(12) INTERNATIONAL APPLICATION PUBLISHED UNDER THE PATENT COOPERATION TREATY (PCT)

(19) World Intellectual Property Organization
International Bureau

(43) International Publication Date
22 November 2012 (22.11.2012)

WIPO | PCT

(10) International Publication Number
WO 2012/158613 Al

(51) **International Patent Classification:**
C07K 14/135 (2006.01)

(21) **International Application Number:**
PCT/US20 12/037773

(22) **International Filing Date:**
14 May 2012 (14.05.2012)

(25) **Filing Language:** English

(26) **Publication Language:** English

(30) **Priority Data:**
61/486,005 13 May 201 1 (13.05.201 1) US

(71) **Applicant** *(for all designated States except US):* **NOVARTIS AG** [CH/CH]; Lichtstrasse 35, CH-4056 Basel (CH).

(72) **Inventors; and**

(75) **Inventors/Applicants** *(for US only):* **SWANSON, Kurt** [US/US]; c/o Novartis Vaccines And Diagonstics, Inc., PO Box 8097, Emeryville, CA 94662-8097 (US). **CARFI, Andrea** [US/US]; c/o Novartis Vaccines And Diagonstics, Inc., PO Box 8097, Emeryville, CA 94662-8097 (US).

(74) **Agents: BAUTISTA, Regina** et al; Novartis Vaccines And Diagnostics, Inc., IP Services M/S X-100B, PO Box 8097, Emeryville, CA 94662-8097 (US).

(81) **Designated States** *(unless otherwise indicated, for every kind of national protection available):* AE, AG, AL, AM, AO, AT, AU, AZ, BA, BB, BG, BH, BR, BW, BY, BZ, CA, CH, CL, CN, CO, CR, CU, CZ, DE, DK, DM, DO, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GT, HN, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LY, MA, MD, ME, MG, MK, MN, MW, MX, MY, MZ, NA, NG, NI, NO, NZ, OM, PE, PG, PH, PL, PT, QA, RO, RS, RU, RW, SC, SD, SE, SG, SK, SL, SM, ST, SV, SY, TH, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW.

(84) **Designated States** *(unless otherwise indicated, for every kind of regional protection available):* ARIPO (BW, GH, GM, KE, LR, LS, MW, MZ, NA, RW, SD, SL, SZ, TZ, UG, ZM, ZW), Eurasian (AM, AZ, BY, KG, KZ, RU, TJ, TM), European (AL, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HR, HU, IE, IS, IT, LT, LU, LV, MC, MK, MT, NL, NO, PL, PT, RO, RS, SE, SI, SK, SM, TR), OAPI (BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG).

Published:

— *with international search report (Art. 21(3))*

— *before the expiration of the time limit for amending the claims and to be republished in the event of receipt of amendments (Rule 48.2(h))*

— *with sequence listing part of description (Rule 5.2(a))*

WO 2012/158613 A1

(54) **Title:** PRE-FUSION RSV F ANTIGENS

(57) **Abstract:** The invention relates to pre-fusion RSV F protein and polypeptides that contain one or more amino acid mutations that stabilize the pre-fusion conformation or destabilize the post-fusion conformation. The invention also relates to methods for inducing an immune response to pre-fusion RSV F.

PRE-FUSION RSV F ANTIGENS

RELATED APPLICATION

[001] This application claims priority to U.S. Provisional Application 61/486,005 filed on May 13, 2011. The entire contents of the foregoing application is incorporated herein by reference.

SEQUENCE LISTING

[002] The instant application contains a Sequence Listing which has been submitted in ASCII format via EFS-Web and is hereby incorporated by reference in its entirety. Said ASCII copy, created on May 11, 2012, is named PAT05457.txt and is 98,385 bytes in size.

