  46.042   2.157  1.00 40.56           O
HETATM 3011 O   HOH S 49   176.760  53.698   2.889  1.00 56.49           O
HETATM 3012 O   HOH S 50   168.790  62.275   2.328  1.00 60.56           O
HETATM 3013 O   HOH S 51   167.855  55.504   4.837  1.00 40.62           O
HETATM 3014 O   HOH S 52   177.579  50.250  -7.113  1.00 55.88           O
HETATM 3015 O   HOH S 53   155.929  68.342  -6.155  1.00 42.77           O
HETATM 3016 O   HOH S 54   187.365  29.710  12.394  1.00 49.65           O
HETATM 3017 O   HOH S 55   185.843  27.691  12.218  1.00 51.08           O
HETATM 3018 O   HOH S 56   190.462  26.460   7.158  1.00 50.01           O
HETATM 3019 O   HOH S 57   163.171  48.532  17.270  1.00 48.75           O
HETATM 3020 O   HOH S 58   164.548  48.001  15.528  1.00 60.23           O
HETATM 3021 O   HOH S 59   143.593  59.258  12.238  1.00 63.87           O
HETATM 3022 O   HOH S 60   144.484  59.906  14.347  1.00 71.48           O
HETATM 3023 O   HOH S 61   152.669  45.115  16.448  1.00 43.47           O
HETATM 3024 O   HOH S 62   160.263  38.016  17.761  1.00 48.84           O
HETATM 3025 O   HOH S 63   152.484  64.476  18.117  1.00 65.15           O
HETATM 3026 O   HOH S 64   149.649  67.575   5.246  1.00 53.28           O
HETATM 3028 O   HOH S 66   154.393  85.153  -5.360  1.00 42.89           O
HETATM 3029 O   HOH S 67   163.677  82.527  -9.406  1.00 55.89           O
HETATM 3030 O   HOH S 68   163.984  77.274  -8.161  1.00 46.95           O
HETATM 3031 O   HOH S 69   176.278  65.478  13.005  1.00 69.67           O
HETATM 3033 O   HOH S 71   149.765  70.612   2.125  1.00 53.58           O
HETATM 3039 S   SO4 E  1   190.873  52.635   2.687  1.00209.77           S
HETATM 3040 O1  SO4 E  1   191.344  51.848   1.550  1.00208.46           O
HETATM 3041 O2  SO4 E  1   189.413  52.472   2.690  1.00210.80           O
HETATM 3042 O3  SO4 E  1   191.451  52.156   3.943  1.00210.05           O
HETATM 3043 O4  SO4 E  1   191.281  54.037   2.527  1.00209.37           O
END
```

Table 9. DMXAA-hSTING$^{S162A/G230I/Q266I}$ complex

```
REMARK   3
REMARK   3 REFINEMENT.
REMARK   3   PROGRAM     : PHENIX (phenix.refine: 1.8.2_1309)
REMARK   3   AUTHORS     : Adams,Afonine,Burnley,Chen,Davis,Echols,Gildea,
REMARK   3               : Gopal,Gros,Grosse-Kunstleve,Headd,Hung,Immormino,
REMARK   3               : Ioerger,McCoy,McKee,Moriarty,Pai,Read,Richardson,
REMARK   3               : Richardson,Romo,Sacchettini,Sauter,Smith,Storoni,
REMARK   3               : Terwilliger,Zwart
REMARK   3
REMARK   3  REFINEMENT TARGET : ML
REMARK   3
REMARK   3  DATA USED IN REFINEMENT.
REMARK   3   RESOLUTION RANGE HIGH (ANGSTROMS) : 2.370
REMARK   3   RESOLUTION RANGE LOW  (ANGSTROMS) : 128.671
REMARK   3   MIN(FOBS/SIGMA_FOBS)              : 1.35
REMARK   3   COMPLETENESS FOR RANGE        (%) : 99.91
REMARK   3   NUMBER OF REFLECTIONS             : 19048
REMARK   3   NUMBER OF REFLECTIONS (NON-ANOMALOUS) : 19048
REMARK   3
REMARK   3  FIT TO DATA USED IN REFINEMENT.
REMARK   3   R VALUE     (WORKING + TEST SET) : 0.1893
REMARK   3   R VALUE           (WORKING SET) : 0.1870
REMARK   3   FREE R VALUE                     : 0.2310
REMARK   3   FREE R VALUE TEST SET SIZE   (%) : 5.15
REMARK   3   FREE R VALUE TEST SET COUNT      : 981
REMARK   3
REMARK   3  FIT TO DATA USED IN REFINEMENT (IN BINS).
REMARK   3   BIN  RESOLUTION RANGE  COMPL.    NWORK NFREE   RWORK
RFREE
REMARK   3     1 128.8606 -  4.5338    1.00     2698   133  0.1721 0.2114
REMARK   3     2  4.5338 -  3.5985    1.00     2593   146  0.1554 0.1881
REMARK   3     3  3.5985 -  3.1436    1.00     2587   136  0.1775 0.2098
REMARK   3     4  3.1436 -  2.8562    1.00     2551   135  0.2056 0.2800
REMARK   3     5  2.8562 -  2.6514    1.00     2559   140  0.2293 0.2668
REMARK   3     6  2.6514 -  2.4951    1.00     2546   142  0.2922 0.3880
REMARK   3     7  2.4951 -  2.3701    1.00     2533   149  0.2916 0.3274
REMARK   3
REMARK   3  BULK SOLVENT MODELLING.
REMARK   3   METHOD USED        : FLAT BULK SOLVENT MODEL
REMARK   3   SOLVENT RADIUS     : 1.11
REMARK   3   SHRINKAGE RADIUS   : 0.90
REMARK   3   GRID STEP FACTOR   : 4.00
REMARK   3
REMARK   3  ERROR ESTIMATES.
REMARK   3   COORDINATE ERROR (MAXIMUM-LIKELIHOOD BASED)     : 0.30
REMARK   3   PHASE ERROR (DEGREES, MAXIMUM-LIKELIHOOD BASED) :
22.08
REMARK   3
REMARK   3  STRUCTURE FACTORS CALCULATION ALGORITHM : FFT
REMARK   3
REMARK   3  DEVIATIONS FROM IDEAL VALUES.
REMARK   3              RMSD     MAX  COUNT
REMARK   3   BOND      : 0.007   0.040  3034
REMARK   3   ANGLE     : 1.203   8.976  4122
REMARK   3   CHIRALITY : 0.075   0.371   448
REMARK   3   PLANARITY : 0.004   0.039   542
REMARK   3   DIHEDRAL  : 18.321  82.369  1138
REMARK   3   MIN NONBONDED DISTANCE : 1.922
REMARK   3
REMARK   3  MOLPROBITY STATISTICS.
REMARK   3   ALL-ATOM CLASHSCORE : 7.67
REMARK   3   RAMACHANDRAN PLOT:
REMARK   3     OUTLIERS : 0.56 %
REMARK   3     ALLOWED  : 3.89 %
REMARK   3     FAVORED  : 95.56 %
REMARK   3   ROTAMER OUTLIERS : 11.71 %
REMARK   3   CBETA DEVIATIONS : 0
REMARK   3
REMARK   3  ATOMIC DISPLACEMENT PARAMETERS.
REMARK   3   WILSON B : 52.20
REMARK   3   RMS(B_ISO_OR_EQUIVALENT_BONDED) : 8.54
REMARK   3   ATOMS         NUMBER OF ATOMS
REMARK   3                 ISO.  ANISO.
REMARK   3   ALL        :  3033    2928
REMARK   3   ALL (NO H) :  3033    2928
REMARK   3   SOLVENT    :  58      0
REMARK   3   NON-SOLVENT :  2975    2928
REMARK   3   HYDROGENS  :  0       0
REMARK   3
REMARK   3  TLS DETAILS.
REMARK   3   NUMBER OF TLS GROUPS: 19
REMARK   3   ORIGIN: CENTER OF MASS
REMARK   3   TLS GROUP : 1
REMARK   3    SELECTION: chain 'A' and (resid  154  through  185 )
REMARK   3    ORIGIN FOR THE GROUP (A): 119.7412 -45.6180   0.9079
REMARK   3   T TENSOR
REMARK   3     T11:  0.4193 T22:  0.4961
REMARK   3     T33:  0.3419 T12:  0.1443
REMARK   3     T13:  0.0895 T23:  0.1533
REMARK   3   L TENSOR
REMARK   3     L11:  4.6250 L22:  6.8599
REMARK   3     L33:  2.9736 L12: -3.3531
REMARK   3     L13:  0.4680 L23: -0.1759
REMARK   3   S TENSOR
REMARK   3     S11: -0.8048 S12: -0.9653 S13: -0.5231
REMARK   3     S21:  1.3663 S22:  0.5796 S23:  0.1655
REMARK   3     S31:  0.2873 S32:  0.2438 S33:  0.2232
REMARK   3   TLS GROUP : 2
REMARK   3    SELECTION: chain 'A' and (resid  186  through  211 )
REMARK   3    ORIGIN FOR THE GROUP (A): 129.3530 -48.7083  -7.1009
REMARK   3   T TENSOR
REMARK   3     T11:  0.4212 T22:  0.6459
REMARK   3     T33:  0.6367 T12:  0.1380
REMARK   3     T13:  0.0329 T23: -0.0528
REMARK   3   L TENSOR
REMARK   3     L11:  3.5990 L22:  9.5628
REMARK   3     L33:  2.8698 L12: -3.6331
REMARK   3     L13:  1.0100 L23: -0.5546
REMARK   3   S TENSOR
REMARK   3     S11: -0.0638 S12:  0.2429 S13: -0.8055
REMARK   3     S21:  0.1232 S22:  0.2133 S23: -0.3000
REMARK   3     S31:  0.5832 S32:  0.3737 S33: -0.0249
REMARK   3   TLS GROUP : 3
REMARK   3    SELECTION: chain 'A' and (resid  212  through  227 )
REMARK   3    ORIGIN FOR THE GROUP (A): 129.1486 -52.5547 -12.8258
REMARK   3   T TENSOR
REMARK   3     T11:  0.4393 T22:  0.5281
REMARK   3     T33:  0.5919 T12:  0.0322
REMARK   3     T13: -0.0127 T23:  0.1194
REMARK   3   L TENSOR
REMARK   3     L11:  5.8586 L22:  9.3215
REMARK   3     L33:  8.1146 L12:  6.4837
REMARK   3     L13: -6.5623 L23: -5.5758
REMARK   3   S TENSOR
REMARK   3     S11: -0.8869 S12:  1.2379 S13: -0.7595
REMARK   3     S21: -0.4167 S22:  1.1681 S23:  0.6136
REMARK   3     S31:  0.0975 S32: -1.4546 S33: -0.1067
REMARK   3   TLS GROUP : 4
REMARK   3    SELECTION: chain 'A' and (resid  228  through  242 )
REMARK   3    ORIGIN FOR THE GROUP (A): 110.4692 -51.7135  -1.3574
REMARK   3   T TENSOR
REMARK   3     T11:  0.7933 T22:  0.5352
REMARK   3     T33:  0.8596 T12: -0.0041
REMARK   3     T13:  0.2322 T23:  0.1112
REMARK   3   L TENSOR
REMARK   3     L11:  7.5537 L22:  2.8609
REMARK   3     L33:  1.4922 L12: -4.5153
REMARK   3     L13: -2.2277 L23:  1.0483
REMARK   3   S TENSOR
REMARK   3     S11: -0.9886 S12: -1.1618 S13: -1.8144
REMARK   3     S21:  0.0203 S22:  0.2433 S23:  0.9635
REMARK   3     S31: -0.0130 S32: -0.0466 S33:  0.4012
REMARK   3   TLS GROUP : 5
REMARK   3    SELECTION: chain 'A' and (resid  243  through  280 )
REMARK   3    ORIGIN FOR THE GROUP (A): 124.7540 -41.4323 -13.6540
REMARK   3   T TENSOR
REMARK   3     T11:  0.3074 T22:  0.3011
REMARK   3     T33:  0.2748 T12: -0.0078
REMARK   3     T13:  0.0100 T23:  0.0303
REMARK   3   L TENSOR
REMARK   3     L11:  3.6448 L22:  2.3155
REMARK   3     L33:  1.7574 L12: -1.9552
REMARK   3     L13: -0.0407 L23: -0.1114
REMARK   3   S TENSOR
REMARK   3     S11: -0.1020 S12: -0.0173 S13: -0.1125
REMARK   3     S21:  0.1136 S22:  0.0133 S23: -0.1586
REMARK   3     S31:  0.0827 S32:  0.2233 S33:  0.0722
REMARK   3   TLS GROUP : 6
REMARK   3    SELECTION: chain 'A' and (resid  281  through  314 )
REMARK   3    ORIGIN FOR THE GROUP (A): 123.3640 -32.6276  -3.4192
REMARK   3   T TENSOR
REMARK   3     T11:  0.4307 T22:  0.4987
REMARK   3     T33:  0.3607 T12:  0.0528
REMARK   3     T13: -0.0232 T23: -0.0691
REMARK   3   L TENSOR
REMARK   3     L11:  5.0093 L22:  6.6833
REMARK   3     L33:  6.8768 L12: -2.5420
REMARK   3     L13: -0.4223 L23: -1.0414
REMARK   3   S TENSOR
REMARK   3     S11: -0.3563 S12: -0.7204 S13: -0.0370
REMARK   3     S21:  1.1416 S22:  0.4752 S23: -0.2161
REMARK   3     S31: -0.6150 S32:  0.5594 S33: -0.1028
REMARK   3   TLS GROUP : 7
REMARK   3    SELECTION: chain 'A' and (resid  315  through  324 )
```

REMARK 3 ORIGIN FOR THE GROUP (A): 136.1529 -33.2184 -19.3637
REMARK 3 T TENSOR
REMARK 3 T11: 1.2099 T22: 1.0982
REMARK 3 T33: 1.0451 T12: -0.0360
REMARK 3 T13: 0.0766 T23: 0.2092
REMARK 3 L TENSOR
REMARK 3 L11: 7.4924 L22: 8.3097
REMARK 3 L33: 3.9134 L12: -7.5601
REMARK 3 L13: -2.5458 L23: 3.9627
REMARK 3 S TENSOR
REMARK 3 S11: 1.0706 S12: 0.5115 S13: 0.7413
REMARK 3 S21: -2.3931 S22: 0.2034 S23: -0.4202
REMARK 3 S31: -1.4970 S32: 1.0416 S33: -1.1149
REMARK 3 TLS GROUP : 8
REMARK 3 SELECTION: chain 'A' and (resid 325 through 335)
REMARK 3 ORIGIN FOR THE GROUP (A): 138.2183 -41.3718 -6.6489
REMARK 3 T TENSOR
REMARK 3 T11: 0.4830 T22: 0.6805
REMARK 3 T33: 0.7524 T12: 0.0984
REMARK 3 T13: 0.0045 T23: -0.1937
REMARK 3 L TENSOR
REMARK 3 L11: 3.9316 L22: 9.9442
REMARK 3 L33: 4.3889 L12: 0.7967
REMARK 3 L13: -3.5976 L23: 2.5293
REMARK 3 S TENSOR
REMARK 3 S11: -0.0798 S12: -1.5666 S13: 2.2980
REMARK 3 S21: 0.1616 S22: 0.8716 S23: 0.0533
REMARK 3 S31: -0.9688 S32: 1.3146 S33: -0.7372
REMARK 3 TLS GROUP : 9
REMARK 3 SELECTION: chain 'B' and (resid 154 through 185)
REMARK 3 ORIGIN FOR THE GROUP (A): 102.7779 -46.2422 -15.6896
REMARK 3 T TENSOR
REMARK 3 T11: 0.3790 T22: 0.4564
REMARK 3 T33: 0.4948 T12: -0.0780
REMARK 3 T13: 0.1193 T23: -0.1808
REMARK 3 L TENSOR
REMARK 3 L11: 5.0670 L22: 9.2284
REMARK 3 L33: 1.9220 L12: 6.1333
REMARK 3 L13: -0.3197 L23: -1.2094
REMARK 3 S TENSOR
REMARK 3 S11: -0.7388 S12: 0.8656 S13: -0.5878
REMARK 3 S21: -0.7892 S22: 0.2346 S23: 0.4003
REMARK 3 S31: 0.4546 S32: -0.3021 S33: 0.5353
REMARK 3 TLS GROUP : 10
REMARK 3 SELECTION: chain 'B' and (resid 186 through 197)
REMARK 3 ORIGIN FOR THE GROUP (A): 89.4343 -60.0520 -14.5866
REMARK 3 T TENSOR
REMARK 3 T11: 0.7926 T22: 0.8090
REMARK 3 T33: 0.7893 T12: -0.2621
REMARK 3 T13: 0.0833 T23: -0.0286
REMARK 3 L TENSOR
REMARK 3 L11: 4.1177 L22: 2.1948
REMARK 3 L33: 4.0533 L12: 3.0564
REMARK 3 L13: -1.0144 L23: -0.7338
REMARK 3 S TENSOR
REMARK 3 S11: -0.2529 S12: 0.1725 S13: -0.4022
REMARK 3 S21: -0.9500 S22: 0.4807 S23: -0.1411
REMARK 3 S31: 1.0844 S32: -1.4521 S33: -0.1682
REMARK 3 TLS GROUP : 11
REMARK 3 SELECTION: chain 'B' and (resid 198 through 227)
REMARK 3 ORIGIN FOR THE GROUP (A): 94.8966 -48.5955 -2.3933
REMARK 3 T TENSOR
REMARK 3 T11: 0.3729 T22: 0.3587
REMARK 3 T33: 0.5199 T12: -0.0317
REMARK 3 T13: 0.0514 T23: -0.0067
REMARK 3 L TENSOR
REMARK 3 L11: 3.2456 L22: 4.8310
REMARK 3 L33: 3.6015 L12: 1.6632
REMARK 3 L13: 0.0335 L23: -0.3002
REMARK 3 S TENSOR
REMARK 3 S11: 0.0959 S12: -0.1614 S13: -0.6866
REMARK 3 S21: 0.3321 S22: -0.1757 S23: -0.1693
REMARK 3 S31: 0.4177 S32: 0.1672 S33: 0.1094
REMARK 3 TLS GROUP : 12
REMARK 3 SELECTION: chain 'B' and (resid 228 through 242)
REMARK 3 ORIGIN FOR THE GROUP (A): 112.4208 -51.6896 -13.1983
REMARK 3 T TENSOR
REMARK 3 T11: 0.7790 T22: 0.5122
REMARK 3 T33: 1.0026 T12: 0.1648
REMARK 3 T13: 0.1659 T23: -0.1220
REMARK 3 L TENSOR
REMARK 3 L11: 3.7366 L22: 2.5001
REMARK 3 L33: 0.7851 L12: 3.0397
REMARK 3 L13: 1.3074 L23: 1.0241
REMARK 3 S TENSOR
REMARK 3 S11: 0.1534 S12: 0.8507 S13: -1.6972
REMARK 3 S21: -0.4068 S22: 0.1129 S23: -0.7964
REMARK 3 S31: -0.8144 S32: -0.0429 S33: -0.2444
REMARK 3 TLS GROUP : 13
REMARK 3 SELECTION: chain 'B' and (resid 243 through 251)
REMARK 3 ORIGIN FOR THE GROUP (A): 85.9333 -53.1198 -4.2411
REMARK 3 T TENSOR
REMARK 3 T11: 0.3714 T22: 0.2747
REMARK 3 T33: 0.5722 T12: -0.0192
REMARK 3 T13: -0.0126 T23: -0.0928
REMARK 3 L TENSOR
REMARK 3 L11: 3.3449 L22: 2.0165
REMARK 3 L33: 5.6917 L12: -1.8933
REMARK 3 L13: 1.8124 L23: 0.8956
REMARK 3 S TENSOR
REMARK 3 S11: 0.4190 S12: 1.2640 S13: -1.7916
REMARK 3 S21: -0.2402 S22: -0.4122 S23: 0.0219
REMARK 3 S31: -0.1884 S32: -0.4293 S33: 0.0260
REMARK 3 TLS GROUP : 14
REMARK 3 SELECTION: chain 'B' and (resid 252 through 262)
REMARK 3 ORIGIN FOR THE GROUP (A): 90.2196 -50.5140 -6.8148
REMARK 3 T TENSOR
REMARK 3 T11: 0.3741 T22: 0.3438
REMARK 3 T33: 0.5056 T12: 0.0020
REMARK 3 T13: 0.0368 T23: -0.0219
REMARK 3 L TENSOR
REMARK 3 L11: 6.9716 L22: 3.5972
REMARK 3 L33: 0.3302 L12: 4.8886
REMARK 3 L13: -0.2250 L23: -0.4021
REMARK 3 S TENSOR
REMARK 3 S11: -0.6307 S12: 0.1548 S13: -0.3940
REMARK 3 S21: -0.4735 S22: 0.4279 S23: -0.0522
REMARK 3 S31: 0.1429 S32: -0.0110 S33: 0.1038
REMARK 3 TLS GROUP : 15
REMARK 3 SELECTION: chain 'B' and (resid 263 through 280)
REMARK 3 ORIGIN FOR THE GROUP (A): 107.3523 -32.3148 3.4381
REMARK 3 T TENSOR
REMARK 3 T11: 0.3575 T22: 0.4111
REMARK 3 T33: 0.2047 T12: 0.0400
REMARK 3 T13: -0.0095 T23: -0.0117
REMARK 3 L TENSOR
REMARK 3 L11: 4.1938 L22: 7.9005
REMARK 3 L33: 7.0490 L12: 3.5052
REMARK 3 L13: 2.3469 L23: 5.1477
REMARK 3 S TENSOR
REMARK 3 S11: -0.0007 S12: -0.7426 S13: 0.1759
REMARK 3 S21: 0.2832 S22: -0.1936 S23: -0.0761
REMARK 3 S31: -0.2331 S32: -0.0177 S33: 0.2045
REMARK 3 TLS GROUP : 16
REMARK 3 SELECTION: chain 'B' and (resid 281 through 300)
REMARK 3 ORIGIN FOR THE GROUP (A): 99.3068 -29.4630 -6.9766
REMARK 3 T TENSOR
REMARK 3 T11: 0.3660 T22: 0.3222
REMARK 3 T33: 0.3279 T12: 0.0265
REMARK 3 T13: 0.0158 T23: 0.0473
REMARK 3 L TENSOR
REMARK 3 L11: 5.4311 L22: 8.2757
REMARK 3 L33: 4.2934 L12: -1.9276
REMARK 3 L13: -1.7369 L23: 5.9517
REMARK 3 S TENSOR
REMARK 3 S11: -0.0824 S12: -0.1743 S13: 0.1487
REMARK 3 S21: -0.2388 S22: -0.3192 S23: 0.1127
REMARK 3 S31: -0.9197 S32: -0.8060 S33: 0.2108
REMARK 3 TLS GROUP : 17
REMARK 3 SELECTION: chain 'B' and (resid 301 through 314)
REMARK 3 ORIGIN FOR THE GROUP (A): 96.0561 -40.1387 -17.0384
REMARK 3 T TENSOR
REMARK 3 T11: 0.5710 T22: 0.5758
REMARK 3 T33: 0.3773 T12: -0.0341
REMARK 3 T13: -0.0190 T23: 0.0308
REMARK 3 L TENSOR
REMARK 3 L11: 9.0583 L22: 4.4916
REMARK 3 L33: 4.0786 L12: 0.9703
REMARK 3 L13: -6.1633 L23: -0.3551
REMARK 3 S TENSOR
REMARK 3 S11: -0.5655 S12: 1.7341 S13: -0.0968
REMARK 3 S21: -0.9309 S22: 0.3457 S23: -0.0561
REMARK 3 S31: 0.6964 S32: -1.2850 S33: 0.1675
REMARK 3 TLS GROUP : 18
REMARK 3 SELECTION: chain 'B' and (resid 315 through 324)
REMARK 3 ORIGIN FOR THE GROUP (A): 85.7637 -36.4903 5.1908
REMARK 3 T TENSOR
REMARK 3 T11: 0.9311 T22: 0.7813
REMARK 3 T33: 0.7808 T12: 0.0715
REMARK 3 T13: 0.1264 T23: -0.2422
REMARK 3 L TENSOR
REMARK 3 L11: 9.5457 L22: 5.3768
REMARK 3 L33: 8.6160 L12: 7.1404
REMARK 3 L13: -0.7572 L23: -0.6912
REMARK 3 S TENSOR
REMARK 3 S11: 0.9085 S12: -1.4752 S13: 1.2802
REMARK 3 S21: 2.8252 S22: 0.2965 S23: -0.1022
REMARK 3 S31: -1.1428 S32: 0.4070 S33: -1.0872
REMARK 3 TLS GROUP : 19
REMARK 3 SELECTION: chain 'B' and (resid 325 through 335)

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REMARK   3   ORIGIN FOR THE GROUP (A):  84.2902 -43.4926  -8.6366
REMARK   3   T TENSOR
REMARK   3     T11:  0.4372 T22:  0.4478
REMARK   3     T33:  0.5271 T12:  -0.0293
REMARK   3     T13:  0.0374 T23:  0.0203
REMARK   3   L TENSOR
REMARK   3     L11:  2.9969 L22:  9.0584
REMARK   3     L33:  2.9310 L12:  2.4391
REMARK   3     L13:  2.1374 L23:  -1.3556
REMARK   3   S TENSOR
REMARK   3     S11: -0.3830 S12:  0.6242 S13:  0.6931
REMARK   3     S21: -0.3255 S22:  0.2273 S23:  0.9659
REMARK   3     S31: -0.6838 S32: -0.4201 S33:  0.0795
REMARK   3
CRYST1  148.576  148.576   36.202  90.00  90.00 120.00 P 6
SCALE1      0.006731  0.003886  0.000000        0.00000
SCALE2      0.000000  0.007772  0.000000        0.00000
SCALE3      0.000000  0.000000  0.027623        0.00000
ATOM      1  N   SER A 154     111.359 -23.888  -5.719  1.00 72.94           N
ANISOU    1  N   SER A 154     9351   8569   9792    361  -1470   -975       N
ATOM      2  CA  SER A 154     112.507 -24.367  -6.476  1.00 64.85           C
ANISOU    2  CA  SER A 154     8208   7554   8878     89  -1489   -800       C
ATOM      3  CB  SER A 154     113.799 -24.176  -5.687  1.00 67.42           C
ANISOU    3  CB  SER A 154     8581   7816   9221     15  -1696   -885       C
ATOM      4  OG  SER A 154     114.906 -24.681  -6.410  1.00 72.11           O
ANISOU    4  OG  SER A 154     9011   8432   9954   -232  -1673   -698       O
ATOM      5  C   SER A 154     112.352 -25.838  -6.840  1.00 64.20           C
ANISOU    5  C   SER A 154     7963   7714   8716     47  -1234   -654       C
ATOM      6  O   SER A 154     111.976 -26.667  -6.008  1.00 54.17           O
ANISOU    6  O   SER A 154     6679   6610   7293    183  -1077   -690       O
ATOM      7  N   VAL A 155     112.663 -26.148  -8.092  1.00 49.48           N
ANISOU    7  N   VAL A 155     5996   5850   6954   -123  -1186   -482       N
ATOM      8  CA  VAL A 155     112.566 -27.503  -8.597  1.00 44.82           C
ANISOU    8  CA  VAL A 155     5269   5442   6319   -166   -990   -371       C
ATOM      9  CB  VAL A 155     112.836 -27.531 -10.105  1.00 56.19           C
ANISOU    9  CB  VAL A 155     6672   6848   7830   -288   -983   -215       C
ATOM     10  CG1 VAL A 155     113.122 -28.948 -10.578  1.00 38.85           C
ANISOU   10  CG1 VAL A 155     4361   4816   5583   -340   -826   -127       C
ATOM     11  CG2 VAL A 155     111.660 -26.930 -10.848  1.00 54.16           C
ANISOU   11  CG2 VAL A 155     6460   6512   7605   -182  -1036   -244       C
ATOM     12  C   VAL A 155     113.542 -28.425  -7.879  1.00 35.93           C
ANISOU   12  C   VAL A 155     4095   4441   5115   -213   -931   -342       C
ATOM     13  O   VAL A 155     113.189 -29.530  -7.466  1.00 41.33           O
ANISOU   13  O   VAL A 155     4719   5270   5717   -143   -760   -326       O
ATOM     14  N   ALA A 156     114.774 -27.953  -7.726  1.00 37.14           N
ANISOU   14  N   ALA A 156     4260   4517   5335   -328  -1082   -325       N
ATOM     15  CA  ALA A 156     115.835 -28.774  -7.162  1.00 39.89           C
ANISOU   15  CA  ALA A 156     4540   4976   5641   -369  -1075   -292       C
ATOM     16  CB  ALA A 156     117.172 -28.110  -7.348  1.00 42.00           C
ANISOU   16  CB  ALA A 156     4741   5116   6103   -539  -1258   -252       C
ATOM     17  C   ALA A 156     115.586 -29.035  -5.685  1.00 56.44           C
ANISOU   17  C   ALA A 156     7168   7157   7538   -166  -1097   -434       C
ATOM     18  O   ALA A 156     115.878 -30.115  -5.166  1.00 56.09           O
ANISOU   18  O   ALA A 156     6677   7262   7374   -105   -986   -385       O
ATOM     19  N   HIS A 157     115.068 -28.017  -5.013  1.00 51.70           N
ANISOU   19  N   HIS A 157     6303   6454   6888    -31  -1238   -604       N
ATOM     20  CA  HIS A 157     114.783 -28.102  -3.592  1.00 55.14           C
ANISOU   20  CA  HIS A 157     6911   6970   7071    231  -1254   -750       C
ATOM     21  CB  HIS A 157     114.165 -26.785  -3.115  1.00 57.97           C
ANISOU   21  CB  HIS A 157     7452   7174   7400    387  -1422   -957       C
ATOM     22  CG  HIS A 157     113.896 -26.742  -1.644  1.00 63.55           C
ANISOU   22  CG  HIS A 157     8394   7962   7789    720  -1447  -1131       C
ATOM     23  ND1 HIS A 157     114.900 -26.800  -0.700  1.00 57.21           N
ANISOU   23  ND1 HIS A 157     7720   7186   6832    816  -1690  -1255       N
ATOM     24  CE1 HIS A 157     114.366 -26.728   0.508  1.00 62.29           C
ANISOU   24  CE1 HIS A 157     8625   7917   7126   1183  -1653  -1398       C
ATOM     25  NE2 HIS A 157     113.055 -26.628   0.379  1.00 68.89           N
ANISOU   25  NE2 HIS A 157     9467   8782   7927   1309  -1358  -1353       N
ATOM     26  CD2 HIS A 157     112.733 -26.635  -0.957  1.00 68.39           C
ANISOU   26  CD2 HIS A 157     9149   8644   8193   1017  -1255  -1200       C
ATOM     27  C   HIS A 157     113.846 -29.279  -3.323  1.00 53.97           C
ANISOU   27  C   HIS A 157     6730   7006   6771    374  -903   -641       C
ATOM     28  O   HIS A 157     114.069 -30.068  -2.408  1.00 49.08           O
ANISOU   28  O   HIS A 157     6182   6519   5949    524  -808   -613       O
ATOM     29  N   GLY A 158     112.813 -29.414  -4.146  1.00 37.40           N
ANISOU   29  N   GLY A 158     4514   4896   4801    328  -722   -568       N
ATOM     30  CA  GLY A 158     111.844 -30.479  -3.969  1.00 44.70           C
ANISOU   30  CA  GLY A 158     5345   5938   5702    425  -398   -464       C
ATOM     31  C   GLY A 158     112.340 -31.826  -4.474  1.00 45.00           C
ANISOU   31  C   GLY A 158     5236   6053   5811    278  -266   -301       C
ATOM     32  O   GLY A 158     111.915 -32.875  -4.007  1.00 48.19           O
ANISOU   32  O   GLY A 158     5590   6536   6185    361   -14   -198       O
ATOM     33  N   LEU A 159     113.243 -31.794  -5.445  1.00 31.81           N
ANISOU   33  N   LEU A 159     3497   4341   4249     73  -414   -264       N
ATOM     34  CA  LEU A 159     113.779 -33.016  -6.032  1.00 34.05           C
ANISOU   34  CA  LEU A 159     3657   4685   4594    -43  -307   -133       C
ATOM     35  CB  LEU A 159     114.551 -32.695  -7.313  1.00 43.51           C
ANISOU   35  CB  LEU A 159     4792   5329   5409   -230  -437    -94       C
ATOM     36  CG  LEU A 159     114.045 -33.149  -8.684  1.00 52.71           C
ANISOU   36  CG  LEU A 159     5868   6976   7185   -307  -369    -48       C
ATOM     37  CD2 LEU A 159     114.661 -32.262  -9.760  1.00 41.60           C
ANISOU   37  CD2 LEU A 159     4488   5498   5821   -412  -498     -6       C
ATOM     38  CD1 LEU A 159     112.535 -33.109  -8.789  1.00 40.55           C
ANISOU   38  CD1 LEU A 159     4288   5399   5721   -227  -312   -119       C
ATOM     39  C   LEU A 159     114.724 -33.670  -5.030  1.00 35.97           C
ANISOU   39  C   LEU A 159     3963   5020   4686     35  -298    -88       C
ATOM     40  O   LEU A 159     114.826 -34.892  -4.941  1.00 37.43           O
ANISOU   40  O   LEU A 159     4091   5265   4866     49  -126     24       O
ATOM     41  N   ALA A 160     115.433 -32.830  -4.286  1.00 32.34           N
ANISOU   41  N   ALA A 160     3625   4547   4117     96  -520    -190       N
ATOM     42  CA  ALA A 160     116.391 -33.302  -3.299  1.00 31.84           C
ANISOU   42  CA  ALA A 160     3639   4569   3891    208  -602    -185       C
ATOM     43  CB  ALA A 160     117.279 -32.169  -2.826  1.00 31.17           C
ANISOU   43  CB  ALA A 160     3633   4413   3798    211  -963    -352       C
ATOM     44  C   ALA A 160     115.671 -33.945  -2.120  1.00 34.93           C
ANISOU   44  C   ALA A 160     4183   5056   4034    478  -386    -145       C
ATOM     45  O   ALA A 160     116.087 -34.991  -1.619  1.00 32.90           O
ANISOU   45  O   ALA A 160     3950   4884   3666    571  -276     -26       O
ATOM     46  N   TRP A 161     114.596 -33.304  -1.672  1.00 33.86           N
ANISOU   46  N   TRP A 161     4155   4899   3811    628  -302    -223       N
ATOM     47  CA  TRP A 161     113.769 -33.868  -0.613  1.00 40.67           C
ANISOU   47  CA  TRP A 161     5148   5849   4454    905   -4   -138       C
ATOM     48  CB  TRP A 161     112.747 -32.853  -0.108  1.00 52.32           C
ANISOU   48  CB  TRP A 161     6244   6993   5642   1101    38    -268       C
ATOM     49  CG  TRP A 161     113.380 -31.898   0.825  1.00 33.73           C
ANISOU   49  CG  TRP A 161     4675   4951   3189   1309  -278   -485       C
ATOM     50  CD1 TRP A 161     113.864 -30.649   0.533  1.00 34.67           C
ANISOU   50  CD1 TRP A 161     4834   4938   3401   1210  -667   -710       C
ATOM     51  NE1 TRP A 161     114.412 -30.085   1.659  1.00 47.90           N
ANISOU   51  NE1 TRP A 161     6792   6626   4780   1471  -941   -912       N
ATOM     52  CE2 TRP A 161     114.299 -30.975   2.700  1.00 43.24           C
ANISOU   52  CE2 TRP A 161     6383   6209   3837   1778  -716   -801       C
ATOM     53  CD2 TRP A 161     113.664 -32.131   2.203  1.00 39.35           C
ANISOU   53  CD2 TRP A 161     5680   5782   3488   1666  -273   -508       C
ATOM     54  CE3 TRP A 161     113.423 -33.199   3.075  1.00 46.01           C
ANISOU   54  CE3 TRP A 161     6650   6766   4065   1926    65   -300       C
ATOM     55  CZ3 TRP A 161     113.824 -33.081   4.402  1.00 48.63           C
ANISOU   55  CZ3 TRP A 161     7350   7205   3924   2328   -47   -387       C
ATOM     56  CH2 TRP A 161     114.460 -31.920   4.866  1.00 46.40           C
ANISOU   56  CH2 TRP A 161     7288   6874   3467   2456  -540   -725       C
ATOM     57  CZ2 TRP A 161     114.704 -30.858   4.033  1.00 52.29           C
ANISOU   57  CZ2 TRP A 161     7878   7446   4543   2165  -881   -938       C
ATOM     58  C   TRP A 161     113.079 -35.146  -1.061  1.00 44.81           C
ANISOU   58  C   TRP A 161     5482   6377   5165    823   361     82       C
ATOM     59  O   TRP A 161     112.957 -36.096  -0.296  1.00 32.05           O
ANISOU   59  O   TRP A 161     3934   4823   3422    986   617    249       O
ATOM     60  N   ALA A 162     112.636 -35.165  -2.313  1.00 38.90           N
ANISOU   60  N   ALA A 162     4511   5541   4729    583   366     79       N
ATOM     61  CA  ALA A 162     111.962 -36.340  -2.848  1.00 32.10           C
ANISOU   61  CA  ALA A 162     3446   4635   4114    484   635    230       C
ATOM     62  CB  ALA A 162     111.342 -36.045  -4.204  1.00 29.26           C
ANISOU   62  CB  ALA A 162     2889   4180   4049    282   544    147       C
ATOM     63  C   ALA A 162     112.934 -37.518  -2.940  1.00 28.12           C
ANISOU   63  C   ALA A 162     2926   4149   3609    420   658    356       C
ATOM     64  O   ALA A 162     112.562 -38.672  -2.727  1.00 43.67           O
ANISOU   64  O   ALA A 162     4827   6083   3683    521   923    521       O
ATOM     65  N   TYR A 163     114.182 -37.219  -3.265  1.00 35.69           N
ANISOU   65  N   TYR A 163     3926   5142   4492    337   387    288       N
ATOM     66  CA  TYR A 163     115.191 -38.263  -3.410  1.00 37.74           C
ANISOU   66  CA  TYR A 163     4154   5425   4761    297   387    391       C
ATOM     67  CB  TYR A 163     116.431 -37.706  -4.095  1.00 38.32           C
ANISOU   67  CB  TYR A 163     4181   5518   4860    160   100    305       C
ATOM     68  CG  TYR A 163     117.442 -38.751  -4.494  1.00 44.80           C
ANISOU   68  CG  TYR A 163     4918   6362   5743    112   113    401       C
ATOM     69  CD1 TYR A 163     117.067 -39.863  -5.243  1.00 40.62           C
ANISOU   69  CD1 TYR A 163     4289   5766   5378    45   299    480       C
ATOM     70  CE1 TYR A 163     117.997 -40.811  -5.620  1.00 38.72           C
ANISOU   70  CE1 TYR A 163     3991   5536   5186    34   312    551       C
ATOM     71  CZ  TYR A 163     119.320 -40.647  -5.246  1.00 43.29           C
ANISOU   71  CZ  TYR A 163     4570   6207   5672    85   148    562       C
ATOM     72  OH  TYR A 163     120.264 -41.579  -5.611  1.00 50.07           O
ANISOU   72  OH  TYR A 163     5349   7082   6592    102   171    634       O
ATOM     73  CE2 TYR A 163     119.709 -39.547  -4.507  1.00 43.52           C
ANISOU   73  CE2 TYR A 163     4662   6296   5577    129   -66    479       C
ATOM     74  CD2 TYR A 163     118.777 -38.609  -4.141  1.00 35.51           C
ANISOU   74  CD2 TYR A 163     3746   5256   4492    145   -88    391       C
ATOM     75  C   TYR A 163     115.549 -38.845  -2.044  1.00 38.96           C
ANISOU   75  C   TYR A 163     4484   5659   4660    543   487    506       C
ATOM     76  O   TYR A 163     115.807 -40.033  -1.901  1.00 41.43           O
ANISOU   76  O   TYR A 163     4783   5959   4999    581   644    664       O
ATOM     77  N   TYR A 164     115.545 -37.991  -1.035  1.00 46.11           N
ANISOU   77  N   TYR A 164     5587   6635   5298   1048   383    420       N
ATOM     78  CA  TYR A 164     115.822 -38.433   0.319  1.00 42.19           C
ANISOU   78  CA  TYR A 164     5326   6231   4471   1050   457   515       C
ATOM     79  CB  TYR A 164     116.127 -37.237   1.217  1.00 35.48           C
ANISOU   79  CB  TYR A 164     4714   5453   3313   1260   172   312       C
ATOM     80  CG  TYR A 164     116.033 -37.561   2.685  1.00 37.98           C
ANISOU   80  CG  TYR A 164     5349   5880   3201   1671   297   398       C
ATOM     81  CD1 TYR A 164     116.852 -38.529   3.256  1.00 44.12           C
ANISOU   81  CD1 TYR A 164     6236   6725   3801   1833   288   542       C
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ATOM 82 CE1 TYR A 164 116.767 -38.833 4.598 1.00 56.67 C
ANISOU 82 CE1 TYR A 164 8169 8423 4941 2261 409 646 C
ATOM 83 CZ TYR A 164 115.851 -38.162 5.389 1.00 64.24 C
ANISOU 83 CZ TYR A 164 9364 9432 5611 2538 570 601 C
ATOM 84 OH TYR A 164 115.771 -38.464 6.723 1.00 75.84 O
ANISOU 84 OH TYR A 164 11222 11026 6569 3019 723 722 O
ATOM 85 CE2 TYR A 164 115.022 -37.192 4.844 1.00 49.80 C
ANISOU 85 CE2 TYR A 164 7404 7535 3982 2375 588 442 C
ATOM 86 CD2 TYR A 164 115.119 -36.898 3.498 1.00 41.28 C
ANISOU 86 CD2 TYR A 164 5982 6338 3363 1939 436 344 C
ATOM 87 C TYR A 164 114.639 -39.219 0.879 1.00 34.16 C
ANISOU 87 C TYR A 164 4349 5193 3439 1204 918 736 C
ATOM 88 O TYR A 164 114.787 -40.337 1.363 1.00 44.10 O
ANISOU 88 O TYR A 164 5666 6451 4638 1324 1136 956 O
ATOM 89 N ILE A 165 113.460 -38.623 0.795 1.00 38.35 N
ANISOU 89 N ILE A 165 4823 5687 4063 1200 1079 695 N
ATOM 90 CA ILE A 165 112.250 -39.226 1.333 1.00 48.87 C
ANISOU 90 CA ILE A 165 6130 6986 5453 1340 1550 914 C
ATOM 91 CB ILE A 165 111.073 -38.225 1.292 1.00 50.77 C
ANISOU 91 CB ILE A 165 6306 7216 5770 1375 1640 802 C
ATOM 92 CG1 ILE A 165 111.337 -37.082 2.265 1.00 44.29 C
ANISOU 92 CG1 ILE A 165 5812 6519 4499 1678 1458 628 C
ATOM 93 CD1 ILE A 165 111.586 -37.560 3.697 1.00 39.10 C
ANISOU 93 CD1 ILE A 165 5490 5984 3380 2084 1659 792 C
ATOM 94 CG2 ILE A 165 109.747 -38.901 1.620 1.00 36.02 C
ANISOU 94 CG2 ILE A 165 4283 5283 4121 1452 2162 1048 C
ATOM 95 C ILE A 165 111.861 -40.515 0.609 1.00 45.97 C
ANISOU 95 C ILE A 165 5495 6467 5505 1121 1798 1107 C
ATOM 96 O ILE A 165 111.359 -41.459 1.219 1.00 50.30 O
ANISOU 96 O ILE A 165 6046 6960 6105 1241 2190 1376 O
ATOM 97 N GLY A 166 112.038 -40.538 -0.695 1.00 44.97 N
ANISOU 97 N GLY A 166 5153 6256 5680 816 1571 972 N
ATOM 98 CA GLY A 166 111.595 -41.651 -1.494 1.00 46.42 C
ANISOU 98 CA GLY A 166 5078 6264 6296 609 1734 1068 C
ATOM 99 C GLY A 166 112.585 -42.674 -1.962 1.00 49.67 C
ANISOU 99 C GLY A 166 5480 6621 6769 510 1629 1113 C
ATOM 100 O GLY A 166 112.254 -43.542 -2.717 1.00 53.06 O
ANISOU 100 O GLY A 166 5720 6885 7556 335 1676 1125 O
ATOM 101 N TYR A 167 113.828 -42.530 -1.579 1.00 50.40 N
ANISOU 101 N TYR A 167 5773 6844 6533 638 1456 1111 N
ATOM 102 CA TYR A 167 114.816 -43.511 -1.956 1.00 48.12 C
ANISOU 102 CA TYR A 167 5471 6516 6297 591 1379 1168 C
ATOM 103 CB TYR A 167 115.468 -43.187 -3.298 1.00 38.31 C
ANISOU 103 CB TYR A 167 4095 5280 5182 373 1082 962 C
ATOM 104 CG TYR A 167 116.491 -44.174 -3.702 1.00 31.13 C
ANISOU 104 CG TYR A 167 3158 4335 4333 353 1032 1011 C
ATOM 105 CD1 TYR A 167 116.136 -45.410 -4.137 1.00 48.17 C
ANISOU 105 CD1 TYR A 167 5228 6304 6772 296 1215 1103 C
ATOM 106 CE1 TYR A 167 117.051 -46.306 -4.499 1.00 29.30 C
ANISOU 106 CE1 TYR A 167 2832 3867 4435 312 1174 1135 C
ATOM 107 CZ TYR A 167 118.347 -45.996 -4.425 1.00 32.82 C
ANISOU 107 CZ TYR A 167 3322 4479 4669 384 966 1094 C
ATOM 108 OH TYR A 167 119.252 -46.919 -4.782 1.00 41.47 O
ANISOU 108 OH TYR A 167 4392 5536 5827 429 943 1128 O
ATOM 109 CE2 TYR A 167 118.735 -44.792 -3.976 1.00 33.13 C
ANISOU 109 CE2 TYR A 167 3411 4700 4478 415 772 1010 C
ATOM 110 CD2 TYR A 167 117.812 -43.884 -3.629 1.00 35.52 C
ANISOU 110 CD2 TYR A 167 3759 5027 4712 401 797 960 C
ATOM 111 C TYR A 167 115.842 -43.763 -0.887 1.00 37.61 C
ANISOU 111 C TYR A 167 4374 5314 4602 841 1308 1265 C
ATOM 112 O TYR A 167 115.980 -44.841 -0.408 1.00 54.20 O
ANISOU 112 O TYR A 167 6559 7357 6679 981 1512 1486 O
ATOM 113 N LEU A 168 116.588 -42.733 -0.580 1.00 44.24 N
ANISOU 113 N LEU A 168 5316 6308 5186 905 994 1095 N
ATOM 114 CA LEU A 168 117.719 -42.803 0.289 1.00 39.59 C
ANISOU 114 CA LEU A 168 4913 5843 4285 1135 800 1115 C
ATOM 115 CB LEU A 168 118.400 -41.456 0.341 1.00 47.60 C
ANISOU 115 CB LEU A 168 5966 6970 5148 1134 394 864 C
ATOM 116 CG LEU A 168 119.233 -41.056 -0.857 1.00 44.06 C
ANISOU 116 CG LEU A 168 5267 6494 4978 839 160 721 C
ATOM 117 CD1 LEU A 168 119.778 -39.714 -0.676 1.00 40.81 C
ANISOU 117 CD1 LEU A 168 4872 6139 4496 820 -216 502 C
ATOM 118 CD2 LEU A 168 120.319 -42.025 -1.031 1.00 39.25 C
ANISOU 118 CD2 LEU A 168 4554 5889 4471 830 132 819 C
ATOM 119 C LEU A 168 117.433 -43.219 1.695 1.00 51.50 C
ANISOU 119 C LEU A 168 6698 7393 5478 1484 1044 1329 C
ATOM 120 O LEU A 168 118.185 -43.944 2.269 1.00 53.79 O
ANISOU 120 O LEU A 168 7112 7701 5626 1672 1059 1486 O
ATOM 121 N ARG A 169 116.360 -42.735 2.272 1.00 49.82 N
ANISOU 121 N ARG A 169 6594 7196 5139 1604 1255 1355 N
ATOM 122 CA ARG A 169 116.081 -43.062 3.641 1.00 58.82 C
ANISOU 122 CA ARG A 169 8044 8402 5903 1998 1521 1575 C
ATOM 123 CB ARG A 169 115.277 -41.978 4.323 1.00 62.17 C
ANISOU 123 CB ARG A 169 8633 8916 6074 2189 1601 1480 C
ATOM 124 CG ARG A 169 113.825 -42.185 4.234 1.00 66.31 C
ANISOU 124 CG ARG A 169 8984 9327 6885 2097 2077 1642 C
ATOM 125 CD ARG A 169 113.106 -40.999 4.735 1.00 71.86 C
ANISOU 125 CD ARG A 169 9823 10112 7367 2285 2094 1497 C
ATOM 126 NE ARG A 169 111.689 -41.138 4.494 1.00 73.35 N
ANISOU 126 NE ARG A 169 9773 10134 7962 2140 2420 1597 N
ATOM 127 CZ ARG A 169 110.751 -40.536 5.196 1.00 73.48 C
ANISOU 127 CZ ARG A 169 9892 10168 7859 2342 2580 1598 C
ATOM 128 NH1 ARG A 169 111.080 -39.747 6.194 1.00 65.58 N
ANISOU 128 NH1 ARG A 169 9251 9327 6338 2708 2434 1478 N
ATOM 129 NH2 ARG A 169 109.488 -40.738 4.889 1.00 74.99 N
ANISOU 129 NH2 ARG A 169 9827 10208 8459 2186 2847 1697 N
ATOM 130 C ARG A 169 115.383 -44.385 3.716 1.00 58.53 C
ANISOU 130 C ARG A 169 7942 8201 6094 1998 2023 1935 C
ATOM 131 O ARG A 169 115.185 -44.908 4.766 1.00 65.30 O
ANISOU 131 O ARG A 169 8993 9016 6800 2265 2206 2100 O
ATOM 132 N LEU A 170 115.026 -44.935 2.579 1.00 64.83 N
ANISOU 132 N LEU A 170 8415 8816 7401 1645 2099 1934 N
ATOM 133 CA LEU A 170 114.442 -46.270 2.522 1.00 66.72 C
ANISOU 133 CA LEU A 170 8536 8788 8027 1561 2373 2135 C
ATOM 134 CB LEU A 170 113.403 -46.378 1.413 1.00 61.59 C
ANISOU 134 CB LEU A 170 7554 7930 7916 1209 2420 2026 C
ATOM 135 CG LEU A 170 112.508 -45.194 1.087 1.00 71.61 C
ANISOU 135 CG LEU A 170 8705 9260 9243 1101 2378 1842 C
ATOM 136 CD1 LEU A 170 111.586 -45.585 -0.051 1.00 68.42 C
ANISOU 136 CD1 LEU A 170 7995 8624 9378 783 2351 1731 C
ATOM 137 CD2 LEU A 170 111.712 -44.780 2.307 1.00 80.57 C
ANISOU 137 CD2 LEU A 170 10009 10444 10158 1362 2602 1955 C
ATOM 138 C LEU A 170 115.515 -47.308 2.240 1.00 69.65 C
ANISOU 138 C LEU A 170 8919 9103 8441 1559 2294 2235 C
ATOM 139 O LEU A 170 115.288 -48.508 2.366 1.00 73.24 O
ANISOU 139 O LEU A 170 9342 9144 1564 2485 2402 O
ATOM 140 N ILE A 171 116.680 -46.842 1.825 1.00 62.81 N
ANISOU 140 N ILE A 171 8068 8400 7397 1538 1937 2067 N
ATOM 141 CA ILE A 171 117.687 -47.747 1.310 1.00 54.15 C
ANISOU 141 CA ILE A 171 6908 7231 6434 1489 1796 2085 C
ATOM 142 CB ILE A 171 117.963 -47.458 -0.177 1.00 52.72 C
ANISOU 142 CB ILE A 171 6569 7015 6569 1155 1555 1813 C
ATOM 143 CG1 ILE A 171 117.425 -48.598 -1.044 1.00 62.70 C
ANISOU 143 CG1 ILE A 171 7536 8004 8283 965 1756 1885 C
ATOM 144 CD1 ILE A 171 118.507 -49.561 -1.529 1.00 57.89 C
ANISOU 144 CD1 ILE A 171 6904 7329 6763 989 1642 1893 C
ATOM 145 CG2 ILE A 171 119.448 -47.210 -0.425 1.00 47.41 C
ANISOU 145 CG2 ILE A 171 5763 6496 5757 1191 1178 1665 C
ATOM 146 C ILE A 171 118.962 -47.701 2.147 1.00 54.13 C
ANISOU 146 C ILE A 171 7132 7413 6022 1790 1530 2094 C
ATOM 147 O ILE A 171 119.615 -48.719 2.362 1.00 63.95 O
ANISOU 147 O ILE A 171 8446 8593 7258 1932 1560 2262 O
ATOM 148 N LEU A 172 119.304 -46.515 2.634 1.00 47.71 N
ANISOU 148 N LEU A 172 6432 6809 4889 1902 1240 1899 N
ATOM 149 CA LEU A 172 120.481 -46.363 3.483 1.00 55.03 C
ANISOU 149 CA LEU A 172 7560 7907 5442 2203 906 1855 C
ATOM 150 CB LEU A 172 120.769 -44.890 3.787 1.00 51.97 C
ANISOU 150 CB LEU A 172 7228 7691 4825 2239 517 1552 C
ATOM 151 CG LEU A 172 121.240 -44.075 2.593 1.00 60.79 C
ANISOU 151 CG LEU A 172 8021 8805 6273 1871 225 1277 C
ATOM 152 CD1 LEU A 172 121.711 -42.716 3.066 1.00 63.38 C
ANISOU 152 CD1 LEU A 172 8423 9256 6403 1942 -202 998 C
ATOM 153 CD2 LEU A 172 122.343 -44.817 1.861 1.00 56.04 C
ANISOU 153 CD2 LEU A 172 7197 8175 5919 1760 96 1295 C
ATOM 154 C LEU A 172 120.473 -47.183 4.785 1.00 65.71 C
ANISOU 154 C LEU A 172 9263 9274 6429 2632 1112 2153 C
ATOM 155 O LEU A 172 121.486 -47.819 5.101 1.00 73.94 O
ANISOU 155 O LEU A 172 10359 10336 7397 2788 927 2172 O
ATOM 156 N PRO A 173 119.359 -47.157 5.551 1.00 63.91 N
ANISOU 156 N PRO A 173 9182 8994 6108 2741 1464 2243 N
ATOM 157 CA PRO A 173 119.343 -47.849 6.847 1.00 72.40 C
ANISOU 157 CA PRO A 173 10522 10049 6939 3086 1637 2389 C
ATOM 158 CB PRO A 173 117.858 -47.878 7.197 1.00 65.42 C
ANISOU 158 CB PRO A 173 9635 9040 6184 3085 2101 2538 C
ATOM 159 CG PRO A 173 117.347 -46.601 6.632 1.00 61.93 C
ANISOU 159 CG PRO A 173 9081 8684 5764 2899 1985 2328 C
ATOM 160 CD PRO A 173 118.106 -46.403 5.343 1.00 64.47 C
ANISOU 160 CD PRO A 173 9175 9037 6281 2597 1689 2202 C
ATOM 161 C PRO A 173 119.890 -49.271 6.823 1.00 75.75 C
ANISOU 161 C PRO A 173 10928 10333 7519 3125 1751 2598 C
ATOM 162 O PRO A 173 120.603 -49.661 7.746 1.00 69.85 O
ANISOU 162 O PRO A 173 10408 9657 6476 3430 1634 2625 O
ATOM 163 N GLU A 174 119.574 -50.033 5.784 1.00 71.87 N
ANISOU 163 N GLU A 174 10180 9635 7494 2829 1952 2717 N
ATOM 164 CA GLU A 174 119.989 -51.424 5.750 1.00 77.47 C
ANISOU 164 CA GLU A 174 10879 10170 8387 2868 2083 2907 C
ATOM 165 CB GLU A 174 118.806 -52.335 5.433 1.00 70.91 C
ANISOU 165 CB GLU A 174 9887 9034 8020 2679 2533 3099 C
ATOM 166 CG GLU A 174 117.692 -52.247 6.445 1.00 76.28 C
ANISOU 166 CG GLU A 174 10687 9682 8616 2845 2871 3235 C
ATOM 167 CD GLU A 174 118.102 -52.781 7.800 1.00106.62 C
ANISOU 167 CD GLU A 174 14852 13588 12071 3264 2965 3408 C
ATOM 168 OE1 GLU A 174 119.003 -53.649 7.853 1.00116.02 O
ANISOU 168 OE1 GLU A 174 16115 14740 13226 3359 2875 3486 O
ATOM 169 OE2 GLU A 174 117.524 -52.331 8.815 1.00111.19 O
ANISOU 169 OE2 GLU A 174 15623 14251 12374 3520 3126 3464 O
ATOM 170 C GLU A 174 121.100 -51.675 4.752 1.00 70.07 C
ANISOU 170 C GLU A 174 9776 9235 7613 2735 1778 2820 C
ATOM 171 O GLU A 174 121.312 -52.807 4.327 1.00 67.57 O
ANISOU 171 O GLU A 174 9378 8720 7575 2678 1900 2947 O

ATOM 172 N LEU A 175 121.815 -50.628 4.370 1.00 66.42 N
ANISOU 172 N LEU A 175 9245 8981 7009 2700 1375 2597 N
ATOM 173 CA LEU A 175 122.786 -50.788 3.303 1.00 68.74 C
ANISOU 173 CA LEU A 175 9304 9274 7539 2573 1111 2515 C
ATOM 174 CB LEU A 175 123.215 -49.449 2.718 1.00 68.07 C
ANISOU 174 CB LEU A 175 9007 9377 7477 2359 733 2150 C
ATOM 175 CG LEU A 175 124.122 -49.686 1.513 1.00 71.76 C
ANISOU 175 CG LEU A 175 9156 9821 8290 2143 555 1995 C
ATOM 176 CD1 LEU A 175 123.326 -50.325 0.383 1.00 69.95 C
ANISOU 176 CD1 LEU A 175 8768 9360 8452 1857 862 2024 C
ATOM 177 CD2 LEU A 175 124.756 -48.395 1.065 1.00 68.69 C
ANISOU 177 CD2 LEU A 175 8560 9610 7929 1976 187 1697 C
ATOM 178 C LEU A 175 124.015 -51.556 3.759 1.00 65.89 C
ANISOU 178 C LEU A 175 9011 8949 7076 2807 904 2530 C
ATOM 179 O LEU A 175 124.388 -52.564 3.158 1.00 69.49 O
ANISOU 179 O LEU A 175 9354 9244 7805 2764 986 2621 O
ATOM 180 N GLN A 176 124.641 -51.066 4.822 1.00 70.35 N
ANISOU 180 N GLN A 176 9761 9708 7259 3057 615 2413 N
ATOM 181 CA GLN A 176 125.846 -51.681 5.358 1.00 74.29 C
ANISOU 181 CA GLN A 176 10324 10257 7646 3288 362 2398 C
ATOM 182 CB GLN A 176 126.271 -50.977 6.632 1.00 74.33 C
ANISOU 182 CB GLN A 176 10570 10451 7223 3555 52 2239 C
ATOM 183 CG GLN A 176 126.088 -49.491 6.565 1.00 81.07 C
ANISOU 183 CG GLN A 176 11365 11450 7989 3441 -207 1973 C
ATOM 184 CD GLN A 176 127.229 -48.750 7.209 1.00 106.05 C
ANISOU 184 CD GLN A 176 14535 14768 10990 3576 -765 1684 C
ATOM 185 OE1 GLN A 176 128.292 -48.586 6.611 1.00 119.42 O
ANISOU 185 OE1 GLN A 176 15926 16500 12951 3450 -1110 1538 O
ATOM 186 NE2 GLN A 176 127.025 -48.311 8.445 1.00 114.32 N
ANISOU 186 NE2 GLN A 176 15909 15889 11639 3841 -844 1595 N
ATOM 187 C GLN A 176 125.631 -53.151 5.654 1.00 71.28 C
ANISOU 187 C GLN A 176 10083 9667 7334 3407 715 2679 C
ATOM 188 O GLN A 176 126.494 -53.978 5.381 1.00 82.45 O
ANISOU 188 O GLN A 176 11416 11018 8892 3466 614 2715 O
ATOM 189 N ALA A 177 124.472 -53.466 6.219 1.00 79.72 N
ANISOU 189 N ALA A 177 11337 10618 8334 3443 1136 2871 N
ATOM 190 CA ALA A 177 124.161 -54.837 6.594 1.00 86.84 C
ANISOU 190 CA ALA A 177 12361 11297 9338 3547 1496 3149 C
ATOM 191 CB ALA A 177 122.863 -54.907 7.367 1.00 62.05 C
ANISOU 191 CB ALA A 177 9383 8074 6121 3609 1934 3329 C
ATOM 192 C ALA A 177 124.083 -55.708 5.354 1.00 83.93 C
ANISOU 192 C ALA A 177 11746 10671 9473 3283 1647 3217 C
ATOM 193 O ALA A 177 124.414 -56.887 5.392 1.00 82.55 O
ANISOU 193 O ALA A 177 11613 10320 9433 3367 1751 3366 O
ATOM 194 N ARG A 178 123.633 -55.122 4.252 1.00 74.77 N
ANISOU 194 N ARG A 178 10342 9475 8590 2979 1647 3095 N
ATOM 195 CA ARG A 178 123.541 -55.858 3.000 1.00 77.32 C
ANISOU 195 CA ARG A 178 10441 9544 9393 2740 1753 3101 C
ATOM 196 CB ARG A 178 122.688 -55.099 2.003 1.00 70.71 C
ANISOU 196 CB ARG A 178 9394 8658 8815 2421 1818 2983 C
ATOM 197 CG ARG A 178 121.235 -55.179 2.331 1.00 70.83 C
ANISOU 197 CG ARG A 178 9426 8515 8971 2286 2188 3091 C
ATOM 198 CD ARG A 178 120.451 -54.248 1.460 1.00 63.52 C
ANISOU 198 CD ARG A 178 8303 7593 8240 1990 2187 2937 C
ATOM 199 NE ARG A 178 120.408 -54.682 0.071 1.00 54.03 N
ANISOU 199 NE ARG A 178 6879 6161 7488 1733 2161 2833 N
ATOM 200 CZ ARG A 178 120.571 -53.870 -0.966 1.00 60.81 C
ANISOU 200 CZ ARG A 178 7533 7161 8411 1504 1907 2490 C
ATOM 201 NH1 ARG A 178 120.797 -52.582 -0.759 1.00 62.71 N
ANISOU 201 NH1 ARG A 178 7770 7707 8349 1502 1700 2333 N
ATOM 202 NH2 ARG A 178 120.511 -54.344 -2.207 1.00 62.39 N
ANISOU 202 NH2 ARG A 178 7557 7179 8969 1301 1857 2304 N
ATOM 203 C ARG A 178 124.917 -56.081 2.422 1.00 76.19 C
ANISOU 203 C ARG A 178 10179 9475 9296 2822 1423 2977 C
ATOM 204 O ARG A 178 125.188 -57.090 1.777 1.00 71.95 O
ANISOU 204 O ARG A 178 9563 8721 9055 2788 1493 3009 O
ATOM 205 N ILE A 179 125.780 -55.109 2.659 1.00 69.81 N
ANISOU 205 N ILE A 179 9332 8969 8224 2930 1049 2805 N
ATOM 206 CA ILE A 179 127.132 -55.157 2.158 1.00 64.05 C
ANISOU 206 CA ILE A 179 8408 8354 7574 2999 716 2654 C
ATOM 207 CB ILE A 179 127.735 -53.763 2.131 1.00 52.00 C
ANISOU 207 CB ILE A 179 6717 7128 5910 2966 332 2414 C
ATOM 208 CG1 ILE A 179 127.131 -52.974 0.972 1.00 55.85 C
ANISOU 208 CG1 ILE A 179 6964 7618 6641 2634 404 2275 C
ATOM 209 CD1 ILE A 179 127.736 -51.607 0.785 1.00 57.56 C
ANISOU 209 CD1 ILE A 179 6966 8087 6818 2505 49 2002 C
ATOM 210 CG2 ILE A 179 129.243 -53.838 2.014 1.00 60.05 C
ANISOU 210 CG2 ILE A 179 7537 8283 6998 3078 -27 2268 C
ATOM 211 C ILE A 179 127.969 -56.090 3.021 1.00 74.21 C
ANISOU 211 C ILE A 179 9866 9625 8705 3289 626 2753 C
ATOM 212 O ILE A 179 128.676 -56.964 2.508 1.00 74.73 O
ANISOU 212 O ILE A 179 9826 9581 8985 3338 601 2760 O
ATOM 213 N ARG A 180 127.874 -55.897 4.334 1.00 74.18 N
ANISOU 213 N ARG A 180 10139 9729 8319 3502 581 2819 N
ATOM 214 CA ARG A 180 128.508 -56.784 5.303 1.00 80.62 C
ANISOU 214 CA ARG A 180 11173 10521 8939 3809 527 2947 C
ATOM 215 CB ARG A 180 128.054 -56.445 6.719 1.00 85.92 C
ANISOU 215 CB ARG A 180 12183 11301 9161 4036 574 3023 C
ATOM 216 CG ARG A 180 128.933 -55.468 7.468 1.00 91.95 C
ANISOU 216 CG ARG A 180 12994 12342 9601 4219 84 2787 C
ATOM 217 CD ARG A 180 128.430 -55.323 8.896 1.00 104.25 C
ANISOU 217 CD ARG A 180 14944 13973 10694 4509 188 2870 C
ATOM 218 NE ARG A 180 129.208 -54.366 9.677 1.00 117.14 N
ANISOU 218 NE ARG A 180 16654 15840 12014 4697 -305 2605 N
ATOM 219 CZ ARG A 180 129.199 -54.309 11.006 1.00 126.76 C
ANISOU 219 CZ ARG A 180 18228 17147 12788 5052 -352 2618 C
ATOM 220 NH1 ARG A 180 129.938 -53.405 11.636 1.00 128.69 N
ANISOU 220 NH1 ARG A 180 18520 17576 12802 5203 -846 2328 N
ATOM 221 NH2 ARG A 180 128.459 -55.158 11.705 1.00 127.17 N
ANISOU 221 NH2 ARG A 180 18580 17087 12651 5265 98 2916 N
ATOM 222 C ARG A 180 128.144 -58.234 5.012 1.00 87.42 C
ANISOU 222 C ARG A 180 12093 11064 10059 3799 888 3183 C
ATOM 223 O ARG A 180 128.988 -59.127 5.034 1.00 94.84 O
ANISOU 223 O ARG A 180 13038 11929 11068 3960 791 3231 O
ATOM 224 N THR A 181 126.866 -58.451 4.740 1.00 86.09 N
ANISOU 224 N THR A 181 11947 10691 10072 3599 1291 3316 N
ATOM 225 CA THR A 181 126.356 -59.771 4.418 1.00 85.37 C
ANISOU 225 CA THR A 181 11877 10246 10313 3527 1631 3511 C
ATOM 226 CB THR A 181 124.822 -59.762 4.401 1.00 88.62 C
ANISOU 226 CB THR A 181 12289 10472 10911 3305 2045 3634 C
ATOM 227 OG1 THR A 181 124.342 -59.442 5.713 1.00 90.82 O
ANISOU 227 OG1 THR A 181 12807 10883 10816 3505 2191 3775 O
ATOM 228 CG2 THR A 181 124.259 -61.106 3.970 1.00 79.42 C
ANISOU 228 CG2 THR A 181 11085 8901 10192 3176 2351 3791 C
ATOM 229 C THR A 181 126.907 -60.281 3.085 1.00 91.37 C
ANISOU 229 C THR A 181 12396 10852 11469 3386 1530 3376 C
ATOM 230 O THR A 181 127.056 -61.486 2.880 1.00 99.93 O
ANISOU 230 O THR A 181 13515 11672 12782 3429 1646 3478 O
ATOM 231 N TYR A 182 127.221 -59.363 2.179 1.00 86.87 N
ANISOU 231 N TYR A 182 11584 10443 10978 3238 1318 3139 N
ATOM 232 CA TYR A 182 127.757 -59.771 0.889 1.00 76.62 C
ANISOU 232 CA TYR A 182 10057 9032 10022 3144 1244 2982 C
ATOM 233 CB TYR A 182 127.691 -58.644 -0.130 1.00 78.14 C
ANISOU 233 CB TYR A 182 9988 9383 10317 2933 1128 2754 C
ATOM 234 CG TYR A 182 128.133 -59.095 -1.500 1.00 64.81 C
ANISOU 234 CG TYR A 182 8089 7578 8959 2858 1113 2575 C
ATOM 235 CD1 TYR A 182 127.226 -59.678 -2.371 1.00 72.08 C
ANISOU 235 CD1 TYR A 182 9003 8169 10215 2668 1334 2537 C
ATOM 236 CE1 TYR A 182 127.611 -60.104 -3.619 1.00 79.90 C
ANISOU 236 CE1 TYR A 182 9852 9055 11451 2640 1306 2327 C
ATOM 237 CZ TYR A 182 128.930 -59.958 -4.010 1.00 75.04 C
ANISOU 237 CZ TYR A 182 9071 8683 10756 2793 1115 2189 C
ATOM 238 OH TYR A 182 129.326 -60.381 -5.254 1.00 70.06 O
ANISOU 238 OH TYR A 182 8325 7977 10316 2797 1125 1973 O
ATOM 239 CE2 TYR A 182 129.860 -59.388 -3.159 1.00 65.52 C
ANISOU 239 CE2 TYR A 182 7811 7793 9290 2944 903 2244 C
ATOM 240 CD2 TYR A 182 129.457 -58.962 -1.912 1.00 59.62 C
ANISOU 240 CD2 TYR A 182 7232 7129 8290 2982 873 2419 C
ATOM 241 C TYR A 182 129.199 -60.182 1.050 1.00 73.36 C
ANISOU 241 C TYR A 182 9603 8742 9528 3399 970 2927 C
ATOM 242 O TYR A 182 129.660 -61.154 0.451 1.00 71.50 O
ANISOU 242 O TYR A 182 9317 8321 9530 3451 998 2904 O
ATOM 243 N ASN A 183 129.908 -59.427 1.879 1.00 75.52 N
ANISOU 243 N ASN A 183 9894 9318 9482 3561 682 2880 N
ATOM 244 CA ASN A 183 131.330 -59.631 2.092 1.00 69.08 C
ANISOU 244 CA ASN A 183 8979 8648 8621 3787 357 2794 C
ATOM 245 CB ASN A 183 131.906 -58.503 2.939 1.00 64.57 C
ANISOU 245 CB ASN A 183 8386 8395 7752 3884 -8 2678 C
ATOM 246 CG ASN A 183 132.200 -57.271 2.126 1.00 72.76 C
ANISOU 246 CG ASN A 183 9081 9637 8927 3668 -202 2431 C
ATOM 247 OD1 ASN A 183 132.154 -57.309 0.899 1.00 77.79 O
ANISOU 247 OD1 ASN A 183 9484 10216 9858 3487 -68 2348 O
ATOM 248 ND2 ASN A 183 132.519 -56.170 2.801 1.00 75.78 N
ANISOU 248 ND2 ASN A 183 9437 10249 9107 3688 -522 2301 N
ATOM 249 C ASN A 183 131.663 -60.965 2.729 1.00 81.86 C
ANISOU 249 C ASN A 183 10818 10075 10210 4039 425 2988 C
ATOM 250 O ASN A 183 132.805 -61.217 3.100 1.00 79.94 O
ANISOU 250 O ASN A 183 10529 9936 9910 4267 152 2949 O
ATOM 251 N GLN A 184 130.651 -61.812 2.850 1.00 98.06 N
ANISOU 251 N GLN A 184 13084 11832 12344 3986 788 3197 N
ATOM 252 CA GLN A 184 130.783 -63.098 3.496 1.00107.67 C
ANISOU 252 CA GLN A 184 14534 12827 13549 4203 908 3421 C
ATOM 253 CB GLN A 184 129.845 -63.171 4.689 1.00 93.19 C
ANISOU 253 CB GLN A 184 13011 10950 11449 4270 1158 3675 C
ATOM 254 CG GLN A 184 130.441 -63.860 5.876 1.00116.71 C
ANISOU 254 CG GLN A 184 16254 13943 14149 4629 1085 3864 C
ATOM 255 CD GLN A 184 130.816 -62.879 6.956 1.00130.90 C
ANISOU 255 CD GLN A 184 18178 16087 15471 4835 818 3801 C
ATOM 256 OE1 GLN A 184 130.085 -62.710 7.930 1.00137.40 O
ANISOU 256 OE1 GLN A 184 19262 16946 15997 4934 1018 3959 O
ATOM 257 NE2 GLN A 184 131.951 -62.210 6.784 1.00131.97 N
ANISOU 257 NE2 GLN A 184 18113 16472 15558 4902 364 3553 N
ATOM 258 C GLN A 184 130.416 -64.214 2.537 1.00116.25 C
ANISOU 258 C GLN A 184 15577 13535 15060 4073 1146 3449 C
ATOM 259 O GLN A 184 131.260 -65.020 2.146 1.00124.03 O
ANISOU 259 O GLN A 184 16506 14415 16206 4215 1038 3401 O
ATOM 260 N HIS A 185 129.139 -64.252 2.171 1.00110.66 N
ANISOU 260 N HIS A 185 14884 12608 14552 3806 1452 3504 N
ATOM 261 C HIS A 185 129.383 -65.406 0.017 1.00 92.33 C
ANISOU 261 C HIS A 185 12318 9864 12900 3635 1469 3216 C

ATOM 262 O HIS A 185 129.521 -66.485 -0.550 1.00 98.64 O
ANISOU 262 O HIS A 185 13138 10359 13983 3667 1510 3178 O
ATOM 263 CA HIS A 185 128.615 -65.303 1.318 1.00104.80 C
ANISOU 263 CA HIS A 185 14115 11454 14250 3652 1655 3503 C
ATOM 264 CB HIS A 185 127.139 -65.062 1.013 1.00112.81 C
ANISOU 264 CB HIS A 185 15091 12281 15489 3324 1935 3529 C
ATOM 265 CG HIS A 185 126.246 -65.249 2.193 1.00126.75 C
ANISOU 265 CG HIS A 185 17047 13979 17133 3339 2220 3828 C
ATOM 266 ND1 HIS A 185 126.578 -64.797 3.455 1.00131.78 N
ANISOU 266 ND1 HIS A 185 17870 14903 17298 3592 2178 3979 N
ATOM 267 CE1 HIS A 185 125.611 -65.104 4.297 1.00133.99 C
ANISOU 267 CE1 HIS A 185 18294 15058 17557 3587 2513 4234 C
ATOM 268 NE2 HIS A 185 124.662 -65.741 3.630 1.00135.39 N
ANISOU 268 NE2 HIS A 185 18348 14872 18224 3310 2756 4257 N
ATOM 269 CD2 HIS A 185 125.037 -65.845 2.314 1.00131.80 C
ANISOU 269 CD2 HIS A 185 17704 14302 18072 3152 2554 3989 C
ATOM 270 N TYR A 186 129.888 -64.273 -0.451 1.00 97.02 N
ANISOU 270 N TYR A 186 12866 8573 15423 3009 47 783 N
ATOM 271 CA TYR A 186 130.601 -64.247 -1.715 1.00 95.33 C
ANISOU 271 CA TYR A 186 12399 8574 15249 3003 -192 278 C
ATOM 272 CB TYR A 186 129.839 -63.409 -2.733 1.00 98.17 C
ANISOU 272 CB TYR A 186 12474 9203 15622 2672 -134 91 C
ATOM 273 CG TYR A 186 128.475 -63.961 -3.053 1.00109.28 C
ANISOU 273 CG TYR A 186 13823 10238 17462 2362 -43 209 C
ATOM 274 CD1 TYR A 186 128.331 -65.017 -3.935 1.00107.32 C
ANISOU 274 CD1 TYR A 186 13548 9632 17598 2305 -239 -55 C
ATOM 275 CE1 TYR A 186 127.093 -65.536 -4.236 1.00108.04 C
ANISOU 275 CE1 TYR A 186 13541 9324 18185 2007 -237 30 C
ATOM 276 CZ TYR A 186 125.969 -64.996 -3.654 1.00111.82 C
ANISOU 276 CZ TYR A 186 13903 9779 18806 1761 30 414 C
ATOM 277 OH TYR A 186 124.734 -65.519 -3.964 1.00113.56 O
ANISOU 277 OH TYR A 186 13941 9566 19641 1451 18 506 O
ATOM 278 CE2 TYR A 186 126.078 -63.939 -2.768 1.00108.67 C
ANISOU 278 CE2 TYR A 186 13559 9758 17974 1843 291 695 C
ATOM 279 CD2 TYR A 186 127.330 -63.429 -2.471 1.00108.19 C
ANISOU 279 CD2 TYR A 186 13640 10074 17392 2142 220 576 C
ATOM 280 C TYR A 186 132.019 -63.730 -1.573 1.00 88.95 C
ANISOU 280 C TYR A 186 11556 8110 14130 3307 -379 80 C
ATOM 281 O TYR A 186 132.646 -63.346 -2.558 1.00 79.91 O
ANISOU 281 O TYR A 186 10159 7254 12948 3310 -476 -285 O
ATOM 282 N ASN A 187 132.522 -63.715 -0.344 1.00 94.49 N
ANISOU 282 N ASN A 187 12515 8757 14629 3581 -431 330 N
ATOM 283 CA ASN A 187 133.897 -63.300 -0.102 1.00100.37 C
ANISOU 283 CA ASN A 187 13199 9752 15186 3887 -692 148 C
ATOM 284 CB ASN A 187 134.194 -63.283 1.396 1.00107.63 C
ANISOU 284 CB ASN A 187 14510 10537 15846 4200 -800 467 C
ATOM 285 CG ASN A 187 135.670 -63.413 1.701 1.00114.91 C
ANISOU 285 CG ASN A 187 15406 11504 16752 4586 -1183 271 C
ATOM 286 OD1 ASN A 187 136.466 -62.528 1.387 1.00111.24 O
ANISOU 286 OD1 ASN A 187 14625 11390 16252 4610 -1357 30 O
ATOM 287 ND2 ASN A 187 136.045 -64.525 2.327 1.00121.75 N
ANISOU 287 ND2 ASN A 187 16583 11983 17693 4893 -1323 390 N
ATOM 288 C ASN A 187 134.878 -64.206 -0.840 1.00102.41 C
ANISOU 288 C ASN A 187 13316 9898 15696 4082 -877 -186 C
ATOM 289 O ASN A 187 135.930 -63.760 -1.297 1.00113.67 O
ANISOU 289 O ASN A 187 14465 11610 17113 4217 -1016 -463 O
ATOM 290 N ASN A 188 134.519 -65.479 -0.963 1.00 93.40 N
ANISOU 290 N ASN A 188 12352 8316 14820 4101 -857 -147 N
ATOM 291 CA ASN A 188 135.336 -66.437 -1.697 1.00101.81 C
ANISOU 291 CA ASN A 188 13336 9222 16127 4308 -1017 -472 C
ATOM 292 CB ASN A 188 134.932 -67.872 -1.346 1.00102.42 C
ANISOU 292 CB ASN A 188 13733 8706 16476 4384 -1043 -307 C
ATOM 293 CG ASN A 188 135.496 -68.324 -0.020 1.00110.24 C
ANISOU 293 CG ASN A 188 15056 9462 17367 4735 -1177 -19 C
ATOM 294 OD1 ASN A 188 136.561 -67.874 0.400 1.00114.87 O
ANISOU 294 OD1 ASN A 188 15584 10284 17776 5024 -1386 -102 O
ATOM 295 ND2 ASN A 188 134.785 -69.225 0.651 1.00 96.05 N
ANISOU 295 ND2 ASN A 188 13615 7167 15712 4725 -1073 333 N
ATOM 296 C ASN A 188 135.243 -66.232 -3.202 1.00 84.41 C
ANISOU 296 C ASN A 188 10844 7225 14004 4133 -947 -860 C
ATOM 297 O ASN A 188 136.102 -66.672 -3.959 1.00 88.71 O
ANISOU 297 O ASN A 188 11265 7791 14649 4351 -1030 -1187 O
ATOM 298 N LEU A 189 134.182 -65.560 -3.625 1.00 92.06 N
ANISOU 298 N LEU A 189 11736 8334 14910 3776 -786 -814 N
ATOM 299 CA LEU A 189 133.913 -65.354 -5.041 1.00 95.19 C
ANISOU 299 CA LEU A 189 11957 8887 15326 3619 -744 -1159 C
ATOM 300 CB LEU A 189 132.409 -65.404 -5.294 1.00 88.17 C
ANISOU 300 CB LEU A 189 11124 7793 14585 3248 -679 -1047 C
ATOM 301 CG LEU A 189 131.920 -64.906 -6.650 1.00 83.74 C
ANISOU 301 CG LEU A 189 10426 7430 13960 3061 -682 -1363 C
ATOM 302 CD1 LEU A 189 132.484 -65.766 -7.773 1.00 81.76 C
ANISOU 302 CD1 LEU A 189 10252 7028 13785 3290 -829 -1794 C
ATOM 303 CD2 LEU A 189 130.402 -64.890 -6.692 1.00 78.74 C
ANISOU 303 CD2 LEU A 189 9796 6570 13554 2691 -673 -1205 C
ATOM 304 C LEU A 189 134.476 -64.020 -5.515 1.00104.41 C
ANISOU 304 C LEU A 189 12847 10608 16216 3602 -650 -1299 C
ATOM 305 O LEU A 189 135.013 -63.908 -6.619 1.00103.93 O
ANISOU 305 O LEU A 189 12643 10736 16110 3698 -609 -1623 O
ATOM 306 N LEU A 190 134.340 -63.006 -4.669 1.00103.74 N
ANISOU 306 N LEU A 190 12716 10757 15943 3499 -596 -1038 N
ATOM 307 CA LEU A 190 134.820 -61.671 -4.986 1.00 95.91 C
ANISOU 307 CA LEU A 190 11460 10243 14740 3450 -524 -1121 C
ATOM 308 CB LEU A 190 134.059 -60.637 -4.161 1.00 87.74 C
ANISOU 308 CB LEU A 190 10475 9357 13507 3235 -462 -822 C
ATOM 309 CG LEU A 190 134.612 -59.218 -4.144 1.00 92.31 C
ANISOU 309 CG LEU A 190 10820 10362 13892 3202 -451 -846 C
ATOM 310 CD1 LEU A 190 133.896 -58.331 -5.146 1.00 86.41 C
ANISOU 310 CD1 LEU A 190 9935 9875 13020 2917 -276 -940 C
ATOM 311 CD2 LEU A 190 134.456 -58.672 -2.758 1.00 97.93 C
ANISOU 311 CD2 LEU A 190 11710 11065 14436 3242 -543 -546 C
ATOM 312 C LEU A 190 136.321 -61.547 -4.736 1.00101.40 C
ANISOU 312 C LEU A 190 11962 11085 15481 3764 -636 -1224 C
ATOM 313 O LEU A 190 137.007 -60.772 -5.406 1.00107.19 O
ANISOU 313 O LEU A 190 12395 12145 16186 3782 -548 -1390 O
ATOM 314 N ARG A 191 136.823 -62.322 -3.775 1.00102.35 N
ANISOU 314 N ARG A 191 12243 10934 15711 4020 -830 -1108 N
ATOM 315 CA ARG A 191 138.241 -62.311 -3.423 1.00 92.68 C
ANISOU 315 CA ARG A 191 10820 9781 14614 4348 -1021 -1202 C
ATOM 316 CB ARG A 191 139.070 -62.902 -4.549 1.00 82.16 C
ANISOU 316 CB ARG A 191 9253 8467 13495 4543 -934 -1528 C
ATOM 317 CG ARG A 191 138.862 -64.381 -4.694 1.00 92.03 C
ANISOU 317 CG ARG A 191 10784 9297 14886 4699 -989 -1602 C
ATOM 318 CD ARG A 191 138.932 -64.798 -6.139 1.00 85.99 C
ANISOU 318 CD ARG A 191 9943 8559 14170 4746 -801 -1933 C
ATOM 319 NE ARG A 191 139.533 -66.117 -6.261 1.00 98.85 N
ANISOU 319 NE ARG A 191 11687 9851 16021 5090 -914 -2097 N
ATOM 320 CZ ARG A 191 140.827 -66.354 -6.078 1.00112.46 C
ANISOU 320 CZ ARG A 191 13216 11667 17849 5318 -939 -2112 C
ATOM 321 NH1 ARG A 191 141.302 -67.586 -6.203 1.00104.32 N
ANISOU 321 NH1 ARG A 191 12332 10363 16942 5534 -997 -2201 N
ATOM 322 NH2 ARG A 191 141.648 -65.361 -5.766 1.00120.30 N
ANISOU 322 NH2 ARG A 191 13851 13000 18856 5312 -921 -2030 N
ATOM 323 C ARG A 191 138.706 -60.903 -3.099 1.00 99.97 C
ANISOU 323 C ARG A 191 11480 11061 15441 4282 -1079 -1157 C
ATOM 324 O ARG A 191 139.677 -60.403 -3.665 1.00100.88 O
ANISOU 324 O ARG A 191 11198 11411 15722 4363 -1053 -1338 O
ATOM 325 N GLY A 192 137.979 -60.268 -2.191 1.00 97.78 N
ANISOU 325 N GLY A 192 11432 10798 14923 4142 -1134 -901 N
ATOM 326 CA GLY A 192 138.250 -58.906 -1.790 1.00 92.08 C
ANISOU 326 CA GLY A 192 10543 10359 14083 4067 -1236 -852 C
ATOM 327 C GLY A 192 137.107 -58.429 -0.924 1.00101.10 C
ANISOU 327 C GLY A 192 12059 11065 14436 3242 -543 -546 C
ATOM 328 O GLY A 192 136.419 -59.231 -0.292 1.00106.23 O
ANISOU 328 O GLY A 192 13090 11818 15455 3977 -1160 -356 O
ATOM 329 N ALA A 193 136.881 -57.124 -0.914 1.00 99.06 N
ANISOU 329 N ALA A 193 11682 11476 14479 3733 -1174 -535 N
ATOM 330 CA ALA A 193 135.786 -56.563 -0.146 1.00 92.70 C
ANISOU 330 CA ALA A 193 11211 10661 13349 3617 -1094 -272 C
ATOM 331 CB ALA A 193 136.239 -56.239 1.268 1.00 85.64 C
ANISOU 331 CB ALA A 193 10620 9667 12252 3914 -1438 -133 C
ATOM 332 C ALA A 193 135.260 -55.317 -0.834 1.00 82.52 C
ANISOU 332 C ALA A 193 9700 9692 11962 3302 -913 -318 C
ATOM 333 O ALA A 193 136.031 -54.500 -1.331 1.00 84.82 O
ANISOU 333 O ALA A 193 9647 10216 12364 3256 -994 -489 O
ATOM 334 N VAL A 194 133.944 -55.176 -0.876 1.00 67.94 N
ANISOU 334 N VAL A 194 8027 7835 9954 3087 -658 -148 N
ATOM 335 CA VAL A 194 133.371 -53.956 -1.400 1.00 69.10 C