BACKGROUND OF THE INVENTION

[003] Respiratory syncytial virus (RSV) is an enveloped non-segmented negative-strand RNA virus in the family *Paramyxoviridae*, genus *Pneumovirus.* It is the most common cause of bronchiolitis and pneumonia among children in their first year of life. RSV also causes repeated infections including severe lower respiratory tract disease, which may occur at any age, especially among the elderly or those with compromised cardiac, pulmonary, or immune systems.

[004] To infect a host cell, paramyxoviruses such as RSV, like other enveloped viruses such as influenza virus and HIV, require fusion of the viral membrane with a host cell's membrane. For RSV the conserved fusion protein (RSV F) fuses the viral and cellular membranes by coupling irreversible protein refolding with juxtaposition of the membranes. In current models, based on paramyxovirus studies, the RSV F protein initially folds into a "pre-fusion" conformation. During cell entry, the pre-fusion conformation undergoes refolding and conformational changes to its "post-fusion" conformation.

[005] The RSV F protein is translated from mRNA into an approximately 574 amino acid protein designated F_o. Post-translational processing of F_o includes removal of an N-terminal signal peptide by a signal peptidase in the endoplasmic reticulum. F_o is also cleaved at two sites (109/110 and 136/137) by cellular proteases (in particular furin) in the trans-Golgi. This cleavage results in the removal of a short intervening sequence and generates

two subunits designated Fi (-50 kDa; C-terminal; approximately residues 137-574) and F_2 (-20 kDa; N- terminal; approximately residues 1-109) that remain associated with each other. Fi contains a hydrophobic fusion peptide at its N-terminus and also two amphipathic heptad-repeat regions (HRA and HRB). HRA is near the fusion peptide and HRB is near the transmembrane domain. Three Fi-F_2 heterodimers are assembled as homotrimers of Fi-F_2 on the surface of the virion.

[006] A vaccine against RSV infection is not currently available, but is desired. Vaccine candidates based on the chief RSV neutralization antigen, the F glycoprotein, have foundered due to problems with stability, purity, reproducibility, and potency. Crystal structures of related parainfluenza F glycoproteins have revealed a large conformational change between the pre-fusion and post-fusion states. The magnitude of the rearrangement suggested that post-fusion F antigens would not efficiently elicit neutralizing antibodies, which presumably must bind epitopes exposed on the pre-fusion conformation. Accordingly, efforts to produce a vaccine against RSV have focused on developing subunit vaccines that contain pre-fusion forms of RSV F. (See, e.g., WO 2010/149745, WO 2010/149743, WO 2009/079796) This focus on pre-fusion forms of RSV F has been corroborated by available models of RSV F.

[007] Pre-fusion F is a "metastable" structure that readily rearranges into the lower energy post-fusion state, which then aggregates due to exposure of a hydrophobic fusion peptide (Begona Ruiz-Arguello, M. et al. *Virology* 298, 317-326 (2002) (142)). Large structural differences between the lollipop-shaped pre-fusion F trimer and the crutch-shaped post-fusion F trimer are apparent even at the resolution of electron microscopy of negatively stained specimens, suggesting that pre-fusion and post-fusion F may be antigenically distinct (Calder, L. J. *et al. Virology* 271, 122-131 (2000) (143)). To prevent viral entry, F-specific neutralizing antibodies presumably must bind the pre-fusion conformation of F on the virion, before the viral envelope fuses with a cellular membrane. However, efforts to generate a soluble, stabilized pre-fusion F subunit antigen have not yet yielded candidates suitable for testing in humans. Furthermore, analysis of a Motavizumab-peptide complex and homology modeling suggested that the dominant neutralizing epitope recognized by Palivizumab and Motavizumab might be buried in trimeric F, requiring at least a local dissociation for surface exposure to allow antibody binding (McLellan, J. S. *et al. Nat Struct Mol Biol* 17, 248-250 (2010)). There is a need for improved RSV F protein compositions and methods for making RSV F protein compositions.

SUMMARY OF THE INVENTION

[008] The invention relates to pre-fusion respiratory syncytial virus (RSV) F polypeptides and pre-fusion chimeric F polypeptides.

[009] In some aspects, the pre-fusion respiratory syncytial virus (RSV) F polypeptide comprises at least two introduced cysteine residues that are in close proximity to one another, and form a disulfide bond that stabilizes the pre-fusion RSV F polypeptide. In particular embodiments, the HRB region contains an introduced cysteine residue and the DI and/or DII region contain an introduced cysteine residue, and a disulfide bond is formed between the introduced cysteine residue in the HRB region and the introduced cysteine residue in the D1 or DII region. In other embodiments, the HRA region contains an introduced cysteine residue and the Dili region contains an introduced cysteine residue, and a disulfide bond is formed between the introduced cysteine residue in the HRA region and the introduced cysteine residue in the III region. In other embodiments, the HRA region contains at least 2 introduced cysteine residues, and a disulfide bond is formed between the introduced cysteine residues in the HRA region.

[010] In other aspects, the pre-fusion respiratory syncytial virus (RSV) F polypeptide comprises a post-fusion modification selected from the group consisting of deletion of the HRA helix, deletion of the HRB helix, introduction of point mutations, addition of glycosylation sites and combinations thereof, wherein said post-fusion modification destabilizes the post-fusion conformation. In some embodiments, the destabilizing post-fusion modification is deletion of the HRB helix, in whole or in part. If desired, the destabilizing post-fusion modification can further comprise deletion of the fusion peptide, in whole or in part. In other embodiments, the destabilizing post-fusion modification includes addition of a glycosylation site, such as glycosylation on a residue selected from the group consisting of position 173, position 175 and position 184.

[011] In another aspect, the invention is a pre-fusion respiratory syncytial virus (RSV) F protein comprising three RSV F monomers, wherein at least two of the monomers contain an introduced cysteine residue, the introduced cysteine residues are in close proximity to one another and form a disulfide bond that stabilizes the pre-fusion RSV F protein.

[012] In another aspect, the invention is a chimeric pre-fusion F protein comprising a stabilized F protein from a virus other than RSV, such as parainfluenza virus F polypeptide

or a metapneumovirus virus F polypeptide, that contains one or more neutralizing epitope of RSV F. Suitable neutralizing epitopes can be selected from the group consisting of the epitopes that are recognized by motavizumab, palivizumab, mAb 11, mAb 151, mAb 1129, mAb 1153, mAb 1200, mAb 1214, mAb 1237, mAb 47F, mAb 7C2, mAb B4, Fab 19, mAb AK13A2, mAb 7.936, mAb 9.936, mAb 19, mAb 20, mAb 101F and combinations thereof.

[013] The invention relates to methods for inducing an anti-respiratory syncytial virus (RSV) immune response in a subject, comprising administering to the subject an effective amount of an immunogenic composition comprising a pre-fusion RSV F protein or a pre-fusion chimeric F protein. Preferably, the induced immune response is characterized by neutralizing antibodies to RSV and/or protective immunity against RSV.

[014] In particular aspects, the invention relates to a method for inducing or raising neutralizing anti-respiratory syncytial virus (RSV) F protein antibodies in a subject, comprising administering to the subject an effective amount of an immunogenic composition comprising a pre-fusion RSV F protein or a pre-fusion chimeric F protein.

[015] In particular aspects, the invention relates to a method for inducing or raising protective immunity against respiratory syncytial virus (RSV) in a subject, comprising administering to the subject an effective amount of an immunogenic composition comprising a pre-fusion RSV F protein or a pre-fusion chimeric F protein.

[016] In particular aspects, the invention relates to immunogenic compositions comprising a pre-fusion respiratory syncytial virus (RSV) F protein or a pre-fusion chimeric F protein.