ANISOU 335 CA VAL A 194 8018 8262 9975 2821 -519 -166 C
ATOM 336 CB VAL A 194 131.990 -54.192 -2.040 1.00 63.56 C
ANISOU 336 CB VAL A 194 7347 7519 9283 2553 -224 -92 C
ATOM 337 CG1 VAL A 194 131.949 -55.557 -2.694 1.00 58.36 C
ANISOU 337 CG1 VAL A 194 6670 6625 8881 2563 -173 -202 C
ATOM 338 CG2 VAL A 194 130.893 -54.095 -1.012 1.00 78.10 C
ANISOU 338 CG2 VAL A 194 9501 9220 10954 2549 -89 236 C
ATOM 339 C VAL A 194 133.304 -52.956 -0.252 1.00 68.18 C
ANISOU 339 C VAL A 194 8123 8202 9581 2921 -671 -1 C
ATOM 340 O VAL A 194 133.091 -53.330 0.905 1.00 70.06 O
ANISOU 340 O VAL A 194 8749 8231 9640 3145 -1053 -1 O
ATOM 341 N SER A 195 133.521 -51.687 -0.574 1.00 62.31 N
ANISOU 341 N SER A 195 7170 7718 8787 2789 -730 -97 N
ATOM 342 CA SER A 195 133.480 -50.635 0.426 1.00 66.35 C
ANISOU 342 CA SER A 195 7899 8274 9039 2890 -925 7 C
ATOM 343 CB SER A 195 133.952 -49.319 -0.179 1.00 65.76 C
ANISOU 343 CB SER A 195 7486 8453 9046 2711 -1018 -151 C
ATOM 344 OG SER A 195 134.845 -49.562 -1.243 1.00 76.90 O
ANISOU 344 OG SER A 195 8462 9955 10800 2629 -985 -353 O
ATOM 345 C SER A 195 132.055 -50.507 0.951 1.00 78.03 C
ANISOU 345 C SER A 195 9723 9700 10227 2841 -653 272 C
ATOM 346 O SER A 195 131.102 -50.967 0.316 1.00 72.71 O
ANISOU 346 O SER A 195 8980 9006 9641 2634 -332 341 O
ATOM 347 N GLN A 196 131.902 -49.867 2.102 1.00 75.77 N
ANISOU 347 N GLN A 196 9804 9369 9615 3051 -789 415 N
ATOM 348 CA GLN A 196 130.637 -49.963 2.815 1.00 95.27 C
ANISOU 348 CA GLN A 196 12658 11728 11812 3115 -472 725 C
ATOM 349 CB GLN A 196 130.886 -50.181 4.307 1.00107.29 C
ANISOU 349 CB GLN A 196 14754 13030 12983 3563 -650 904 C
ATOM 350 CG GLN A 196 129.989 -51.235 4.926 1.00117.21 C
ANISOU 350 CG GLN A 196 16367 14021 14147 3700 -255 1260 C
ATOM 351 CD GLN A 196 130.726 -52.107 5.920 1.00131.08 C
ANISOU 351 CD GLN A 196 18557 15502 15747 4122 -492 1348 C

ATOM 352 OE1 GLN A 196 131.505 -52.981 5.539 1.00131.50 O
ANISOU 352 OE1 GLN A 196 18420 15455 16088 4126 -678 1202 O
ATOM 353 NE2 GLN A 196 130.490 -51.867 7.206 1.00139.63 N
ANISOU 353 NE2 GLN A 196 20266 16448 16341 4524 -490 1584 N
ATOM 354 C GLN A 196 129.672 -48.796 2.598 1.00 96.40 C
ANISOU 354 C GLN A 196 12760 12066 11802 2921 -267 787 C
ATOM 355 O GLN A 196 128.565 -48.804 3.132 1.00105.45 O
ANISOU 355 O GLN A 196 14161 13133 12773 2970 54 1058 O
ATOM 356 N ARG A 197 130.077 -47.801 1.818 1.00 74.18 N
ANISOU 356 N ARG A 197 9617 9488 9081 2715 -421 561 N
ATOM 357 CA ARG A 197 129.212 -46.655 1.585 1.00 65.60 C
ANISOU 357 CA ARG A 197 8499 8575 7852 2547 -266 606 C
ATOM 358 CB ARG A 197 129.997 -45.349 1.706 1.00 78.79 C
ANISOU 358 CB ARG A 197 10127 10376 9435 2574 -627 432 C
ATOM 359 CG ARG A 197 130.910 -45.302 2.922 1.00 86.12 C
ANISOU 359 CG ARG A 197 11394 11139 10188 2946 -1055 401 C
ATOM 360 CD ARG A 197 130.852 -43.954 3.628 1.00 98.27 C
ANISOU 360 CD ARG A 197 13203 12701 11433 3083 -1308 376 C
ATOM 361 NE ARG A 197 131.678 -42.934 2.985 1.00111.48 N
ANISOU 361 NE ARG A 197 14490 14493 13375 2876 -1615 140 N
ATOM 362 CZ ARG A 197 131.689 -41.650 3.331 1.00110.43 C
ANISOU 362 CZ ARG A 197 14483 14374 13101 2908 -1868 73 C
ATOM 363 NH1 ARG A 197 132.476 -40.796 2.691 1.00112.62 N
ANISOU 363 NH1 ARG A 197 14356 14716 13718 2688 -2115 -109 N
ATOM 364 NH2 ARG A 197 130.910 -41.218 4.314 1.00 95.25 N
ANISOU 364 NH2 ARG A 197 13098 12379 10712 3176 -1847 202 N
ATOM 365 C ARG A 197 128.520 -46.746 0.230 1.00 60.72 C
ANISOU 365 C ARG A 197 7503 8088 7481 2186 2 545 C
ATOM 366 O ARG A 197 128.893 -47.552 -0.617 1.00 60.04 O
ANISOU 366 O ARG A 197 7172 7984 7657 2070 17 411 O
ATOM 367 N LEU A 198 127.499 -45.918 0.039 1.00 53.27 N
ANISOU 367 N LEU A 198 6547 7257 6435 2048 187 630 N
ATOM 368 CA LEU A 198 126.854 -45.814 -1.255 1.00 59.13 C
ANISOU 368 CA LEU A 198 6969 8125 7374 1738 345 540 C
ATOM 369 CB LEU A 198 125.347 -45.638 -1.105 1.00 62.03 C
ANISOU 369 CB LEU A 198 7383 8456 7729 1665 635 752 C
ATOM 370 CG LEU A 198 124.412 -46.093 -2.233 1.00 57.38 C
ANISOU 370 CG LEU A 198 6510 7850 7442 1397 780 708 C
ATOM 371 CD1 LEU A 198 123.314 -45.059 -2.436 1.00 61.47 C
ANISOU 371 CD1 LEU A 198 6959 8487 7910 1287 898 784 C
ATOM 372 CD2 LEU A 198 125.127 -46.373 -3.550 1.00 49.71 C
ANISOU 372 CD2 LEU A 198 5311 6971 6607 1246 614 413 C
ATOM 373 C LEU A 198 127.437 -44.595 -1.938 1.00 54.18 C
ANISOU 373 C LEU A 198 6163 7726 6698 1613 176 352 C
ATOM 374 O LEU A 198 127.406 -43.495 -1.394 1.00 58.50 O
ANISOU 374 O LEU A 198 6844 8340 7042 1678 78 391 O
ATOM 375 N TYR A 199 127.970 -44.794 -3.133 1.00 48.96 N
ANISOU 375 N TYR A 199 5225 7158 6219 1455 160 160 N
ATOM 376 CA TYR A 199 128.545 -43.689 -3.867 1.00 47.41 C
ANISOU 376 CA TYR A 199 4847 7153 6014 1333 78 30 C
ATOM 377 CB TYR A 199 129.894 -44.078 -4.435 1.00 45.79 C
ANISOU 377 CB TYR A 199 4415 6969 6015 1355 -2 -134 C
ATOM 378 CG TYR A 199 130.883 -44.256 -3.329 1.00 52.57 C
ANISOU 378 CG TYR A 199 5336 7703 6935 1568 -261 -129 C
ATOM 379 CD1 TYR A 199 131.008 -45.480 -2.673 1.00 59.93 C
ANISOU 379 CD1 TYR A 199 6415 8452 7904 1754 -303 -90 C
ATOM 380 CE1 TYR A 199 131.898 -45.638 -1.640 1.00 64.77 C
ANISOU 380 CE1 TYR A 199 7136 8931 8541 1993 -598 -94 C
ATOM 381 CZ TYR A 199 132.662 -44.556 -1.235 1.00 67.32 C
ANISOU 381 CZ TYR A 199 7394 9286 8897 2033 -898 -158 C
ATOM 382 OH TYR A 199 133.558 -44.706 -0.208 1.00 80.49 O
ANISOU 382 OH TYR A 199 9180 10788 10613 2295 -1290 -197 O
ATOM 383 CE2 TYR A 199 132.545 -43.331 -1.863 1.00 63.93 C
ANISOU 383 CE2 TYR A 199 6789 9017 8483 1820 -850 -189 C
ATOM 384 CD2 TYR A 199 131.651 -43.186 -2.896 1.00 59.32 C
ANISOU 384 CD2 TYR A 199 6130 8583 7825 1597 -512 -162 C
ATOM 385 C TYR A 199 127.585 -43.202 -4.930 1.00 46.13 C
ANISOU 385 C TYR A 199 4598 7116 5811 1127 238 10 C
ATOM 386 O TYR A 199 127.218 -43.929 -5.845 1.00 44.02 O
ANISOU 386 O TYR A 199 4247 6834 5644 1042 339 -73 O
ATOM 387 N ILE A 200 127.155 -41.961 -4.761 1.00 45.87 N
ANISOU 387 N ILE A 200 4623 7180 5624 1077 215 73 N
ATOM 388 CA ILE A 200 126.173 -41.375 -5.640 1.00 46.13 C
ANISOU 388 CA ILE A 200 4610 7319 5599 917 321 69 C
ATOM 389 CB ILE A 200 125.079 -40.694 -4.846 1.00 46.93 C
ANISOU 389 CB ILE A 200 4867 7403 5563 959 364 234 C
ATOM 390 CG1 ILE A 200 124.409 -41.706 -3.930 1.00 39.39 C
ANISOU 390 CG1 ILE A 200 4026 6271 4670 1083 493 393 C
ATOM 391 CD1 ILE A 200 123.399 -41.100 -3.017 1.00 41.61 C
ANISOU 391 CD1 ILE A 200 4478 6520 4811 1193 620 595 C
ATOM 392 CG2 ILE A 200 124.067 -40.075 -5.785 1.00 37.87 C
ANISOU 392 CG2 ILE A 200 3641 6352 4396 808 428 217 C
ATOM 393 C ILE A 200 126.831 -40.376 -6.574 1.00 46.59 C
ANISOU 393 C ILE A 200 4549 7532 5622 808 292 -28 C
ATOM 394 O ILE A 200 127.385 -39.372 -6.139 1.00 45.64 O
ANISOU 394 O ILE A 200 4438 7441 5463 819 179 0 O
ATOM 395 N LEU A 201 126.780 -40.688 -7.864 1.00 37.61 N
ANISOU 395 N LEU A 201 3326 6461 4505 723 392 -139 N
ATOM 396 CA LEU A 201 127.345 -39.838 -8.895 1.00 44.66 C
ANISOU 396 CA LEU A 201 4146 7486 5337 647 458 -190 C
ATOM 397 CB LEU A 201 127.619 -40.653 -10.148 1.00 52.73 C
ANISOU 397 CB LEU A 201 5143 8533 6357 671 588 -332 C
ATOM 398 CG LEU A 201 128.661 -41.745 -9.991 1.00 51.94 C
ANISOU 398 CG LEU A 201 4934 8362 6440 785 623 -411 C
ATOM 399 CD1 LEU A 201 128.547 -42.706 -11.158 1.00 40.25 C
ANISOU 399 CD1 LEU A 201 3528 6863 4902 854 720 -576 C
ATOM 400 CD2 LEU A 201 130.033 -41.109 -9.943 1.00 47.80 C
ANISOU 400 CD2 LEU A 201 4209 7891 6061 797 686 -373 C
ATOM 401 C LEU A 201 126.384 -38.714 -9.246 1.00 50.88 C
ANISOU 401 C LEU A 201 5031 8352 5951 556 449 -130 C
ATOM 402 O LEU A 201 125.201 -38.949 -9.483 1.00 36.89 O
ANISOU 402 O LEU A 201 3332 6560 4127 535 434 -136 O
ATOM 403 N LEU A 202 126.913 -37.497 -9.299 1.00 56.46 N
ANISOU 403 N LEU A 202 5711 9118 6624 502 440 -70 N
ATOM 404 CA LEU A 202 126.125 -36.319 -9.620 1.00 34.24 C
ANISOU 404 CA LEU A 202 3003 6362 3646 432 419 -6 C
ATOM 405 CB LEU A 202 125.970 -35.446 -8.399 1.00 40.78 C
ANISOU 405 CB LEU A 202 3898 7132 4466 459 265 88 C
ATOM 406 CG LEU A 202 124.996 -35.957 -7.365 1.00 54.27 C
ANISOU 406 CG LEU A 202 5717 8772 6131 566 225 137 C
ATOM 407 CD1 LEU A 202 125.599 -35.774 -5.999 1.00 60.13 C
ANISOU 407 CD1 LEU A 202 6550 9414 6884 697 76 177 C
ATOM 408 CD2 LEU A 202 123.724 -35.159 -7.497 1.00 52.67 C
ANISOU 408 CD2 LEU A 202 5610 8604 5797 553 232 200 C
ATOM 409 C LEU A 202 126.765 -35.491 -10.713 1.00 37.34 C
ANISOU 409 C LEU A 202 3369 6828 3990 361 548 15 C
ATOM 410 O LEU A 202 127.434 -34.496 -10.430 1.00 44.17 O
ANISOU 410 O LEU A 202 4167 7667 4950 302 519 99 O
ATOM 411 N PRO A 203 126.581 -35.912 -11.967 1.00 46.49 N
ANISOU 411 N PRO A 203 4605 8049 5009 386 687 -57 N
ATOM 412 CA PRO A 203 127.074 -35.119 -13.096 1.00 46.65 C
ANISOU 412 CA PRO A 203 4684 8135 4908 367 883 5 C
ATOM 413 CB PRO A 203 126.863 -36.040 -14.295 1.00 39.98 C
ANISOU 413 CB PRO A 203 4001 7329 3860 490 995 -130 C
ATOM 414 CG PRO A 203 125.775 -36.991 -13.870 1.00 38.12 C
ANISOU 414 CG PRO A 203 3803 7031 3648 513 756 -262 C
ATOM 415 CD PRO A 203 125.997 -37.195 -12.392 1.00 36.53 C
ANISOU 415 CD PRO A 203 3410 6766 3702 583 539 -200 C
ATOM 416 C PRO A 203 126.244 -33.852 -13.255 1.00 43.70 C
ANISOU 416 C PRO A 203 4467 7776 4363 306 794 99 C
ATOM 417 O PRO A 203 125.024 -33.921 -13.421 1.00 44.20 O
ANISOU 417 O PRO A 203 4676 7849 4268 337 647 41 O
ATOM 418 N LEU A 204 126.916 -32.705 -13.205 1.00 52.75 N
ANISOU 418 N LEU A 204 5554 8894 5596 221 866 243 N
ATOM 419 CA LEU A 204 126.239 -31.415 -13.250 1.00 50.34 C
ANISOU 419 CA LEU A 204 5398 8569 5161 168 766 343 C
ATOM 420 CB LEU A 204 127.192 -30.290 -12.859 1.00 61.50 C
ANISOU 420 CB LEU A 204 6672 9876 6819 48 787 491 C
ATOM 421 CG LEU A 204 127.599 -30.326 -11.389 1.00 57.99 C
ANISOU 421 CG LEU A 204 6061 9327 6647 25 534 447 C
ATOM 422 CD1 LEU A 204 128.215 -29.000 -10.980 1.00 47.40 C
ANISOU 422 CD1 LEU A 204 4645 7824 5541 -89 412 557 C
ATOM 423 CD2 LEU A 204 126.396 -30.648 -10.518 1.00 43.15 C
ANISOU 423 CD2 LEU A 204 4336 7469 4592 317 317 447 C
ATOM 424 C LEU A 204 125.604 -31.132 -14.605 1.00 51.32 C
ANISOU 424 C LEU A 204 5780 8572 4611 245 709 378 O
ATOM 425 O LEU A 204 124.617 -30.404 -14.702 1.00 49.91 O
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ANISOU 426 N ASP A 205 5014 7956 3983 323 1118 335 N
ATOM 427 CA ASP A 205 125.586 -31.612 -16.990 1.00 48.53 C
ANISOU 427 CA ASP A 205 5863 8496 4081 466 1179 312 C
ATOM 428 CB ASP A 205 126.604 -32.012 -18.052 1.00 46.12 C
ANISOU 428 CB ASP A 205 5655 8224 3645 597 1578 357 C
ATOM 429 CG ASP A 205 127.179 -33.391 -17.799 1.00111.60 C
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ANISOU 430 OD1 ASP A 205 13641 16737 12727 539 1698 255 O
ATOM 431 OD2 ASP A 205 126.750 -34.354 -18.469 1.00108.99 O
ANISOU 431 OD2 ASP A 205 13659 16220 11531 834 1568 5 O
ATOM 432 C ASP A 205 124.358 -32.514 -17.096 1.00 41.86 C
ANISOU 432 C ASP A 205 5142 7661 3102 563 869 85 C
ATOM 433 O ASP A 205 123.716 -32.582 -18.145 1.00 47.54 O
ANISOU 433 O ASP A 205 6174 8386 3501 712 781 -2 O
ATOM 434 N CYS A 206 124.067 -33.229 -16.009 1.00 45.24 N
ANISOU 434 N CYS A 206 5329 8059 3801 491 696 -3 N
ATOM 435 CA CYS A 206 122.873 -34.066 -15.891 1.00 42.51 C
ANISOU 435 CA CYS A 206 4991 7609 3552 413 -173 C
ATOM 436 CB CYS A 206 121.609 -33.207 -15.929 1.00 38.59 C
ANISOU 436 CB CYS A 206 4586 7155 2922 529 176 -146 C
ATOM 437 SG CYS A 206 121.490 -32.044 -14.559 1.00 48.70 S
ANISOU 437 SG CYS A 206 5700 8427 4375 412 172 43 S
ATOM 438 C CYS A 206 122.785 -35.158 -16.948 1.00 45.62 C
ANISOU 438 C CYS A 206 5568 8037 3727 683 367 -376 C
ATOM 439 O CYS A 206 121.700 -35.652 -17.243 1.00 70.57 O
ANISOU 439 O CYS A 206 8796 11121 6896 732 69 -531 O
ATOM 440 N GLY A 207 123.920 -35.504 -17.541 1.00 52.22 N
ANISOU 440 N GLY A 207 6484 8914 4444 775 648 -379 N
ATOM 441 CA GLY A 207 123.960 -36.591 -18.498 1.00 46.68 C
ANISOU 441 CA GLY A 207 6007 8172 3556 970 620 -593 C

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ATOM 443 O GLY A 207 125.078 -38.220 -17.140 1.00 63.85 O
ANISOU 443 O GLY A 207 7722 10288 6251 886 756 -652 O
ATOM 444 N VAL A 208 122.975 -38.687 -17.787 1.00 52.82 N
ANISOU 444 N VAL A 208 6568 8734 4765 938 175 -909 N
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ANISOU 445 CA VAL A 208 5532 7767 4261 899 82 -1016 C
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ANISOU 446 CB VAL A 208 6151 8536 5511 729 -143 -957 C
ATOM 447 CG1 VAL A 208 121.841 -41.481 -15.477 1.00 56.27 C
ANISOU 447 CG1 VAL A 208 6369 8756 6255 698 -195 -1028 C
ATOM 448 CG2 VAL A 208 121.977 -39.015 -15.065 1.00 45.69 C
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ATOM 449 C VAL A 208 122.828 -41.084 -18.167 1.00 53.32 C
ANISOU 449 C VAL A 208 6692 8534 5034 1092 -101 -1302 C
ATOM 450 O VAL A 208 121.869 -41.111 -18.931 1.00 64.85 O
ANISOU 450 O VAL A 208 8364 9894 6382 1171 -443 -1470 O
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ANISOU 451 N PRO A 209 6313 8132 4679 1197 87 -1378 N
ATOM 452 CA PRO A 209 123.884 -43.032 -19.223 1.00 59.62 C
ANISOU 452 CA PRO A 209 7803 9175 5673 1441 -50 -1669 C
ATOM 453 CB PRO A 209 125.335 -43.508 -19.131 1.00 60.97 C
ANISOU 453 CB PRO A 209 7916 9423 5827 1560 360 -1630 C
ATOM 454 CG PRO A 209 125.688 -43.293 -17.706 1.00 64.35 C
ANISOU 454 CG PRO A 209 7903 9901 6644 1317 491 -1396 C
ATOM 455 CD PRO A 209 124.975 -42.026 -17.301 1.00 46.90 C
ANISOU 455 CD PRO A 209 5604 7786 4430 1128 423 -1206 C
ATOM 456 C PRO A 209 122.949 -44.203 -18.973 1.00 53.38 C
ANISOU 456 C PRO A 209 6928 8107 5249 1379 -481 -1875 C
ATOM 457 O PRO A 209 122.583 -44.527 -17.841 1.00 56.65 O
ANISOU 457 O PRO A 209 6987 8430 6109 1162 -528 -1754 O
ATOM 458 N ASP A 210 122.580 -44.828 -20.081 1.00 58.64 N
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ATOM 459 CA ASP A 210 121.848 -46.079 -20.114 1.00 79.31 C
ANISOU 459 CA ASP A 210 10558 10893 8683 1592 -1243 -2442 C
ATOM 460 CB ASP A 210 121.899 -46.590 -21.542 1.00 93.89 C
ANISOU 460 CB ASP A 210 12963 12612 10101 1955 -1507 -2807 C
ATOM 461 CG ASP A 210 123.154 -46.128 -22.264 1.00106.02 C
ANISOU 461 CG ASP A 210 14853 14408 11024 2253 -1004 -2753 C
ATOM 462 OD2 ASP A 210 123.089 -45.087 -22.957 1.00103.95 O
ANISOU 462 OD2 ASP A 210 14874 14310 10314 2376 -911 -2680 O
ATOM 463 OD1 ASP A 210 124.210 -46.782 -22.109 1.00100.76 O
ANISOU 463 OD1 ASP A 210 14155 13769 10362 2365 -669 -2754 O
ATOM 464 C ASP A 210 122.498 -47.102 -19.192 1.00 82.20 C
ANISOU 464 C ASP A 210 10650 11163 9421 1507 -1055 -2384 C
ATOM 465 O ASP A 210 121.834 -47.724 -18.363 1.00 68.23 O
ANISOU 465 O ASP A 210 8573 9176 8176 1297 -1239 -2336 O
ATOM 466 N ASN A 211 123.805 -47.277 -19.353 1.00 90.27 N
ANISOU 466 N ASN A 211 11784 12328 10185 1691 -668 -2371 N
ATOM 467 CA ASN A 211 124.582 -48.145 -18.478 1.00 91.11 C
ANISOU 467 CA ASN A 211 11646 12371 10602 1652 -471 -2302 C
ATOM 468 CB ASN A 211 124.858 -49.495 -19.139 1.00103.18 C
ANISOU 468 CB ASN A 211 13438 13650 12116 1902 -645 -2627 C
ATOM 469 CG ASN A 211 123.642 -50.394 -19.140 1.00110.52 C
ANISOU 469 CG ASN A 211 14359 14191 13442 1793 -1195 -2829 C
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ANISOU 470 OD1 ASN A 211 15002 14416 13669 1888 -1603 -3075 O
ATOM 471 ND2 ASN A 211 123.496 -51.192 -18.087 1.00109.03 N
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ANISOU 472 C ASN A 211 10878 12051 9873 1672 39 -2059 C
ATOM 473 O ASN A 211 126.714 -47.099 -18.843 1.00 78.01 O
ANISOU 473 O ASN A 211 10028 11165 8448 1891 331 -2080 O
ATOM 474 N LEU A 212 126.013 -47.361 -16.712 1.00 95.19 N
ANISOU 474 N LEU A 212 11488 13442 10128 1488 -1249 3688 N
ATOM 475 CA LEU A 212 127.161 -46.730 -16.080 1.00 95.93 C
ANISOU 475 CA LEU A 212 10852 13931 11664 946 -919 3289 C
ATOM 476 CB LEU A 212 127.042 -46.883 -14.567 1.00 93.98 C
ANISOU 476 CB LEU A 212 10752 13167 11791 1472 -519 3285 C
ATOM 477 CG LEU A 212 128.290 -46.769 -13.704 1.00 80.74 C
ANISOU 477 CG LEU A 212 9712 10871 10095 1658 -263 2763 C
ATOM 478 CD1 LEU A 212 128.974 -45.427 -13.906 1.00 82.58 C
ANISOU 478 CD1 LEU A 212 10387 10897 10091 1814 -122 2675 C
ATOM 479 CD2 LEU A 212 127.877 -46.939 -12.263 1.00 76.72 C
ANISOU 479 CD2 LEU A 212 9312 9974 9864 1925 90 2733 C
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ANISOU 480 C LEU A 212 12023 14495 12207 434 -987 2476 C
ATOM 481 O LEU A 212 129.452 -46.763 -16.803 1.00101.04 O
ANISOU 481 O LEU A 212 12333 14146 11913 496 -923 2195 O
ATOM 482 N SER A 213 128.320 -48.714 -16.706 1.00110.74 N
ANISOU 482 N SER A 213 13007 15688 13381 -84 -1045 2124 N
ATOM 483 CA SER A 213 129.394 -49.551 -17.201 1.00108.19 C
ANISOU 483 CA SER A 213 13017 15118 12974 -596 -956 1401 C
ATOM 484 CB SER A 213 128.859 -50.970 -17.357 1.00103.95 C
ANISOU 484 CB SER A 213 12287 14695 12513 -1179 -922 1174 C
ATOM 485 OG SER A 213 127.614 -51.105 -16.692 1.00 91.43 O
ANISOU 485 OG SER A 213 10259 13360 11122 -952 -1005 1685 O
ATOM 486 C SER A 213 129.922 -49.042 -18.539 1.00101.82 C
ANISOU 486 C SER A 213 12421 14545 11719 -1058 -1124 1227 C
ATOM 487 O SER A 213 131.061 -49.313 -18.911 1.00 91.58 O
ANISOU 487 O SER A 213 11498 12915 10385 -1297 -936 665 O
ATOM 488 N MET A 214 129.086 -48.292 -19.251 1.00106.88 N
ANISOU 488 N MET A 214 12792 15761 12056 -1169 -1455 1782 N
ATOM 489 CA MET A 214 129.434 -47.781 -20.570 1.00100.93 C
ANISOU 489 CA MET A 214 12223 15322 10803 -1680 -1675 1718 C
ATOM 490 CB MET A 214 128.275 -48.012 -21.537 1.00113.49 C
ANISOU 490 CB MET A 214 13386 17726 12008 -2403 -2121 2191 C
ATOM 491 CG MET A 214 127.606 -49.373 -21.387 1.00126.03 C
ANISOU 491 CG MET A 214 14750 19473 13662 -2973 -2119 2023 C
ATOM 492 SD MET A 214 128.517 -50.735 -22.140 1.00157.08 S
ANISOU 492 SD MET A 214 19295 23060 17327 -4014 -1779 961 S
ATOM 493 CE MET A 214 128.777 -51.803 -20.729 1.00105.49 C
ANISOU 493 CE MET A 214 12781 15799 11503 -3486 -1264 575 C
ATOM 494 C MET A 214 129.796 -46.296 -20.533 1.00 96.96 C
ANISOU 494 C MET A 214 11883 14720 10237 -1067 -1664 2050 C
ATOM 495 O MET A 214 130.165 -45.716 -21.552 1.00 91.46 O
ANISOU 495 O MET A 214 11382 14228 9139 -1387 -1820 2027 O
ATOM 496 N ALA A 215 129.681 -45.679 -19.360 1.00111.58 N
ANISOU 496 N ALA A 215 13723 16223 12448 -244 -1420 2344 N
ATOM 497 CA ALA A 215 130.025 -44.262 -19.200 1.00107.97 C
ANISOU 497 CA ALA A 215 13536 15552 11935 326 -1256 2620 C
ATOM 498 CB ALA A 215 129.447 -43.715 -17.907 1.00106.55 C
ANISOU 498 CB ALA A 215 13305 15026 12155 1078 -897 3020 C
ATOM 499 C ALA A 215 131.537 -44.066 -19.224 1.00 92.13 C
ANISOU 499 C ALA A 215 12125 13085 9795 259 -1078 1935 C
ATOM 500 O ALA A 215 132.047 -43.073 -19.736 1.00 79.93 O
ANISOU 500 O ALA A 215 10876 11503 7990 328 -1053 1961 O
ATOM 501 N ASP A 216 132.239 -45.022 -18.631 1.00 79.82 N
ANISOU 501 N ASP A 216 10690 11176 8460 143 -935 1394 N
ATOM 502 CA ASP A 216 133.684 -45.089 -18.678 1.00 66.06 C
ANISOU 502 CA ASP A 216 9346 9056 6699 6 -783 812 C
ATOM 503 CB ASP A 216 134.294 -44.525 -17.389 1.00 65.42 C
ANISOU 503 CB ASP A 216 9539 8543 6774 510 -560 837 C
ATOM 504 CG ASP A 216 135.828 -44.647 -17.340 1.00 70.81 C
ANISOU 504 CG ASP A 216 10500 8909 7496 342 -456 359 C
ATOM 505 OD1 ASP A 216 136.381 -45.682 -17.750 1.00 74.00 O
ANISOU 505 OD1 ASP A 216 10776 9234 8107 -2 -412 -7 O
ATOM 506 OD2 ASP A 216 136.479 -43.690 -16.862 1.00 61.37 O
ANISOU 506 OD2 ASP A 216 9651 7523 6143 540 -362 388 O
ATOM 507 C ASP A 216 133.961 -46.570 -18.809 1.00 67.30 C
ANISOU 507 C ASP A 216 9372 9111 7088 -437 -713 365 C
ATOM 508 O ASP A 216 133.339 -47.379 -18.123 1.00 67.08 O
ANISOU 508 O ASP A 216 9086 9061 7340 -358 -680 466 O
ATOM 509 N PRO A 217 134.882 -46.941 -19.706 1.00 66.02 N
ANISOU 509 N PRO A 217 9420 8830 6834 -911 -599 -130 N
ATOM 510 CA PRO A 217 135.176 -48.368 -19.827 1.00 64.08 C
ANISOU 510 CA PRO A 217 9116 8350 6883 -1313 -340 -551 C
ATOM 511 CB PRO A 217 135.888 -48.464 -21.173 1.00 48.60 C
ANISOU 511 CB PRO A 217 7463 6347 4654 -1938 -174 -1014 C
ATOM 512 CG PRO A 217 136.568 -47.138 -21.307 1.00 59.06 C
ANISOU 512 CG PRO A 217 9013 7671 5756 -1645 -285 -928 C
ATOM 513 CD PRO A 217 135.602 -46.143 -20.714 1.00 60.33 C
ANISOU 513 CD PRO A 217 9020 8151 5751 -1145 -614 -321 C
ATOM 514 C PRO A 217 136.084 -48.884 -18.709 1.00 63.77 C
ANISOU 514 C PRO A 217 9035 7806 7389 -926 -71 -659 C
ATOM 515 O PRO A 217 136.365 -50.077 -18.673 1.00 75.95 O
ANISOU 515 O PRO A 217 10495 9060 9303 -1134 241 -919 O
ATOM 516 N ASN A 218 136.551 -48.011 -17.824 1.00 58.53 N
ANISOU 516 N ASN A 218 8446 7036 6757 -433 -161 -426 N
ATOM 517 CA ASN A 218 137.290 -48.472 -16.651 1.00 57.92 C
ANISOU 517 CA ASN A 218 8269 6617 7121 -144 -31 -365 C
ATOM 518 CB ASN A 218 138.402 -47.496 -16.269 1.00 51.91 C
ANISOU 518 CB ASN A 218 7721 5747 6256 27 -80 -310 C
ATOM 519 CG ASN A 218 139.519 -47.476 -17.274 1.00 56.93 C
ANISOU 519 CG ASN A 218 8447 6253 6932 -265 99 -655 C
ATOM 520 OD1 ASN A 218 139.944 -48.518 -17.760 1.00 57.84 O
ANISOU 520 OD1 ASN A 218 8408 6135 7433 -494 408 -906 O
ATOM 521 ND2 ASN A 218 139.988 -46.277 -17.618 1.00 60.95 N
ANISOU 521 ND2 ASN A 218 9250 6855 7054 -270 -2 -680 N
ATOM 522 C ASN A 218 136.364 -48.698 -15.467 1.00 51.59 C
ANISOU 522 C ASN A 218 7309 5852 6439 178 -128 -14 C
ATOM 523 O ASN A 218 136.807 -48.853 -14.335 1.00 51.21 O
ANISOU 523 O ASN A 218 7233 5606 6620 413 -112 158 O
ATOM 524 N ILE A 219 135.071 -48.695 -15.748 1.00 53.47 N
ANISOU 524 N ILE A 219 7431 6381 6503 140 -239 141 N
ATOM 525 CA ILE A 219 134.069 -48.994 -14.747 1.00 47.84 C
ANISOU 525 CA ILE A 219 6537 5699 5942 412 -262 461 C
ATOM 526 CB ILE A 219 133.148 -47.801 -14.501 1.00 56.94 C
ANISOU 526 CB ILE A 219 7753 7063 6819 744 -356 889 C
ATOM 527 CG1 ILE A 219 133.968 -46.593 -14.070 1.00 53.02 C
ANISOU 527 CG1 ILE A 219 7676 6368 6099 981 -293 933 C
ATOM 528 CD1 ILE A 219 133.121 -45.397 -13.681 1.00 52.89 C
ANISOU 528 CD1 ILE A 219 7831 6379 5887 1363 -169 1365 C
ATOM 529 CG2 ILE A 219 132.127 -48.122 -13.426 1.00 52.12 C
ANISOU 529 CG2 ILE A 219 6967 6415 6419 1033 -276 1218 C
ATOM 530 C ILE A 219 133.268 -50.179 -15.245 1.00 54.28 C
ANISOU 530 C ILE A 219 7070 6656 6898 54 -221 343 C
ATOM 531 O ILE A 219 132.538 -50.070 -16.227 1.00 49.64 O
ANISOU 531 O ILE A 219 6385 6448 6026 -281 -366 373 O

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ATOM   532 N  ARG A 220    133.437 -51.318 -14.578 1.00 52.26           N
ANISOU 532 N  ARG A 220     6696  6109  7052    60    -22    241       N
ATOM   533 CA ARG A 220    132.825 -52.567 -15.009 1.00 50.66           C
ANISOU 533 CA ARG A 220     6322  5932  6995  -359    137     44       C
ATOM   534 CB ARG A 220    133.894 -53.609 -15.309 1.00 63.82           C
ANISOU 534 CB ARG A 220     8077  7136  9034  -606    557   -360       C
ATOM   535 CG ARG A 220    134.474 -53.532 -16.697 1.00 76.30           C
ANISOU 535 CG ARG A 220     9888  8715 10386 -1116    717   -766       C
ATOM   536 CD ARG A 220    135.968 -53.766 -16.654 1.00 76.49           C
ANISOU 536 CD ARG A 220     9990  8230 10842  -977   1090   -943       C
ATOM   537 NE ARG A 220    136.386 -54.937 -17.413 1.00 83.48           N
ANISOU 537 NE ARG A 220    11006  8688 12026 -1449   1725 -1376       N
ATOM   538 CZ ARG A 220    136.970 -56.008 -16.885 1.00 85.77           C
ANISOU 538 CZ ARG A 220    11164  8425 13000 -1276   2248 -1366       C
ATOM   539 NH1 ARG A 220    137.314 -57.031 -17.662 1.00 95.16           N
ANISOU 539 NH1 ARG A 220    12547  9173 14437 -1706   2971 -1764       N
ATOM   540 NH2 ARG A 220    137.210 -56.063 -15.583 1.00 69.97           N
ANISOU 540 NH2 ARG A 220     8857  6328 11400  -687   2084   -911       N
ATOM   541 C  ARG A 220    131.885 -53.121 -13.957 1.00 50.13           C
ANISOU 541 C  ARG A 220     6036  5858  7155  -128    144    315       C
ATOM   542 O  ARG A 220    132.194 -53.117 -12.765 1.00 46.16           O
ANISOU 542 O  ARG A 220     5553  5089  6895   293    190    507       O
ATOM   543 N  PHE A 221    130.743 -53.615 -14.410 1.00 45.38           N
ANISOU 543 N  PHE A 221     5231  5579  6433  -487     88    349       N
ATOM   544 CA PHE A 221    129.805 -54.256 -13.516 1.00 51.00           C
ANISOU 544 CA PHE A 221     5715  6286  7377  -344    140    569       C
ATOM   545 CB PHE A 221    128.479 -54.512 -14.229 1.00 65.56           C
ANISOU 545 CB PHE A 221     7268  8671  8971  -832    -37    706       C
ATOM   546 CG PHE A 221    127.575 -55.445 -13.488 1.00 59.67           C
ANISOU 546 CG PHE A 221     6292  7898  8483  -853     92    818       C
ATOM   547 CD1 PHE A 221    126.753 -54.972 -12.478 1.00 60.92           C
ANISOU 547 CD1 PHE A 221     6222  8136  8790  -322     17   1304       C
ATOM   548 CE1 PHE A 221    125.919 -55.829 -11.786 1.00 58.77           C
ANISOU 548 CE1 PHE A 221     5744  7826  8759  -349    159   1402       C
ATOM   549 CZ  PHE A 221    125.908 -57.180 -12.102 1.00 58.77           C
ANISOU 549 CZ  PHE A 221     5788  7703  8841  -922    378   1003       C
ATOM   550 CE2 PHE A 221    126.734 -57.665 -13.109 1.00 65.13           C
ANISOU 550 CE2 PHE A 221     6873  8370  9503 -1465    529    504       C
ATOM   551 CD2 PHE A 221    127.558 -56.797 -13.793 1.00 58.19           C
ANISOU 551 CD2 PHE A 221     6176  7535  8398 -1422    385    417       C
ATOM   552 C  PHE A 221    130.392 -55.567 -13.005 1.00 56.52           C
ANISOU 552 C  PHE A 221     6480  6473  8520  -401    525    293       C
ATOM   553 O  PHE A 221    130.897 -56.378 -13.775 1.00 52.12           O
ANISOU 553 O  PHE A 221     6048  5706  8047  -856    828   -112       O
ATOM   554 N  LEU A 222    130.321 -55.763 -11.697 1.00 62.61           N
ANISOU 554 N  LEU A 222     7201  7004  9585    50    579    544       N
ATOM   555 CA LEU A 222    130.802 -56.987 -11.089 1.00 64.09           C
ANISOU 555 CA LEU A 222     7389  6716 10246    75    932    436       C
ATOM   556 CB LEU A 222    131.618 -56.685 -9.836 1.00 64.99           C
ANISOU 556 CB LEU A 222     7566  6552 10577   585    870    747       C
ATOM   557 CG LEU A 222    133.117 -56.490 -10.030 1.00 69.45           C
ANISOU 557 CG LEU A 222     8202  6882 11304   656    920    706       C
ATOM   558 CD2 LEU A 222    133.673 -57.553 -10.968 1.00 42.04           C
ANISOU 558 CD2 LEU A 222     4693  3085  8195   330   1391    348       C
ATOM   559 CD1 LEU A 222    133.810 -56.551 -8.682 1.00 64.59           C
ANISOU 559 CD1 LEU A 222     7558  6052 10930   997    839   1120       C
ATOM   560 C  LEU A 222    129.642 -57.889 -10.719 1.00 72.27           C
ANISOU 560 C  LEU A 222     8266  7798 11397   -84   1061   474       C
ATOM   561 O  LEU A 222    129.511 -59.002 -11.226 1.00 72.79           O
ANISOU 561 O  LEU A 222     8350  7698 11609  -531   1403   166       O
ATOM   562 N  ASP A 223    128.795 -57.393 -9.830 1.00 68.75           N
ANISOU 562 N  ASP A 223     7710  7534 10878   250    863   841       N
ATOM   563 CA ASP A 223    127.782 -58.227 -9.222 1.00 62.67           C
ANISOU 563 CA ASP A 223     6779  6747 10284   196   1007   937       C
ATOM   564 CB ASP A 223    128.443 -59.128 -8.175 1.00 69.82           C
ANISOU 564 CB ASP A 223     7794  7108 11625   434   1289   966       C
ATOM   565 CG ASP A 223    127.536 -60.248 -7.702 1.00 79.32           C
ANISOU 565 CG ASP A 223     8887  8197 13052   282   1546   956       C
ATOM   566 OD1 ASP A 223    126.316 -60.185 -7.956 1.00 87.51           O
ANISOU 566 OD1 ASP A 223     9744  9603 13901   -81   1503   894       O
ATOM   567 OD2 ASP A 223    128.058 -61.195 -7.079 1.00 81.50           O
ANISOU 567 OD2 ASP A 223     9232  8043 13690   496   1775  1063       O
ATOM   568 C  ASP A 223    126.687 -57.377 -8.585 1.00 60.35           C
ANISOU 568 C  ASP A 223     6333  6754  9844   515   814  1362       C
ATOM   569 O  ASP A 223    126.847 -56.172 -8.404 1.00 49.51           O
ANISOU 569 O  ASP A 223     5064  5468  8281   851   655  1589       O
ATOM   570 N  LYS A 224    125.570 -58.014 -8.261 1.00 54.11           N
ANISOU 570 N  LYS A 224     5312  6076  9172   394   915  1474       N
ATOM   571 CA LYS A 224    124.482 -57.340 -7.579 1.00 67.24           C
ANISOU 571 CA LYS A 224     6786  7933 10830   732   879  1925       C
ATOM   572 CB LYS A 224    123.136 -57.840 -8.100 1.00 79.72           C
ANISOU 572 CB LYS A 224     7895  9982 12412   328   833  2063       C
ATOM   573 CG LYS A 224    122.806 -57.387 -9.501 1.00 89.53           C
ANISOU 573 CG LYS A 224     8845 11840 13333  -117   507  2136       C
ATOM   574 CD LYS A 224    122.770 -55.881 -9.551 1.00 91.80           C
ANISOU 574 CD LYS A 224     9068 12298 13512   380   350  2572       C
ATOM   575 CE LYS A 224    121.471 -55.372 -10.129 1.00 94.90           C
ANISOU 575 CE LYS A 224     8831 13364 13862   269   131  3181       C
ATOM   576 NZ LYS A 224    121.041 -54.144 -9.407 1.00 96.27           N
ANISOU 576 NZ LYS A 224     8924 13410 14244  1037   329  3763       N
ATOM   577 C  LYS A 224    124.581 -57.612 -6.087 1.00 61.88           C
ANISOU 577 C  LYS A 224     6350  6786 10376  1114  1117  2043       C
ATOM   578 O  LYS A 224    125.084 -58.649 -5.677 1.00 79.58           O
ANISOU 578 O  LYS A 224     8721  8686 12830  1012  1274  1843       O
ATOM   579 N  LEU A 225    124.096 -56.673 -5.283 1.00 68.38           N
ANISOU 579 N  LEU A 225     7268  7563 11151  1526  1203  2402       N
ATOM   580 CA LEU A 225    123.941 -56.898 -3.853 1.00 68.91           C
ANISOU 580 CA LEU A 225     7622  7278 11283  1717  1448  2491       C
ATOM   581 CB LEU A 225    123.782 -55.567 -3.120 1.00 68.40           C
ANISOU 581 CB LEU A 225     7909  7268 10811  1852  1549  2539       C
ATOM   582 CG LEU A 225    125.045 -54.815 -2.728 1.00 58.28           C
ANISOU 582 CG LEU A 225     7121  5890  9132  1795  1397  2308       C
ATOM   583 CD1 LEU A 225    124.669 -53.663 -1.823 1.00 54.77           C
ANISOU 583 CD1 LEU A 225     7025  5370  8416  1902  1670  2372       C
ATOM   584 CD2 LEU A 225    126.007 -55.751 -2.021 1.00 61.54           C
ANISOU 584 CD2 LEU A 225     7722  6109  9552  1632  1261  2151       C
ATOM   585 C  LEU A 225    122.714 -57.776 -3.604 1.00 76.72           C
ANISOU 585 C  LEU A 225     8255  8306 12590  1655  1653  2635       C
ATOM   586 O  LEU A 225    121.908 -57.986 -4.513 1.00 83.49           O
ANISOU 586 O  LEU A 225     8638  9600 13483  1389  1550  2676       O
ATOM   587 N  PRO A 226    122.566 -58.299 -2.374 1.00 78.29           N
ANISOU 587 N  PRO A 226     8707  8191 12847  1708  1882  2634       N
ATOM   588 CA PRO A 226    121.321 -59.007 -2.060 1.00 81.39           C
ANISOU 588 CA PRO A 226     8775  9060 13085  1469  1776  2860       C
ATOM   589 CB PRO A 226    121.573 -59.574 -0.659 1.00 75.37           C
ANISOU 589 CB PRO A 226     8452  7482 12703  1672  2316  2686       C
ATOM   590 CG PRO A 226    122.683 -58.741 -0.099 1.00 79.28           C
ANISOU 590 CG PRO A 226     9438  7991 12693  1671  2115  2509       C
ATOM   591 CD PRO A 226    123.544 -58.411 -1.279 1.00 80.52           C
ANISOU 591 CD PRO A 226     9497  8278 12818  1631  1832  2408       C
ATOM   592 C  PRO A 226    120.129 -58.057 -2.034 1.00 83.17           C
ANISOU 592 C  PRO A 226     8712  9065 13825  1929  2300  3224       C
ATOM   593 O  PRO A 226    120.241 -56.911 -1.600 1.00 84.84           O
ANISOU 593 O  PRO A 226     9271  9276 13688  2047  2394  3232       O
ATOM   594 N  GLN A 227    118.988 -58.552 -2.492 1.00 81.13           N
ANISOU 594 N  GLN A 227     7853  9178 13794  1740  2316  3406       N
ATOM   595 CA GLN A 227    117.816 -57.716 -2.663 1.00 87.79           C
ANISOU 595 CA GLN A 227     8191 10348 14817  1983  2456  3967       C
ATOM   596 CB GLN A 227    116.797 -58.424 -3.534 1.00 87.19           C
ANISOU 596 CB GLN A 227     7349 10919 14861  1497  2230  4131       C
ATOM   597 CG GLN A 227    117.308 -58.689 -4.919 1.00 87.65           C
ANISOU 597 CG GLN A 227     7247 11452 14602   929  1726  3858       C
ATOM   598 CD GLN A 227    116.409 -59.620 -5.679 1.00 95.42           C
ANISOU 598 CD GLN A 227     7657 13039 15559   197  1516  3898       C
ATOM   599 OE1 GLN A 227    115.568 -60.302 -5.092 1.00 88.00           O
ANISOU 599 OE1 GLN A 227     6499 12083 14854    98  1744  4006       O
ATOM   600 NE2 GLN A 227    116.570 -59.654 -6.997 1.00 98.48           N
ANISOU 600 NE2 GLN A 227     7835 13979 15603  -410  1088  3808       N
ATOM   601 C  GLN A 227    117.172 -57.293 -1.356 1.00 90.29           C
ANISOU 601 C  GLN A 227     8902 10264 15140  2216  2954  4135       C
ATOM   602 O  GLN A 227    117.273 -57.975 -0.335 1.00 77.69           O
ANISOU 602 O  GLN A 227     7658  8284 13578  2191  3201  3924       O
ATOM   603 N  GLN A 228    116.505 -56.150 -1.414 1.00 77.76           N
ANISOU 603 N  GLN A 228     9247  7639 11657    16  3681  2587       N
ATOM   604 CA GLN A 228    115.783 -55.635 -0.276 1.00 77.20           C
ANISOU 604 CA GLN A 228     9022 11081   427  3334  2626       C
ATOM   605 CB GLN A 228    116.422 -54.346  0.218 1.00 81.32           C
ANISOU 605 CB GLN A 228     9794  9022 11081   427  3334  2626       C
ATOM   606 CG GLN A 228    115.781 -53.786  1.468 1.00 88.52           C
ANISOU 606 CG GLN A 228     9794  9022 11081   427  3334  2626       C
ATOM   607 CD GLN A 228    116.645 -52.741  2.132 1.00 92.39           C
ANISOU 607 CD GLN A 228     9794  9022 11081   427  3334  2626       C
ATOM   608 OE1 GLN A 228    117.699 -52.374  1.615 1.00 95.36           O
ANISOU 608 OE1 GLN A 228     9794  9022 11081   427  3334  2626       O
ATOM   609 NE2 GLN A 228    116.207 -52.258  3.288 1.00 90.21           N
ANISOU 609 NE2 GLN A 228     9794  9022 11081   427  3334  2626       N
ATOM   610 C  GLN A 228    114.357 -55.380 -0.712 1.00 77.10           C
ANISOU 610 C  GLN A 228     9794  9022 11081   427  3334  2626       C
ATOM   611 O  GLN A 228    114.115 -54.766 -1.752 1.00 78.09           O
ANISOU 611 O  GLN A 228     9794  9022 11081   427  3334  2626       O
ATOM   612 N  THR A 229    113.413 -55.867  0.082 1.00 72.46           N
ANISOU 612 N  THR A 229     9081  7055 11395   366  3933  2803       N
ATOM   613 CA THR A 229    112.008 -55.659 -0.211 1.00 86.25           C
ANISOU 613 CA THR A 229     9794  9022 11081   427  3334  2626       C
ATOM   614 CB THR A 229    111.200 -56.928  0.020 1.00 98.72           C
ANISOU 614 CB THR A 229     9794  9022 11081   427  3334  2626       C
ATOM   615 OG1 THR A 229    112.053 -58.067 -0.143 1.00102.25           O
ANISOU 615 OG1 THR A 229     9794  9022 11081   427  3334  2626       O
ATOM   616 CG2 THR A 229    110.051 -57.005 -0.971 1.00 97.67           C
ANISOU 616 CG2 THR A 229     9794  9022 11081   427  3334  2626       C
ATOM   617 C  THR A 229    111.494 -54.551  0.686 1.00 85.87           C
ANISOU 617 C  THR A 229     9794  9022 11081   427  3334  2626       C
ATOM   618 O  THR A 229    111.907 -54.431  1.839 1.00 79.18           O
ANISOU 618 O  THR A 229     9794  9022 11081   427  3334  2626       O
ATOM   619 N  ILE A 230    110.597 -53.732  0.156 1.00 94.96           N
ANISOU 619 N  ILE A 230     9794  9022 11081   427  3334  2626       N
ATOM   620 CA ILE A 230    110.200 -52.537  0.879 1.00105.12           C
ANISOU 620 CA ILE A 230     9794  9022 11081   427  3334  2626       C
ATOM   621 C  ILE A 230    108.769 -52.585  1.373 1.00107.19           C
ANISOU 621 C  ILE A 230     9794  9022 11081   427  3334  2626       C
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ATOM 622 O ILE A 230 107.856 -53.005 0.660 1.00107.09 O
ANISOU 622 O ILE A 230 13315 11579 15797 430 3165 1872 O
ATOM 623 CB ILE A 230 110.426 -51.286 0.051 1.00107.83 C
ANISOU 623 CB ILE A 230 14193 12202 14576 289 2422 1455 C
ATOM 624 CG1 ILE A 230 111.719 -51.434 -0.722 1.00107.90 C
ANISOU 624 CG1 ILE A 230 14414 12089 14496 101 2332 1344 C
ATOM 625 CG2 ILE A 230 110.525 -50.077 0.959 1.00112.84 C
ANISOU 625 CG2 ILE A 230 14946 13370 14559 518 2181 1429 C
ATOM 626 CD1 ILE A 230 112.956 -51.437 0.152 1.00110.78 C
ANISOU 626 CD1 ILE A 230 14767 12860 14464 318 2447 1666 C
ATOM 627 N ASP A 231 108.598 -52.124 2.606 1.00110.83 N
ANISOU 627 N ASP A 231 13839 12998 15272 1012 3209 2410 N
ATOM 628 CA ASP A 231 107.360 -52.282 3.346 1.00116.69 C
ANISOU 628 CA ASP A 231 14294 13784 16261 1241 3468 2665 C
ATOM 629 CB ASP A 231 107.620 -53.164 4.571 1.00133.15 C
ANISOU 629 CB ASP A 231 16048 16128 18415 1698 4061 3410 C
ATOM 630 CG ASP A 231 108.717 -52.605 5.486 1.00138.60 C
ANISOU 630 CG ASP A 231 16865 17521 18274 2067 3947 3591 C
ATOM 631 OD1 ASP A 231 109.623 -53.378 5.859 1.00135.24 O
ANISOU 631 OD1 ASP A 231 16323 17215 17847 2271 4284 4010 O
ATOM 632 OD2 ASP A 231 108.680 -51.407 5.849 1.00141.48 O
ANISOU 632 OD2 ASP A 231 17416 18330 18010 2176 3528 3296 O
ATOM 633 C ASP A 231 106.821 -50.946 3.821 1.00103.91 C
ANISOU 633 C ASP A 231 12842 12591 14047 1381 3078 2422 C
ATOM 634 O ASP A 231 106.187 -50.861 4.868 1.00113.64 O
ANISOU 634 O ASP A 231 13874 14146 15158 1743 3278 2747 O
ATOM 635 N ARG A 232 107.104 -49.894 3.075 1.00 90.06 N
ANISOU 635 N ARG A 232 11449 10847 11923 1130 2550 1877 N
ATOM 636 CA ARG A 232 106.747 -48.565 3.524 1.00 84.45 C
ANISOU 636 CA ARG A 232 10908 10529 10652 1261 2180 1625 C
ATOM 637 CB ARG A 232 107.794 -47.560 3.052 1.00 86.13 C
ANISOU 637 CB ARG A 232 11477 10867 10382 1103 1748 1225 C
ATOM 638 CG ARG A 232 108.805 -47.142 4.063 1.00 88.53 C
ANISOU 638 CG ARG A 232 11769 11727 10140 1407 1711 1353 C
ATOM 639 CD ARG A 232 108.377 -45.821 4.631 1.00 99.52 C
ANISOU 639 CD ARG A 232 13251 13494 11069 1569 1373 1061 C
ATOM 640 NE ARG A 232 109.487 -45.080 5.203 1.00106.19 N
ANISOU 640 NE ARG A 232 14153 14783 11413 1732 1156 887 N
ATOM 641 CZ ARG A 232 109.384 -44.328 6.291 1.00110.50 C
ANISOU 641 CZ ARG A 232 14594 15886 11504 2097 1016 807 C
ATOM 642 NH1 ARG A 232 108.219 -44.232 6.915 1.00106.89 N
ANISOU 642 NH1 ARG A 232 14002 15609 11004 2342 1094 948 N
ATOM 643 NH2 ARG A 232 110.443 -43.677 6.755 1.00111.84 N
ANISOU 643 NH2 ARG A 232 14767 16444 11285 2232 797 554 N
ATOM 644 C ARG A 232 105.388 -48.196 2.966 1.00 82.28 C
ANISOU 644 C ARG A 232 10644 9980 10638 1094 2011 1314 C
ATOM 645 O ARG A 232 104.746 -48.994 2.282 1.00 92.01 O
ANISOU 645 O ARG A 232 11719 10754 12487 896 2177 1272 O
ATOM 646 N ALA A 233 104.954 -46.979 3.266 1.00 73.11 N
ANISOU 646 N ALA A 233 9645 9110 9025 1187 1676 1060 N
ATOM 647 CA ALA A 233 103.758 -46.433 2.651 1.00 69.97 C
ANISOU 647 CA ALA A 233 9318 8497 8769 1032 1441 703 C
ATOM 648 CB ALA A 233 103.304 -45.206 3.392 1.00 60.26 C
ANISOU 648 CB ALA A 233 8188 7685 7023 1253 1186 578 C
ATOM 649 C ALA A 233 104.075 -46.087 1.205 1.00 74.76 C
ANISOU 649 C ALA A 233 10230 8754 9422 674 1117 230 C
ATOM 650 O ALA A 233 105.183 -45.653 0.889 1.00 69.64 O
ANISOU 650 O ALA A 233 9829 8161 8472 588 947 110 O
ATOM 651 N GLY A 234 103.092 -46.279 0.332 1.00 73.78 N
ANISOU 651 N GLY A 234 10063 8294 9678 503 1042 -43 N
ATOM 652 CA GLY A 234 103.243 -45.975 -1.077 1.00 66.19 C
ANISOU 652 CA GLY A 234 9364 7058 8727 255 744 -490 C
ATOM 653 C GLY A 234 104.168 -46.939 -1.791 1.00 74.82 C
ANISOU 653 C GLY A 234 10444 7875 10108 81 889 -458 C
ATOM 654 O GLY A 234 104.506 -46.738 -2.956 1.00 87.48 O
ANISOU 654 O GLY A 234 12278 9299 11662 -76 668 -786 O
ATOM 655 N ILE A 235 104.566 -48.005 -1.107 1.00 74.45 N
ANISOU 655 N ILE A 235 10121 7802 10363 146 1286 -41 N
ATOM 656 CA ILE A 235 105.611 -48.862 -1.639 1.00 77.16 C
ANISOU 656 CA ILE A 235 10470 7928 10919 7 1439 38 C
ATOM 657 CB ILE A 235 106.970 -48.134 -1.548 1.00 74.77 C
ANISOU 657 CB ILE A 235 10490 7877 10042 20 1269 72 C
ATOM 658 CG1 ILE A 235 108.119 -48.954 -2.107 1.00 86.24 C
ANISOU 658 CG1 ILE A 235 11973 9129 11664 -117 1413 159 C
ATOM 659 CD1 ILE A 235 109.442 -48.277 -1.864 1.00 91.15 C
ANISOU 659 CD1 ILE A 235 12842 10011 11778 -86 1288 219 C
ATOM 660 CG2 ILE A 235 107.257 -47.726 -0.138 1.00 75.09 C
ANISOU 660 CG2 ILE A 235 10459 8372 9699 294 1365 404 C
ATOM 661 C ILE A 235 105.604 -50.247 -0.975 1.00 86.08 C
ANISOU 661 C ILE A 235 11190 8912 12603 89 1959 495 C
ATOM 662 O ILE A 235 106.509 -50.637 -0.235 1.00 96.17 O
ANISOU 662 O ILE A 235 12415 10372 13752 233 2215 915 O
ATOM 663 N LYS A 236 104.538 -50.983 -1.247 1.00 82.69 N
ANISOU 663 N LYS A 236 10441 8147 12830 20 2134 404 N
ATOM 664 CA LYS A 236 104.439 -52.363 -0.816 1.00 92.51 C
ANISOU 664 CA LYS A 236 11254 9111 14783 62 2679 797 C
ATOM 665 CB LYS A 236 102.984 -52.699 -0.520 1.00102.01 C
ANISOU 665 CB LYS A 236 12069 10118 16570 110 2883 798 C
ATOM 666 CG LYS A 236 102.037 -52.223 -1.606 1.00104.79 C
ANISOU 666 CG LYS A 236 12479 10290 17047 -92 2459 110 C
ATOM 667 CD LYS A 236 100.598 -52.449 -1.207 1.00111.37 C
ANISOU 667 CD LYS A 236 12914 10977 18423 -29 2646 107 C
ATOM 668 CE LYS A 236 100.180 -51.487 -0.105 1.00113.51 C
ANISOU 668 CE LYS A 236 13299 11714 18117 243 2601 410 C
ATOM 669 NZ LYS A 236 98.967 -51.970 0.613 1.00115.08 N
ANISOU 669 NZ LYS A 236 13036 11775 18915 378 2986 661 N
ATOM 670 C LYS A 236 104.972 -53.286 -1.910 1.00 89.98 C
ANISOU 670 C LYS A 236 10882 8355 14950 -191 2730 558 C
ATOM 671 O LYS A 236 104.772 -53.029 -3.100 1.00 77.11 O
ANISOU 671 O LYS A 236 9400 6556 13340 -389 2365 -16 O
ATOM 672 N ASP A 237 105.656 -54.351 -1.496 1.00 91.80 N
ANISOU 672 N ASP A 237 10898 8438 15545 -139 3190 1004 N
ATOM 673 CA ASP A 237 106.115 -55.404 -2.402 1.00 95.15 C
ANISOU 673 CA ASP A 237 11191 8408 16554 -355 3329 827 C
ATOM 674 CB ASP A 237 104.928 -56.186 -2.968 1.00104.62 C
ANISOU 674 CB ASP A 237 11959 9100 18692 -508 3462 469 C
ATOM 675 CG ASP A 237 104.312 -57.136 -1.955 1.00119.66 C
ANISOU 675 CG ASP A 237 13346 10767 21353 -357 4113 1010 C
ATOM 676 OD1 ASP A 237 104.162 -56.744 -0.779 1.00124.16 O
ANISOU 676 OD1 ASP A 237 13914 11692 21568 -75 4308 1537 O
ATOM 677 OD2 ASP A 237 103.981 -58.278 -2.343 1.00118.27 O
ANISOU 677 OD2 ASP A 237 12744 10043 22150 -495 4449 903 O
ATOM 678 C ASP A 237 106.980 -54.907 -3.556 1.00 91.77 C
ANISOU 678 C ASP A 237 11179 8020 15671 -539 2872 377 C
ATOM 679 O ASP A 237 106.742 -55.236 -4.714 1.00 94.08 O
ANISOU 679 O ASP A 237 11433 8004 16309 -728 2691 -141 O
ATOM 680 N ARG A 238 107.987 -54.114 -3.233 1.00 92.74 N
ANISOU 680 N ARG A 238 11668 8535 15033 -452 2697 560 N
ATOM 681 CA ARG A 238 108.866 -53.577 -4.252 1.00 81.27 C
ANISOU 681 CA ARG A 238 10608 7122 13149 -595 2323 217 C
ATOM 682 CB ARG A 238 108.889 -52.059 -4.158 1.00 73.09 C
ANISOU 682 CB ARG A 238 9947 6466 11358 -529 1911 62 C
ATOM 683 CG ARG A 238 109.509 -51.365 -5.343 1.00 73.97 C
ANISOU 683 CG ARG A 238 10447 6566 11093 -651 1535 -326 C
ATOM 684 CD ARG A 238 108.553 -50.322 -5.883 1.00 67.88 C
ANISOU 684 CD ARG A 238 9848 5867 10075 -634 1162 -739 C
ATOM 685 NE ARG A 238 109.168 -49.007 -5.968 1.00 65.06 N
ANISOU 685 NE ARG A 238 9885 5756 9080 -595 889 -788 N
ATOM 686 CZ ARG A 238 108.552 -47.920 -6.421 1.00 75.03 C
ANISOU 686 CZ ARG A 238 11363 7105 10038 -547 583 -1082 C
ATOM 687 NH1 ARG A 238 107.293 -47.990 -6.833 1.00 52.39 N
ANISOU 687 NH1 ARG A 238 8366 4155 7387 -521 470 -1377 N
ATOM 688 NH2 ARG A 238 109.202 -46.766 -6.463 1.00 49.24 N
ANISOU 688 NH2 ARG A 238 8419 3997 6293 -516 407 -1089 N
ATOM 689 C ARG A 238 110.249 -54.142 -3.998 1.00 75.31 C
ANISOU 689 C ARG A 238 9901 6405 12310 -576 2562 590 C
ATOM 690 O ARG A 238 110.682 -54.223 -2.852 1.00 72.82 O
ANISOU 690 O ARG A 238 9502 6357 11811 -376 2821 1088 O
ATOM 691 N VAL A 239 110.942 -54.549 -5.053 1.00 59.22 N
ANISOU 691 N VAL A 239 7982 4137 10383 -742 2478 349 N
ATOM 692 CA VAL A 239 112.260 -55.138 -4.865 1.00 58.90 C
ANISOU 692 CA VAL A 239 7976 4113 10292 -731 2711 694 C
ATOM 693 CB VAL A 239 112.363 -56.510 -5.508 1.00 61.22 C
ANISOU 693 CB VAL A 239 8009 3944 11307 -859 2990 637 C
ATOM 694 CG1 VAL A 239 113.670 -57.158 -5.114 1.00 61.20 C
ANISOU 694 CG1 VAL A 239 8009 3985 11259 -804 3295 1087 C
ATOM 695 CG2 VAL A 239 111.184 -57.376 -5.091 1.00 65.00 C
ANISOU 695 CG2 VAL A 239 8013 4113 12573 -833 3342 717 C
ATOM 696 C VAL A 239 113.365 -54.256 -5.413 1.00 55.71 C
ANISOU 696 C VAL A 239 7999 3917 9252 -788 2380 545 C
ATOM 697 O VAL A 239 113.400 -53.965 -6.606 1.00 59.88 O
ANISOU 697 O VAL A 239 8737 4304 9710 -915 2095 121 O
ATOM 698 N TYR A 240 114.267 -53.842 -4.528 1.00 84.46 N
ANISOU 698 N TYR A 240 11737 7909 12444 -658 2436 892 N
ATOM 699 CA TYR A 240 115.387 -52.978 -4.896 1.00 77.39 C
ANISOU 699 CA TYR A 240 11188 7198 11018 -709 2173 780 C
ATOM 700 CB TYR A 240 115.518 -51.822 -3.921 1.00 51.23 C
ANISOU 700 CB TYR A 240 7970 4322 7174 -555 2013 859 C
ATOM 701 CG TYR A 240 114.507 -50.734 -4.114 1.00 64.11 C
ANISOU 701 CG TYR A 240 9737 5998 8622 -565 1701 531 C
ATOM 702 CD1 TYR A 240 114.735 -49.704 -5.006 1.00 60.79 C
ANISOU 702 CD1 TYR A 240 9645 5529 7924 -674 1376 189 C
ATOM 703 CE1 TYR A 240 113.811 -48.700 -5.175 1.00 60.29 C
ANISOU 703 CE1 TYR A 240 9707 5508 7692 -653 1119 -79 C
ATOM 704 CZ TYR A 240 112.639 -48.720 -4.448 1.00 65.08 C
ANISOU 704 CZ TYR A 240 10111 6217 8399 -543 1155 -37 C
ATOM 705 OH TYR A 240 111.708 -47.725 -4.613 1.00 61.22 O
ANISOU 705 OH TYR A 240 9745 5777 7738 -513 900 -303 O
ATOM 706 CE2 TYR A 240 112.394 -49.734 -3.550 1.00 73.96 C
ANISOU 706 CE2 TYR A 240 10902 7390 9810 -436 1482 305 C
ATOM 707 CD2 TYR A 240 113.329 -50.733 -3.393 1.00 74.48 C
ANISOU 707 CD2 TYR A 240 10845 7402 10052 -438 1766 600 C
ATOM 708 C TYR A 240 116.706 -53.716 -4.877 1.00 75.28 C
ANISOU 708 C TYR A 240 10907 6914 10781 -719 2395 1050 C
ATOM 709 O TYR A 240 117.012 -54.437 -3.930 1.00 83.55 O
ANISOU 709 O TYR A 240 11717 8088 11942 -560 2734 1478 O
ATOM 710 N SER A 241 117.507 -53.509 -5.908 1.00 64.59 N
ANISOU 710 N SER A 241 9809 5433 9298 -865 2223 832 N
ATOM 711 CA SER A 241 118.841 -54.068 -5.899 1.00 78.88 C
ANISOU 711 CA SER A 241 11635 7260 11076 -876 2399 1072 C

ATOM 712 CB SER A 241 119.007 -55.117 -6.997 1.00 90.36 C
ANISOU 712 CB SER A 241 13061 8312 12959 -1015 2514 950 C
ATOM 713 OG SER A 241 119.087 -54.504 -8.266 1.00 96.85 O
ANISOU 713 OG SER A 241 14176 9015 13606 -1124 2203 547 O
ATOM 714 C SER A 241 119.844 -52.944 -6.086 1.00 70.46 C
ANISOU 714 C SER A 241 10863 6399 9510 -910 2145 959 C
ATOM 715 O SER A 241 119.499 -51.852 -6.520 1.00 73.41 O
ANISOU 715 O SER A 241 11451 6790 9651 -954 1856 669 O
ATOM 716 N ASN A 242 121.089 -53.225 -5.743 1.00 70.78 N
ANISOU 716 N ASN A 242 10885 6579 9430 -876 2283 1197 N
ATOM 717 CA ASN A 242 122.160 -52.283 -5.963 1.00 54.31 C
ANISOU 717 CA ASN A 242 9019 4624 6991 -930 2092 1082 C
ATOM 718 CB ASN A 242 122.653 -51.712 -4.643 1.00 62.00 C
ANISOU 718 CB ASN A 242 9857 6054 7644 -754 2074 1215 C
ATOM 719 CG ASN A 242 121.621 -50.840 -3.971 1.00 71.36 C
ANISOU 719 CG ASN A 242 11003 7444 8668 -649 1900 1075 C
ATOM 720 OD1 ASN A 242 120.672 -51.336 -3.355 1.00 73.27 O
ANISOU 720 OD1 ASN A 242 11052 7755 9033 -513 2036 1236 O
ATOM 721 ND2 ASN A 242 121.794 -49.526 -4.090 1.00 60.48 N
ANISOU 721 ND2 ASN A 242 9790 6136 7052 -704 1623 781 N
ATOM 722 C ASN A 242 123.284 -53.011 -6.655 1.00 66.02 C
ANISOU 722 C ASN A 242 10565 5934 8588 -1021 2233 1184 C
ATOM 723 O ASN A 242 123.385 -54.234 -6.571 1.00 74.94 O
ANISOU 723 O ASN A 242 11428 7066 9981 -947 2396 1349 O
ATOM 724 N SER A 243 124.136 -52.261 -7.333 1.00 43.84 N
ANISOU 724 N SER A 243 5896 4842 5919 675 745 1234 N
ATOM 725 CA SER A 243 125.180 -52.889 -8.107 1.00 47.87 C
ANISOU 725 CA SER A 243 6383 5303 6504 703 699 1144 C
ATOM 726 CB SER A 243 125.067 -52.500 -9.567 1.00 60.70 C
ANISOU 726 CB SER A 243 7964 6912 8185 564 626 916 C
ATOM 727 OG SER A 243 123.978 -53.173 -10.135 1.00 68.49 O
ANISOU 727 OG SER A 243 8935 7696 9394 471 688 871 O
ATOM 728 C SER A 243 126.553 -52.564 -7.592 1.00 46.65 C
ANISOU 728 C SER A 243 6230 5334 6162 835 614 1167 C
ATOM 729 O SER A 243 126.809 -51.474 -7.092 1.00 45.37 O
ANISOU 729 O SER A 243 6070 5362 5807 846 529 1145 O
ATOM 730 N ILE A 244 127.436 -53.535 -7.747 1.00 57.68 N
ANISOU 730 N ILE A 244 7616 6662 7638 937 630 1197 N
ATOM 731 CA ILE A 244 128.815 -53.388 -7.351 1.00 49.88 C
ANISOU 731 CA ILE A 244 6604 5842 6508 1071 546 1212 C
ATOM 732 CB ILE A 244 129.272 -54.603 -6.571 1.00 41.30 C
ANISOU 732 CB ILE A 244 5548 4674 5470 1262 625 1401 C
ATOM 733 CG1 ILE A 244 128.400 -54.778 -5.332 1.00 45.71 C
ANISOU 733 CG1 ILE A 244 6174 5211 5983 1339 728 1618 C
ATOM 734 CD1 ILE A 244 128.660 -56.085 -4.583 1.00 40.06 C
ANISOU 734 CD1 ILE A 244 5496 4374 5349 1533 847 1854 C
ATOM 735 CG2 ILE A 244 130.712 -54.450 -6.159 1.00 42.72 C
ANISOU 735 CG2 ILE A 244 5686 5047 5498 1413 521 1407 C
ATOM 736 C ILE A 244 129.637 -53.269 -8.611 1.00 47.66 C
ANISOU 736 C ILE A 244 6254 5587 6267 1016 477 1033 C
ATOM 737 O ILE A 244 129.478 -54.059 -9.535 1.00 45.99 O
ANISOU 737 O ILE A 244 6039 5215 6221 986 525 961 O
ATOM 738 N TYR A 245 130.510 -52.272 -8.649 1.00 45.91 N
ANISOU 738 N TYR A 245 5970 5569 5903 1009 364 960 N
ATOM 739 CA TYR A 245 131.357 -52.080 -9.809 1.00 42.18 C
ANISOU 739 CA TYR A 245 5416 5151 5458 971 320 824 C
ATOM 740 CB TYR A 245 131.110 -50.725 -10.458 1.00 46.75 C
ANISOU 740 CB TYR A 245 5955 5832 5976 815 259 707 C
ATOM 741 CG TYR A 245 129.739 -50.614 -11.047 1.00 47.21 C
ANISOU 741 CG TYR A 245 6070 5772 6095 689 312 650 C
ATOM 742 CD1 TYR A 245 128.654 -50.262 -10.249 1.00 41.72 C
ANISOU 742 CD1 TYR A 245 5438 5045 5369 644 329 712 C
ATOM 743 CE1 TYR A 245 127.388 -50.169 -10.775 1.00 55.30 C
ANISOU 743 CE1 TYR A 245 7190 6664 7158 532 373 660 C
ATOM 744 CZ TYR A 245 127.193 -50.440 -12.117 1.00 54.69 C
ANISOU 744 CZ TYR A 245 7089 6522 7170 472 383 529 C
ATOM 745 OH TYR A 245 125.930 -50.347 -12.646 1.00 57.29 O
ANISOU 745 OH TYR A 245 7436 6765 7568 370 404 460 O
ATOM 746 CE2 TYR A 245 128.256 -50.801 -12.932 1.00 59.41 C
ANISOU 746 CE2 TYR A 245 7639 7157 7776 531 367 460 C
ATOM 747 CD2 TYR A 245 129.520 -50.889 -12.391 1.00 47.48 C
ANISOU 747 CD2 TYR A 245 6089 5741 6209 635 341 529 C
ATOM 748 C TYR A 245 132.824 -52.223 -9.499 1.00 45.55 C
ANISOU 748 C TYR A 245 5764 5713 5832 1106 259 854 C
ATOM 749 O TYR A 245 133.273 -52.022 -8.374 1.00 41.16 O
ANISOU 749 O TYR A 245 5200 5268 5169 1205 198 939 O
ATOM 750 N GLU A 246 133.553 -52.561 -10.549 1.00 55.77 N
ANISOU 750 N GLU A 246 6991 7009 7191 1122 272 773 N
ATOM 751 CA GLU A 246 134.985 -52.700 -10.521 1.00 56.36 C
ANISOU 751 CA GLU A 246 6958 7214 7241 1242 225 784 C
ATOM 752 CB GLU A 246 135.347 -53.881 -11.404 1.00 62.62 C
ANISOU 752 CB GLU A 246 7752 7896 8147 1337 305 748 C
ATOM 753 CG GLU A 246 136.669 -54.532 -11.134 1.00 83.10 C
ANISOU 753 CG GLU A 246 10266 10565 10741 1523 289 804 C
ATOM 754 CD GLU A 246 136.916 -55.681 -12.094 1.00 95.97 C
ANISOU 754 CD GLU A 246 11911 12066 12488 1623 373 742 C
ATOM 755 OE1 GLU A 246 137.880 -56.444 -11.878 1.00 96.93 O
ANISOU 755 OE1 GLU A 246 11988 12208 12634 1802 380 796 O
ATOM 756 OE2 GLU A 246 136.135 -55.817 -13.062 1.00 96.30 O
ANISOU 756 OE2 GLU A 246 12007 11990 12593 1537 421 626 O
ATOM 757 C GLU A 246 135.520 -51.428 -11.149 1.00 48.85 C
ANISOU 757 C GLU A 246 5888 6427 6245 1125 158 694 C
ATOM 758 O GLU A 246 135.039 -51.015 -12.198 1.00 50.43 O
ANISOU 758 O GLU A 246 6090 6600 6470 1011 197 610 O
ATOM 759 N LEU A 247 136.498 -50.797 -10.510 1.00 51.24 N
ANISOU 759 N LEU A 247 6081 6895 6494 1159 55 715 N
ATOM 760 CA LEU A 247 137.141 -49.625 -11.096 1.00 38.62 C
ANISOU 760 CA LEU A 247 4337 5428 4908 1046 1 650 C
ATOM 761 CB LEU A 247 137.228 -48.488 -10.096 1.00 38.08 C
ANISOU 761 CB LEU A 247 4226 5457 4785 984 -138 636 C
ATOM 762 CG LEU A 247 135.914 -48.101 -9.444 1.00 42.78 C
ANISOU 762 CG LEU A 247 4972 5976 5308 920 -149 636 C
ATOM 763 CD1 LEU A 247 136.193 -47.165 -8.296 1.00 48.05 C
ANISOU 763 CD1 LEU A 247 5598 6757 5901 924 -307 605 C
ATOM 764 CD2 LEU A 247 135.003 -47.438 -10.466 1.00 47.25 C
ANISOU 764 CD2 LEU A 247 5578 6465 5911 750 -82 580 C
ATOM 765 C LEU A 247 138.536 -50.008 -11.545 1.00 48.91 C
ANISOU 765 C LEU A 247 5484 6838 6262 1150 6 659 C
ATOM 766 O LEU A 247 139.318 -50.554 -10.770 1.00 52.80 O
ANISOU 766 O LEU A 247 5928 7392 6740 1296 -49 709 O
ATOM 767 N LEU A 248 138.844 -49.714 -12.799 1.00 42.05 N
ANISOU 767 N LEU A 248 4531 6004 5441 1092 78 619 N
ATOM 768 CA LEU A 248 140.098 -50.146 -13.366 1.00 37.95 C
ANISOU 768 CA LEU A 248 3860 5589 4968 1205 117 635 C
ATOM 769 CB LEU A 248 139.897 -50.721 -14.763 1.00 48.54 C
ANISOU 769 CB LEU A 248 5240 6886 6315 1246 255 589 C
ATOM 770 CG LEU A 248 138.936 -51.887 -14.968 1.00 57.93 C
ANISOU 770 CG LEU A 248 6621 7890 7500 1317 317 540 C
ATOM 771 CD1 LEU A 248 139.121 -52.358 -16.391 1.00 58.89 C
ANISOU 771 CD1 LEU A 248 6728 8028 7619 1395 422 463 C
ATOM 772 CD2 LEU A 248 139.185 -53.027 -13.978 1.00 40.68 C
ANISOU 772 CD2 LEU A 248 4491 5621 5343 1474 293 599 C
ATOM 773 C LEU A 248 141.097 -49.016 -13.441 1.00 42.46 C
ANISOU 773 C LEU A 248 5212 6321 5600 1121 57 648 C
ATOM 774 O LEU A 248 140.742 -47.863 -13.664 1.00 48.42 O
ANISOU 774 O LEU A 248 6082 7082 6379 954 38 632 O
ATOM 775 N GLU A 249 142.358 -49.382 -13.278 1.00 47.07 N
ANISOU 775 N GLU A 249 6023 6682 7023 1242 32 682 N
ATOM 776 CA GLU A 249 143.466 -48.465 -13.426 1.00 52.66 C
ANISOU 776 CA GLU A 249 6507 7881 7045 1175 -13 702 C
ATOM 777 CB GLU A 249 143.935 -47.978 -12.061 1.00 59.35 C
ANISOU 777 CB GLU A 249 7212 8394 8369 1261 -212 681 C
ATOM 778 CG GLU A 249 144.424 -46.544 -12.043 1.00 76.50 C
ANISOU 778 CG GLU A 249 9232 10232 11029 1104 -270 655 C
ATOM 779 CD GLU A 249 144.712 -46.040 -10.638 1.00 94.55 C
ANISOU 779 CD GLU A 249 11371 12252 13727 1191 -534 581 C
ATOM 780 OE1 GLU A 249 145.351 -46.778 -9.855 1.00108.42 O
ANISOU 780 OE1 GLU A 249 13033 13871 15717 1382 -625 582 O
ATOM 781 OE2 GLU A 249 144.292 -44.907 -10.317 1.00 88.03 O
ANISOU 781 OE2 GLU A 249 10603 11745 12527 979 -534 581 C
ATOM 782 C GLU A 249 144.544 -49.285 -14.106 1.00 53.35 C
ANISOU 782 C GLU A 249 6507 7984 7203 1104 78 619 N
ATOM 783 O GLU A 249 144.938 -50.332 -13.601 1.00 52.21 O
ANISOU 783 O GLU A 249 6339 7928 6990 1523 61 756 O
ATOM 784 N ASN A 250 144.992 -48.824 -15.268 1.00 53.02 N
ANISOU 784 N ASN A 250 6855 7985 6729 1341 -84 780 N
ATOM 785 CA ASN A 250 145.932 -49.575 -16.087 1.00 56.11 C
ANISOU 785 CA ASN A 250 7126 8604 7589 1470 -331 819 C
ATOM 786 CB ASN A 250 147.318 -49.574 -15.453 1.00 64.54 C
ANISOU 786 CB ASN A 250 8243 9821 8766 1544 -243 864 C
ATOM 787 CG ASN A 250 147.893 -48.194 -15.355 1.00 68.44 C
ANISOU 787 CG ASN A 250 8702 10232 9377 1353 -181 902 C
ATOM 788 OD1 ASN A 250 148.170 -47.557 -16.372 1.00 71.32 O
ANISOU 788 OD1 ASN A 250 9276 10825 9304 1276 -318 974 O
ATOM 789 ND2 ASN A 250 148.061 -47.705 -14.128 1.00 59.14 N
ANISOU 789 ND2 ASN A 250 7411 9224 8303 1281 -25 855 N
ATOM 790 C ASN A 250 145.516 -51.014 -16.362 1.00 55.12 C
ANISOU 790 C ASN A 250 7200 8544 7199 1524 -259 780 C
ATOM 791 O ASN A 250 146.357 -51.902 -16.422 1.00 55.68 O
ANISOU 791 O ASN A 250 7191 8518 7441 1860 437 785 O
ATOM 792 N GLY A 251 144.216 -51.239 -16.510 1.00 60.10 N
ANISOU 792 N GLY A 251 7605 8552 7679 1614 -422 705 N
ATOM 793 CA GLY A 251 143.715 -52.544 -16.896 1.00 55.11 C
ANISOU 793 CA GLY A 251 7622 8392 6924 1622 -1096 784 C
ATOM 794 C GLY A 251 143.413 -53.484 -15.741 1.00 63.57 C
ANISOU 794 C GLY A 251 8307 8643 8203 1845 -1 643 C
ATOM 795 O GLY A 251 142.845 -54.553 -15.945 1.00 64.09 O
ANISOU 795 O GLY A 251 8307 8643 8399 1961 -589 589 O
ATOM 796 N GLN A 252 143.790 -53.097 -14.527 1.00 54.87 N
ANISOU 796 N GLN A 252 7656 8644 5545 1832 -1375 1234 N
ATOM 797 CA GLN A 252 143.572 -53.959 -13.375 1.00 44.68 C
ANISOU 797 CA GLN A 252 6486 6578 4910 1949 -1220 1234 C
ATOM 798 CB GLN A 252 144.889 -54.274 -12.673 1.00 50.42 C
ANISOU 798 CB GLN A 252 6928 7028 6198 1949 -1220 1234 C
ATOM 799 CG GLN A 252 146.029 -54.672 -13.602 1.00 49.88 C
ANISOU 799 CG GLN A 252 6928 7028 5993 1949 -1220 1234 C
ATOM 800 CD GLN A 252 145.885 -56.080 -14.176 1.00 59.65 C
ANISOU 800 CD GLN A 252 8193 8268 7202 1949 -1220 1234 C
ATOM 801 OE1 GLN A 252 145.065 -56.877 -13.714 1.00 59.49 O
ANISOU 801 OE1 GLN A 252 8193 8268 7142 1949 -1220 1234 O

ATOM 802 NE2 GLN A 252 146.693 -56.390 -15.189 1.00 68.03 N
ANISOU 802 NE2 GLN A 252 7125 9756 8969 2571 446 756 N
ATOM 803 C GLN A 252 142.609 -53.317 -12.392 1.00 49.03 C
ANISOU 803 C GLN A 252 5149 7065 6417 1809 127 765 C
ATOM 804 O GLN A 252 142.416 -52.103 -12.390 1.00 50.15 O
ANISOU 804 O GLN A 252 5230 7275 6550 1631 71 738 O
ATOM 805 N ARG A 253 142.009 -54.149 -11.556 1.00 60.02 N
ANISOU 805 N ARG A 253 6702 8320 7783 1901 121 819 N
ATOM 806 CA ARG A 253 141.120 -53.659 -10.522 1.00 65.27 C
ANISOU 806 CA ARG A 253 7476 8942 8380 1815 49 852 C
ATOM 807 CB ARG A 253 140.506 -54.822 -9.759 1.00 68.74 C
ANISOU 807 CB ARG A 253 8087 9215 8815 1955 97 951 C
ATOM 808 CG ARG A 253 139.560 -54.393 -8.663 1.00 74.55 C
ANISOU 808 CG ARG A 253 8938 9924 9462 1901 50 1011 C
ATOM 809 CD ARG A 253 138.892 -55.606 -8.071 1.00 78.34 C
ANISOU 809 CD ARG A 253 9579 10215 9973 2033 145 1143 C
ATOM 810 NE ARG A 253 138.380 -56.489 -9.114 1.00 78.20 N
ANISOU 810 NE ARG A 253 9633 9970 10108 2006 274 1096 N
ATOM 811 CZ ARG A 253 137.801 -57.662 -8.881 1.00 79.41 C
ANISOU 811 CZ ARG A 253 9909 9895 10369 2097 376 1191 C
ATOM 812 NH1 ARG A 253 137.662 -58.092 -7.635 1.00 65.59 N
ANISOU 812 NH1 ARG A 253 8225 8125 8570 2232 389 1375 N
ATOM 813 NH2 ARG A 253 137.363 -58.404 -9.896 1.00 73.08 N
ANISOU 813 NH2 ARG A 253 9157 8882 9728 2063 465 1100 N
ATOM 814 C ARG A 253 141.880 -52.757 -9.557 1.00 46.24 C
ANISOU 814 C ARG A 253 4925 6733 5911 1814 -113 864 C
ATOM 815 O ARG A 253 142.989 -53.072 -9.142 1.00 51.02 O
ANISOU 815 O ARG A 253 5403 7467 6516 1966 -177 899 O
ATOM 816 N ALA A 254 141.276 -51.632 -9.204 1.00 53.21 N
ANISOU 816 N ALA A 254 5826 7640 6751 1649 -189 818 N
ATOM 817 CA ALA A 254 141.905 -50.708 -8.279 1.00 61.18 C
ANISOU 817 CA ALA A 254 6707 8820 7718 1639 -368 786 C
ATOM 818 CB ALA A 254 142.315 -49.441 -8.997 1.00 49.86 C
ANISOU 818 CB ALA A 254 5099 7459 6385 1441 -409 699 C
ATOM 819 C ALA A 254 140.954 -50.387 -7.142 1.00 66.62 C
ANISOU 819 C ALA A 254 7549 9484 8279 1637 -441 797 C
ATOM 820 O ALA A 254 141.312 -49.697 -6.194 1.00 69.58 O
ANISOU 820 O ALA A 254 7858 9996 8584 1664 -609 751 O
ATOM 821 N GLY A 255 139.730 -50.881 -7.255 1.00 61.93 N
ANISOU 821 N GLY A 255 7151 8721 7660 1612 -316 848 N
ATOM 822 CA GLY A 255 138.712 -50.586 -6.273 1.00 52.05 C
ANISOU 822 CA GLY A 255 6044 7443 6289 1611 -347 878 C
ATOM 823 C GLY A 255 137.405 -51.265 -6.611 1.00 45.40 C
ANISOU 823 C GLY A 255 5381 6393 5478 1570 -180 945 C
ATOM 824 O GLY A 255 137.177 -51.692 -7.741 1.00 48.88 O
ANISOU 824 O GLY A 255 5831 6705 6035 1494 -69 918 O
ATOM 825 N THR A 256 136.545 -51.353 -5.611 1.00 51.64 N
ANISOU 825 N THR A 256 6301 7158 6163 1631 -168 1029 N