[017] The pre-fusion RSV F protein that is used in the invention can be full length or truncated, such as a soluble ectodomain that lacks the cytoplasmic and transmembrane domains. The pre-fusion RSV F protein, e.g., full length or soluble ectodomain, may comprise functional furin cleavage sites at positions 109/110 and 136/137. In some preferred embodiments, that pre-fusion RSV F protein (e.g., full length or soluble ecto-domain) contains the amino acid sequence of the corresponding portion (e.g., ecto-domain) of a naturally occurring RSV F protein. In any of the aspects of the invention, the pre-fusion RSV F protein can be administered with or without an adjuvant as desired, and the immunogenic composition can comprise an adjuvant if desired.

BRIEF DESCRIPTION OF THE DRAWINGS

[018] FIG. 1 shows a structure-based sequence alignment of four F proteins, secondary assignment, and key features. The alignment of RSV (SEQ ID NO:33), Newcastle disease virus (NDV) (SEQ ID NO:34), PIV3 (SEQ ID NO:36) and PIV5 (SEQ ID NO:35) Fs was generated with ClustalW2 (http://www.ebi.ac.uk/Tools/msa/clustalw2/), adjusted manually based on structural superposition using Lsqkab from the CCP4 suite of programs and displayed using ESPript version 2.2 (http://espript.ibcp.fr/ESPript/ESPript/). Features of RSV F are indicated above the sequences; features of PIV3 F are indicated below the sequences. *CHO indicates RSV F glycosylation sites. Secondary structure elements are indicated, with arrows parallel to the sequences designating β-sheets, cylinders designating a-helices, "TT" designating turns, and coils designating 3_{10} helices. The domain location of secondary structure symbols are indicated (DI, DII, Dili), except for RSV helices αι5 and αι6, which are labeled to indicate that they form the Motavizumab binding site and β20 and β21, which are labeled to indicate that they form the 10 IF binding site. Circled numbers (RSV) or triangled numbers (PIV3) designate residues that form disulfide bonds, with the same number for each partner in a disulfide-linked pair. The furin cleavage sites for RSV F and PIV3 F are indicated by vertical arrows labeled Fr. The RSV F p27 region released from the protein after furin cleavage is indicated by a black bar. The fusion peptides of RSV F and PIV3 F are labeled. The arrow in the fusion peptide indicates the first residue of the Fl fragment in the fusion peptide deletion construct used in this study. Residues that are identical in all four proteins are indicated by shaded boxes. Peptides used to investigate neutralizing binding sites are in open boxes and resistance mutations are indicated by asterisks.

[019] FIG. 2 shows electron microscopy and circular dichroism analysis of the RSV F post-fusion trimer. In FIG. 2A an electron micrograph of the RSV F protein shows a field of uniform crutch phenotypes consistent with the structure of post-fusion F proteins. FIG. 2B shows a CD melting curve of the post-fusion RSV F trimer observed at 210 nm, the observed spectral minimum of the folded RSV F protein. The CD absorption, y-axis, is plotted against temperature, x-axis. FIG. 2C shows a CD spectra of the post-fusion RSV F trimer at 20° and 95°C. The spectra were recorded from 320 to 190 nm and show at both temperatures characteristic helical minima for a folded protein.

[020] FIG. 3 shows representative electron densities of the crystallized RSV F protein. FIG. 3A is a side view of the original molecular replacement solution model, which contains the PIV3 post-fusion head in-frame with the 6-helix bundle of RSV F, shown in the initial electron density map (1σ) calculated after iterative real-space NCS three-fold

averaging, histogram matching, and solvent flattening with phase extension from 7.0 to 3.2 Å and no phase recombination. The head region fits poorly in the electron density. FIG. 3B Side view. The final model of RSV F shown in the averaged electron density map as described in FIG. 4A. FIG. 3C shows a top view of the RSV F protein structure shown in FIG. 4A. FIG. 3D shows a top view of B. Model and electron density depicted as in FIG. 4B. FIG. 3E is a close up of a representative averaged electron density (gray) with the final model in stick representation. FIG. 3F shows the same view as in FIG. 4E but with final *2mFo-dFc* electron density map contoured at 1.5σ.