ATOM 826 CA THR A 256 135.270 -52.018 -5.751 1.00 61.33 C
ANISOU 826 CA THR A 256 7675 8183 7442 1596 -11 1114 C
ATOM 827 CB THR A 256 135.332 -53.424 -5.158 1.00 63.03 C
ANISOU 827 CB THR A 256 7965 8308 7677 1805 88 1295 C
ATOM 828 OG1 THR A 256 136.433 -54.136 -5.732 1.00 74.47 O
ANISOU 828 OG1 THR A 256 9328 9754 9214 1895 89 1282 O
ATOM 829 CG2 THR A 256 134.056 -54.173 -5.430 1.00 57.25 C
ANISOU 829 CG2 THR A 256 7352 7328 7073 1743 257 1377 C
ATOM 830 C THR A 256 134.277 -51.194 -4.963 1.00 61.39 C
ANISOU 830 C THR A 256 7765 8230 7328 1545 -39 1120 C
ATOM 831 O THR A 256 134.575 -50.783 -3.850 1.00 69.11 O
ANISOU 831 O THR A 256 8744 9370 8143 1669 -146 1141 O
ATOM 832 N CYS A 257 133.103 -50.935 -5.524 1.00 53.53 N
ANISOU 832 N CYS A 257 6836 7103 6401 1382 45 1088 N
ATOM 833 CA CYS A 257 132.154 -50.096 -4.807 1.00 49.19 C
ANISOU 833 CA CYS A 257 6357 6600 5734 1342 23 1088 C
ATOM 834 CB CYS A 257 132.606 -48.629 -4.828 1.00 46.30 C
ANISOU 834 CB CYS A 257 5910 6383 5297 1245 -145 922 C
ATOM 835 SG CYS A 257 132.342 -47.808 -6.413 1.00 61.31 S
ANISOU 835 SG CYS A 257 7749 8198 7347 985 -130 775 S
ATOM 836 C CYS A 257 130.722 -50.188 -5.315 1.00 49.36 C
ANISOU 836 C CYS A 257 6456 6449 5849 1204 154 1105 C
ATOM 837 O CYS A 257 130.464 -50.511 -6.479 1.00 41.68 O
ANISOU 837 O CYS A 257 5464 5339 5031 1082 217 1043 O
ATOM 838 N VAL A 258 129.798 -49.885 -4.409 1.00 36.44 N
ANISOU 838 N VAL A 258 4900 4840 4107 1242 185 1180 N
ATOM 839 CA VAL A 258 128.404 -49.750 -4.766 1.00 44.98 C
ANISOU 839 CA VAL A 258 6032 5793 5264 1110 289 1187 C
ATOM 840 CB VAL A 258 127.488 -49.987 -3.570 1.00 49.65 C
ANISOU 840 CB VAL A 258 6708 6398 5758 1231 388 1362 C
ATOM 841 CG2 VAL A 258 127.825 -51.324 -2.933 1.00 46.49 C
ANISOU 841 CG2 VAL A 258 6338 5941 5388 1417 494 1572 C
ATOM 842 CG1 VAL A 258 126.033 -49.959 -4.008 1.00 43.15 C
ANISOU 842 CG1 VAL A 258 5908 5429 5058 1086 507 1377 C
ATOM 843 C VAL A 258 128.223 -48.350 -5.319 1.00 48.92 C
ANISOU 843 C VAL A 258 6498 6361 5728 950 184 1008 C
ATOM 844 O VAL A 258 128.511 -47.352 -4.656 1.00 48.72 O
ANISOU 844 O VAL A 258 6469 6486 5557 985 64 945 O
ATOM 845 N LEU A 259 127.750 -48.290 -6.551 1.00 45.19 N
ANISOU 845 N LEU A 259 6001 5773 5396 785 225 922 N
ATOM 846 CA LEU A 259 127.833 -47.072 -7.316 1.00 45.45 C
ANISOU 846 CA LEU A 259 5987 5860 5422 644 137 771 C
ANISOU 846 CA LEU A 259 5987 5860 5422 644 137 771 C
ATOM 847 CB LEU A 259 129.008 -47.189 -8.280 1.00 51.44 C
ANISOU 847 CB LEU A 259 6653 6638 6253 616 94 698 C
ATOM 848 CG LEU A 259 129.582 -45.924 -8.894 1.00 62.42 C
ANISOU 848 CG LEU A 259 7963 8116 7639 509 -3 585 C
ATOM 849 CD1 LEU A 259 130.145 -45.051 -7.797 1.00 65.76 C
ANISOU 849 CD1 LEU A 259 8361 8664 7959 560 -137 559 C
ATOM 850 CD2 LEU A 259 130.663 -46.299 -9.890 1.00 58.33 C
ANISOU 850 CD2 LEU A 259 7347 7613 7202 506 6 556 C
ATOM 851 C LEU A 259 126.549 -46.860 -8.103 1.00 50.61 C
ANISOU 851 C LEU A 259 6653 6408 6155 508 208 730 C
ATOM 852 O LEU A 259 126.047 -47.780 -8.747 1.00 48.96 O
ANISOU 852 O LEU A 259 6462 6065 6076 476 299 745 O
ATOM 853 N GLU A 260 126.016 -45.646 -8.054 1.00 44.73 N
ANISOU 853 N GLU A 260 5934 5718 5344 433 155 663 N
ATOM 854 CA GLU A 260 124.886 -45.318 -8.905 1.00 43.78 C
ANISOU 854 CA GLU A 260 5822 5521 5290 311 203 611 C
ATOM 855 CB GLU A 260 123.586 -45.918 -8.360 1.00 44.32 C
ANISOU 855 CB GLU A 260 5940 5506 5392 331 312 705 C
ATOM 856 CG GLU A 260 123.180 -45.451 -6.976 1.00 47.56 C
ANISOU 856 CG GLU A 260 6406 6003 5659 429 314 786 C
ATOM 857 CD GLU A 260 122.004 -46.249 -6.430 1.00 73.21 C
ANISOU 857 CD GLU A 260 9682 9169 8967 467 461 929 C
ATOM 858 OE1 GLU A 260 122.096 -47.496 -6.404 1.00 87.23 O
ANISOU 858 OE1 GLU A 260 11446 10836 10860 505 551 1032 O
ATOM 859 OE2 GLU A 260 120.985 -45.632 -6.057 1.00 81.40 O
ANISOU 859 OE2 GLU A 260 10740 10236 9952 457 493 943 O
ATOM 860 C GLU A 260 124.747 -43.823 -9.127 1.00 49.13 C
ANISOU 860 C GLU A 260 6493 6268 5908 230 120 519 C
ATOM 861 O GLU A 260 125.290 -43.009 -8.376 1.00 47.87 O
ANISOU 861 O GLU A 260 6333 6197 5659 268 26 494 O
ATOM 862 N TYR A 261 124.029 -43.484 -10.191 1.00 47.32 N
ANISOU 862 N TYR A 261 6253 5991 5736 127 147 461 N
ATOM 863 CA TYR A 261 123.708 -42.107 -10.503 1.00 40.20 C
ANISOU 863 CA TYR A 261 5350 5125 4798 54 92 397 C
ATOM 864 CB TYR A 261 123.388 -41.964 -11.979 1.00 42.64 C
ANISOU 864 CB TYR A 261 5627 5405 5168 -29 120 344 C
ATOM 865 CG TYR A 261 124.596 -41.918 -12.869 1.00 50.21 C
ANISOU 865 CG TYR A 261 6518 6404 6155 -42 101 323 C
ATOM 866 CD1 TYR A 261 125.237 -40.711 -13.125 1.00 41.41 C
ANISOU 866 CD1 TYR A 261 5359 5336 5038 -88 48 312 C
ATOM 867 CE1 TYR A 261 126.336 -40.652 -13.944 1.00 49.19 C
ANISOU 867 CE1 TYR A 261 6262 6365 6062 -97 55 322 C
ATOM 868 CZ TYR A 261 126.815 -41.813 -14.522 1.00 46.48 C
ANISOU 868 CZ TYR A 261 5892 6033 5734 -41 107 323 C
ATOM 869 OH TYR A 261 127.917 -41.749 -15.339 1.00 56.84 O
ANISOU 869 OH TYR A 261 7115 7409 7072 -29 129 342 O
ATOM 870 CE2 TYR A 261 126.195 -43.031 -14.284 1.00 50.48 C
ANISOU 870 CE2 TYR A 261 6454 6477 6248 8 144 310 C
ATOM 871 CD2 TYR A 261 125.091 -43.077 -13.460 1.00 50.53 C
ANISOU 871 CD2 TYR A 261 6531 6427 6242 -1 145 319 C
ATOM 872 C TYR A 261 122.494 -41.680 -9.705 1.00 41.89 C
ANISOU 872 C TYR A 261 5626 5336 4955 72 112 417 C
ATOM 873 O TYR A 261 121.621 -42.488 -9.412 1.00 43.11 O
ANISOU 873 O TYR A 261 5802 5441 5136 98 199 480 O
ATOM 874 N ALA A 262 122.440 -40.403 -9.354 1.00 42.04 N
ANISOU 874 N ALA A 262 5665 5399 4911 61 37 366 N
ATOM 875 CA ALA A 262 121.255 -39.871 -8.705 1.00 38.91 C
ANISOU 875 CA ALA A 262 5325 5010 4449 91 59 372 C
ATOM 876 CB ALA A 262 121.563 -38.572 -8.003 1.00 34.70 C
ANISOU 876 CB ALA A 262 4821 4526 3838 122 -53 296 C
ATOM 877 C ALA A 262 120.181 -39.662 -9.763 1.00 38.08 C
ANISOU 877 C ALA A 262 5205 4853 4410 4 112 351 C
ATOM 878 O ALA A 262 120.383 -38.933 -10.729 1.00 31.85 O
ANISOU 878 O ALA A 262 4391 4056 3656 -66 74 298 O
ATOM 879 N THR A 263 119.035 -40.303 -9.570 1.00 37.56 N
ANISOU 879 N THR A 263 5144 4758 4368 19 202 404 N
ATOM 880 CA THR A 263 117.941 -40.260 -10.543 1.00 39.32 C
ANISOU 880 CA THR A 263 5334 4942 4665 -52 241 373 C
ATOM 881 CB THR A 263 116.840 -41.265 -10.170 1.00 41.91 C
ANISOU 881 CB THR A 263 5635 5220 5071 -40 346 446 C
ATOM 882 OG1 THR A 263 116.357 -40.986 -8.846 1.00 38.62 O
ANISOU 882 OG1 THR A 263 5259 4852 4562 52 392 527 O
ATOM 883 CG2 THR A 263 117.401 -42.674 -10.235 1.00 24.77 C
ANISOU 883 CG2 THR A 263 3436 2975 3000 -37 392 491 C
ATOM 884 C THR A 263 117.307 -38.897 -10.867 1.00 29.26 C
ANISOU 884 C THR A 263 4076 3696 3344 -74 198 318 C
ATOM 885 O THR A 263 116.885 -38.682 -12.006 1.00 45.79 O
ANISOU 885 O THR A 263 6137 5781 5481 -129 192 274 O
ATOM 886 N PRO A 264 117.205 -37.985 -9.877 1.00 37.40 N
ANISOU 886 N PRO A 264 5161 4766 4282 -13 164 315 N
ATOM 887 CA PRO A 264 116.598 -36.690 -10.218 1.00 39.64 C
ANISOU 887 CA PRO A 264 5464 5053 4544 -26 125 262 C
ATOM 888 CB PRO A 264 116.688 -35.905 -8.907 1.00 41.04 C
ANISOU 888 CB PRO A 264 5709 5266 4617 69 77 238 C
ATOM 889 CG PRO A 264 116.664 -36.968 -7.843 1.00 40.43 C
ANISOU 889 CG PRO A 264 5644 5235 4483 156 143 316 C
ATOM 890 CD PRO A 264 117.445 -38.104 -8.423 1.00 32.06 C
ANISOU 890 CD PRO A 264 4534 4138 3507 96 178 355 C
ATOM 891 C PRO A 264 117.315 -35.911 -11.322 1.00 36.77 C
ANISOU 891 C PRO A 264 5083 4663 4224 -97 63 218 C

ATOM 892 O PRO A 264 116.735 -34.978 -11.884 1.00 38.64 O
ANISOU 892 O PRO A 264 5327 4888 4466 -110 50 199 O
ATOM 893 N LEU A 265 118.559 -36.263 -11.625 1.00 40.12 N
ANISOU 893 N LEU A 265 5479 5083 4682 -129 35 221 N
ATOM 894 CA LEU A 265 119.262 -35.598 -12.722 1.00 50.24 C
ANISOU 894 CA LEU A 265 6725 6349 6014 -188 8 216 C
ATOM 895 CB LEU A 265 120.760 -35.868 -12.665 1.00 46.07 C
ANISOU 895 CB LEU A 265 6154 5826 5524 -207 -27 224 C
ATOM 896 CG LEU A 265 121.381 -35.385 -11.364 1.00 38.99 C
ANISOU 896 CG LEU A 265 5278 4925 4612 -175 -114 184 C
ATOM 897 CD1 LEU A 265 122.825 -35.793 -11.307 1.00 52.56 C
ANISOU 897 CD1 LEU A 265 6930 6663 6377 -187 -154 189 C
ATOM 898 CD2 LEU A 265 121.257 -33.873 -11.269 1.00 39.29 C
ANISOU 898 CD2 LEU A 265 5335 4906 4689 -199 -181 138 C
ATOM 899 C LEU A 265 118.700 -36.029 -14.072 1.00 45.73 C
ANISOU 899 C LEU A 265 6120 5798 5456 -208 62 225 C
ATOM 900 O LEU A 265 118.782 -35.302 -15.061 1.00 51.66 O
ANISOU 900 O LEU A 265 6856 6557 6214 -225 62 241 O
ATOM 901 N ILE A 266 118.150 -37.234 -14.105 1.00 43.38 N
ANISOU 901 N ILE A 266 5807 5508 5168 -197 106 216 N
ATOM 902 CA ILE A 266 117.415 -37.682 -15.267 1.00 38.42 C
ANISOU 902 CA ILE A 266 5143 4901 4554 -203 129 182 C
ATOM 903 CB ILE A 266 116.915 -39.107 -15.094 1.00 34.90 C
ANISOU 903 CB ILE A 266 4666 4421 4174 -204 165 158 C
ATOM 904 CG1 ILE A 266 118.098 -40.054 -14.979 1.00 45.29 C
ANISOU 904 CG1 ILE A 266 5974 5714 5521 -197 175 169 C
ATOM 905 CD1 ILE A 266 117.727 -41.437 -14.501 1.00 41.97 C
ANISOU 905 CD1 ILE A 266 5533 5219 5194 -194 221 175 C
ATOM 906 CG2 ILE A 266 116.038 -39.514 -16.268 1.00 27.36 C
ANISOU 906 CG2 ILE A 266 3661 3486 3249 -208 157 79 C
ATOM 907 C ILE A 266 116.229 -36.747 -15.462 1.00 42.72 C
ANISOU 907 C ILE A 266 5699 5462 5069 -191 121 173 C
ATOM 908 O ILE A 266 115.934 -36.306 -16.568 1.00 36.17 O
ANISOU 908 O ILE A 266 4855 4677 4213 -178 111 159 O
ATOM 909 N THR A 267 115.570 -36.425 -14.359 1.00 33.13 N
ANISOU 909 N THR A 267 4514 4227 3846 -172 129 188 N
ATOM 910 CA THR A 267 114.407 -35.566 -14.408 1.00 30.75 C
ANISOU 910 CA THR A 267 4221 3942 3519 -145 127 181 C
ATOM 911 CB THR A 267 113.633 -35.587 -13.088 1.00 33.04 C
ANISOU 911 CB THR A 267 4530 4227 3795 -103 161 201 C
ATOM 912 OG1 THR A 267 113.045 -36.879 -12.919 1.00 33.06 O
ANISOU 912 OG1 THR A 267 4471 4223 3865 -118 222 217 O
ATOM 913 CG2 THR A 267 112.539 -34.506 -13.077 1.00 22.10 C
ANISOU 913 CG2 THR A 267 3159 2863 2377 -56 156 191 C
ATOM 914 C THR A 267 114.789 -34.136 -14.809 1.00 39.63 C
ANISOU 914 C THR A 267 5387 5057 4615 -135 87 195 C
ATOM 915 O THR A 267 114.108 -33.509 -15.628 1.00 36.59 O
ANISOU 915 O THR A 267 4993 4698 4212 -110 83 198 O
ATOM 916 N LEU A 268 115.891 -33.636 -14.252 1.00 34.13 N
ANISOU 916 N LEU A 268 4723 4315 3929 -151 54 206 N
ATOM 917 CA LEU A 268 116.391 -32.311 -14.632 1.00 41.26 C
ANISOU 917 CA LEU A 268 5646 5168 4862 -161 21 230 C
ATOM 918 CB LEU A 268 117.632 -31.917 -13.827 1.00 31.47 C
ANISOU 918 CB LEU A 268 4415 3866 3674 -192 -35 214 C
ATOM 919 CG LEU A 268 117.405 -31.509 -12.379 1.00 45.22 C
ANISOU 919 CG LEU A 268 6215 5581 5386 -143 -92 144 C
ATOM 920 CD1 LEU A 268 118.726 -31.172 -11.722 1.00 55.89 C
ANISOU 920 CD1 LEU A 268 7555 6884 6797 -171 -177 100 C
ATOM 921 CD2 LEU A 268 116.463 -30.321 -12.303 1.00 47.05 C
ANISOU 921 CD2 LEU A 268 6497 5765 5616 -97 -107 122 C
ATOM 922 C LEU A 268 116.713 -32.249 -16.123 1.00 36.09 C
ANISOU 922 C LEU A 268 4950 4548 4214 -174 53 286 C
ATOM 923 O LEU A 268 116.436 -31.256 -16.799 1.00 31.94 O
ANISOU 923 O LEU A 268 4435 4007 3694 -150 61 335 O
ATOM 924 N PHE A 269 117.316 -33.312 -16.632 1.00 23.63 N
ANISOU 924 N PHE A 269 3328 3021 2628 -190 76 285 N
ATOM 925 CA PHE A 269 117.644 -33.349 -18.048 1.00 35.81 C
ANISOU 925 CA PHE A 269 4835 4630 4141 -167 112 331 C
ATOM 926 CB PHE A 269 118.478 -34.582 -18.391 1.00 32.84 C
ANISOU 926 CB PHE A 269 4416 4301 3758 -173 132 309 C
ATOM 927 CG PHE A 269 119.047 -34.525 -19.766 1.00 37.72 C
ANISOU 927 CG PHE A 269 5000 5004 4327 -125 177 364 C
ATOM 928 CD1 PHE A 269 120.199 -33.790 -20.009 1.00 36.51 C
ANISOU 928 CD1 PHE A 269 4815 4833 4224 -146 216 473 C
ATOM 929 CE1 PHE A 269 120.731 -33.714 -21.266 1.00 39.02 C
ANISOU 929 CE1 PHE A 269 5095 5247 4485 -82 285 557 C
ATOM 930 CZ PHE A 269 120.100 -34.370 -22.324 1.00 48.35 C
ANISOU 930 CZ PHE A 269 6284 6558 5529 23 295 501 C
ATOM 931 CE2 PHE A 269 118.936 -35.102 -22.095 1.00 44.60 C
ANISOU 931 CE2 PHE A 269 5836 6090 5020 33 228 358 C
ATOM 932 CD2 PHE A 269 118.415 -35.167 -20.818 1.00 31.93 C
ANISOU 932 CD2 PHE A 269 4255 4374 3501 -49 181 306 C
ATOM 933 C PHE A 269 116.383 -33.332 -18.908 1.00 30.08 C
ANISOU 933 C PHE A 269 3909 3979 3341 -102 116 308 C
ATOM 934 O PHE A 269 116.265 -32.554 -19.851 1.00 35.59 O
ANISOU 934 O PHE A 269 4808 4718 3995 -50 136 374 O
ATOM 935 N ALA A 270 115.440 -34.200 -18.567 1.00 38.93 N
ANISOU 935 N ALA A 270 5216 5119 4458 -100 98 222 N
ATOM 936 CA ALA A 270 114.193 -34.310 -19.316 1.00 34.22 C
ANISOU 936 CA ALA A 270 4591 4598 3813 -43 79 170 C
ATOM 937 CB ALA A 270 113.300 -35.395 -18.728 1.00 38.08 C
ANISOU 937 CB ALA A 270 5035 5071 4363 -73 67 81 C
ATOM 938 C ALA A 270 113.446 -32.982 -19.346 1.00 36.08 C
ANISOU 938 C ALA A 270 4857 4830 4021 4 74 223 C
ATOM 939 O ALA A 270 112.927 -32.568 -20.384 1.00 43.81 O
ANISOU 939 O ALA A 270 5824 5893 4928 82 65 237 O
ATOM 940 N MET A 271 113.394 -32.311 -18.201 1.00 41.65 N
ANISOU 940 N MET A 271 5607 5445 4774 -23 76 246 N
ATOM 941 CA MET A 271 112.701 -31.029 -18.121 1.00 38.79 C
ANISOU 941 CA MET A 271 5282 5055 4402 30 69 285 C
ATOM 942 CB MET A 271 112.669 -30.495 -16.696 1.00 34.05 C
ANISOU 942 CB MET A 271 4734 4358 3846 15 58 268 C
ATOM 943 CG MET A 271 111.765 -31.276 -15.775 1.00 25.98 C
ANISOU 943 CG MET A 271 3688 3368 2816 23 70 208 C
ATOM 944 SD MET A 271 111.843 -30.648 -14.097 1.00 40.35 S
ANISOU 944 SD MET A 271 5583 5115 4634 52 59 185 S
ATOM 945 CE MET A 271 110.878 -29.152 -14.233 1.00 42.12 C
ANISOU 945 CE MET A 271 5848 5309 4847 144 44 189 C
ATOM 946 C MET A 271 113.316 -29.994 -19.053 1.00 30.50 C
ANISOU 946 C MET A 271 4256 3989 3345 63 88 390 C
ATOM 947 O MET A 271 112.623 -29.125 -19.572 1.00 45.40 O
ANISOU 947 O MET A 271 6159 5891 5201 141 91 439 O
ATOM 948 N SER A 272 114.621 -30.087 -19.268 1.00 33.34 N
ANISOU 948 N SER A 272 4609 4318 3741 13 112 443 N
ATOM 949 CA SER A 272 115.280 -29.148 -20.163 1.00 33.40 C
ANISOU 949 CA SER A 272 4619 4305 3768 40 158 579 C
ATOM 950 CB SER A 272 116.791 -29.090 -19.909 1.00 32.18 C
ANISOU 950 CB SER A 272 4438 4068 3719 -48 181 632 C
ATOM 951 OG SER A 272 117.427 -30.312 -20.239 1.00 35.55 O
ANISOU 951 OG SER A 272 4819 4591 4096 -62 196 598 O
ATOM 952 C SER A 272 115.211 -28.724 -22.534 1.00 46.64 O
ANISOU 952 C SER A 272 6270 6169 5282 215 247 759 O
ATOM 953 O SER A 272 114.519 -30.740 -21.848 1.00 36.29 N
ANISOU 953 N GLN A 273 4922 4946 3921 161 155 497 N
ATOM 954 CA GLN A 273 114.224 -31.178 -23.208 1.00 41.96 C
ANISOU 955 CA GLN A 273 5610 5836 4496 278 155 485 C
ATOM 955 CB GLN A 273 114.628 -32.637 -23.435 1.00 41.92 C
ANISOU 956 CB GLN A 273 5564 5899 4464 260 132 362 C
ATOM 956 CG GLN A 273 116.120 -32.871 -23.342 1.00 54.73 C
ANISOU 957 CG GLN A 273 7181 7482 6132 206 193 430 C
ATOM 957 CD GLN A 273 116.930 -31.817 -24.094 1.00 74.29 C
ANISOU 958 CD GLN A 273 9663 9981 8584 261 283 624 C
ATOM 958 OE1 GLN A 273 116.672 -31.534 -25.270 1.00 76.76 O
ANISOU 959 OE1 GLN A 273 9975 10432 8757 400 314 688 O
ATOM 959 NE2 GLN A 273 117.908 -31.223 -23.409 1.00 58.93 N
ANISOU 960 NE2 GLN A 273 7712 7900 6780 160 325 723 N
ATOM 960 C GLN A 273 112.762 -30.964 -23.600 1.00 43.54 C
ANISOU 961 C GLN A 273 5802 6124 4619 375 100 428 C
ATOM 961 O GLN A 273 112.441 -30.846 -24.781 1.00 45.57 O
ANISOU 962 O GLN A 273 6046 6530 4737 511 93 450 O
ATOM 962 N TYR A 274 111.875 -30.917 -22.613 1.00 36.43 N
ANISOU 963 N TYR A 274 4898 5149 3795 322 60 358 N
ATOM 963 CA TYR A 274 110.453 -30.750 -22.906 1.00 28.45 C
ANISOU 964 CA TYR A 274 3852 4225 2732 408 5 298 C
ATOM 964 CB TYR A 274 109.591 -31.682 -22.059 1.00 26.63 C
ANISOU 965 CB TYR A 274 3557 3972 2588 333 -40 156 C
ATOM 965 CG TYR A 274 109.815 -33.130 -22.395 1.00 41.07 C
ANISOU 966 CG TYR A 274 5324 5847 4434 291 -76 29 C
ATOM 966 CD1 TYR A 274 109.300 -33.668 -23.560 1.00 58.75 C
ANISOU 967 CD1 TYR A 274 7500 8232 6591 382 -151 -80 C
ATOM 967 CE1 TYR A 274 109.513 -34.984 -23.885 1.00 77.16 C
ANISOU 968 CE1 TYR A 274 9776 10583 8957 350 -198 -223 C
ATOM 968 CZ TYR A 274 110.257 -35.783 -23.039 1.00 72.59 C
ANISOU 969 CZ TYR A 274 9209 9875 8498 227 -153 -229 C
ATOM 969 OH TYR A 274 110.466 -37.100 -23.370 1.00 71.71 O
ANISOU 970 OH TYR A 274 9045 9758 8441 203 -197 -371 O
ATOM 970 CE2 TYR A 274 110.790 -35.267 -21.872 1.00 59.23 C
ANISOU 971 CE2 TYR A 274 7579 8059 6868 145 -75 -105 C
ATOM 971 CD2 TYR A 274 110.571 -33.947 -21.561 1.00 55.88 C
ANISOU 972 CD2 TYR A 274 7206 7618 6406 177 -45 9 C
ATOM 972 C TYR A 274 109.949 -29.319 -22.782 1.00 43.31 C
ANISOU 973 C TYR A 274 5783 6057 4614 477 27 412 C
ATOM 973 O TYR A 274 110.124 -28.675 -21.752 1.00 45.27 O
ANISOU 974 O TYR A 274 6080 6157 4962 413 53 450 O
ATOM 974 N SER A 275 109.312 -28.854 -23.852 1.00 39.73 N
ANISOU 975 N SER A 275 5318 5734 4042 626 8 453 N
ATOM 975 CA SER A 275 108.706 -27.529 -23.922 1.00 47.48 C
ANISOU 976 CA SER A 275 6342 6684 5013 726 27 567 C
ATOM 976 CB SER A 275 107.915 -27.383 -25.222 1.00 30.05 C
ANISOU 977 CB SER A 275 4081 4595 2741 838 -15 582 C
ATOM 977 OG SER A 275 108.776 -27.447 -26.329 1.00 50.82 O
ANISOU 978 OG SER A 275 6750 7413 5147 998 29 678 O
ATOM 978 C SER A 275 107.763 -27.265 -22.764 1.00 39.47 C
ANISOU 979 C SER A 275 5321 5582 4093 688 1 497 C
ATOM 979 O SER A 275 107.732 -26.173 -22.206 1.00 51.70 O
ANISOU 980 O SER A 275 6935 6999 5708 703 34 577 O
ATOM 981 N GLN A 276 106.976 -28.276 -22.433 1.00 35.92 N
ANISOU 981 N GLN A 276 4784 5205 3658 649 -55 346 N

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ATOM 983 CB GLN A 276 105.093 -29.386 -21.364 1.00 59.82 C
ANISOU 983 CB GLN A 276 7645 8290 6793 596 -116 145 C
ATOM 984 CG GLN A 276 103.709 -29.194 -21.890 1.00 77.52 C
ANISOU 984 CG GLN A 276 9786 10668 9001 712 -178 96 C
ATOM 985 CD GLN A 276 102.693 -29.937 -21.075 1.00 82.36 C
ANISOU 985 CD GLN A 276 10269 11287 9737 647 -184 1 C
ATOM 986 OE1 GLN A 276 102.540 -31.148 -21.217 1.00 94.25 O
ANISOU 986 OE1 GLN A 276 11666 12824 11319 565 -224 -110 O
ATOM 987 NE2 GLN A 276 102.000 -29.223 -20.195 1.00 81.23 N
ANISOU 987 NE2 GLN A 276 10131 11105 9629 688 -136 49 N
ATOM 988 C GLN A 276 106.459 -27.798 -20.068 1.00 40.32 C
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ATOM 989 O GLN A 276 105.746 -27.258 -19.240 1.00 41.86 O
ANISOU 989 O GLN A 276 5588 5706 4611 585 -1 303 O
ATOM 990 N ALA A 277 107.713 -28.150 -19.830 1.00 41.85 N
ANISOU 990 N ALA A 277 5621 5667 4611 448 12 328 N
ATOM 991 CA ALA A 277 108.318 -27.992 -18.518 1.00 42.30 C
ANISOU 991 CA ALA A 277 5739 5586 4746 368 36 319 C
ATOM 992 CB ALA A 277 109.478 -28.963 -18.349 1.00 36.84 C
ANISOU 992 CB ALA A 277 5043 4871 4083 255 44 298 C
ATOM 993 C ALA A 277 108.779 -26.555 -18.274 1.00 44.78 C
ANISOU 993 C ALA A 277 6150 5759 5105 402 46 397 C
ATOM 994 O ALA A 277 109.032 -26.170 -17.136 1.00 45.54 O
ANISOU 994 O ALA A 277 6300 5745 5258 375 41 359 O
ATOM 995 N GLY A 278 108.900 -25.776 -19.348 1.00 45.02 N
ANISOU 995 N GLY A 278 6199 5791 5115 471 60 503 N
ATOM 996 CA GLY A 278 109.313 -24.381 -19.258 1.00 46.08 C
ANISOU 996 CA GLY A 278 6412 5760 5336 501 78 597 C
ATOM 997 C GLY A 278 110.633 -24.218 -18.522 1.00 38.88 C
ANISOU 997 C GLY A 278 5538 4686 4548 379 75 588 C
ATOM 998 O GLY A 278 110.755 -23.459 -17.565 1.00 60.48 O
ANISOU 998 O GLY A 278 8331 7270 7380 369 45 540 O
ATOM 999 N PHE A 279 111.635 -24.948 -18.984 1.00 39.91 N
ANISOU 999 N PHE A 279 5629 4858 4676 297 96 620 N
ATOM 1000 CA PHE A 279 112.846 -25.144 -18.221 1.00 40.74 C
ANISOU 1000 CA PHE A 279 5738 4858 4883 177 78 582 C
ATOM 1001 CB PHE A 279 112.742 -26.482 -17.497 1.00 47.68 C
ANISOU 1001 CB PHE A 279 6588 5835 5692 130 52 458 C
ATOM 1002 CG PHE A 279 113.749 -26.663 -16.416 1.00 57.08 C
ANISOU 1002 CG PHE A 279 7792 6938 6959 42 14 392 C
ATOM 1003 CD1 PHE A 279 113.635 -25.960 -15.228 1.00 55.52 C
ANISOU 1003 CD1 PHE A 279 7651 6633 6809 60 -41 308 C
ATOM 1004 CE1 PHE A 279 114.557 -26.131 -14.217 1.00 50.65 C
ANISOU 1004 CE1 PHE A 279 7044 5959 6241 4 -99 228 C
ATOM 1005 CZ PHE A 279 115.612 -27.026 -14.390 1.00 54.57 C
ANISOU 1005 CZ PHE A 279 7485 6498 6750 -79 -92 247 C
ATOM 1006 CE2 PHE A 279 115.727 -27.743 -15.573 1.00 39.80 C
ANISOU 1006 CE2 PHE A 279 5560 4723 4839 -99 -24 337 C
ATOM 1007 CD2 PHE A 279 114.798 -27.556 -16.577 1.00 49.04 C
ANISOU 1007 CD2 PHE A 279 6727 5957 5949 -35 23 400 C
ATOM 1008 C PHE A 279 114.007 -25.174 -19.192 1.00 51.53 C
ANISOU 1008 C PHE A 279 7065 6223 6292 131 134 710 C
ATOM 1009 O PHE A 279 114.105 -26.075 -20.023 1.00 46.48 O
ANISOU 1009 O PHE A 279 6379 5736 5544 148 165 732 O
ATOM 1010 N SER A 280 114.877 -24.177 -19.091 1.00 34.46 N
ANISOU 1010 N SER A 280 4911 3884 4299 80 147 790 N
ATOM 1011 CA SER A 280 115.967 -24.039 -20.043 1.00 39.56 C
ANISOU 1011 CA SER A 280 5501 4518 5011 45 227 954 C
ATOM 1012 CB SER A 280 116.271 -22.569 -20.303 1.00 38.02 C
ANISOU 1012 CB SER A 280 5318 4120 5010 47 272 1105 C
ATOM 1013 OG SER A 280 116.895 -21.991 -19.174 1.00 52.77 O
ANISOU 1013 OG SER A 280 7188 5773 7090 -62 193 1005 O
ATOM 1014 C SER A 280 117.246 -24.735 -19.590 1.00 49.26 C
ANISOU 1014 C SER A 280 6670 5733 6315 -78 210 907 C
ATOM 1015 O SER A 280 117.397 -25.136 -18.433 1.00 57.66 O
ANISOU 1015 O SER A 280 7745 6762 7403 -140 125 752 O
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ANISOU 1021 NE ARG A 281 11910 12185 10732 -35 1244 205 N
ATOM 1022 CZ ARG A 281 124.162 -27.596 -22.130 1.00 91.29 C
ANISOU 1022 CZ ARG A 281 11617 12380 10689 31 1159 22 C
ATOM 1023 NH1 ARG A 281 125.333 -27.998 -21.652 1.00 85.14 N
ANISOU 1023 NH1 ARG A 281 10564 11695 10090 -176 1255 -29 N
ATOM 1024 NH2 ARG A 281 123.342 -28.481 -22.684 1.00 87.43 N
ANISOU 1024 NH2 ARG A 281 11155 12028 10038 307 959 -119 N
ATOM 1025 C ARG A 281 120.253 -24.674 -19.186 1.00 54.25 C
ANISOU 1025 C ARG A 281 7557 6772 6283 246 785 126 C
ATOM 1026 O ARG A 281 121.030 -25.287 -18.454 1.00 59.98 O
ANISOU 1026 O ARG A 281 8076 7558 7157 20 760 -18 O

ATOM 1027 N GLU A 282 120.033 -23.369 -19.061 1.00 57.06 N
ANISOU 1027 N GLU A 282 8241 6824 6614 273 907 270 N
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ANISOU 1028 CA GLU A 282 8661 6786 7033 -10 995 226 C
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ANISOU 1032 OE1 GLU A 282 13627 11413 11056 146 1507 886 O
ATOM 1033 OE2 GLU A 282 119.623 -21.337 -20.997 1.00 97.16 O
ANISOU 1033 OE2 GLU A 282 14001 11587 11328 600 1204 782 O
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ANISOU 1034 C GLU A 282 8955 7093 7475 74 862 57 C
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ANISOU 1036 N ASP A 283 8951 7159 7418 431 798 102 N
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ANISOU 1037 CA ASP A 283 7622 5964 6273 565 727 -7 C
ATOM 1038 CB ASP A 283 116.482 -23.427 -15.870 1.00 57.22 C
ANISOU 1038 CB ASP A 283 8151 6718 6872 964 680 101 C
ATOM 1039 CG ASP A 283 115.847 -22.081 -16.175 1.00 77.24 C
ANISOU 1039 CG ASP A 283 11051 8999 9297 1243 794 271 C
ATOM 1040 OD1 ASP A 283 116.478 -21.047 -15.878 1.00 87.58 O
ANISOU 1040 OD1 ASP A 283 12745 9954 10577 1114 926 277 O
ATOM 1041 OD2 ASP A 283 114.709 -22.065 -16.704 1.00 74.73 O
ANISOU 1041 OD2 ASP A 283 10631 8825 8940 1595 735 399 O
ATOM 1042 C ASP A 283 118.495 -24.662 -15.045 1.00 62.44 C
ANISOU 1042 C ASP A 283 8558 7498 7667 384 616 -163 C
ATOM 1043 O ASP A 283 118.592 -24.889 -13.841 1.00 61.88 O
ANISOU 1043 O ASP A 283 8467 7394 7650 333 597 -271 O
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ATOM 1046 CB ARG A 284 119.418 -27.783 -16.843 1.00 46.88 C
ANISOU 1046 CB ARG A 284 5875 6182 5755 242 376 -322 C
ATOM 1047 CG ARG A 284 119.637 -29.240 -16.475 1.00 42.76 C
ANISOU 1047 CG ARG A 284 5077 5809 5360 190 269 -456 C
ATOM 1048 CD ARG A 284 119.893 -30.075 -17.701 1.00 37.32 C
ANISOU 1048 CD ARG A 284 4298 5286 4596 233 202 -522 C
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ANISOU 1052 NH2 ARG A 284 6256 7332 5976 413 233 -531 N
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ANISOU 1053 C ARG A 284 6893 6789 6718 -62 466 -402 C
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ANISOU 1054 O ARG A 284 6167 6244 6188 -84 398 -491 O
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ANISOU 1055 N LEU A 285 6756 6466 6453 -270 554 -367 N
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ANISOU 1056 CA LEU A 285 6506 6334 6398 -558 527 -463 C
ATOM 1057 CB LEU A 285 123.973 -25.575 -15.433 1.00 50.95 C
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ATOM 1060 CD2 LEU A 285 126.356 -24.847 -15.613 1.00 70.27 C
ANISOU 1060 CD2 LEU A 285 8752 8808 9139 -1421 791 -330 C
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ATOM 1062 O LEU A 285 123.423 -26.018 -12.267 1.00 56.94 O
ANISOU 1062 O LEU A 285 7381 7010 7242 -733 334 -689 O
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ANISOU 1063 N GLU A 286 6591 5396 5878 -505 529 -514 N
ATOM 1064 CA GLU A 286 121.859 -23.820 -11.833 1.00 53.04 C
ANISOU 1064 CA GLU A 286 7631 5927 6594 -510 478 -640 C
ATOM 1065 CB GLU A 286 121.171 -22.448 -11.969 1.00 61.87 C
ANISOU 1065 CB GLU A 286 9192 6673 7643 -385 602 -572 C
ATOM 1066 CG GLU A 286 119.653 -22.492 -12.099 1.00 89.48 C
ANISOU 1066 CG GLU A 286 12746 10195 11056 60 692 -452 C
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ANISOU 1067 CD GLU A 286 15995 12583 13740 264 808 -422 C
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ANISOU 1068 OE1 GLU A 286 16788 12698 14181 48 793 -552 O
ATOM 1069 OE2 GLU A 286 117.793 -21.004 -12.168 1.00115.73 O
ANISOU 1069 OE2 GLU A 286 16574 13157 14242 647 901 -275 O
ATOM 1070 C GLU A 286 121.100 -24.711 -10.847 1.00 51.37 C
ANISOU 1070 C GLU A 286 7317 7317 6324 -693 422 -693 C
ATOM 1071 O GLU A 286 121.416 -24.749 -9.659 1.00 47.88 O
ANISOU 1071 O GLU A 286 6964 5414 5816 -290 327 -832 O

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ATOM  1072  N  GLN A 287     120.105 -25.439 -11.348  1.00 42.68           N
ANISOU 1072  N  GLN A 287     6028  4942  5247   -6   474   -575       N
ATOM  1073  CA  GLN A 287    119.291 -26.262 -10.480  1.00 37.21           C
ANISOU 1073  CA  GLN A 287     5215  4375  4548   215   479   -566       C
ATOM  1074  CB  GLN A 287    117.971 -26.641 -11.141  1.00 54.31           C
ANISOU 1074  CB  GLN A 287     7209  6642  6785   467   544   -418       C
ATOM  1075  CG  GLN A 287    116.986 -25.494 -11.232  1.00 40.90           C
ANISOU 1075  CG  GLN A 287     5760  4769  5013   722   665   -325       C
ATOM  1076  CD  GLN A 287    116.608 -24.946  -9.871  1.00 49.59           C
ANISOU 1076  CD  GLN A 287     7125  5720  5995   902   776   -368       C
ATOM  1077  OE1 GLN A 287    116.041 -25.657  -9.041  1.00 57.21           O
ANISOU 1077  OE1 GLN A 287     7942  6821  6973  1052   840   -330       O
ATOM  1078  NE2 GLN A 287    116.924 -23.676  -9.632  1.00 61.68           N
ANISOU 1078  NE2 GLN A 287     9086  6949  7401   895   816   -445       N
ATOM  1079  C  GLN A 287     120.053 -27.503 -10.052  1.00 39.52           C
ANISOU 1079  C  GLN A 287     5240  4876  4898    91   369   -630       C
ATOM  1080  O  GLN A 287     119.861 -28.007  -8.952  1.00 51.16           O
ANISOU 1080  O  GLN A 287     6716  6400  6322   198   365   -645       O
ATOM  1081  N  ALA A 288     120.920 -27.994 -10.927  1.00 38.41           N
ANISOU 1081  N  ALA A 288     4893  4860  4842   -91   305   -647       N
ATOM  1082  CA  ALA A 288    121.717 -29.174 -10.602  1.00 42.79           C
ANISOU 1082  CA  ALA A 288     5199  5604  5457   -162   209   -698       C
ATOM  1083  CB  ALA A 288    122.464 -29.677 -11.811  1.00 40.86           C
ANISOU 1083  CB  ALA A 288     4738  5495  5291   -272   199   -698       C
ATOM  1084  C  ALA A 288     122.692 -28.881  -9.469  1.00 49.91           C
ANISOU 1084  C  ALA A 288     6183  6500  6279   -291    94   -813       C
ATOM  1085  O  ALA A 288     122.952 -29.733  -8.618  1.00 42.56           O
ANISOU 1085  O  ALA A 288     5158  5692  5322   -218    14   -831       O
ATOM  1086  N  LYS A 289     123.234 -27.669  -9.467  1.00 42.44           N
ANISOU 1086  N  LYS A 289     5428  5399  5296   -487    66   -888       N
ATOM  1087  CA  LYS A 289    124.145 -27.260  -8.415  1.00 46.34           C
ANISOU 1087  CA  LYS A 289     6015  5872  5719   -652   -111  -1043       C
ATOM  1088  CB  LYS A 289    124.819 -25.943  -8.764  1.00 60.14           C
ANISOU 1088  CB  LYS A 289     7921  7405  7524   -968   -136  -1117       C
ATOM  1089  CG  LYS A 289    125.754 -26.015  -9.944  1.00 74.27           C
ANISOU 1089  CG  LYS A 289     9406  9313  9500  -1217   -79  -1036       C
ATOM  1090  CD  LYS A 289    126.266 -24.628 -10.259  1.00 80.93           C
ANISOU 1090  CD  LYS A 289     10445  9874 10431  -1548   -47  -1057       C
ATOM  1091  CE  LYS A 289    127.138 -24.608 -11.492  1.00 84.18           C
ANISOU 1091  CE  LYS A 289     10566 10400 11019  -1781    96   -913       C
ATOM  1092  NZ  LYS A 289    127.295 -23.213 -11.996  1.00 88.82           N
ANISOU 1092  NZ  LYS A 289     11424 10629 11694  -2052   226   -843       N
ATOM  1093  C  LYS A 289     123.386 -27.105  -7.106  1.00 49.67           C
ANISOU 1093  C  LYS A 289     6201  6201  5933   -419   -128  -1100       C
ATOM  1094  O  LYS A 289     123.873 -27.471  -6.037  1.00 56.99           O
ANISOU 1094  O  LYS A 289     7684  7237  6732   -390   -291  -1195       O
ATOM  1095  N  LEU A 290     122.186 -26.551  -7.206  1.00 40.29           N
ANISOU 1095  N  LEU A 290     5789  4832  4688   -212    51  -1027       N
ATOM  1096  CA  LEU A 290    121.362 -26.305  -6.037  1.00 38.30           C
ANISOU 1096  CA  LEU A 290     5843  4490  4220    69   117  -1054       C
ATOM  1097  CB  LEU A 290    120.198 -25.388  -6.399  1.00 36.13           C
ANISOU 1097  CB  LEU A 290     5815  3989  3923   275   326   -975       C
ATOM  1098  CG  LEU A 290    119.167 -25.024  -5.338  1.00 52.76           C
ANISOU 1098  CG  LEU A 290     8237  6000  5807   648   486   -967       C
ATOM  1099  CD1 LEU A 290    119.844 -24.496  -4.081  1.00 51.15           C
ANISOU 1099  CD1 LEU A 290     8424  5681  5330   618   327  -1213       C
ATOM  1100  CD2 LEU A 290    118.237 -23.977  -5.920  1.00 56.81           C
ANISOU 1100  CD2 LEU A 290     8966  6277  6340   836   669   -892       C
ATOM  1101  C  LEU A 290     120.863 -27.627  -5.448  1.00 44.57           C
ANISOU 1101  C  LEU A 290     6434  5514  4987   305   183   -922       C
ATOM  1102  O  LEU A 290     120.674 -27.760  -4.240  1.00 55.20           O
ANISOU 1102  O  LEU A 290     7974  6888  6112   500   191   -946       O
ATOM  1103  N  PHE A 291     120.667 -28.606  -6.319  1.00 38.51           N
ANISOU 1103  N  PHE A 291     5308  4889  4435   287   234   -781       N
ATOM  1104  CA  PHE A 291     120.258 -29.941  -5.911  1.00 34.50           C
ANISOU 1104  CA  PHE A 291     4592  4537  3981   445   299   -639       C
ATOM  1105  CB  PHE A 291     119.939 -30.779  -7.155  1.00 38.37           C
ANISOU 1105  CB  PHE A 291     4748  5092  4739   382   332   -541       C
ATOM  1106  CG  PHE A 291     119.667 -32.226  -6.858  1.00 30.11           C
ANISOU 1106  CG  PHE A 291     3492  4134  3814   471   374   -413       C
ATOM  1107  CD1 PHE A 291     118.412 -32.640  -6.435  1.00 28.88           C
ANISOU 1107  CD1 PHE A 291     3288  3953  3733   645   564   -234       C
ATOM  1108  CE1 PHE A 291     118.156 -33.982  -6.164  1.00 29.10           C
ANISOU 1108  CE1 PHE A 291     3138  4000  3921   682   626   -89       C
ATOM  1109  CZ  PHE A 291     119.174 -34.925  -6.313  1.00 32.34           C
ANISOU 1109  CZ  PHE A 291     3461  4445  4384   599   485   -138       C
ATOM  1110  CE2 PHE A 291     120.435 -34.513  -6.740  1.00 40.72           C
ANISOU 1110  CE2 PHE A 291     4543  5578  5350   476   296   -322       C
ATOM  1111  CD2 PHE A 291     120.671 -33.170  -7.011  1.00 35.92           C
ANISOU 1111  CD2 PHE A 291     4071  4962  4616   385   246   -450       C
ATOM  1112  C  PHE A 291     121.351 -30.614  -5.066  1.00 46.79           C
ANISOU 1112  C  PHE A 291     6119  6231  5427   408   124   -703       C
ATOM  1113  O  PHE A 291     121.070 -31.207  -4.025  1.00 49.14           O
ANISOU 1113  O  PHE A 291     6497  6589  5585   616   180   -612       O
ATOM  1114  N  CYS A 292     122.599 -30.510  -5.518  1.00 41.14           N
ANISOU 1114  N  CYS A 292     5274  5587  4770   168   -76   -832       N
ATOM  1115  CA  CYS A 292     123.730 -31.085  -4.794  1.00 46.08           C
ANISOU 1115  CA  CYS A 292     5812  6390  5309   146   -289   -896       C
ATOM  1116  CB  CYS A 292     125.036 -30.921  -5.574  1.00 44.22           C
ANISOU 1116  CB  CYS A 292     5316  6261  5225   -138   -458  -1004       C
ATOM  1117  SG  CYS A 292     125.052 -31.770  -7.150  1.00 80.54           S
ANISOU 1117  SG  CYS A 292     9573 10925 10105   -177   -314   -893       S
ATOM  1118  C  CYS A 292     123.891 -30.465  -3.413  1.00 41.93           C
ANISOU 1118  C  CYS A 292     5622  5847  4463   238   -425  -1018       C
ATOM  1119  O  CYS A 292     124.062 -31.168  -2.418  1.00 46.09           O
ANISOU 1119  O  CYS A 292     6393  6488  4804   438   -495   -968       O
ATOM  1120  N  ARG A 293     123.844 -29.141  -3.365  1.00 51.13           N
ANISOU 1120  N  ARG A 293     7060  6826  5541   109   -466  -1183       N
ATOM  1121  CA  ARG A 293     123.970 -28.419  -2.107  1.00 52.73           C
ANISOU 1121  CA  ARG A 293     7666  6963  5407   193   -621  -1367       C
ATOM  1122  CB  ARG A 293     123.996 -26.918  -2.355  1.00 50.13           C
ANISOU 1122  CB  ARG A 293     7634  6338  5075   -19   -665  -1569       C
ATOM  1123  CG  ARG A 293     125.325 -26.421  -2.858  1.00 66.91           C
ANISOU 1123  CG  ARG A 293     9563  8464  7394   -467   -940  -1736       C
ATOM  1124  CD  ARG A 293     125.309 -24.922  -3.035  1.00 90.67           C
ANISOU 1124  CD  ARG A 293     12931 11099 10421   -696   -963  -1917       C
ATOM  1125  NE  ARG A 293     124.939 -24.540  -4.394  1.00102.36           N
ANISOU 1125  NE  ARG A 293     14300 12418 12173   -816   -708  -1754       N
ATOM  1126  CZ  ARG A 293     124.160 -23.508  -4.694  1.00106.89           C
ANISOU 1126  CZ  ARG A 293     15243 12642 12728   -754   -526  -1751       C
ATOM  1127  NH1 ARG A 293     123.882 -23.231  -5.962  1.00103.74           N
ANISOU 1127  NH1 ARG A 293     14732 12141 12544   -831   -319  -1573       N
ATOM  1128  NH2 ARG A 293     123.658 -22.755  -3.725  1.00113.36           N
ANISOU 1128  NH2 ARG A 293     16574 13216 13281   -567   -547  -1922       N
ATOM  1129  C  ARG A 293     122.848 -28.760  -1.131  1.00 58.02           C
ANISOU 1129  C  ARG A 293     8611  7630  5806   613   -395  -1231       C
ATOM  1130  O  ARG A 293     123.069 -28.895   0.075  1.00 57.30           O
ANISOU 1130  O  ARG A 293     8764  7634  5374   807   -518  -1297       O
ATOM  1131  N  THR A 294     121.638 -28.891  -1.660  1.00 48.76           N
ANISOU 1131  N  THR A 294     7381  6368  4776   764   -60  -1030       N
ATOM  1132  CA  THR A 294     120.489 -29.133  -0.811  1.00 44.14           C
ANISOU 1132  CA  THR A 294     6996  5786  4014   227   -855  -1227       C
ATOM  1133  CB  THR A 294     119.174 -28.883  -1.542  1.00 47.37           C
ANISOU 1133  CB  THR A 294     7308  6081  4610  1257   550   -686       C
ATOM  1134  OG1 THR A 294     119.208 -27.588  -2.147  1.00 51.55           O
ANISOU 1134  OG1 THR A 294     8025  6392  5167  1127   496   -861       O
ATOM  1135  CG2 THR A 294     118.002 -28.957  -0.560  1.00 41.42           C
ANISOU 1135  CG2 THR A 294     6750  5347  3641  1671   887   -503       C
ATOM  1136  C  THR A 294     120.522 -30.556  -0.287  1.00 40.40           C
ANISOU 1136  C  THR A 294     6331  5516  3504  1305   285   -634       C
ATOM  1137  O  THR A 294     120.199 -30.820   0.870  1.00 50.45           O
ANISOU 1137  O  THR A 294     7849  6856  4462  1609   400   -537       O
ATOM  1138  N  LEU A 295     120.925 -31.472  -1.153  1.00 37.85           N
ANISOU 1138  N  LEU A 295     5607  5269  3506  1119   223   -543       N
ATOM  1139  CA  LEU A 295     121.016 -32.873  -0.773  1.00 48.68           C
ANISOU 1139  CA  LEU A 295     6813  6765  4920  1251   276   -325       C
ATOM  1140  CB  LEU A 295     121.273 -33.752  -1.993  1.00 38.11           C
ANISOU 1140  CB  LEU A 295     5068  5429  3985  1047   245   -265       C
ATOM  1141  CG  LEU A 295     121.290 -35.246  -1.706  1.00 43.40           C
ANISOU 1141  CG  LEU A 295     5599  6135  4756  1181   324   -33       C
ATOM  1142  CD1 LEU A 295     119.971 -35.656  -1.068  1.00 50.64           C
ANISOU 1142  CD1 LEU A 295     6601  6969  5671  1391   678   250       C
ATOM  1143  CD2 LEU A 295     121.527 -36.018  -2.993  1.00 40.05           C
ANISOU 1143  CD2 LEU A 295     4842  5665  4710   994   280   -41       C
ATOM  1144  C  LEU A 295     122.107 -33.083   0.279  1.00 40.58           C
ANISOU 1144  C  LEU A 295     5955  5901  3562  1355   4   -414       C
ATOM  1145  O  LEU A 295     121.937 -33.857   1.223  1.00 68.34           O
ANISOU 1145  O  LEU A 295     9595  9498  6874  1634   104   -216       O
ATOM  1146  N  GLU A 296     123.226 -32.387   0.106  1.00 59.18           N
ANISOU 1146  N  GLU A 296     8301  8313  5872  1129   -344   -693       N
ATOM  1147  CA  GLU A 296     124.305 -32.402   1.088  1.00 54.90           C
ANISOU 1147  CA  GLU A 296     7888  7960  5013  1198   -694   -834       C
ATOM  1148  CB  GLU A 296     125.433 -31.460   0.676  1.00 62.30           C
ANISOU 1148  CB  GLU A 296     8723  8922  6027   833  -1062  -1154       C
ATOM  1149  CG  GLU A 296     126.691 -32.166   0.242  1.00 83.26           C
ANISOU 1149  CG  GLU A 296     10937 11809  8888   688  -1318  -1157       C
ATOM  1150  CD  GLU A 296     127.875 -31.848   1.130  1.00103.45           C
ANISOU 1150  CD  GLU A 296     13523 14587 11195   645  -1790  -1381       C
ATOM  1151  OE1 GLU A 296     127.991 -30.685   1.575  1.00112.17           O
ANISOU 1151  OE1 GLU A 296     14915 15588 12116   486  -1992  -1654       O
ATOM  1152  OE2 GLU A 296     128.687 -32.765   1.388  1.00111.35           O
ANISOU 1152  OE2 GLU A 296     14268 15855 12184   782  -1982  -1292       O
ATOM  1153  C  GLU A 296     123.794 -31.990   2.463  1.00 53.69           C
ANISOU 1153  C  GLU A 296     8239  7803  4359  1523   -647   -854       C
ATOM  1154  O  GLU A 296     124.059 -32.657   3.462  1.00 60.30           O
ANISOU 1154  O  GLU A 296     9218  8811  4882  1807   -725   -747       O
ATOM  1155  N  ASP A 297     123.064 -30.879   2.500  1.00 55.94           N
ANISOU 1155  N  ASP A 297     8824  7888  4541  1524   -506   -985       N
ATOM  1156  CA  ASP A 297     122.544 -30.348   3.755  1.00 63.40           C
ANISOU 1156  CA  ASP A 297     9977  8744  5369  1808   -428  -1046       C
ATOM  1157  CB  ASP A 297     121.808 -29.029   3.541  1.00 69.36           C
ANISOU 1157  CB  ASP A 297     9365  8649  6339  1849   -273  -1221       C
ATOM  1158  CG  ASP A 297     122.731 -27.903   3.151  1.00 99.54           C
ANISOU 1158  CG  ASP A 297    15271 12961  9589  1459   -667  -1613       C
ATOM  1159  OD1 ASP A 297     123.961 -28.072   3.278  1.00110.44           O
ANISOU 1159  OD1 ASP A 297    16501 14496 10965  1230  -1092  -1781       O
ATOM  1160  OD2 ASP A 297     122.215 -26.844   2.726  1.00109.93           O
ANISOU 1160  OD2 ASP A 297    16794 13995 10981  1387   -542  -1734       O
ATOM  1161  C  ASP A 297     121.599 -31.331   4.420  1.00 54.00           C
ANISOU 1161  C  ASP A 297     9182  7704  3633  2284   -656   -656       C
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ATOM 1162 O ASP A 297 121.615 -31.505 5.630 1.00 66.19 O
ANISOU 1162 O ASP A 297 11089 9371 4689 2632 -20 -612 O
ATOM 1163 N ILE A 298 120.766 -31.966 3.610 1.00 54.21 N
ANISOU 1163 N ILE A 298 8857 7659 4082 2233 335 -366 N
ATOM 1164 CA ILE A 298 119.820 -32.929 4.131 1.00 51.45 C
ANISOU 1164 CA ILE A 298 8490 7349 3708 2541 761 43 C
ATOM 1165 CB ILE A 298 118.871 -33.421 3.046 1.00 51.13 C
ANISOU 1165 CB ILE A 298 8013 7190 4222 2374 1073 279 C
ATOM 1166 CG1 ILE A 298 117.975 -32.280 2.591 1.00 47.60 C
ANISOU 1166 CG1 ILE A 298 7620 6614 3852 2364 1250 176 C
ATOM 1167 CD1 ILE A 298 117.042 -32.659 1.474 1.00 46.35 C
ANISOU 1167 CD1 ILE A 298 7010 6379 4220 2200 1475 368 C
ATOM 1168 CG2 ILE A 298 118.014 -34.568 3.568 1.00 60.58 C
ANISOU 1168 CG2 ILE A 298 9122 8408 5489 2603 1489 727 C
ATOM 1169 C ILE A 298 120.531 -34.113 4.767 1.00 52.33 C
ANISOU 1169 C ILE A 298 8583 7623 3674 2685 641 227 C
ATOM 1170 O ILE A 298 120.211 -34.515 5.882 1.00 61.86 O
ANISOU 1170 O ILE A 298 10088 8919 4497 3062 842 452 O
ATOM 1171 N LEU A 299 121.514 -34.654 4.060 1.00 57.38 N
ANISOU 1171 N LEU A 299 8895 8310 4598 2428 331 148 N
ATOM 1172 CA LEU A 299 122.212 -35.848 4.521 1.00 51.71 C
ANISOU 1172 CA LEU A 299 8118 7725 3804 2591 217 345 C
ATOM 1173 CB LEU A 299 123.093 -36.432 3.421 1.00 48.81 C
ANISOU 1173 CB LEU A 299 7306 7365 3874 2302 -24 270 C
ATOM 1174 CG LEU A 299 122.363 -36.971 2.200 1.00 66.13 C
ANISOU 1174 CG LEU A 299 9155 9351 6621 2078 249 409 C
ATOM 1175 CD1 LEU A 299 123.325 -37.735 1.310 1.00 63.97 C
ANISOU 1175 CD1 LEU A 299 8537 9103 6665 1918 33 355 C
ATOM 1176 CD2 LEU A 299 121.208 -37.862 2.634 1.00 58.44 C
ANISOU 1176 CD2 LEU A 299 8242 8238 5726 2279 697 814 C
ATOM 1177 C LEU A 299 123.061 -35.587 5.755 1.00 63.98 C
ANISOU 1177 C LEU A 299 10042 9504 4762 2858 -120 206 C
ATOM 1178 O LEU A 299 123.257 -36.475 6.579 1.00 70.06 O
ANISOU 1178 O LEU A 299 10956 10393 5271 3185 -91 463 O
ATOM 1179 N ALA A 300 123.578 -34.370 5.867 1.00 64.53 N
ANISOU 1179 N ALA A 300 10282 9618 4619 2713 -463 -202 N
ATOM 1180 CA ALA A 300 124.483 -34.035 6.956 1.00 72.54 C
ANISOU 1180 CA ALA A 300 11622 10856 5084 2900 -904 -424 C
ATOM 1181 CB ALA A 300 124.997 -32.619 6.814 1.00 62.85 C
ANISOU 1181 CB ALA A 300 10519 9576 3784 2595 -1285 -918 C
ATOM 1182 C ALA A 300 123.805 -34.222 8.309 1.00 83.96 C
ANISOU 1182 C ALA A 300 13605 12371 5925 3426 -651 -214 C
ATOM 1183 O ALA A 300 124.443 -34.604 9.290 1.00 88.19 O
ANISOU 1183 O ALA A 300 14294 13079 6134 3660 -891 -188 O
ATOM 1184 N ASP A 301 122.505 -33.961 8.354 1.00 76.83 N
ANISOU 1184 N ASP A 301 12878 11291 5025 3561 -124 -40 N
ATOM 1185 CA ASP A 301 121.778 -34.046 9.609 1.00 75.30 C
ANISOU 1185 CA ASP A 301 13036 11068 4508 3957 202 175 C
ATOM 1186 CB ASP A 301 121.098 -32.708 9.929 1.00 95.50 C
ANISOU 1186 CB ASP A 301 15894 13447 6944 3974 312 -78 C
ATOM 1187 CG ASP A 301 121.805 -31.941 11.037 1.00120.84 C
ANISOU 1187 CG ASP A 301 19495 16700 9719 4069 -107 -425 C
ATOM 1188 OD1 ASP A 301 123.053 -31.965 11.087 1.00128.34 O
ANISOU 1188 OD1 ASP A 301 20373 17799 10592 3887 -654 -674 O
ATOM 1189 OD2 ASP A 301 121.102 -31.317 11.863 1.00128.05 O
ANISOU 1189 OD2 ASP A 301 20764 17506 10382 4330 109 -441 O
ATOM 1190 C ASP A 301 120.739 -35.166 9.637 1.00 71.55 C
ANISOU 1190 C ASP A 301 12425 10533 4226 4170 814 737 C
ATOM 1191 O ASP A 301 119.971 -35.278 10.582 1.00 87.78 O
ANISOU 1191 O ASP A 301 14694 12542 6118 4477 1169 965 O
ATOM 1192 N ALA A 302 120.706 -35.997 8.604 1.00 73.18 N
ANISOU 1192 N ALA A 302 12245 10710 4852 3973 934 962 N
ATOM 1193 CA ALA A 302 119.666 -37.019 8.538 1.00 71.92 C
ANISOU 1193 CA ALA A 302 11904 10420 5002 4064 1516 1488 C
ATOM 1194 CB ALA A 302 119.262 -37.292 7.104 1.00 60.51 C
ANISOU 1194 CB ALA A 302 9898 8763 4328 3608 1608 1501 C
ATOM 1195 C ALA A 302 120.060 -38.313 9.241 1.00 86.36 C
ANISOU 1195 C ALA A 302 13798 12291 6725 4315 1561 1854 C
ATOM 1196 O ALA A 302 121.096 -38.901 8.929 1.00 87.89 O
ANISOU 1196 O ALA A 302 13858 12552 6983 4247 1190 1810 O
ATOM 1197 N PRO A 303 119.223 -38.754 10.199 1.00 90.87 N
ANISOU 1197 N PRO A 303 14508 12782 7237 4584 2004 2185 N
ATOM 1198 CA PRO A 303 119.346 -39.984 10.993 1.00 95.18 C
ANISOU 1198 CA PRO A 303 15137 13299 7728 4838 2173 2566 C
ATOM 1199 CB PRO A 303 117.906 -40.241 11.447 1.00 83.53 C
ANISOU 1199 CB PRO A 303 13619 11663 6456 4945 2822 2941 C
ATOM 1200 CG PRO A 303 117.231 -38.892 11.421 1.00 80.65 C
ANISOU 1200 CG PRO A 303 13319 11330 5996 4931 2879 2672 C
ATOM 1201 CD PRO A 303 118.129 -37.910 10.704 1.00 87.77 C
ANISOU 1201 CD PRO A 303 14250 12335 6763 4709 2340 2163 C
ATOM 1202 C PRO A 303 119.839 -41.197 10.208 1.00 90.58 C
ANISOU 1202 C PRO A 303 14281 12599 7537 4674 2120 2807 C
ATOM 1203 O PRO A 303 120.660 -41.961 10.711 1.00 87.61 O
ANISOU 1203 O PRO A 303 14015 12278 6994 4871 1921 2899 O
ATOM 1204 N GLU A 304 119.335 -41.373 8.993 1.00 85.28 N
ANISOU 1204 N GLU A 304 13260 11744 7398 4332 2289 2905 N
ATOM 1205 CA GLU A 304 119.609 -42.584 8.231 1.00 95.23 C
ANISOU 1205 CA GLU A 304 14249 12770 9164 4150 2287 3131 C
ATOM 1206 CB GLU A 304 118.454 -42.883 7.269 1.00 93.31 C
ANISOU 1206 CB GLU A 304 13592 12223 9639 3745 2661 3267 C
ATOM 1207 CG GLU A 304 117.079 -42.904 7.920 1.00 99.39 C
ANISOU 1207 CG GLU A 304 14390 12928 10447 3840 3265 3634 C
ATOM 1208 CD GLU A 304 116.443 -41.521 8.013 1.00100.29 C
ANISOU 1208 CD GLU A 304 14523 13230 10352 3865 3332 3379 C
ATOM 1209 OE1 GLU A 304 115.216 -41.448 8.231 1.00 98.49 O
ANISOU 1209 OE1 GLU A 304 14123 12925 10373 3845 3744 3565 O
ATOM 1210 OE2 GLU A 304 117.168 -40.513 7.862 1.00100.65 O
ANISOU 1210 OE2 GLU A 304 14738 13479 10027 3899 2941 2974 O
ATOM 1211 C GLU A 304 120.911 -42.497 7.442 1.00 89.63 C
ANISOU 1211 C GLU A 304 13327 12146 8582 3960 1677 2705 C
ATOM 1212 O GLU A 304 121.421 -43.504 6.962 1.00 78.68 O
ANISOU 1212 O GLU A 304 11775 10601 7521 3906 1584 2809 O
ATOM 1213 N SER A 305 121.446 -41.290 7.320 1.00 85.74 N
ANISOU 1213 N SER A 305 12848 11888 7842 3869 1288 2236 N
ATOM 1214 CA SER A 305 122.467 -41.022 6.322 1.00 87.73 C
ANISOU 1214 CA SER A 305 12775 12204 8355 3568 805 1829 C
ATOM 1215 CB SER A 305 122.027 -39.862 5.445 1.00 95.11 C
ANISOU 1215 CB SER A 305 13514 13099 9523 3191 774 1478 C
ATOM 1216 OG SER A 305 122.247 -38.645 6.132 1.00100.27 O
ANISOU 1216 OG SER A 305 14466 13955 9676 3295 567 1198 O
ATOM 1217 C SER A 305 123.813 -40.652 6.909 1.00 89.66 C
ANISOU 1217 C SER A 305 13155 12776 8136 3756 263 1572 C
ATOM 1218 O SER A 305 124.580 -39.915 6.287 1.00 81.56 O
ANISOU 1218 O SER A 305 11905 11877 7208 3487 -135 1166 O
ATOM 1219 N GLN A 306 124.098 -41.135 8.109 1.00 86.88 N
ANISOU 1219 N GLN A 306 13259 12575 7855 3518 1818 N
ATOM 1220 CA GLN A 306 125.373 -40.818 8.724 1.00 88.90 C
ANISOU 1220 CA GLN A 306 13520 13186 7071 4412 -339 1572 C
ATOM 1221 CB GLN A 306 125.223 -40.565 10.227 1.00106.68 C
ANISOU 1221 CB GLN A 306 16223 15550 8761 4738 -295 1591 C
ATOM 1222 CG GLN A 306 125.659 -39.164 10.673 1.00122.35 C
ANISOU 1222 CG GLN A 306 18365 17726 10398 4623 -718 1078 C
ATOM 1223 CD GLN A 306 124.735 -38.051 10.183 1.00136.76 C
ANISOU 1223 CD GLN A 306 20271 19405 12288 4382 -504 881 C
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ANISOU 1224 OE1 GLN A 306 20950 19941 13286 4336 -3 1155 O
ATOM 1225 NE2 GLN A 306 125.147 -36.805 10.399 1.00138.57 N
ANISOU 1225 NE2 GLN A 306 20623 19709 12318 4209 -880 408 N
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ANISOU 1232 OD1 ASN A 307 16042 17858 11427 4934 -1993 1452 O
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ATOM 1238 CB ASN A 308 126.024 -45.626 5.200 1.00 79.22 C
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ATOM 1239 CG ASN A 308 124.826 -44.874 5.730 1.00 83.81 C
ANISOU 1239 CG ASN A 308 11968 11438 8438 4020 484 2392 C
ATOM 1240 OD1 ASN A 308 124.714 -43.664 5.548 1.00 61.56 O
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ATOM 1241 ND2 ASN A 308 123.926 -45.585 6.398 1.00 95.78 N
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ATOM 1244 N CYS A 309 127.064 -42.984 2.973 1.00 55.06 N
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ATOM 1245 CA CYS A 309 126.673 -42.362 1.736 1.00 50.64 C
ANISOU 1245 CA CYS A 309 6479 7608 5152 2763 -417 933 C
ATOM 1246 CB CYS A 309 125.306 -41.706 1.899 1.00 55.78 C
ANISOU 1246 CB CYS A 309 7323 8091 5781 2596 -118 975 C
ATOM 1247 SG CYS A 309 124.592 -41.092 0.370 1.00109.82 S
ANISOU 1247 SG CYS A 309 13897 14750 13079 2128 10 742 S
ATOM 1248 C CYS A 309 127.720 -41.323 1.391 1.00 62.38 C
ANISOU 1248 C CYS A 309 7714 9419 6568 2568 -806 567 C
ATOM 1249 O CYS A 309 128.319 -40.719 2.275 1.00 61.60 O
ANISOU 1249 O CYS A 309 7710 9600 6094 2674 -1105 463 O
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ANISOU 1250 N ARG A 310 7089 9066 6614 2275 -807 372 N
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ANISOU 1254 CD ARG A 310 12907 16637 12963 1800 -1940 -385 C
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ATOM 1282 N TYR A 314 130.514 -33.670 -10.078 1.00 52.80 N
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ATOM 1283 CA TYR A 314 131.604 -33.358 -10.988 1.00 59.38 C
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ATOM 1284 CB TYR A 314 132.372 -34.618 -11.378 1.00 46.79 C
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ANISOU 1287 CE1 TYR A 314 4922 8865 7761 446 -89 -830 C
ATOM 1288 CZ TYR A 314 129.950 -37.672 -13.162 1.00 52.64 C
ANISOU 1288 CZ TYR A 314 4433 8329 7239 471 96 -875 C
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ANISOU 1289 OH TYR A 314 6127 9606 8725 663 145 -934 O
ATOM 1290 CE2 TYR A 314 130.612 -36.765 -13.974 1.00 45.51 C
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ANISOU 1291 CD2 TYR A 314 2665 7282 5899 42 156 -815 C
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ANISOU 1292 C TYR A 314 4237 8415 7276 -763 -55 -833 C
ATOM 1293 O TYR A 314 129.976 -32.799 -12.659 1.00 53.17 O
ANISOU 1293 O TYR A 314 4627 8305 7270 -629 41 -826 O
ATOM 1294 N GLN A 315 132.004 -31.835 -12.789 1.00 73.26 N
ANISOU 1294 N GLN A 315 8269 9110 10457 141 -456 2692 N
ATOM 1295 CA GLN A 315 131.682 -31.071 -13.970 1.00 75.45 C
ANISOU 1295 CA GLN A 315 9227 8921 10520 5 -355 2863 C
ATOM 1296 CB GLN A 315 131.782 -29.587 -13.667 1.00 77.58 C
ANISOU 1296 CB GLN A 315 9717 8958 10803 -265 73 2800 C
ATOM 1297 CG GLN A 315 130.827 -28.728 -14.453 1.00 90.47 C
ANISOU 1297 CG GLN A 315 12046 10035 12292 -175 41 3173 C
ATOM 1298 CD GLN A 315 130.637 -27.372 -13.810 1.00 93.01 C
ANISOU 1298 CD GLN A 315 12461 10118 12762 -349 350 3165 C
ATOM 1299 OE1 GLN A 315 131.018 -27.164 -12.656 1.00 89.11 O
ANISOU 1299 OE1 GLN A 315 11435 9905 12517 -458 452 2878 O
ATOM 1300 NE2 GLN A 315 130.048 -26.438 -14.551 1.00 94.84 N
ANISOU 1300 NE2 GLN A 315 13385 9837 12813 -307 487 3452 N
ATOM 1301 C GLN A 315 132.660 -31.460 -15.058 1.00 85.58 C
ANISOU 1301 C GLN A 315 10745 10280 11491 -159 -133 2667 C
ATOM 1302 O GLN A 315 133.872 -31.346 -14.887 1.00 87.44 O
ANISOU 1302 O GLN A 315 10754 10784 11686 -458 292 2283 O
ATOM 1303 N GLU A 316 132.122 -31.948 -16.167 1.00 93.06 N
ANISOU 1303 N GLU A 316 12110 11010 12238 87 -449 2879 N
ATOM 1304 CA GLU A 316 132.944 -32.378 -17.282 1.00105.24 C
ANISOU 1304 CA GLU A 316 13941 12627 13416 48 -282 2736 C
ATOM 1305 CB GLU A 316 132.120 -33.240 -18.235 1.00114.41 C
ANISOU 1305 CB GLU A 316 15363 13652 14455 500 -893 2893 C
ATOM 1306 CG GLU A 316 132.753 -34.573 -18.582 1.00122.92 C
ANISOU 1306 CG GLU A 316 16147 15063 15495 591 -1104 2657 C
ATOM 1307 CD GLU A 316 131.724 -35.676 -18.747 1.00123.98 C
ANISOU 1307 CD GLU A 316 16060 15103 15943 1008 -1852 2711 C
ATOM 1308 OE1 GLU A 316 131.525 -36.142 -19.889 1.00123.64 O
ANISOU 1308 OE1 GLU A 316 16358 14968 15652 1322 -2192 2638 O
ATOM 1309 OE2 GLU A 316 131.115 -36.076 -17.731 1.00119.92 O
ANISOU 1309 OE2 GLU A 316 15014 14589 15959 1055 -2075 2803 O
ATOM 1310 C GLU A 316 133.463 -31.157 -18.014 1.00109.60 C
ANISOU 1310 C GLU A 316 15117 12873 13653 -194 381 2771 C
ATOM 1311 O GLU A 316 132.674 -30.320 -18.457 1.00113.83 O
ANISOU 1311 O GLU A 316 16227 12983 14038 -35 395 3075 O
ATOM 1312 N PRO A 317 134.796 -31.031 -18.125 1.00111.73 N
ANISOU 1312 N PRO A 317 15265 13325 13864 -561 985 2455 N
ATOM 1313 CA PRO A 317 135.320 -29.971 -18.987 1.00120.18 C
ANISOU 1313 CA PRO A 317 16968 14005 14689 -768 1748 2540 C
ATOM 1314 CB PRO A 317 136.828 -30.205 -18.945 1.00119.13 C
ANISOU 1314 CB PRO A 317 16423 14183 14659 -1174 2309 2077 C
ATOM 1315 CG PRO A 317 137.060 -30.809 -17.601 1.00110.79 C
ANISOU 1315 CG PRO A 317 14465 13637 13996 -1270 1934 1685 C
ATOM 1316 CD PRO A 317 135.864 -31.697 -17.360 1.00106.48 C
ANISOU 1316 CD PRO A 317 13857 13183 13418 -798 1078 1990 C
ATOM 1317 C PRO A 317 134.795 -30.149 -20.404 1.00127.42 C
ANISOU 1317 C PRO A 317 18712 14665 15039 -290 1592 2901 C
ATOM 1318 O PRO A 317 134.416 -31.255 -20.787 1.00130.44 O
ANISOU 1318 O PRO A 317 19028 15274 15261 91 939 2897 O
ATOM 1319 N ALA A 318 134.757 -29.066 -21.167 1.00135.01 N
ANISOU 1319 N ALA A 318 20452 15141 15705 -245 2186 3191 N
ATOM 1320 CA ALA A 318 134.265 -29.136 -22.533 1.00144.52 C
ANISOU 1320 CA ALA A 318 22543 16124 16244 366 2063 3528 C
ATOM 1321 CB ALA A 318 133.292 -28.005 -22.800 1.00144.93 C
ANISOU 1321 CB ALA A 318 23324 15649 16095 667 2151 3940 C
ATOM 1322 C ALA A 318 135.436 -29.077 -23.502 1.00155.29 C
ANISOU 1322 C ALA A 318 24319 17450 17233 299 2881 3522 C
ATOM 1323 O ALA A 318 135.313 -29.458 -24.665 1.00156.58 O
ANISOU 1323 O ALA A 318 25121 17609 16763 871 2760 3699 O
ATOM 1324 N ASP A 319 136.572 -28.598 -23.004 1.00164.45 N
ANISOU 1324 N ASP A 319 25077 18591 18815 -365 3714 3270 N
ATOM 1325 CA ASP A 319 137.777 -28.445 -23.812 1.00174.36 C
ANISOU 1325 CA ASP A 319 26611 19754 19884 -538 4665 3234 C
ATOM 1326 CB ASP A 319 138.796 -27.551 -23.098 1.00176.94 C
ANISOU 1326 CB ASP A 319 26440 19871 20918 -1328 5629 2910 C
ATOM 1327 CG ASP A 319 138.650 -27.587 -21.584 1.00170.39 C
ANISOU 1327 CG ASP A 319 24650 19336 20753 -1725 5120 2467 C
ATOM 1328 OD2 ASP A 319 139.444 -28.288 -20.921 1.00164.19 O
ANISOU 1328 OD2 ASP A 319 23021 19069 20293 -2021 4963 1922 O
ATOM 1329 OD1 ASP A 319 137.743 -26.908 -21.058 1.00170.65 O
ANISOU 1329 OD1 ASP A 319 24803 19101 20937 -1670 4881 2663 O
ATOM 1330 C ASP A 319 138.404 -29.787 -24.182 1.00175.38 C
ANISOU 1330 C ASP A 319 26406 20445 19784 -403 4303 2948 C
ATOM 1331 O ASP A 319 138.652 -30.063 -25.356 1.00179.26 O
ANISOU 1331 O ASP A 319 27527 20911 19672 19 4527 3145 O
ATOM 1332 N ASP A 320 138.666 -30.620 -23.180 1.00169.60 N
ANISOU 1332 N ASP A 320 24722 20225 19495 -693 3761 2491 N
ATOM 1333 CA ASP A 320 139.199 -31.953 -23.439 1.00162.15 C
ANISOU 1333 CA ASP A 320 23426 19811 18372 -543 3347 2209 C
ATOM 1334 CB ASP A 320 140.477 -32.211 -22.624 1.00154.29 C
ANISOU 1334 CB ASP A 320 21538 19212 17872 -1132 3716 1629 C
ATOM 1335 CG ASP A 320 140.195 -32.517 -21.160 1.00140.41 C
ANISOU 1335 CG ASP A 320 18937 17780 16633 -1309 3124 1322 C
ATOM 1336 OD1 ASP A 320 139.993 -31.568 -20.374 1.00134.61 O
ANISOU 1336 OD1 ASP A 320 18030 16823 16294 -1597 3353 1281 O
ATOM 1337 OD2 ASP A 320 140.174 -33.713 -20.801 1.00131.89 O
ANISOU 1337 OD2 ASP A 320 17395 17166 15551 -1107 2456 1135 O
ATOM 1338 C ASP A 320 138.136 -33.015 -23.166 1.00156.49 C
ANISOU 1338 C ASP A 320 22479 19354 17626 -97 2212 2232 C
ATOM 1339 O ASP A 320 137.556 -33.072 -22.080 1.00152.48 O
ANISOU 1339 O ASP A 320 21451 18919 17564 -218 1719 2167 O
ATOM 1340 N SER A 321 137.865 -33.850 -24.162 1.00155.79 N
ANISOU 1340 N SER A 321 22770 19372 17050 454 1703 2309 N
ATOM 1341 CA SER A 321 136.912 -34.938 -23.984 1.00148.13 C
ANISOU 1341 CA SER A 321 21503 18582 16198 857 631 2243 C

ATOM 1342 CB SER A 321 136.269 -35.331 -25.316 1.00152.02 C
ANISOU 1342 CB SER A 321 22697 18968 16095 1607 146 2375 C
ATOM 1343 OG SER A 321 134.886 -35.022 -25.325 1.00150.99 O
ANISOU 1343 OG SER A 321 22817 18534 16020 2000 -450 2573 O
ATOM 1344 C SER A 321 137.605 -36.140 -23.355 1.00139.27 C
ANISOU 1344 C SER A 321 19565 17956 15395 653 363 1848 C
ATOM 1345 O SER A 321 137.255 -37.286 -23.631 1.00137.43 O
ANISOU 1345 O SER A 321 19169 17894 15154 1018 -332 1729 O
ATOM 1346 N SER A 322 138.595 -35.862 -22.512 1.00134.09 N
ANISOU 1346 N SER A 322 18387 17516 15045 106 914 1599 N
ATOM 1347 CA SER A 322 139.367 -36.898 -21.837 1.00124.46 C
ANISOU 1347 CA SER A 322 16413 16805 14070 -41 738 1198 C
ATOM 1348 CB SER A 322 140.782 -36.974 -22.410 1.00125.86 C
ANISOU 1348 CB SER A 322 16587 17235 14000 -264 1379 898 C
ATOM 1349 OG SER A 322 141.628 -37.737 -21.569 1.00121.45 O
ANISOU 1349 OG SER A 322 15247 17188 13711 -452 1301 443 O
ATOM 1350 C SER A 322 139.427 -36.670 -20.327 1.00114.51 C
ANISOU 1350 C SER A 322 14458 15717 13333 -350 751 1020 C
ATOM 1351 O SER A 322 140.499 -36.490 -19.751 1.00117.25 O
ANISOU 1351 O SER A 322 14345 16365 13840 -700 1196 622 O
ATOM 1352 N PHE A 323 138.257 -36.666 -19.701 1.00 98.14 N
ANISOU 1352 N PHE A 323 12304 13459 11525 -161 255 1278 N
ATOM 1353 CA PHE A 323 138.142 -36.610 -18.256 1.00 90.65 C
ANISOU 1353 CA PHE A 323 10743 12699 11000 -267 166 1173 C
ATOM 1354 CB PHE A 323 136.985 -35.680 -17.878 1.00 81.28 C
ANISOU 1354 CB PHE A 323 9788 11097 9997 -237 72 1529 C
ATOM 1355 CG PHE A 323 136.132 -36.180 -16.747 1.00 77.40 C
ANISOU 1355 CG PHE A 323 8840 10672 9894 4 -398 1673 C
ATOM 1356 CD2 PHE A 323 136.348 -35.732 -15.454 1.00 80.07 C
ANISOU 1356 CD2 PHE A 323 8731 11228 10463 -103 -218 1522 C
ATOM 1357 CE2 PHE A 323 135.564 -36.177 -14.410 1.00 73.12 C
ANISOU 1357 CE2 PHE A 323 7494 10402 9888 204 -554 1723 C
ATOM 1358 CZ PHE A 323 134.541 -37.076 -14.655 1.00 71.61 C
ANISOU 1358 CZ PHE A 323 7327 9974 9908 535 -1030 2064 C
ATOM 1359 CE1 PHE A 323 134.309 -37.530 -15.943 1.00 72.94 C
ANISOU 1359 CE1 PHE A 323 7862 9910 9941 601 -1280 2120 C
ATOM 1360 CD1 PHE A 323 135.093 -37.073 -16.981 1.00 75.71 C
ANISOU 1360 CD1 PHE A 323 8637 10275 9854 379 -989 1936 C
ATOM 1361 C PHE A 323 137.896 -38.043 -17.798 1.00 78.80 C
ANISOU 1361 C PHE A 323 8792 11471 9679 72 -411 1148 C
ATOM 1362 O PHE A 323 137.410 -38.862 -18.574 1.00 78.84 O
ANISOU 1362 O PHE A 323 8994 11346 9615 363 -837 1277 O
ATOM 1363 N SER A 324 138.221 -38.354 -16.550 1.00 76.66 N
ANISOU 1363 N SER A 324 7929 11553 9646 98 -416 963 N
ATOM 1364 CA SER A 324 138.120 -39.735 -16.096 1.00 86.20 C
ANISOU 1364 CA SER A 324 8743 12992 11019 457 -816 971 C
ATOM 1365 CB SER A 324 139.505 -40.310 -15.804 1.00 75.19 C
ANISOU 1365 CB SER A 324 6950 12173 9445 429 -614 484 C
ATOM 1366 OG SER A 324 139.434 -41.708 -15.608 1.00 81.29 O
ANISOU 1366 OG SER A 324 7464 13098 10323 810 -968 532 O
ATOM 1367 C SER A 324 137.213 -39.905 -14.884 1.00 79.88 C
ANISOU 1367 C SER A 324 7631 12116 10603 736 -1025 1258 C
ATOM 1368 O SER A 324 137.592 -39.579 -13.760 1.00 75.64 O
ANISOU 1368 O SER A 324 6754 11893 10092 778 -827 1102 O
ATOM 1369 N LEU A 325 136.015 -40.425 -15.131 1.00 60.54 N
ANISOU 1369 N LEU A 325 8649 4434 9918 -162 -384 1802 N
ATOM 1370 CA LEU A 325 135.062 -40.708 -14.071 1.00 59.04 C