[021] FIG. 4 shows the RSV F ectodomain structure. 4A is a linear diagram. Listed residue numbers correspond to the N-terminus of each segment, the furin cleavage sites (arrow heads), and the C-terminus. DI-III, domains I-III; p27, excised peptide; FP, fusion peptide; HRA, B, and C, heptad repeats A, B, and C. 4B shows a ribbon representation of one subunit of the RSV F ectodomain trimer. Domains are labeled and shaded as in 4A, glycans are shown in black. 4C shows surface representation of the RSV F ectodomain trimer. The domains of one subunit are labeled and shaded as in 4A, the other two subunits are white and gray.

[022] FIG. 5 shows superposition of domains I and II of RSV F and PIV3 F. FIG. 5A shows a ribbon diagram of domain I from RSV and PIV3 superimposed by matching the common β-sheets. FIG 5B shows a ribbon diagram of domain II from RSV F and PIV3 F superimposed based on common β-strands. The secondary structure elements of RSV F are labeled.

[023] FIG. 6 illustrates a comparison between RSV and PIV3. FIG. 6A is a ribbon diagram of RSV F domain III. FIG. 6B shows a ribbon diagram of the PIV3 domain III oriented to match orientation shown in FIG. 6A. FIG. 6C shows the detail of the RSV and PIV3 (which are shaded differently) domain III helical bundles superimposed based on domain III β-sheets. FIG. 6D shows RSV and PIV3 F ectodomain trimers (shaded as in A and B) superimposed based on their six-helix bundles. The image on the left shows a ribbon diagram viewed perpendicular to the three-fold axis; the image on the right is a surface representation viewed along the three-fold axis from the top of the head.

[024] FIG. 7 illustrates the Motavizumab epitope. FIG. 7A is a superposition of the Motavizumab-binding helices, α5 and α6, from the RSV F post-fusion trimer and the peptide-Motavizumab complex (PDB code 3ΓXT). The post fusion trimer structure and the peptide-motavizumab complex structure are shaded differently. RSV residues bound by

Motavizumab are shown in stick representation. Asterisks denote Palivizumab escape mutations. FIG. 7B shows a ribbon representation modeling a Motavizumab-RSV F post-fusion trimer complex. The V_H and V_L domains of the Fab are labeled; helices α5 and α6 from the RSV F structure and the peptide-Motavizumab structure are shaded differently; a glycan on RSV F is black; and the remainder of RSV F is white.

[025] FIG. 8 illustrates RSV F conformational changes, antigenic structure and Palivizumab binding. FIG. 8A is a surface representation of the post-fusion structure. Antigenic sites A and C are outlined and labeled. Asterisks indicate residues selected in neutralization escape variants or forming contacts with an antibody in the determined structures of neutralizing antibody-peptide complexes. The HRA and HRB surfaces are shaded. FIG. 8B is a surface representation of a pre-fusion model, annotated as in A. FIG. 8C is a graph showing inhibition of Palivizumab binding to post-fusion RSV F by pooled sera from un-immunized mice or mice immunized with the RSV F antigen. Palivizumab binding (percentage of ELISA signal without competing sera) is plotted as a function of the dilution of competing pooled sera.

[026] FIG. 9 shows the exposure of the Motaviuzumab epitope in the post-fusion RSV F structure (A) and pre-fusion RSV F model (B). Fig. 9A shows Domain III of one subunit from the post-fusion structure shaded black and grey while the remaining parts of RSV F are in white. Structural elements that do not significantly change betweeen pre- and post-fusion are in black while HRA (labeled with arrow), which refolds in the transition from the pre- to post-fusion conformation, is lighter grey. Motavizumab epitopes on two subunits are also labeled. A third Motavizumab epitope is present on the trimer surface, but is not easily visible in this orientation. The Motavizumab epitope a5 and a6 helices are labeled on one example. Fig. 9B shows Domain III of the pre-fusion model shaded as in A. The fusion peptide region is shaded and labeled FP. The HRA region is broken into structural elements al, a2, a3, βï and β2; labeled and shaded grey for one subunit. In both the pre-fusion and post-fusion structures, the a5 and a6 helices of the Motavizumab epitope are surface exposed. However, in the pre-fusion model, the HRC loop may need to shift to accommodate antibody binding (as indicated by the arrow).