ANISOU 1370 CA LEU A 325 8051 4428 9952 254 -549 1741 C
ATOM 1371 CB LEU A 325 133.762 -41.238 -14.661 1.00 61.51 C
ANISOU 1371 CB LEU A 325 8508 5067 9797 450 -714 1932 C
ATOM 1372 CG LEU A 325 132.661 -41.391 -13.621 1.00 67.24 C
ANISOU 1372 CG LEU A 325 8863 5932 10755 782 -784 1807 C
ATOM 1373 CD1 LEU A 325 132.447 -40.052 -12.940 1.00 64.62 C
ANISOU 1373 CD1 LEU A 325 8330 5070 11151 844 -696 1593 C
ATOM 1374 CD2 LEU A 325 131.382 -41.873 -14.271 1.00 68.04 C
ANISOU 1374 CD2 LEU A 325 9071 6235 10546 866 -892 1916 C
ATOM 1375 C LEU A 325 135.644 -41.755 -13.135 1.00 50.75 C
ANISOU 1375 C LEU A 325 6643 4106 8532 416 -481 1465 C
ATOM 1376 O LEU A 325 135.478 -41.701 -11.919 1.00 52.59 O
ANISOU 1376 O LEU A 325 6502 4681 8800 661 -393 1008 O
ATOM 1377 N SER A 326 136.329 -42.710 -13.744 1.00 50.97 N
ANISOU 1377 N SER A 326 6839 4463 8062 276 -478 1686 N
ATOM 1378 CA SER A 326 137.016 -43.768 -13.032 1.00 53.85 C
ANISOU 1378 CA SER A 326 6923 5627 7911 432 -389 1420 C
ATOM 1379 CB SER A 326 137.823 -44.606 -14.018 1.00 52.10 C
ANISOU 1379 CB SER A 326 6967 5539 7289 182 -320 1724 C
ATOM 1380 OG SER A 326 137.857 -45.951 -13.610 1.00 76.36 O
ANISOU 1380 OG SER A 326 9910 9235 9869 470 -335 1817 O
ATOM 1381 C SER A 326 137.956 -43.191 -11.980 1.00 50.22 C
ANISOU 1381 C SER A 326 6308 5780 7746 390 -202 656 C
ATOM 1382 O SER A 326 137.951 -43.607 -10.818 1.00 51.82 O
ANISOU 1382 O SER A 326 5945 6293 7452 706 -216 308 O
ATOM 1383 N GLN A 327 138.766 -42.229 -12.406 1.00 44.35 N
ANISOU 1383 N GLN A 327 5357 4444 7050 -20 -19 383 N
ATOM 1384 CA GLN A 327 139.746 -41.596 -11.530 1.00 48.33 C
ANISOU 1384 CA GLN A 327 5451 5257 7655 -156 155 -408 C
ATOM 1385 CB GLN A 327 140.732 -40.777 -12.354 1.00 52.93 C
ANISOU 1385 CB GLN A 327 6157 5404 8548 -697 437 -601 C
ATOM 1386 CG GLN A 327 141.742 -41.643 -13.058 1.00 50.52 C
ANISOU 1386 CG GLN A 327 5894 5379 7921 -894 534 -477 C
ATOM 1387 CD GLN A 327 142.638 -42.363 -12.073 1.00 51.89 C
ANISOU 1387 CD GLN A 327 5503 6448 7764 -693 463 -999 C
ATOM 1388 OE1 GLN A 327 143.172 -41.750 -11.144 1.00 57.63 O
ANISOU 1388 OE1 GLN A 327 5794 7460 8640 -727 482 -1712 O
ATOM 1389 NE2 GLN A 327 142.793 -43.671 -12.255 1.00 51.46 N
ANISOU 1389 NE2 GLN A 327 5466 6838 7248 -467 363 -651 N
ATOM 1390 C GLN A 327 139.107 -40.706 -10.476 1.00 51.08 C
ANISOU 1390 C GLN A 327 5588 5492 8328 4 173 -833 C
ATOM 1391 O GLN A 327 139.614 -40.573 -9.363 1.00 63.13 O
ANISOU 1391 O GLN A 327 6739 7520 9726 76 205 -1483 O
ATOM 1392 N GLU A 328 138.005 -40.072 -10.851 1.00 56.97 N
ANISOU 1392 N GLU A 328 6587 5554 9506 52 149 -475 N
ATOM 1393 CA GLU A 328 137.294 -39.186 -9.945 1.00 67.32 C
ANISOU 1393 CA GLU A 328 7726 6626 11226 195 239 -835 C
ATOM 1394 CB GLU A 328 136.176 -38.447 -10.684 1.00 55.41 C
ANISOU 1394 CB GLU A 328 6519 4231 10304 222 198 -331 C
ATOM 1395 CG GLU A 328 135.508 -37.357 -9.869 1.00 72.04 C
ANISOU 1395 CG GLU A 328 8455 5935 12983 316 387 -718 C
ATOM 1396 CD GLU A 328 136.427 -36.182 -9.603 1.00 92.77 C
ANISOU 1396 CD GLU A 328 10997 8350 15903 -82 739 -1378 C
ATOM 1397 OE1 GLU A 328 136.622 -35.838 -8.416 1.00 98.81 O
ANISOU 1397 OE1 GLU A 328 11445 9428 16668 -70 920 -2077 O
ATOM 1398 OE2 GLU A 328 136.951 -35.601 -10.580 1.00100.16 O
ANISOU 1398 OE2 GLU A 328 12597 9165 17434 -431 864 -1219 O
ATOM 1399 C GLU A 328 136.721 -40.008 -8.791 1.00 67.22 C
ANISOU 1399 C GLU A 328 7284 8850 9761 1399 C GLU A 328 7484 7207 10850 642 137 -969 C
ATOM 1400 O GLU A 328 136.815 -39.625 -7.625 1.00 67.33 O
ANISOU 1400 O GLU A 328 7250 7484 10848 718 262 -1581 O
ATOM 1401 N VAL A 329 136.133 -41.149 -9.128 1.00 50.73 N
ANISOU 1401 N VAL A 329 5528 5305 8443 911 -53 -408 N
ATOM 1402 CA VAL A 329 135.567 -42.031 -8.118 1.00 50.22 C
ANISOU 1402 CA VAL A 329 5332 5743 8006 1331 -73 -474 C
ATOM 1403 CB VAL A 329 134.715 -43.143 -8.748 1.00 44.05 C
ANISOU 1403 CB VAL A 329 4741 4938 7057 1557 -227 217 C
ATOM 1404 CG1 VAL A 329 134.264 -44.134 -7.685 1.00 48.29 C
ANISOU 1404 CG1 VAL A 329 5192 5743 8006 1331 -73 -474 C
ATOM 1405 CG2 VAL A 329 133.503 -42.532 -9.433 1.00 41.12 C
ANISOU 1405 CG2 VAL A 329 4484 3797 7344 1559 -325 627 C
ATOM 1406 C VAL A 329 136.660 -42.615 -7.220 1.00 54.37 C
ANISOU 1406 C VAL A 329 5660 7097 7901 1410 -64 -962 C
ATOM 1407 O VAL A 329 136.498 -42.721 -6.004 1.00 45.85 O
ANISOU 1407 O VAL A 329 4460 6389 6573 1661 1 -1368 O
ATOM 1408 N LEU A 330 137.783 -42.980 -7.824 1.00 46.41 N
ANISOU 1408 N LEU A 330 4633 6359 6642 1202 -131 -931 N
ATOM 1409 CA LEU A 330 138.899 -43.505 -7.056 1.00 55.29 C
ANISOU 1409 CA LEU A 330 5503 8263 7241 1298 -194 -1388 C
ATOM 1410 CB LEU A 330 139.995 -44.038 -7.971 1.00 54.46 C
ANISOU 1410 CB LEU A 330 5374 8336 6982 1078 -228 -1214 C
ATOM 1411 CG LEU A 330 139.686 -45.380 -8.611 1.00 56.73 C
ANISOU 1411 CG LEU A 330 5905 8749 6899 1291 -276 -534 C
ATOM 1412 CD1 LEU A 330 140.641 -45.619 -9.758 1.00 53.07 C
ANISOU 1412 CD1 LEU A 330 5500 8198 6467 944 -201 -341 C
ATOM 1413 CD2 LEU A 330 139.812 -46.483 -7.573 1.00 51.48 C
ANISOU 1413 CD2 LEU A 330 5132 8823 5603 1778 -364 -622 C
ATOM 1414 C LEU A 330 139.468 -42.433 -6.141 1.00 57.39 C
ANISOU 1414 C LEU A 330 5486 8649 7671 1129 -136 -2203 C
ATOM 1415 O LEU A 330 139.975 -42.730 -5.061 1.00 63.33 O
ANISOU 1415 O LEU A 330 6037 10055 7971 1333 -246 -2678 O
ATOM 1416 N ARG A 331 139.387 -41.185 -6.586 1.00 54.75 N
ANISOU 1416 N ARG A 331 5169 7669 7965 752 36 -2366 N
ATOM 1417 CA ARG A 331 139.896 -40.072 -5.798 1.00 64.26 C
ANISOU 1417 CA ARG A 331 6120 8892 9405 511 162 -3176 C
ATOM 1418 CB ARG A 331 139.832 -38.764 -6.588 1.00 67.85 C
ANISOU 1418 CB ARG A 331 6681 8494 10603 66 428 -3211 C
ATOM 1419 CG ARG A 331 139.639 -37.542 -5.719 1.00 87.83 C
ANISOU 1419 CG ARG A 331 9083 10770 13517 -84 661 -3885 C
ATOM 1420 CD ARG A 331 139.642 -36.251 -6.518 1.00 98.56 C
ANISOU 1420 CD ARG A 331 10587 11239 15622 -513 982 -3907 C
ATOM 1421 NE ARG A 331 138.468 -35.422 -6.244 1.00108.78 N
ANISOU 1421 NE ARG A 331 12029 11870 17433 -402 1183 -3845 N
ATOM 1422 CZ ARG A 331 138.194 -34.852 -5.071 1.00112.55 C
ANISOU 1422 CZ ARG A 331 12344 12422 17999 -363 1361 -4467 C
ATOM 1423 NH1 ARG A 331 139.002 -35.018 -4.030 1.00107.37 N
ANISOU 1423 NH1 ARG A 331 11405 12520 16872 -421 1296 -5206 N
ATOM 1424 NH2 ARG A 331 137.099 -34.115 -4.937 1.00116.88 N
ANISOU 1424 NH2 ARG A 331 13021 12277 19112 -257 1597 -4358 N
ATOM 1425 C ARG A 331 139.125 -39.947 -4.483 1.00 82.42 C
ANISOU 1425 C ARG A 331 8406 11367 11544 816 197 -3512 C
ATOM 1426 O ARG A 331 139.704 -39.666 -3.433 1.00 98.29 O
ANISOU 1426 O ARG A 331 10200 13848 13298 793 165 -4224 O
ATOM 1427 N HIS A 332 137.817 -40.166 -4.540 1.00 75.79 N
ANISOU 1427 N HIS A 332 7801 10141 10853 1087 270 -3025 N
ATOM 1428 CA HIS A 332 137.010 -40.170 -3.329 1.00 66.73 C
ANISOU 1428 CA HIS A 332 6692 9106 9556 1382 395 -3300 C
ATOM 1429 CB HIS A 332 135.526 -40.028 -3.659 1.00 67.38 C
ANISOU 1429 CB HIS A 332 6943 8490 10167 1548 561 -2806 C
ATOM 1430 CG HIS A 332 135.154 -38.666 -4.151 1.00 80.98 C
ANISOU 1430 CG HIS A 332 8649 9378 12744 1259 756 -2871 C
ATOM 1431 ND1 HIS A 332 135.535 -38.196 -5.387 1.00 93.26 N
ANISOU 1431 ND1 HIS A 332 10274 10483 14679 959 684 -2552 N

ATOM 1432 CE1 HIS A 332 135.073 -36.966 -5.545 1.00 95.60 C
ANISOU 1432 CE1 HIS A 332 10592 10025 15705 791 915 -2663 C
ATOM 1433 NE2 HIS A 332 134.416 -36.625 -4.454 1.00 93.80 N
ANISOU 1433 NE2 HIS A 332 10268 9751 15620 953 1149 -3070 N
ATOM 1434 CD2 HIS A 332 134.454 -37.670 -3.560 1.00 86.16 C
ANISOU 1434 CD2 HIS A 332 9267 9531 13939 1232 1063 -3217 C
ATOM 1435 C HIS A 332 137.234 -41.443 -2.529 1.00 67.50 C
ANISOU 1435 C HIS A 332 6838 10015 8795 1781 225 -3299 C
ATOM 1436 O HIS A 332 137.463 -41.396 -1.322 1.00 69.48 O
ANISOU 1436 O HIS A 332 7066 10714 8618 1903 235 -3861 O
ATOM 1437 N LEU A 333 137.162 -42.575 -3.223 1.00 63.88 N
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ATOM 1438 CA LEU A 333 137.325 -43.892 -2.612 1.00 74.05 C
ANISOU 1438 CA LEU A 333 7893 11682 8561 2398 -34 -2526 C
ATOM 1439 CB LEU A 333 137.459 -44.967 -3.690 1.00 69.09 C
ANISOU 1439 CB LEU A 333 7355 11111 7785 2470 -148 -1833 C
ATOM 1440 CG LEU A 333 136.282 -45.907 -3.924 1.00 73.24 C
ANISOU 1440 CG LEU A 333 8146 11437 8246 2764 -16 -1218 C
ATOM 1441 CD1 LEU A 333 136.734 -47.344 -3.775 1.00 81.65 C
ANISOU 1441 CD1 LEU A 333 9440 12971 8612 2889 -138 -869 C
ATOM 1442 CD2 LEU A 333 135.169 -45.619 -2.955 1.00 75.23 C
ANISOU 1442 CD2 LEU A 333 8537 11425 8624 2879 218 -1382 C
ATOM 1443 C LEU A 333 138.525 -43.981 -1.675 1.00 82.19 C
ANISOU 1443 C LEU A 333 8752 13481 8997 2462 -251 -3141 C
ATOM 1444 O LEU A 333 138.441 -44.549 -0.587 1.00 89.91 O
ANISOU 1444 O LEU A 333 9904 14840 9419 2726 -323 -3194 O
ATOM 1445 N ARG A 334 139.646 -43.421 -2.102 1.00 75.04 N
ANISOU 1445 N ARG A 334 7536 12681 8297 2109 -403 -3472 N
ATOM 1446 CA ARG A 334 140.856 -43.471 -1.300 1.00 86.72 C
ANISOU 1446 CA ARG A 334 8741 14906 9302 2144 -689 -4099 C
ATOM 1447 CB ARG A 334 142.073 -43.093 -2.142 1.00 79.76 C
ANISOU 1447 CB ARG A 334 7469 14055 8782 1734 -799 -4300 C
ATOM 1448 CG ARG A 334 142.540 -44.219 -3.038 1.00 71.60 C
ANISOU 1448 CG ARG A 334 6425 13204 7575 1872 -901 -3710 C
ATOM 1449 CD ARG A 334 142.931 -43.711 -4.406 1.00 78.55 C
ANISOU 1449 CD ARG A 334 7218 13530 9098 1370 -716 -3528 C
ATOM 1450 NE ARG A 334 143.455 -44.775 -5.257 1.00 79.10 N
ANISOU 1450 NE ARG A 334 7290 13766 8998 1452 -755 -3027 N
ATOM 1451 CZ ARG A 334 143.721 -44.629 -6.550 1.00 84.77 C
ANISOU 1451 CZ ARG A 334 8077 13998 10136 1065 -553 -2716 C
ATOM 1452 NH1 ARG A 334 143.501 -43.461 -7.139 1.00 93.59 N
ANISOU 1452 NH1 ARG A 334 9290 14426 11845 605 -324 -2816 N
ATOM 1453 NH2 ARG A 334 144.200 -45.650 -7.251 1.00 63.69 N
ANISOU 1453 NH2 ARG A 334 5432 11492 7275 1140 -542 -2298 N
ATOM 1454 C ARG A 334 140.765 -42.597 -0.053 1.00106.79 C
ANISOU 1454 C ARG A 334 11265 17540 11770 2063 -659 -4808 C
ATOM 1455 O ARG A 334 141.549 -41.661 0.094 1.00120.52 O
ANISOU 1455 O ARG A 334 12685 19344 13764 1690 -715 -5470 O
ATOM 1456 N GLN A 335 139.790 -42.919 0.807 1.00106.24 N
ANISOU 1456 N GLN A 335 11563 17353 11451 2318 -531 -4541 N
ATOM 1457 CA GLN A 335 139.553 -42.335 2.141 1.00109.47 C
ANISOU 1457 CA GLN A 335 12109 17782 11704 2260 -455 -4970 C
ATOM 1458 CB GLN A 335 139.856 -40.839 2.213 1.00106.86 C
ANISOU 1458 CB GLN A 335 11521 17201 11878 1789 -310 -5741 C
ATOM 1459 CG GLN A 335 138.927 -39.988 1.380 1.00100.18 C
ANISOU 1459 CG GLN A 335 10712 15519 11833 1588 131 -5734 C
ATOM 1460 CD GLN A 335 139.678 -39.126 0.389 1.00105.46 C
ANISOU 1460 CD GLN A 335 11038 15898 13134 1133 156 -6015 C
ATOM 1461 OE1 GLN A 335 139.183 -38.088 -0.048 1.00113.37 O
ANISOU 1461 OE1 GLN A 335 12049 16138 14888 827 490 -6049 O
ATOM 1462 NE2 GLN A 335 140.884 -39.548 0.033 1.00103.48 N
ANISOU 1462 NE2 GLN A 335 10504 16175 12640 1055 -178 -6101 N
ATOM 1463 C GLN A 335 138.098 -42.552 2.541 1.00110.98 C
ANISOU 1463 C GLN A 335 12751 17492 11923 2440 -78 -4603 C
ATOM 1464 O GLN A 335 137.744 -43.571 3.133 1.00109.72 O
ANISOU 1464 O GLN A 335 12908 17475 11306 2730 -97 -4162 O
TER 1465 GLN A 335
HETATM 1465 OAD DRG C 1 113.462 -38.019 -10.559 1.00 29.78 O
HETATM 1466 CAQ DRG C 1 113.397 -39.177 -10.166 1.00 40.86 C
HETATM 1467 CAS DRG C 1 113.580 -40.249 -11.022 1.00 40.22 C
HETATM 1468 CAJ DRG C 1 113.855 -40.035 -12.369 1.00 32.92 C
HETATM 1469 CAH DRG C 1 114.057 -41.134 -13.196 1.00 29.54 C
HETATM 1470 CAN DRG C 1 113.982 -42.436 -12.689 1.00 41.38 C
HETATM 1471 CAA DRG C 1 114.183 -43.537 -13.518 1.00 29.25 C
HETATM 1472 CAO DRG C 1 113.710 -42.644 -11.336 1.00 32.01 C
HETATM 1473 CAB DRG C 1 113.622 -43.906 -10.750 1.00 33.55 C
HETATM 1474 CAT DRG C 1 113.499 -41.553 -10.532 1.00 36.06 C
HETATM 1475 OAL DRG C 1 113.267 -41.828 -9.235 1.00 35.96 O
HETATM 1476 CAU DRG C 1 113.112 -40.793 -8.373 1.00 29.79 C
HETATM 1477 CAR DRG C 1 113.191 -39.466 -8.835 1.00 38.79 C
HETATM 1478 CAI DRG C 1 113.048 -38.423 -7.930 1.00 35.14 C
HETATM 1479 CAF DRG C 1 112.818 -38.723 -6.595 1.00 40.44 C
HETATM 1480 CAG DRG C 1 112.741 -40.042 -6.150 1.00 36.18 C
HETATM 1481 CAP DRG C 1 112.879 -41.100 -7.040 1.00 36.02 C
HETATM 1482 CAK DRG C 1 112.792 -42.415 -6.569 1.00 35.27 C
HETATM 1483 CAM DRG C 1 114.002 -43.331 -6.858 1.00 42.08 C
HETATM 1484 OAE DRG C 1 115.083 -42.798 -7.202 1.00 51.70 O
HETATM 1485 OAC DRG C 1 113.797 -44.559 -6.713 1.00 41.96 O
HETATM 1486 OAD DRG C 2 108.474 -38.473 -3.971 1.00 36.96 O
HETATM 1487 CAQ DRG C 2 108.627 -39.628 -4.372 1.00 49.22 C
HETATM 1488 CAS DRG C 2 108.520 -40.709 -3.521 1.00 43.19 C
HETATM 1489 CAJ DRG C 2 108.227 -40.522 -2.176 1.00 31.16 C
HETATM 1490 CAH DRG C 2 108.129 -41.637 -1.347 1.00 32.15 C
HETATM 1491 CAN DRG C 2 108.311 -42.932 -1.845 1.00 47.34 C
HETATM 1492 CAA DRG C 2 108.213 -44.057 -1.015 1.00 30.55 C
HETATM 1493 CAO DRG C 2 108.594 -43.114 -3.197 1.00 44.08 C
HETATM 1494 CAB DRG C 2 108.784 -44.373 -3.763 1.00 31.60 C
HETATM 1495 CAT DRG C 2 108.702 -42.002 -4.005 1.00 44.81 C
HETATM 1496 OAL DRG C 2 108.961 -42.249 -5.314 1.00 40.22 O
HETATM 1497 CAU DRG C 2 109.053 -41.199 -6.163 1.00 34.93 C
HETATM 1498 CAR DRG C 2 108.884 -39.890 -5.703 1.00 42.08 C
HETATM 1499 CAI DRG C 2 108.976 -38.828 -6.597 1.00 36.30 C
HETATM 1500 CAF DRG C 2 109.251 -39.098 -7.930 1.00 38.45 C
HETATM 1501 CAG DRG C 2 109.418 -40.405 -8.378 1.00 43.73 C
HETATM 1502 CAP DRG C 2 109.326 -41.476 -7.499 1.00 34.19 C
HETATM 1503 CAK DRG C 2 109.511 -42.771 -7.991 1.00 41.63 C
HETATM 1504 CAM DRG C 2 108.391 -43.779 -7.682 1.00 52.21 C
HETATM 1505 OAE DRG C 2 107.239 -43.341 -7.449 1.00 53.23 O
HETATM 1506 OAC DRG C 2 108.735 -44.980 -7.713 1.00 50.44 O
ATOM 1507 N SER B 154 109.380 -24.066 -8.178 1.00 59.21 N
ANISOU 1507 N SER B 154 8214 7141 7141 -67 -526 997 N
ATOM 1508 CA SER B 154 108.231 -24.663 -7.508 1.00 59.32 C
ANISOU 1508 CA SER B 154 8128 6918 7492 -96 -101 651 C
ATOM 1509 CB SER B 154 106.967 -24.499 -8.351 1.00 61.82 C
ANISOU 1509 CB SER B 154 7950 7074 8464 137 -192 514 C
ATOM 1510 OG SER B 154 105.850 -25.104 -7.726 1.00 66.10 O
ANISOU 1510 OG SER B 154 8348 7382 9384 112 240 177 O
ATOM 1511 C SER B 154 108.484 -26.143 -7.259 1.00 62.75 C
ANISOU 1511 C SER B 154 8644 7550 7646 -177 -8 653 C
ATOM 1512 O SER B 154 108.929 -26.861 -8.158 1.00 53.14 O
ANISOU 1512 O SER B 154 7288 6606 6298 -61 -286 817 O
ATOM 1513 N VAL B 155 108.195 -26.610 -6.049 1.00 47.86 N
ANISOU 1513 N VAL B 155 7000 5505 5681 -413 406 460 N
ATOM 1514 CA VAL B 155 108.467 -28.004 -5.756 1.00 42.30 C
ANISOU 1514 CA VAL B 155 6380 4949 4742 -515 452 512 C
ATOM 1515 CB VAL B 155 108.588 -28.294 -4.234 1.00 62.29 C
ANISOU 1515 CB VAL B 155 9366 7333 6968 -935 800 445 C
ATOM 1516 CG2 VAL B 155 107.236 -28.588 -3.609 1.00 50.37 C
ANISOU 1516 CG2 VAL B 155 7802 5561 5775 -1037 1306 19 C
ATOM 1517 CG1 VAL B 155 109.261 -27.125 -3.530 1.00 48.01 C
ANISOU 1517 CG1 VAL B 155 7957 5430 4853 -1197 815 551 C
ATOM 1518 C VAL B 155 107.453 -28.916 -6.449 1.00 42.87 C
ANISOU 1518 C VAL B 155 6060 5037 5190 -311 495 315 C
ATOM 1519 O VAL B 155 107.811 -29.985 -6.934 1.00 49.65 O
ANISOU 1519 O VAL B 155 6838 6094 5933 -248 348 423 O
ATOM 1520 N ALA B 156 106.198 -28.481 -6.524 1.00 38.64 N
ANISOU 1520 N ALA B 156 5258 4264 5158 -215 695 33 N
ATOM 1521 CA ALA B 156 105.155 -29.313 -7.118 1.00 46.04 C
ANISOU 1521 CA ALA B 156 5817 5192 6484 -67 716 -137 C
ATOM 1522 CB ALA B 156 103.788 -28.716 -6.886 1.00 40.11 C
ANISOU 1522 CB ALA B 156 4766 4085 6388 -15 1012 -439 C
ATOM 1523 C ALA B 156 105.398 -29.502 -8.609 1.00 37.09 C
ANISOU 1523 C ALA B 156 4426 4318 5347 136 221 70 C
ATOM 1524 O ALA B 156 105.096 -30.543 -9.183 1.00 35.58 O
ANISOU 1524 O ALA B 156 4079 4255 5185 178 152 30 O
ATOM 1525 N HIS B 157 105.945 -28.472 -9.230 1.00 37.65 N
ANISOU 1525 N HIS B 157 4496 4459 5351 209 -105 281 N
ATOM 1526 CA HIS B 157 106.222 -28.514 -10.655 1.00 48.59 C
ANISOU 1526 CA HIS B 157 5718 6092 6651 301 -565 479 C
ATOM 1527 CB HIS B 157 106.718 -27.139 -11.112 1.00 49.34 C
ANISOU 1527 CB HIS B 157 5844 6191 6711 334 -884 704 C
ATOM 1528 CG HIS B 157 107.091 -27.075 -12.565 1.00 34.29 C
ANISOU 1528 CG HIS B 157 3856 4553 4620 329 -1359 926 C
ATOM 1529 ND1 HIS B 157 108.357 -26.779 -12.980 1.00 44.41 N
ANISOU 1529 ND1 HIS B 157 5403 6038 5433 275 -1345 986 N
ATOM 1530 CE1 HIS B 157 108.386 -26.771 -14.314 1.00 40.71 C
ANISOU 1530 CE1 HIS B 157 4907 5692 4869 236 -1437 919 C
ATOM 1531 NE2 HIS B 157 107.182 -27.055 -14.747 1.00 41.99 N
ANISOU 1531 NE2 HIS B 157 4825 5799 5329 211 -1634 927 N
ATOM 1532 CD2 HIS B 157 106.334 -27.254 -13.677 1.00 29.33 C
ANISOU 1532 CD2 HIS B 157 2991 3973 4181 307 -1638 933 C
ATOM 1533 C HIS B 157 107.265 -29.588 -10.924 1.00 41.92 C
ANISOU 1533 C HIS B 157 5056 5536 5334 246 -592 584 C
ATOM 1534 O HIS B 157 107.106 -30.418 -11.822 1.00 49.38 O
ANISOU 1534 O HIS B 157 5875 6636 6253 253 -709 553 O
ATOM 1535 N GLY B 158 108.329 -29.572 -10.132 1.00 29.40 N
ANISOU 1535 N GLY B 158 3763 3988 3421 161 -477 711 N
ATOM 1536 CA GLY B 158 109.407 -30.533 -10.283 1.00 38.06 C
ANISOU 1536 CA GLY B 158 4966 5275 4218 -488 851 C
ATOM 1537 C GLY B 158 108.967 -31.929 -9.875 1.00 38.76 C
ANISOU 1537 C GLY B 158 5013 5304 4409 89 -237 684 C
ATOM 1538 O GLY B 158 109.416 -32.930 -10.421 1.00 37.24 O
ANISOU 1538 O GLY B 158 4761 5227 4161 110 -238 703 O
ATOM 1539 N LEU B 159 108.061 -31.994 -8.910 1.00 29.75 N
ANISOU 1539 N LEU B 159 3906 3954 3445 17 22 496 N
ATOM 1540 CA LEU B 159 107.623 -33.272 -8.373 1.00 31.76 C
ANISOU 1540 CA LEU B 159 4161 4131 3775 -60 267 352 C
ATOM 1541 CB LEU B 159 106.827 -33.073 -7.083 1.00 28.85 C
ANISOU 1541 CB LEU B 159 3939 3521 3503 -237 606 165 C
ATOM 1542 CG LEU B 159 107.459 -33.468 -5.751 1.00 46.24 C

ANISOU 1542 CG LEU B 159 6523 5642 5404 -537 764 293 C
ATOM 1543 CD2 LEU B 159 106.741 -32.721 -4.652 1.00 45.94 C
ANISOU 1543 CD2 LEU B 159 6701 5371 5384 -774 1116 73 C
ATOM 1544 CD1 LEU B 159 108.940 -33.159 -5.699 1.00 54.73 C
ANISOU 1544 CD1 LEU B 159 7794 6840 6162 -595 483 677 C
ATOM 1545 C LEU B 159 106.771 -33.993 -9.415 1.00 34.06 C
ANISOU 1545 C LEU B 159 4156 4484 4300 59 222 167 C
ATOM 1546 O LEU B 159 106.878 -35.206 -9.605 1.00 33.81 O
ANISOU 1546 O LEU B 159 4095 4495 4256 47 294 124 O
ATOM 1547 N ALA B 160 105.922 -33.227 -10.089 1.00 29.30 N
ANISOU 1547 N ALA B 160 3333 3857 3943 145 75 81 N
ATOM 1548 CA ALA B 160 105.052 -33.767 -11.118 1.00 33.09 C
ANISOU 1548 CA ALA B 160 3545 4392 4634 184 -60 -42 C
ATOM 1549 CB ALA B 160 104.076 -32.714 -11.606 1.00 28.13 C
ANISOU 1549 CB ALA B 160 2647 3652 4388 242 -281 -49 C
ATOM 1550 C ALA B 160 105.875 -34.325 -12.283 1.00 38.04 C
ANISOU 1550 C ALA B 160 4223 5270 4960 161 -263 57 C
ATOM 1551 O ALA B 160 105.629 -35.430 -12.770 1.00 31.69 O
ANISOU 1551 O ALA B 160 3368 4518 4154 111 -199 -73 O
ATOM 1552 N TRP B 161 106.852 -33.551 -12.731 1.00 30.18 N
ANISOU 1552 N TRP B 161 3343 4413 3712 168 -463 261 N
ATOM 1553 CA TRP B 161 107.751 -34.033 -13.763 1.00 36.31 C
ANISOU 1553 CA TRP B 161 4195 5402 4199 102 -544 316 C
ATOM 1554 CB TRP B 161 108.682 -32.927 -14.240 1.00 34.27 C
ANISOU 1554 CB TRP B 161 4043 5282 3696 87 -778 544 C
ATOM 1555 CG TRP B 161 107.969 -32.038 -15.169 1.00 24.91 C
ANISOU 1555 CG TRP B 161 2762 4152 2551 15 -1150 599 C
ATOM 1556 CD1 TRP B 161 107.358 -30.854 -14.875 1.00 29.59 C
ANISOU 1556 CD1 TRP B 161 3250 4604 3391 82 -1357 700 C
ATOM 1557 NE1 TRP B 161 106.771 -30.339 -16.000 1.00 32.70 N
ANISOU 1557 NE1 TRP B 161 3575 5001 3848 -12 -1640 717 N
ATOM 1558 CE2 TRP B 161 106.977 -31.208 -17.047 1.00 33.34 C
ANISOU 1558 CE2 TRP B 161 3753 5261 3652 -195 -1662 641 C
ATOM 1559 CD2 TRP B 161 107.720 -32.293 -16.546 1.00 40.53 C
ANISOU 1559 CD2 TRP B 161 4737 6301 4363 -188 -1381 572 C
ATOM 1560 CE3 TRP B 161 108.073 -33.331 -17.420 1.00 26.85 C
ANISOU 1560 CE3 TRP B 161 3113 4721 2366 -374 -1249 424 C
ATOM 1561 CZ3 TRP B 161 107.675 -33.251 -18.742 1.00 37.79 C
ANISOU 1561 CZ3 TRP B 161 4569 6222 3567 -656 -1518 416 C
ATOM 1562 CH2 TRP B 161 106.932 -32.154 -19.213 1.00 41.76 C
ANISOU 1562 CH2 TRP B 161 5014 6560 4292 -635 -1803 533 C
ATOM 1563 CZ2 TRP B 161 106.576 -31.122 -18.382 1.00 37.46 C
ANISOU 1563 CZ2 TRP B 161 4319 5834 4082 -396 -1863 637 C
ATOM 1564 C TRP B 161 108.548 -35.254 -13.328 1.00 34.70 C
ANISOU 1564 C TRP B 161 4073 5172 3940 107 -245 280 C
ATOM 1565 O TRP B 161 108.729 -36.192 -14.098 1.00 32.00 O
ANISOU 1565 O TRP B 161 3712 4896 3550 44 -146 156 O
ATOM 1566 N ALA B 162 109.029 -35.241 -12.093 1.00 28.82 N
ANISOU 1566 N ALA B 162 3426 4299 3224 141 -109 403 N
ATOM 1567 CA ALA B 162 109.778 -36.380 -11.572 1.00 29.10 C
ANISOU 1567 CA ALA B 162 3499 4249 3309 128 94 458 C
ATOM 1568 CB ALA B 162 110.371 -36.060 -10.219 1.00 27.34 C
ANISOU 1568 CB ALA B 162 3440 3905 3045 69 102 702 C
ATOM 1569 C ALA B 162 108.896 -37.634 -11.483 1.00 31.94 C
ANISOU 1569 C ALA B 162 3772 4499 3865 105 294 220 C
ATOM 1570 O ALA B 162 109.353 -38.754 -11.702 1.00 46.58 O
ANISOU 1570 O ALA B 162 5582 6299 5818 103 447 182 O
ATOM 1571 N TYR B 163 107.632 -37.438 -11.138 1.00 33.94 N
ANISOU 1571 N TYR B 163 3977 4685 4233 85 316 57 N
ATOM 1572 CA TYR B 163 106.722 -38.560 -10.979 1.00 36.48 C
ANISOU 1572 CA TYR B 163 4215 4901 4743 42 499 -163 C
ATOM 1573 CB TYR B 163 105.448 -38.111 -10.268 1.00 27.18 C
ANISOU 1573 CB TYR B 163 2977 3601 3750 9 577 -303 C
ATOM 1574 CG TYR B 163 104.498 -39.234 -9.938 1.00 35.21 C
ANISOU 1574 CG TYR B 163 3914 4498 4967 -61 790 -517 C
ATOM 1575 CD1 TYR B 163 104.943 -40.378 -9.274 1.00 44.03 C
ANISOU 1575 CD1 TYR B 163 5156 5515 6059 -140 967 -479 C
ATOM 1576 CE1 TYR B 163 104.073 -41.407 -8.967 1.00 35.72 C
ANISOU 1576 CE1 TYR B 163 4046 4349 5178 -225 1155 -666 C
ATOM 1577 CZ TYR B 163 102.739 -41.290 -9.323 1.00 36.72 C
ANISOU 1577 CZ TYR B 163 3964 4468 5522 -226 1179 -900 C
ATOM 1578 OH TYR B 163 101.861 -42.295 -9.025 1.00 44.92 O
ANISOU 1578 OH TYR B 163 4932 5397 6738 -324 1368 -1085 O
ATOM 1579 CE2 TYR B 163 102.278 -40.159 -9.981 1.00 41.54 C
ANISOU 1579 CE2 TYR B 163 4403 5154 6225 -144 980 -913 C
ATOM 1580 CD2 TYR B 163 103.154 -39.144 -10.283 1.00 32.94 C
ANISOU 1580 CD2 TYR B 163 3398 4172 4946 -64 782 -720 C
ATOM 1581 C TYR B 163 106.416 -39.157 -12.352 1.00 42.75 C
ANISOU 1581 C TYR B 163 4894 5812 5537 22 445 -339 C
ATOM 1582 O TYR B 163 106.279 -40.373 -12.519 1.00 36.33 O
ANISOU 1582 O TYR B 163 4055 4934 4813 -21 617 -486 O
ATOM 1583 N TYR B 164 106.339 -38.282 -13.344 1.00 39.30 N
ANISOU 1583 N TYR B 164 4423 5535 4973 3 192 -311 N
ATOM 1584 CA TYR B 164 106.093 -38.716 -14.702 1.00 38.13 C
ANISOU 1584 CA TYR B 164 4256 5521 4711 -136 96 -451 C
ATOM 1585 CB TYR B 164 105.678 -37.534 -15.568 1.00 37.79 C
ANISOU 1585 CB TYR B 164 4173 5618 4566 -221 -297 -347 C
ATOM 1586 CG TYR B 164 105.746 -37.817 -17.043 1.00 45.68 C
ANISOU 1586 CG TYR B 164 5275 6799 5280 -485 -443 -426 C
ATOM 1587 CD1 TYR B 164 104.855 -38.696 -17.646 1.00 41.06 C
ANISOU 1587 CD1 TYR B 164 4663 6212 4724 -684 -458 -619 C
ATOM 1588 CE1 TYR B 164 104.921 -38.952 -19.000 1.00 52.04 C
ANISOU 1588 CE1 TYR B 164 6235 7769 5767 -1035 -582 -704 C
ATOM 1589 CZ TYR B 164 105.891 -38.321 -19.762 1.00 57.32 C
ANISOU 1589 CZ TYR B 164 7106 8610 6063 -1183 -657 -610 C
ATOM 1590 OH TYR B 164 105.974 -38.562 -21.110 1.00 66.85 O
ANISOU 1590 OH TYR B 164 8569 9985 6847 -1631 -735 -721 O
ATOM 1591 CE2 TYR B 164 106.785 -37.443 -19.178 1.00 53.77 C
ANISOU 1591 CE2 TYR B 164 6639 8165 5627 -943 -642 -411 C
ATOM 1592 CD2 TYR B 164 106.708 -37.200 -17.831 1.00 49.78 C
ANISOU 1592 CD2 TYR B 164 5960 7492 5463 -599 -553 -313 C
ATOM 1593 C TYR B 164 107.324 -39.409 -15.280 1.00 40.21 C
ANISOU 1593 C TYR B 164 4641 5838 4801 -184 297 -483 C
ATOM 1594 O TYR B 164 107.243 -40.521 -15.804 1.00 37.31 O
ANISOU 1594 O TYR B 164 4291 5434 4452 -291 499 -697 O
ATOM 1595 N ILE B 165 108.462 -38.752 -15.180 1.00 30.92 N
ANISOU 1595 N ILE B 165 3529 4712 3507 -113 275 -281 N
ATOM 1596 CA ILE B 165 109.696 -39.275 -15.703 1.00 31.32 C
ANISOU 1596 CA ILE B 165 3629 4780 3490 -151 497 -299 C
ATOM 1597 CB ILE B 165 110.793 -38.200 -15.709 1.00 33.02 C
ANISOU 1597 CB ILE B 165 3889 5094 3562 -96 368 -34 C
ATOM 1598 CG1 ILE B 165 110.470 -37.098 -16.706 1.00 35.79 C
ANISOU 1598 CG1 ILE B 165 4333 5673 3593 -242 45 -3 C
ATOM 1599 CD1 ILE B 165 110.094 -37.550 -18.016 1.00 30.89 C
ANISOU 1599 CD1 ILE B 165 3822 5188 2728 -534 92 -246 C
ATOM 1600 CG2 ILE B 165 112.142 -38.783 -15.962 1.00 26.33 C
ANISOU 1600 CG2 ILE B 165 3006 4189 2810 -97 672 -29 C
ATOM 1601 C ILE B 165 110.202 -40.535 -15.024 1.00 39.00 C
ANISOU 1601 C ILE B 165 4520 5510 4789 -56 826 -330 C
ATOM 1602 O ILE B 165 110.686 -41.435 -15.667 1.00 47.32 O
ANISOU 1602 O ILE B 165 5550 6484 5945 -118 1123 -510 O
ATOM 1603 N GLY B 166 110.100 -40.567 -13.712 1.00 40.03 N
ANISOU 1603 N GLY B 166 4619 5493 5098 54 783 -152 N
ATOM 1604 CA GLY B 166 110.625 -41.640 -12.925 1.00 36.59 C
ANISOU 1604 CA GLY B 166 4110 4803 4991 108 982 -58 C
ATOM 1605 C GLY B 166 109.706 -42.758 -12.547 1.00 40.38 C
ANISOU 1605 C GLY B 166 4563 5121 5657 70 1120 -238 C
ATOM 1606 O GLY B 166 110.115 -43.643 -11.873 1.00 43.27 O
ANISOU 1606 O GLY B 166 4876 5247 6316 88 1229 -114 O
ATOM 1607 N TYR B 167 108.455 -42.676 -12.935 1.00 31.17 N
ANISOU 1607 N TYR B 167 3417 4065 4361 -4 1079 -491 N
ATOM 1608 CA TYR B 167 107.505 -43.715 -12.650 1.00 39.43 C
ANISOU 1608 CA TYR B 167 4429 4969 5583 -60 1221 -681 C
ATOM 1609 CB TYR B 167 106.820 -43.484 -11.323 1.00 28.55 C
ANISOU 1609 CB TYR B 167 3086 3508 4253 -71 1158 -563 C
ATOM 1610 CG TYR B 167 105.890 -44.568 -10.958 1.00 34.39 C
ANISOU 1610 CG TYR B 167 3796 4100 5172 -153 1315 -741 C
ATOM 1611 CD1 TYR B 167 106.352 -45.820 -10.638 1.00 41.93 C
ANISOU 1611 CD1 TYR B 167 4740 4829 6362 -171 1485 -710 C
ATOM 1612 CE1 TYR B 167 105.513 -46.806 -10.317 1.00 30.94 C
ANISOU 1612 CE1 TYR B 167 3336 3295 5124 -267 1619 -864 C
ATOM 1613 CZ TYR B 167 104.189 -46.571 -10.310 1.00 40.47 C
ANISOU 1613 CZ TYR B 167 4518 4595 6263 -346 1604 -1061 C
ATOM 1614 OH TYR B 167 103.337 -47.567 -9.970 1.00 50.37 O
ANISOU 1614 OH TYR B 167 5752 5717 7670 -460 1746 -1216 O
ATOM 1615 CE2 TYR B 167 103.699 -45.345 -10.614 1.00 36.07 C
ANISOU 1615 CE2 TYR B 167 3918 4230 5555 -313 1445 -1087 C
ATOM 1616 CD2 TYR B 167 104.542 -44.358 -10.939 1.00 39.25 C
ANISOU 1616 CD2 TYR B 167 4356 4764 5791 -218 1291 -923 C
ATOM 1617 C TYR B 167 106.501 -44.020 -13.752 1.00 39.73 C
ANISOU 1617 C TYR B 167 4455 5126 5516 -192 1212 -995 C
ATOM 1618 O TYR B 167 106.489 -45.079 -14.286 1.00 49.78 O
ANISOU 1618 O TYR B 167 5733 6312 6869 -281 1422 -1216 O
ATOM 1619 N LEU B 168 105.650 -43.069 -14.059 1.00 38.42 N
ANISOU 1619 N LEU B 168 4266 5126 5205 -231 951 -994 N
ATOM 1620 CA LEU B 168 104.580 -43.235 -14.996 1.00 43.70 C
ANISOU 1620 CA LEU B 168 4899 5896 5809 -408 819 -1197 C
ATOM 1621 CB LEU B 168 103.733 -41.984 -15.022 1.00 35.81 C
ANISOU 1621 CB LEU B 168 3785 5003 4818 -408 467 -1082 C
ATOM 1622 CG LEU B 168 102.958 -41.719 -13.757 1.00 49.06 C
ANISOU 1622 CG LEU B 168 5326 6527 6789 -282 526 -1041 C
ATOM 1623 CD1 LEU B 168 102.083 -40.540 -13.960 1.00 52.56 C
ANISOU 1623 CD1 LEU B 168 5772 6998 7203 -223 -971 C
ATOM 1624 CD2 LEU B 168 102.148 -42.900 -13.390 1.00 47.62 C
ANISOU 1624 CD2 LEU B 168 5087 6197 6809 -343 756 -1233 C
ATOM 1625 C LEU B 168 104.998 -43.560 -16.408 1.00 46.97 C
ANISOU 1625 C LEU B 168 5452 6424 5969 -620 869 -1363 C
ATOM 1626 O LEU B 168 104.392 -44.352 -17.051 1.00 42.91 O
ANISOU 1626 O LEU B 168 4986 5889 5430 -823 955 -1599 O
ATOM 1627 N ARG B 169 106.029 -42.934 -16.907 1.00 44.92 N
ANISOU 1627 N ARG B 169 5291 6281 5497 -627 845 -1264 N
ATOM 1628 CA ARG B 169 106.448 -43.261 -18.265 1.00 51.77 C
ANISOU 1628 CA ARG B 169 6345 7255 5069 -915 963 -1469 C
ATOM 1629 CB ARG B 169 107.262 -42.140 -18.904 1.00 47.70 C
ANISOU 1629 CB ARG B 169 5942 6904 5278 -1317 1243 -1243 C
ATOM 1630 CG ARG B 169 108.733 -42.167 -18.591 1.00 48.59 C
ANISOU 1630 CG ARG B 169 6032 6960 5470 -810 1118 -1243 C
ATOM 1631 CD ARG B 169 109.431 -41.113 -19.415 1.00 54.09 C
ANISOU 1631 CD ARG B 169 6869 7877 5806 -964 976 -1141 C
ATOM 1632 NE ARG B 169 110.850 -41.013 -19.107 1.00 63.98 N

ANISOU 1632 NE ARG B 169 8050 9045 7216 -791 1245 -1030 N
ATOM 1633 CZ ARG B 169 111.715 -40.276 -19.792 1.00 60.86 C
ANISOU 1633 CZ ARG B 169 7759 8802 6562 -921 1255 -972 C
ATOM 1634 NH1 ARG B 169 111.303 -39.568 -20.832 1.00 49.23 N
ANISOU 1634 NH1 ARG B 169 6515 7583 4609 -1258 985 -1003 N
ATOM 1635 NH2 ARG B 169 112.994 -40.253 -19.436 1.00 58.96 N
ANISOU 1635 NH2 ARG B 169 7386 8447 6569 -748 1506 -851 N
ATOM 1636 C ARG B 169 107.197 -44.600 -18.308 1.00 48.60 C
ANISOU 1636 C ARG B 169 5973 6632 5859 -912 1484 -1706 C
ATOM 1637 O ARG B 169 107.495 -45.130 -19.377 1.00 52.89 O
ANISOU 1637 O ARG B 169 6691 7190 6213 -1190 1738 -1981 O
ATOM 1638 N LEU B 170 107.479 -45.151 -17.133 1.00 40.85 N
ANISOU 1638 N LEU B 170 4830 5415 5278 -637 1647 -1596 N
ATOM 1639 CA LEU B 170 108.114 -46.457 -17.049 1.00 47.41 C
ANISOU 1639 CA LEU B 170 5611 5952 6450 -600 2094 -1763 C
ATOM 1640 CB LEU B 170 109.108 -46.521 -15.892 1.00 53.57 C
ANISOU 1640 CB LEU B 170 6211 6509 7634 -313 2155 -1449 C
ATOM 1641 CG LEU B 170 110.097 -45.373 -15.710 1.00 66.77 C
ANISOU 1641 CG LEU B 170 7851 8301 9217 -194 1992 -1146 C
ATOM 1642 CD1 LEU B 170 111.146 -45.791 -14.706 1.00 70.69 C
ANISOU 1642 CD1 LEU B 170 8158 8504 10196 4 2080 -844 C
ATOM 1643 CD2 LEU B 170 110.744 -44.956 -17.016 1.00 73.81 C
ANISOU 1643 CD2 LEU B 170 8847 9352 9847 -358 2148 -1323 C
ATOM 1644 C LEU B 170 107.084 -47.565 -16.869 1.00 51.00 C
ANISOU 1644 C LEU B 170 6061 6262 7055 -684 2185 -1972 C
ATOM 1645 O LEU B 170 107.252 -48.677 -17.360 1.00 70.42 O
ANISOU 1645 O LEU B 170 8563 8526 9668 -802 2553 -2255 O
ATOM 1646 N ILE B 171 106.017 -47.257 -16.153 1.00 45.67 N
ANISOU 1646 N ILE B 171 5326 5657 6370 -635 1891 -1850 N
ATOM 1647 CA ILE B 171 105.061 -48.283 -15.781 1.00 49.10 C
ANISOU 1647 CA ILE B 171 5723 5940 6992 -694 1975 -2002 C
ATOM 1648 CB ILE B 171 104.490 -48.060 -14.356 1.00 52.70 C
ANISOU 1648 CB ILE B 171 6063 6330 7632 -535 1822 -1772 C
ATOM 1649 CG1 ILE B 171 104.171 -49.392 -13.688 1.00 60.42 C
ANISOU 1649 CG1 ILE B 171 7006 7035 8916 -549 2038 -1852 C
ATOM 1650 CD1 ILE B 171 105.350 -49.985 -12.959 1.00 64.40 C
ANISOU 1650 CD1 ILE B 171 7470 7257 9741 -408 2211 -1650 C
ATOM 1651 CG2 ILE B 171 103.253 -47.167 -14.380 1.00 59.21 C
ANISOU 1651 CG2 ILE B 171 6827 7354 8315 -599 1513 -1760 C
ATOM 1652 C ILE B 171 103.921 -48.394 -16.792 1.00 50.43 C
ANISOU 1652 C ILE B 171 5985 6272 6902 -996 1834 -2246 C
ATOM 1653 O ILE B 171 103.399 -49.482 -17.031 1.00 66.95 O
ANISOU 1653 O ILE B 171 8121 8236 9078 -1153 2010 -2485 O
ATOM 1654 N LEU B 172 103.542 -47.270 -17.390 1.00 46.26 N
ANISOU 1654 N LEU B 172 5487 6008 6080 -1109 1476 -2151 N
ATOM 1655 CA LEU B 172 102.349 -47.229 -18.242 1.00 50.22 C
ANISOU 1655 CA LEU B 172 6032 6659 6390 -1430 1186 -2258 C
ATOM 1656 CB LEU B 172 101.850 -45.795 -18.449 1.00 40.37 C
ANISOU 1656 CB LEU B 172 4685 5623 5029 -1447 682 -1997 C
ATOM 1657 CG LEU B 172 101.233 -45.088 -17.243 1.00 47.35 C
ANISOU 1657 CG LEU B 172 5283 6438 6268 -1147 529 -1783 C
ATOM 1658 CD1 LEU B 172 100.701 -43.735 -17.671 1.00 50.62 C
ANISOU 1658 CD1 LEU B 172 5573 7000 6662 -1202 42 -1556 C
ATOM 1659 CD2 LEU B 172 100.125 -45.923 -16.591 1.00 51.57 C
ANISOU 1659 CD2 LEU B 172 5651 6817 7127 -1146 626 -1902 C
ATOM 1660 C LEU B 172 102.434 -47.940 -19.592 1.00 52.94 C
ANISOU 1660 C LEU B 172 6660 7050 6403 -1859 1328 -2559 C
ATOM 1661 O LEU B 172 101.421 -48.466 -20.054 1.00 64.79 O
ANISOU 1661 O LEU B 172 8209 8570 7838 -2151 1192 -2691 O
ATOM 1662 N PRO B 173 103.616 -47.930 -20.252 1.00 69.07 N
ANISOU 1662 N PRO B 173 8908 9107 8229 -1952 1615 -2678 N
ATOM 1663 CA PRO B 173 103.661 -48.552 -21.580 1.00 65.54 C
ANISOU 1663 CA PRO B 173 8804 8699 7398 -2463 1818 -3022 C
ATOM 1664 CB PRO B 173 105.138 -48.449 -21.958 1.00 60.37 C
ANISOU 1664 CB PRO B 173 8274 7993 6672 -2436 2257 -3137 C
ATOM 1665 CG PRO B 173 105.592 -47.229 -21.283 1.00 58.34 C
ANISOU 1665 CG PRO B 173 7812 7855 6498 -2075 1961 -2746 C
ATOM 1666 CD PRO B 173 104.876 -47.216 -19.965 1.00 64.01 C
ANISOU 1666 CD PRO B 173 8223 8476 7621 -1692 1733 -2509 C
ATOM 1667 C PRO B 173 103.226 -50.011 -21.602 1.00 68.20 C
ANISOU 1667 C PRO B 173 9201 8801 7913 -2595 2165 -3337 C
ATOM 1668 O PRO B 173 102.507 -50.404 -22.513 1.00 81.18 O
ANISOU 1668 O PRO B 173 11047 10538 9261 -3017 2041 -3425 O
ATOM 1669 N GLU B 174 103.648 -50.802 -20.624 1.00 68.37 N
ANISOU 1669 N GLU B 174 9005 8525 8450 -2209 2503 -3321 N
ATOM 1670 CA GLU B 174 103.288 -52.215 -20.620 1.00 73.99 C
ANISOU 1670 CA GLU B 174 9711 9000 9401 -2283 2767 -3462 C
ATOM 1671 CB GLU B 174 104.510 -53.097 -20.349 1.00 77.89 C
ANISOU 1671 CB GLU B 174 10088 9154 10354 -2066 3216 -3429 C
ATOM 1672 CG GLU B 174 105.588 -53.013 -21.418 1.00 97.84 C
ANISOU 1672 CG GLU B 174 12772 11666 12736 -2273 3506 -3539 C
ATOM 1673 CD GLU B 174 105.165 -53.638 -22.742 1.00121.13 C
ANISOU 1673 CD GLU B 174 16029 14678 15317 -2805 3698 -3828 C
ATOM 1674 OE1 GLU B 174 104.366 -54.601 -22.726 1.00129.64 O
ANISOU 1674 OE1 GLU B 174 17134 15665 16458 -2927 3758 -3949 O
ATOM 1675 OE2 GLU B 174 105.637 -53.164 -23.800 1.00125.30 O
ANISOU 1675 OE2 GLU B 174 16790 15349 15471 -3131 3789 -3917 O
ATOM 1676 C GLU B 174 102.180 -52.544 -19.621 1.00 77.17 C
ANISOU 1676 C GLU B 174 9931 9331 10061 -2139 2576 -3424 C
ATOM 1677 O GLU B 174 102.010 -53.698 -19.232 1.00 80.47 O
ANISOU 1677 O GLU B 174 10278 9517 10782 -2082 2794 -3464 O
ATOM 1678 N LEU B 175 101.427 -51.535 -19.206 1.00 58.22 N
ANISOU 1678 N LEU B 175 7398 7131 7591 -2072 2125 -3231 N
ATOM 1679 CA LEU B 175 100.394 -51.754 -18.205 1.00 59.56 C
ANISOU 1679 CA LEU B 175 7330 7233 8065 -1918 1957 -3105 C
ATOM 1680 CB LEU B 175 99.976 -50.447 -17.542 1.00 57.85 C
ANISOU 1680 CB LEU B 175 6882 7185 7913 -1699 1564 -2771 C
ATOM 1681 CG LEU B 175 98.934 -50.659 -16.447 1.00 64.25 C
ANISOU 1681 CG LEU B 175 7449 7894 9069 -1571 1506 -2694 C
ATOM 1682 CD1 LEU B 175 99.555 -51.412 -15.279 1.00 71.52 C
ANISOU 1682 CD1 LEU B 175 8359 8557 10258 -1332 1862 -2669 C
ATOM 1683 CD2 LEU B 175 98.362 -49.337 -15.991 1.00 55.00 C
ANISOU 1683 CD2 LEU B 175 6043 6853 8000 -1432 1174 -2446 C
ATOM 1684 C LEU B 175 99.163 -52.435 -18.795 1.00 69.82 C
ANISOU 1684 C LEU B 175 8693 8559 9275 -2292 1820 -3293 C
ATOM 1685 O LEU B 175 98.629 -53.389 -18.225 1.00 68.12 O
ANISOU 1685 O LEU B 175 8402 8155 9326 -2267 1978 -3392 O
ATOM 1686 N GLN B 176 98.708 -51.932 -19.937 1.00 64.96 N
ANISOU 1686 N GLN B 176 8229 8177 8276 -2684 1482 -3307 N
ATOM 1687 CA GLN B 176 97.522 -52.481 -20.571 1.00 69.72 C
ANISOU 1687 CA GLN B 176 8898 8824 8767 -3117 1247 -3420 C
ATOM 1688 CB GLN B 176 97.018 -51.579 -21.695 1.00 75.31 C
ANISOU 1688 CB GLN B 176 9713 9816 9084 -3507 679 -3217 C
ATOM 1689 CG GLN B 176 96.046 -50.522 -21.210 1.00 91.17 C
ANISOU 1689 CG GLN B 176 11299 11921 11419 -3375 117 -2869 C
ATOM 1690 CD GLN B 176 95.520 -49.646 -22.327 1.00103.56 C
ANISOU 1690 CD GLN B 176 12935 13709 12706 -3779 -538 -2589 C
ATOM 1691 OE1 GLN B 176 96.021 -49.686 -23.451 1.00105.79 O
ANISOU 1691 OE1 GLN B 176 13637 14101 12459 -4079 -549 -2590 O
ATOM 1692 NE2 GLN B 176 94.499 -48.849 -22.024 1.00102.03 N
ANISOU 1692 NE2 GLN B 176 12303 13533 12931 -3721 -1061 -2277 N
ATOM 1693 C GLN B 176 97.769 -53.895 -21.075 1.00 66.42 C
ANISOU 1693 C GLN B 176 8748 8250 8237 -3259 1689 -3652 C
ATOM 1694 O GLN B 176 96.835 -54.673 -21.233 1.00 72.91 O
ANISOU 1694 O GLN B 176 9587 9034 9084 -3456 1615 -3705 O
ATOM 1695 N ALA B 177 99.032 -54.226 -21.319 1.00 70.71 N
ANISOU 1695 N ALA B 177 9453 8688 8727 -3157 2155 -3765 N
ATOM 1696 CA ALA B 177 99.380 -55.580 -21.725 1.00 75.96 C
ANISOU 1696 CA ALA B 177 10273 9151 9438 -3264 2635 -3964 C
ATOM 1697 CB ALA B 177 100.761 -55.625 -22.350 1.00 66.79 C
ANISOU 1697 CB ALA B 177 9253 7919 8207 -3285 3059 -4044 C
ATOM 1698 C ALA B 177 99.315 -56.490 -20.509 1.00 70.57 C
ANISOU 1698 C ALA B 177 9334 8182 9297 -2911 2861 -3944 C
ATOM 1699 O ALA B 177 98.792 -57.604 -20.572 1.00 73.01 O
ANISOU 1699 O ALA B 177 9686 8361 9694 -3036 3009 -4062 O
ATOM 1700 N ARG B 178 99.851 -56.000 -19.397 1.00 64.80 N
ANISOU 1700 N ARG B 178 8361 7359 8902 -2498 2859 -3760 N
ATOM 1701 CA ARG B 178 99.839 -56.752 -18.150 1.00 73.39 C
ANISOU 1701 CA ARG B 178 9230 8187 10466 -2202 2995 -3642 C
ATOM 1702 CB ARG B 178 100.587 -55.999 -17.051 1.00 78.71 C
ANISOU 1702 CB ARG B 178 9717 8800 11391 -1823 2937 -3374 C
ATOM 1703 CG ARG B 178 102.080 -56.233 -17.029 1.00 77.77 C
ANISOU 1703 CG ARG B 178 9568 8477 11503 -1648 3197 -3259 C
ATOM 1704 CD ARG B 178 102.759 -55.204 -16.133 1.00 75.05 C
ANISOU 1704 CD ARG B 178 9097 8154 11263 -1343 3036 -2969 C
ATOM 1705 NE ARG B 178 102.770 -55.582 -14.718 1.00 65.21 N
ANISOU 1705 NE ARG B 178 7704 6691 10380 -1140 3006 -2729 N
ATOM 1706 CZ ARG B 178 102.641 -54.718 -13.717 1.00 65.38 C
ANISOU 1706 CZ ARG B 178 7662 6784 10397 -982 2810 -2517 C
ATOM 1707 NH1 ARG B 178 102.474 -53.432 -13.978 1.00 75.96 N
ANISOU 1707 NH1 ARG B 178 9018 8408 11437 -951 2622 -2513 N
ATOM 1708 NH2 ARG B 178 102.672 -55.140 -12.456 1.00 66.60 N
ANISOU 1708 NH2 ARG B 178 7752 6710 10842 -892 2824 -2321 N
ATOM 1709 C ARG B 178 98.418 -57.030 -17.681 1.00 73.50 C
ANISOU 1709 C ARG B 178 9158 8238 10530 -2295 2775 -3665 C
ATOM 1710 O ARG B 178 98.140 -58.063 -17.089 1.00 79.88 O
ANISOU 1710 O ARG B 178 9899 8851 11600 -2241 2929 -3662 O
ATOM 1711 N ILE B 179 97.514 -56.102 -17.933 1.00 62.83 N
ANISOU 1711 N ILE B 179 7772 7120 8978 -2456 2384 -3658 N
ATOM 1712 CA ILE B 179 96.158 -56.274 -17.449 1.00 71.25 C
ANISOU 1712 CA ILE B 179 8663 8203 10205 -2541 2158 -3632 C
ATOM 1713 CB ILE B 179 95.443 -54.925 -17.314 1.00 65.73 C
ANISOU 1713 CB ILE B 179 7729 7703 9544 -2572 1720 -3486 C
ATOM 1714 CG1 ILE B 179 95.988 -54.192 -16.090 1.00 60.28 C
ANISOU 1714 CG1 ILE B 179 6854 6973 9077 -2138 1800 -3251 C
ATOM 1715 CD1 ILE B 179 95.409 -52.812 -15.887 1.00 59.09 C
ANISOU 1715 CD1 ILE B 179 6440 7012 9000 -2035 1437 -3008 C
ATOM 1716 CG2 ILE B 179 93.937 -55.110 -17.199 1.00 56.99 C
ANISOU 1716 CG2 ILE B 179 6394 6637 8624 -2740 1452 -3434 C
ATOM 1717 C ILE B 179 95.393 -57.269 -18.322 1.00 81.45 C
ANISOU 1717 C ILE B 179 10125 9508 11315 -2894 2140 -3785 C
ATOM 1718 O ILE B 179 94.633 -58.109 -17.822 1.00 76.25 O
ANISOU 1718 O ILE B 179 9376 8734 10860 -2906 2191 -3808 O
ATOM 1719 N ARG B 180 95.630 -57.197 -19.626 1.00 89.48 N
ANISOU 1719 N ARG B 180 11422 10661 11915 -3209 2083 -3882 N
ATOM 1720 CA ARG B 180 95.027 -58.141 -20.557 1.00 90.84 C
ANISOU 1720 CA ARG B 180 11836 10840 11839 -3599 2025 -4025 C
ATOM 1721 CB ARG B 180 95.281 -57.728 -21.999 1.00 93.73 C
ANISOU 1721 CB ARG B 180 12543 11408 11662 -4006 1950 -4061 C
ATOM 1722 CG ARG B 180 94.506 -56.502 -22.397 1.00 99.35 C

ANISOU 1722 CG ARG B 180 13166 12380 12201 -4212 1280 -3807 C
ATOM 1723 CD ARG B 180 94.511 -56.305 -23.887 1.00116.30 C
ANISOU 1723 CD ARG B 180 15704 14718 13768 -4718 1066 -3777 C
ATOM 1724 NE ARG B 180 93.754 -55.121 -24.266 1.00123.66 N
ANISOU 1724 NE ARG B 180 16497 15864 14624 -4896 332 -3426 N
ATOM 1725 CZ ARG B 180 93.266 -54.910 -25.482 1.00130.00 C
ANISOU 1725 CZ ARG B 180 17556 16830 15009 -5382 -88 -3258 C
ATOM 1726 NH1 ARG B 180 93.452 -55.812 -26.437 1.00119.89 N
ANISOU 1726 NH1 ARG B 180 16728 15547 13276 -5784 212 -3459 N
ATOM 1727 NH2 ARG B 180 92.586 -53.802 -25.743 1.00138.81 N
ANISOU 1727 NH2 ARG B 180 18456 18085 16200 -5470 -790 -2866 N
ATOM 1728 C ARG B 180 95.532 -59.554 -20.316 1.00 77.93 C
ANISOU 1728 C ARG B 180 10281 8932 10398 -3496 2620 -4195 C
ATOM 1729 O ARG B 180 94.776 -60.517 -20.407 1.00 73.54 O
ANISOU 1729 O ARG B 180 9780 8296 9866 -3672 2647 -4286 O
ATOM 1730 N THR B 181 96.817 -59.669 -20.011 1.00 76.75 N
ANISOU 1730 N THR B 181 10101 8620 10439 -3221 3005 -4200 N
ATOM 1731 CA THR B 181 97.389 -60.967 -19.704 1.00 84.43 C
ANISOU 1731 CA THR B 181 11052 9284 11742 -3102 3455 -4281 C
ATOM 1732 CB THR B 181 98.907 -60.897 -19.502 1.00 85.82 C
ANISOU 1732 CB THR B 181 11138 9278 12194 -2839 3780 -4210 C
ATOM 1733 OG1 THR B 181 99.547 -60.747 -20.775 1.00 89.45 O
ANISOU 1733 OG1 THR B 181 11837 9810 12342 -3115 3992 -4384 O
ATOM 1734 CG2 THR B 181 99.414 -62.170 -18.838 1.00 69.58 C
ANISOU 1734 CG2 THR B 181 8933 6848 10657 -2657 4116 -4188 C
ATOM 1735 C THR B 181 96.728 -61.548 -18.464 1.00 78.25 C
ANISOU 1735 C THR B 181 10046 8352 11333 -2892 3393 -4166 C
ATOM 1736 O THR B 181 96.349 -62.718 -18.434 1.00 91.21 O
ANISOU 1736 O THR B 181 11729 9828 13096 -2988 3560 -4268 O
ATOM 1737 N TYR B 182 96.574 -60.715 -17.444 1.00 65.42 N
ANISOU 1737 N TYR B 182 8204 6785 9868 -2640 3165 -3957 N
ATOM 1738 CA TYR B 182 95.981 -61.170 -16.195 1.00 65.09 C
ANISOU 1738 CA TYR B 182 7978 6614 10140 -2485 3132 -3828 C
ATOM 1739 CB TYR B 182 96.085 -60.090 -15.123 1.00 62.91 C
ANISOU 1739 CB TYR B 182 7510 6397 9994 -2237 2962 -3601 C
ATOM 1740 CG TYR B 182 95.529 -60.536 -13.799 1.00 70.58 C
ANISOU 1740 CG TYR B 182 8348 7241 11227 -2143 2973 -3461 C
ATOM 1741 CD1 TYR B 182 96.340 -61.170 -12.865 1.00 74.18 C
ANISOU 1741 CD1 TYR B 182 8794 7438 11954 -1969 3144 -3287 C
ATOM 1742 CE1 TYR B 182 95.834 -61.582 -11.659 1.00 70.79 C
ANISOU 1742 CE1 TYR B 182 8317 6901 11681 -1955 3134 -3147 C
ATOM 1743 CZ TYR B 182 94.494 -61.366 -11.384 1.00 73.73 C
ANISOU 1743 CZ TYR B 182 8611 7431 11971 -2090 3020 -3207 C
ATOM 1744 OH TYR B 182 93.947 -61.771 -10.196 1.00 75.59 O
ANISOU 1744 OH TYR B 182 8831 7581 12307 -2121 3050 -3086 O
ATOM 1745 CE2 TYR B 182 93.676 -60.746 -12.296 1.00 67.69 C
ANISOU 1745 CE2 TYR B 182 7780 6896 11043 -2223 2857 -3371 C
ATOM 1746 CD2 TYR B 182 94.190 -60.337 -13.490 1.00 64.00 C
ANISOU 1746 CD2 TYR B 182 7398 6531 10389 -2265 2798 -3483 C
ATOM 1747 C TYR B 182 94.521 -61.577 -16.391 1.00 70.13 C
ANISOU 1747 C TYR B 182 8623 7343 10678 -2744 2943 -3929 C
ATOM 1748 O TYR B 182 94.052 -62.560 -15.816 1.00 74.03 O
ANISOU 1748 O TYR B 182 9080 7682 11367 -2746 3046 -3931 O
ATOM 1749 N ASN B 183 93.808 -60.813 -17.211 1.00 66.39 N
ANISOU 1749 N ASN B 183 8187 7114 9923 -2987 2620 -3976 N
ATOM 1750 CA ASN B 183 92.408 -61.092 -17.485 1.00 66.46 C
ANISOU 1750 CA ASN B 183 8157 7210 9885 -3269 2347 -4006 C
ATOM 1751 CB ASN B 183 91.748 -59.914 -18.191 1.00 75.57 C
ANISOU 1751 CB ASN B 183 9235 8623 10856 -3488 1859 -3907 C
ATOM 1752 CG ASN B 183 91.284 -58.850 -17.227 1.00 70.44 C
ANISOU 1752 CG ASN B 183 8196 8035 10532 -3258 1658 -3709 C
ATOM 1753 OD1 ASN B 183 91.136 -59.101 -16.030 1.00 69.33 O
ANISOU 1753 OD1 ASN B 183 7878 7765 10698 -3018 1864 -3665 O
ATOM 1754 ND2 ASN B 183 91.045 -57.648 -17.744 1.00 73.30 N
ANISOU 1754 ND2 ASN B 183 8430 8589 10833 -3354 1257 -3567 N
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ATOM 1756 O ASN B 183 91.109 -62.822 -18.523 1.00 75.62 O
ANISOU 1756 O ASN B 183 9582 8309 10840 -3810 2306 -4220 O
ATOM 1757 N GLN B 184 93.343 -62.868 -18.802 1.00 78.87 N
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ATOM 1759 CB GLN B 184 94.504 -64.036 -20.592 1.00 97.79 C
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ATOM 1760 CG GLN B 184 94.217 -64.700 -21.911 1.00109.17 C
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ATOM 1761 CD GLN B 184 93.268 -63.878 -22.753 1.00112.28 C
ANISOU 1761 CD GLN B 184 15483 13020 14159 -4810 3025 -4846 C
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ANISOU 1762 OE1 GLN B 184 15502 13424 14423 -4690 2577 -4626 O
ATOM 1763 NE2 GLN B 184 92.900 -64.404 -23.915 1.00 99.14 N
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ANISOU 1764 C GLN B 184 10785 8565 11874 -3596 3451 -4557 C
ATOM 1765 O GLN B 184 92.702 -66.206 -18.724 1.00 85.55 O
ANISOU 1765 O GLN B 184 11272 8913 12321 -3774 3452 -4642 O
ATOM 1766 N HIS B 185 94.555 -65.236 -17.900 1.00 78.95 N
ANISOU 1766 N HIS B 185 10212 7980 11805 -3235 3671 -4433 N
ATOM 1767 C HIS B 185 94.223 -66.709 -15.909 1.00100.85 C
ANISOU 1767 C HIS B 185 12734 10354 15229 -2939 3793 -4232 C
ATOM 1768 O HIS B 185 94.040 -67.867 -15.533 1.00 95.59 O
ANISOU 1768 O HIS B 185 12077 9458 14787 -2956 3934 -4255 O
ATOM 1769 CA HIS B 185 94.997 -66.425 -17.194 1.00 99.08 C
ANISOU 1769 CA HIS B 185 12681 10195 14771 -3067 3965 -4409 C
ATOM 1770 CB HIS B 185 96.499 -66.349 -16.931 1.00110.66 C
ANISOU 1770 CB HIS B 185 14033 11454 16557 -2791 4224 -4305 C
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ANISOU 1772 ND1 HIS B 185 17811 15031 19214 -3339 4466 -4733 N
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ANISOU 1773 CE1 HIS B 185 18375 15439 19570 -3455 4773 -4870 C
ATOM 1774 NE2 HIS B 185 98.884 -66.053 -19.708 1.00138.79 N
ANISOU 1774 NE2 HIS B 185 17918 14972 19845 -3127 4992 -4734 N
ATOM 1775 CD2 HIS B 185 98.657 -66.202 -18.365 1.00132.42 C
ANISOU 1775 CD2 HIS B 185 16870 14050 19395 -2814 4788 -4485 C
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ATOM 1777 CA TYR B 186 93.012 -65.832 -14.008 1.00 88.87 C
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ANISOU 1781 CE2 TYR B 186 14749 10161 15820 -2157 1746 -278 C
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ANISOU 1783 OH TYR B 186 16276 10854 17956 -1555 2152 -395 O
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ANISOU 1787 O TYR B 186 11448 9134 10905 -3350 1081 -398 O
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ANISOU 1792 OD1 ASN B 187 14898 13560 12646 -4661 690 -457 O
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ATOM 1797 CA ASN B 188 88.124 -68.517 -14.243 1.00 93.86 C
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ATOM 1798 CB ASN B 188 88.709 -69.924 -14.299 1.00102.50 C
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ANISOU 1799 CG ASN B 188 16043 10993 12913 -5740 1181 -729 C
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ANISOU 1800 OD1 ASN B 188 17406 12836 13835 -6133 1043 -736 O
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ANISOU 1801 ND2 ASN B 188 15242 9042 12011 -5688 1495 -952 N
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ANISOU 1806 CB LEU B 189 11687 9468 11601 -3612 821 76 C
ATOM 1807 CG LEU B 189 90.891 -66.449 -9.106 1.00 82.39 C
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ATOM 1811 O LEU B 189 87.726 -65.612 -9.615 1.00 91.88 O
ANISOU 1811 O LEU B 189 11584 11729 11599 -3960 326 352 O
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ANISOU 1813 CA LEU B 190 10671 11079 10640 -3540 467 101 C
ATOM 1814 CB LEU B 190 88.553 -62.632 -12.411 1.00 82.74 C
ANISOU 1814 CB LEU B 190 10418 10612 10407 -3214 621 -54 C
ATOM 1815 CG LEU B 190 88.942 -61.384 -11.635 1.00 91.81 C
ANISOU 1815 CG LEU B 190 11193 11945 11746 -2748 662 -23 C
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ANISOU 1816 CD1 LEU B 190 11859 11957 12590 -2429 878 -142 C
ATOM 1817 CD2 LEU B 190 88.436 -60.139 -12.341 1.00 89.58 C
ANISOU 1817 CD2 LEU B 190 10716 11992 11330 -2587 626 -23 C
ATOM 1818 C LEU B 190 86.355 -63.568 -11.715 1.00 86.28 C
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ANISOU 1824 CD ARG B 191 13536 15343 12065 -5813 -356 609 C
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ANISOU 1825 NE ARG B 191 15706 17159 13545 -6421 -416 579 N
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ANISOU 1827 NH1 ARG B 191 15127 16980 12056 -7393 -643 637 N
ATOM 1828 NH2 ARG B 191 80.056 -66.890 -12.257 1.00110.51 N
ANISOU 1828 NH2 ARG B 191 13488 16927 11575 -6575 -751 827 N
ATOM 1829 C ARG B 191 84.166 -62.728 -13.366 1.00105.34 C
ANISOU 1829 C ARG B 191 12743 15134 12147 -4303 -56 371 C
ATOM 1830 O ARG B 191 83.151 -62.240 -12.875 1.00107.31 O
ANISOU 1830 O ARG B 191 12561 15943 12271 -4307 -220 538 O
ATOM 1831 N GLY B 192 85.053 -62.018 -14.053 1.00 94.81 N
ANISOU 1831 N GLY B 192 11541 13508 10973 -3981 101 242 N
ATOM 1832 CA GLY B 192 84.883 -60.604 -14.307 1.00 91.69 C
ANISOU 1832 CA GLY B 192 10819 13403 10615 -3615 76 309 C
ATOM 1833 C GLY B 192 86.065 -60.117 -15.112 1.00 98.42 C
ANISOU 1833 C GLY B 192 11952 13810 11633 -3352 276 133 C
ATOM 1834 O GLY B 192 86.650 -60.875 -15.885 1.00112.65 O
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ATOM 1835 N ALA B 193 86.422 -58.853 -14.926 1.00 86.23 N
ANISOU 1835 N ALA B 193 10161 12318 10282 -2888 339 145 N
ATOM 1836 CA ALA B 193 87.583 -58.291 -15.597 1.00 77.82 C
ANISOU 1836 CA ALA B 193 9332 10857 9378 -2623 531 -17 C
ATOM 1837 CB ALA B 193 87.293 -58.039 -17.066 1.00 68.40 C
ANISOU 1837 CB ALA B 193 8314 9751 7926 -2834 471 1 C
ATOM 1838 C ALA B 193 88.019 -57.005 -14.925 1.00 83.28 C
ANISOU 1838 C ALA B 193 9723 11585 10333 -2106 619 -7 C
ATOM 1839 O ALA B 193 87.217 -56.098 -14.700 1.00 84.05 O
ANISOU 1839 O ALA B 193 9448 12074 10411 -1944 513 146 O
ATOM 1840 N VAL B 194 89.303 -56.940 -14.604 1.00 81.14 N
ANISOU 1840 N VAL B 194 9612 10898 10318 -1854 828 -175 N
ATOM 1841 CA VAL B 194 89.907 -55.712 -14.134 1.00 70.74 C
ANISOU 1841 CA VAL B 194 8097 9552 9228 -1408 952 -210 C
ATOM 1842 CB VAL B 194 91.371 -55.939 -13.788 1.00 65.98 C
ANISOU 1842 CB VAL B 194 7703 8496 8871 -1228 1171 -388 C
ATOM 1843 CG1 VAL B 194 91.958 -54.709 -13.131 1.00 59.23 C
ANISOU 1843 CG1 VAL B 194 6627 7657 8222 -822 1298 -425 C
ATOM 1844 CG2 VAL B 194 91.499 -57.138 -12.874 1.00 76.21 C
ANISOU 1844 CG2 VAL B 194 9034 9684 10240 -1398 1156 -372 C
ATOM 1845 C VAL B 194 89.817 -54.670 -15.239 1.00 64.76 C
ANISOU 1845 C VAL B 194 7361 8853 8394 -1286 943 -181 C
ATOM 1846 O VAL B 194 89.892 -55.000 -16.421 1.00 65.28 O
ANISOU 1846 O VAL B 194 7715 8806 8282 -1518 925 -217 O
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ANISOU 1847 N SER B 195 7646 9605 9107 -944 964 -114 N
ATOM 1848 CA SER B 195 89.638 -52.316 -15.805 1.00 66.53 C
ANISOU 1848 CA SER B 195 7293 9263 8724 -782 958 -52 C
ATOM 1849 CB SER B 195 89.080 -51.065 -15.141 1.00 69.69 C
ANISOU 1849 CB SER B 195 7284 9909 9286 -430 958 64 C
ATOM 1850 OG SER B 195 88.063 -51.425 -14.230 1.00 75.90 O
ANISOU 1850 OG SER B 195 7741 11051 10046 -512 848 166 O
ATOM 1851 C SER B 195 91.040 -52.052 -16.344 1.00 59.01 C
ANISOU 1851 C SER B 195 6670 7878 7872 -652 1165 -250 C
ATOM 1852 O SER B 195 92.037 -52.414 -15.722 1.00 61.64 O
ANISOU 1852 O SER B 195 7115 7935 8370 -562 1334 -422 O
ATOM 1853 N GLN B 196 91.102 -51.402 -17.498 1.00 74.21 N
ANISOU 1853 N GLN B 196 8728 9775 9693 -654 1140 -203 N
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ANISOU 1857 CD GLN B 196 15693 16129 15118 -1566 876 -49 C
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ANISOU 1858 OE1 GLN B 196 15722 16699 15485 -1349 733 211 O
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ATOM 1861 O GLN B 196 94.516 -50.305 -17.820 1.00 88.19 O
ANISOU 1861 O GLN B 196 11019 10666 11825 -178 1712 -700 O
ATOM 1862 N ARG B 197 92.757 -49.160 -17.038 1.00 79.93 N
ANISOU 1862 N ARG B 197 9413 10127 10828 52 1488 -369 N
ATOM 1863 CA ARG B 197 93.562 -48.006 -16.644 1.00 78.97 C
ANISOU 1863 CA ARG B 197 9257 9833 10913 392 1679 -461 C
ATOM 1864 CB ARG B 197 92.709 -46.737 -16.661 1.00 72.37 C
ANISOU 1864 CB ARG B 197 8155 9187 10156 630 1608 -263 C
ATOM 1865 CG ARG B 197 92.229 -46.344 -18.046 1.00 73.78 C
ANISOU 1865 CG ARG B 197 8435 9432 10165 523 1440 -57 C
ATOM 1866 CD ARG B 197 91.120 -45.318 -17.970 1.00 83.46 C
ANISOU 1866 CD ARG B 197 9317 10895 11499 752 1321 214 C
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ANISOU 1867 NE ARG B 197 12285 13622 14387 890 1315 347 N
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ANISOU 1868 CZ ARG B 197 12610 14306 15136 1159 1250 595 C
ATOM 1869 NH1 ARG B 197 90.863 -42.135 -19.783 1.00100.40 N
ANISOU 1869 NH1 ARG B 197 11442 12845 13859 1262 1237 737 N
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ANISOU 1870 NH2 ARG B 197 12934 15283 16011 1324 1207 706 N
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ANISOU 1871 C ARG B 197 8629 9219 10583 538 1853 -626 C
ATOM 1872 O ARG B 197 93.941 -49.028 -14.497 1.00 80.15 O
ANISOU 1872 O ARG B 197 9185 10011 11259 420 1801 -621 O
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ANISOU 1873 N LEU B 198 8102 8167 8604 -545 849 -1462 N
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ATOM 1875 CB LEU B 198 97.296 -46.739 -13.831 1.00 57.48 C
ANISOU 1875 CB LEU B 198 6846 7234 7759 -343 1010 -1307 C
ATOM 1876 CG LEU B 198 98.280 -47.200 -12.746 1.00 53.82 C
ANISOU 1876 CG LEU B 198 6216 6712 7522 -184 1066 -1220 C
ATOM 1877 CD1 LEU B 198 99.415 -46.191 -12.608 1.00 46.13 C
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ATOM 1878 CD2 LEU B 198 97.620 -47.456 -11.394 1.00 45.39 C
ANISOU 1878 CD2 LEU B 198 5119 5539 6590 -148 931 -1072 C
ATOM 1879 C LEU B 198 95.087 -46.002 -13.026 1.00 56.37 C
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ATOM 1880 O LEU B 198 94.959 -44.909 -13.573 1.00 57.67 O
ANISOU 1880 O LEU B 198 6961 7349 7603 -529 651 -1104 O
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ANISOU 1881 N TYR B 199 5751 6046 6813 -406 664 -1044 N
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ANISOU 1882 CA TYR B 199 5213 5597 6297 -430 567 -912 C
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ANISOU 1892 O TYR B 199 4196 4644 5531 -303 626 -744 O
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ANISOU 1894 CA ILE B 200 3491 4159 4593 -380 568 -633 C
ATOM 1895 CB ILE B 200 97.070 -42.029 -9.779 1.00 39.12 C
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ATOM 1896 CG1 ILE B 200 97.812 -42.953 -10.734 1.00 45.54 C
ANISOU 1896 CG1 ILE B 200 5131 5978 6196 -389 709 -744 C
ATOM 1897 CD1 ILE B 200 98.732 -42.234 -11.650 1.00 55.86 C
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ATOM 1901 N LEU B 201 95.451 -42.209 -6.781 1.00 35.53 N
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ATOM 1904 CG LEU B 201 93.553 -43.426 -4.773 1.00 41.07 C
ANISOU 1904 CG LEU B 201 4674 5070 5862 -409 571 -419 C
ATOM 1905 CD1 LEU B 201 93.647 -44.434 -3.664 1.00 38.22 C
ANISOU 1905 CD1 LEU B 201 4344 4640 5539 -422 589 -331 C
ATOM 1906 CD2 LEU B 201 92.156 -42.855 -4.854 1.00 44.79 C
ANISOU 1906 CD2 LEU B 201 5132 5530 6357 -433 602 -467 C
ATOM 1907 C LEU B 201 95.595 -40.211 -5.365 1.00 40.53 C
ANISOU 1907 C LEU B 201 4669 5205 5525 -479 477 -392 C
ATOM 1908 O LEU B 201 96.786 -40.310 -5.083 1.00 35.98 O
ANISOU 1908 O LEU B 201 4058 4687 4927 -499 448 -339 O
ATOM 1909 N LEU B 202 94.932 -39.058 -5.354 1.00 29.97 N
ANISOU 1909 N LEU B 202 3403 3842 4143 -503 475 -411 N
ATOM 1910 CA LEU B 202 95.571 -37.795 -5.019 1.00 27.75 C
ANISOU 1910 CA LEU B 202 3204 3577 3761 -574 447 -384 C
ATOM 1911 CB LEU B 202 95.606 -36.902 -6.244 1.00 45.84 C
ANISOU 1911 CB LEU B 202 5522 5873 6022 -592 410 -394 C
ATOM 1912 CG LEU B 202 96.581 -37.346 -7.319 1.00 61.91 C
ANISOU 1912 CG LEU B 202 7487 8006 8029 -618 405 -389 C
ATOM 1913 CD1 LEU B 202 96.067 -36.976 -8.692 1.00 72.29 C
ANISOU 1913 CD1 LEU B 202 8843 9317 9308 -623 376 -408 C
ATOM 1914 CD2 LEU B 202 97.886 -36.663 -7.055 1.00 66.93 C
ANISOU 1914 CD2 LEU B 202 8127 8713 8592 -720 388 -338 C
ATOM 1915 C LEU B 202 94.854 -37.062 -3.897 1.00 37.45 C
ANISOU 1915 C LEU B 202 4541 4729 4959 -593 491 -403 C
ATOM 1916 O LEU B 202 94.128 -36.092 -4.147 1.00 42.77 O
ANISOU 1916 O LEU B 202 5269 5326 5654 -568 507 -441 O
ATOM 1917 N PRO B 203 95.027 -37.532 -2.655 1.00 45.89 N
ANISOU 1917 N PRO B 203 5651 5808 5978 -634 517 -376 N
ATOM 1918 CA PRO B 203 94.434 -36.812 -1.525 1.00 50.82 C
ANISOU 1918 CA PRO B 203 6413 6368 6527 -678 597 -419 C
ATOM 1919 CB PRO B 203 94.665 -37.750 -0.340 1.00 29.70 C
ANISOU 1919 CB PRO B 203 3779 3732 3775 -738 607 -360 C
ATOM 1920 CG PRO B 203 95.810 -38.620 -0.755 1.00 38.03 C
ANISOU 1920 CG PRO B 203 4722 4865 4862 -732 483 -264 C
ATOM 1921 CD PRO B 203 95.664 -38.790 -2.239 1.00 42.42 C
ANISOU 1921 CD PRO B 203 5148 5420 5550 -637 482 -304 C
ATOM 1922 C PRO B 203 95.149 -35.487 -1.307 1.00 41.70 C
ANISOU 1922 C PRO B 203 5391 5194 5257 -773 552 -434 C
ATOM 1923 O PRO B 203 96.365 -35.440 -1.130 1.00 37.45 O
ANISOU 1923 O PRO B 203 4863 4736 4632 -873 450 -372 O
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ANISOU 1924 N LEU B 204 5391 4987 5192 -742 623 -515 N
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ATOM 1926 CB LEU B 204 93.904 -32.034 -1.615 1.00 57.77 C
ANISOU 1926 CB LEU B 204 7729 6873 7347 -730 659 -617 C
ATOM 1927 CG LEU B 204 93.551 -32.085 -3.095 1.00 59.91 C
ANISOU 1927 CG LEU B 204 7865 7141 7757 -624 579 -558 C
ATOM 1928 CD1 LEU B 204 92.730 -30.868 -3.465 1.00 65.80 C
ANISOU 1928 CD1 LEU B 204 8683 7696 8621 -530 594 -592 C
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ANISOU 1930 C LEU B 204 6810 6021 6007 -994 585 -564 C
ATOM 1931 O LEU B 204 96.436 -31.907 0.211 1.00 55.16 O
ANISOU 1931 O LEU B 204 7630 6713 6615 -1130 504 -561 O
ATOM 1932 N ASP B 205 95.138 -33.474 1.140 1.00 39.52 N
ANISOU 1932 N ASP B 205 5575 4776 4665 -1007 670 -583 N
ATOM 1933 CA ASP B 205 95.722 -33.301 2.463 1.00 53.70 C
ANISOU 1933 CA ASP B 205 7567 6605 6233 -1187 648 -592 C
ATOM 1934 CB ASP B 205 94.779 -33.840 3.541 1.00 47.75 C
ANISOU 1934 CB ASP B 205 6906 5837 5399 -1187 820 -647 C
ATOM 1935 CG ASP B 205 94.300 -35.246 3.237 1.00 80.95 C
ANISOU 1935 CG ASP B 205 10916 10109 9733 -1079 839 -556 C
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ANISOU 1936 OD1 ASP B 205 12978 12278 12161 -923 922 -593 O
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ANISOU 1937 OD2 ASP B 205 11327 10604 10037 -1158 750 -438 O
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ANISOU 1941 CA CYS B 206 6171 6045 5422 -1223 201 -216 C
ATOM 1942 CB CYS B 206 99.877 -34.577 1.504 1.00 45.91 C
ANISOU 1942 CB CYS B 206 6143 6042 5260 -1403 57 -185 C
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ATOM 1944 C CYS B 206 98.732 -36.603 2.395 1.00 52.46 C
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ATOM 1945 O CYS B 206 99.825 -37.019 2.784 1.00 51.74 O
ANISOU 1945 O CYS B 206 6792 6869 5996 -1320 -30 11 O
ATOM 1946 N GLY B 207 97.574 -37.080 2.845 1.00 45.94 N
ANISOU 1946 N GLY B 207 6207 5967 5282 -1190 294 -160 N
ATOM 1947 CA GLY B 207 97.528 -38.172 3.802 1.00 42.54 C
ANISOU 1947 CA GLY B 207 5825 5564 4776 -1226 259 -48 C
ATOM 1948 C GLY B 207 97.568 -39.547 3.152 1.00 39.71 C
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ANISOU 1949 O GLY B 207 7254 7168 6775 -980 368 -2 O
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ANISOU 1951 CA VAL B 208 5732 6018 5687 -913 11 266 C
ATOM 1952 CB VAL B 208 100.157 -41.451 1.525 1.00 45.13 C
ANISOU 1952 CB VAL B 208 5403 5990 5753 -833 -88 292 C
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ANISOU 1953 CG1 VAL B 208 3838 4523 4587 -660 -85 345 C