[027] FIG. 10 shows a model of neutralizing antibody 101F bound to the post-fusion RSV F trimer. FIG. 10A shows the peptide (residues 431-435) (SEQ ID NO:37) from the 101F Fab-peptide complex structure (PDB code 3041 [21]) superposed on equivalent residues of the RSV F structure (β-strand 20 to β-strand 21). FIG. 10B is a ribbon representation of a

model of the 101F Fab bound to the RSV F post-fusion trimer. 101F Fab V_H and V_L domains are labeled; RSV F β-strand 20 and β-strand 21 and labeled as in A. The remaining parts of RSV F are in white. FIG. 10B discloses "IIKTF" as SEQ ID NO: 37.

[028] FIGS. 11A-C show that residues within appropriate distances to form disulfides can be identified, based on the current model of RSV F pre-fusion, can be identified. FIG. 11A (Center), The pre-fusion RSV F model is shaded/colored to show structural features which are labeled (HRB, HRA, Dili). FIG. 11B (Left) is a zoom-in view of the packing of HRA on domain III in the pre-fusion model. The paired numbers indicate residues in close proximity which, if mutated to cysteines could form a disulfide bond. FIG. llC (Right) is a zoom-in view of the packing of the HRB-stalk on domains I and III (white). The paired numbers indicate residues which, if mutated to cysteines could form a disulfide bond. Amino acid residues 165 and 296, and 56 and 164 are not at ideal distances to one another, in the pre-fusion model, to form disulfide bonds, but are in correct orientation and can form disulfides if the model is biased by the PIV5 structure, on which the model was built.

[029] FIG. 12 shows a negative stained electron micrograph of the HRB-deleted RSV F construct (RSV F delHRB HIS, SEQ ID NO:28). Electron microscopy of the HRB-deleted RSV F construct demonstrated the RSV F protein formed rosettes, likely through the fusion peptide. The formation of rosettes through the fusion peptide is a feature of post-fusion RSV F rather than a predicted behavior of pre-fusion F proteins (Ruiz-Arguello et al. 2004 (142) and Connolly et al, 2006 (144)). This result shows the HRB-deleted RSV F construct does not appreciably stabilize the protein in the desired pre-fusion conformation.

[030] FIG. 13 shows the structure of RSV F protein in which certain mutations are introduced to inhibit 6-helix bundle formation. Shown is the RSV F post-fusion structure in which the HRB helix has been removed and replaced with a hypothetical random coil (represented by the lines). The elongated HRA helix of the post-fusion RSV F is labeled. The numbers represent potential sites for introduced glycosylation sites or other mutations which interfere with formation of the 6-helix bundle characteristic of the post-fusion structure. A mutation on the HRA helix which interferes with HRB interaction would destabilize the post-fusion conformation, which in turn would cause the protein to remain in the favored pre-fusion conformation.

[031] FIGs. 14 A and B are western blots of cell lysates (14A, showing total expression) or media (14B, showing secreted protein) under boiled and reducing conditions using an anti-His tag antibody. The westerns show the expression of RSV-F proteins, and

that proteins with engineered cysteine residues were expressed and contained intra-chain disulfide bonds. Cleavage of RSV F protein from F0 to F1/F2 and secretion from the cell is evidence of proper protein folding of the RSV F proteins. Migrations for uncleaved F0 and cleaved F1 are indicated. The key for gel lane labeling is shown above the blots. (A) Western blot of cell lysate indicating total protein expression. Each protein construct was well expressed by the cell. (B) Western blot of RSV F secreted into the media. The secreted protein was predominantly cleaved (F1) and the amount of secretion varied among proteins. The results of this analysis indicate that the T58C & V164C, K168C & V296C and M396C & F483C protein constructs were the best expressed/secreted protein constructs. R049: RSV-F fus del R429S I432T K433T S436F trunc (SEQ ID NO:39); R050: RSV-F HRA Disulfide2 I57C S190C trun (SEQ ID NO:40); R051: RSV-F HRA Disulfide3 T58C V164C trunc (SEQ ID NO:6); R052: RSV-F HRA Disulfide5 K168C V296C trunc (SEQ ID NO:8); R053: RSV-F fus del N262Y N268I K272M R429S I432T K433T S436F trunc (SEQ ID NO:41); R054 RSV-F HRA Disulfidel V56C V164C trunc (SEQ ID NO:4); R055 RSV-F HRA Disulfide4 N165C V296C trunc (SEQ ID NO: 7); R056 RSV-F HRB Disulfide M396C F483C trunc (SEQ ID NO:9).

[032] FIGs. 15 A - C show SEC analysis of RSV F intra-chain disulfide. Postfusion F rosettes and fusion peptide deleted RSV F trimers were used to develop an HPLC-SEC assay to differentiate between rosettes and trimers. (FIG. 15 A) Fusion peptide-stabilized RSV F rosettes migrated with the void volume by SEC (retention time of 5 minutes on Bio-Sil 250 SEC column). Anti-HIS-tag western blotting confirmed that the protein was in the void volume peak. (FIG. 15 B) Fusion peptide-deletion RSV F trimers migrated with an SEC retention time of approximately 6.5 minutes. Anti-HIS-tag western blot similarly confirmed that the protein was in the included volume trimer peak. Although the void peak is larger than the included volume peak, the anti-HIS western shows approximately equal amounts of RSV F are in the two peaks. (FIG. 15 C) These data show that the RSV F T58C V164C construct had a population of cleaved RSV F that was in the form of monodispersed trimers rather than rosettes, suggesting that population of the protein construct was in the prefusion form.

[033] FIGs. 16 A - C show purification and analysis of RSV F protein constructs that contain engineered cysteins. FIG 16 A shows purification of the RSV F N165C/V296C construct. Columns are labeled for flow-through (FT), wash (W), elution (E) and resin (R) from a chelating purification. Unlike other protein constructs that contained introduced disulfide mutations and were expressed in insect cells, N165C/V296C secreted as a cleaved

species, similar to its profile when expressed in mammalian cells. FIG. 16 B shows a gel-shift analysis of the K168C/V296C and M396C/F483C RSV F protein constructs. On the left side of the standards are the two constructs run with boiling and reducing agent present. On the right side of the standards, the two constructs are run after boiling with no reducing agent (b/nr) or no boiling and no reducing agent (nb/nr). The western blot shows the protein is largely uncleaved, but that unexpectedly no inter-chain disulfide bonds were formed. K168C/V296C without boiling shifted to the trimer band, while non-boiled M396C/F483C ran as a monomer band. FIG. 16 C shows a coomasie-stained gel of the K168C/V296C and M396C/F483C RSV F protein constructs with reducing and boiling. Approximately 50% of the material was cleaved.

[034] FIG. 17(A) shows electron microscopy analysis of NDV F (prefusion) with the expected spherical heads for prefusion F, with a few rosette-like aggregates. FIG. 17(B) shows NDV prefusion F forms rod-like crystals. An isolated rod was analyzed and a dataset with -95% completion to -3.7 angstroms was recorded. FIG, 17 (C) shows NDV prefusion F forms bipiramidal crystals (50x50x50 μιη size).

[035] FIGs. 18 A-E show analysis of several RSV F protein constructs. FIG. 18A shows EM analysis of RSV F Del-HRB showing that 100% formed rosettes. The protein eluted from the SEC column in the void/rosette retention peak. FIG. 18(B) shows analysis/purification of the Del-HRB Del-FP RSV F construct. The protein was found in both the void and trimer retention peaks. FIG. 18C shows gel-analysis, which suggests that there was partially cleaved RSV F Del-HRB Del-FP present in both the void and trimer peaks. FIG. 18D shows EM of NDV F (prefusion), which shows the expected spherical heads for pre-fusion F with a few rosette-like aggregates. FIG. 18E shows that RSV F Del-HRB from the SEC trimer peak contains a heterogeneous mix of rosette-like structures, post-fusion crutches and pre-fusion head-like spherical species.