ATOM 1954 CG2 VAL B 208 99.971 -40.428 0.429 1.00 46.87 C
ANISOU 1954 CG2 VAL B 208 5587 6231 5990 -825 21 140 C
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ANISOU 1958 CA PRO B 209 6777 6651 6484 -940 -83 650 C
ATOM 1959 CB PRO B 209 96.817 -45.156 4.468 1.00 41.71 C
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ANISOU 1963 O PRO B 209 7653 7873 8206 -644 -236 715 O
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ANISOU 1965 CA ASP B 210 8895 8875 9309 -681 -626 1205 C
ATOM 1966 CB ASP B 210 101.076 -47.947 6.402 1.00 82.95 C
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ATOM 1967 CG ASP B 210 101.898 -46.963 7.202 1.00102.87 C
ANISOU 1967 CG ASP B 210 13098 13052 12934 -960 -1091 1580 C
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ANISOU 1975 CG ASN B 211 14090 13150 15221 -289 -395 1343 C
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ATOM 1979 O ASN B 211 95.852 -49.084 3.842 1.00 64.14 O
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ANISOU 1982 CB LEU B 212 9299 9010 10587 -356 381 234 C
ATOM 1983 CG LEU B 212 94.558 -48.641 -1.346 1.00 68.59 C
ANISOU 1983 CG LEU B 212 8326 8091 9644 -395 508 43 C
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ANISOU 1984 CD1 LEU B 212 8010 7874 9114 -496 564 13 C
ATOM 1985 CD2 LEU B 212 95.125 -48.414 -2.726 1.00 68.54 C
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ANISOU 1989 CA SER B 213 11643 10451 12535 -678 451 644 C
ATOM 1990 CB SER B 213 94.194 -53.505 2.313 1.00 89.16 C
ANISOU 1990 CB SER B 213 11458 9955 12463 -597 328 816 C
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ANISOU 1991 OG SER B 213 10851 9452 12194 -377 247 744 O
ATOM 1992 C SER B 213 92.837 -51.724 3.411 1.00 99.55 C
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ANISOU 1994 N MET B 214 13374 12177 13580 -915 436 855 N
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ATOM 1996 CB MET B 214 94.116 -50.419 6.593 1.00109.32 C
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ATOM 1997 CG MET B 214 95.015 -51.628 6.728 1.00112.85 C
ANISOU 1997 CG MET B 214 14976 13403 14500 -1073 73 1395 C
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ANISOU 1998 SD MET B 214 20954 18975 20439 -1175 162 1535 S
ATOM 1999 CE MET B 214 95.400 -54.289 7.379 1.00 83.56 C
ANISOU 1999 CE MET B 214 11464 9225 11058 -1040 -175 1862 C
ATOM 2000 C MET B 214 92.251 -49.257 5.451 1.00 87.09 C
ANISOU 2000 C MET B 214 11502 10430 11157 -1175 711 726 C
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ANISOU 2001 O MET B 214 12341 11204 11665 -1342 876 722 O
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ATOM 2009 CB ASP B 216 87.973 -47.329 2.175 1.00 79.26 C
ANISOU 2009 CB ASP B 216 9820 9590 10707 -1055 1287 -39 C
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ANISOU 2011 OD1 ASP B 216 9294 9220 10596 -1249 1552 -88 O
ATOM 2012 OD2 ASP B 216 85.993 -46.155 1.529 1.00 86.81 O
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ANISOU 2015 N PRO B 217 6345 5674 6852 -1472 1536 272 N
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ATOM 2025 CG ASN B 218 82.390 -50.120 1.431 1.00 55.11 C
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ANISOU 2029 O ASN B 218 5821 5572 7896 -1265 1145 -216 O
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ANISOU 2030 N ILE B 219 6486 5985 8033 -1168 1143 -21 N
ATOM 2031 CA ILE B 219 88.066 -51.251 -0.715 1.00 52.95 C
ANISOU 2031 CA ILE B 219 6377 5781 7960 -1020 982 -66 C
ATOM 2032 CB ILE B 219 88.979 -50.059 -0.953 1.00 51.96 C
ANISOU 2032 CB ILE B 219 6228 5798 7717 -872 917 -107 C
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ANISOU 2033 CG1 ILE B 219 5490 5352 7121 -862 963 -238 C
ATOM 2034 CD1 ILE B 219 89.008 -47.738 -1.954 1.00 58.34 C
ANISOU 2034 CD1 ILE B 219 6879 6863 8426 -735 889 -287 C
ATOM 2035 CG2 ILE B 219 90.076 -50.417 -1.940 1.00 46.64 C
ANISOU 2035 CG2 ILE B 219 5556 5060 7107 -732 795 -157 C
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ANISOU 2036 C ILE B 219 7438 6484 8891 -1017 918 85 C
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ANISOU 2037 O ILE B 219 8088 7008 9293 -1045 914 254 O
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ATOM 2040 CB ARG B 220 88.401 -55.766 -0.421 1.00 54.31 C
ANISOU 2040 CB ARG B 220 6939 5164 8531 -1195 881 200 C
ATOM 2041 CG ARG B 220 87.702 -55.672 0.916 1.00 75.74 C
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ATOM 2054 CE1 PHE B 221 96.826 -57.089 -3.314 1.00 53.24 C
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ATOM 2061 CA LEU B 222 92.231 -59.110 -4.164 1.00 68.04 C
ANISOU 2061 CA LEU B 222 8879 5968 11004 -446 679 -253 C
ATOM 2062 CB LEU B 222 90.978 -59.146 -5.051 1.00 76.03 C
ANISOU 2062 CB LEU B 222 9903 7013 11971 -665 730 -470 C
ATOM 2063 CG LEU B 222 90.785 -58.221 -6.245 1.00 80.72 C
ANISOU 2063 CG LEU B 222 10387 7857 12425 -673 748 -708 C
ATOM 2064 CD1 LEU B 222 91.619 -58.685 -7.416 1.00 94.02 C
ANISOU 2064 CD1 LEU B 222 12131 9409 14185 -524 798 -936 C
ATOM 2065 CD2 LEU B 222 89.320 -58.216 -6.626 1.00 77.29 C
ANISOU 2065 CD2 LEU B 222 9939 7481 11948 -939 736 -801 C
ATOM 2066 C LEU B 222 93.429 -59.821 -4.797 1.00 71.25 C
ANISOU 2066 C LEU B 222 9307 6193 11573 -350 650 -350 C
ATOM 2067 O LEU B 222 93.618 -61.001 -4.561 1.00 74.79 O
ANISOU 2067 O LEU B 222 9890 6327 12202 -283 627 -283 O
ATOM 2068 N ASP B 223 94.247 -59.118 -5.573 1.00 66.22 N
ANISOU 2068 N ASP B 223 8536 5691 10931 -31 738 -500 N
ATOM 2069 CA ASP B 223 95.335 -59.798 -6.270 1.00 59.33 C
ANISOU 2069 CA ASP B 223 7658 4613 10271 210 809 -635 C
ATOM 2070 CB ASP B 223 94.774 -60.584 -7.456 1.00 59.87 C
ANISOU 2070 CB ASP B 223 7880 4473 10396 124 920 -938 C
ATOM 2071 CG ASP B 223 95.583 -61.829 -7.767 1.00 74.59 C
ANISOU 2071 CG ASP B 223 9836 5940 12566 338 1001 -1030 C
ATOM 2072 OD1 ASP B 223 96.762 -61.893 -7.376 1.00 82.90 O
ANISOU 2072 OD1 ASP B 223 10813 6864 13819 561 946 -822 O
ATOM 2073 OD2 ASP B 223 95.025 -62.754 -8.391 1.00 86.26 O
ANISOU 2073 OD2 ASP B 223 11467 7222 14087 280 1111 -1312 O
ATOM 2074 C ASP B 223 96.432 -58.861 -6.758 1.00 70.26 C
ANISOU 2074 C ASP B 223 8846 6254 11594 389 855 -709 C
ATOM 2075 O ASP B 223 96.220 -57.662 -6.906 1.00 64.39 O
ANISOU 2075 O ASP B 223 8011 5839 10617 296 843 -728 O
ATOM 2076 N LYS B 224 97.606 -59.429 -7.008 1.00 70.51 N
ANISOU 2076 N LYS B 224 8808 6121 11863 646 915 -748 N
ATOM 2077 CA LYS B 224 98.702 -58.696 -7.620 1.00 62.10 C
ANISOU 2077 CA LYS B 224 7540 5274 10782 810 1005 -853 C
ATOM 2078 CB LYS B 224 100.034 -59.179 -7.070 1.00 65.25 C
ANISOU 2078 CB LYS B 224 7771 5534 11486 1101 968 -693 C
ATOM 2079 CG LYS B 224 100.210 -58.921 -5.615 1.00 73.13 C
ANISOU 2079 CG LYS B 224 8710 6597 12479 1093 732 -321 C
ATOM 2080 CD LYS B 224 101.192 -57.805 -5.389 1.00 74.58 C
ANISOU 2080 CD LYS B 224 8637 7112 12586 1164 674 -224 C
ATOM 2081 CE LYS B 224 100.803 -57.048 -4.143 1.00 82.74 C
ANISOU 2081 CE LYS B 224 9706 8341 13391 987 465 53 C
ATOM 2082 NZ LYS B 224 101.882 -56.169 -3.643 1.00 94.62 N

ANISOU 2082 NZ LYS B 224 10981 10100 14871 1054 344 209 N
ATOM 2083 C LYS B 224 98.705 -58.926 -9.118 1.00 66.42 C
ANISOU 2083 C LYS B 224 8155 5778 11303 814 1217 -1220 C
ATOM 2084 O LYS B 224 98.303 -59.984 -9.592 1.00 81.46 O
ANISOU 2084 O LYS B 224 10244 7378 13329 799 1296 -1385 O
ATOM 2085 N LEU B 225 99.175 -57.935 -9.860 1.00 64.32 N
ANISOU 2085 N LEU B 225 7766 5810 10862 814 1312 -1347 N
ATOM 2086 CA LEU B 225 99.482 -58.150 -11.259 1.00 70.84 C
ANISOU 2086 CA LEU B 225 8648 6612 11656 845 1542 -1685 C
ATOM 2087 CB LEU B 225 99.605 -56.820 -11.996 1.00 71.30 C
ANISOU 2087 CB LEU B 225 8629 7056 11406 729 1596 -1770 C
ATOM 2088 CG LEU B 225 98.321 -56.174 -12.496 1.00 67.37 C
ANISOU 2088 CG LEU B 225 8294 6722 10580 440 1508 -1836 C
ATOM 2089 CD1 LEU B 225 98.667 -55.064 -13.470 1.00 57.97 C
ANISOU 2089 CD1 LEU B 225 7063 5840 9121 363 1600 -1954 C
ATOM 2090 CD2 LEU B 225 97.438 -57.215 -13.164 1.00 70.99 C
ANISOU 2090 CD2 LEU B 225 9004 6927 11042 318 1546 -2055 C
ATOM 2091 C LEU B 225 100.805 -58.895 -11.325 1.00 68.45 C
ANISOU 2091 C LEU B 225 8201 6111 11696 1159 1694 -1735 C
ATOM 2092 O LEU B 225 101.602 -58.820 -10.392 1.00 71.97 O
ANISOU 2092 O LEU B 225 8436 6570 12341 1335 1589 -1485 O
ATOM 2093 N PRO B 226 101.051 -59.625 -12.424 1.00 70.55 N
ANISOU 2093 N PRO B 226 8577 6190 12039 1232 1941 -2063 N
ATOM 2094 CA PRO B 226 102.406 -60.162 -12.549 1.00 78.63 C
ANISOU 2094 CA PRO B 226 9400 7069 13409 1562 2130 -2129 C
ATOM 2095 CB PRO B 226 102.320 -61.084 -13.763 1.00 66.61 C
ANISOU 2095 CB PRO B 226 8111 5323 11874 1561 2381 -2503 C
ATOM 2096 CG PRO B 226 101.226 -60.545 -14.557 1.00 64.39 C
ANISOU 2096 CG PRO B 226 8071 5189 11204 1235 2397 -2704 C
ATOM 2097 CD PRO B 226 100.211 -60.000 -13.571 1.00 75.76 C
ANISOU 2097 CD PRO B 226 9529 6760 12497 1033 2067 -2390 C
ATOM 2098 C PRO B 226 103.378 -59.023 -12.806 1.00 75.65 C
ANISOU 2098 C PRO B 226 8733 7078 12933 1612 2220 -2107 C
ATOM 2099 O PRO B 226 103.097 -58.075 -13.545 1.00 70.96 O
ANISOU 2099 O PRO B 226 8190 6786 11984 1404 2285 -2226 O
ATOM 2100 N GLN B 227 104.530 -59.137 -12.168 1.00 83.72 N
ANISOU 2100 N GLN B 227 9444 8078 14285 1883 2204 -1933 N
ATOM 2101 CA GLN B 227 105.486 -58.057 -12.099 1.00 96.43 C
ANISOU 2101 CA GLN B 227 10732 10053 15854 1917 2221 -1828 C
ATOM 2102 CB GLN B 227 106.650 -58.469 -11.218 1.00101.85 C
ANISOU 2102 CB GLN B 227 11075 10637 16986 2229 2130 -1595 C
ATOM 2103 CG GLN B 227 106.222 -58.821 -9.827 1.00105.43 C
ANISOU 2103 CG GLN B 227 11586 10929 17542 2235 1768 -1238 C
ATOM 2104 CD GLN B 227 107.067 -59.915 -9.237 1.00119.40 C
ANISOU 2104 CD GLN B 227 13189 12390 19786 2564 1696 -1084 C
ATOM 2105 OE1 GLN B 227 107.463 -60.853 -9.930 1.00130.45 O
ANISOU 2105 OE1 GLN B 227 14650 13607 21307 2705 1879 -1276 O
ATOM 2106 NE2 GLN B 227 107.363 -59.799 -7.950 1.00121.33 N
ANISOU 2106 NE2 GLN B 227 13280 12642 20180 2628 1374 -700 N
ATOM 2107 C GLN B 227 106.022 -57.594 -13.438 1.00104.22 C
ANISOU 2107 C GLN B 227 11674 11254 16670 1874 2552 -2132 C
ATOM 2108 O GLN B 227 105.692 -58.126 -14.501 1.00108.64 O
ANISOU 2108 O GLN B 227 12491 11721 17068 1796 2742 -2414 O
ATOM 2109 N GLN B 228 106.878 -56.591 -13.346 1.00 93.61 N
ANISOU 2109 N GLN B 228 10600 9446 15523 2340 917 -1613 N
ATOM 2110 CA GLN B 228 107.514 -56.000 -14.494 1.00 86.82 C
ANISOU 2110 CA GLN B 228 9901 8736 14349 2298 1170 -1914 C
ATOM 2111 CB GLN B 228 106.707 -54.792 -14.958 1.00 85.38 C
ANISOU 2111 CB GLN B 228 10238 8831 13373 2431 1262 -1824 C
ATOM 2112 CG GLN B 228 106.961 -54.372 -16.389 1.00 89.04 C
ANISOU 2112 CG GLN B 228 10847 9525 13461 2385 1482 -2172 C
ATOM 2113 CD GLN B 228 106.183 -53.131 -16.764 1.00 92.22 C
ANISOU 2113 CD GLN B 228 11773 10151 13116 2499 1504 -2015 C
ATOM 2114 OE1 GLN B 228 105.145 -52.837 -16.174 1.00103.63 O
ANISOU 2114 OE1 GLN B 228 13377 11611 14388 2674 1360 -1760 O
ATOM 2115 NE2 GLN B 228 106.689 -52.386 -17.739 1.00 96.81 N
ANISOU 2115 NE2 GLN B 228 12615 10902 13267 2383 1674 -2170 N
ATOM 2116 C GLN B 228 108.881 -55.565 -14.001 1.00 84.86 C
ANISOU 2116 C GLN B 228 9704 8308 14231 2110 1226 -1792 C
ATOM 2117 O GLN B 228 108.990 -54.751 -13.088 1.00 93.99 O
ANISOU 2117 O GLN B 228 11170 9413 15129 2084 1171 -1409 O
ATOM 2118 N THR B 229 109.927 -56.140 -14.573 1.00 81.28 N
ANISOU 2118 N THR B 229 8919 7752 14212 1970 1333 -2136 N
ATOM 2119 CA THR B 229 111.269 -55.713 -14.242 1.00 79.42 C
ANISOU 2119 CA THR B 229 8718 7358 14101 1788 1407 -2073 C
ATOM 2120 CB THR B 229 112.264 -56.862 -14.382 1.00 88.46 C
ANISOU 2120 CB THR B 229 9283 8254 16076 1643 1380 -2385 C
ATOM 2121 OG1 THR B 229 111.609 -58.094 -14.065 1.00 90.20 O
ANISOU 2121 OG1 THR B 229 9155 8442 16676 1623 1099 -2312 O
ATOM 2122 CG2 THR B 229 113.443 -56.660 -13.447 1.00 91.06 C
ANISOU 2122 CG2 THR B 229 9568 8289 16742 1483 1301 -2139 C
ATOM 2123 C THR B 229 111.603 -54.609 -15.226 1.00 88.04 C
ANISOU 2123 C THR B 229 10206 8714 14530 1741 1685 -2244 C
ATOM 2124 O THR B 229 111.261 -54.708 -16.401 1.00 94.87 O
ANISOU 2124 O THR B 229 11060 9814 15174 1759 1837 -2606 O
ATOM 2125 N ILE B 230 112.244 -53.545 -14.759 1.00 83.19 N
ANISOU 2125 N ILE B 230 9957 8078 13574 1659 1975 N
ATOM 2126 CA ILE B 230 112.514 -52.424 -15.652 1.00 90.88 C
ANISOU 2126 CA ILE B 230 11349 9303 13879 1597 1969 -2085 C
ATOM 2127 C ILE B 230 113.997 -52.207 -15.947 1.00 88.68 C
ANISOU 2127 C ILE B 230 11003 8961 13729 1363 2558 -2282 C
ATOM 2128 O ILE B 230 114.834 -52.194 -15.044 1.00 84.49 O
ANISOU 2128 O ILE B 230 10391 8183 13527 1275 2088 -2076 O
ATOM 2129 CB ILE B 230 111.848 -51.128 -15.165 1.00 98.08 C
ANISOU 2129 CB ILE B 230 12833 10318 14114 1711 1912 -1660 C
ATOM 2130 CG1 ILE B 230 110.335 -51.236 -15.323 1.00 97.19 C
ANISOU 2130 CG1 ILE B 230 12803 10352 13772 1933 1793 -1609 C
ATOM 2131 CG2 ILE B 230 112.318 -49.949 -15.991 1.00 93.96 C
ANISOU 2131 CG2 ILE B 230 12738 9999 12964 1605 2108 -1725 C
ATOM 2132 CD1 ILE B 230 109.891 -51.216 -16.779 1.00 91.06 C
ANISOU 2132 CD1 ILE B 230 12085 9855 12659 1942 1923 -1964 C
ATOM 2133 N ASP B 231 114.292 -52.030 -17.233 1.00102.37 N
ANISOU 2133 N ASP B 231 12776 10940 15182 1241 2396 -2688 N
ATOM 2134 CA ASP B 231 115.650 -51.931 -17.750 1.00121.49 C
ANISOU 2134 CA ASP B 231 15077 13362 17720 988 2623 -3002 C
ATOM 2135 CB ASP B 231 115.845 -53.015 -18.803 1.00134.17 C
ANISOU 2135 CB ASP B 231 16187 15055 19738 880 2778 -3621 C
ATOM 2136 CG ASP B 231 114.577 -53.277 -19.606 1.00142.54 C
ANISOU 2136 CG ASP B 231 17298 16375 20487 1000 2765 -3768 C
ATOM 2137 OD1 ASP B 231 114.134 -52.374 -20.351 1.00145.88 O
ANISOU 2137 OD1 ASP B 231 18169 17105 20155 960 2858 -3736 O
ATOM 2138 OD2 ASP B 231 114.017 -54.387 -19.486 1.00142.66 O
ANISOU 2138 OD2 ASP B 231 16903 16276 21024 1126 2640 -3899 O
ATOM 2139 C ASP B 231 115.924 -50.573 -18.399 1.00123.54 C
ANISOU 2139 C ASP B 231 15884 13889 17166 855 2805 -2952 C
ATOM 2140 O ASP B 231 115.877 -50.446 -19.620 1.00131.14 O
ANISOU 2140 O ASP B 231 16914 15143 17771 718 2991 -3301 O
ATOM 2141 N ARG B 232 116.224 -49.560 -17.596 1.00111.30 N
ANISOU 2141 N ARG B 232 14723 12246 15320 866 2744 -2519 N
ATOM 2142 CA ARG B 232 116.472 -48.236 -18.151 1.00107.25 C
ANISOU 2142 CA ARG B 232 14743 11956 14053 741 2879 -2429 C
ATOM 2143 CB ARG B 232 115.217 -47.376 -18.073 1.00 97.93 C
ANISOU 2143 CB ARG B 232 14039 10899 12270 942 2724 -2072 C
ATOM 2144 CG ARG B 232 114.249 -47.566 -19.209 1.00104.03 C
ANISOU 2144 CG ARG B 232 14847 11947 12732 976 2737 -2309 C
ATOM 2145 CD ARG B 232 112.938 -46.921 -18.845 1.00115.18 C
ANISOU 2145 CD ARG B 232 16616 13382 13764 1232 2520 -1930 C
ATOM 2146 NE ARG B 232 112.423 -46.043 -19.890 1.00122.63 N
ANISOU 2146 NE ARG B 232 17976 14596 14022 1172 2527 -1934 N
ATOM 2147 CZ ARG B 232 112.880 -44.818 -20.135 1.00121.90 C
ANISOU 2147 CZ ARG B 232 18338 14581 13396 1030 2564 -1760 C
ATOM 2148 NH1 ARG B 232 113.880 -44.324 -19.417 1.00117.50 N
ANISOU 2148 NH1 ARG B 232 17878 13865 12904 945 2629 -1591 N
ATOM 2149 NH2 ARG B 232 112.343 -44.091 -21.106 1.00122.63 N
ANISOU 2149 NH2 ARG B 232 18730 14846 12840 957 2517 -1741 N
ATOM 2150 C ARG B 232 117.612 -47.519 -17.455 1.00104.78 C
ANISOU 2150 C ARG B 232 14599 11483 13729 612 2927 -2205 C
ATOM 2151 O ARG B 232 118.258 -48.073 -16.571 1.00111.40 O
ANISOU 2151 O ARG B 232 15127 12039 15159 603 2858 -2134 O
ATOM 2152 N ALA B 233 117.855 -46.279 -17.862 1.00 91.19 N
ANISOU 2152 N ALA B 233 13375 9937 11337 497 3024 -2080 N
ATOM 2153 CA ALA B 233 118.847 -45.460 -17.190 1.00 86.90 C
ANISOU 2153 CA ALA B 233 13059 9258 10699 387 3062 -1827 C
ATOM 2154 CB ALA B 233 119.032 -44.144 -17.911 1.00 84.49 C
ANISOU 2154 CB ALA B 233 13295 9192 9615 234 3173 -1754 C
ATOM 2155 C ALA B 233 118.366 -45.223 -15.772 1.00 88.14 C
ANISOU 2155 C ALA B 233 13341 9172 10975 602 2829 -1325 C
ATOM 2156 O ALA B 233 117.165 -45.093 -15.530 1.00 83.02 O
ANISOU 2156 O ALA B 233 12850 8559 10137 818 2670 -1118 O
ATOM 2157 N GLY B 234 119.304 -45.195 -14.831 1.00 87.94 N
ANISOU 2157 N GLY B 234 13227 8908 11276 521 2810 -1148 N
ATOM 2158 CA GLY B 234 118.976 -44.946 -13.441 1.00 80.20 C
ANISOU 2158 CA GLY B 234 12367 7718 10386 650 2606 -678 C
ATOM 2159 C GLY B 234 118.126 -46.036 -12.825 1.00 79.87 C
ANISOU 2159 C GLY B 234 11966 7546 10835 813 2403 -625 C
ATOM 2160 O GLY B 234 117.729 -45.959 -11.663 1.00 80.49 O
ANISOU 2160 O GLY B 234 12105 7480 10995 891 2226 -257 O
ATOM 2161 N ILE B 235 117.842 -47.072 -13.595 1.00 88.05 N
ANISOU 2161 N ILE B 235 12617 8643 12196 839 2430 -1002 N
ATOM 2162 CA ILE B 235 117.014 -48.135 -13.071 1.00 91.27 C
ANISOU 2162 CA ILE B 235 12679 8975 13027 1076 2162 -867 C
ATOM 2163 CB ILE B 235 115.506 -47.840 -13.313 1.00110.98 C
ANISOU 2163 CB ILE B 235 15428 11625 15114 1207 2153 -867 C
ATOM 2164 CG1 ILE B 235 114.640 -48.518 -12.260 1.00107.58 C
ANISOU 2164 CG1 ILE B 235 15428 11625 15114 1207 2153 -867 C
ATOM 2165 CD1 ILE B 235 113.213 -48.646 -12.691 1.00107.37 C
ANISOU 2165 CD1 ILE B 235 15428 11625 15114 1207 2153 -867 C
ATOM 2166 CG2 ILE B 235 115.066 -48.185 -14.725 1.00119.64 C
ANISOU 2166 CG2 ILE B 235 16435 12963 16059 1231 2277 -1288 C
ATOM 2167 C ILE B 235 117.501 -49.495 -13.578 1.00 94.55 C
ANISOU 2167 C ILE B 235 12492 9244 14190 907 2256 -1387 C
ATOM 2168 O ILE B 235 117.456 -49.810 -14.766 1.00101.51 O
ANISOU 2168 O ILE B 235 13240 10311 15018 875 2421 -1819 O
ATOM 2169 N LYS B 236 118.042 -50.288 -12.671 1.00 86.81 N
ANISOU 2169 N LYS B 236 11134 7955 13894 846 2089 -1276 N
ATOM 2170 CA LYS B 236 118.524 -51.584 -13.090 1.00 97.56 C
ANISOU 2170 CA LYS B 236 11887 9165 16015 781 2082 -1684 C
ATOM 2171 CB LYS B 236 120.056 -51.633 -13.158 1.00100.49 C
ANISOU 2171 CB LYS B 236 12033 9365 16784 563 2199 -1882 C
ATOM 2172 CG LYS B 236 120.764 -52.015 -11.878 1.00102.42 C

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ANISOU 2172 CG LYS B 236 12047 9225 17641 473 1947 -1550 C
ATOM 2173 CD LYS B 236 122.237 -51.735 -12.014 1.00 99.28 C
ANISOU 2173 CD LYS B 236 11554 8711 17458 268 2098 -1720 C
ATOM 2174 CE LYS B 236 122.893 -52.677 -13.013 1.00102.27 C
ANISOU 2174 CE LYS B 236 11372 9042 18445 180 2252 -2368 C
ATOM 2175 NZ LYS B 236 124.104 -52.048 -13.607 1.00100.60 N
ANISOU 2175 NZ LYS B 236 11226 8914 18084 -19 2544 -2656 N
ATOM 2176 C LYS B 236 117.947 -52.672 -12.213 1.00 95.84 C
ANISOU 2176 C LYS B 236 11304 8705 16406 865 1771 -1495 C
ATOM 2177 O LYS B 236 117.988 -52.590 -10.981 1.00 98.10 O
ANISOU 2177 O LYS B 236 11653 8794 16827 831 1549 -1045 O
ATOM 2178 N ASP B 237 117.362 -53.662 -12.879 1.00 91.49 N
ANISOU 2178 N ASP B 237 10392 8194 16174 953 1757 -1838 N
ATOM 2179 CA ASP B 237 116.823 -54.837 -12.225 1.00 95.99 C
ANISOU 2179 CA ASP B 237 10555 8538 17379 1017 1462 -1731 C
ATOM 2180 CB ASP B 237 117.963 -55.762 -11.807 1.00105.52 C
ANISOU 2180 CB ASP B 237 11221 9356 19516 857 1313 -1829 C
ATOM 2181 CG ASP B 237 118.515 -56.561 -12.968 1.00114.21 C
ANISOU 2181 CG ASP B 237 11859 10529 21005 772 1468 -2438 C
ATOM 2182 OD1 ASP B 237 119.007 -55.946 -13.939 1.00116.12 O
ANISOU 2182 OD1 ASP B 237 12245 10939 20936 734 1816 -2821 O
ATOM 2183 OD2 ASP B 237 118.452 -57.806 -12.904 1.00115.88 O
ANISOU 2183 OD2 ASP B 237 11579 10673 21775 691 1231 -2518 O
ATOM 2184 C ASP B 237 115.963 -54.475 -11.023 1.00 93.55 C
ANISOU 2184 C ASP B 237 10545 8208 16791 1088 1228 -1161 C
ATOM 2185 O ASP B 237 116.207 -54.932 -9.908 1.00 99.80 O
ANISOU 2185 O ASP B 237 11156 8727 18037 987 959 -834 O
ATOM 2186 N ARG B 238 114.980 -53.616 -11.250 1.00 76.68 N
ANISOU 2186 N ARG B 238 8868 6365 13904 1233 1326 -1049 N
ATOM 2187 CA ARG B 238 114.047 -53.272 -10.197 1.00 69.59 C
ANISOU 2187 CA ARG B 238 8230 5488 12724 1303 1143 -593 C
ATOM 2188 CB ARG B 238 113.797 -51.777 -10.156 1.00 70.10 C
ANISOU 2188 CB ARG B 238 8899 5768 11970 1357 1293 -387 C
ATOM 2189 CG ARG B 238 113.268 -51.311 -8.833 1.00 67.37 C
ANISOU 2189 CG ARG B 238 8794 5384 11420 1340 1128 88 C
ATOM 2190 CD ARG B 238 114.172 -50.240 -8.288 1.00 67.24 C
ANISOU 2190 CD ARG B 238 9114 5316 11119 1201 1207 333 C
ATOM 2191 NE ARG B 238 113.574 -48.918 -8.410 1.00 63.62 N
ANISOU 2191 NE ARG B 238 9181 5075 9916 1321 1339 443 N
ATOM 2192 CZ ARG B 238 114.216 -47.781 -8.173 1.00 63.81 C
ANISOU 2192 CZ ARG B 238 9576 5108 9561 1242 1449 608 C
ATOM 2193 NH1 ARG B 238 115.486 -47.803 -7.798 1.00 56.77 N
ANISOU 2193 NH1 ARG B 238 8595 4035 8939 1040 1456 687 N
ATOM 2194 NH2 ARG B 238 113.581 -46.627 -8.301 1.00 56.26 N
ANISOU 2194 NH2 ARG B 238 9066 4324 7986 1366 1534 696 N
ATOM 2195 C ARG B 238 112.755 -53.993 -10.487 1.00 74.07 C
ANISOU 2195 C ARG B 238 8637 6168 13339 1476 1049 -705 C
ATOM 2196 O ARG B 238 112.357 -54.119 -11.642 1.00 85.97 O
ANISOU 2196 O ARG B 238 10111 7866 14689 1589 1203 -1072 O
ATOM 2197 N VAL B 239 112.097 -54.476 -9.444 1.00 71.98 N
ANISOU 2197 N VAL B 239 8273 5800 13277 1468 795 -389 N
ATOM 2198 CA VAL B 239 110.855 -55.194 -9.649 1.00 62.35 C
ANISOU 2198 CA VAL B 239 6889 4681 12121 1622 693 -481 C
ATOM 2199 CB VAL B 239 110.853 -56.539 -8.930 1.00 72.47 C
ANISOU 2199 CB VAL B 239 7681 5695 14160 1514 389 -375 C
ATOM 2200 CG1 VAL B 239 109.843 -57.459 -9.577 1.00 60.93 C
ANISOU 2200 CG1 VAL B 239 5949 4333 12869 1671 341 -642 C
ATOM 2201 CG2 VAL B 239 112.238 -57.155 -8.999 1.00 62.14 C
ANISOU 2201 CG2 VAL B 239 5996 4110 13503 1330 337 -514 C
ATOM 2202 C VAL B 239 109.682 -54.350 -9.201 1.00 60.71 C
ANISOU 2202 C VAL B 239 7100 4692 11273 1747 694 -224 C
ATOM 2203 O VAL B 239 109.561 -53.997 -8.030 1.00 56.77 O
ANISOU 2203 O VAL B 239 6760 4141 10669 1644 570 158 O
ATOM 2204 N TYR B 240 108.834 -54.006 -10.159 1.00 66.99 N
ANISOU 2204 N TYR B 240 8067 5736 11648 1951 835 -454 N
ATOM 2205 CA TYR B 240 107.634 -53.246 -9.878 1.00 69.02 C
ANISOU 2205 CA TYR B 240 8675 6191 11359 2103 831 -281 C
ATOM 2206 CB TYR B 240 107.432 -52.162 -10.924 1.00 72.04 C
ANISOU 2206 CB TYR B 240 9444 6795 11133 2244 1037 -447 C
ATOM 2207 CG TYR B 240 108.358 -50.991 -10.766 1.00 69.93 C
ANISOU 2207 CG TYR B 240 9539 6506 10527 2141 1164 -300 C
ATOM 2208 CD1 TYR B 240 108.059 -49.967 -9.876 1.00 56.94 C
ANISOU 2208 CD1 TYR B 240 8255 4879 8503 2150 1142 20 C
ATOM 2209 CE1 TYR B 240 108.894 -48.891 -9.728 1.00 62.14 C
ANISOU 2209 CE1 TYR B 240 9245 5510 8856 2058 1253 155 C
ATOM 2210 CZ TYR B 240 110.050 -48.823 -10.475 1.00 64.12 C
ANISOU 2210 CZ TYR B 240 9475 5727 9161 1945 1390 -24 C
ATOM 2211 OH TYR B 240 110.883 -47.744 -10.325 1.00 56.47 O
ANISOU 2211 OH TYR B 240 8842 4735 7878 1845 1497 118 O
ATOM 2212 CE2 TYR B 240 110.373 -49.834 -11.369 1.00 69.67 C
ANISOU 2212 CE2 TYR B 240 9809 6426 10237 1920 1430 -368 C
ATOM 2213 CD2 TYR B 240 109.530 -50.905 -11.509 1.00 65.13 C
ANISOU 2213 CD2 TYR B 240 8898 5865 9981 2022 1317 -507 C
ATOM 2214 C TYR B 240 106.417 -54.151 -9.862 1.00 78.62 C
ANISOU 2214 C TYR B 240 9642 7469 12760 2226 687 -345 C
ATOM 2215 O TYR B 240 106.264 -55.027 -10.713 1.00 74.15 O
ANISOU 2215 O TYR B 240 8772 6917 12485 2293 692 -655 O
ATOM 2216 N SER B 241 105.549 -53.926 -8.888 1.00 79.96 N
ANISOU 2216 N SER B 241 9938 7688 12755 2238 573 -71 N
ATOM 2217 CA SER B 241 104.311 -54.671 -8.795 1.00 85.85 C
ANISOU 2217 CA SER B 241 10488 8519 13613 2346 443 -111 C
ATOM 2218 CB SER B 241 104.354 -55.608 -7.596 1.00 93.06 C
ANISOU 2218 CB SER B 241 11102 9260 14999 2131 199 146 C
ATOM 2219 OG SER B 241 104.571 -54.861 -6.416 1.00 98.91 O
ANISOU 2219 OG SER B 241 12095 9981 15507 1955 171 497 O
ATOM 2220 C SER B 241 103.155 -53.700 -8.629 1.00 76.19 C
ANISOU 2220 C SER B 241 9620 7508 11821 2511 498 -33 C
ATOM 2221 O SER B 241 103.314 -52.613 -8.082 1.00 77.14 O
ANISOU 2221 O SER B 241 10080 7654 11575 2472 568 159 O
ATOM 2222 N ASN B 242 101.987 -54.102 -9.103 1.00 70.47 N
ANISOU 2222 N ASN B 242 8796 6924 11055 2696 462 -197 N
ATOM 2223 CA ASN B 242 100.792 -53.321 -8.885 1.00 60.34 C
ANISOU 2223 CA ASN B 242 7773 5817 9337 2856 480 -145 C
ATOM 2224 CB ASN B 242 100.332 -52.679 -10.187 1.00 66.79 C
ANISOU 2224 CB ASN B 242 8805 6785 9789 3099 593 -386 C
ATOM 2225 CG ASN B 242 101.357 -51.718 -10.743 1.00 70.58 C
ANISOU 2225 CG ASN B 242 9583 7239 9997 3061 738 -396 C
ATOM 2226 OD1 ASN B 242 102.406 -52.133 -11.239 1.00 78.16 O
ANISOU 2226 OD1 ASN B 242 10406 8115 11175 2943 798 -509 O
ATOM 2227 ND2 ASN B 242 101.072 -50.423 -10.647 1.00 53.57 N
ANISOU 2227 ND2 ASN B 242 7821 5147 7387 3149 791 -289 N
ATOM 2228 C ASN B 242 99.697 -54.184 -8.290 1.00 67.60 C
ANISOU 2228 C ASN B 242 8435 6790 10460 2860 327 -112 C
ATOM 2229 O ASN B 242 99.581 -55.360 -8.615 1.00 74.28 O
ANISOU 2229 O ASN B 242 8928 7591 11703 2855 227 -237 O
ATOM 2230 N SER B 243 98.902 -53.594 -7.408 1.00 59.32 N
ANISOU 2230 N SER B 243 5998 7665 8876 -134 596 -1377 N
ATOM 2231 CA SER B 243 97.854 -54.342 -6.739 1.00 52.84 C
ANISOU 2231 CA SER B 243 5275 6302 8498 -89 391 -1463 C
ATOM 2232 CB SER B 243 97.819 -54.017 -5.251 1.00 63.15 C
ANISOU 2232 CB SER B 243 6853 7101 10042 -341 337 -985 C
ATOM 2233 OG SER B 243 98.998 -54.463 -4.620 1.00 81.25 O
ANISOU 2233 OG SER B 243 8983 9267 12621 -373 290 -958 O
ATOM 2234 C SER B 243 96.496 -54.082 -7.360 1.00 52.84 C
ANISOU 2234 C SER B 243 5421 6386 8269 0 386 -1569 C
ATOM 2235 O SER B 243 96.218 -52.994 -7.853 1.00 46.24 O
ANISOU 2235 O SER B 243 4794 5862 6914 -48 535 -1365 O
ATOM 2236 N ILE B 244 95.648 -55.100 -7.313 1.00 57.53 N
ANISOU 2236 N ILE B 244 5912 6802 9243 -55.100 -7.313 1.00 57.53 N
ANISOU 2236 N ILE B 244 5912 6686 9261 126 197 -1892 N
ATOM 2237 CA ILE B 244 94.307 -55.003 -7.852 1.00 47.95 C
ANISOU 2237 CA ILE B 244 4775 5545 7897 219 155 -2054 C
ATOM 2238 CB ILE B 244 93.994 -56.186 -8.741 1.00 59.70 C
ANISOU 2238 CB ILE B 244 5947 7103 9633 489 -9 -2687 C
ATOM 2239 CG1 ILE B 244 95.138 -56.437 -9.710 1.00 59.82 C
ANISOU 2239 CG1 ILE B 244 6138 7103 9490 -9 -2687 C
ATOM 2240 CD1 ILE B 244 94.917 -57.652 -10.559 1.00 51.94 C
ANISOU 2240 CD1 ILE B 244 4391 6621 8723 1029 -151 -3677 C
ATOM 2241 CG2 ILE B 244 92.718 -55.944 -9.514 1.00 58.22 C
ANISOU 2241 CG2 ILE B 244 5802 7137 9183 615 -34 -2897 C
ATOM 2242 C ILE B 244 93.309 -54.994 -6.713 1.00 55.72 C
ANISOU 2242 C ILE B 244 5976 6044 9152 34 63 -1760 C
ATOM 2243 O ILE B 244 93.399 -55.805 -5.795 1.00 51.52 O
ANISOU 2243 O ILE B 244 5395 5043 9138 -61 -66 -1717 O
ATOM 2244 N TYR B 245 92.347 -54.083 -6.785 1.00 50.99 N
ANISOU 2244 N TYR B 245 5619 5579 8177 7 126 -1559 N
ATOM 2245 CA TYR B 245 91.394 -53.921 -5.705 1.00 43.63 C
ANISOU 2245 CA TYR B 245 4887 4286 7404 -146 65 -1248 C
ATOM 2246 CB TYR B 245 91.556 -52.555 -5.060 1.00 46.69 C
ANISOU 2246 CB TYR B 245 5658 4697 7385 -282 186 -699 C
ATOM 2247 CG TYR B 245 92.882 -52.387 -4.376 1.00 52.34 C
ANISOU 2247 CG TYR B 245 6424 5253 8211 -437 236 -414 C
ATOM 2248 CD1 TYR B 245 93.999 -51.957 -5.082 1.00 52.62 C
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ATOM 2249 CE1 TYR B 245 95.220 -51.810 -4.457 1.00 50.43 C
ANISOU 2249 CE1 TYR B 245 6125 5243 7794 -586 398 -203 C
ATOM 2250 CZ TYR B 245 95.329 -52.102 -3.108 1.00 52.64 C
ANISOU 2250 CZ TYR B 245 6490 5050 8461 -712 296 54 C
ATOM 2251 OH TYR B 245 96.537 -51.964 -2.470 1.00 59.11 O
ANISOU 2251 OH TYR B 245 7297 5774 9387 -843 310 263 O
ATOM 2252 CE2 TYR B 245 94.231 -52.535 -2.389 1.00 56.61 C
ANISOU 2252 CE2 TYR B 245 7076 5202 9232 -706 183 106 C
ATOM 2253 CD2 TYR B 245 93.019 -52.678 -3.024 1.00 56.85 C
ANISOU 2253 CD2 TYR B 245 7075 5363 9162 -588 160 -124 C
ATOM 2254 C TYR B 245 89.956 -54.115 -6.141 1.00 47.73 C
ANISOU 2254 C TYR B 245 5349 4896 7889 -43 -19 -1499 C
ATOM 2255 O TYR B 245 89.575 -53.781 -7.257 1.00 49.86 O
ANISOU 2255 O TYR B 245 5585 5585 7774 151 13 -1766 O
ATOM 2256 N GLU B 246 89.174 -54.667 -5.227 1.00 50.03 N
ANISOU 2256 N GLU B 246 5620 4809 8581 -179 -125 -1402 N
ATOM 2257 CA GLU B 246 87.739 -54.776 -5.381 1.00 48.26 C
ANISOU 2257 CA GLU B 246 5333 4659 8344 -146 -199 -1555 C
ATOM 2258 CB GLU B 246 87.264 -56.047 -4.695 1.00 70.53 C
ANISOU 2258 CB GLU B 246 7940 7024 11833 -315 -351 -1658 C
ATOM 2259 CG GLU B 246 85.778 -56.266 -4.698 1.00 86.28 C
ANISOU 2259 CG GLU B 246 9811 9074 13898 -356 -430 -1788 C
ATOM 2260 CD GLU B 246 85.394 -57.518 -3.925 1.00 95.68 C
ANISOU 2260 CD GLU B 246 10856 10003 15495 -497 -511 -1651 C
ATOM 2261 OE1 GLU B 246 84.559 -58.297 -4.432 1.00101.97 O
ANISOU 2261 OE1 GLU B 246 11412 10833 16501 -490 -625 -1986 O
ATOM 2262 OE2 GLU B 246 85.930 -57.725 -2.814 1.00 83.50 O
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ATOM 2263 C GLU B 246 87.115 -53.572 -4.694 1.00 46.20 C
ANISOU 2263 C GLU B 246 5402 4477 7675 -189 -112 -1092 C
ATOM 2264 O GLU B 246 87.529 -53.191 -3.603 1.00 50.39 O
ANISOU 2264 O GLU B 246 6144 4748 8253 -336 -68 -644 O
ATOM 2265 N LEU B 247 86.132 -52.960 -5.338 1.00 36.17 N
ANISOU 2265 N LEU B 247 4186 3576 5981 -23 -108 -1219 N
ATOM 2266 CA LEU B 247 85.415 -51.852 -4.733 1.00 40.20 C
ANISOU 2266 CA LEU B 247 5010 4184 6082 1 -64 -838 C
ATOM 2267 CB LEU B 247 85.445 -50.659 -5.664 1.00 46.44 C
ANISOU 2267 CB LEU B 247 6070 5403 6174 230 10 -841 C
ATOM 2268 CG LEU B 247 86.857 -50.403 -6.176 1.00 58.80 C
ANISOU 2268 CG LEU B 247 7717 7017 7607 206 115 -793 C
ATOM 2269 CD1 LEU B 247 86.784 -49.502 -7.364 1.00 59.30 C
ANISOU 2269 CD1 LEU B 247 7965 7540 7028 437 184 -901 C
ATOM 2270 CD2 LEU B 247 87.707 -49.771 -5.084 1.00 47.38 C
ANISOU 2270 CD2 LEU B 247 6565 5277 6161 4 174 -266 C
ATOM 2271 C LEU B 247 83.978 -52.264 -4.468 1.00 52.15 C
ANISOU 2271 C LEU B 247 6335 5734 7745 -1 -155 -969 C
ATOM 2272 O LEU B 247 83.276 -52.702 -5.377 1.00 49.19 O
ANISOU 2272 O LEU B 247 5709 5607 7372 124 -230 -1417 O
ATOM 2273 N LEU B 248 83.542 -52.131 -3.220 1.00 47.06 N
ANISOU 2273 N LEU B 248 5791 4870 7218 -142 -151 -584 N
ATOM 2274 CA LEU B 248 82.192 -52.538 -2.856 1.00 48.85 C
ANISOU 2274 CA LEU B 248 5798 5165 7599 -187 -215 -660 C
ATOM 2275 CB LEU B 248 82.159 -53.202 -1.486 1.00 45.80 C
ANISOU 2275 CB LEU B 248 5341 4351 7708 -465 -214 -327 C
ATOM 2276 CG LEU B 248 83.064 -54.373 -1.171 1.00 58.11 C
ANISOU 2276 CG LEU B 248 6748 5426 9903 -690 -250 -360 C
ATOM 2277 CD1 LEU B 248 82.969 -54.607 0.319 1.00 69.12 C
ANISOU 2277 CD1 LEU B 248 8261 6737 11267 -785 -198 96 C
ATOM 2278 CD2 LEU B 248 82.628 -55.607 -1.934 1.00 53.15 C
ANISOU 2278 CD2 LEU B 248 5724 4748 9723 -769 -372 -871 C
ATOM 2279 C LEU B 248 81.249 -51.357 -2.806 1.00 53.88 C
ANISOU 2279 C LEU B 248 6660 6188 7624 37 -199 -514 C
ATOM 2280 O LEU B 248 81.626 -50.257 -2.409 1.00 46.37 O
ANISOU 2280 O LEU B 248 6113 5256 6249 139 -147 -155 O
ATOM 2281 N GLU B 249 80.005 -51.614 -3.177 1.00 50.45 N
ANISOU 2281 N GLU B 249 5959 6053 7158 114 -266 -808 N
ATOM 2282 CA GLU B 249 78.949 -50.645 -2.991 1.00 48.20 C
ANISOU 2282 CA GLU B 249 5822 6151 6341 344 -275 -695 C
ATOM 2283 CB GLU B 249 78.628 -49.948 -4.302 1.00 59.95 C
ANISOU 2283 CB GLU B 249 7413 8099 7267 697 -317 -1039 C
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ATOM 2285 CD GLU B 249 77.440 -48.074 -5.461 1.00 96.99 C
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ANISOU 2286 OE1 GLU B 249 13319 14783 11949 1411 -428 -1673 O
ATOM 2287 OE2 GLU B 249 77.176 -46.854 -5.424 1.00105.18 O
ANISOU 2287 OE2 GLU B 249 13986 14841 11139 1684 -419 -1031 O
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ANISOU 2289 O GLU B 249 4989 6260 7013 80 -393 -1204 O
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ATOM 2291 CA ASN B 250 76.014 -51.503 -0.745 1.00 43.22 C
ANISOU 2291 CA ASN B 250 4507 5794 6122 33 -286 -394 C
ATOM 2292 CB ASN B 250 74.801 -51.247 -1.651 1.00 46.23 C
ANISOU 2292 CB ASN B 250 4653 6764 6148 287 -371 -829 C
ATOM 2293 CG ASN B 250 73.474 -51.393 -0.922 1.00 41.47 C
ANISOU 2293 CG ASN B 250 3716 6488 5551 221 -362 -753 C
ATOM 2294 OD1 ASN B 250 73.378 -51.167 0.282 1.00 45.28 O
ANISOU 2294 OD1 ASN B 250 4298 6892 6012 148 -280 -299 O
ATOM 2295 ND2 ASN B 250 72.439 -51.779 -1.662 1.00 45.40 N
ANISOU 2295 ND2 ASN B 250 3791 7392 6067 254 -448 -1212 N
ATOM 2296 C ASN B 250 76.211 -53.006 -0.489 1.00 42.69 C
ANISOU 2296 C ASN B 250 4059 5301 6860 -405 -292 -476 C
ATOM 2297 O ASN B 250 75.294 -53.812 -0.657 1.00 41.49 O
ANISOU 2297 O ASN B 250 3469 5274 7021 -585 -344 -736 O
ATOM 2298 N GLY B 251 77.432 -53.371 -0.118 1.00 37.96 N
ANISOU 2298 N GLY B 251 3641 4192 6591 -570 -259 -268 N
ATOM 2299 CA GLY B 251 77.765 -54.748 0.185 1.00 42.65 C
ANISOU 2299 CA GLY B 251 3974 4305 7925 -944 -287 -308 C
ATOM 2300 C GLY B 251 78.122 -55.607 -1.022 1.00 55.81 C
ANISOU 2300 C GLY B 251 5420 5863 9923 -978 -407 -855 C
ATOM 2301 O GLY B 251 78.469 -56.772 -0.867 1.00 60.68 O
ANISOU 2301 O GLY B 251 5867 6043 11146 -1248 -469 -935 O
ATOM 2302 N GLN B 252 78.037 -55.044 -2.225 1.00 57.71 N
ANISOU 2302 N GLN B 252 6371 6718 8837 269 228 206 N
ATOM 2303 CA GLN B 252 78.251 -55.824 -3.445 1.00 47.13 C
ANISOU 2303 CA GLN B 252 5182 5256 7468 162 238 251 C
ATOM 2304 CB GLN B 252 77.011 -55.806 -4.341 1.00 35.35 C
ANISOU 2304 CB GLN B 252 3722 3678 6030 25 121 284 C
ATOM 2305 CG GLN B 252 75.704 -55.814 -3.586 1.00 42.44 C
ANISOU 2305 CG GLN B 252 4482 4598 7044 81 94 301 C
ATOM 2306 CD GLN B 252 75.534 -57.055 -2.731 1.00 46.86 C
ANISOU 2306 CD GLN B 252 5017 5227 7563 142 240 334 C
ATOM 2307 OE1 GLN B 252 75.869 -58.165 -3.150 1.00 48.46 O
ANISOU 2307 OE1 GLN B 252 5311 5371 7733 97 326 379 O
ATOM 2308 NE2 GLN B 252 75.026 -56.869 -1.515 1.00 40.28 N
ANISOU 2308 NE2 GLN B 252 4036 4516 6752 214 279 303 N
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ANISOU 2309 C GLN B 252 6252 6190 8373 108 223 208 C
ATOM 2310 O GLN B 252 79.715 -54.110 -4.252 1.00 55.07 O
ANISOU 2310 O GLN B 252 6258 6251 8416 128 120 177 O
ATOM 2311 N ARG B 253 80.094 -56.218 -4.949 1.00 54.78 N
ANISOU 2311 N ARG B 253 6354 6119 8342 21 344 184 N
ATOM 2312 CA ARG B 253 81.185 -55.836 -5.828 1.00 47.37 C
ANISOU 2312 CA ARG B 253 5513 5153 7330 -82 367 106 C
ATOM 2313 CB ARG B 253 81.846 -57.055 -6.453 1.00 54.90 C
ANISOU 2313 CB ARG B 253 6528 6001 8330 -187 585 12 C
ATOM 2314 CG ARG B 253 82.962 -56.693 -7.413 1.00 62.33 C
ANISOU 2314 CG ARG B 253 7563 6928 9189 -342 652 -122 C
ATOM 2315 CD ARG B 253 83.685 -57.933 -7.900 1.00 66.37 C
ANISOU 2315 CD ARG B 253 8075 7296 9847 -439 938 -284 C
ATOM 2316 NE ARG B 253 84.199 -58.733 -6.792 1.00 70.49 N
ANISOU 2316 NE ARG B 253 8427 7708 10647 -192 1051 -190 N
ATOM 2317 CZ ARG B 253 85.023 -59.764 -6.936 1.00 73.56 C
ANISOU 2317 CZ ARG B 253 8722 7903 11325 -200 1295 -287 C
ATOM 2318 NH1 ARG B 253 85.433 -60.114 -8.145 1.00 76.44 N
ANISOU 2318 NH1 ARG B 253 9161 8175 11707 -453 1509 -561 N
ATOM 2319 NH2 ARG B 253 85.443 -60.438 -5.869 1.00 67.09 N
ANISOU 2319 NH2 ARG B 253 7707 6982 10804 7 1328 -107 N
ATOM 2320 C ARG B 253 80.664 -54.916 -6.923 1.00 53.87 C
ANISOU 2320 C ARG B 253 6415 5990 8062 -291 178 118 C
ATOM 2321 O ARG B 253 79.709 -55.237 -7.623 1.00 52.06 O
ANISOU 2321 O ARG B 253 6233 5742 7804 -473 112 158 O
ATOM 2322 N ALA B 254 81.300 -53.764 -7.063 1.00 50.63 N
ANISOU 2322 N ALA B 254 6003 5615 7618 -288 66 120 N
ATOM 2323 CA ALA B 254 80.839 -52.765 -8.003 1.00 51.58 C
ANISOU 2323 CA ALA B 254 6147 5742 7708 -496 -173 210 C
ATOM 2324 CB ALA B 254 80.459 -51.496 -7.266 1.00 56.68 C
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ATOM 2325 C ALA B 254 81.928 -52.478 -9.018 1.00 60.20 C
ANISOU 2325 C ALA B 254 7368 6883 8622 -712 -164 155 C
ATOM 2326 O ALA B 254 81.681 -51.887 -10.064 1.00 56.75 O
ANISOU 2326 O ALA B 254 6985 6427 8151 -1002 -359 256 O
ATOM 2327 N GLY B 255 83.144 -52.891 -8.702 1.00 59.44 N
ANISOU 2327 N GLY B 255 7303 6786 8497 -599 50 18 N
ATOM 2328 CA GLY B 255 84.248 -52.653 -9.601 1.00 49.63 C
ANISOU 2328 CA GLY B 255 6166 5588 7102 -801 105 -78 C
ATOM 2329 C GLY B 255 85.532 -53.306 -9.156 1.00 49.48 C
ANISOU 2329 C GLY B 255 6132 5517 7152 -648 375 -229 C
ATOM 2330 O GLY B 255 85.707 -53.659 -7.992 1.00 41.45 O
ANISOU 2330 O GLY B 255 5003 4452 6293 -360 450 -192 O
ATOM 2331 N THR B 256 86.432 -53.463 -10.112 1.00 57.87 N
ANISOU 2331 N THR B 256 7288 6596 8105 -885 515 -387 N
ATOM 2332 CA THR B 256 87.754 -53.988 -9.851 1.00 65.81 C
ANISOU 2332 CA THR B 256 8246 7514 9247 -772 770 -536 C
ATOM 2333 CB THR B 256 87.862 -55.449 -10.273 1.00 69.36 C
ANISOU 2333 CB THR B 256 8680 7828 9847 -899 1090 -740 C
ATOM 2334 OG1 THR B 256 87.021 -56.250 -9.438 1.00 68.47 O
ANISOU 2334 OG1 THR B 256 8473 7626 9918 -697 1095 -623 O
ATOM 2335 CG2 THR B 256 89.287 -55.923 -10.147 1.00 70.16 C
ANISOU 2335 CG2 THR B 256 8681 7787 10188 -816 1357 -896 C
ATOM 2336 C THR B 256 88.750 -53.168 -10.652 1.00 62.48 C
ANISOU 2336 C THR B 256 7905 7177 8655 -968 758 -629 C
ATOM 2337 O THR B 256 88.592 -53.002 -11.858 1.00 61.14 O
ANISOU 2337 O THR B 256 7860 7116 8254 -1342 1193 -1044 O
ATOM 2338 N CYS B 257 89.774 -52.647 -9.990 1.00 55.13 N
ANISOU 2338 N CYS B 257 6905 6228 7813 -740 600 -600 N
ATOM 2339 CA CYS B 257 90.733 -51.812 -10.691 1.00 53.17 C
ANISOU 2339 CA CYS B 257 6729 6066 7406 -910 734 -676 C
ATOM 2340 CB CYS B 257 90.239 -50.369 -10.750 1.00 63.85 C
ANISOU 2340 CB CYS B 257 8116 7542 8600 -937 377 -475 C
ATOM 2341 SG CYS B 257 90.235 -49.558 -9.139 1.00 69.92 S
ANISOU 2341 SG CYS B 257 8736 8282 9548 -487 220 -307 S
ATOM 2342 C CYS B 257 92.109 -51.849 -10.055 1.00 47.80 C
ANISOU 2342 C CYS B 257 5951 5304 6906 -684 884 -729 C
ATOM 2343 O CYS B 257 92.261 -52.213 -8.890 1.00 49.64 O
ANISOU 2343 O CYS B 257 6049 5453 7358 -374 908 -618 O
ATOM 2344 N VAL B 258 93.108 -51.464 -10.843 1.00 48.03 N
ANISOU 2344 N VAL B 258 6040 5379 6829 -882 970 -877 N
ATOM 2345 CA VAL B 258 94.462 -51.280 -10.342 1.00 49.66 C
ANISOU 2345 CA VAL B 258 6154 5522 7193 -693 1071 -905 C
ATOM 2346 CB VAL B 258 95.503 -51.479 -11.438 1.00 49.79 C
ANISOU 2346 CB VAL B 258 6213 5529 7176 -991 1328 -1191 C
ATOM 2347 CG2 VAL B 258 95.360 -52.863 -12.043 1.00 51.67 C
ANISOU 2347 CG2 VAL B 258 6413 5626 7594 -1193 1679 -1464 C
ATOM 2348 CG1 VAL B 258 96.905 -51.272 -10.877 1.00 46.87 C
ANISOU 2348 CG1 VAL B 258 5720 5071 7016 -775 1418 -1193 C
ATOM 2349 C VAL B 258 94.569 -49.869 -9.786 1.00 51.60 C
ANISOU 2349 C VAL B 258 6413 5891 7300 -537 771 -707 C
ATOM 2350 O VAL B 258 94.215 -48.897 -10.446 1.00 53.05 O
ANISOU 2350 O VAL B 258 6701 6202 7252 -658 562 -658 O
ATOM 2351 N LEU B 259 95.078 -49.769 -8.570 1.00 51.23 N
ANISOU 2351 N LEU B 259 6239 5806 7419 -220 748 -583 N
ATOM 2352 CA LEU B 259 94.884 -48.583 -7.778 1.00 45.06 C

ANISOU 2352 CA LEU B 259 5439 5133 6550 -54 495 -423 C
ATOM 2353 CB LEU B 259 93.711 -48.845 -6.845 1.00 51.48 C
ANISOU 2353 CB LEU B 259 6181 5954 7425 99 409 -302 C
ATOM 2354 CG LEU B 259 92.928 -47.726 -6.191 1.00 49.50 C
ANISOU 2354 CG LEU B 259 5895 5791 7122 191 184 -215 C
ATOM 2355 CD1 LEU B 259 92.333 -46.868 -7.271 1.00 59.28 C
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ATOM 2356 CD2 LEU B 259 91.833 -48.350 -5.349 1.00 57.62 C
ANISOU 2356 CD2 LEU B 259 6844 6821 8228 294 194 -154 C
ATOM 2357 C LEU B 259 96.127 -48.317 -6.947 1.00 46.73 C
ANISOU 2357 C LEU B 259 5551 5350 6853 135 530 -372 C
ATOM 2358 O LEU B 259 96.697 -49.243 -6.382 1.00 51.04 O
ANISOU 2358 O LEU B 259 5976 5804 7613 249 683 -333 O
ATOM 2359 N GLU B 260 96.544 -47.059 -6.864 1.00 42.49 N
ANISOU 2359 N GLU B 260 5043 4910 6191 153 371 -344 N
ATOM 2360 CA GLU B 260 97.584 -46.684 -5.914 1.00 52.74 C
ANISOU 2360 CA GLU B 260 6244 6253 7540 326 366 -270 C
ATOM 2361 CB GLU B 260 98.954 -47.186 -6.367 1.00 53.94 C
ANISOU 2361 CB GLU B 260 6367 6316 7812 289 553 -341 C
ATOM 2362 CG GLU B 260 99.379 -46.736 -7.745 1.00 60.18 C
ANISOU 2362 CG GLU B 260 7290 7113 8464 49 593 -514 C
ATOM 2363 CD GLU B 260 100.622 -47.460 -8.207 1.00 88.97 C
ANISOU 2363 CD GLU B 260 10872 10636 12296 -12 859 -655 C
ATOM 2364 OE1 GLU B 260 100.622 -48.712 -8.179 1.00 98.16 O
ANISOU 2364 OE1 GLU B 260 11930 11637 13730 3 1076 -712 O
ATOM 2365 OE2 GLU B 260 101.606 -46.778 -8.564 1.00 96.06 O
ANISOU 2365 OE2 GLU B 260 11798 11579 13123 -72 860 -714 O
ATOM 2366 C GLU B 260 97.634 -45.186 -5.633 1.00 49.13 C
ANISOU 2366 C GLU B 260 5805 5909 6953 357 164 -248 C
ATOM 2367 O GLU B 260 97.057 -44.384 -6.361 1.00 42.11 O
ANISOU 2367 O GLU B 260 4991 5027 5983 235 19 -275 O
ATOM 2368 N TYR B 261 98.324 -44.832 -4.555 1.00 43.08 N
ANISOU 2368 N TYR B 261 4945 5225 6197 497 147 -179 N
ATOM 2369 CA TYR B 261 98.510 -43.445 -4.176 1.00 34.37 C
ANISOU 2369 CA TYR B 261 3831 4217 5010 525 2 -198 C
ATOM 2370 CB TYR B 261 98.760 -43.330 -2.683 1.00 39.73 C
ANISOU 2370 CB TYR B 261 4387 5041 5667 630 7 -134 C
ATOM 2371 CG TYR B 261 97.520 -43.403 -1.831 1.00 54.69 C
ANISOU 2371 CG TYR B 261 6211 7010 7561 645 -8 -152 C
ATOM 2372 CD1 TYR B 261 96.721 -42.276 -1.642 1.00 45.87 C
ANISOU 2372 CD1 TYR B 261 5057 5906 6466 630 -93 -285 C
ATOM 2373 CE1 TYR B 261 95.584 -42.332 -0.853 1.00 56.76 C
ANISOU 2373 CE1 TYR B 261 6344 7342 7878 624 -65 -353 C
ATOM 2374 CZ TYR B 261 95.238 -43.527 -0.237 1.00 54.20 C
ANISOU 2374 CZ TYR B 261 5989 7100 7503 622 20 -252 C
ATOM 2375 OH TYR B 261 94.115 -43.592 0.550 1.00 58.38 O
ANISOU 2375 OH TYR B 261 6429 7714 8039 586 61 -334 O
ATOM 2376 CE2 TYR B 261 96.019 -44.660 -0.409 1.00 55.68 C
ANISOU 2376 CE2 TYR B 261 6207 7266 7683 643 71 -73 C
ATOM 2377 CD2 TYR B 261 97.154 -44.593 -1.201 1.00 57.17 C
ANISOU 2377 CD2 TYR B 261 6462 7361 7899 660 71 -41 C
ATOM 2378 C TYR B 261 99.690 -42.835 -4.922 1.00 39.48 C
ANISOU 2378 C TYR B 261 4543 4853 5605 462 -12 -235 C
ATOM 2379 O TYR B 261 100.658 -43.526 -5.243 1.00 44.83 O
ANISOU 2379 O TYR B 261 5221 5482 6329 446 128 -237 O
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ANISOU 2380 N ALA B 262 4416 4726 5406 419 -175 -266 N
ATOM 2381 CA ALA B 262 100.711 -40.792 -5.777 1.00 36.25 C
ANISOU 2381 CA ALA B 262 4210 4484 5080 353 -218 -284 C
ATOM 2382 CB ALA B 262 100.226 -39.478 -6.349 1.00 33.76 C
ANISOU 2382 CB ALA B 262 3910 4144 4774 253 -441 -274 C
ATOM 2383 C ALA B 262 101.788 -40.545 -4.727 1.00 43.22 C
ANISOU 2383 C ALA B 262 5013 5456 5953 488 -173 -258 C
ATOM 2384 O ALA B 262 101.588 -39.777 -3.791 1.00 40.65 O
ANISOU 2384 O ALA B 262 4611 5211 5625 559 -245 -270 O
ATOM 2385 N THR B 263 102.935 -41.191 -4.896 1.00 38.65 N
ANISOU 2385 N THR B 263 5349 5034 4300 356 491 413 N
ATOM 2386 CA THR B 263 104.028 -41.086 -3.928 1.00 42.76 C
ANISOU 2386 CA THR B 263 5842 5580 4824 397 473 492 C
ATOM 2387 CB THR B 263 105.189 -42.018 -4.288 1.00 38.33 C
ANISOU 2387 CB THR B 263 5272 4888 4404 428 499 529 C
ATOM 2388 OG1 THR B 263 105.640 -41.737 -5.620 1.00 43.17 O
ANISOU 2388 OG1 THR B 263 5897 5442 5063 377 586 411 O
ATOM 2389 CG2 THR B 263 104.745 -43.451 -4.179 1.00 30.88 C
ANISOU 2389 CG2 THR B 263 4395 3835 3502 403 510 613 C
ATOM 2390 C THR B 263 104.604 -39.697 -3.620 1.00 35.14 C
ANISOU 2390 C THR B 263 4863 4671 3817 436 403 439 C
ATOM 2391 O THR B 263 105.086 -39.485 -2.507 1.00 35.41 O
ANISOU 2391 O THR B 263 4855 4786 3813 460 358 477 O
ATOM 2392 N PRO B 264 104.596 -38.759 -4.593 1.00 31.58 N
ANISOU 2392 N PRO B 264 4508 4147 3343 410 368 361 N
ATOM 2393 CA PRO B 264 105.191 -37.467 -4.231 1.00 34.29 C
ANISOU 2393 CA PRO B 264 4893 4500 3636 406 296 319 C
ATOM 2394 CB PRO B 264 105.153 -36.675 -5.541 1.00 28.58 C
ANISOU 2394 CB PRO B 264 4414 3609 2836 301 238 278 C
ATOM 2395 CG PRO B 264 105.182 -37.709 -6.602 1.00 32.01 C
ANISOU 2395 CG PRO B 264 4888 3991 3285 255 294 294 C
ATOM 2396 CD PRO B 264 104.346 -38.840 -6.043 1.00 30.64 C
ANISOU 2396 CD PRO B 264 4538 3900 3202 329 379 329 C
ATOM 2397 C PRO B 264 104.419 -36.711 -3.159 1.00 35.41 C
ANISOU 2397 C PRO B 264 4977 4742 3737 497 195 250 C
ATOM 2398 O PRO B 264 104.956 -35.763 -2.580 1.00 40.47 O
ANISOU 2398 O PRO B 264 5633 5403 4343 500 139 210 O
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ANISOU 2399 N LEU B 265 4814 4750 3675 542 195 180 N
ATOM 2400 CA LEU B 265 102.416 -36.503 -1.811 1.00 43.01 C
ANISOU 2400 CA LEU B 265 5720 5939 4682 590 171 14 C
ATOM 2401 CB LEU B 265 100.955 -36.949 -1.840 1.00 40.16 C
ANISOU 2401 CB LEU B 265 5196 5689 4374 594 208 -169 C
ATOM 2402 CG LEU B 265 100.206 -36.452 -3.072 1.00 46.21 C
ANISOU 2402 CG LEU B 265 5992 6294 5274 732 -6 -301 C
ATOM 2403 CD1 LEU B 265 98.808 -37.026 -3.111 1.00 46.11 C
ANISOU 2403 CD1 LEU B 265 5733 6429 5359 730 29 -537 C
ATOM 2404 CD2 LEU B 265 100.149 -34.926 -3.083 1.00 48.20 C
ANISOU 2404 CD2 LEU B 265 6313 6410 5589 905 -266 -461 C
ATOM 2405 C LEU B 265 103.060 -36.815 -0.457 1.00 29.42 C
ANISOU 2405 C LEU B 265 3967 4371 2839 503 264 99 C
ATOM 2406 O LEU B 265 102.961 -36.041 0.495 1.00 39.52 O
ANISOU 2406 O LEU B 265 5198 5769 4048 504 251 -28 O
ATOM 2407 N ILE B 266 103.720 -37.964 -0.385 1.00 40.28 N
ANISOU 2407 N ILE B 266 5399 5715 4192 435 317 183 N
ATOM 2408 CA ILE B 266 104.473 -38.355 0.802 1.00 40.42 C
ANISOU 2408 CA ILE B 266 5469 5799 4092 373 287 424 C
ATOM 2409 CB ILE B 266 105.012 -39.777 0.669 1.00 40.60 C
ANISOU 2409 CB ILE B 266 5584 5688 4154 358 251 621 C
ATOM 2410 CG1 ILE B 266 103.855 -40.765 0.694 1.00 45.98 C
ANISOU 2410 CG1 ILE B 266 6341 6380 4748 210 371 652 C
ATOM 2411 CD1 ILE B 266 104.236 -42.162 0.275 1.00 37.46 C
ANISOU 2411 CD1 ILE B 266 5389 5087 3758 215 319 820 C
ATOM 2412 CG2 ILE B 266 105.999 -40.102 1.790 1.00 36.79 C
ANISOU 2412 CG2 ILE B 266 5202 5192 3585 358 73 758 C
ATOM 2413 C ILE B 266 105.619 -37.375 1.041 1.00 31.18 C
ANISOU 2413 C ILE B 266 4278 4623 2946 438 178 400 C
ATOM 2414 O ILE B 266 105.906 -36.975 2.165 1.00 39.97 O
ANISOU 2414 O ILE B 266 5410 5850 3927 397 121 388 O
ATOM 2415 N THR B 267 106.253 -36.967 -0.045 1.00 30.03 N
ANISOU 2415 N THR B 267 4114 4354 2942 484 170 370 N
ATOM 2416 CA THR B 267 107.335 -36.007 0.044 1.00 37.75 C
ANISOU 2416 CA THR B 267 5069 5330 3946 470 112 306 C
ATOM 2417 CB THR B 267 108.117 -35.941 -1.260 1.00 36.41 C
ANISOU 2417 CB THR B 267 4901 5041 3892 405 183 264 C
ATOM 2418 OG1 THR B 267 108.875 -37.145 -1.394 1.00 46.07 O
ANISOU 2418 OG1 THR B 267 5991 6258 4255 446 202 295 O
ATOM 2419 CG2 THR B 267 109.058 -34.737 -1.262 1.00 29.75 C
ANISOU 2419 CG2 THR B 267 4071 4199 3034 473 121 151 C
ATOM 2420 C THR B 267 106.841 -34.614 0.472 1.00 36.14 C
ANISOU 2420 C THR B 267 4920 5156 3655 467 64 171 C
ATOM 2421 O THR B 267 107.432 -33.979 1.349 1.00 45.07 O
ANISOU 2421 O THR B 267 6030 6369 4727 441 4 121 O
ATOM 2422 N LEU B 268 105.744 -34.164 -0.130 1.00 33.93 N
ANISOU 2422 N LEU B 268 4705 4792 3394 518 49 81 N
ATOM 2423 CA LEU B 268 105.091 -32.917 0.275 1.00 32.75 C
ANISOU 2423 CA LEU B 268 4586 4624 3233 587 -54 -113 C
ATOM 2424 CB LEU B 268 103.822 -32.654 -0.541 1.00 28.79 C
ANISOU 2424 CB LEU B 268 4118 3992 2831 712 -162 -244 C
ATOM 2425 CG LEU B 268 103.999 -32.226 -1.991 1.00 41.80 C
ANISOU 2425 CG LEU B 268 6034 5345 4504 693 -309 -167 C
ATOM 2426 CD1 LEU B 268 102.649 -31.984 -2.643 1.00 43.30 C
ANISOU 2426 CD1 LEU B 268 6250 5396 4804 870 -529 -318 C
ATOM 2427 CD2 LEU B 268 104.851 -30.970 -2.068 1.00 44.86 C
ANISOU 2427 CD2 LEU B 268 6664 5547 4832 603 -421 -172 C
ATOM 2428 C LEU B 268 104.723 -32.933 1.751 1.00 43.95 C
ANISOU 2428 C LEU B 268 5872 6282 4546 574 5 -226 C
ATOM 2429 O LEU B 268 104.898 -31.943 2.462 1.00 48.04 O
ANISOU 2429 O LEU B 268 6398 6832 5022 579 -51 -372 O
ATOM 2430 N PHE B 269 104.189 -34.053 2.214 1.00 33.23 N
ANISOU 2430 N PHE B 269 4436 5081 3107 507 130 -172 N
ATOM 2431 CA PHE B 269 103.848 -34.146 3.622 1.00 35.51 C
ANISOU 2431 CA PHE B 269 4683 5609 3199 380 226 -272 C
ATOM 2432 CB PHE B 269 103.114 -35.444 3.925 1.00 39.82 C
ANISOU 2432 CB PHE B 269 5232 6281 3616 216 385 -202 C
ATOM 2433 CG PHE B 269 102.636 -35.524 5.338 1.00 49.03 C
ANISOU 2433 CG PHE B 269 6426 7709 4493 -29 536 -337 C
ATOM 2434 CD1 PHE B 269 101.497 -34.838 5.728 1.00 48.61 C
ANISOU 2434 CD1 PHE B 269 6162 7857 4449 -71 697 -758 C
ATOM 2435 CE1 PHE B 269 101.049 -34.891 7.029 1.00 42.52 C
ANISOU 2435 CE1 PHE B 269 5415 7374 3367 -380 909 -950 C
ATOM 2436 CZ PHE B 269 101.749 -35.641 7.965 1.00 50.97 C
ANISOU 2436 CZ PHE B 269 6649 8484 4059 -659 897 -642 C
ATOM 2437 CE2 PHE B 269 102.897 -36.331 7.585 1.00 50.48 C
ANISOU 2437 CE2 PHE B 269 6984 8167 4027 -547 638 -193 C
ATOM 2438 CD2 PHE B 269 103.336 -36.261 6.279 1.00 40.10 C
ANISOU 2438 CD2 PHE B 269 5545 6615 3077 -230 492 -83 C
ATOM 2439 C PHE B 269 105.104 -34.057 4.492 1.00 34.85 C
ANISOU 2439 C PHE B 269 4702 5569 2972 305 138 -129 C
ATOM 2440 O PHE B 269 105.151 -33.328 5.481 1.00 42.26 O
ANISOU 2440 O PHE B 269 5646 6639 3772 240 135 -279 O
ATOM 2441 N ALA B 270 106.124 -34.814 4.114 1.00 35.80 N
ANISOU 2441 N ALA B 270 4873 5581 3148 324 -34 114 N
ATOM 2442 CA ALA B 270 107.367 -34.807 4.867 1.00 40.47 C

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ANISOU 2442 CA ALA B 270 5503 6202 3670 298 -114 209 C
ATOM 2443 CB ALA B 270 108.351 -35.815 4.305 1.00 37.17 C
ANISOU 2443 CB ALA B 270 5055 5651 3417 379 -233 385 C
ATOM 2444 C ALA B 270 107.990 -33.411 4.893 1.00 38.88 C
ANISOU 2444 C ALA B 270 5248 5998 3528 318 -168 43 C
ATOM 2445 O ALA B 270 108.531 -32.983 5.903 1.00 44.04 O
ANISOU 2445 O ALA B 270 5925 6762 4047 253 -267 -1 O
ATOM 2446 N MET B 271 107.913 -32.705 3.774 1.00 30.86 N
ANISOU 2446 N MET B 271 4215 4828 2681 370 -125 -41 N
ATOM 2447 CA MET B 271 108.488 -31.375 3.711 1.00 35.37 C
ANISOU 2447 CA MET B 271 4823 5330 3286 331 -181 -183 C
ATOM 2448 CB MET B 271 108.464 -30.821 2.292 1.00 30.14 C
ANISOU 2448 CB MET B 271 4275 4426 2749 316 -164 -199 C
ATOM 2449 CG MET B 271 109.551 -31.419 1.397 1.00 26.56 C
ANISOU 2449 CG MET B 271 3767 3935 2391 212 -94 -108 C
ATOM 2450 SD MET B 271 109.342 -30.946 -0.321 1.00 39.72 S
ANISOU 2450 SD MET B 271 5687 5328 4076 87 -36 -101 S
ATOM 2451 CE MET B 271 110.352 -29.479 -0.419 1.00 34.88 C
ANISOU 2451 CE MET B 271 5256 4599 3396 -184 -51 -227 C
ATOM 2452 C MET B 271 107.820 -30.413 4.685 1.00 40.64 C
ANISOU 2452 C MET B 271 5525 6078 3840 336 -200 -391 C
ATOM 2453 O MET B 271 108.469 -29.522 5.233 1.00 37.95 O
ANISOU 2453 O MET B 271 5212 5753 3456 269 -271 -498 O
ATOM 2454 N SER B 272 106.526 -30.597 4.913 1.00 35.02 N
ANISOU 2454 N SER B 272 4775 5437 3093 396 -120 -507 N
ATOM 2455 CA SER B 272 105.831 -29.730 5.857 1.00 36.53 C
ANISOU 2455 CA SER B 272 4930 5741 3207 398 -94 -813 C
ATOM 2456 CB SER B 272 104.319 -29.727 5.627 1.00 37.08 C
ANISOU 2456 CB SER B 272 4869 5836 3385 512 -13 -1068 C
ATOM 2457 OG SER B 272 103.752 -30.989 5.911 1.00 49.49 O
ANISOU 2457 OG SER B 272 6365 7613 4825 389 166 -983 O
ATOM 2458 C SER B 272 106.151 -30.095 7.315 1.00 34.75 C
ANISOU 2458 C SER B 272 4719 5795 2689 211 -36 -806 C
ATOM 2459 O SER B 272 105.932 -29.294 8.217 1.00 52.91 O
ANISOU 2459 O SER B 272 7011 8216 4877 152 -6 -1070 O
ATOM 2460 N GLN B 273 106.656 -31.303 7.551 1.00 40.74 N
ANISOU 2460 N GLN B 273 5542 6628 3310 113 -55 -518 N
ATOM 2461 CA GLN B 273 106.995 -31.709 8.917 1.00 35.92 C
ANISOU 2461 CA GLN B 273 5066 6221 2361 -90 -95 -455 C
ATOM 2462 CB GLN B 273 106.833 -33.215 9.119 1.00 41.55 C
ANISOU 2462 CB GLN B 273 5931 6960 2898 -210 -97 -177 C
ATOM 2463 CG GLN B 273 105.458 -33.749 8.785 1.00 55.27 C
ANISOU 2463 CG GLN B 273 7620 8756 4624 -284 166 -270 C
ATOM 2464 CD GLN B 273 104.368 -33.161 9.664 1.00 82.05 C
ANISOU 2464 CD GLN B 273 10955 12415 7805 -488 424 -653 C
ATOM 2465 OE1 GLN B 273 103.658 -32.234 9.261 1.00 80.01 O
ANISOU 2465 OE1 GLN B 273 10450 12168 7780 -335 525 -1008 O
ATOM 2466 NE2 GLN B 273 104.230 -33.698 10.877 1.00 86.40 N
ANISOU 2466 NE2 GLN B 273 11751 13154 7923 -842 508 -612 N
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ANISOU 2467 C GLN B 273 5272 6369 2532 -85 -337 -374 C
ATOM 2468 O GLN B 273 108.720 -31.045 10.443 1.00 50.96 O
ANISOU 2468 O GLN B 273 7113 8255 3996 -235 -419 -432 O
ATOM 2469 N TYR B 274 109.298 -31.267 8.292 1.00 46.42 N
ANISOU 2469 N TYR B 274 6317 7350 3971 50 -441 -279 N
ATOM 2470 CA TYR B 274 110.703 -30.974 8.546 1.00 37.77 C
ANISOU 2470 CA TYR B 274 5158 6261 2933 38 -656 -269 C
ATOM 2471 CB TYR B 274 111.619 -31.813 7.653 1.00 39.92 C
ANISOU 2471 CB TYR B 274 5281 6420 3469 148 -758 -128 C
ATOM 2472 CG TYR B 274 111.542 -33.285 7.976 1.00 47.25 C
ANISOU 2472 CG TYR B 274 6300 7331 4322 208 -905 108 C
ATOM 2473 CD1 TYR B 274 111.898 -33.749 9.232 1.00 60.08 C
ANISOU 2473 CD1 TYR B 274 8098 9035 5697 151 -1188 216 C
ATOM 2474 CE1 TYR B 274 111.814 -35.088 9.549 1.00 72.23 C
ANISOU 2474 CE1 TYR B 274 9841 10474 7129 178 -1389 464 C
ATOM 2475 CZ TYR B 274 111.364 -35.985 8.598 1.00 70.01 C
ANISOU 2475 CZ TYR B 274 9535 10038 7027 273 -1265 577 C
ATOM 2476 OH TYR B 274 111.286 -37.318 8.921 1.00 75.36 O
ANISOU 2476 OH TYR B 274 10474 10559 7600 284 -1492 827 O
ATOM 2477 CE2 TYR B 274 110.993 -35.550 7.337 1.00 55.52 C
ANISOU 2477 CE2 TYR B 274 7480 8171 5446 334 -953 450 C
ATOM 2478 CD2 TYR B 274 111.080 -34.204 7.033 1.00 50.56 C
ANISOU 2478 CD2 TYR B 274 6704 7619 4888 297 -794 232 C
ATOM 2479 C TYR B 274 111.031 -29.494 8.423 1.00 36.33 C
ANISOU 2479 C TYR B 274 4934 6035 2833 -8 -625 -508 C
ATOM 2480 O TYR B 274 110.680 -28.849 7.442 1.00 46.63 O
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ANISOU 2481 N SER B 275 4976 6192 2721 -112 -771 -610 N
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ANISOU 2482 CA SER B 275 6464 7618 4235 -198 -751 -857 C
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ANISOU 2483 CB SER B 275 5947 7244 3399 -330 -897 -978 C
ATOM 2484 OG SER B 275 113.543 -27.860 11.314 1.00 61.31 O
ANISOU 2484 OG SER B 275 8086 9584 5624 -342 -1166 -848 O
ATOM 2485 C SER B 275 113.071 -27.096 8.506 1.00 53.01 C
ANISOU 2485 C SER B 275 6956 8087 5099 -258 -765 -890 C
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ANISOU 2498 CB ALA B 277 4459 4988 3030 -53 -326 -467 C
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ANISOU 2502 CA GLY B 278 8515 7909 6279 -270 -556 -1035 C
ATOM 2503 C GLY B 278 109.834 -24.449 4.307 1.00 57.23 C
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ANISOU 2504 O GLY B 278 9728 8031 7134 -87 -731 -1019 O
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ANISOU 2505 N PHE B 279 8755 8162 6644 156 -558 -1012 N
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ATOM 2512 CE2 PHE B 279 105.113 -28.285 1.162 1.00 50.79 C
ANISOU 2512 CE2 PHE B 279 7262 6458 5578 733 -570 -692 C
ATOM 2513 CD2 PHE B 279 105.934 -28.056 2.246 1.00 49.48 C
ANISOU 2513 CD2 PHE B 279 7015 6476 5308 616 -474 -720 C
ATOM 2514 C PHE B 279 106.577 -25.691 5.020 1.00 45.23 C
ANISOU 2514 C PHE B 279 6456 6100 4629 538 -556 -1270 C
ATOM 2515 O PHE B 279 106.591 -26.547 5.898 1.00 58.42 O
ANISOU 2515 O PHE B 279 7940 8107 6151 468 -397 -1233 O
ATOM 2516 N SER B 280 105.603 -24.798 4.897 1.00 40.10 N
ANISOU 2516 N SER B 280 5857 5235 4145 744 -716 -1564 N
ATOM 2517 CA SER B 280 104.515 -24.734 5.862 1.00 37.26 C
ANISOU 2517 CA SER B 280 5230 5103 3824 880 -632 -1954 C
ATOM 2518 CB SER B 280 104.022 -23.296 6.025 1.00 53.38 C
ANISOU 2518 CB SER B 280 7352 6860 6071 1082 -868 -2370 C
ATOM 2519 OG SER B 280 103.224 -22.914 4.923 1.00 60.97 O
ANISOU 2519 OG SER B 280 8427 7430 7310 1361 -1175 -2449 O
ATOM 2520 C SER B 280 103.347 -25.629 5.454 1.00 40.92 C
ANISOU 2520 C SER B 280 5468 5685 4395 1017 -553 -2018 C
ATOM 2521 O SER B 280 103.287 -26.146 4.337 1.00 58.09 O
ANISOU 2521 O SER B 280 7734 7693 6643 1067 -634 -1767 O
ATOM 2522 N ARG B 281 102.396 -25.774 6.369 1.00 50.87 N
ANISOU 2522 N ARG B 281 8326 8383 5659 1120 -812 -887 N
ATOM 2523 CA ARG B 281 101.235 -26.607 6.123 1.00 70.75 C
ANISOU 2523 CA ARG B 281 9909 9979 6992 1011 -459 -575 C
ATOM 2524 CB ARG B 281 100.511 -26.891 7.427 1.00 86.15 C
ANISOU 2524 CB ARG B 281 12102 12238 8391 1134 -289 -585 C
ATOM 2525 CG ARG B 281 100.183 -28.348 7.605 1.00100.97 C
ANISOU 2525 CG ARG B 281 14348 14284 10112 1060 -6 -192 C
ATOM 2526 CD ARG B 281 98.703 -28.489 7.883 1.00107.82 C
ANISOU 2526 CD ARG B 281 15104 15175 10687 949 478 -209 C
ATOM 2527 NE ARG B 281 98.343 -29.316 9.039 1.00113.76 N
ANISOU 2527 NE ARG B 281 16275 16081 10868 994 793 -33 N
ATOM 2528 CZ ARG B 281 98.924 -29.303 10.240 1.00119.33 C
ANISOU 2528 CZ ARG B 281 17373 16937 11029 1244 616 -36 C
ATOM 2529 NH1 ARG B 281 98.459 -30.105 11.188 1.00126.50 N
ANISOU 2529 NH1 ARG B 281 18751 17936 11376 1272 1003 182 N
ATOM 2530 NH2 ARG B 281 99.958 -28.514 10.515 1.00113.49 N
ANISOU 2530 NH2 ARG B 281 16584 16246 10290 1478 80 -280 N
ATOM 2531 C ARG B 281 100.293 -25.943 5.128 1.00 68.75 C
ANISOU 2531 C ARG B 281 9456 9608 7057 907 -283 -635 C
ATOM 2532 O ARG B 281 99.464 -26.594 4.497 1.00 72.07 O
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ANISOU 2532 O  ARG B 281    9821 10037  7527   794   -39   -450       O
ATOM  2533 N  GLU B 282     100.433 -24.633  4.991  1.00 69.45           N
ANISOU 2533 N  GLU B 282    9441  9570  7375   977   -425   -930       N
ATOM  2534 CA GLU B 282     99.634 -23.881  4.044  1.00 59.33           C
ANISOU 2534 CA GLU B 282    8047  8124  6370   971   -337   -992       C
ATOM  2535 CB GLU B 282     99.539 -22.410  4.446  1.00 67.43           C
ANISOU 2535 CB GLU B 282    9028  9077  7517  1114   -450  -1367       C
ATOM  2536 CG GLU B 282     98.709 -22.168  5.693  1.00 86.43           C
ANISOU 2536 CG GLU B 282   11418 11822  9600  1236   -383  -1621       C
ATOM  2537 CD GLU B 282     99.280 -22.849  6.933  1.00 95.29           C
ANISOU 2537 CD GLU B 282   12688 13223 10295  1269   -431  -1611       C
ATOM  2538 OE1 GLU B 282     98.500 -23.489  7.671  1.00 99.31           O
ANISOU 2538 OE1 GLU B 282   13303 14017 10415  1275   -207  -1555       O
ATOM  2539 OE2 GLU B 282     100.507 -22.753  7.154  1.00 97.80           O
ANISOU 2539 OE2 GLU B 282   13034 13458 10669  1305   -681  -1684       O
ATOM  2540 C  GLU B 282     100.282 -24.002  2.682  1.00 59.46           C
ANISOU 2540 C  GLU B 282    8057  7811  6724   847   -365   -794       C
ATOM  2541 O  GLU B 282     99.603 -24.094  1.660  1.00 58.58           O
ANISOU 2541 O  GLU B 282    7923  7609  6726   834   -269   -669       O
ATOM  2542 N  ASP B 283     101.609 -24.001  2.676  1.00 58.22           N
ANISOU 2542 N  ASP B 283    7913  7483  6723   771   -501   -819       N
ATOM  2543 CA ASP B 283     102.340 -24.235  1.449  1.00 58.57           C
ANISOU 2543 CA ASP B 283    7959  7219  7074   605   -462   -653       C
ATOM  2544 CB ASP B 283     103.848 -24.182  1.687  1.00 76.12           C
ANISOU 2544 CB ASP B 283   10116  9284  9523   519   -607   -830       C
ATOM  2545 CG ASP B 283     104.351 -22.777  1.925  1.00 96.28           C
ANISOU 2545 CG ASP B 283   12630 11604 12346   551   -655  -1215       C
ATOM  2546 OD1 ASP B 283     103.641 -21.819  1.550  1.00108.82           O
ANISOU 2546 OD1 ASP B 283   14309 13033 14007   610   -544  -1247       O
ATOM  2547 OD2 ASP B 283     105.465 -22.636  2.483  1.00 95.53           O
ANISOU 2547 OD2 ASP B 283   12400 11471 12425   536   -815  -1526       O
ATOM  2548 C  ASP B 283     101.959 -25.600  0.892  1.00 62.66           C
ANISOU 2548 C  ASP B 283    8464  7857  7485   504   -343   -322       C
ATOM  2549 O  ASP B 283     101.898 -25.798 -0.318  1.00 64.84           O
ANISOU 2549 O  ASP B 283    8748  7959  7928   409   -248   -162       O
ATOM  2550 N  ARG B 284     101.682 -26.532  1.796  1.00 53.69           N
ANISOU 2550 N  ARG B 284    7340  7005  6054   536   -323   -232       N
ATOM  2551 CA ARG B 284     101.449 -27.909  1.409  1.00 49.47           C
ANISOU 2551 CA ARG B 284    6789  6540  5467   419   -175    56       C
ATOM  2552 CB ARG B 284     101.394 -28.822  2.631  1.00 52.96           C
ANISOU 2552 CB ARG B 284    7364  7205  5552   478   -136   161       C
ATOM  2553 CG ARG B 284     101.430 -30.292  2.261  1.00 45.17           C
ANISOU 2553 CG ARG B 284    6388  6191  4583   345    20   465       C
ATOM  2554 CD ARG B 284     101.369 -31.155  3.494  1.00 43.81           C
ANISOU 2554 CD ARG B 284    6474  6163  4010   437   104   620       C
ATOM  2555 NE ARG B 284     100.024 -31.210  4.042  1.00 54.85           N
ANISOU 2555 NE ARG B 284    7934  7744  5163   423   459   600       N
ATOM  2556 CZ ARG B 284     99.751 -31.465  5.313  1.00 58.27           C
ANISOU 2556 CZ ARG B 284    8670  8328  5143   531   599   647       C
ATOM  2557 NH1 ARG B 284     98.489 -31.500  5.730  1.00 60.64           N
ANISOU 2557 NH1 ARG B 284    8985  8770  5285   459  1012   571       N
ATOM  2558 NH2 ARG B 284     100.739 -31.680  6.163  1.00 57.40           N
ANISOU 2558 NH2 ARG B 284    8853  8228  4730   730   328   731       N
ATOM  2559 C  ARG B 284     100.186 -28.111  0.578  1.00 51.26           C
ANISOU 2559 C  ARG B 284    6917  6819  5739   387   33   118       C
ATOM  2560 O  ARG B 284     100.183 -28.855 -0.410  1.00 37.73           O
ANISOU 2560 O  ARG B 284    5126  5030  4179   267   115   278       O
ATOM  2561 N  LEU B 285     99.099 -27.474  0.989  1.00 47.68           N
ANISOU 2561 N  LEU B 285    6430  6516  5171   513   100   -71       N
ATOM  2562 CA LEU B 285     97.849 -27.670  0.278  1.00 47.01           C
ANISOU 2562 CA LEU B 285    6185  6516  5162   534   248   -131       C
ATOM  2563 CB LEU B 285     96.657 -27.142  1.072  1.00 50.69           C
ANISOU 2563 CB LEU B 285    6563  7198  5500   659   355   -418       C
ATOM  2564 CG LEU B 285     95.343 -27.319  0.305  1.00 63.69           C
ANISOU 2564 CG LEU B 285    7956  8941  7302   718   461   -608       C
ATOM  2565 CD1 LEU B 285     94.990 -28.802  0.131  1.00 58.52           C
ANISOU 2565 CD1 LEU B 285    7154  8389  6692   510   758   -495       C
ATOM  2566 CD2 LEU B 285     94.223 -26.563  0.983  1.00 60.14           C
ANISOU 2566 CD2 LEU B 285    7368  8664  6817   869   520   -996       C
ATOM  2567 C  LEU B 285     97.923 -26.992 -1.089  1.00 50.47           C
ANISOU 2567 C  LEU B 285    6634  6727  5816   615    98   -138       C
ATOM  2568 O  LEU B 285     97.437 -27.517 -2.091  1.00 56.28           O
ANISOU 2568 O  LEU B 285    7267  7472  6644   608   140   -96       O
ATOM  2569 N  GLU B 286     98.541 -25.817 -1.110  1.00 42.73           N
ANISOU 2569 N  GLU B 286    5809  5525  4902   702   -59   -210       N
ATOM  2570 CA GLU B 286     98.719 -25.069 -2.339  1.00 52.03           C
ANISOU 2570 CA GLU B 286    7140  6401  6228   788   -142   -169       C
ATOM  2571 CB GLU B 286     99.444 -23.760 -2.047  1.00 57.33           C
ANISOU 2571 CB GLU B 286    7989  6783  7008   837   -217   -285       C
ATOM  2572 CG GLU B 286     99.940 -23.030 -3.273  1.00 83.87           C
ANISOU 2572 CG GLU B 286   11629  9716 10520   859   -192   -176       C
ATOM  2573 CD GLU B 286     100.840 -21.865 -2.916  1.00103.03           C
ANISOU 2573 CD GLU B 286   14201 11794 13152   814   -161   -322       C
ATOM  2574 OE1 GLU B 286     100.465 -20.710 -3.216  1.00103.70           O
ANISOU 2574 OE1 GLU B 286   14505 11606 13292  1010   -173   -393       O
ATOM  2575 OE2 GLU B 286     101.920 -22.107 -2.330  1.00105.76           O
ANISOU 2575 OE2 GLU B 286   14428 12126 13632   603   -135   -405       O
ATOM  2576 C  GLU B 286     99.518 -25.905 -3.340  1.00 50.59           C
ANISOU 2576 C  GLU B 286    6998  6080  6144   594   -77    74       C
ATOM  2577 O  GLU B 286     99.150 -26.033 -4.509  1.00 49.40           O
ANISOU 2577 O  GLU B 286    6905  5862  6001   661   -77   150       O
ATOM  2578 N  GLN B 287     100.606 -26.493 -2.857  1.00 42.52           N
ANISOU 2578 N  GLN B 287    5937  5034  5183   385   -48   154       N
ATOM  2579 CA GLN B 287     101.494 -27.274 -3.706  1.00 39.34           C
ANISOU 2579 CA GLN B 287    5530  4488  4929   178    18   324       C
ATOM  2580 CB GLN B 287     102.814 -27.553 -2.994  1.00 39.44           C
ANISOU 2580 CB GLN B 287    5491  4427  5068    24   -35   286       C
ATOM  2581 CG GLN B 287     103.701 -26.323 -2.893  1.00 43.54           C
ANISOU 2581 CG GLN B 287    6111  4651  5780     7   -69    84       C
ATOM  2582 CD GLN B 287     104.124 -25.806 -4.259  1.00 50.36           C
ANISOU 2582 CD GLN B 287    7154  5142  6838   -109   105   142       C
ATOM  2583 OE1 GLN B 287     104.876 -26.471 -4.972  1.00 68.26           O
ANISOU 2583 OE1 GLN B 287    9379  7292  9265   -315   210   215       O
ATOM  2584 NE2 GLN B 287     103.631 -24.629 -4.637  1.00 42.48           N
ANISOU 2584 NE2 GLN B 287    6395  3935  5808    36   157   113       N
ATOM  2585 C  GLN B 287     100.861 -28.576 -4.183  1.00 42.81           C
ANISOU 2585 C  GLN B 287    5803  5135  5328   118   108   452       C
ATOM  2586 O  GLN B 287     101.124 -29.034 -5.287  1.00 47.47           O
ANISOU 2586 O  GLN B 287    6395  5626  6015    22   164   551       O
ATOM  2587 N  ALA B 288     100.028 -29.175 -3.344  1.00 45.27           N
ANISOU 2587 N  ALA B 288    5972  5719  5509   156   167   418       N
ATOM  2588 CA ALA B 288     99.344 -30.405 -3.723  1.00 37.77           C
ANISOU 2588 CA ALA B 288    4825  4934  4591    73   322   472       C
ATOM  2589 CB ALA B 288     98.655 -31.035 -2.528  1.00 34.71           C
ANISOU 2589 CB ALA B 288    4354  4762  4071    51   497   443       C
ATOM  2590 C  ALA B 288     98.343 -30.178 -4.856  1.00 29.67           C
ANISOU 2590 C  ALA B 288    3708  3966  3599   219   295   335       C
ATOM  2591 O  ALA B 288     98.193 -31.015 -5.739  1.00 38.34           O
ANISOU 2591 O  ALA B 288    4665  5104  4800   144   200   335       O
ATOM  2592 N  LYS B 289     97.643 -29.050 -4.810  1.00 39.21           N
ANISOU 2592 N  LYS B 289    4990  5187  4720   467   170   155       N
ATOM  2593 CA LYS B 289     96.711 -28.694 -5.874  1.00 35.85           C
ANISOU 2593 CA LYS B 289    4531  4806  4286   721    41   -14       C
ATOM  2594 CB LYS B 289     95.947 -27.432 -5.519  1.00 35.55           C
ANISOU 2594 CB LYS B 289    4570  4766  4169  1027   -121   -238       C
ATOM  2595 CG LYS B 289     94.896 -27.584 -4.461  1.00 47.66           C
ANISOU 2595 CG LYS B 289    5808  6578  5722  1052   -15   -526       C
ATOM  2596 CD LYS B 289     94.315 -26.216 -4.150  1.00 44.17           C
ANISOU 2596 CD LYS B 289    5456  6090  5239  1360   -205   -762       C
ATOM  2597 CE LYS B 289     93.598 -26.191 -2.823  1.00 51.37           C
ANISOU 2597 CE LYS B 289    6139  7234  6145  1313   -39  -1030       C
ATOM  2598 NZ LYS B 289     93.470 -24.796 -2.308  1.00 65.38           N
ANISOU 2598 NZ LYS B 289    8051  8904  7888  1540   -207  -1198       N
ATOM  2599 C  LYS B 289     97.475 -28.433 -7.166  1.00 41.91           C
ANISOU 2599 C  LYS B 289    5574  5320  5030   744   -45   167       C
ATOM  2600 O  LYS B 289     97.028 -28.769 -8.262  1.00 50.27           O
ANISOU 2600 O  LYS B 289    6602  6442  6056   869   -116   110       O
ATOM  2601 N  LEU B 290     98.631 -27.804 -7.012  1.00 37.60           N
ANISOU 2601 N  LEU B 290    5300  4482  4502   623   -17   337       N
ATOM  2602 CA LEU B 290     99.471 -27.437 -8.135  1.00 41.11           C
ANISOU 2602 CA LEU B 290    6038  4668  4938   584    17   500       C
ATOM  2603 CB LEU B 290     100.554 -26.468 -7.652  1.00 49.46           C
ANISOU 2603 CB LEU B 290    7362  5331  6099   463    92   547       C
ATOM  2604 CG LEU B 290     101.642 -25.958 -8.586  1.00 57.21           C
ANISOU 2604 CG LEU B 290    8697  5888  7153   319   269   675       C
ATOM  2605 CD1 LEU B 290     101.047 -25.551 -9.915  1.00 47.75           C
ANISOU 2605 CD1 LEU B 290    7877  4563  5704   587   243   779       C
ATOM  2606 CD2 LEU B 290     102.305 -24.767 -7.920  1.00 58.82           C
ANISOU 2606 CD2 LEU B 290    9067  5772  7512   276   337   584       C
ATOM  2607 C  LEU B 290     100.080 -28.696 -8.753  1.00 37.59           C
ANISOU 2607 C  LEU B 290    5468  4218  4597   315   147   610       C
ATOM  2608 O  LEU B 290     100.195 -28.829 -9.979  1.00 35.56           O
ANISOU 2608 O  LEU B 290    5370  3875  4265   343   173   673       O
ATOM  2609 N  PHE B 291     100.455 -29.630 -7.889  1.00 30.95           N
ANISOU 2609 N  PHE B 291    4346  3511  3904    82   224   627       N
ATOM  2610 CA PHE B 291     101.006 -30.906 -8.329  1.00 36.22           C
ANISOU 2610 CA PHE B 291    4822  4215  4725   -164   337   708       C
ATOM  2611 CB PHE B 291     101.418 -31.750 -7.116  1.00 34.95           C
ANISOU 2611 CB PHE B 291    4458  4138  4682   -334   382   753       C
ATOM  2612 CG PHE B 291     101.689 -33.187 -7.456  1.00 29.81           C
ANISOU 2612 CG PHE B 291    3577  3539  4210  -535   493   820       C
ATOM  2613 CD1 PHE B 291     102.925 -33.570 -7.952  1.00 29.81           C
ANISOU 2613 CD1 PHE B 291    3573  3345  4409  -739   522   874       C
ATOM  2614 CE1 PHE B 291     103.177 -34.892 -8.283  1.00 27.32           C
ANISOU 2614 CE1 PHE B 291    3072  3086  4223  -869   577   841       C
ATOM  2615 CZ PHE B 291     102.174 -35.848 -8.115  1.00 30.12           C
ANISOU 2615 CZ PHE B 291    3242  3632  4571  -843   661   811       C
ATOM  2616 CE2 PHE B 291     100.934 -35.468 -7.625  1.00 35.87           C
ANISOU 2616 CE2 PHE B 291    3893  4520  5217  -724   737   823       C
ATOM  2617 CD2 PHE B 291     100.696 -34.147 -7.301  1.00 28.40           C
ANISOU 2617 CD2 PHE B 291    3159  3574  4057  -534   606   776       C
ATOM  2618 C  PHE B 291     99.975 -31.662 -9.179  1.00 42.91           C
ANISOU 2618 C  PHE B 291    5471  5294  5536   -66   336   609       C
ATOM  2619 O  PHE B 291     100.282 -32.202 -10.238  1.00 38.58           O
ANISOU 2619 O  PHE B 291    4910  4719  5030   -150   385   632       O
ATOM  2620 N  CYS B 292     98.742 -31.686 -8.694  1.00 29.28           N
ANISOU 2620 N  CYS B 292    3559  3808  3759   112   290   433       N
ATOM  2621 CA CYS B 292     97.654 -32.361 -9.384  1.00 37.25           C
ANISOU 2621 CA CYS B 292    4283  5064  4808   228   276   202       C
ATOM  2622 CB CYS B 292     96.392 -32.323 -8.522  1.00 30.38           C
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ANISOU 2622 CB CYS B 292 3154 4422 3968 357 303 -64 C
ATOM 2623 SG CYS B 292 94.895 -32.847 -9.370 1.00 79.76 S
ANISOU 2623 SG CYS B 292 8981 10986 10340 583 230 -545 S
ATOM 2624 C CYS B 292 97.362 -31.736 -10.756 1.00 41.82 C
ANISOU 2624 C CYS B 292 5080 5620 5188 527 66 119 C
ATOM 2625 O CYS B 292 97.132 -32.424 -11.750 1.00 38.69 O
ANISOU 2625 O CYS B 292 4542 5349 4808 557 42 -1 O
ATOM 2626 N ARG B 293 97.358 -30.416 -10.808 1.00 41.69 N
ANISOU 2626 N ARG B 293 5447 5433 4963 780 -89 173 N
ATOM 2627 CA ARG B 293 97.061 -29.738 -12.056 1.00 32.22 C
ANISOU 2627 CA ARG B 293 4596 4158 3489 1139 -296 146 C
ATOM 2628 CB ARG B 293 96.725 -28.284 -11.794 1.00 44.75 C
ANISOU 2628 CB ARG B 293 6549 5558 4897 1476 -472 154 C
ATOM 2629 CG ARG B 293 95.439 -28.153 -11.064 1.00 54.97 C
ANISOU 2629 CG ARG B 293 7486 7128 6272 1718 -644 -196 C
ATOM 2630 CD ARG B 293 95.009 -26.736 -10.991 1.00 91.56 C
ANISOU 2630 CD ARG B 293 12471 11578 10741 2123 -874 -239 C
ATOM 2631 NE ARG B 293 93.968 -26.578 -9.985 1.00108.10 N
ANISOU 2631 NE ARG B 293 14167 13912 12993 2243 -956 -594 N
ATOM 2632 CZ ARG B 293 94.134 -25.922 -8.844 1.00102.89 C
ANISOU 2632 CZ ARG B 293 13525 13154 12414 2140 -864 -572 C
ATOM 2633 NH1 ARG B 293 93.134 -25.837 -7.980 1.00 99.36 N
ANISOU 2633 NH1 ARG B 293 12707 12948 12095 2237 -896 -936 N
ATOM 2634 NH2 ARG B 293 95.298 -25.342 -8.579 1.00 96.55 N
ANISOU 2634 NH2 ARG B 293 13085 12015 11585 1937 -722 -247 N
ATOM 2635 C ARG B 293 98.192 -29.847 -13.069 1.00 46.65 C
ANISOU 2635 C ARG B 293 6770 5740 5214 964 -152 399 C
ATOM 2636 O ARG B 293 97.958 -29.937 -14.269 1.00 49.04 O
ANISOU 2636 O ARG B 293 7257 6089 5288 1180 -257 356 O
ATOM 2637 N THR B 294 99.421 -29.834 -12.576 1.00 39.86 N
ANISOU 2637 N THR B 294 5992 4628 4524 587 88 614 N
ATOM 2638 CA THR B 294 100.570 -29.946 -13.452 1.00 42.36 C
ANISOU 2638 CA THR B 294 6579 4688 4829 351 302 785 C
ATOM 2639 CB THR B 294 101.872 -29.689 -12.707 1.00 42.27 C
ANISOU 2639 CB THR B 294 6601 4379 5080 -15 524 900 C
ATOM 2640 OG1 THR B 294 101.811 -28.405 -12.076 1.00 44.36 O
ANISOU 2640 OG1 THR B 294 7136 4429 5288 137 480 925 O
ATOM 2641 CG2 THR B 294 103.044 -29.736 -13.679 1.00 30.60 C
ANISOU 2641 CG2 THR B 294 5380 2605 3641 -283 807 994 C
ATOM 2642 C THR B 294 100.628 -31.335 -14.075 1.00 36.59 C
ANISOU 2642 C THR B 294 5498 4188 4215 170 364 697 C
ATOM 2643 O THR B 294 100.810 -31.497 -15.282 1.00 32.95 O
ANISOU 2643 O THR B 294 5247 3700 3571 210 411 709 O
ATOM 2644 N LEU B 295 100.465 -32.338 -13.228 1.00 36.55 N
ANISOU 2644 N LEU B 295 4990 4393 4505 -21 386 607 N
ATOM 2645 CA LEU B 295 100.498 -33.723 -13.670 1.00 39.13 C
ANISOU 2645 CA LEU B 295 4931 4902 5034 -215 473 503 C
ATOM 2646 CB LEU B 295 100.369 -34.661 -12.482 1.00 29.39 C
ANISOU 2646 CB LEU B 295 3269 3781 4117 -417 555 477 C
ATOM 2647 CG LEU B 295 100.553 -36.124 -12.854 1.00 38.69 C
ANISOU 2647 CG LEU B 295 4066 5051 5583 -658 696 396 C
ATOM 2648 CD1 LEU B 295 101.923 -36.352 -13.491 1.00 26.99 C
ANISOU 2648 CD1 LEU B 295 2700 3346 4209 -917 811 510 C
ATOM 2649 CD2 LEU B 295 100.389 -36.970 -11.616 1.00 44.70 C
ANISOU 2649 CD2 LEU B 295 4571 5848 6566 -802 795 419 C
ATOM 2650 C LEU B 295 99.375 -34.009 -14.669 1.00 39.86 C
ANISOU 2650 C LEU B 295 4910 5282 4953 89 305 246 C
ATOM 2651 O LEU B 295 99.567 -34.678 -15.681 1.00 42.15 O
ANISOU 2651 O LEU B 295 5131 5649 5234 30 348 159 O
ATOM 2652 N GLU B 296 98.193 -33.504 -14.343 1.00 37.31 N
ANISOU 2652 N GLU B 296 4526 5135 4515 430 94 60 N
ATOM 2653 CA GLU B 296 97.043 -33.523 -15.237 1.00 40.92 C
ANISOU 2653 CA GLU B 296 4887 5872 4789 840 -170 -280 C
ATOM 2654 CB GLU B 296 95.962 -32.623 -14.645 1.00 42.77 C
ANISOU 2654 CB GLU B 296 5128 6196 4926 1218 -410 -463 C
ATOM 2655 CG GLU B 296 94.609 -32.687 -15.281 1.00 59.21 C
ANISOU 2655 CG GLU B 296 6952 8611 6933 1681 -740 -956 C
ATOM 2656 CD GLU B 296 93.714 -31.549 -14.808 1.00 84.41 C
ANISOU 2656 CD GLU B 296 10262 11814 9996 2108 -1019 -1120 C
ATOM 2657 OE1 GLU B 296 92.542 -31.498 -15.245 1.00101.08 O
ANISOU 2657 OE1 GLU B 296 12123 14202 12082 2552 -1352 -1610 O
ATOM 2658 OE2 GLU B 296 94.182 -30.705 -14.009 1.00 63.58 O
ANISOU 2658 OE2 GLU B 296 7932 8913 7312 2017 -925 -817 O
ATOM 2659 C GLU B 296 97.437 -33.006 -16.631 1.00 45.45 C
ANISOU 2659 C GLU B 296 5996 6334 4937 1072 -280 -174 C
ATOM 2660 O GLU B 296 97.088 -33.592 -17.657 1.00 48.51 O
ANISOU 2660 O GLU B 296 6273 6946 5214 1228 -396 -409 O
ATOM 2661 N ASP B 297 98.177 -31.903 -16.653 1.00 43.27 N
ANISOU 2661 N ASP B 297 6326 5693 4420 1090 -206 164 N
ATOM 2662 CA ASP B 297 98.568 -31.261 -17.900 1.00 50.57 C
ANISOU 2662 CA ASP B 297 7916 6416 4881 1307 -213 329 C
ATOM 2663 CB ASP B 297 99.013 -29.820 -17.655 1.00 51.85 C
ANISOU 2663 CB ASP B 297 8731 6133 4835 1408 -133 641 C
ATOM 2664 CG ASP B 297 97.857 -28.851 -17.672 1.00 83.05 C
ANISOU 2664 CG ASP B 297 12942 10131 8484 2025 -531 534 C
ATOM 2665 OD1 ASP B 297 96.761 -29.250 -18.119 1.00100.07 O
ANISOU 2665 OD1 ASP B 297 14841 12666 10515 2427 -896 194 O
ATOM 2666 OD2 ASP B 297 98.053 -27.689 -17.248 1.00 88.28 O
ANISOU 2666 OD2 ASP B 297 14033 10438 9071 2119 -488 737 O
ATOM 2667 C ASP B 297 99.656 -32.020 -18.651 1.00 47.97 C
ANISOU 2667 C ASP B 297 7624 5999 4605 911 105 431 C
ATOM 2668 O ASP B 297 99.683 -32.037 -19.876 1.00 43.96 O
ANISOU 2668 O ASP B 297 7470 5518 3715 1101 82 415 O
ATOM 2669 N ILE B 298 100.556 -32.636 -17.900 1.00 38.67 N
ANISOU 2669 N ILE B 298 6094 4715 3883 391 385 510 N
ATOM 2670 CA ILE B 298 101.586 -33.463 -18.495 1.00 48.88 C
ANISOU 2670 CA ILE B 298 7292 5937 5342 -9 675 526 C
ATOM 2671 CB ILE B 298 102.581 -33.962 -17.452 1.00 40.21 C
ANISOU 2671 CB ILE B 298 5832 4677 4769 -495 896 599 C
ATOM 2672 CG1 ILE B 298 103.377 -32.794 -16.890 1.00 44.24 C
ANISOU 2672 CG1 ILE B 298 6739 4786 5285 -599 1050 806 C
ATOM 2673 CD1 ILE B 298 104.380 -33.218 -15.841 1.00 47.74 C
ANISOU 2673 CD1 ILE B 298 6823 5098 6218 -988 1172 800 C
ATOM 2674 CG2 ILE B 298 103.542 -34.975 -18.072 1.00 40.72 C
ANISOU 2674 CG2 ILE B 298 5678 4708 5086 -879 1145 524 C
ATOM 2675 C ILE B 298 100.975 -34.666 -19.207 1.00 46.53 C
ANISOU 2675 C ILE B 298 6557 6034 5089 56 553 221 C
ATOM 2676 O ILE B 298 101.329 -34.981 -20.343 1.00 58.33 O
ANISOU 2676 O ILE B 298 8224 7557 6383 31 653 166 O
ATOM 2677 N LEU B 299 100.047 -35.329 -18.530 1.00 39.73 N
ANISOU 2677 N LEU B 299 5126 5464 4505 125 378 -13 N
ATOM 2678 CA LEU B 299 99.469 -36.563 -19.044 1.00 40.75 C
ANISOU 2678 CA LEU B 299 4716 5936 4830 120 319 -378 C
ATOM 2679 CB LEU B 299 98.721 -37.321 -17.950 1.00 35.84 C
ANISOU 2679 CB LEU B 299 3465 5480 4675 14 323 -572 C
ATOM 2680 CG LEU B 299 99.515 -37.784 -16.729 1.00 51.31 C
ANISOU 2680 CG LEU B 299 5245 7205 7047 -422 587 -317 C
ATOM 2681 CD1 LEU B 299 98.539 -38.354 -15.707 1.00 40.79 C
ANISOU 2681 CD1 LEU B 299 3450 6022 6026 -433 622 -497 C
ATOM 2682 CD2 LEU B 299 100.579 -38.820 -17.086 1.00 45.08 C
ANISOU 2682 CD2 LEU B 299 4263 6298 6566 -816 819 -276 C
ATOM 2683 C LEU B 299 98.524 -36.300 -20.208 1.00 54.10 C
ANISOU 2683 C LEU B 299 6574 7912 6068 642 -5 -671 C
ATOM 2684 O LEU B 299 98.267 -37.178 -21.021 1.00 63.33 O
ANISOU 2684 O LEU B 299 7433 9348 7282 671 -54 -999 O
ATOM 2685 N ALA B 300 97.981 -35.095 -20.269 1.00 49.93 N
ANISOU 2685 N ALA B 300 6529 7333 5109 1098 -264 -591 N
ATOM 2686 CA ALA B 300 97.076 -34.761 -21.352 1.00 58.46 C
ANISOU 2686 CA ALA B 300 7846 8672 5694 1709 -663 -874 C
ATOM 2687 CB ALA B 300 96.430 -33.414 -21.113 1.00 56.31 C
ANISOU 2687 CB ALA B 300 8056 8285 5056 2221 -971 -775 C
ATOM 2688 C ALA B 300 97.821 -34.764 -22.681 1.00 68.16 C
ANISOU 2688 C ALA B 300 9616 9824 6459 1734 -551 -741 C
ATOM 2689 O ALA B 300 97.268 -35.126 -23.719 1.00 82.19 O
ANISOU 2689 O ALA B 300 11378 11922 7928 2099 -816 -1082 O
ATOM 2690 N ASP B 301 99.086 -34.366 -22.639 1.00 72.40 N
ANISOU 2690 N ASP B 301 9533 10764 7212 747 309 2417 N
ATOM 2691 CA ASP B 301 99.865 -34.183 -23.855 1.00 79.42 C
ANISOU 2691 CA ASP B 301 10585 11781 7808 745 556 2545 C
ATOM 2692 CB ASP B 301 100.628 -32.863 -23.779 1.00101.48 C
ANISOU 2692 CB ASP B 301 13287 14125 11148 1181 856 2956 C
ATOM 2693 CG ASP B 301 100.669 -32.134 -25.103 1.00128.45 C
ANISOU 2693 CG ASP B 301 16668 17969 14170 1334 1022 3494 C
ATOM 2694 OD1 ASP B 301 100.183 -32.681 -26.115 1.00137.19 O
ANISOU 2694 OD1 ASP B 301 17833 19793 14501 1075 870 3519 O
ATOM 2695 OD2 ASP B 301 101.192 -30.999 -25.120 1.00137.22 O
ANISOU 2695 OD2 ASP B 301 17679 18710 15746 1703 1338 3888 O
ATOM 2696 C ASP B 301 100.867 -35.309 -24.052 1.00 68.04 C
ANISOU 2696 C ASP B 301 9504 10022 6326 450 772 1969 C
ATOM 2697 O ASP B 301 101.744 -35.222 -24.901 1.00 69.68 O
ANISOU 2697 O ASP B 301 9894 10156 6424 447 1058 1983 O
ATOM 2698 N ALA B 302 100.749 -36.360 -23.252 1.00 63.48 N
ANISOU 2698 N ALA B 302 9022 9214 5884 226 694 1496 N
ATOM 2699 CA ALA B 302 101.793 -37.372 -23.222 1.00 55.49 C
ANISOU 2699 CA ALA B 302 8307 7738 5038 43 984 1020 C
ATOM 2700 CB ALA B 302 102.111 -37.772 -21.798 1.00 47.46 C
ANISOU 2700 CB ALA B 302 6267 6152 4613 166 966 807 C
ATOM 2701 C ALA B 302 101.481 -38.602 -24.060 1.00 75.31 C
ANISOU 2701 C ALA B 302 11032 10603 6979 -459 1074 596 C
ATOM 2702 O ALA B 302 100.387 -39.166 -23.968 1.00 68.11 O
ANISOU 2702 O ALA B 302 10038 10099 5741 -734 852 429 O
ATOM 2703 N PRO B 303 102.461 -39.025 -24.875 1.00 72.71 N
ANISOU 2703 N PRO B 303 10970 10095 6561 -611 1451 375 N
ATOM 2704 CA PRO B 303 102.386 -40.233 -25.702 1.00 83.59 C
ANISOU 2704 CA PRO B 303 12597 11691 7471 -1141 1690 -136 C
ATOM 2705 CB PRO B 303 103.795 -40.341 -26.288 1.00 80.66 C
ANISOU 2705 CB PRO B 303 12489 10851 7309 -1108 2173 -249 C
ATOM 2706 CG PRO B 303 104.287 -38.935 -26.330 1.00 59.10 C
ANISOU 2706 CG PRO B 303 9612 8042 4802 -634 2103 304 C
ATOM 2707 CD PRO B 303 103.714 -38.282 -25.102 1.00 62.98 C
ANISOU 2707 CD PRO B 303 9802 8431 5696 -297 1728 593 C
ATOM 2708 C PRO B 303 102.076 -41.481 -24.880 1.00 84.86 C
ANISOU 2708 C PRO B 303 12825 11533 7883 -1385 1768 -602 C
ATOM 2709 O PRO B 303 101.283 -42.301 -25.320 1.00 85.87 O
ANISOU 2709 O PRO B 303 13001 12071 7551 -1823 1694 -1010 O
ATOM 2710 N GLU B 304 102.693 -41.627 -23.713 1.00 80.16 N
ANISOU 2710 N GLU B 304 12216 10251 7992 -1077 1845 -573 N
ATOM 2711 CA GLU B 304 102.485 -42.820 -22.894 1.00 83.48 C
ANISOU 2711 CA GLU B 304 12704 10312 8702 -1234 1994 -920 C
ATOM 2712 CB GLU B 304 103.617 -42.993 -21.881 1.00 90.31 C

ANISOU 2712 CB GLU B 304 13580 10431 10302 -854 2195 -827 C
ATOM 2713 CG GLU B 304 104.979 -43.214 -22.495 1.00102.89 C
ANISOU 2713 CG GLU B 304 15358 11606 12130 -823 2658 -917 C
ATOM 2714 CD GLU B 304 105.765 -41.926 -22.639 1.00111.99 C
ANISOU 2714 CD GLU B 304 16390 12722 13438 -459 2539 -550 C
ATOM 2715 OE1 GLU B 304 107.009 -42.001 -22.722 1.00119.36 O
ANISOU 2715 OE1 GLU B 304 17383 13195 14773 -305 2870 -556 O
ATOM 2716 OE2 GLU B 304 105.140 -40.843 -22.663 1.00108.90 O
ANISOU 2716 OE2 GLU B 304 15823 12733 12821 -323 2164 -251 O
ATOM 2717 C GLU B 304 101.162 -42.812 -22.137 1.00 81.29 C
ANISOU 2717 C GLU B 304 12218 10345 8325 -1266 1601 -868 C
ATOM 2718 O GLU B 304 100.667 -43.857 -21.724 1.00 81.38 O
ANISOU 2718 O GLU B 304 12290 10227 8406 -1515 1740 -1198 O
ATOM 2719 N SER B 305 100.598 -41.628 -21.949 1.00 87.98 N
ANISOU 2719 N SER B 305 12813 11549 9067 -1004 1176 -444 N
ATOM 2720 CA SER B 305 99.522 -41.448 -20.984 1.00 85.33 C
ANISOU 2720 CA SER B 305 12252 11352 8819 -913 830 -316 C
ATOM 2721 CB SER B 305 99.676 -40.106 -20.284 1.00 94.70 C
ANISOU 2721 CB SER B 305 13217 12427 10337 -428 585 164 C
ATOM 2722 OG SER B 305 101.048 -39.772 -20.225 1.00 99.41 O
ANISOU 2722 OG SER B 305 13620 13590 10560 -382 359 517 O
ATOM 2723 C SER B 305 98.126 -41.470 -21.580 1.00 75.03 C
ANISOU 2723 C SER B 305 10778 10799 6933 -1241 556 -356 C
ATOM 2724 O SER B 305 97.157 -41.202 -20.876 1.00 77.92 O
ANISOU 2724 O SER B 305 10917 11326 7362 -1157 264 -205 O
ATOM 2725 N GLN B 306 97.999 -41.751 -22.869 1.00 72.67 N
ANISOU 2725 N GLN B 306 10552 11013 6045 -1619 638 -551 N
ATOM 2726 CA GLN B 306 96.682 -41.627 -23.480 1.00 83.69 C
ANISOU 2726 CA GLN B 306 11693 13286 6819 -1910 305 -524 C
ATOM 2727 CB GLN B 306 96.770 -41.348 -24.983 1.00 89.69 C
ANISOU 2727 CB GLN B 306 12464 14757 6855 -2139 304 -473 C
ATOM 2728 CG GLN B 306 97.738 -40.222 -25.362 1.00 88.91 C
ANISOU 2728 CG GLN B 306 12414 14492 6877 -1680 370 50 C
ATOM 2729 CD GLN B 306 97.183 -38.826 -25.134 1.00 87.21 C
ANISOU 2729 CD GLN B 306 11843 14560 6733 -1200 16 783 C
ATOM 2730 OE1 GLN B 306 96.444 -38.299 -25.970 1.00 75.15 O
ANISOU 2730 OE1 GLN B 306 10070 13869 4616 -1234 -230 1135 O
ATOM 2731 NE2 GLN B 306 97.551 -38.211 -24.006 1.00 63.98 N
ANISOU 2731 NE2 GLN B 306 8850 10943 4515 -751 26 1029 N
ATOM 2732 C GLN B 306 95.820 -42.851 -23.191 1.00 96.38 C
ANISOU 2732 C GLN B 306 13301 14974 8346 -2391 370 -1080 C
ATOM 2733 O GLN B 306 96.202 -43.983 -23.496 1.00 97.12 O
ANISOU 2733 O GLN B 306 13657 14822 8423 -2794 788 -1645 O
ATOM 2734 N ASN B 307 94.674 -42.600 -22.562 1.00 99.08 N
ANISOU 2734 N ASN B 307 13340 15588 8717 -2335 22 -914 N
ATOM 2735 CA ASN B 307 93.634 -43.602 -22.362 1.00 97.27 C
ANISOU 2735 CA ASN B 307 13023 15569 8368 -2807 37 -1399 C
ATOM 2736 CB ASN B 307 93.266 -44.260 -23.695 1.00115.55 C
ANISOU 2736 CB ASN B 307 15329 18632 9942 -3472 120 -1900 C
ATOM 2737 CG ASN B 307 91.855 -43.956 -24.121 1.00132.77 C
ANISOU 2737 CG ASN B 307 17004 21635 11807 -3595 -313 -1726 C
ATOM 2738 OD1 ASN B 307 91.103 -44.855 -24.503 1.00138.43 O
ANISOU 2738 OD1 ASN B 307 17574 22601 12423 -4070 -202 -2189 O
ATOM 2739 ND2 ASN B 307 91.476 -42.688 -24.043 1.00135.98 N
ANISOU 2739 ND2 ASN B 307 17112 22420 12135 -3143 -745 -1026 N
ATOM 2740 C ASN B 307 93.951 -44.681 -21.330 1.00 83.66 C
ANISOU 2740 C ASN B 307 11549 12992 7248 -2847 443 -1779 C
ATOM 2741 O ASN B 307 93.215 -45.659 -21.211 1.00 79.29 O
ANISOU 2741 O ASN B 307 10976 12485 6664 -3279 606 -2257 O
ATOM 2742 N ASN B 308 95.028 -44.517 -20.575 1.00 59.59 N
ANISOU 2742 N ASN B 308 8701 9188 4752 -2398 628 -1554 N
ATOM 2743 CA ASN B 308 95.424 -45.586 -19.670 1.00 61.32 C
ANISOU 2743 CA ASN B 308 9141 8651 5506 -2392 1052 -1826 C
ATOM 2744 CB ASN B 308 96.572 -46.370 -20.276 1.00 66.55 C
ANISOU 2744 CB ASN B 308 10125 8895 6266 -2559 1594 -2145 C
ATOM 2745 CG ASN B 308 97.788 -45.508 -20.503 1.00 77.08 C
ANISOU 2745 CG ASN B 308 11531 10048 7706 -2149 1549 -1767 C
ATOM 2746 OD1 ASN B 308 97.709 -44.283 -20.426 1.00 76.57 O
ANISOU 2746 OD1 ASN B 308 11276 10264 7554 -1815 1127 -1312 O
ATOM 2747 ND2 ASN B 308 98.924 -46.139 -20.787 1.00 80.65 N
ANISOU 2747 ND2 ASN B 308 12242 9994 8407 -2173 2043 -1955 N
ATOM 2748 C ASN B 308 95.816 -45.139 -18.269 1.00 66.14 C
ANISOU 2748 C ASN B 308 9729 8722 6679 -1823 950 -1412 C
ATOM 2749 O ASN B 308 96.478 -45.877 -17.540 1.00 66.00 O
ANISOU 2749 O ASN B 308 9892 8079 7105 -1681 1302 -1481 O
ATOM 2750 N CYS B 309 95.414 -43.937 -17.889 1.00 57.64 N
ANISOU 2750 N CYS B 309 8409 7910 5581 -1500 504 -975 N
ATOM 2751 CA CYS B 309 95.788 -43.419 -16.590 1.00 54.76 C
ANISOU 2751 CA CYS B 309 8006 7120 5682 -1022 410 -648 C
ATOM 2752 CB CYS B 309 97.161 -42.763 -16.660 1.00 48.32 C
ANISOU 2752 CB CYS B 309 7269 6026 5065 -681 469 -420 C
ATOM 2753 SG CYS B 309 97.792 -42.250 -15.068 1.00 71.58 S
ANISOU 2753 SG CYS B 309 10146 8523 8527 -182 390 -139 S
ATOM 2754 C CYS B 309 94.754 -42.419 -16.107 1.00 64.21 C
ANISOU 2754 C CYS B 309 8904 8648 6844 -861 6 -337 C
ATOM 2755 O CYS B 309 94.331 -41.543 -16.856 1.00 73.26 O
ANISOU 2755 O CYS B 309 9852 10282 7702 -862 -242 -112 O
ATOM 2756 N ARG B 310 94.348 -42.544 -14.850 1.00 50.79 N
ANISOU 2756 N ARG B 310 7165 6683 5451 -702 -20 -285 N
ATOM 2757 CA ARG B 310 93.315 -41.663 -14.343 1.00 40.48 C
ANISOU 2757 CA ARG B 310 5581 5629 4170 -576 -325 -27 C
ATOM 2758 CB ARG B 310 91.988 -42.391 -14.279 1.00 60.53 C
ANISOU 2758 CB ARG B 310 8013 8405 6580 -909 -349 -253 C
ATOM 2759 CG ARG B 310 90.812 -41.458 -14.239 1.00 81.13 C
ANISOU 2759 CG ARG B 310 10263 11443 9119 -853 -674 30 C
ATOM 2760 CD ARG B 310 90.295 -41.168 -15.630 1.00 95.03 C
ANISOU 2760 CD ARG B 310 11797 13909 10400 -1092 -879 87 C
ATOM 2761 NE ARG B 310 88.857 -40.939 -15.584 1.00113.74 N
ANISOU 2761 NE ARG B 310 13794 16743 12680 -1209 -1119 198 N
ATOM 2762 CZ ARG B 310 88.303 -39.768 -15.293 1.00119.62 C
ANISOU 2762 CZ ARG B 310 14230 17634 13584 -893 -1325 681 C
ATOM 2763 NH1 ARG B 310 86.982 -39.648 -15.255 1.00119.18 N
ANISOU 2763 NH1 ARG B 310 13805 17997 13483 -1003 -1516 786 N
ATOM 2764 NH2 ARG B 310 89.072 -38.716 -15.043 1.00120.92 N
ANISOU 2764 NH2 ARG B 310 14434 17507 14002 -480 -1292 1045 N
ATOM 2765 C ARG B 310 93.660 -41.082 -12.978 1.00 45.85 C
ANISOU 2765 C ARG B 310 6244 5932 5243 -193 -354 184 C
ATOM 2766 O ARG B 310 93.970 -41.807 -12.040 1.00 49.88 O
ANISOU 2766 O ARG B 310 6910 6080 5964 -123 -183 72 O
ATOM 2767 N LEU B 311 93.593 -39.762 -12.878 1.00 49.02 N
ANISOU 2767 N LEU B 311 6442 6446 5738 48 -534 497 N
ATOM 2768 CA LEU B 311 93.890 -39.084 -11.631 1.00 43.12 C
ANISOU 2768 CA LEU B 311 5648 5407 5328 340 -539 622 C
ATOM 2769 CB LEU B 311 94.539 -37.737 -11.889 1.00 44.46 C
ANISOU 2769 CB LEU B 311 5686 5560 5646 575 -561 862 C
ATOM 2770 CG LEU B 311 95.934 -37.814 -12.484 1.00 56.98 C
ANISOU 2770 CG LEU B 311 7425 6994 7229 634 -433 803 C
ATOM 2771 CD1 LEU B 311 96.606 -36.453 -12.360 1.00 47.40 C
ANISOU 2771 CD1 LEU B 311 6067 5651 6293 880 -383 984 C
ATOM 2772 CD2 LEU B 311 96.744 -38.908 -11.794 1.00 51.52 C
ANISOU 2772 CD2 LEU B 311 6948 6007 6620 636 -301 571 C
ATOM 2773 C LEU B 311 92.644 -38.874 -10.800 1.00 42.01 C
ANISOU 2773 C LEU B 311 5342 5329 5290 334 -630 684 C
ATOM 2774 O LEU B 311 91.672 -38.280 -11.253 1.00 44.08 O
ANISOU 2774 O LEU B 311 5364 5894 5492 291 -762 867 O
ATOM 2775 N ILE B 312 92.693 -39.347 -9.566 1.00 41.91 N
ANISOU 2775 N ILE B 312 5441 5048 5435 400 -542 572 N
ATOM 2776 CA ILE B 312 91.583 -39.157 -8.662 1.00 36.06 C
ANISOU 2776 CA ILE B 312 4577 4309 4816 401 -574 611 C
ATOM 2777 CB ILE B 312 91.105 -40.489 -8.120 1.00 47.47 C
ANISOU 2777 CB ILE B 312 6186 5628 6222 247 -439 411 C
ATOM 2778 CG1 ILE B 312 90.933 -41.467 -9.271 1.00 45.65 C
ANISOU 2778 CG1 ILE B 312 6026 5543 5777 -52 -377 217 C
ATOM 2779 CD1 ILE B 312 90.289 -42.752 -8.856 1.00 58.25 C
ANISOU 2779 CD1 ILE B 312 7744 6983 7405 -259 -155 -14 C
ATOM 2780 CG2 ILE B 312 89.792 -40.315 -7.375 1.00 41.61 C
ANISOU 2780 CG2 ILE B 312 5296 4919 5596 203 -456 445 C
ATOM 2781 C ILE B 312 91.995 -38.236 -7.527 1.00 34.48 C
ANISOU 2781 C ILE B 312 4329 3923 4850 635 -546 683 C
ATOM 2782 O ILE B 312 92.630 -38.660 -6.567 1.00 45.48 O
ANISOU 2782 O ILE B 312 5870 5142 6268 727 -469 582 O
ATOM 2783 N ALA B 313 91.651 -36.964 -7.662 1.00 35.57 N
ANISOU 2783 N ALA B 313 4234 4124 5156 727 -576 864 N
ATOM 2784 CA ALA B 313 91.977 -35.984 -6.637 1.00 44.62 C
ANISOU 2784 CA ALA B 313 5308 5090 6557 875 -474 849 C
ATOM 2785 CB ALA B 313 92.466 -34.698 -7.260 1.00 34.12 C
ANISOU 2785 CB ALA B 313 3804 3732 5430 997 -401 1007 C
ATOM 2786 C ALA B 313 90.766 -35.716 -5.764 1.00 44.06 C
ANISOU 2786 C ALA B 313 5121 4981 6640 844 -410 871 C
ATOM 2787 O ALA B 313 89.652 -35.593 -6.257 1.00 46.95 O
ANISOU 2787 O ALA B 313 5307 5481 7049 787 -451 1041 O
ATOM 2788 N TYR B 314 90.991 -35.614 -4.462 1.00 45.87 N
ANISOU 2788 N TYR B 314 5427 5070 6933 876 -308 701 N
ATOM 2789 CA TYR B 314 89.894 -35.391 -3.540 1.00 48.33 C
ANISOU 2789 CA TYR B 314 5664 5310 7389 833 -192 684 C
ATOM 2790 CB TYR B 314 89.212 -36.709 -3.187 1.00 35.91 C
ANISOU 2790 CB TYR B 314 4252 3762 5629 735 -224 631 C
ATOM 2791 CG TYR B 314 90.161 -37.760 -2.650 1.00 34.89 C
ANISOU 2791 CG TYR B 314 4393 3612 5251 776 -232 506 C
ATOM 2792 CD1 TYR B 314 90.884 -38.577 -3.516 1.00 30.60 C
ANISOU 2792 CD1 TYR B 314 3970 3101 4556 770 -303 514 C
ATOM 2793 CE1 TYR B 314 91.753 -39.529 -3.040 1.00 34.50 C
ANISOU 2793 CE1 TYR B 314 4669 3542 4899 857 -251 479 C
ATOM 2794 CZ TYR B 314 91.902 -39.692 -1.673 1.00 48.14 C
ANISOU 2794 CZ TYR B 314 6473 5270 6546 963 -178 469 C
ATOM 2795 OH TYR B 314 92.762 -40.652 -1.190 1.00 52.05 O
ANISOU 2795 OH TYR B 314 7125 5765 6889 1110 -117 543 O
ATOM 2796 CE2 TYR B 314 91.197 -38.895 -0.786 1.00 36.52 C
ANISOU 2796 CE2 TYR B 314 4910 3822 5143 932 -134 414 C
ATOM 2797 CD2 TYR B 314 90.331 -37.934 -1.278 1.00 33.36 C
ANISOU 2797 CD2 TYR B 314 4315 3387 4972 832 -135 414 C
ATOM 2798 C TYR B 314 90.355 -34.690 -2.273 1.00 48.00 C
ANISOU 2798 C TYR B 314 5634 5157 7445 859 -28 481 C
ATOM 2799 O TYR B 314 91.491 -34.849 -1.823 1.00 42.97 O
ANISOU 2799 O TYR B 314 5108 4829 7390 1023 167 -1 O
ATOM 2800 N GLN B 315 89.448 -33.912 -1.705 1.00 59.28 N
ANISOU 2800 N GLN B 315 7275 9962 -655 546 -2539 N
ATOM 2801 CA GLN B 315 89.703 -33.222 -0.460 1.00 57.58 C
ANISOU 2801 CA GLN B 315 5768 6696 9414 -642 589 -2977 C
ATOM 2802 CB GLN B 315 89.345 -31.750 -0.599 1.00 61.20 C

ANISOU 2802 CB GLN B 315 6516 6556 10180 -785 1109 -2953 C
ATOM 2803 CG GLN B 315 90.256 -30.815 0.155 1.00 89.53 C
ANISOU 2803 CG GLN B 315 10610 9882 13524 -1154 1002 -3613 C
ATOM 2804 CD GLN B 315 90.389 -29.473 -0.536 1.00 94.49 C
ANISOU 2804 CD GLN B 315 11252 10043 14608 -1511 1279 -3599 C
ATOM 2805 OE1 GLN B 315 89.766 -29.230 -1.572 1.00 97.90 O
ANISOU 2805 OE1 GLN B 315 11292 10353 15555 -1464 1525 -3023 O
ATOM 2806 NE2 GLN B 315 91.210 -28.594 0.031 1.00 97.65 N
ANISOU 2806 NE2 GLN B 315 12113 10192 14799 -1936 1211 -4193 N
ATOM 2807 C GLN B 315 88.831 -33.875 0.595 1.00 58.08 C
ANISOU 2807 C GLN B 315 6297 6678 9091 -204 767 -2828 C
ATOM 2808 O GLN B 315 87.622 -33.983 0.429 1.00 71.31 O
ANISOU 2808 O GLN B 315 7977 8210 10908 106 1248 -2339 O
ATOM 2809 N GLU B 316 89.452 -34.321 1.676 1.00 90.11 N
ANISOU 2809 N GLU B 316 10714 10894 12631 -233 349 -3212 N
ATOM 2810 CA GLU B 316 88.724 -35.019 2.722 1.00 93.60 C
ANISOU 2810 CA GLU B 316 11616 11348 12600 61 428 -3070 C
ATOM 2811 CB GLU B 316 89.582 -36.144 3.300 1.00105.57 C
ANISOU 2811 CB GLU B 316 13094 13285 13734 35 -356 -3200 C
ATOM 2812 CG GLU B 316 88.816 -37.169 4.111 1.00115.39 C
ANISOU 2812 CG GLU B 316 14680 14624 14540 304 -397 -2875 C
ATOM 2813 CD GLU B 316 89.676 -38.361 4.501 1.00119.83 C
ANISOU 2813 CD GLU B 316 15103 15530 14896 326 -1247 -2859 C
ATOM 2814 OE1 GLU B 316 90.445 -38.849 3.644 1.00119.94 O
ANISOU 2814 OE1 GLU B 316 14482 15730 15359 359 -1653 -2888 O
ATOM 2815 OE2 GLU B 316 89.586 -38.803 5.665 1.00118.84 O
ANISOU 2815 OE2 GLU B 316 15485 15488 14180 292 -1505 -2812 O
ATOM 2816 C GLU B 316 88.316 -34.033 3.806 1.00 92.26 C
ANISOU 2816 C GLU B 316 12193 10764 12099 -12 922 -3393 C
ATOM 2817 O GLU B 316 89.149 -33.275 4.305 1.00 95.73 O
ANISOU 2817 O GLU B 316 12943 11098 12331 -384 785 -3923 O
ATOM 2818 N PRO B 317 87.021 -34.024 4.163 1.00 95.43 N
ANISOU 2818 N PRO B 317 12868 10949 12444 303 1546 -3115 N
ATOM 2819 CA PRO B 317 86.580 -33.105 5.211 1.00102.12 C
ANISOU 2819 CA PRO B 317 14411 11385 13003 237 2132 -3519 C
ATOM 2820 CB PRO B 317 85.055 -33.279 5.225 1.00 99.20 C
ANISOU 2820 CB PRO B 317 14039 10885 12767 684 2829 -3068 C
ATOM 2821 CG PRO B 317 84.721 -34.108 4.012 1.00 92.31 C
ANISOU 2821 CG PRO B 317 12445 10318 12312 918 2615 -2382 C
ATOM 2822 CD PRO B 317 85.937 -34.918 3.727 1.00 85.93 C
ANISOU 2822 CD PRO B 317 11366 9927 11358 677 1744 -2484 C
ATOM 2823 C PRO B 317 87.150 -33.588 6.527 1.00112.78 C
ANISOU 2823 C PRO B 317 16298 13054 13501 -68 1692 -3909 C
ATOM 2824 O PRO B 317 87.177 -34.796 6.753 1.00114.74 O
ANISOU 2824 O PRO B 317 16441 13739 13415 19 1188 -3608 O
ATOM 2825 N ALA B 318 87.605 -32.676 7.376 1.00120.72 N
ANISOU 2825 N ALA B 318 17879 13842 14148 -472 1859 -4539 N
ATOM 2826 CA ALA B 318 88.154 -33.069 8.668 1.00131.67 C
ANISOU 2826 CA ALA B 318 19789 15612 14629 -899 1418 -4878 C
ATOM 2827 CB ALA B 318 89.649 -32.802 8.714 1.00129.55 C
ANISOU 2827 CB ALA B 318 19451 15578 14193 -1403 706 -5258 C
ATOM 2828 C ALA B 318 87.443 -32.358 9.818 1.00147.32 C
ANISOU 2828 C ALA B 318 22552 17316 16106 -1116 2192 -5357 C
ATOM 2829 O ALA B 318 87.590 -31.149 9.986 1.00150.36 O
ANISOU 2829 O ALA B 318 23290 17228 16610 -1373 2705 -5914 O
ATOM 2830 N ASP B 319 86.682 -33.106 10.616 1.00158.28 N
ANISOU 2830 N ASP B 319 24226 18992 16920 -1063 2301 -5177 N
ATOM 2831 CA ASP B 319 86.553 -34.551 10.455 1.00162.22 C
ANISOU 2831 CA ASP B 319 24382 19987 17266 -818 1656 -4513 C
ATOM 2832 CB ASP B 319 87.586 -35.275 11.330 1.00167.60 C
ANISOU 2832 CB ASP B 319 25290 21220 17169 -1309 682 -4556 C
ATOM 2833 CG ASP B 319 87.745 -36.739 10.961 1.00164.73 C
ANISOU 2833 CG ASP B 319 24478 21224 16889 -1011 -124 -3867 C
ATOM 2834 OD1 ASP B 319 87.355 -37.604 11.773 1.00169.02 O
ANISOU 2834 OD1 ASP B 319 25222 21942 17057 -909 -64 -3482 O
ATOM 2835 OD2 ASP B 319 88.263 -37.028 9.861 1.00157.65 O
ANISOU 2835 OD2 ASP B 319 23029 20427 16444 -900 -793 -3738 O
ATOM 2836 C ASP B 319 85.144 -35.029 10.811 1.00166.37 C
ANISOU 2836 C ASP B 319 25075 20562 17578 -540 2251 -4203 C
ATOM 2837 O ASP B 319 84.951 -35.697 11.826 1.00171.36 O
ANISOU 2837 O ASP B 319 26132 21587 17391 -830 2045 -4163 O
ATOM 2838 N ASP B 320 84.157 -34.672 9.991 1.00162.47 N
ANISOU 2838 N ASP B 320 24229 19716 17786 -35 2971 -3951 N
ATOM 2839 CA ASP B 320 82.827 -35.260 10.122 1.00158.27 C
ANISOU 2839 CA ASP B 320 23664 19337 17132 269 3459 -3536 C
ATOM 2840 CB ASP B 320 81.783 -34.451 9.346 1.00157.98 C
ANISOU 2840 CB ASP B 320 23262 18840 17923 773 4387 -3386 C
ATOM 2841 CG ASP B 320 80.381 -34.580 9.933 1.00160.12 C
ANISOU 2841 CG ASP B 320 23687 19221 17932 960 5184 -3297 C
ATOM 2842 OD1 ASP B 320 79.741 -35.636 9.744 1.00157.27 O
ANISOU 2842 OD1 ASP B 320 23082 19295 17379 1102 5014 -2702 O
ATOM 2843 OD2 ASP B 320 79.918 -33.612 10.575 1.00161.79 O
ANISOU 2843 OD2 ASP B 320 24047 19168 18259 907 5697 -3668 O
ATOM 2844 C ASP B 320 82.956 -36.662 9.546 1.00145.06 C
ANISOU 2844 C ASP B 320 21570 18082 15464 424 2691 -2844 C
ATOM 2845 O ASP B 320 82.335 -37.614 10.021 1.00147.51 O
ANISOU 2845 O ASP B 320 22039 18743 15265 402 2602 -2500 O
ATOM 2846 N SER B 321 83.802 -36.765 8.523 1.00128.64 N
ANISOU 2846 N SER B 321 18971 15947 13961 530 2157 -2690 N
ATOM 2847 CA SER B 321 84.242 -38.039 7.953 1.00111.60 C
ANISOU 2847 CA SER B 321 16410 14104 11889 624 1371 -2209 C
ATOM 2848 CB SER B 321 85.016 -38.864 8.981 1.00105.77 C
ANISOU 2848 CB SER B 321 16063 13693 10433 296 550 -2265 C
ATOM 2849 OG SER B 321 85.343 -38.091 10.112 1.00109.17 O
ANISOU 2849 OG SER B 321 17093 14123 10263 -135 660 -2816 O
ATOM 2850 C SER B 321 83.123 -38.891 7.380 1.00106.37 C
ANISOU 2850 C SER B 321 15449 13590 11376 932 1622 -1574 C
ATOM 2851 O SER B 321 83.075 -40.098 7.608 1.00105.37 O
ANISOU 2851 O SER B 321 15389 13738 10908 901 1142 -1224 O
ATOM 2852 N SER B 322 82.225 -38.274 6.627 1.00103.49 N
ANISOU 2852 N SER B 322 14748 13040 11533 1200 2347 -1381 N
ATOM 2853 CA SER B 322 81.231 -39.056 5.919 1.00 99.85 C
ANISOU 2853 CA SER B 322 13897 12801 11240 1418 2544 -737 C
ATOM 2854 CB SER B 322 79.954 -38.249 5.711 1.00102.64 C
ANISOU 2854 CB SER B 322 14086 13017 11895 1678 3486 -554 C
ATOM 2855 OG SER B 322 78.853 -39.113 5.499 1.00104.22 O
ANISOU 2855 OG SER B 322 14091 13580 11927 1775 3694 31 O
ATOM 2856 C SER B 322 81.823 -39.476 4.580 1.00 91.47 C
ANISOU 2856 C SER B 322 12193 11796 10763 1452 2113 -479 C
ATOM 2857 O SER B 322 81.146 -40.059 3.734 1.00 78.84 O
ANISOU 2857 O SER B 322 10176 10394 9386 1540 2248 35 O
ATOM 2858 N PHE B 323 83.102 -39.175 4.400 1.00 56.42 N
ANISOU 2858 N PHE B 323 7669 7241 6528 1311 1614 -874 N
ATOM 2859 CA PHE B 323 83.759 -39.411 3.132 1.00 54.89 C
ANISOU 2859 CA PHE B 323 6840 7121 6896 1274 1283 -775 C
ATOM 2860 CB PHE B 323 85.122 -38.729 3.103 1.00 53.29 C
ANISOU 2860 CB PHE B 323 6582 6790 6875 1079 880 -1320 C
ATOM 2861 CG PHE B 323 85.891 -38.992 1.852 1.00 53.28 C
ANISOU 2861 CG PHE B 323 5908 6939 7396 972 542 -1317 C
ATOM 2862 CD1 PHE B 323 85.511 -38.400 0.658 1.00 46.58 C
ANISOU 2862 CD1 PHE B 323 4572 6071 7056 903 942 -1079 C
ATOM 2863 CE1 PHE B 323 86.217 -38.641 -0.507 1.00 46.77 C
ANISOU 2863 CE1 PHE B 323 3975 6317 7480 683 671 -1124 C
ATOM 2864 CZ PHE B 323 87.323 -39.484 -0.482 1.00 45.64 C
ANISOU 2864 CZ PHE B 323 3650 6366 7323 625 37 -1463 C
ATOM 2865 CE2 PHE B 323 87.711 -40.087 0.712 1.00 50.47 C
ANISOU 2865 CE2 PHE B 323 4710 6940 7528 789 -405 -1640 C
ATOM 2866 CD2 PHE B 323 86.993 -39.838 1.868 1.00 53.46 C
ANISOU 2866 CD2 PHE B 323 5749 7147 7415 913 -174 -1539 C
ATOM 2867 C PHE B 323 83.915 -40.894 2.864 1.00 51.27 C
ANISOU 2867 C PHE B 323 6207 6926 6347 1281 773 -500 C
ATOM 2868 O PHE B 323 84.216 -41.676 3.762 1.00 61.61 O
ANISOU 2868 O PHE B 323 7906 8292 7210 1268 310 -543 O
ATOM 2869 N SER B 324 83.697 -41.270 1.611 1.00 52.95 N
ANISOU 2869 N SER B 324 5844 7283 6991 1256 867 -200 N
ATOM 2870 CA SER B 324 83.920 -42.637 1.171 1.00 53.22 C
ANISOU 2870 CA SER B 324 5667 7485 7068 1227 457 -34 C
ATOM 2871 CB SER B 324 82.621 -43.275 0.704 1.00 50.70 C
ANISOU 2871 CB SER B 324 5251 7371 6642 1206 884 544 C
ATOM 2872 OG SER B 324 82.895 -44.471 0.002 1.00 62.56 O
ANISOU 2872 OG SER B 324 6478 8981 8311 1095 583 628 O
ATOM 2873 C SER B 324 84.932 -42.650 0.035 1.00 51.81 C
ANISOU 2873 C SER B 324 4862 7378 7445 1074 191 -307 C
ATOM 2874 O SER B 324 84.710 -42.049 -1.012 1.00 43.28 O
ANISOU 2874 O SER B 324 3325 6410 6711 899 546 -200 O
ATOM 2875 N LEU B 325 86.043 -43.344 0.246 1.00 53.65 N
ANISOU 2875 N LEU B 325 7977 5221 7187 -189 1536 -759 N
ATOM 2876 CA LEU B 325 87.075 -43.425 -0.771 1.00 45.96 C
ANISOU 2876 CA LEU B 325 6870 4368 6224 -331 1251 -585 C
ATOM 2877 CB LEU B 325 88.379 -43.974 -0.196 1.00 51.17 C
ANISOU 2877 CB LEU B 325 7750 4907 6786 -598 1099 -572 C
ATOM 2878 CG LEU B 325 89.561 -43.890 -1.160 1.00 48.90 C
ANISOU 2878 CG LEU B 325 7319 4692 6568 -733 869 -390 C
ATOM 2879 CD1 LEU B 325 89.785 -42.442 -1.565 1.00 39.94 C
ANISOU 2879 CD1 LEU B 325 6311 3392 5471 -654 731 -224 C
ATOM 2880 CD2 LEU B 325 90.810 -44.455 -0.521 1.00 54.14 C
ANISOU 2880 CD2 LEU B 325 8125 5189 7258 -980 705 -366 C
ATOM 2881 C LEU B 325 86.616 -44.297 -1.938 1.00 42.53 C
ANISOU 2881 C LEU B 325 5996 4310 5853 -332 1245 -549 C
ATOM 2882 O LEU B 325 86.960 -44.042 -3.090 1.00 44.88 O
ANISOU 2882 O LEU B 325 6146 4738 6168 -357 1085 -403 O
ATOM 2883 N SER B 326 85.851 -45.339 -1.637 1.00 38.02 N
ANISOU 2883 N SER B 326 5260 3899 5288 -337 1408 -674 N
ATOM 2884 CA SER B 326 85.358 -46.219 -2.687 1.00 41.93 C
ANISOU 2884 CA SER B 326 5390 4711 5830 -355 1362 -646 C
ATOM 2885 CB SER B 326 84.818 -47.528 -2.113 1.00 39.92 C
ANISOU 2885 CB SER B 326 5026 4582 5561 -440 1495 -779 C
ATOM 2886 OG SER B 326 83.830 -47.272 -1.143 1.00 57.38 O
ANISOU 2886 OG SER B 326 7277 6688 7838 -320 1751 -864 O
ATOM 2887 C SER B 326 84.293 -45.533 -3.554 1.00 48.03 C
ANISOU 2887 C SER B 326 6767 -161 1318 -539 C
ATOM 2888 O SER B 326 84.179 -45.823 -4.741 1.00 53.17 O
ANISOU 2888 O SER B 326 6384 6408 7409 -208 1151 -439 O
ATOM 2889 N GLN B 327 83.509 -44.634 -2.962 1.00 34.97 N
ANISOU 2889 N GLN B 327 4301 3713 5274 50 1456 -563 N
ATOM 2890 CA GLN B 327 82.537 -43.864 -3.736 1.00 50.89 C
ANISOU 2890 CA GLN B 327 6070 5721 7544 250 1355 -438 C
ATOM 2891 CB GLN B 327 81.669 -42.983 -2.840 1.00 43.63 C
ANISOU 2891 CB GLN B 327 5167 4543 6868 519 1599 -530 C
ATOM 2892 CG GLN B 327 80.448 -43.685 -2.277 1.00 69.58 C

ANISOU 2892 CG GLN B 327 8154 7920 10361 615 1908 -644 C
ATOM 2893 CD GLN B 327 79.598 -44.342 -3.357 1.00 76.84 C
ANISOU 2893 CD GLN B 327 8607 9088 11501 598 1706 -496 C
ATOM 2894 OE1 GLN B 327 78.858 -43.669 -4.080 1.00 87.42 O
ANISOU 2894 OE1 GLN B 327 9685 10364 13167 762 1523 -348 O
ATOM 2895 NE2 GLN B 327 79.707 -45.662 -3.475 1.00 71.13 N
ANISOU 2895 NE2 GLN B 327 7800 8612 10614 383 1686 -522 N
ATOM 2896 C GLN B 327 83.261 -42.983 -4.738 1.00 57.49 C
ANISOU 2896 C GLN B 327 7021 6512 8312 204 1051 -247 C
ATOM 2897 O GLN B 327 82.832 -42.802 -5.879 1.00 56.04 O
ANISOU 2897 O GLN B 327 6653 6431 8207 207 817 -82 O
ATOM 2898 N GLU B 328 84.377 -42.432 -4.290 1.00 55.93 N
ANISOU 2898 N GLU B 328 7153 6138 7960 125 1028 -247 N
ATOM 2899 CA GLU B 328 85.125 -41.490 -5.098 1.00 58.25 C
ANISOU 2899 CA GLU B 328 7578 6357 8196 57 768 -46 C
ATOM 2900 CB GLU B 328 86.137 -40.743 -4.237 1.00 43.81 C
ANISOU 2900 CB GLU B 328 6118 4238 6289 13 758 -56 C
ATOM 2901 CG GLU B 328 86.706 -39.521 -4.912 1.00 51.35 C
ANISOU 2901 CG GLU B 328 7214 5045 7251 -23 485 173 C
ATOM 2902 CD GLU B 328 85.628 -38.562 -5.416 1.00 69.56 C
ANISOU 2902 CD GLU B 328 9415 7232 9784 202 343 271 C
ATOM 2903 OE1 GLU B 328 85.900 -37.848 -6.403 1.00 69.95 O
ANISOU 2903 OE1 GLU B 328 9487 7273 9817 116 61 509 O
ATOM 2904 OE2 GLU B 328 84.517 -38.516 -4.831 1.00 78.20 O
ANISOU 2904 OE2 GLU B 328 10392 8224 11096 452 512 123 O
ATOM 2905 C GLU B 328 85.818 -42.176 -6.272 1.00 57.13 C
ANISOU 2905 C GLU B 328 7349 6499 7861 -181 640 63 C
ATOM 2906 O GLU B 328 85.968 -41.603 -7.350 1.00 52.82 O
ANISOU 2906 O GLU B 328 6810 5999 7261 -251 431 258 O
ATOM 2907 N VAL B 329 86.240 -43.411 -6.051 1.00 35.43 N
ANISOU 2907 N VAL B 329 4545 3919 4997 -315 775 -73 N
ATOM 2908 CA VAL B 329 86.878 -44.178 -7.101 1.00 41.84 C
ANISOU 2908 CA VAL B 329 5282 4981 5636 -513 731 -34 C
ATOM 2909 CB VAL B 329 87.690 -45.347 -6.522 1.00 44.73 C
ANISOU 2909 CB VAL B 329 5643 5401 5952 -642 874 -201 C
ATOM 2910 CG1 VAL B 329 88.324 -46.150 -7.623 1.00 38.21 C
ANISOU 2910 CG1 VAL B 329 4732 4807 4981 -808 889 -207 C
ATOM 2911 CG2 VAL B 329 88.767 -44.813 -5.595 1.00 40.56 C
ANISOU 2911 CG2 VAL B 329 5322 4618 5472 -698 873 -183 C
ATOM 2912 C VAL B 329 85.817 -44.677 -8.076 1.00 47.35 C
ANISOU 2912 C VAL B 329 5785 5888 6318 -496 636 -3 C
ATOM 2913 O VAL B 329 86.004 -44.648 -9.293 1.00 43.12 O
ANISOU 2913 O VAL B 329 5278 5492 5614 -628 505 119 O
ATOM 2914 N LEU B 330 84.689 -45.119 -7.531 1.00 47.31 N
ANISOU 2914 N LEU B 330 5603 5888 6484 -359 696 -97 N
ATOM 2915 CA LEU B 330 83.591 -45.603 -8.359 1.00 51.28 C
ANISOU 2915 CA LEU B 330 5892 6545 7046 -351 545 -36 C
ATOM 2916 CB LEU B 330 82.451 -46.156 -7.501 1.00 46.75 C
ANISOU 2916 CB LEU B 330 5074 5962 6725 -212 680 -143 C
ATOM 2917 CG LEU B 330 82.684 -47.558 -6.942 1.00 54.79 C
ANISOU 2917 CG LEU B 330 6064 7114 7639 -332 840 -329 C
ATOM 2918 CD1 LEU B 330 81.655 -47.889 -5.881 1.00 51.25 C
ANISOU 2918 CD1 LEU B 330 5424 6622 7424 -216 1039 -415 C
ATOM 2919 CD2 LEU B 330 82.636 -48.579 -8.064 1.00 53.00 C
ANISOU 2919 CD2 LEU B 330 5779 7105 7255 -500 656 -314 C
ATOM 2920 C LEU B 330 83.068 -44.524 -9.307 1.00 54.99 C
ANISOU 2920 C LEU B 330 6359 6940 7595 -308 259 201 C
ATOM 2921 O LEU B 330 82.610 -44.819 -10.408 1.00 57.84 O
ANISOU 2921 O LEU B 330 6677 7423 7876 -419 19 321 O
ATOM 2922 N ARG B 331 83.141 -43.272 -8.873 1.00 44.63 N
ANISOU 2922 N ARG B 331 5135 5388 6434 -164 241 276 N
ATOM 2923 CA ARG B 331 82.640 -42.173 -9.685 1.00 51.18 C
ANISOU 2923 CA ARG B 331 5965 6085 7395 -116 -81 517 C
ATOM 2924 CB ARG B 331 82.627 -40.871 -8.892 1.00 58.29 C
ANISOU 2924 CB ARG B 331 6949 6662 8535 103 -54 533 C
ATOM 2925 CG ARG B 331 81.979 -39.723 -9.635 1.00 73.21 C
ANISOU 2925 CG ARG B 331 8801 8353 10661 189 -428 780 C
ATOM 2926 CD ARG B 331 82.192 -38.401 -8.920 1.00 80.82 C
ANISOU 2926 CD ARG B 331 9928 8966 11814 384 -423 785 C
ATOM 2927 NE ARG B 331 83.533 -37.869 -9.145 1.00 94.70 N
ANISOU 2927 NE ARG B 331 12034 10698 13251 172 -503 890 N
ATOM 2928 CZ ARG B 331 83.867 -36.590 -8.994 1.00103.81 C
ANISOU 2928 CZ ARG B 331 13398 11548 14497 234 -680 1009 C
ATOM 2929 NH1 ARG B 331 82.956 -35.701 -8.618 1.00109.37 N
ANISOU 2929 NH1 ARG B 331 14018 11930 15609 533 -782 1005 N
ATOM 2930 NH2 ARG B 331 85.115 -36.200 -9.227 1.00 92.59 N
ANISOU 2968 NE2 GLN B 335 14547 13709 13810 -1216 -1618 1735 N
ATOM 2969 C GLN B 335 84.930 -44.716 -18.000 1.00 99.77 C
ANISOU 2969 C GLN B 335 13688 13356 10864 -1980 -778 1016 C
ATOM 2970 O GLN B 335 85.207 -45.909 -18.035 1.00 94.32 O
ANISOU 2970 O GLN B 335 13052 12823 9963 -2046 -563 777 O
TER 2974 GLN B 335
HETATM 2971 O HOH S 1 110.319 -45.601 -9.573 1.00 39.14 O
HETATM 2972 O HOH S 2 112.398 -45.393 -4.628 1.00 48.56 O
HETATM 2973 O HOH S 3 123.141 -29.303 -16.515 1.00 49.19 O
HETATM 2974 O HOH S 4 92.690 -51.029 -13.033 1.00 53.52 O
HETATM 2975 O HOH S 5 93.030 -41.555 0.913 1.00 51.01 O
HETATM 2976 O HOH S 6 128.910 -39.669 -15.753 1.00 51.84 O
HETATM 2977 O HOH S 7 106.614 -30.842 12.237 1.00 54.53 O
HETATM 2978 O HOH S 8 109.156 -39.164 -21.771 1.00 54.08 O

ANISOU 2930 NH2 ARG B 331 12254 10127 12798 -2 -754 1136 N
ATOM 2931 C ARG B 331 83.488 -42.005 -10.946 1.00 61.47 C
ANISOU 2931 C ARG B 331 7509 7510 8338 -393 -287 695 C
ATOM 2932 O ARG B 331 82.986 -41.671 -12.019 1.00 62.26 O
ANISOU 2932 O ARG B 331 7631 7614 8410 -486 -621 908 O
ATOM 2933 N HIS B 332 84.771 -42.292 -10.848 1.00 59.85 N
ANISOU 2933 N HIS B 332 7487 7383 7868 -544 -86 619 N
ATOM 2934 CA HIS B 332 85.656 -42.259 -11.992 1.00 56.95 C
ANISOU 2934 CA HIS B 332 7331 7158 7150 -822 -152 755 C
ATOM 2935 CB HIS B 332 87.080 -42.058 -11.532 1.00 50.51 C
ANISOU 2935 CB HIS B 332 6645 6305 6242 -915 65 723 C
ATOM 2936 CG HIS B 332 87.377 -40.661 -11.139 1.00 56.42 C
ANISOU 2936 CG HIS B 332 7528 6783 7126 -857 -86 900 C
ATOM 2937 ND1 HIS B 332 88.018 -39.781 -11.969 1.00 64.51 N
ANISOU 2937 ND1 HIS B 332 8741 7788 7983 -1057 -253 1159 N
ATOM 2938 CE1 HIS B 332 88.131 -38.619 -11.364 1.00 60.89 C
ANISOU 2938 CE1 HIS B 332 8384 7036 7716 -956 -407 1277 C
ATOM 2939 NE2 HIS B 332 87.571 -38.711 -10.179 1.00 54.89 N
ANISOU 2939 NE2 HIS B 332 7537 6105 7214 -689 -312 1078 N
ATOM 2940 CD2 HIS B 332 87.093 -39.977 -10.014 1.00 53.58 C
ANISOU 2940 CD2 HIS B 332 7181 6142 7036 -634 -100 852 C
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HETATM 3033  O4  SO4 D  1     123.399 -62.594  -7.442  1.00141.27           O
END
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Equivalents

[0329] Those skilled in the art will recognize, or be able to ascertain using no more than routine experimentation, many equivalents to the specific embodiments of the invention described herein. The scope of the present invention is not intended to be limited to the above Description, but rather is as set forth in the following claims:

CLAIMS

We claim:

1. A STING modulator whose structure is an analog of c[G(2',5')pA(3',5')p], DMXAA, or CMA, and includes a moiety that interacts with a residue corresponding to Gly230, Gln266, Ser162, or Ile165 of hSTING, or a combination thereof.

2. A STING modulator whose structure is an analog of c[G(2',5')pA(3',5')p], DMXAA, or CMA, and includes a moiety that interacts with a residue corresponding to Ser162 and/or Ile165 of hSTING.

3. The STING modulator of claim 1 or 2 that modulates hSTING.

4. The STING modulator of any one of the preceding claims, which STING modulator is specific to hSTING as compared with mSTING.

5. The STING modulator of any one of preceding claims, wherein the STING modulator includes a moiety that interacts with a residue corresponding to Gln266 of hSTING.

6. The STING modulator of any one of preceding claims, wherein the STING modulator includes a moiety that interacts with a residue corresponding to Gly230 of hSTING.

7. The STING modulator of any one of preceding claims, wherein the STING modulator includes a moiety that interacts with a residue corresponding to Ser162 of hSTING.

8. The STING modulator of any one of the preceding claims, which STING modulator comprises one or more of the following features:

i.) direct hydrogen bonds to the side chain of Thr267 of hSTING;

ii.) direct hydrogen bonds to the side chain of Arg238 of hSTING; and

iii.) direct hydrogen bonds to the side chain of Thr263 of hSTING.

9. The STING modulator of any one of the preceding claims, which STING modulator comprises one or more of the following features:

i) direct hydrogen bonds to the side chain of Arg238 of hSTING; and

ii) water-mediated hydrogen bonds to Tyr240 of hSTING.

10. The STING modulator of any one of the preceding claims, which STING modulator comprises one or more of the following features:

i) hydrophobic interactions with a residue corresponding to Leu170 of hSTING;

ii) hydrophobic interactions with a residue corresponding to Ile235 of hSTING; and

iii) hydrophobic interactions with a residue corresponding to Ile165 of hSTING.

11. The STING modulator of any one of the preceding claims, wherein upon binding hSTING, an antiparallel β-pleated sheet forms over the binding pocket indicative of formation of a closed STING conformation.

12. A method of designing or characterizing a STING modulator comprising the steps of:

providing an image of a STING crystal that includes at least one potential interaction site;

docking in the image at least one moiety that is a potential STING modulator structural element; and

assessing one or more features of a potential moiety-interaction site interaction.

13. The method of claim 12, wherein the at least one potential interaction site includes a site of hSTING selected from the group consisting of Ser162, Ile165, Arg238, Thr263, Thr267, and combinations thereof.

14. The method of claim 12 or 13, wherein the at least one potential interaction site includes a site of hSTING selected from the group consisting of Gly230, Gln266, Tyr240, Leu170, Ile235, and combinations thereof.

15. The method of claim 12, wherein the at least one potential interaction site is Ser162.

16. The method of claim 12, wherein the at least one potential interaction site is Ile165.

17. The method of claim 12, wherein the at least one potential interaction site is Gly230.

18. The method of any one of claims 12-17, wherein the one or more features include at least one feature selected from the group consisting of: spatial separation between the moiety and the potential interaction site; energy of the potential moiety-interaction site interaction, and/or combinations thereof.

19. The method of any one of claims 12-18, further comprising a step of providing an image of a potential STING modulator comprising the moiety docked with the image of the STING crystal.

20. The method of claim 19, further comprising a step of comparing the image with that of a STING crystal including a bound known modulator.

21. A system comprising a computer or computer readable medium in which a STING crystal structure, or coordinates thereof, is embedded and/or displayed.

22. A method of designing and/or characterizing a STING modulator, which method comprises steps of:

(i) using the sytem of claim 21 to assess one or more structural features of the STING modulator; and

(ii) performing one or more *in vitro, in vivo* or cell-based assays to characterize the STING modulator.

23. The method of claim 22, wherein the one or more structure features of the STING modulator comprise a moiety that interacts with a residue corresponding to Ser162 and/or Ile165 of hSTING.

24. The method of claim 22 or 23, wherein the one or more structure features of the STING modulator comprise a moiety that interacts with a residue corresponding to Gly230 of hSTING.

25. The method of claim 22, 23, or 24, wherein the one or more structure features of the STING modulator comprise a moiety that interacts with a residue corresponding to Arg238, Thr263, Thr267, Gln266, Tyr240, Leu170, Ile235 of hSTING, or a combination thereof.

26. A method of designing and/or characterizing a STING modulator, which method comprises steps of:

(i) determining the STING modulator binds in the binding pocket having a three-dimensional structure characterized by the structure coordinates of any one of Tables 1, 2, 3, 4, 5, 6, 7, 8, and/or 9; and

(ii) assessing one or more structure features of the STING modulator.

27. The method of claim 26, wherein the method further comprises the step:

(iii) defining the three-dimensional shape of the modulator.

28. The method of claim 26 or 27, wherein the three-dimensional shape of the modulator includes a moiety that interacts with a residue corresponding to Ser162 and/or Ile165 of hSTING.

29. The method of claim 26, 27, or 28, wherein the three-dimensional shape of the modulator includes a moiety that interacts with a residue corresponding to Gly230 of hSTING.

30. The method of any one of claims 26-29, wherein the three-dimensional shape of the modulator includes a moiety that interacts with a residue corresponding to Arg238, Thr263, Thr267, Gln266, Tyr240, Leu170, Ile235 of hSTING, or a combination thereof.

31. A designed STING modulator, comprising the crystallography coordinates of any one of Tables 1-9, wherein the crystallography coordinates are within about a root mean square deviation of not more than about 1.5 Å from the backbone atoms of the amino acids according to Tables 1, 2, 3, 4, 5, 6, 7, 8, and/or 9.

32. A computer system containing a set of information to perform a design or characterization of a STING modulator having a user interface comprising a display unit, the set of information comprising:

(i) logic for inputting an information regarding a binding of a STING protein to a moiety known to bind STING protein;

(ii) logic for designing a candidate STING modulator based on the binding of the STING protein to the moiety known to bind STING protein;

(iii) logic for determing an information regarding a binding of the STING protein to the candidate STING modulator; and

(iv) logic for making a conclusion regarding a STING agonist or antagonist properties of the candidate STING modulator based on the determination of step (iii).

33. A computer-readable storage medium containing a set of information for a general purpose computer having a user interface comprising, a display unit, the set of information comprising:

(i) logic for inputting an information regarding a binding of a STING protein to a chemical known to binding STING protein;

(ii) logic for design a candidate STING modulator based on the binding of the STING protein to the chemical known to bind STING protein;

(iii) logic for determining an information regarding a binding of the STING protein to the candidate STING modulator; and

(iv) logic for making a conclusion regarding a STING agonist or antagonist properties of the candidate STING modulator based on the determination step of step (iii).

34. An electronic signal or carrier wave that is propagated over the internet between computers comprising a set of information for a general purpose computer having a user interface comprising a display unit, the set of information comprising a computer-readable storage medium containing a set of information for a general purpose computer having a user interface comprising a display unit, the set of information comprising:

(i) logic for inputting an information regarding a binding of a STING protein to an agent known to bind STING protein;

(ii) logic for designing a candidate STING modulator based on the binding of the STING protein to the agent known to bind STING protein;

(iii) logic for determining an information regarding a binding of the STING protein to the candidate STING modulator; and

(iv) logic for making a conclusion regarding a STING agonist or antagonist properties of the candidate STING modulator based on the determination of step (iii).

35. A method of modulating activity of a STING polypeptide, the method comprising steps of: contacting the STING polypeptide with a modulating agent of any one of claims 1-11 which modulating agent is not a known modulator.

36. A crystalline or crystallizable composition comprising or consisting of a STING polypeptide.

37. A method of making the composition of claim 36.

38. A method of using the composition of claim 36.

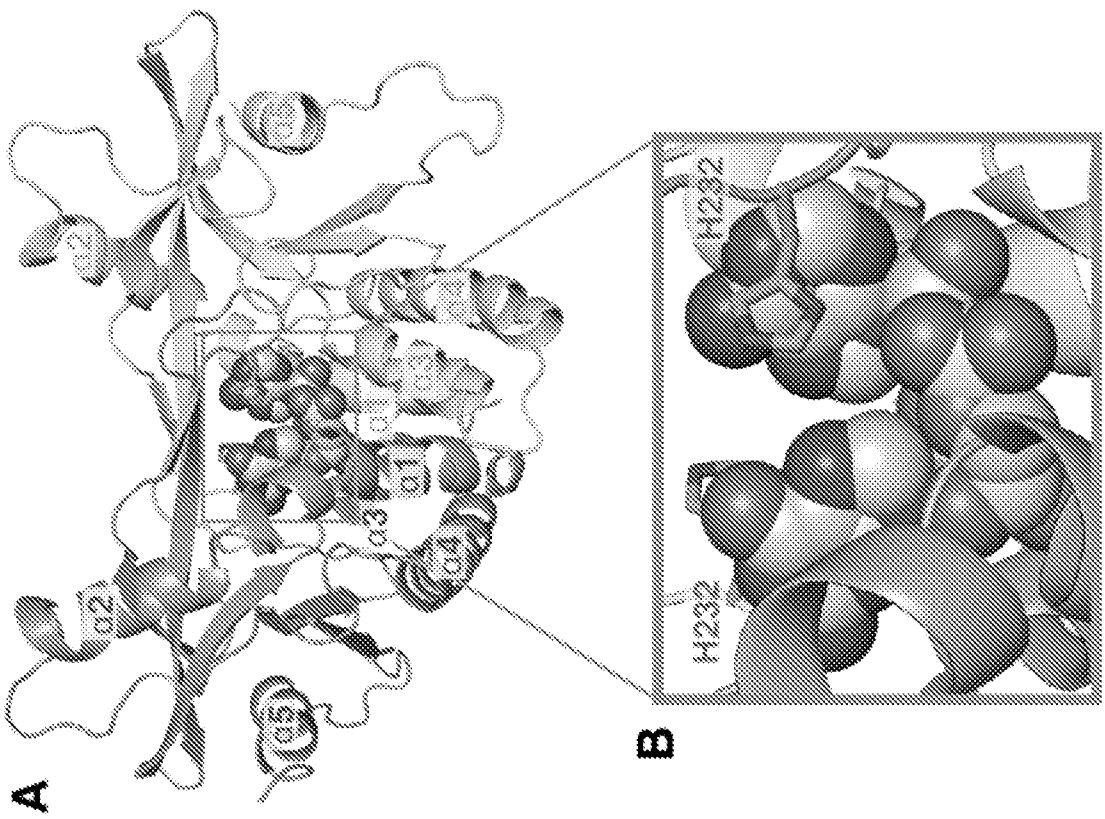


Figure 1A

Figure 1B

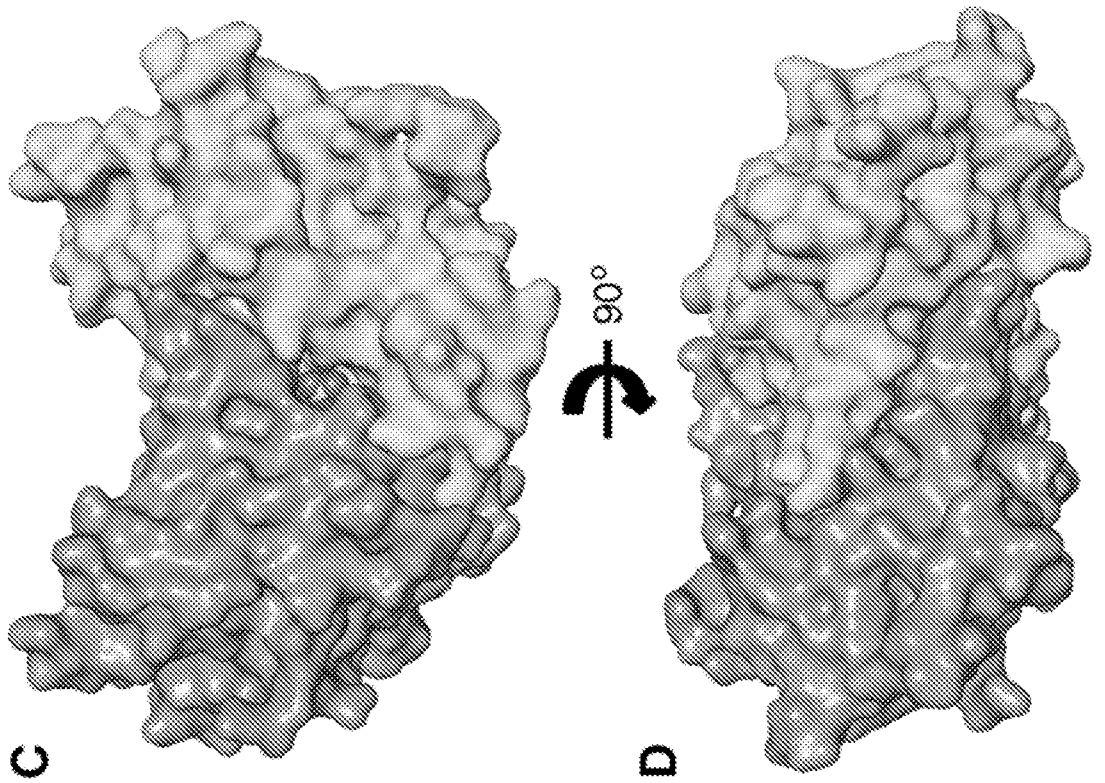


Figure 1C

Figure 1D

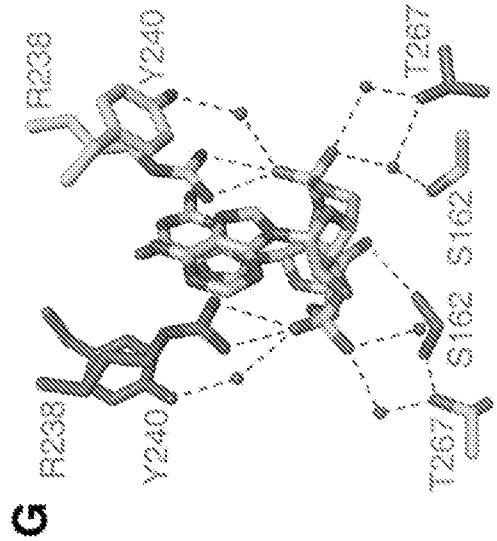


Figure 1G

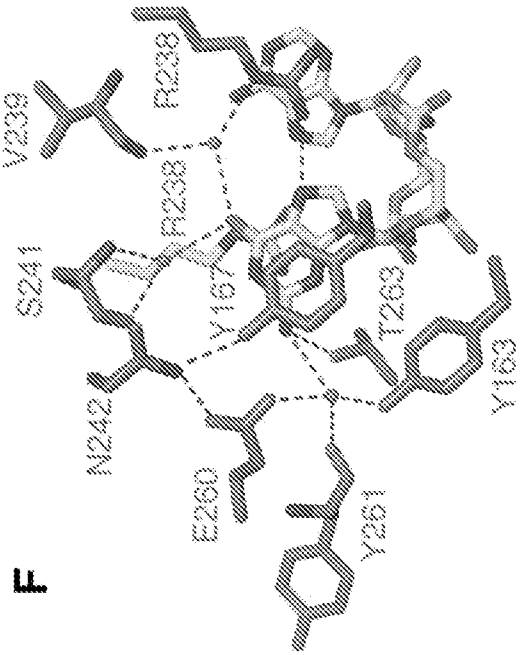


Figure 1F

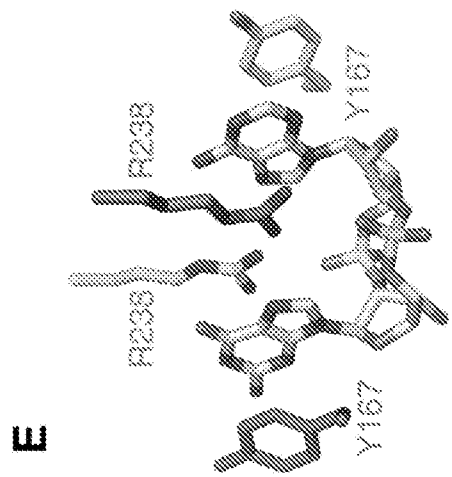


Figure 1E

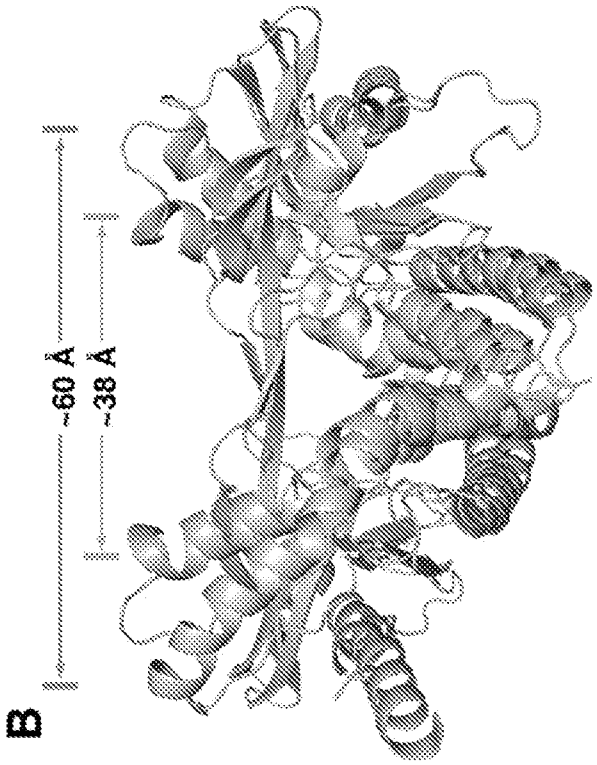


Figure 2B

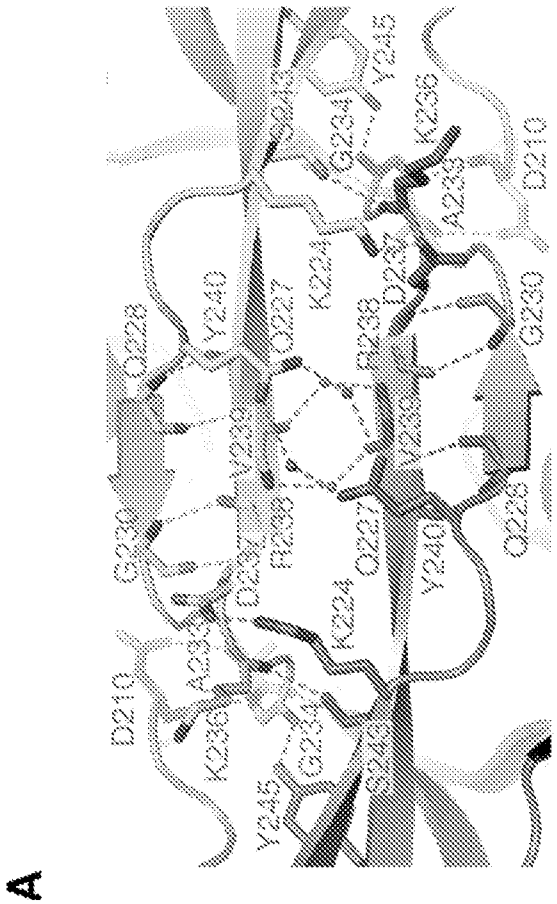
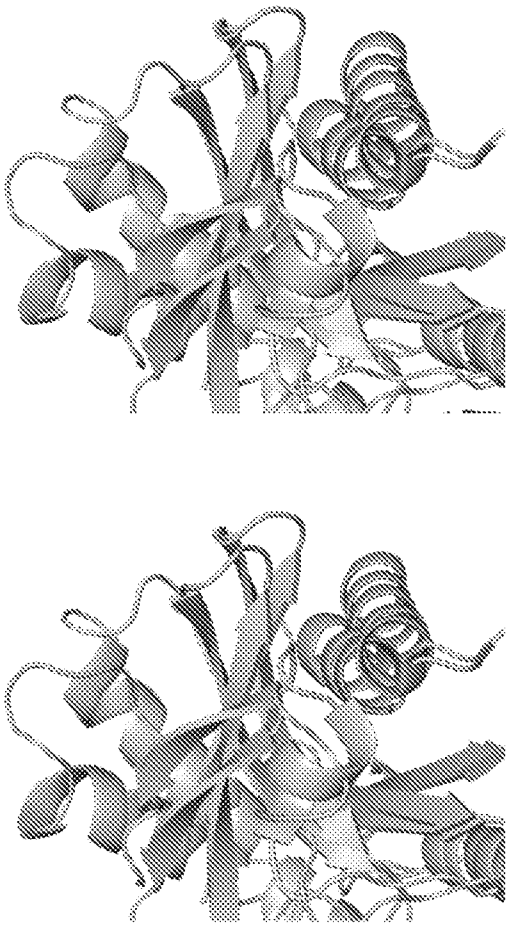


Figure 2A



D

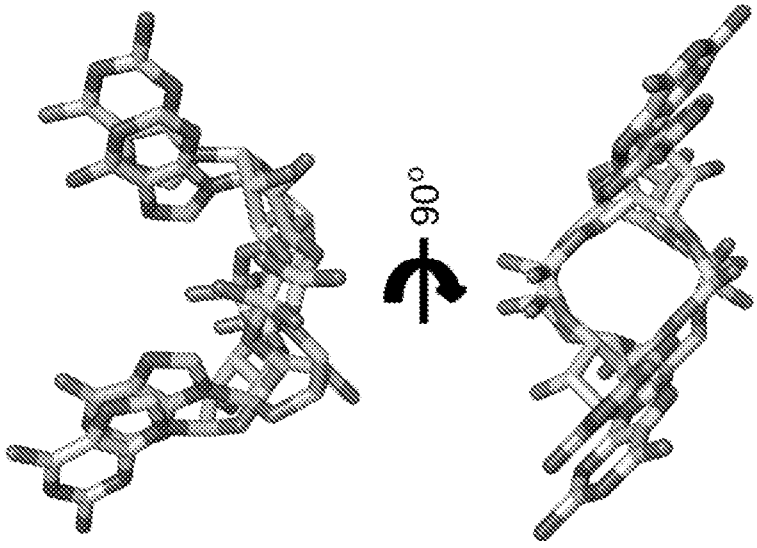


Figure 2D

Figure 2C

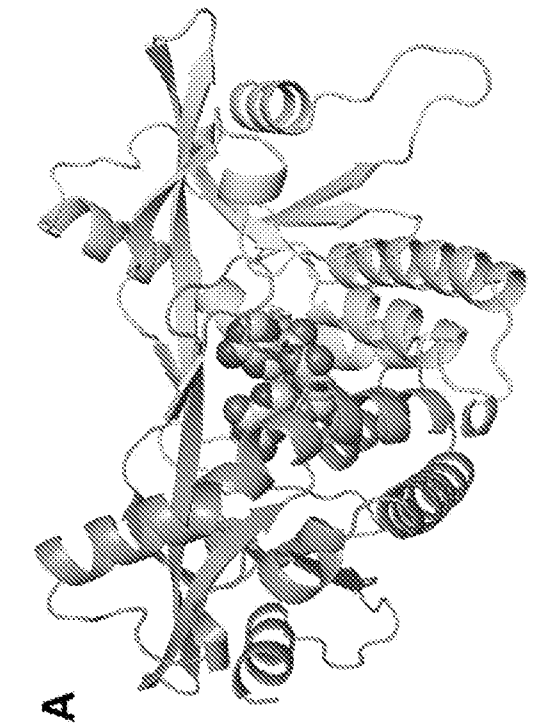


Figure 3A

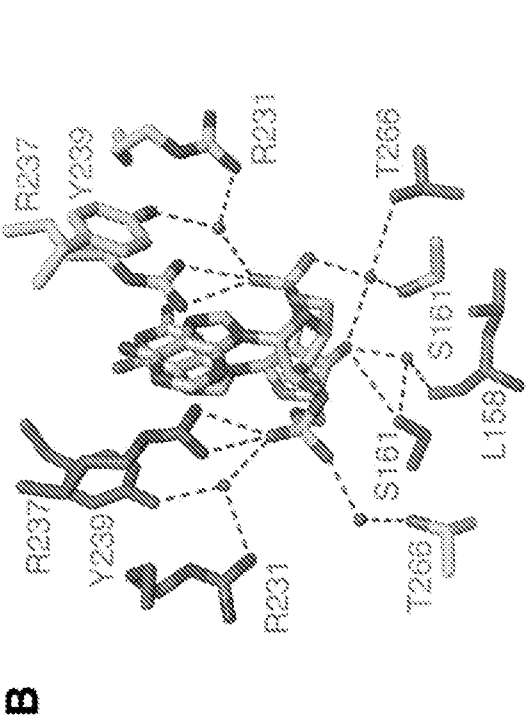


Figure 3B

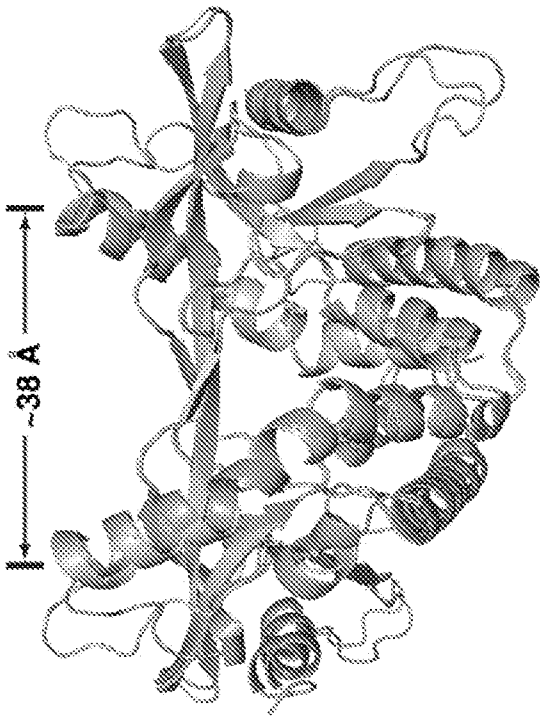


Figure 3C

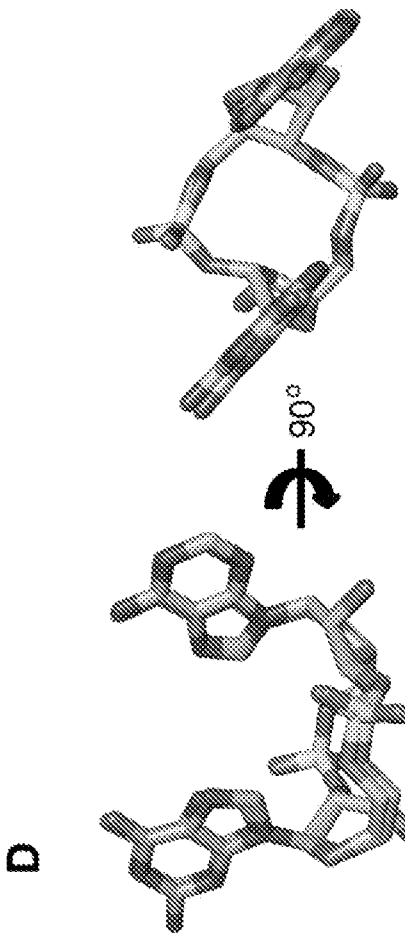


Figure 3D

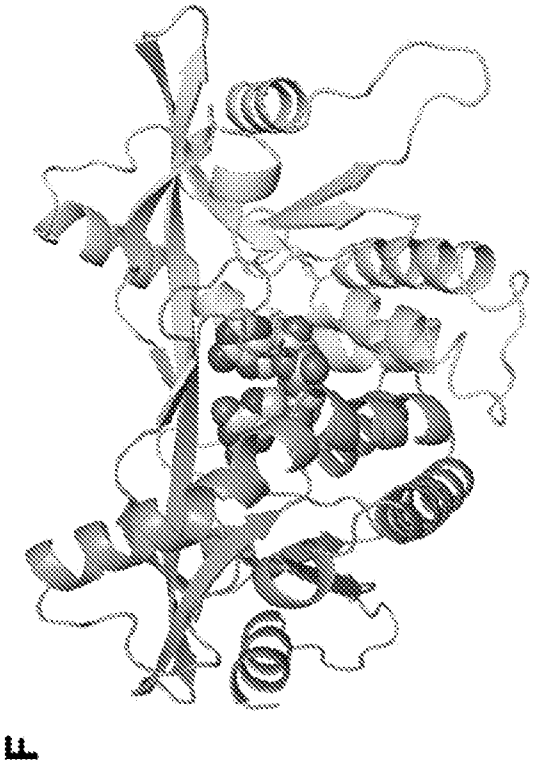


Figure 3F

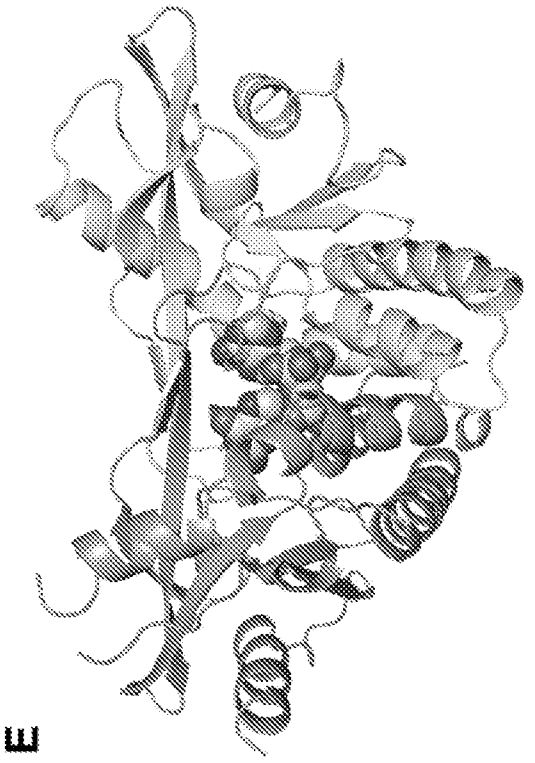


Figure 3E

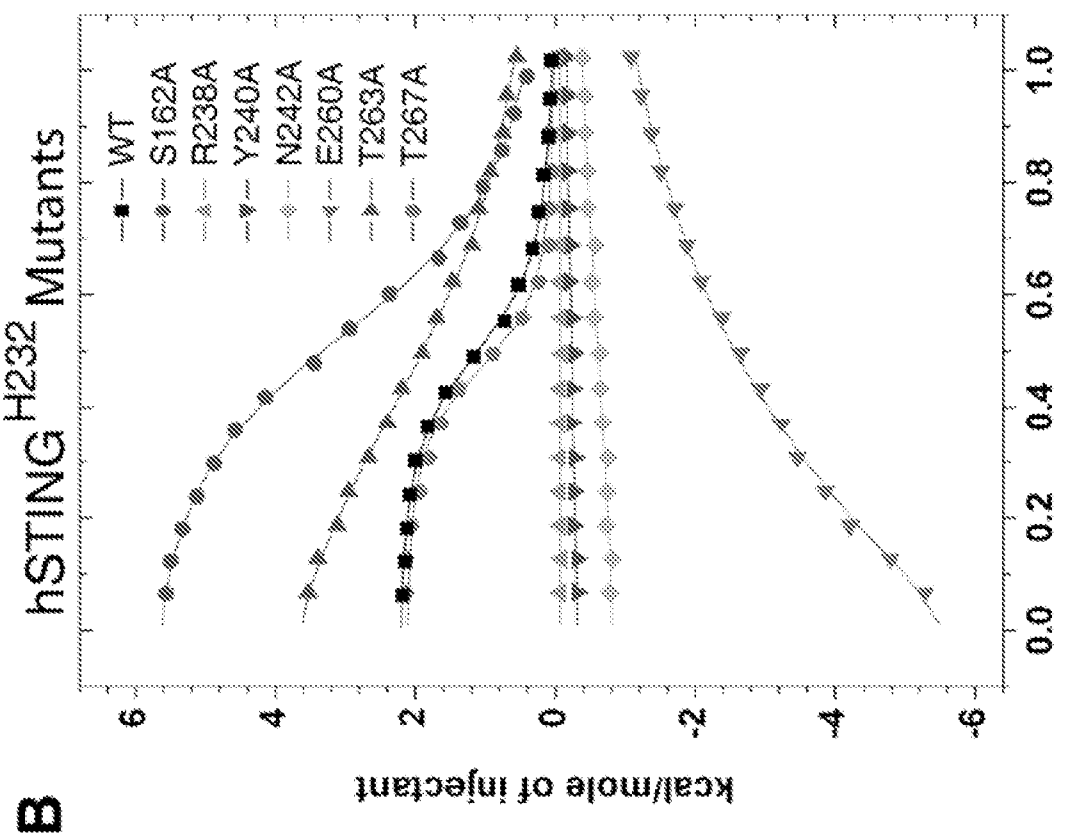


Figure 4B

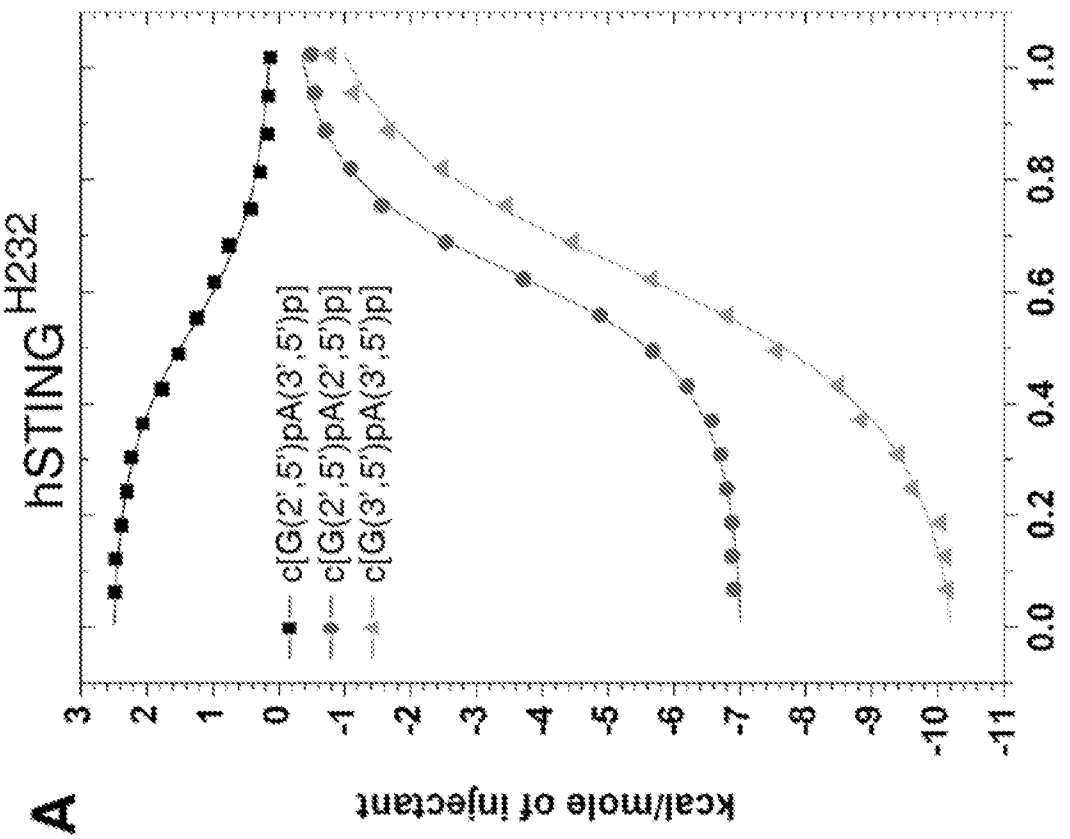


Figure 4A

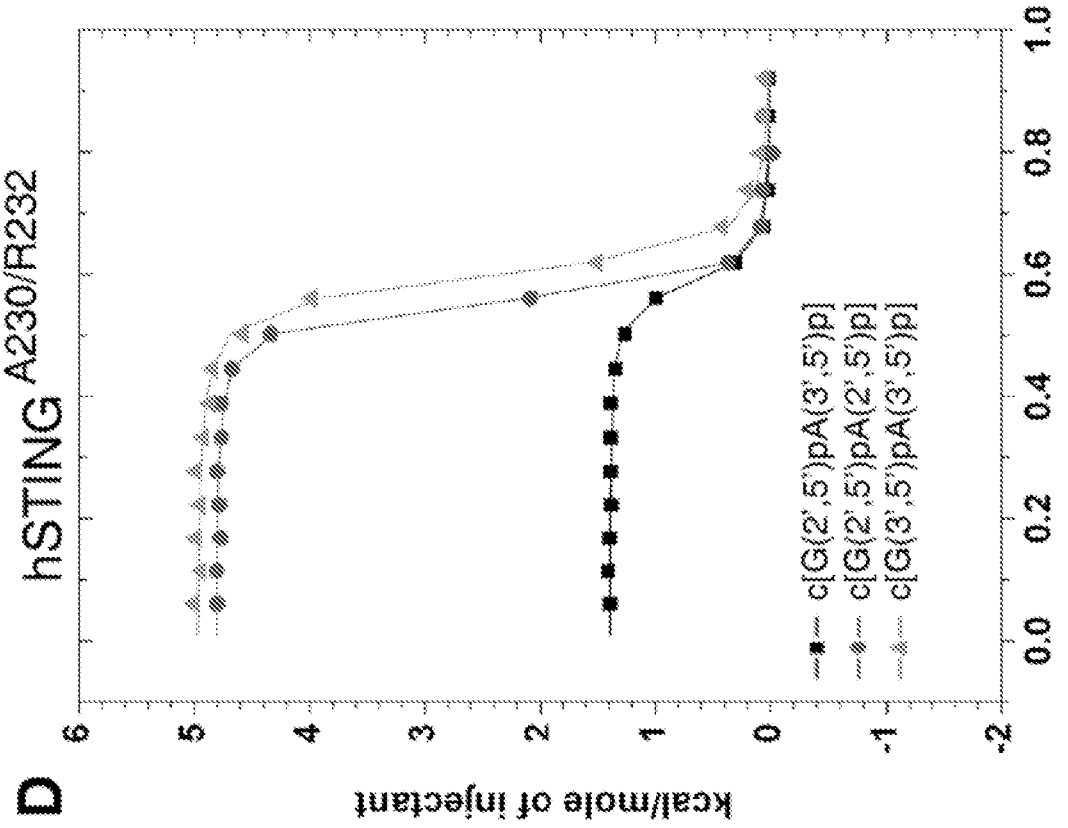


Figure 4D

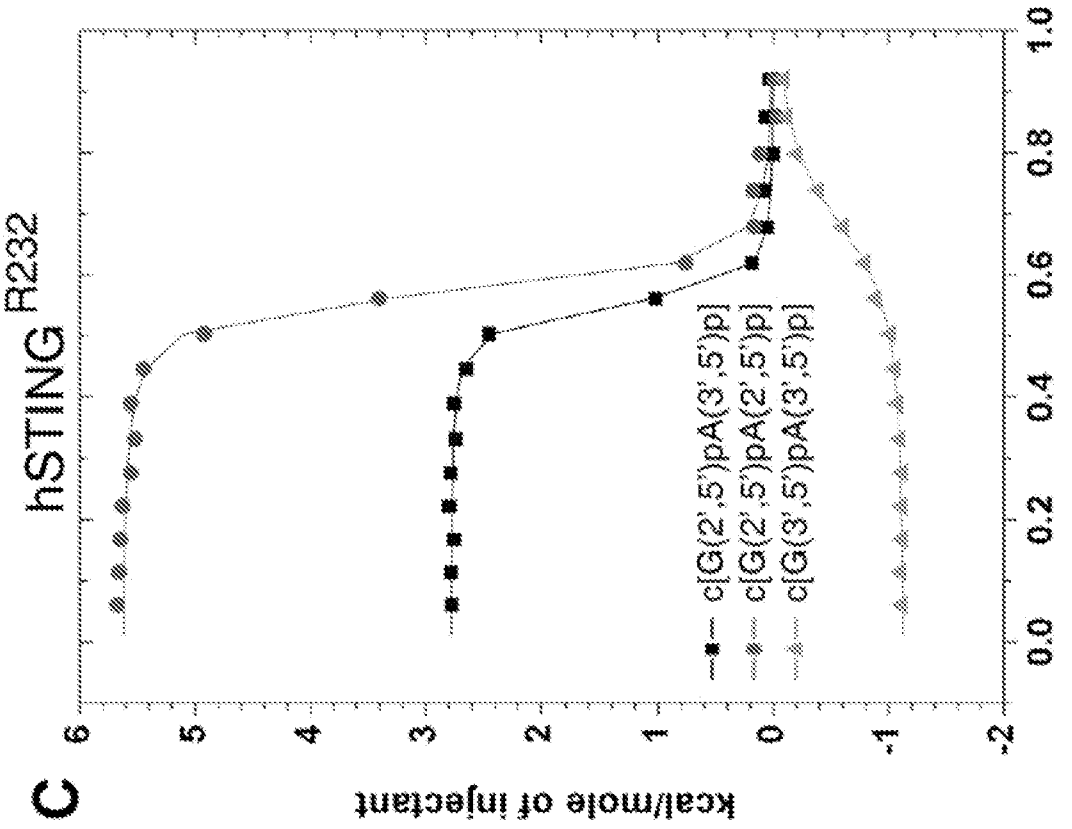


Figure 4C

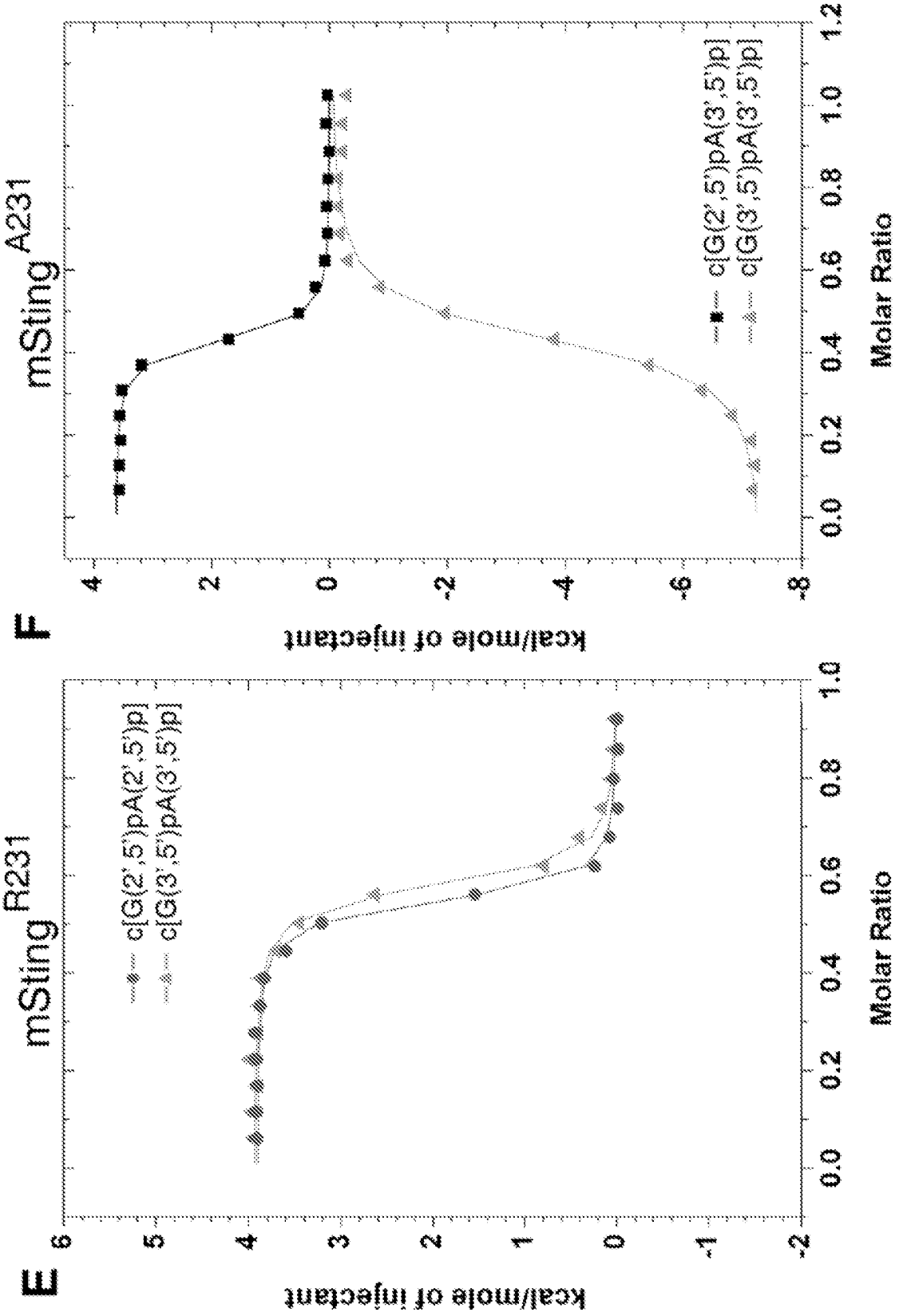


Figure 4F

Figure 4E

Figure 5A

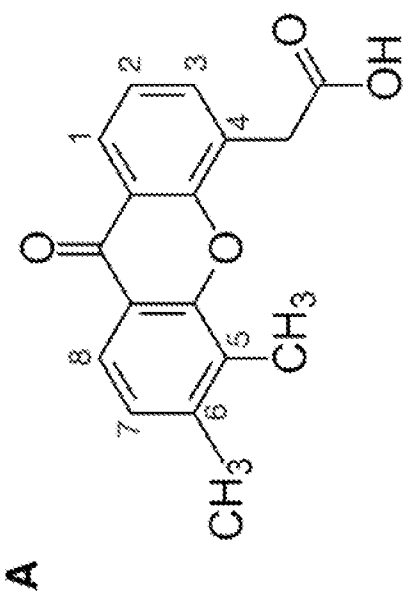


Figure 5B

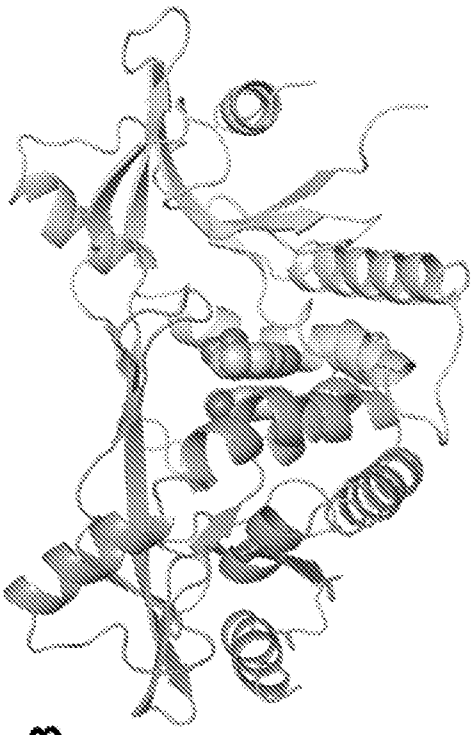
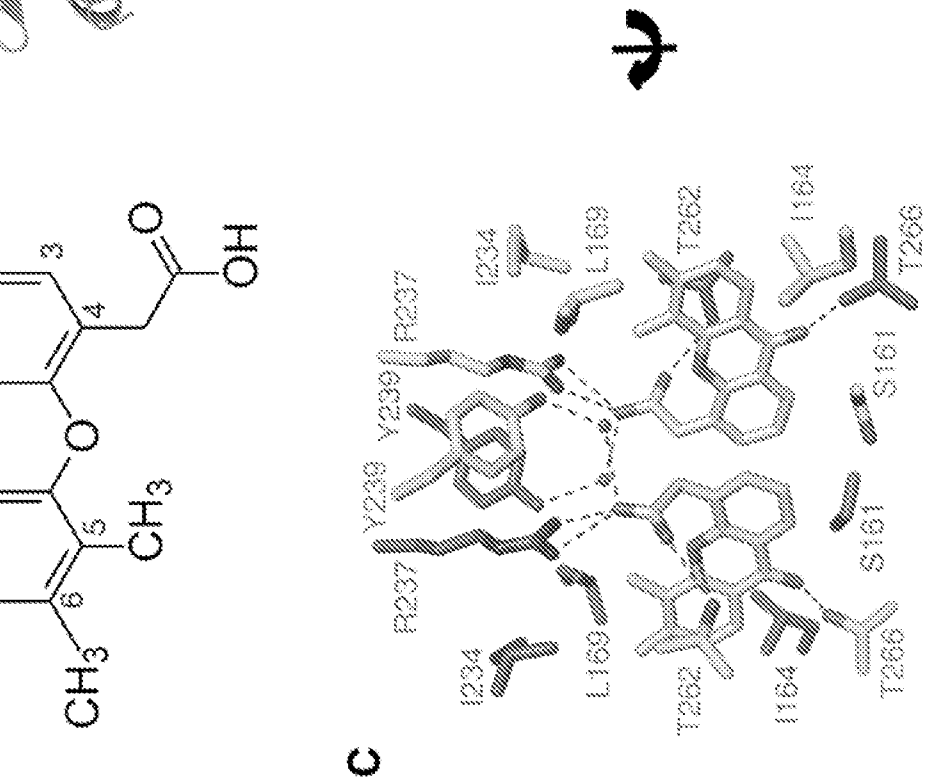


Figure 5C



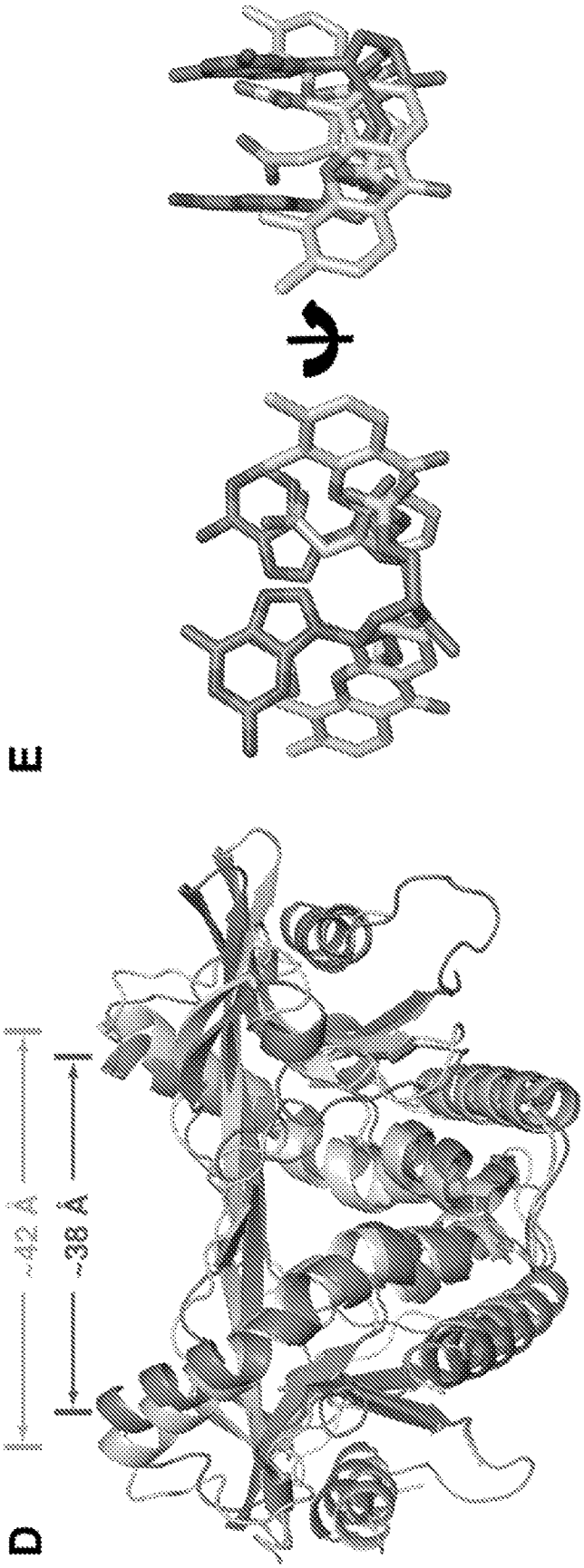


Figure 5D

Figure 5E

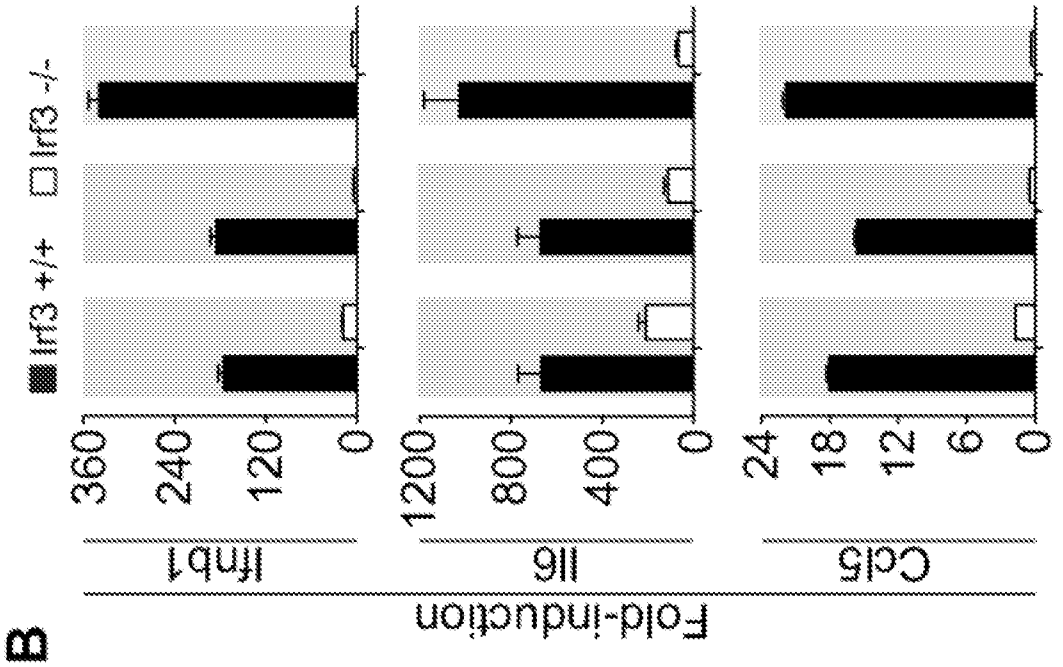


Figure 6B

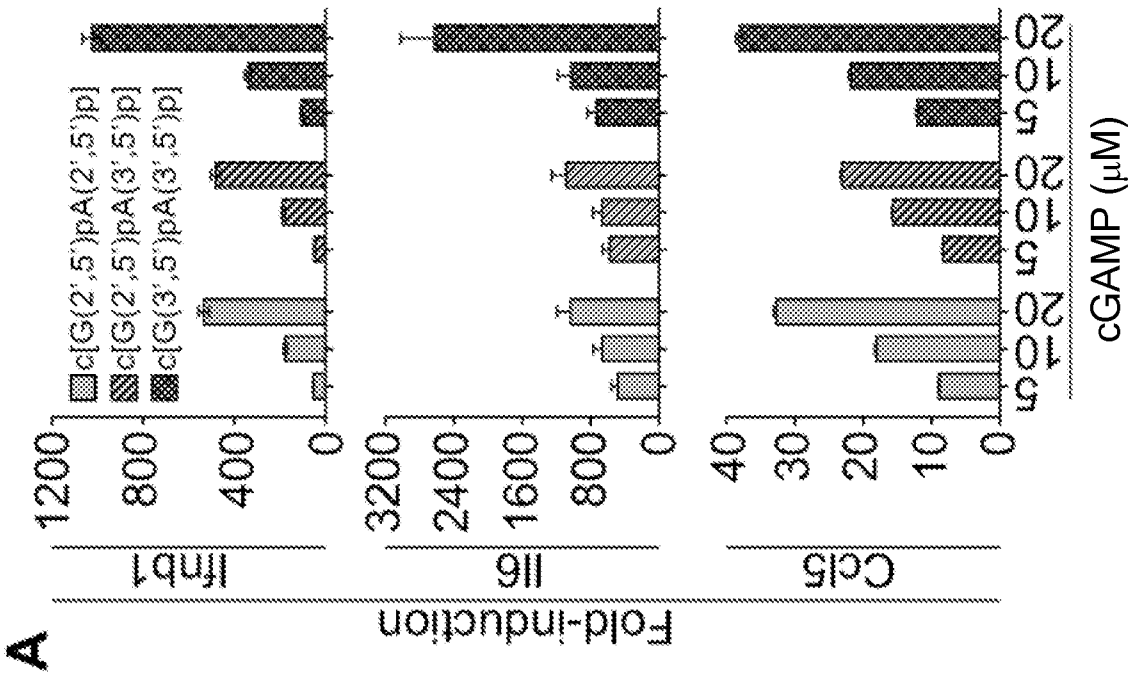


Figure 6A

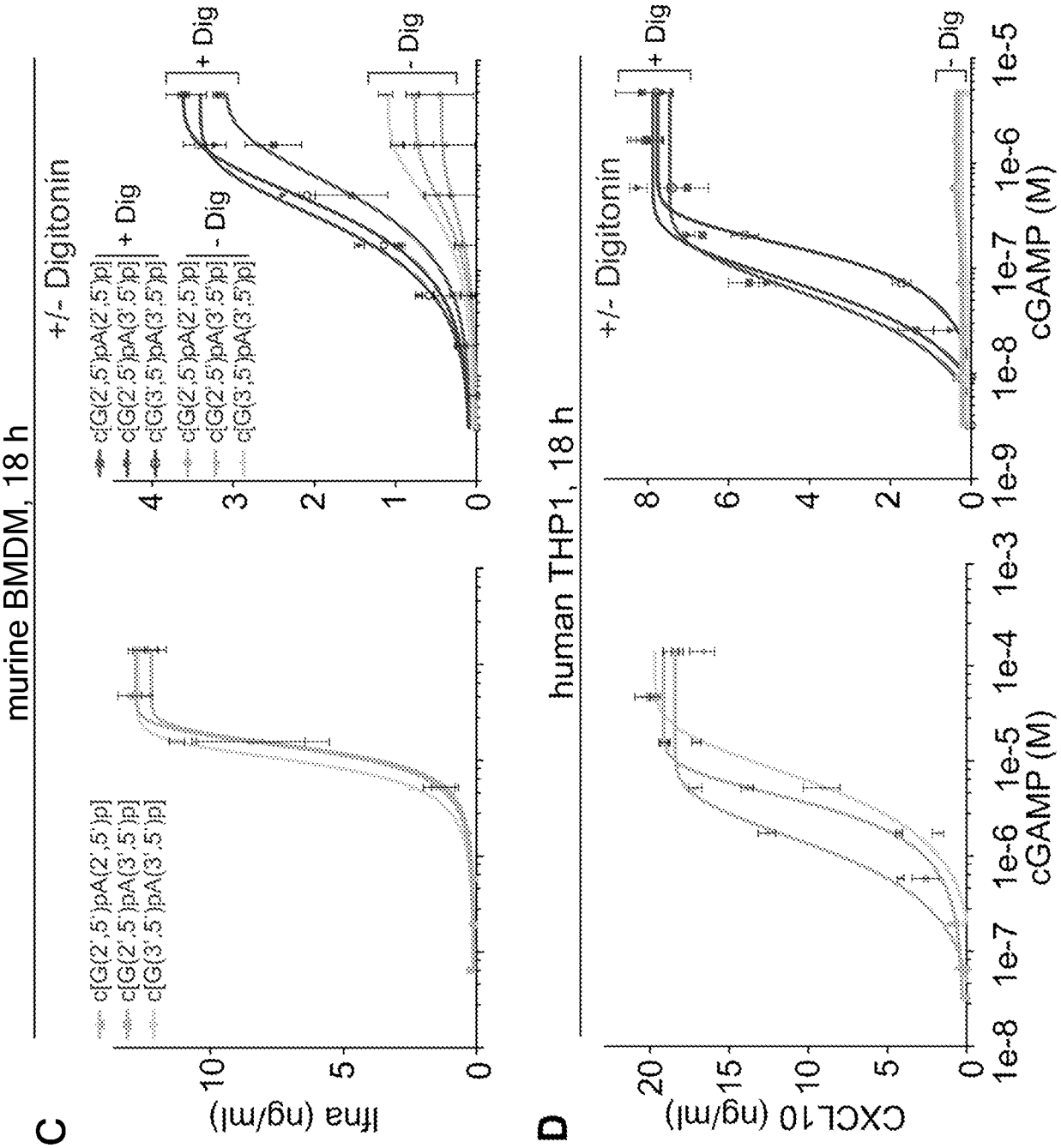


Figure 6C

Figure 6D

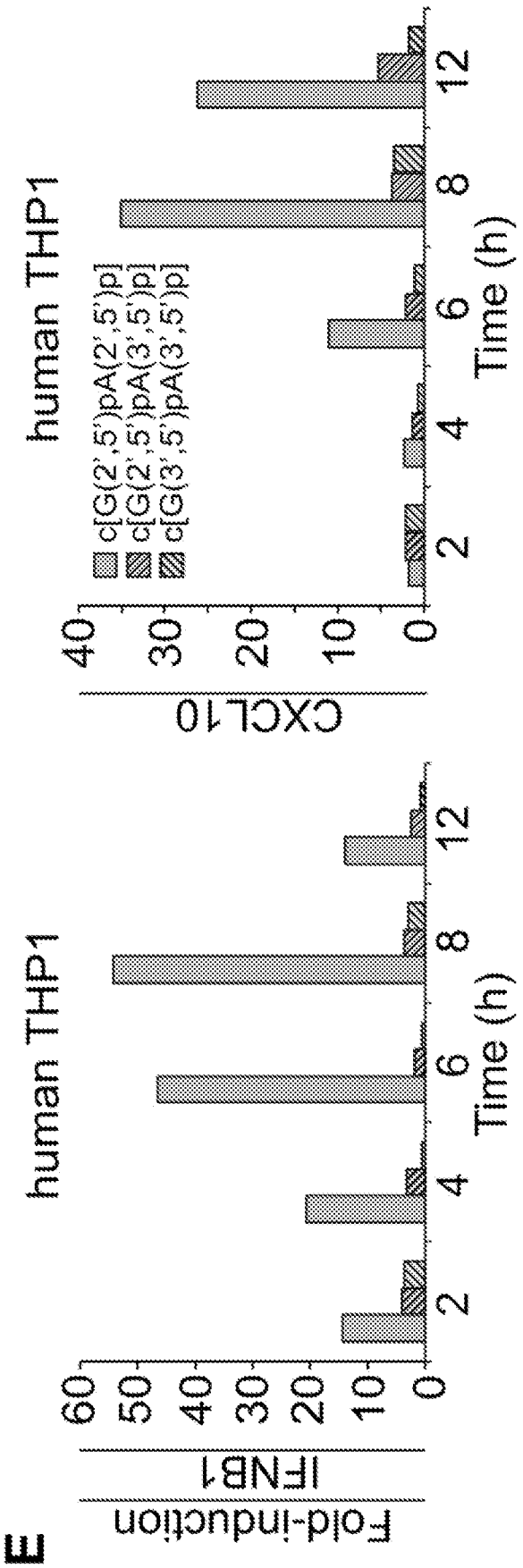

E
Fold-induction
IFNB1
human THP1
Time (h)
CXCL10
human THP1
c[G(2',5')pA(2',5')p]
c[G(2',5')pA(3',5')p]
c[G(3',5')pA(3',5')p]
Time (h)

Figure 6E

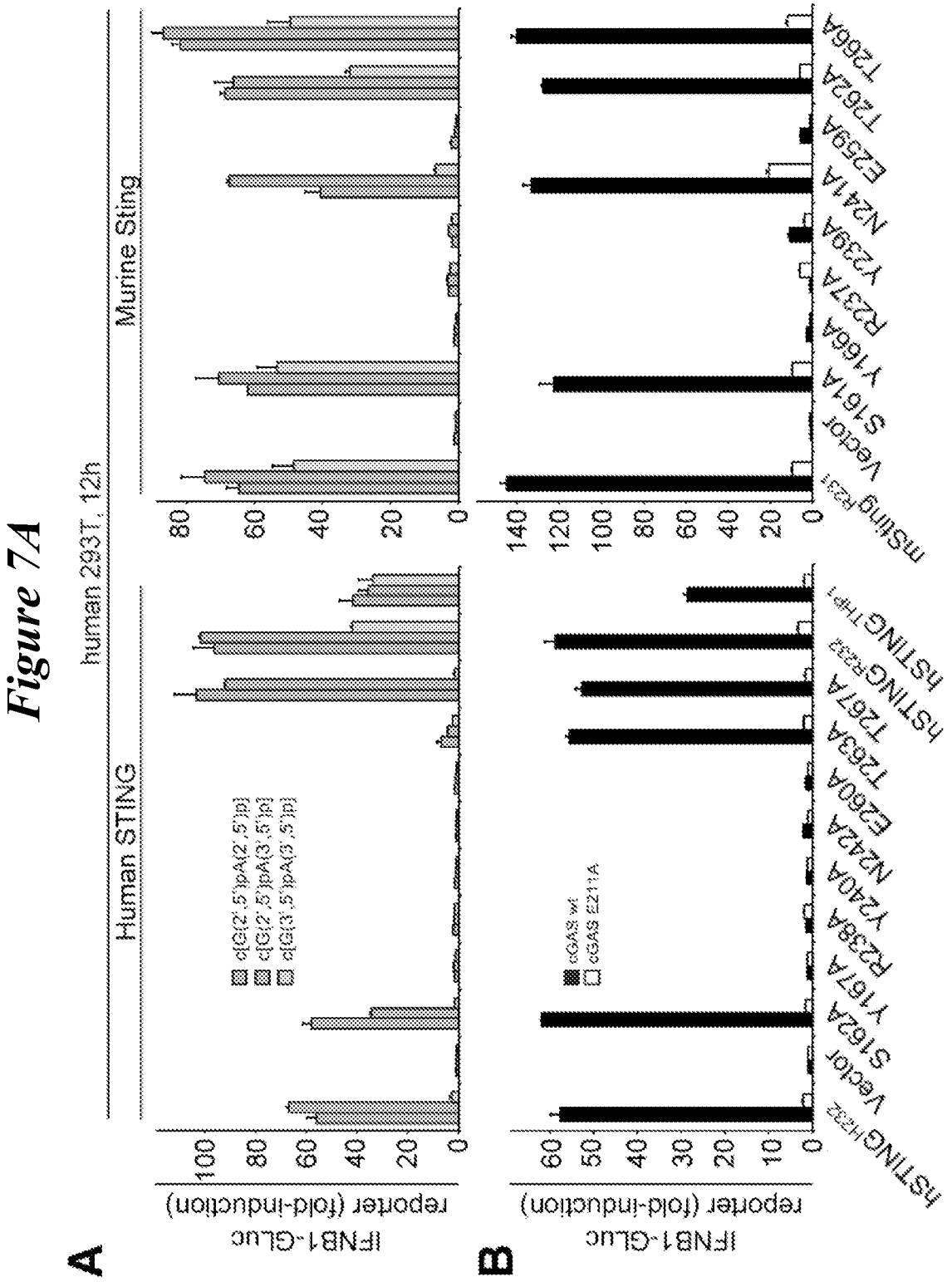


Figure 7A

Figure 7B

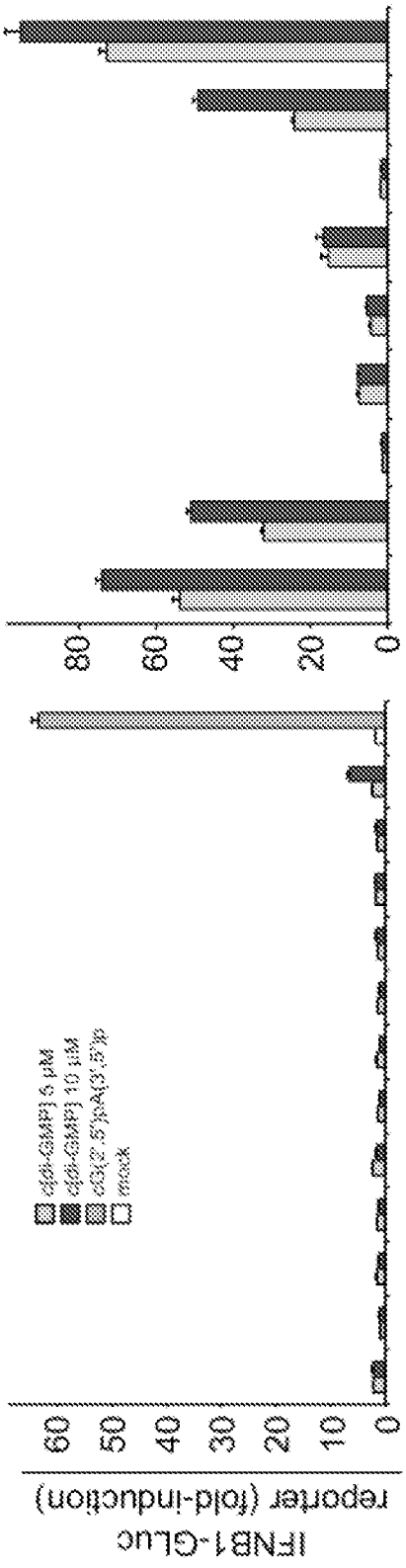


Figure 7C

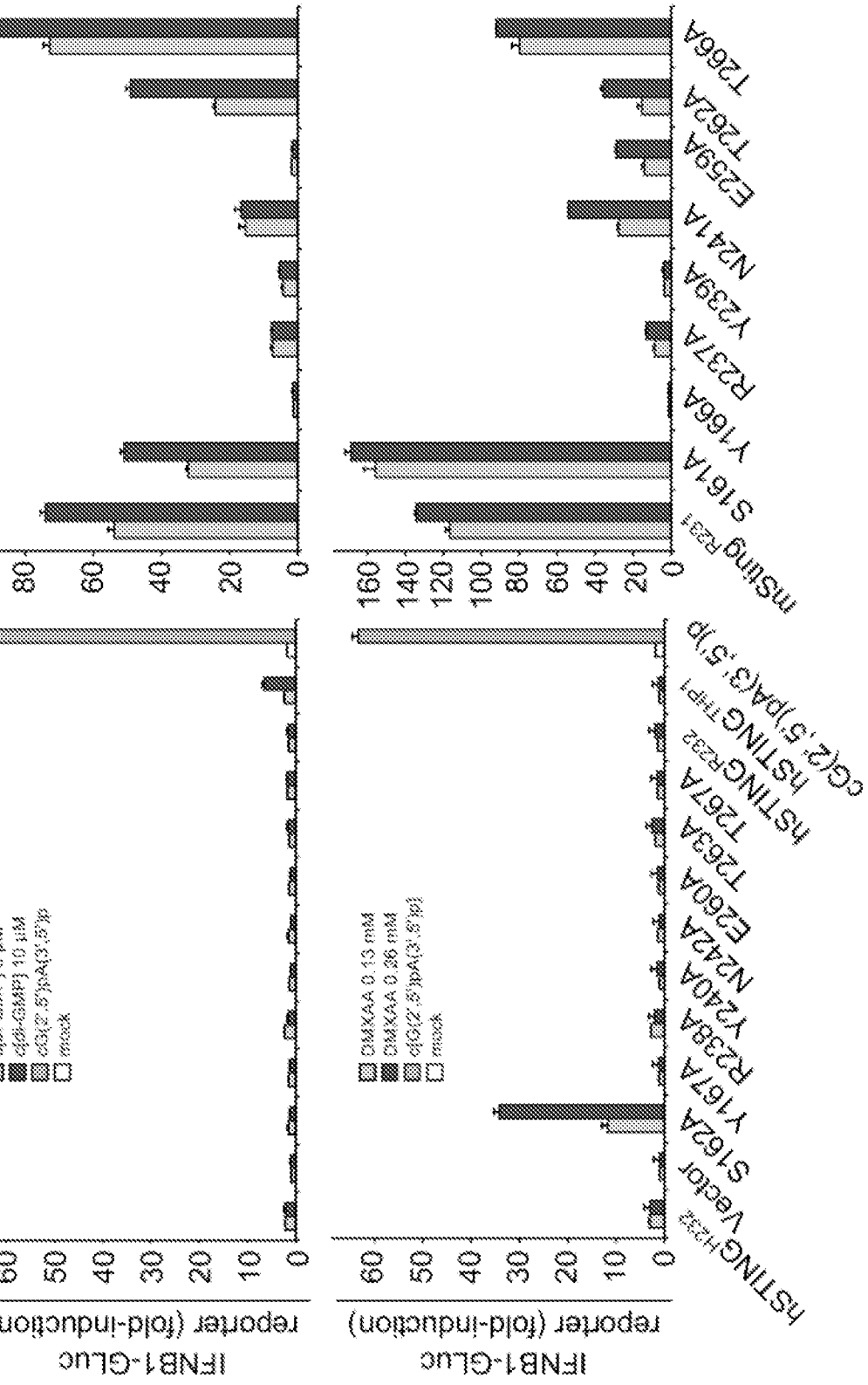


Figure 7D

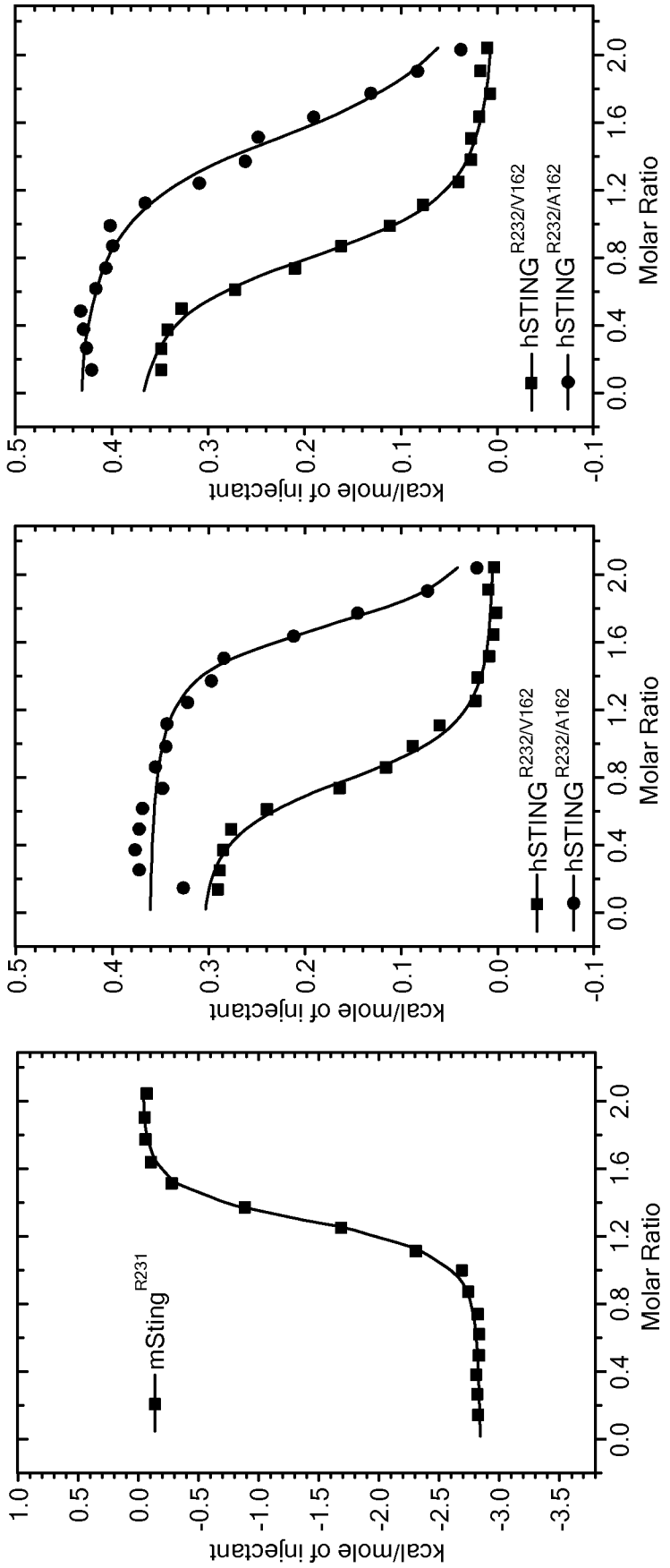


Figure 7E *Figure 7F* *Figure 7G*

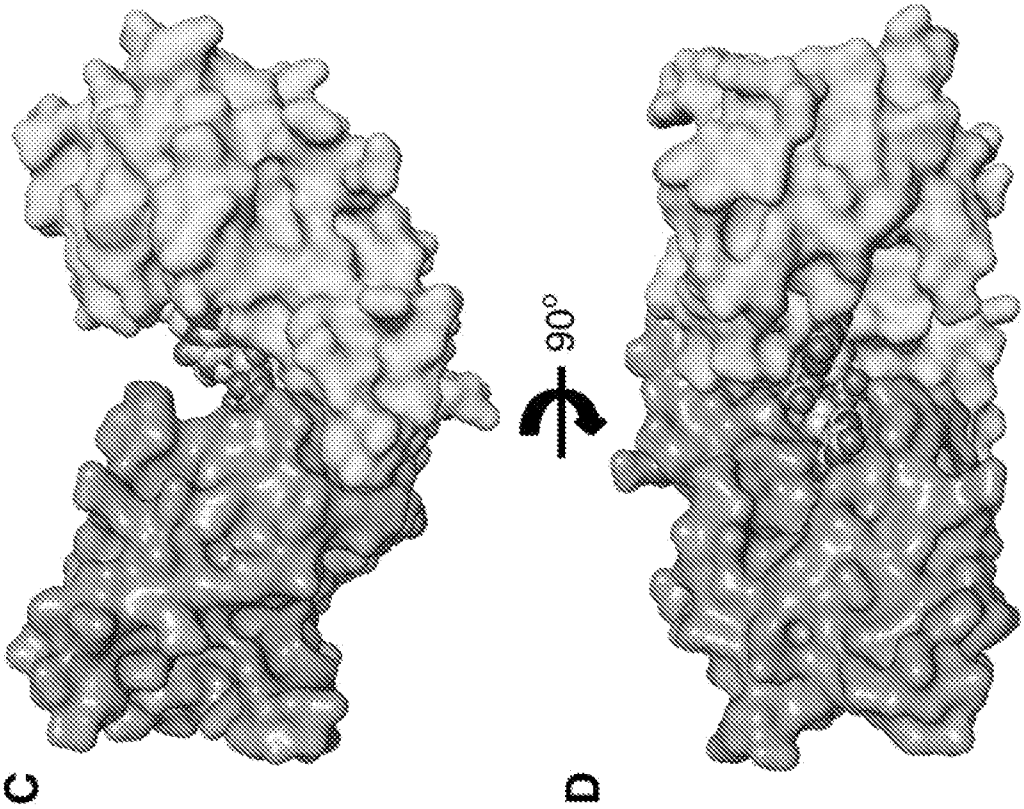


Figure 8C

Figure 8D

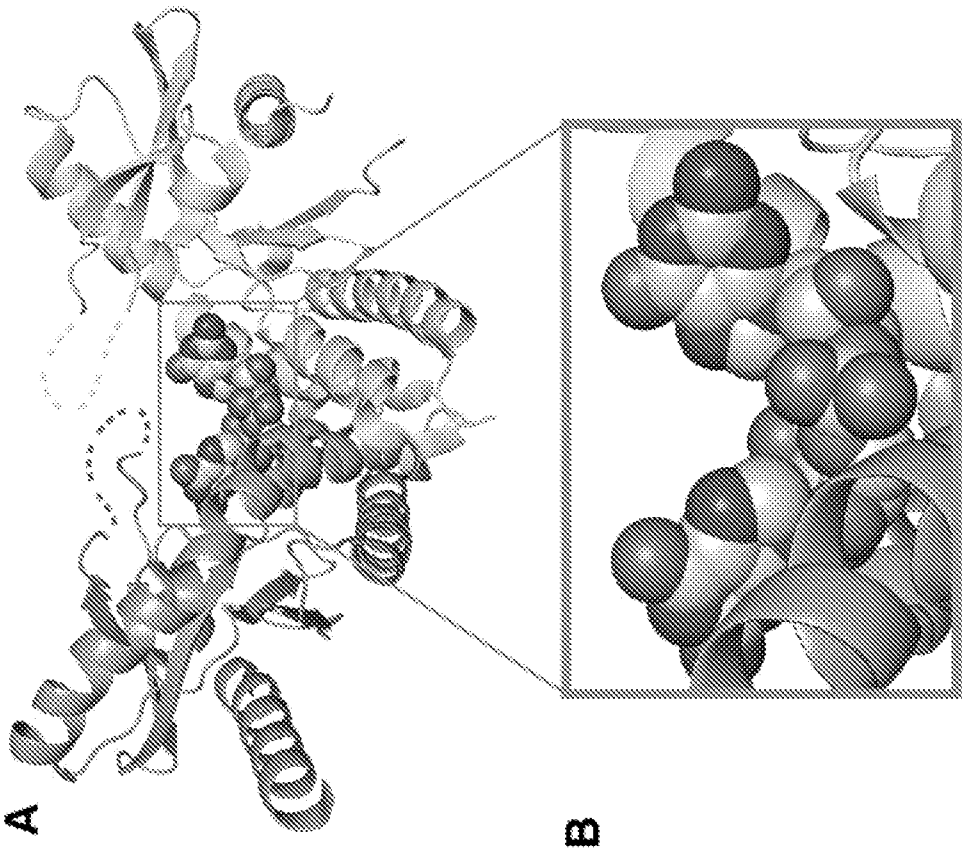


Figure 8A

Figure 8B

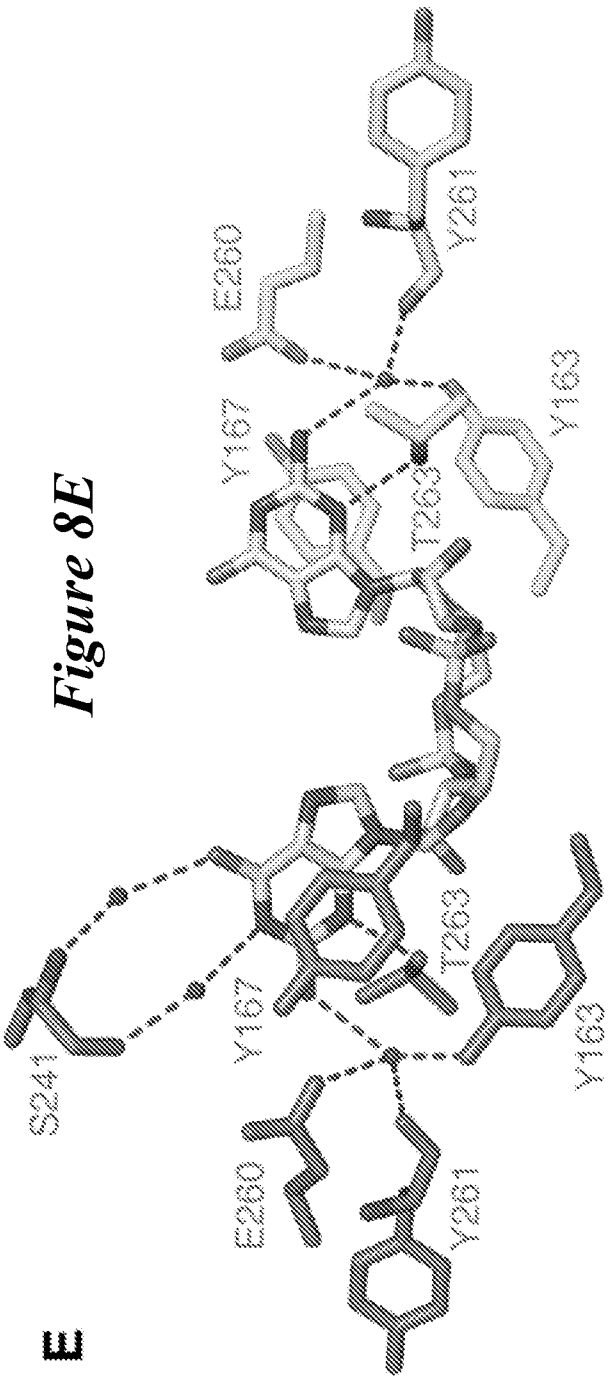


Figure 8E

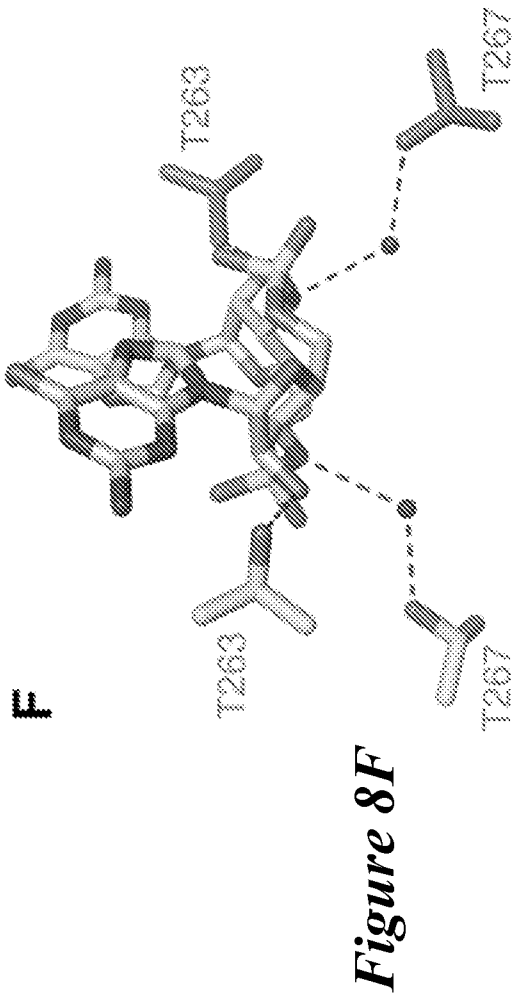


Figure 8F

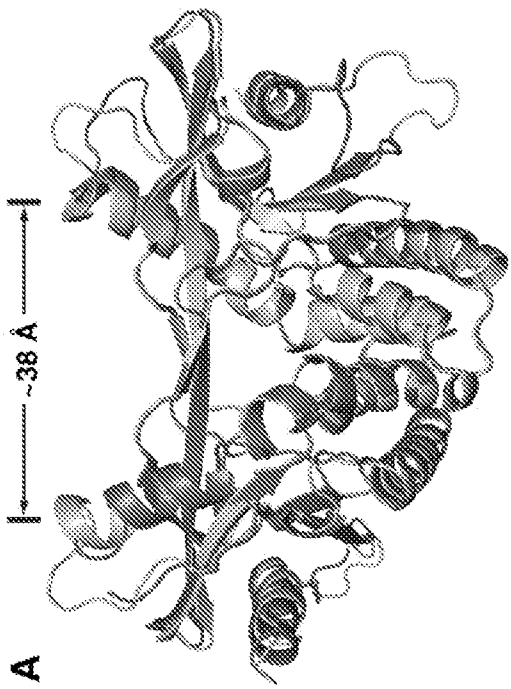


Figure 9A

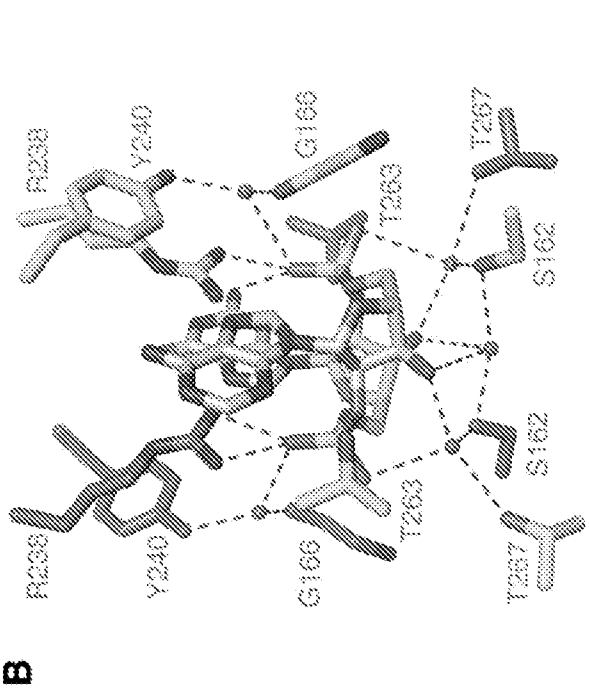


Figure 9B

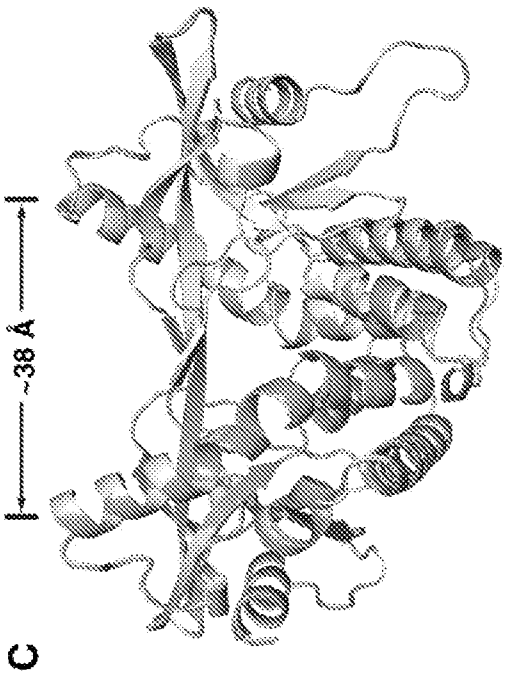


Figure 9C

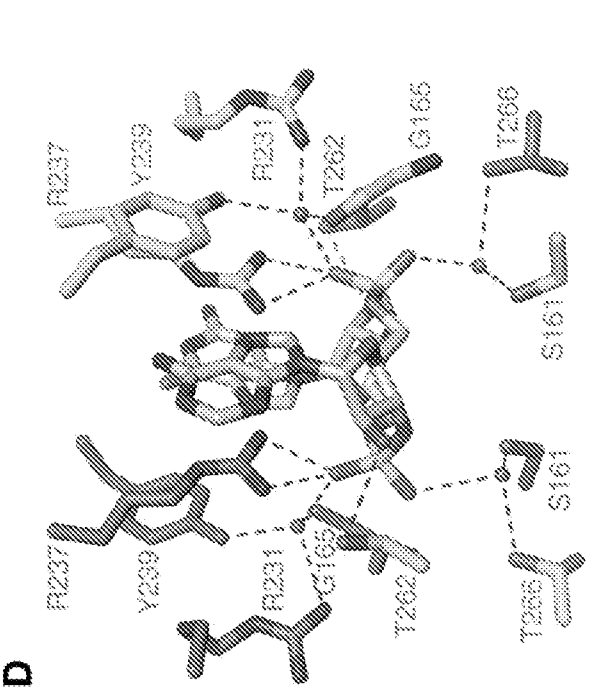


Figure 9D

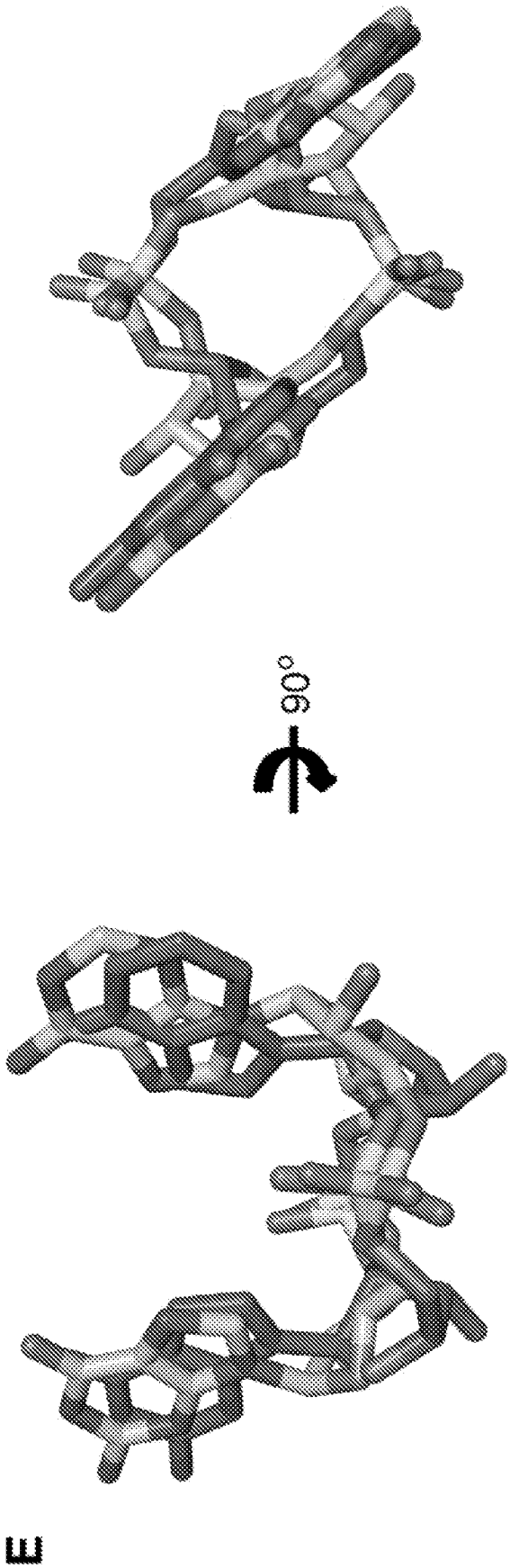


Figure 9E

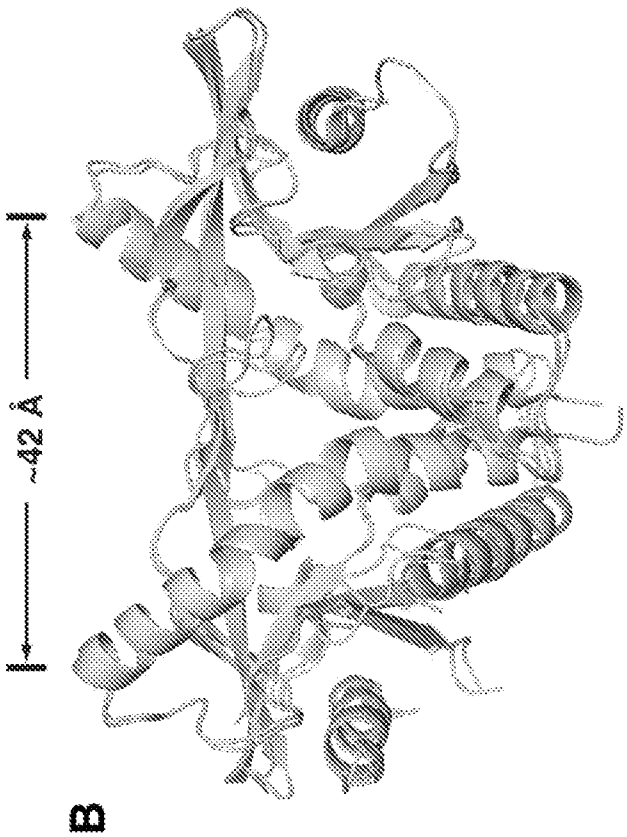


Figure 10B

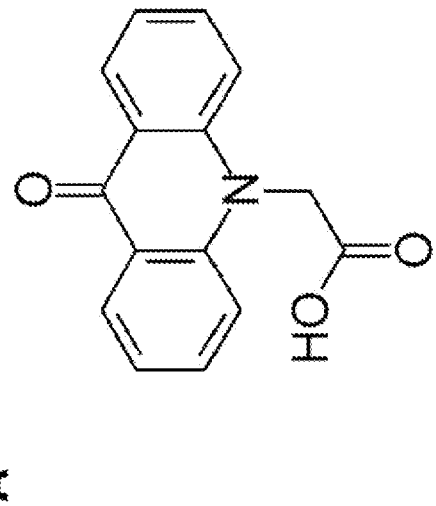


Figure 10A

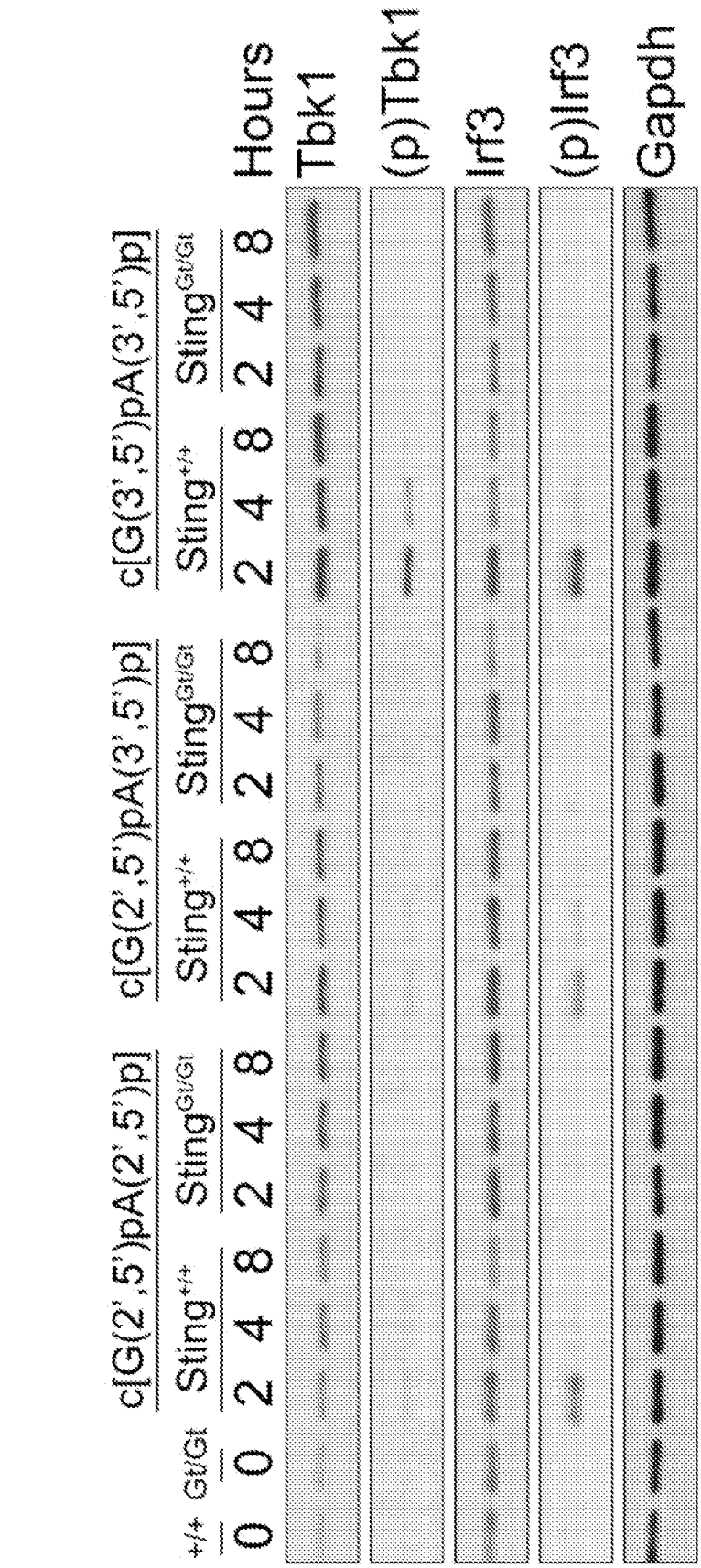

c[G(2',5')pA(2',5')p]
c[G(2',5')pA(3',5')p]
c[G(3',5')pA(3',5')p]
+/+ Gt/Gt Sting+/+ StingGt/Gt Sting+/+ StingGt/Gt Sting+/+ StingGt/Gt
0 0 2 4 8 2 4 8 2 4 8 2 4 8 2 4 8 2 4 8 Hours
Tbk1
(p)Tbk1
Irf3
(p)Irf3
Gapdh

Figure 11

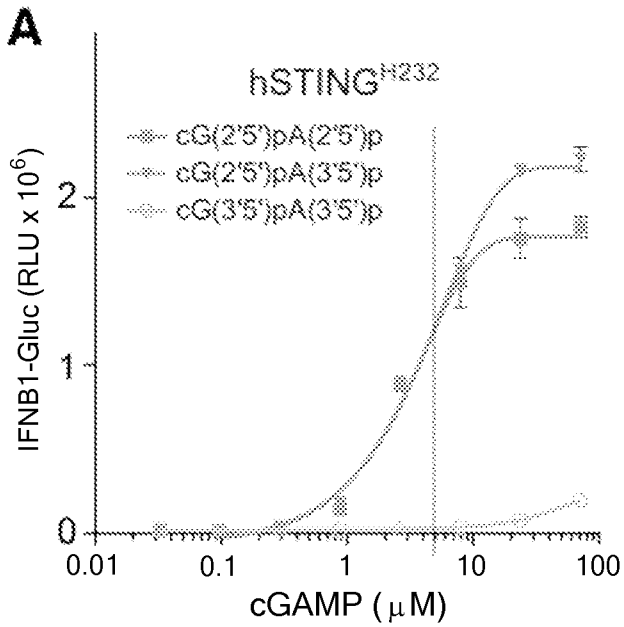


Figure 12A

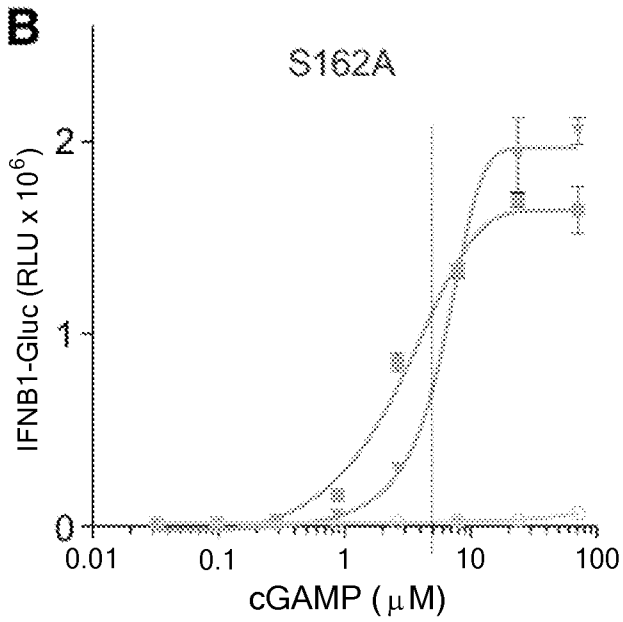


Figure 12B

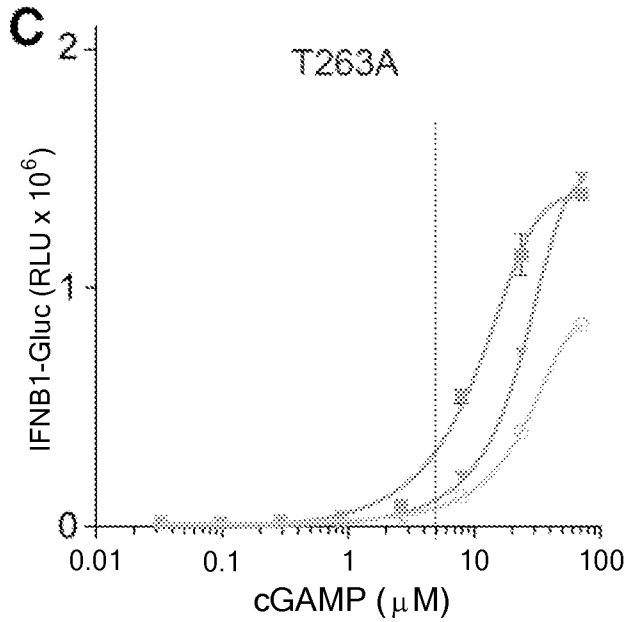


Figure 12C

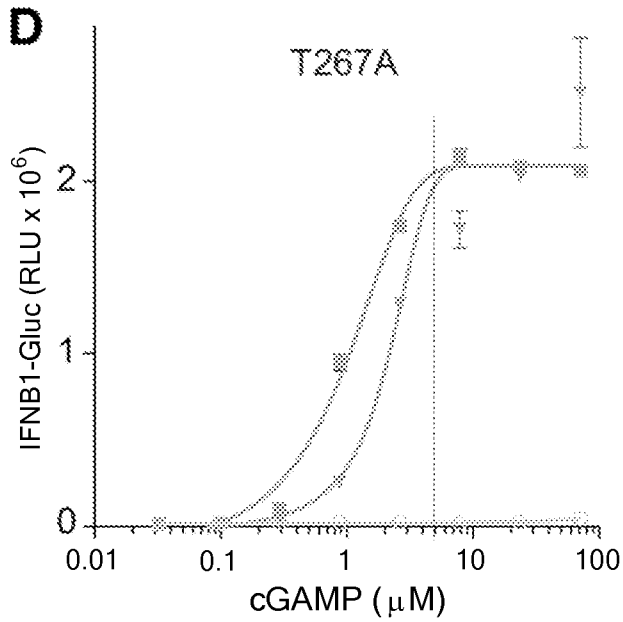


Figure 12D

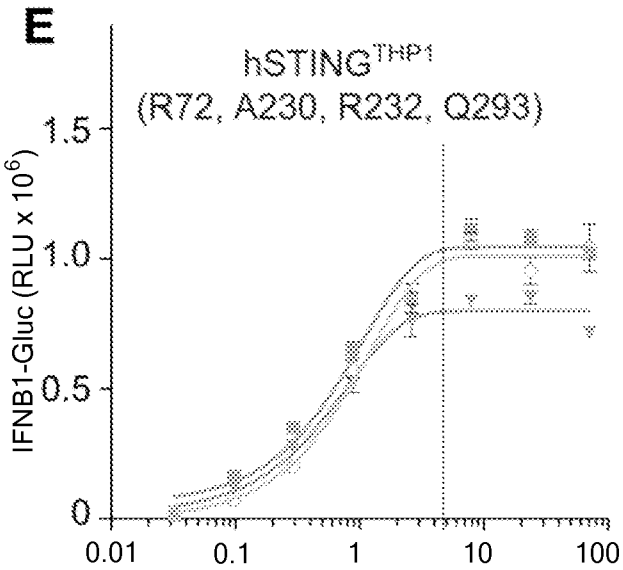


Figure 12E

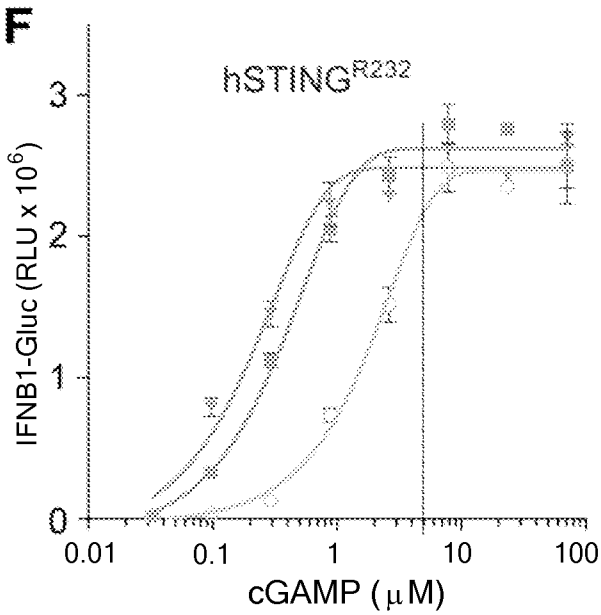


Figure 12F

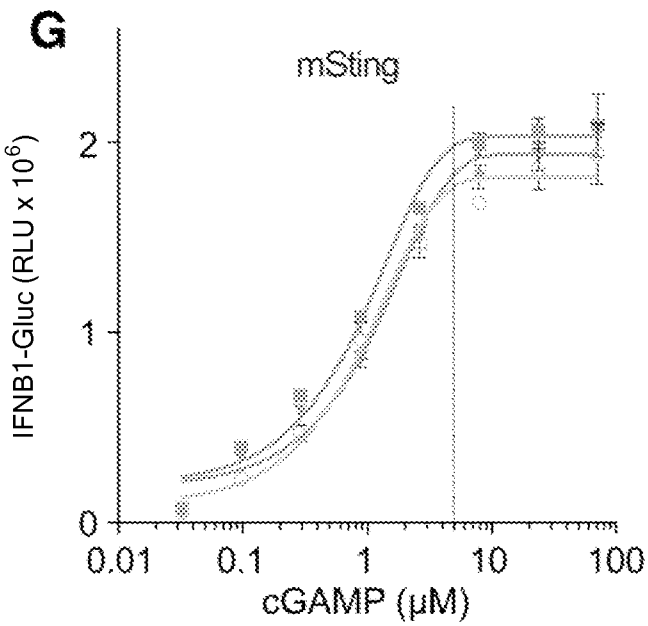


Figure 12G

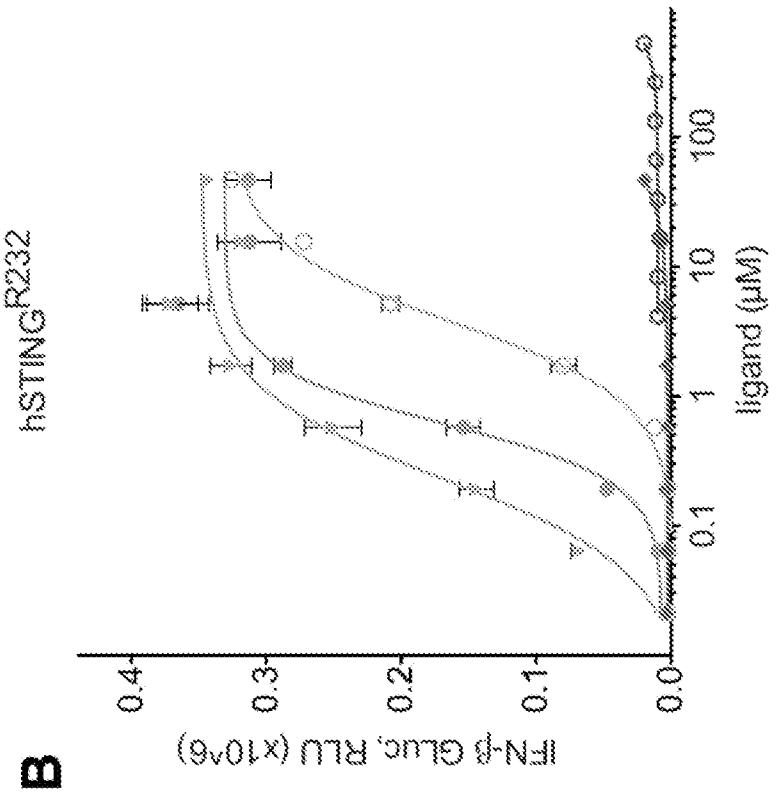


Figure 13B

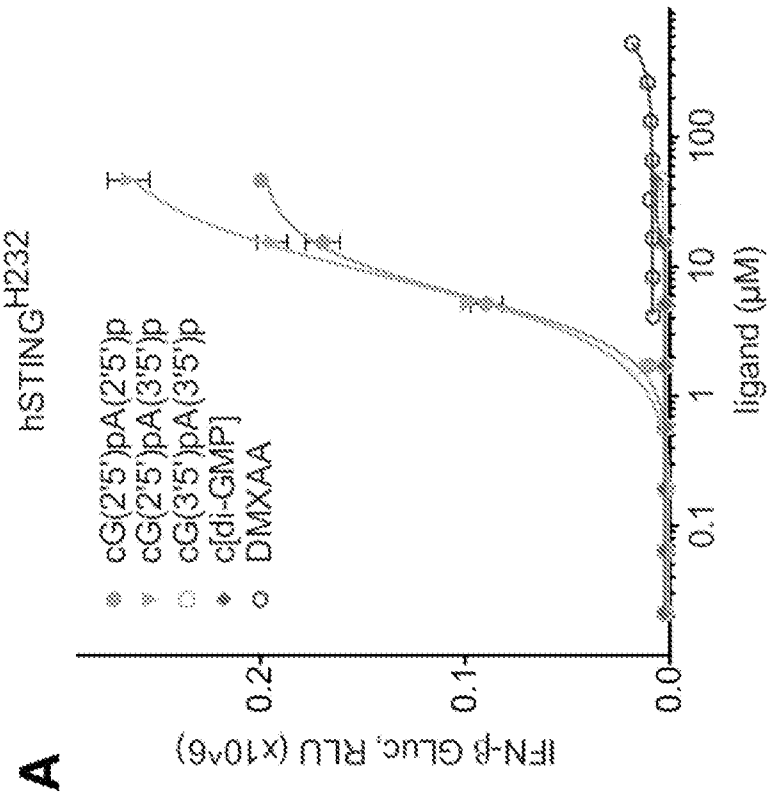


Figure 13A

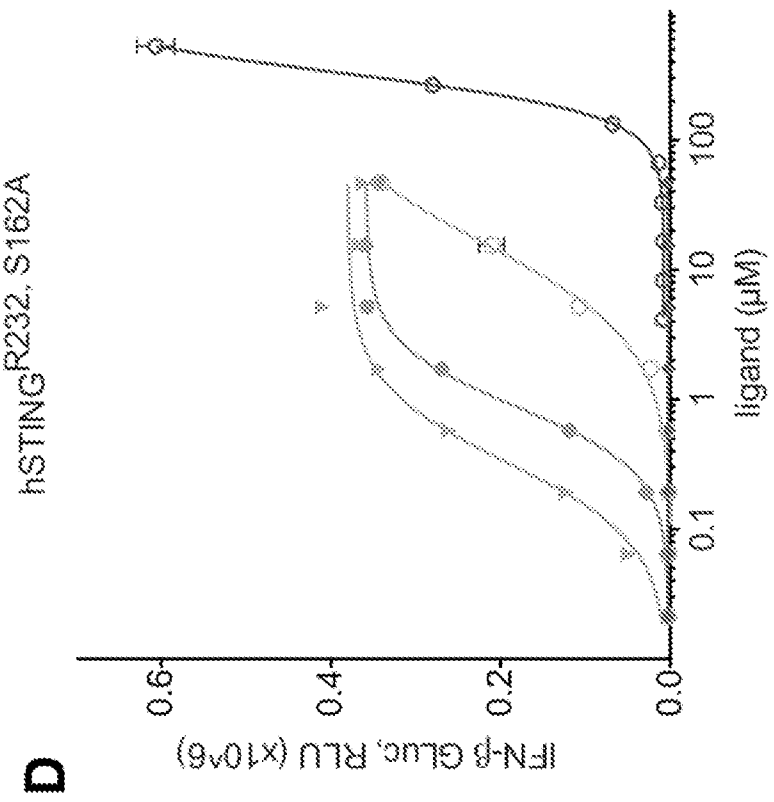


Figure 13D

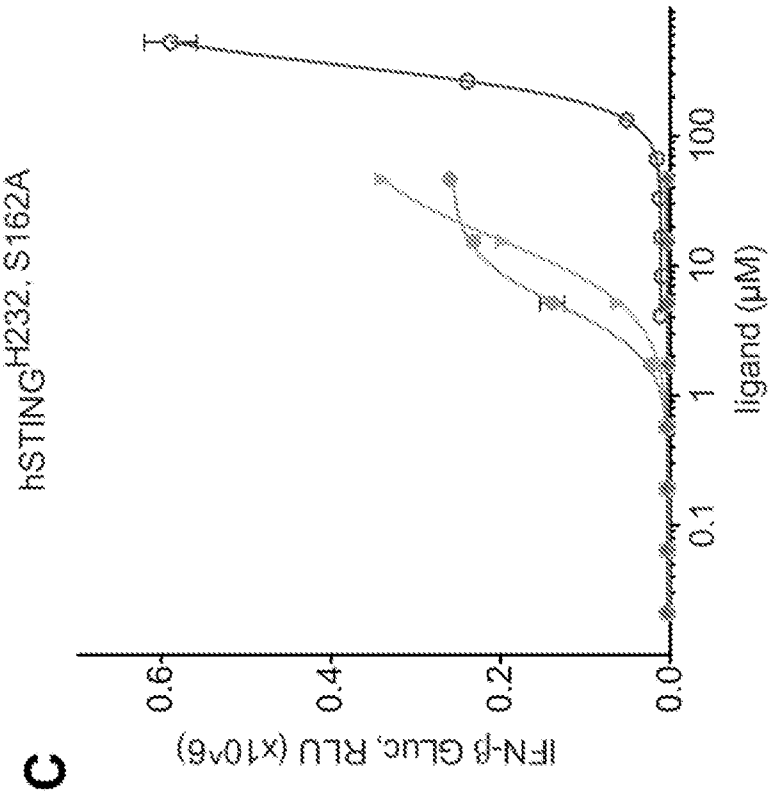


Figure 13C

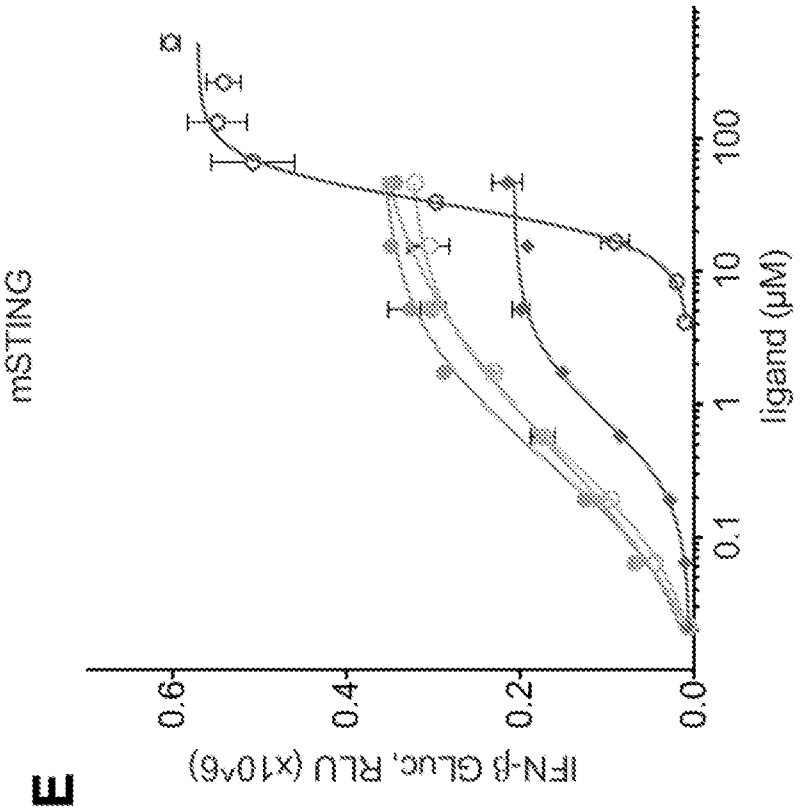


Figure 13E

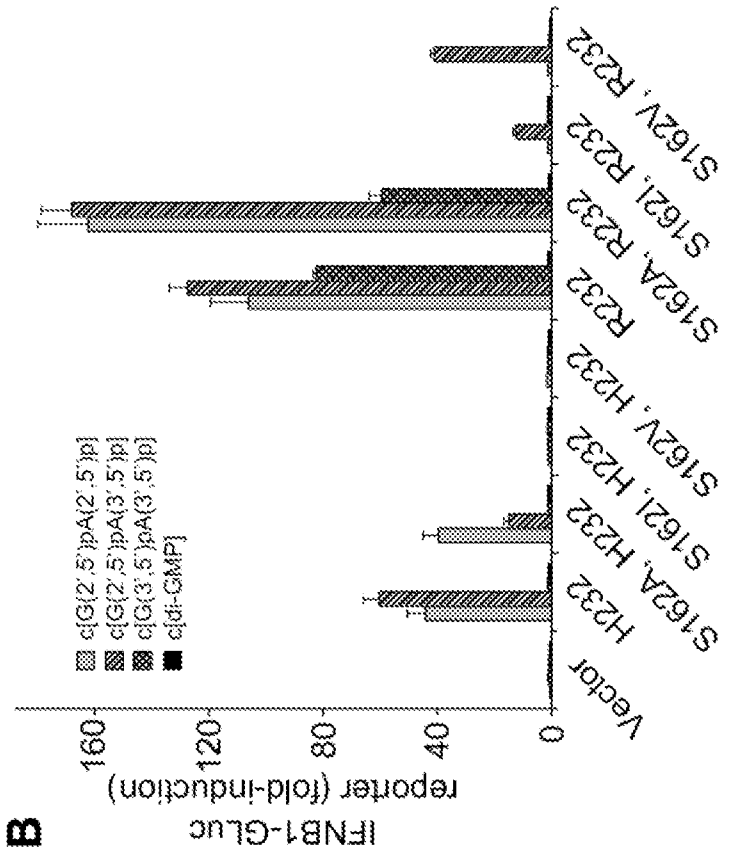


Figure 14B

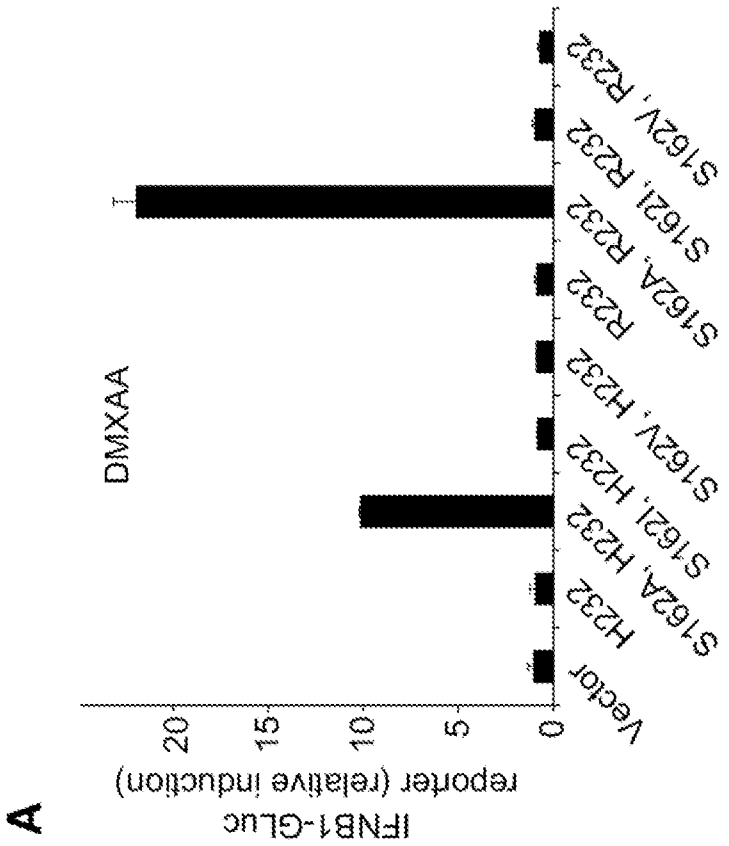


Figure 14A

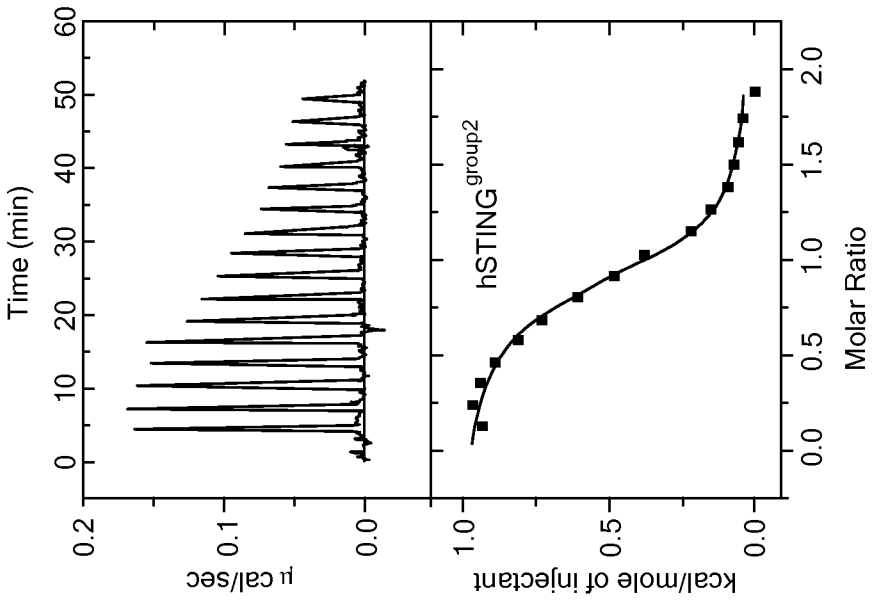


Figure 15C

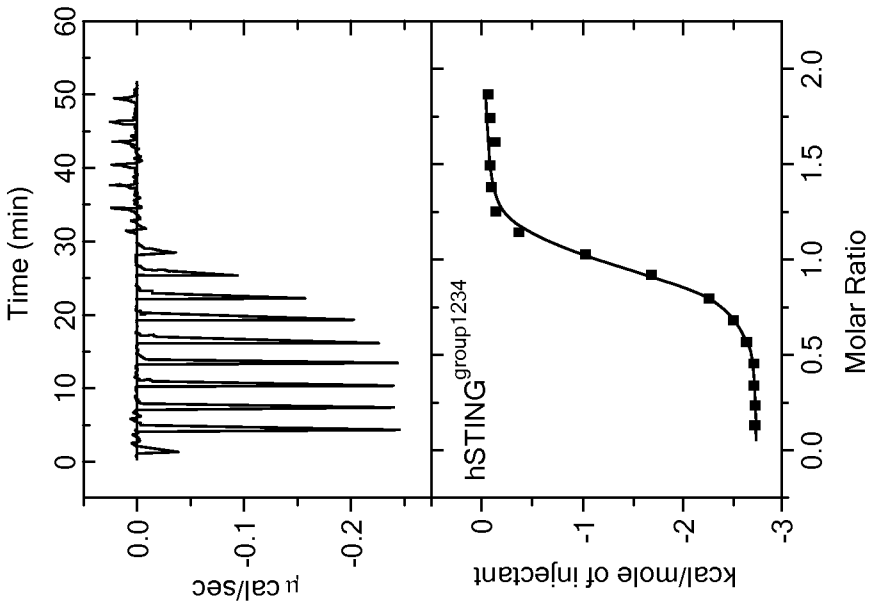


Figure 15B

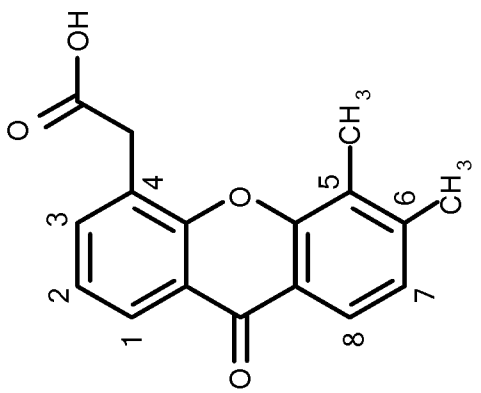


Figure 15A

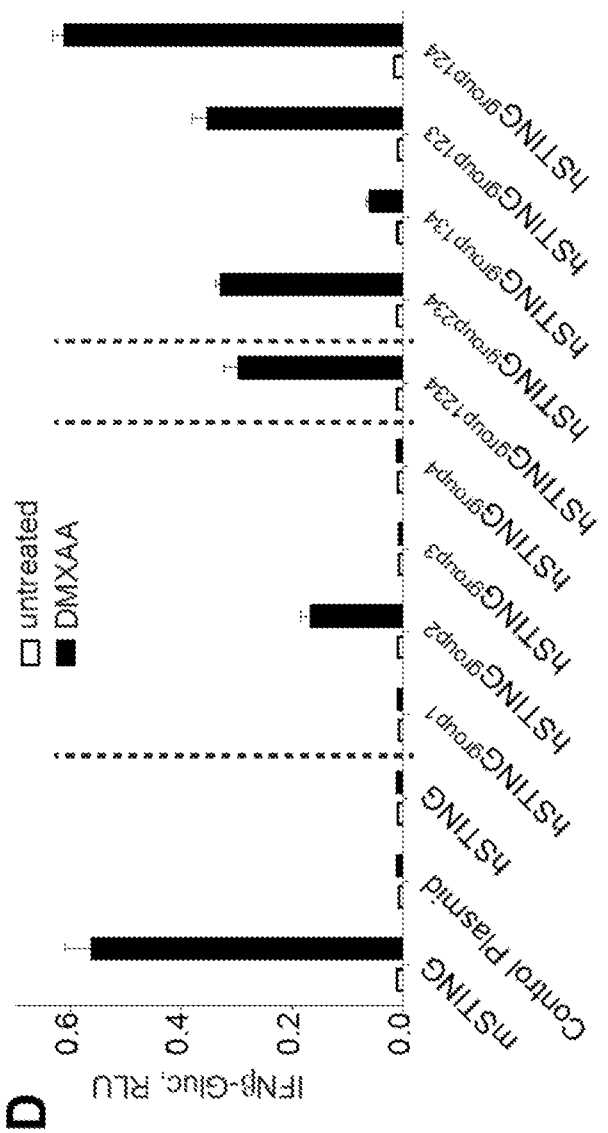


Figure 15D

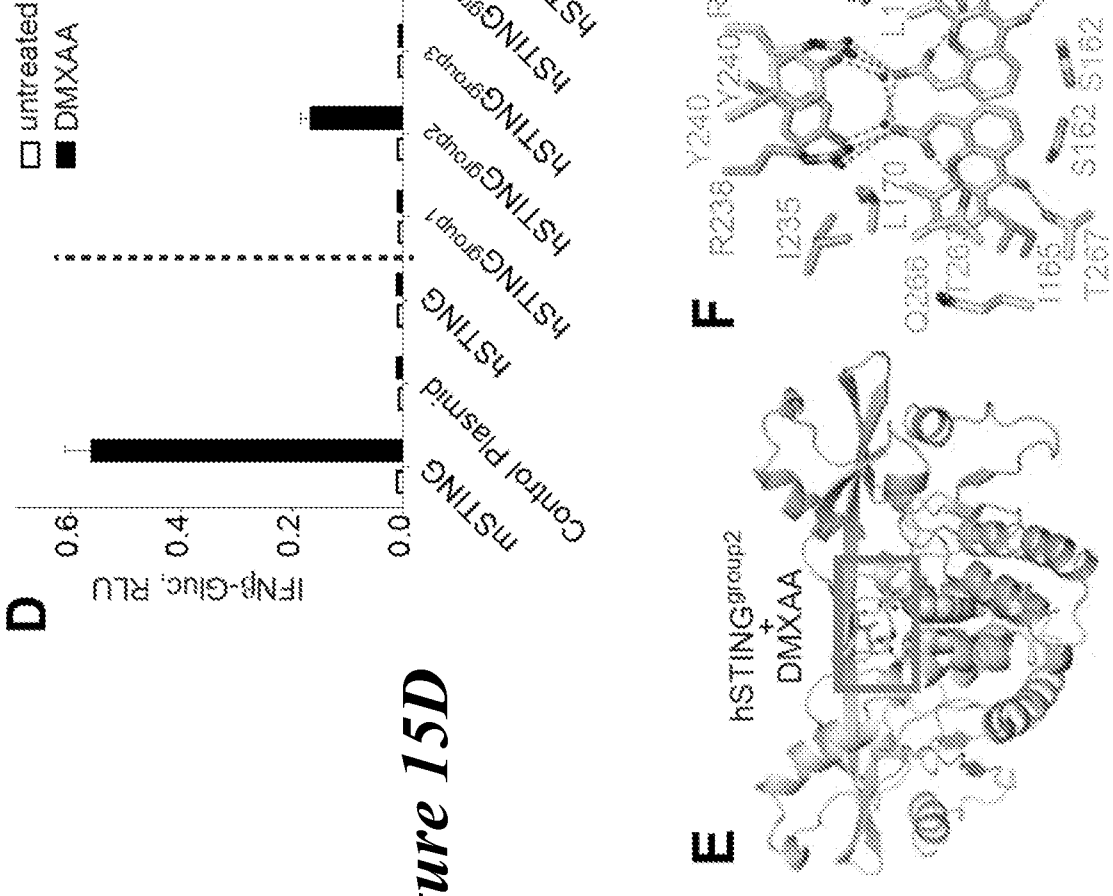


Figure 15E

Figure 15F

Figure 15G

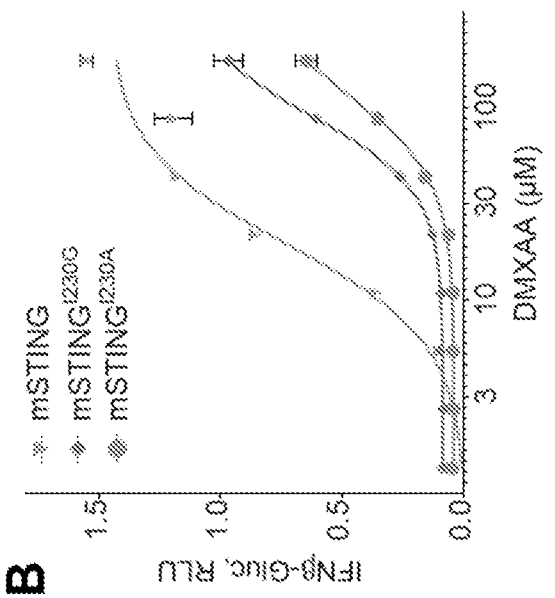


Figure 16A

Figure 16B

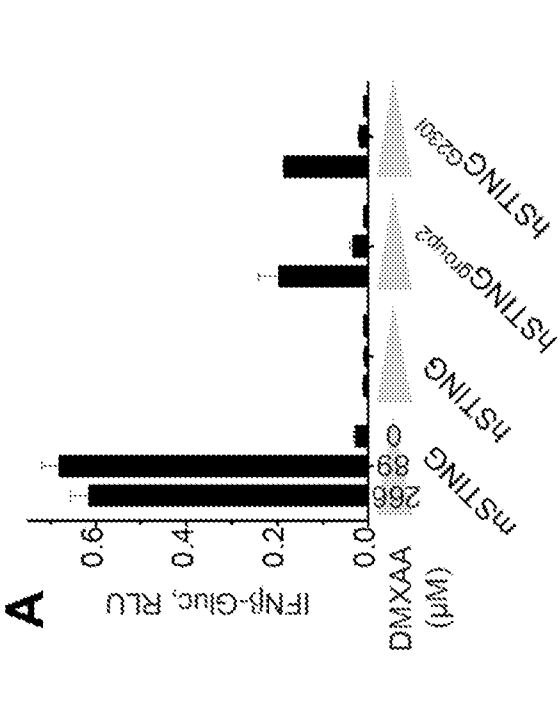


Figure 16C

Figure 16D

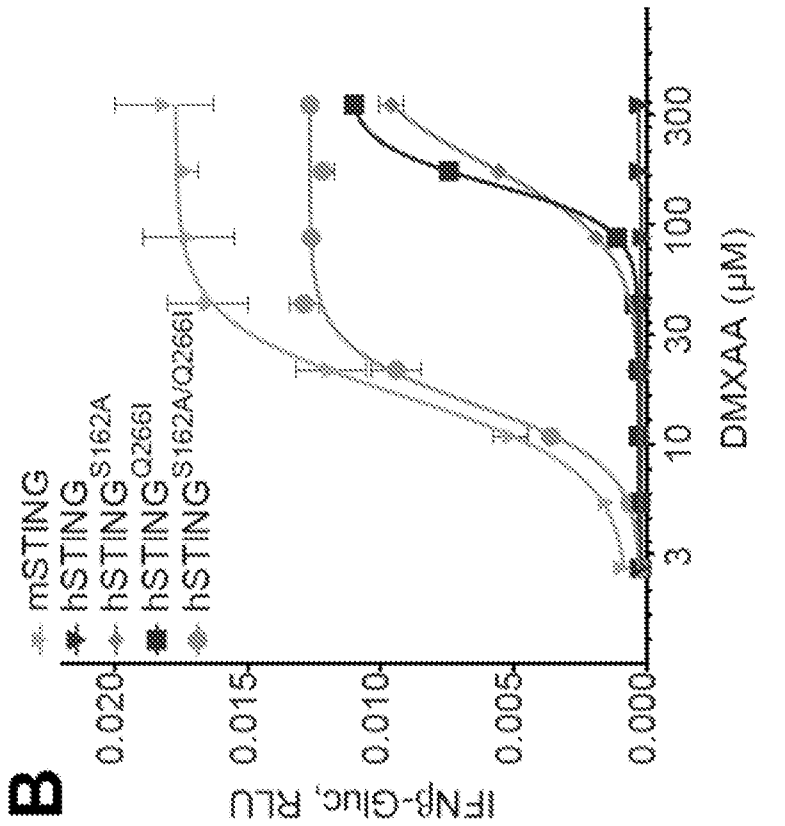


Figure 17B

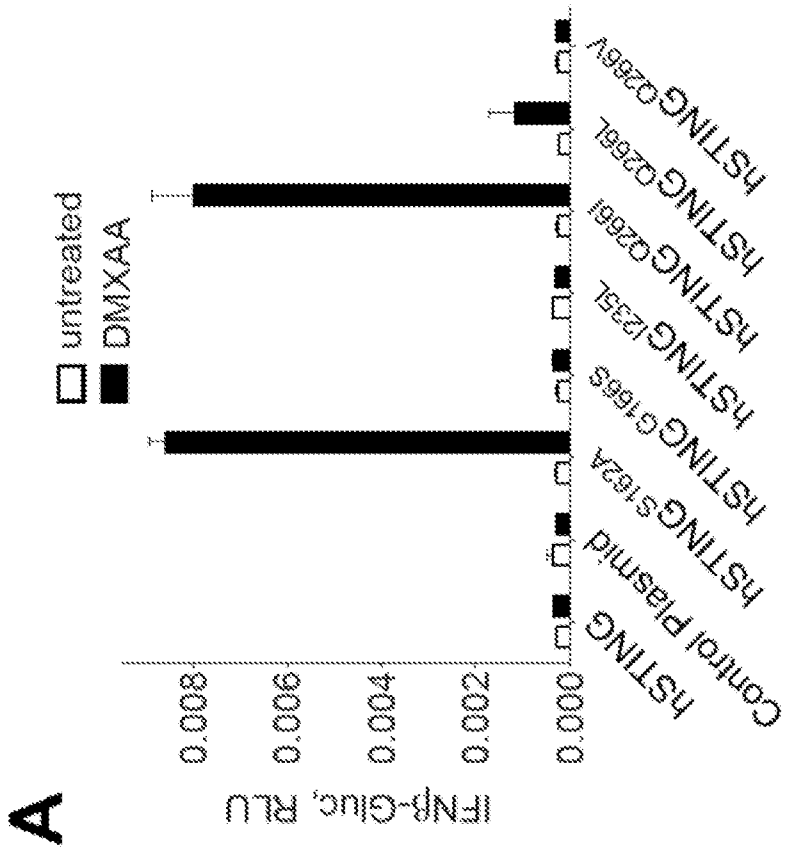


Figure 17A

hSTING Variants	Residue Positions			
	71	230	232	293
R232	R	G	R	R
HAQ	H	A	R	Q
H232	R	G	H	R
AQ	R	A	R	Q
Q293	R	G	R	Q

Figure 17D

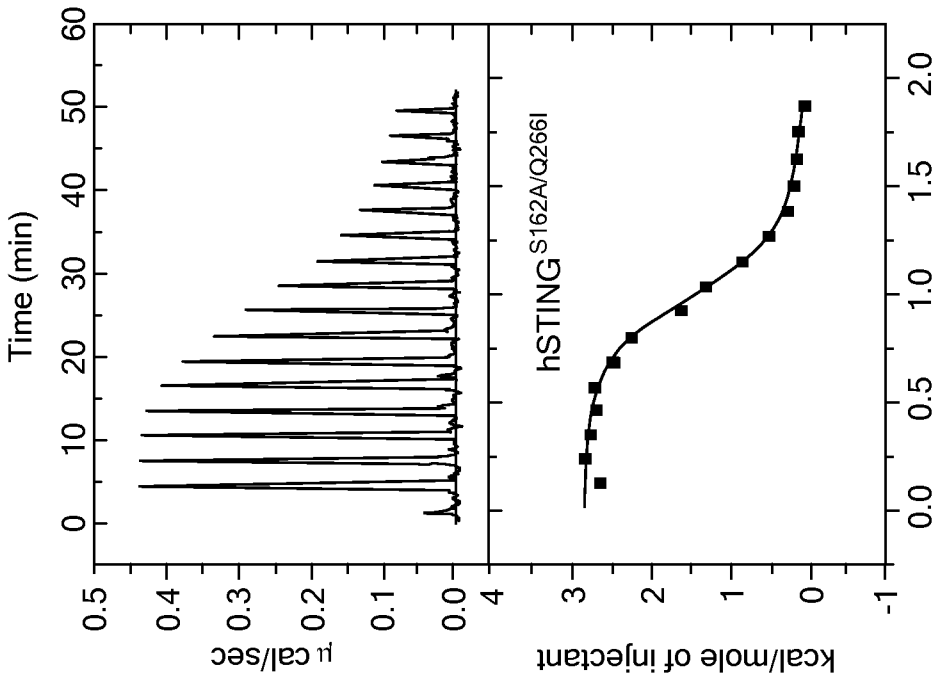


Figure 17C

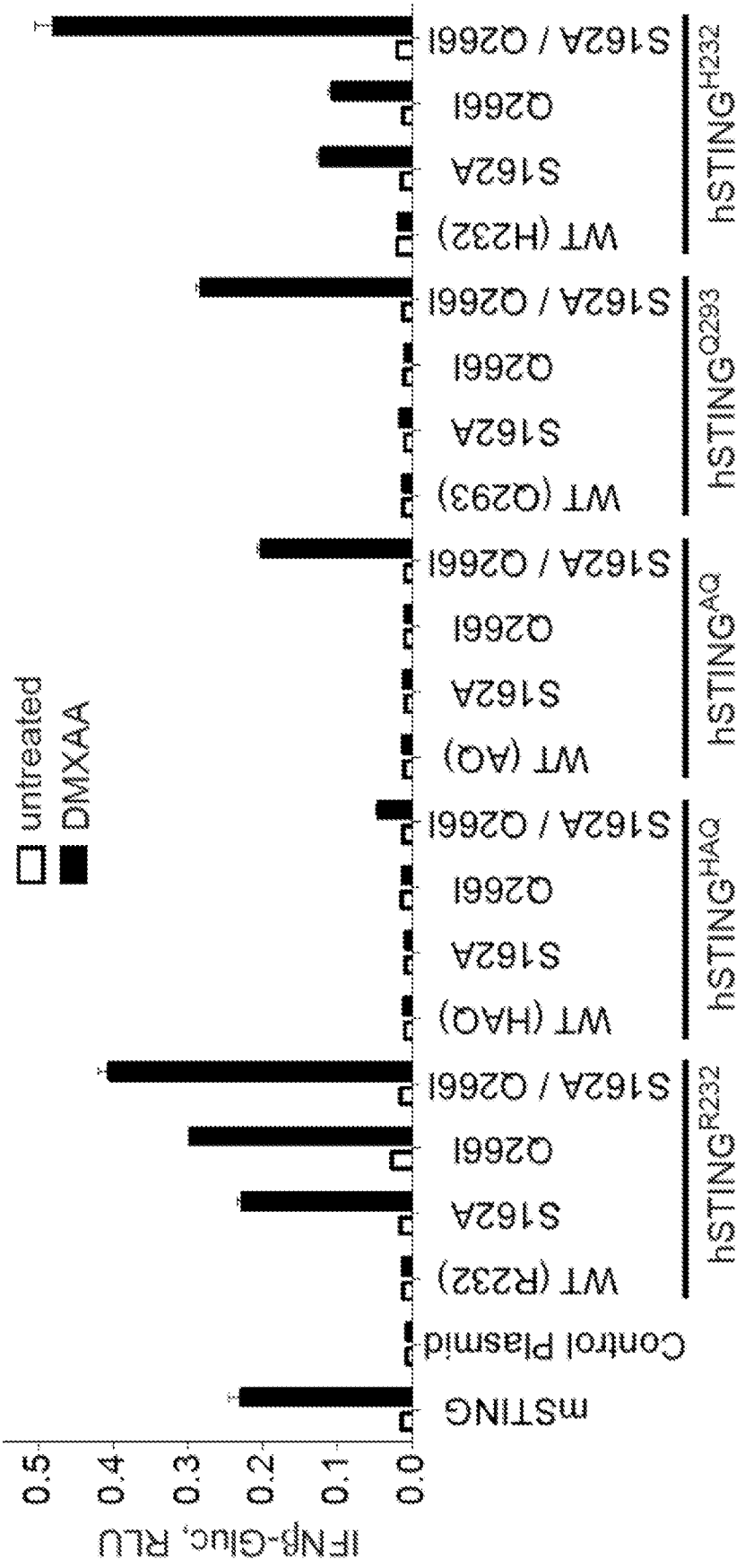

IFNβ-Gluc, RLU
0.0
0.1
0.2
0.3
0.4
0.5
untreated
DMXAA
mSTING
Control Plasmid
hSTING^R232
WT (R232)
S162A
Q266I
S162A / Q266I
hSTING^HAQ
WT (HAQ)
S162A
Q266I
S162A / Q266I
hSTING^AQ
WT (AQ)
S162A
Q266I
S162A / Q266I
hSTING^Q293
WT (Q293)
S162A
Q266I
S162A / Q266I
hSTING^H232
WT (H232)
S162A
Q266I
S162A / Q266I

Figure 17E

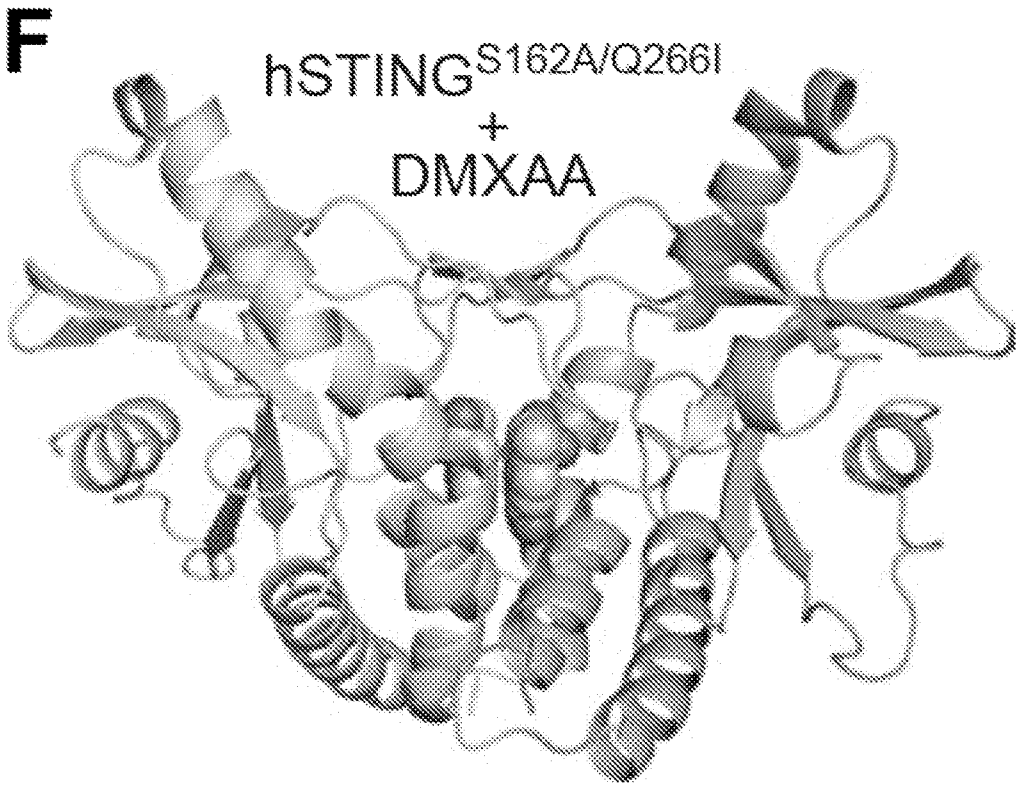


Figure 17F

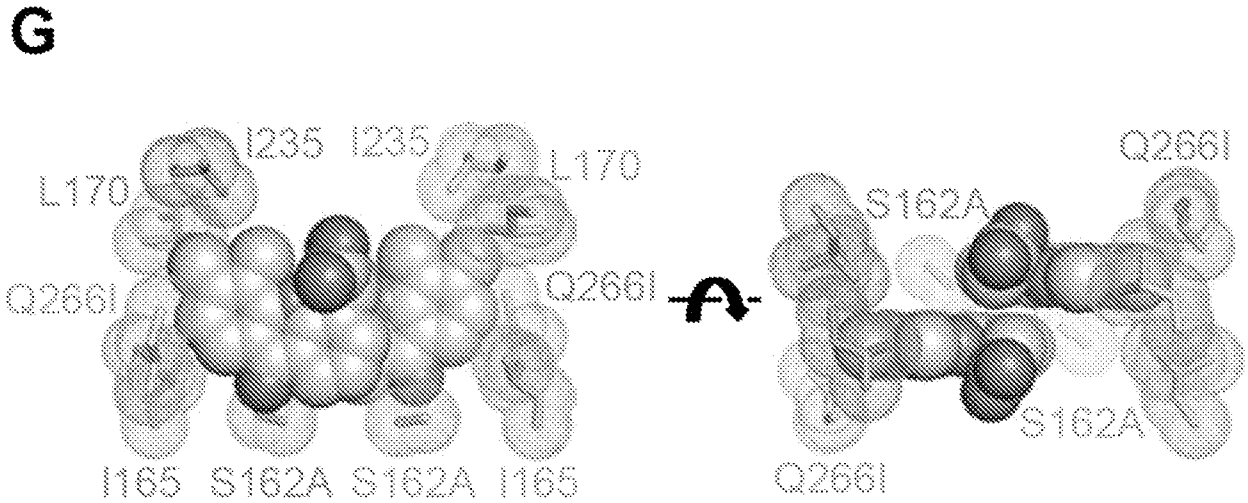


Figure 17G

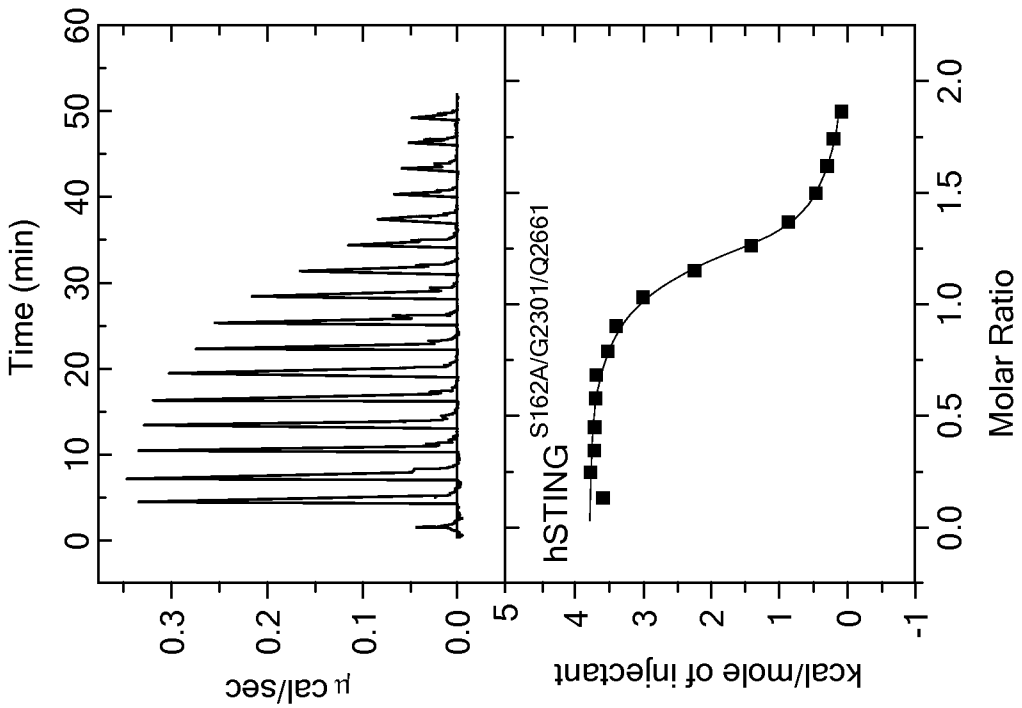


Figure 18A

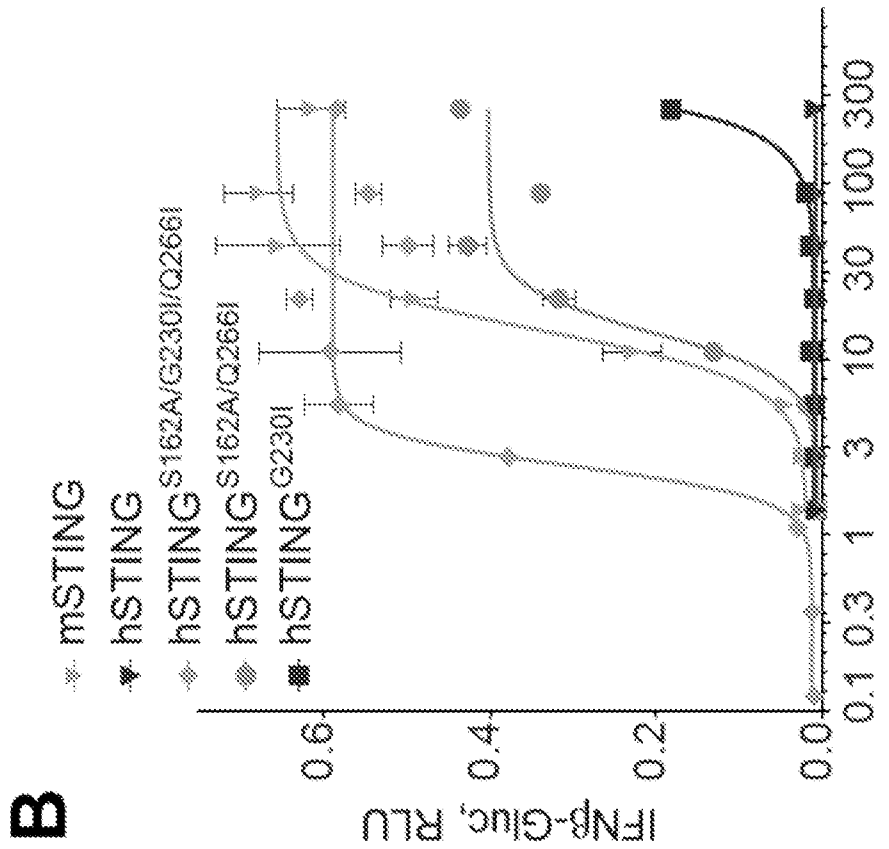


Figure 18B

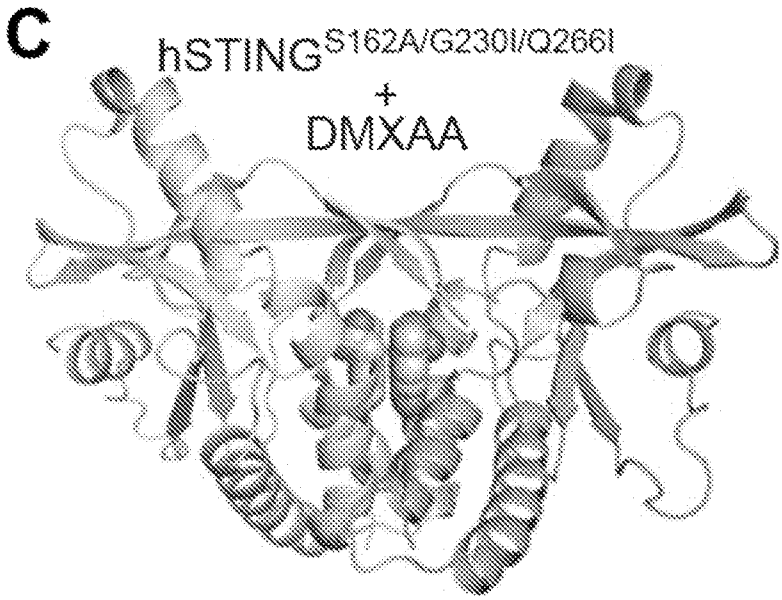


Figure 18C

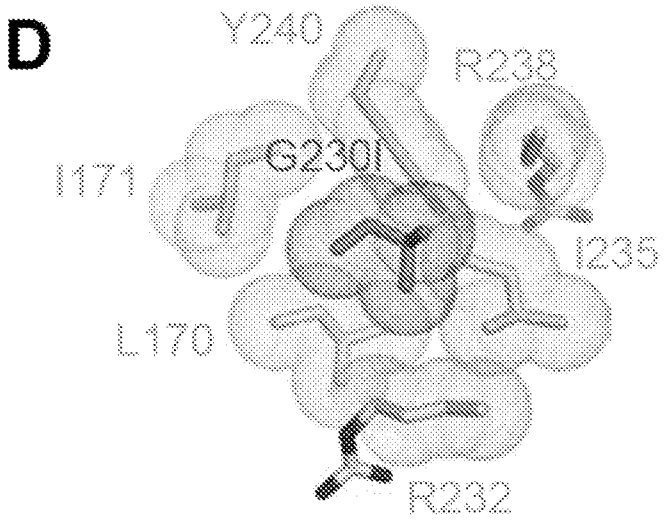


Figure 18D

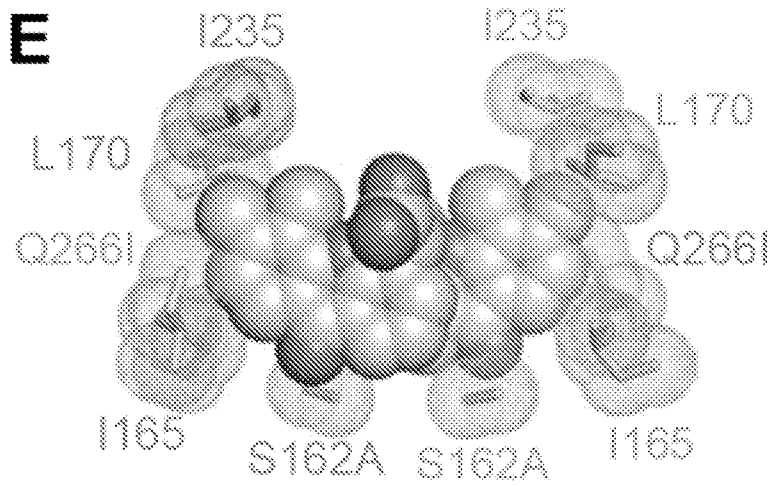


Figure 18E

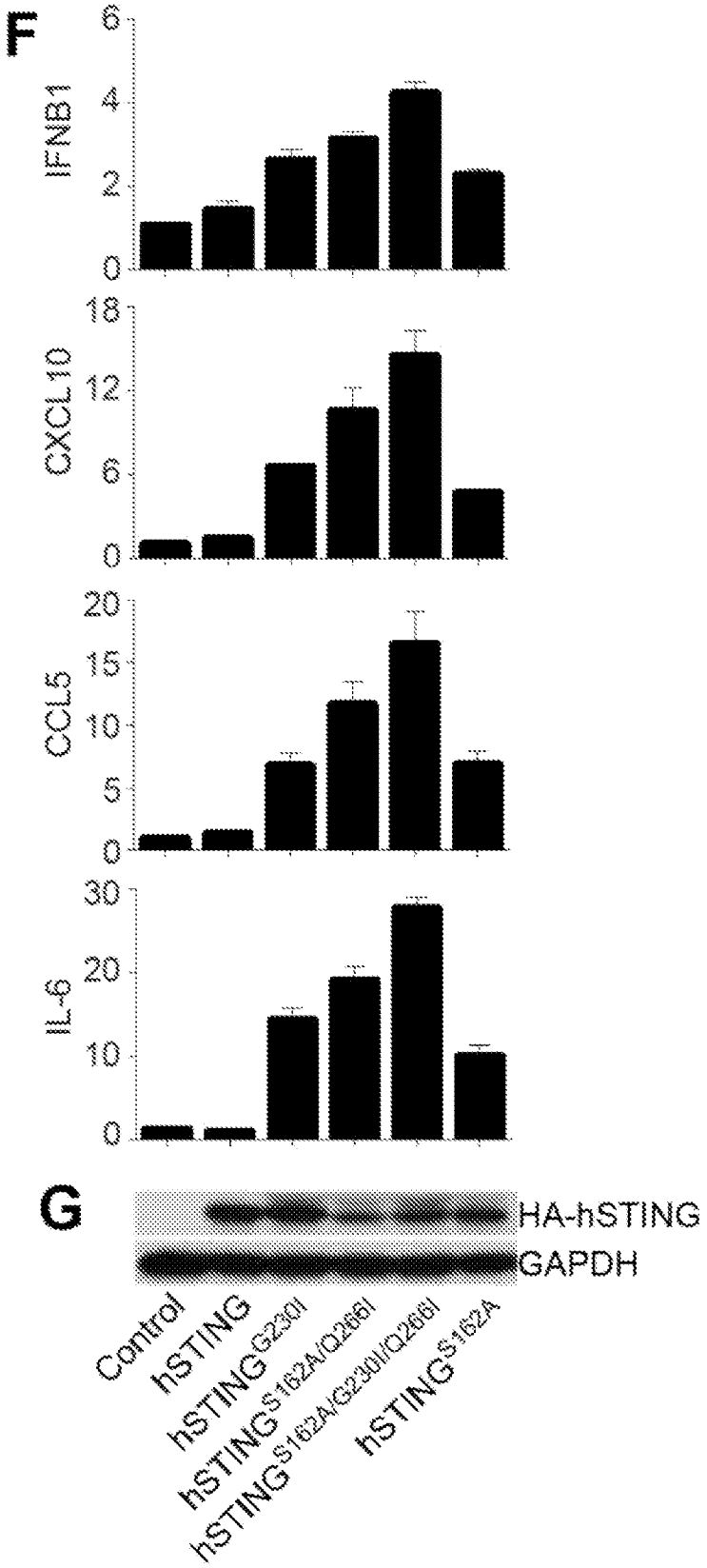


Figure 18F

Figure 18G


hSTING MPRSSLRPSIPCPRGHGAQKAALVLLSACLVTLWGLGEPPEHTLRYLVLHLASLQLGLLL 60
mSTING MPYSNLHDAIPRPRGHRSKYVALTFLVASLMILPVAKDPPNETLRYLALHLASHELGLLL 60
hSTING NGVCSLAEELRHIHSRYRGSYWRTVRACLGCPLRRGALLLLSIYFYYSLPNAVGPPFTWM 120
mSTING KNLCCLAEELCHVQSRYQGSYWKAVRACLGCPIRCHAMILLSSYFYF-LQNTADIYLSWM 119
S162
G166
hSTING LALLGLSQAINTLLGLKGLAPAEISAVCEKGNFNVAHGLAWSYYIGYLRLILPELQARIR 180
mSTING PGLLVLYRSLSMLLGLQSLTPAEVSAVCEEKKLNVAHGLAWSYYIGYLRLILPGLQARIR 179
I235
hSTING TYNQHYNNLLRGAVSQRLYILLPLDCGVPDNLSMADPNIRFLDKLPQQTGDRAGIKDRVY 240
mSTING MFNQLHNNMLSGAGSRRLYILFPLDCGVPDNLSVVDPNIRFRDMLPQQNIDRAGIKNRVY 239
Q266
hSTING SNSIYELLENGQRAGTCVLEYATPLQTLFAMSQYSQAGFSREDRLEQAKLFCRTLEDILA 300
mSTING SNSVYEILENGQPAGVCILEYATPLQTLFAMSQDAKAGFSREDRLEQAKLFCRTLEEILE 299
hSTING DAPESQNNCRLIAYQEPADDSSFSLSQEVLRHLRQEEKEEVTVGSLKTSAVPSTSTMSQE 360
mSTING DVPESRNNCRLIVYQEPTDGNSFSLSQEVLRHIRQEEKEEVTMNAPMTSVAPPPSVLSQE 359
hSTING PELLISGMEKPLPLRTDFS 379 (SEQ. ID. No. 103)
mSTING PRLLISGMDQPLPLRTDLI 378 (SEQ. ID. No. 2)
group1 (E174G / T181M / Y182F / H185L / Y186H / L189M / R191S / V194G / Q196R)
group2 (L222R / K224M / T229N / G230I / D237N / I244V)
group3 (Y274D / S275A / Q276K / D297E / A300E / A302V / Q306R)
group4 (V343M / G344N / S345A / L346P / K347M / A350V / V351A / S353P / T354P / T356V / M357L / E362R / E369D / K370Q / F378L / S379I)
Mutations in ligand-binding pocket

Figure 19

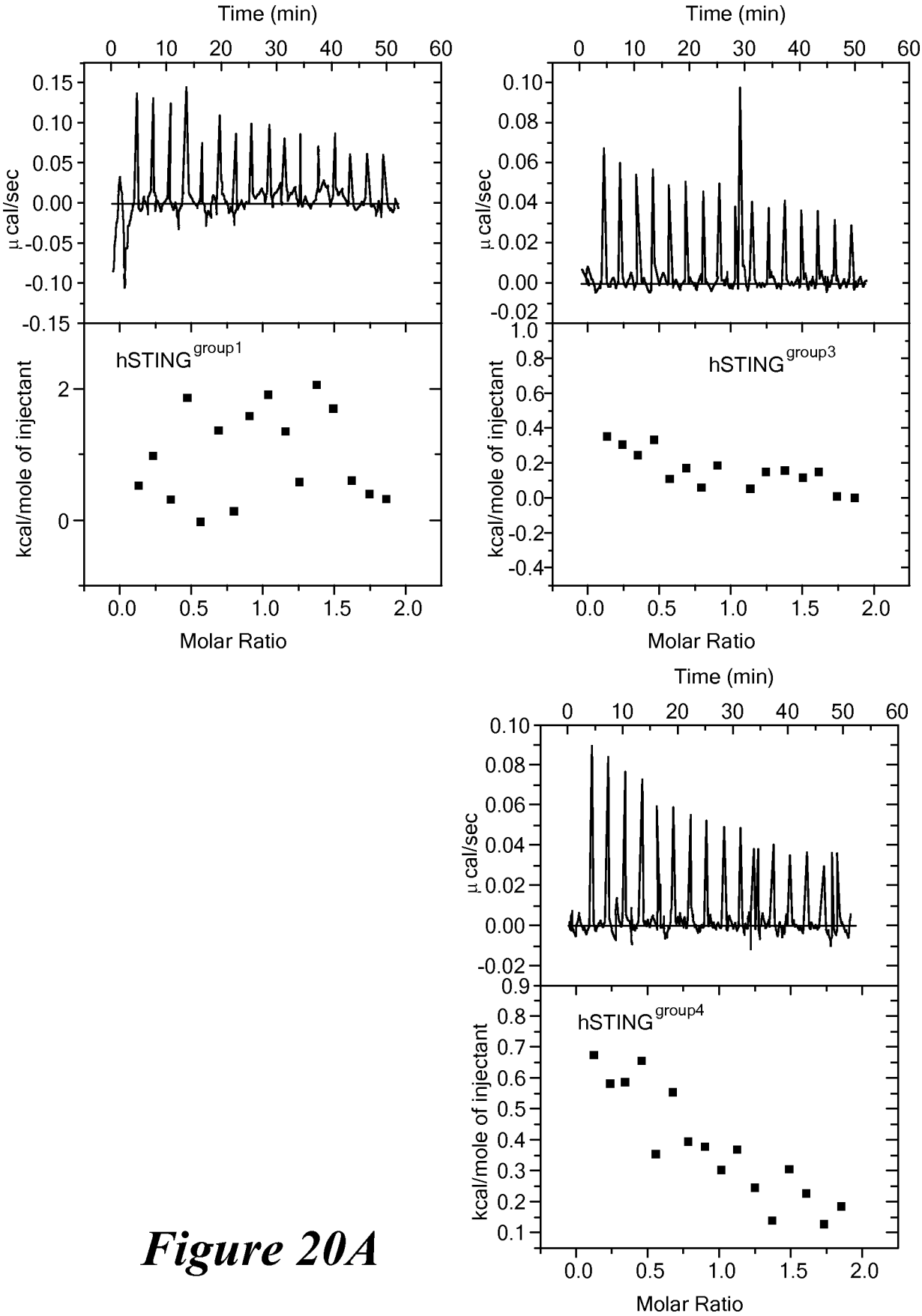

Time (min)
0 10 20 30 40 50 60
µcal/sec
0.15 0.10 0.05 0.00 -0.05 -0.10 -0.15
kcal/mole of injectant
hSTING group1
2 0
0.0 0.5 1.0 1.5 2.0
Molar Ratio
Time (min)
0 10 20 30 40 50 60
µcal/sec
0.10 0.08 0.06 0.04 0.02 0.00 -0.02
kcal/mole of injectant
hSTING group3
1.0 0.8 0.6 0.4 0.2 0.0 -0.2 -0.4
0.0 0.5 1.0 1.5 2.0
Molar Ratio
Time (min)
0 10 20 30 40 50 60
µcal/sec
0.10 0.08 0.06 0.04 0.02 0.00 -0.02
kcal/mole of injectant
hSTING group4
0.9 0.8 0.7 0.6 0.5 0.4 0.3 0.2 0.1
0.0 0.5 1.0 1.5 2.0
Molar Ratio

Figure 20A

B

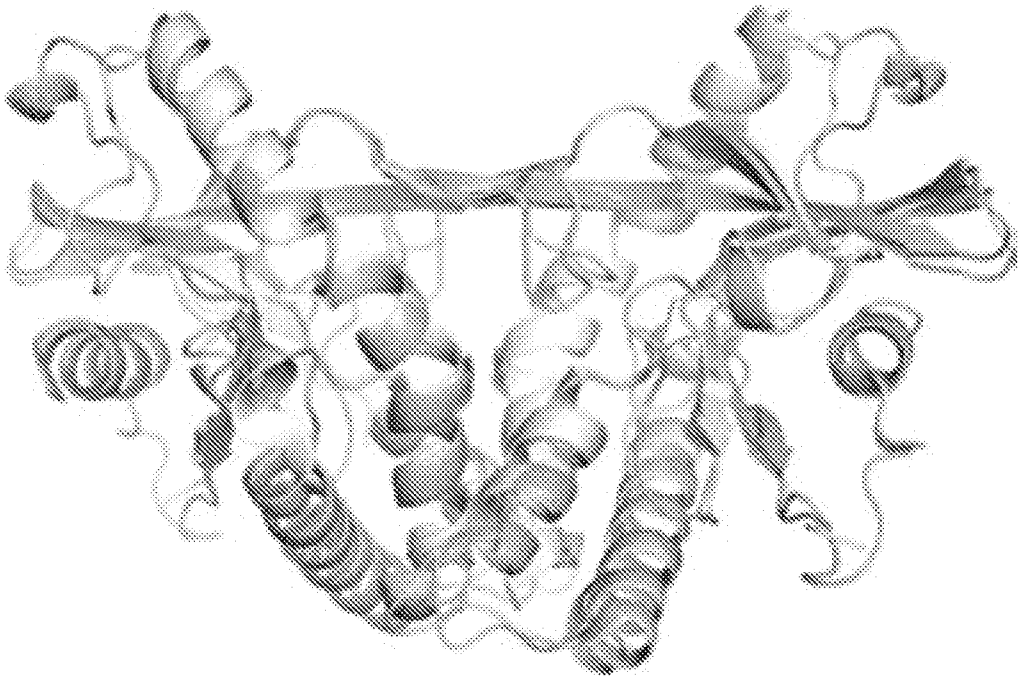


Figure 20B

C

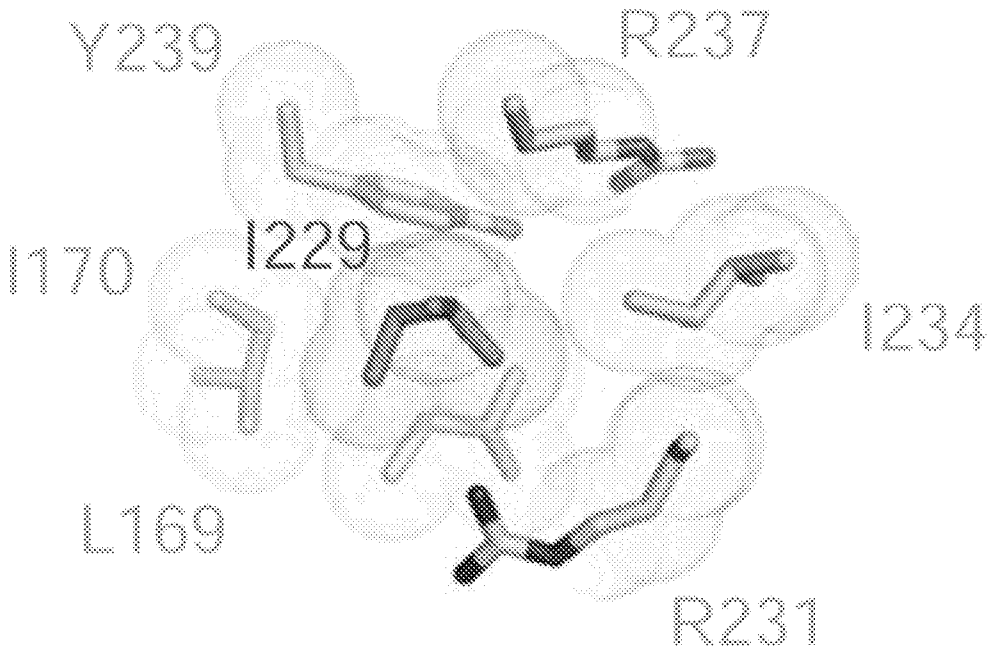


Figure 20C

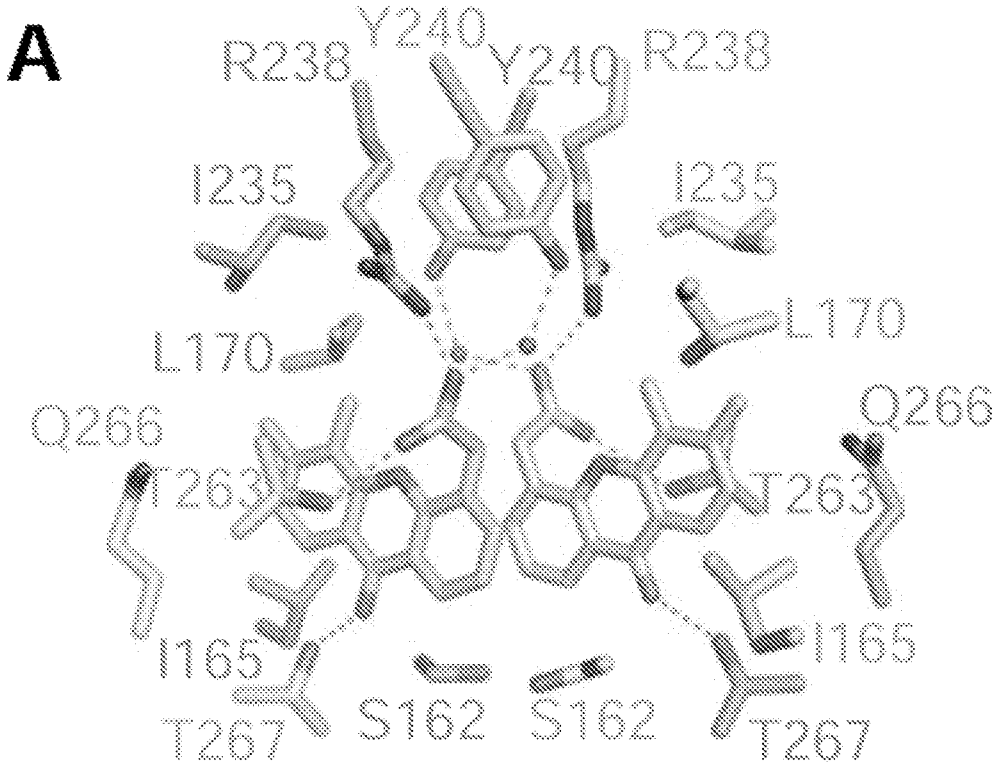
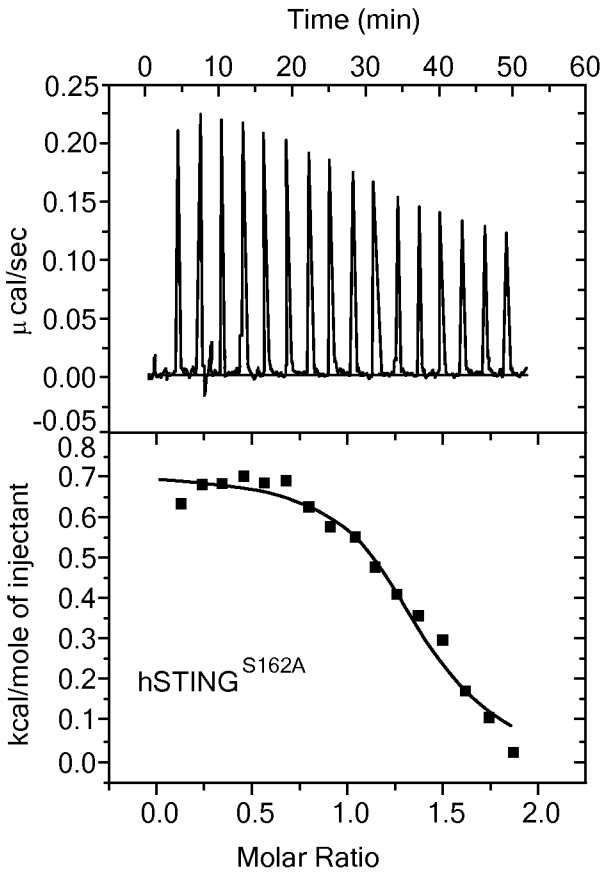


Figure 21A



Figure 21B



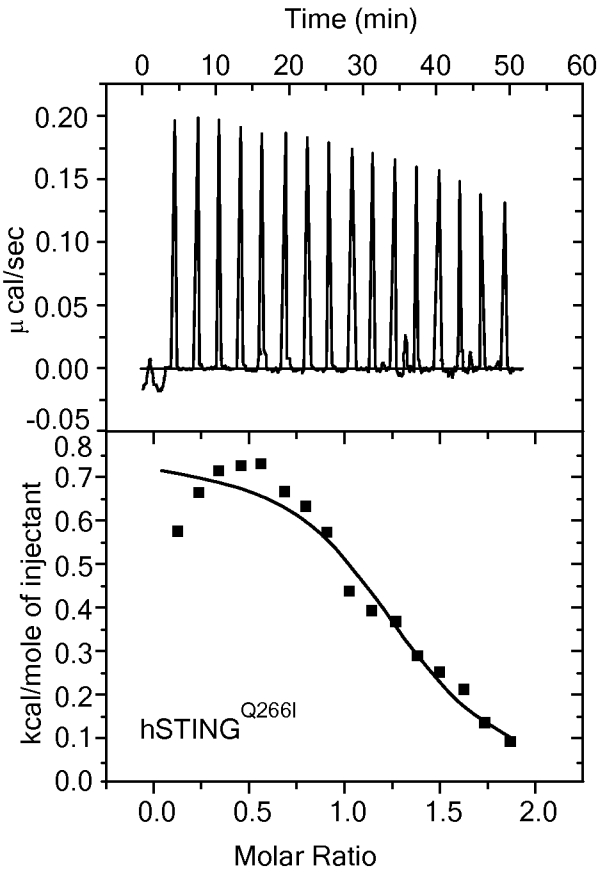


Figure 21C

Figure 21D

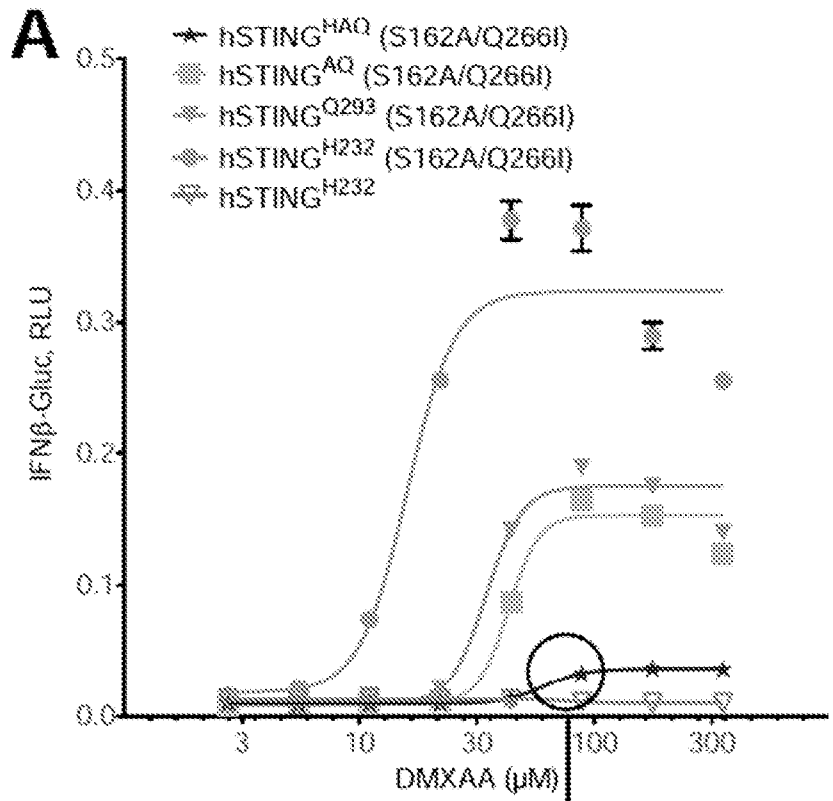


Figure 22A

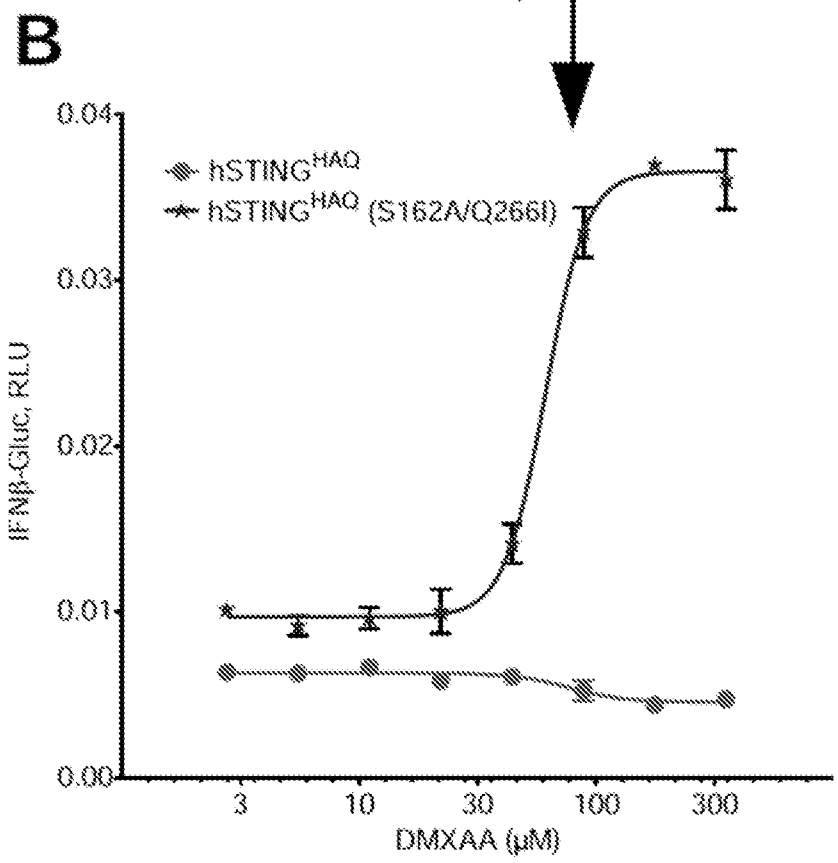


Figure 22B

C

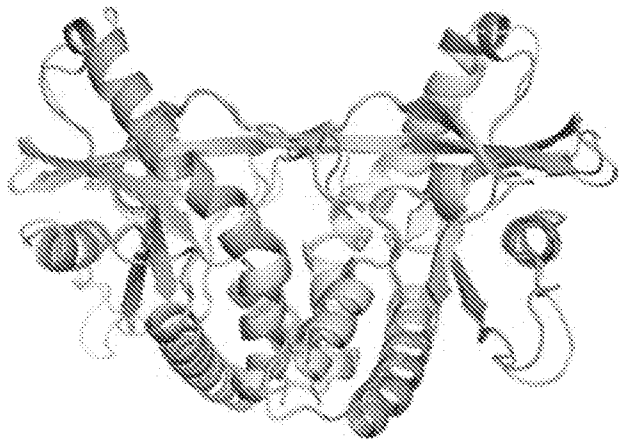


Figure 22C

E

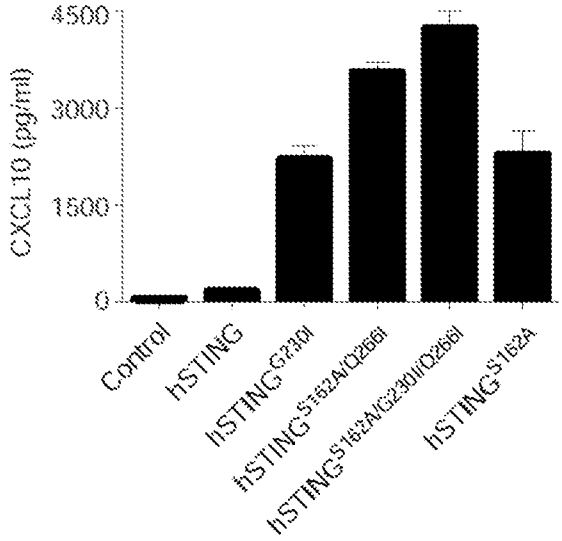


Figure 22E

D

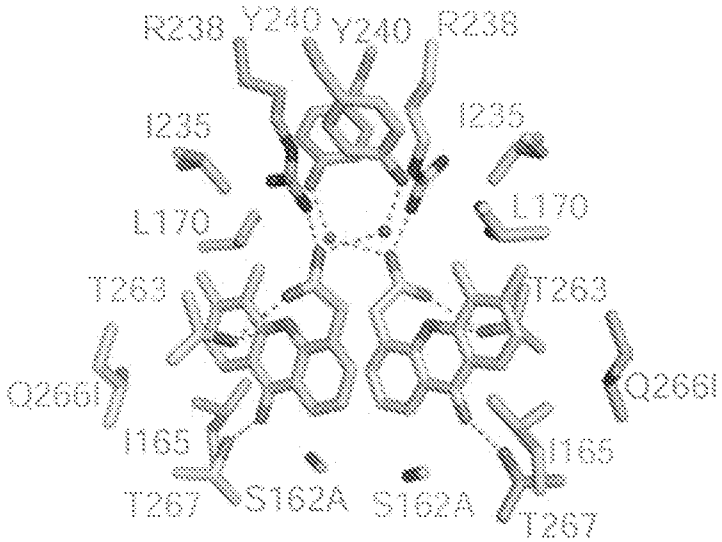


Figure 22D

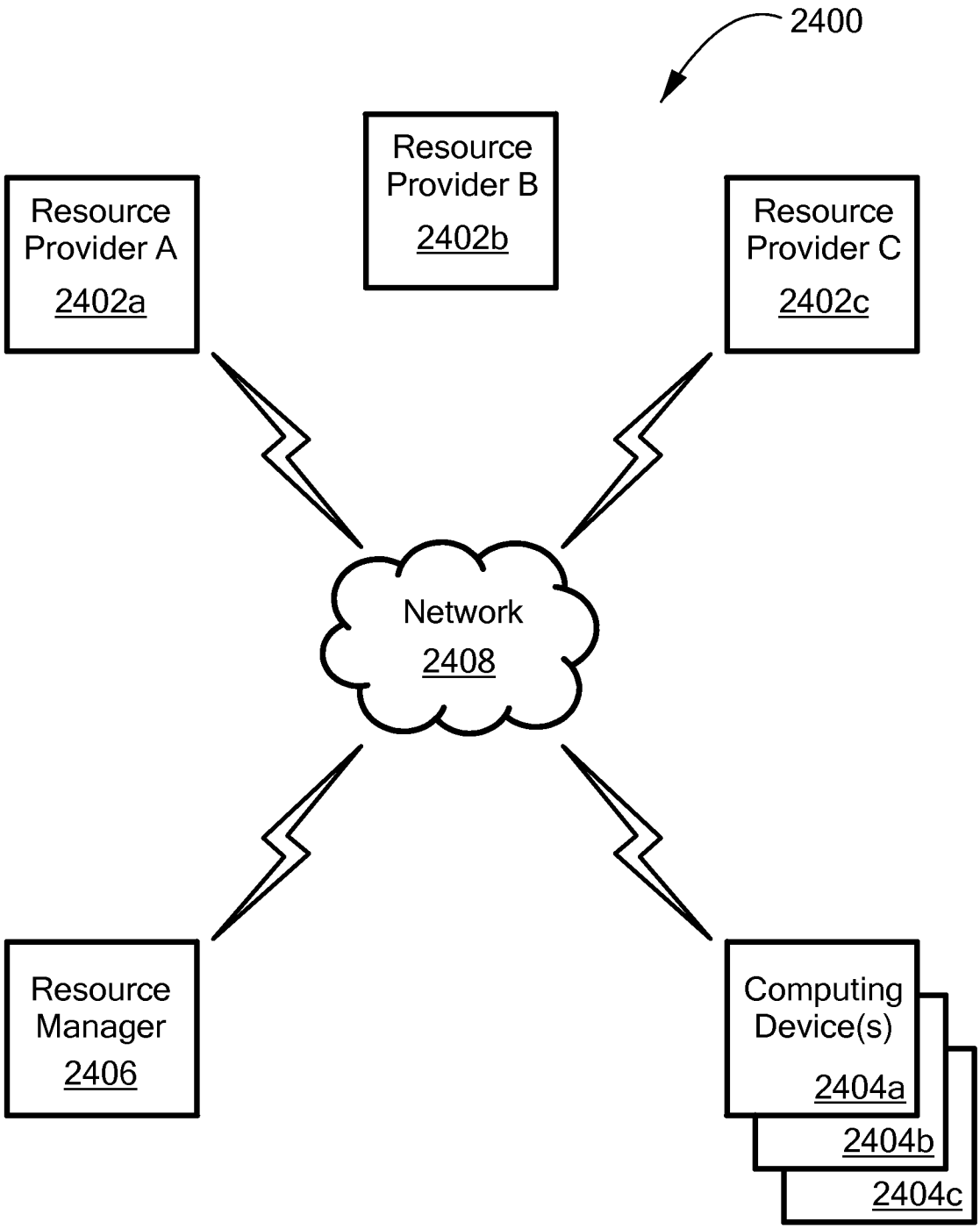

2400
Resource Provider A 2402a
Resource Provider B 2402b
Resource Provider C 2402c
Network 2408
Resource Manager 2406
Computing Device(s) 2404a
2404b
2404c

Figure 23

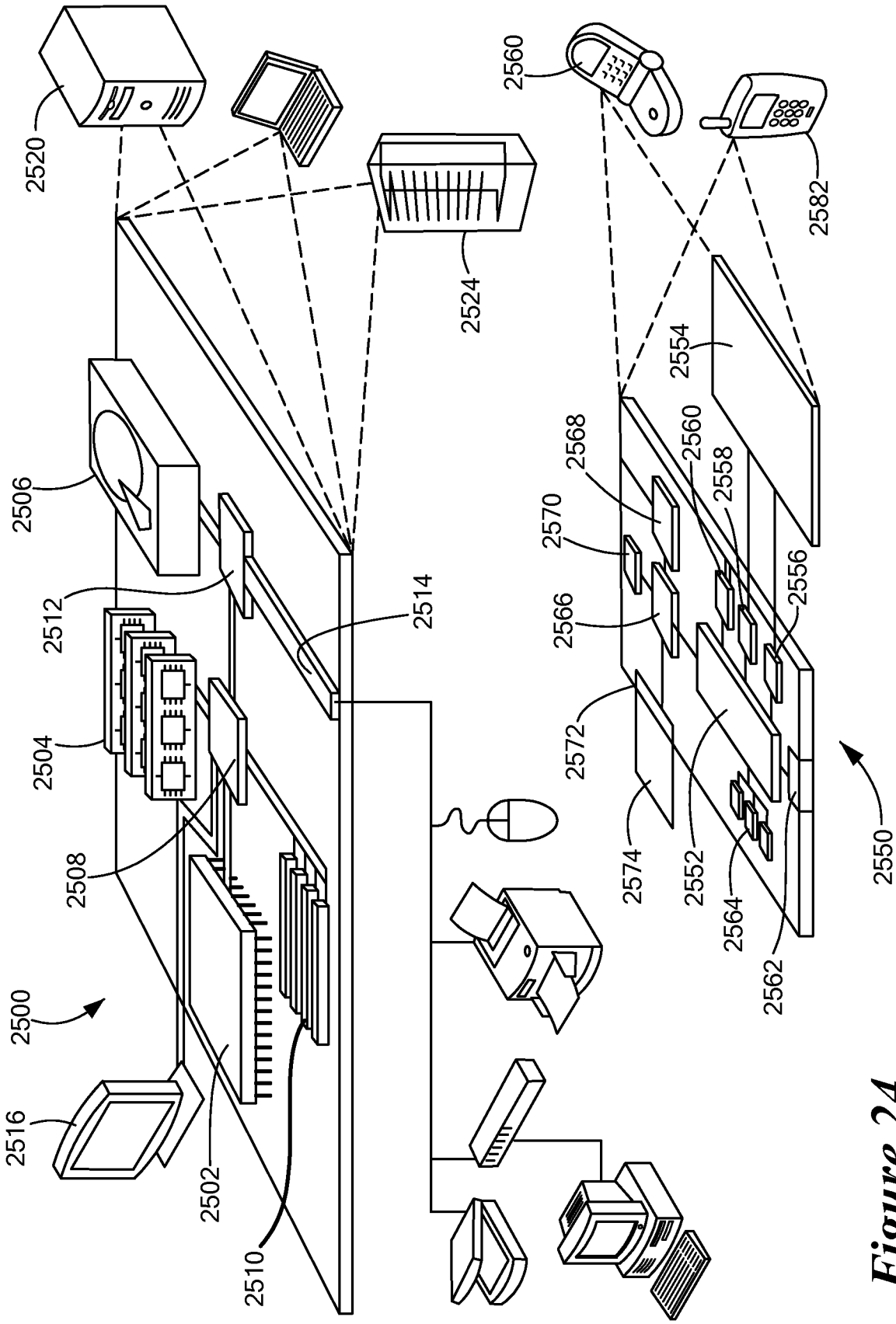

2520
2524
2560
2582
2554
2506
2568
2560
2558
2570
2556
2512
2514
2566
2504
2572
2508
2574
2552
2564
2562
2550
2500
2516
2502
2510

Figure 24

INTERNATIONAL SEARCH REPORT

International application No.
PCT/US2014/049140

A. CLASSIFICATION OF SUBJECT MATTER
IPC(8) - A61K 48/00 (2014.01)
CPC - A61K 48/00 (2014.09)
According to International Patent Classification (IPC) or to both national classification and IPC

B. FIELDS SEARCHED

Minimum documentation searched (classification system followed by classification symbols)
IPC(8) - A01N 1/02; A61K 38/00, 38/06, 38/07, 38/08, 38/12, 38/13, 47/42, 47/48, 48/00; A61P 7/02, 9/10, 43/00 (2014.01)
CPC - A61K 38/06, 38/07, 38/08, 38/13, 48/00

Documentation searched other than minimum documentation to the extent that such documents are included in the fields searched
CPC - A61K 38/06, 38/07, 38/08, 38/13, 48/00 (Keyword Delimited)
US Classes - 514/15.1, 21.9; 530/330

Electronic data base consulted during the international search (name of data base and, where practicable, search terms used)

PatBase, Google Patents, Google, PubMed
Search Terms - cGAMP, hSTING, mSTING, STING, binding, computer, assay, crystal, DMXAA

C. DOCUMENTS CONSIDERED TO BE RELEVANT

Category*	Citation of document, with indication, where appropriate, of the relevant passages	Relevant to claim No.
X -- Y	ZHANG et al. "Cyclic GMP-AMP Containing Mixed Phosphodiester Linkages Is An Endogenous High-Affinity Ligand for STING," Molecular Cell, 25 July 2013 (25.07.2013), Vol. 51, Pgs. 226-235. entire document	12-15, 21-23, 26-28, 31-33, 36-38 ---------- 16, 17, 24, 34
Y	TIJONO et al. "Identification of human-selective analogues of the vascular-disrupting agent 5,6-dimethylxanthenone-4-acetic acid (DMXAA)," British Journal of Cancer, 12 March 2013 (12.03.2013), Vol. 108, Pgs. 1036-1315. entire document	1-3
Y	OUYANG et al. "Structural Analysis of the STING Adaptor Protein Reveals a Hydrophobic Dimer Interface and Mode of Cyclic di-GMP Binding," Immunity, 29 June 2012 (29.06.2012), Vol. 36, Pg. 1073-1086. entire document	1-3
Y	SHU et al. "Structure of STING bound to cyclic di-GMP reveals the mechanism of cyclic dinucleotide recognition by the immune system," Nature Structural & Molecular Biology, 1 July 2012 (01.07.2012), Vol. 19, No. 7, Pgs. 722-725. entire document	16
Y	JIN et al. "Identification and Characterization of a Loss-of-Function Human MPYS Variant," Genes Immun, 01 December 2011 (01.12.2011), Vol. 12, No. 4, Pgs. 263-269. entire document	17, 24
Y	US 2008/0076778 A1 (OSSOVSKAYA et al) 27 March 2008 (27.03.2008) entire document	34
P, X	GAO et al. "Structure-Function Analysis of STING Activation by c[G(20,50)pA(30,50)p] and Targeting by Antiviral DMXAA," Cell, 15 August 2013 (15.08.2013), Vol. 154, Pgs. 748-762. entire document	1-3, 12-17, 21-24, 26-28, 31-34, 36-38

☒ Further documents are listed in the continuation of Box C. ☐

* Special categories of cited documents:
"A" document defining the general state of the art which is not considered to be of particular relevance
"E" earlier application or patent but published on or after the international filing date
"L" document which may throw doubts on priority claim(s) or which is cited to establish the publication date of another citation or other special reason (as specified)
"O" document referring to an oral disclosure, use, exhibition or other means
"P" document published prior to the international filing date but later than the priority date claimed
"T" later document published after the international filing date or priority date and not in conflict with the application but cited to understand the principle or theory underlying the invention
"X" document of particular relevance; the claimed invention cannot be considered novel or cannot be considered to involve an inventive step when the document is taken alone
"Y" document of particular relevance; the claimed invention cannot be considered to involve an inventive step when the document is combined with one or more other such documents, such combination being obvious to a person skilled in the art
"&" document member of the same patent family

Date of the actual completion of the international search	Date of mailing of the international search report
07 November 2014	22 DEC 2014
Name and mailing address of the ISA/US Mail Stop PCT, Attn: ISA/US, Commissioner for Patents P.O. Box 1450, Alexandria, Virginia 22313-1450 Facsimile No. 571-273-3201	Authorized officer: Blaine R. Copenheaver PCT Helpdesk: 571-272-4300 PCT OSP: 571-272-7774

Form PCT/ISA/210 (second sheet) (July 2009)

INTERNATIONAL SEARCH REPORT

International application No.
PCT/US2014/049140

C (Continuation). DOCUMENTS CONSIDERED TO BE RELEVANT

Category*	Citation of document, with indication, where appropriate, of the relevant passages	Relevant to claim No.
P, X	YI et al. "Single Nucleotide Polymorphisms of Human STING Can Affect Innate Immune Response to Cyclic Dinucleotides," Plos One, 21 October 2013 (21.10.2013), Vol. 8, Iss. 10, Pgs. 1-16. entire document	1-3, 12-17, 21-24, 26-28, 31-34, 36-38

INTERNATIONAL SEARCH REPORT

International application No.
PCT/US2014/049140

Box No. II Observations where certain claims were found unsearchable (Continuation of item 2 of first sheet)

This international search report has not been established in respect of certain claims under Article 17(2)(a) for the following reasons:

1. ☐ Claims Nos.:
because they relate to subject matter not required to be searched by this Authority, namely:

2. ☐ Claims Nos.:
because they relate to parts of the international application that do not comply with the prescribed requirements to such an extent that no meaningful international search can be carried out, specifically:

3. ☒ Claims Nos.: 4-11, 18-20, 25, 29, 30, 35
because they are dependent claims and are not drafted in accordance with the second and third sentences of Rule 6.4(a).

Box No. III Observations where unity of invention is lacking (Continuation of item 3 of first sheet)

This International Searching Authority found multiple inventions in this international application, as follows:

1. ☐ As all required additional search fees were timely paid by the applicant, this international search report covers all searchable claims.

2. ☐ As all searchable claims could be searched without effort justifying additional fees, this Authority did not invite payment of additional fees.

3. ☐ As only some of the required additional search fees were timely paid by the applicant, this international search report covers only those claims for which fees were paid, specifically claims Nos.:

4. ☐ No required additional search fees were timely paid by the applicant. Consequently, this international search report is restricted to the invention first mentioned in the claims; it is covered by claims Nos.:

Remark on Protest

☐ The additional search fees were accompanied by the applicant's protest and, where applicable, the payment of a protest fee.

☐ The additional search fees were accompanied by the applicant's protest but the applicable protest fee was not paid within the time limit specified in the invitation.

☐ No protest accompanied the payment of additional search fees.