[036] FIG. 19 shows SDS-PAGE analysis of chimeric RSV F/NDV and RSV F/PIV5 F protein constructs. The supernatant from cells transfected with one of the six constructs (1: RSV-F NDV HRB del fus trunc; 2: RSV-F NDV HRB trunc; 3: RSV-F NDV HRB2 del fus trunc; 4: RSV-F NDV HRB2 trunc; 5: RSV-F PIV5 HRB del fus trunc; 6: RSV-F PIV5 HRB trunc) was analyzed by SDS-PAGE. The constructs were engineered with or without (del fus) fusion peptide. The proteins either had an NDV HRB, an NDV HRB with an additional glycine residue as a linker (HRB2) or PIV5 HRB as indicated. For each construct, a cleaved F1 protein was observed consistent with a processed F protein. One liter expressions of each protein was performed.

DETAILED DESCRIPTION OF THE INVENTION

Definitions

[037] As used herein, "pre-fusion" RSV F proteins are RSV F proteins that share general structural architecture more similar to the PIV5 pre-fusion structure rather than the RSV F post-fusion structure. Pre-fusion RSV F proteins include the following characteristics: the HRA region is packed against domain III in the RSV F head region and/or the HRB region forms a trimer coil-coil stalk in proximity to domains I and II rather than associating with the HRA region in the context of the 6-helix bundle.

[038] As used herein, "post-fusion conformation" of RSV F protein are RSV F proteins that share more general structural architecture with the RSV F post-fusion structure rather than the PIV5 pre-fusion structure. Post-fusion RSV F proteins include an HRA-HRB 6-helix bundle.

[039] As used herein, HRA region in prefusion RSV F is approximately residues 137-239 of RSV F protein (SEQ ID NOS: 1 and 2) and comprises the fusion peptide, helix α1, helix α2, helix α3, helix α4, strand β1 and strand β2. See, FIG. 9B.

[040] As used herein, the HRA helix in post fusion RSV F is formed by approximately residues 155-226 of RSV F protein (SEQ ID NOS: 1 and 2).

[041] As used herein, the fusion peptide is defined by residues 137-154 of RSV F protein (SEQ ID NOS: 1 and 2).

[042] As used herein, helix α1 in the prefusion RSV F HRA region is formed by approximately residues 145-157 of RSV F protein (SEQ ID NOS: 1 and 2).

[043] As used herein, helix α2 in the prefusion RSV F HRA region is formed by approximately residues 158-167 of RSV F protein (SEQ ID NOS: 1 and 2).

[044] As used herein, helix α3 in the prefusion RSV F HRA region is formed by approximately residues 168-176 of RSV F protein (SEQ ID NOS: 1 and 2).

[045] As used herein, helix α4 in the prefusion RSV F HRA region is formed by approximately residues 194-212 of RSV F protein (SEQ ID NOS: 1 and 2).

[046] As used herein, strand β1 in the prefusion RSV F HRA region is formed by approximately residues 177-184 of RSV F protein (SEQ ID NOS: 1 and 2).

[047] As used herein, strand β2 in the prefusion RSV F HRA region is formed by approximately residues 185-193 of RSV F protein (SEQ ID NOS: 1 and 2).

[048] As used herein, HRB region in RSV F is approximately residues 461-515 of RSV F protein (SEQ ID NOS: 1 and 2) and includes the HRB helix and the HRB linker

[049] As used herein, the HRB helix in RSV F is formed by approximately residues 485-515 of RSV F protein (SEQ ID NOS: 1 and 2).

[050] As used herein, the HRB linker in RSV F is formed by approximately residues 461 - 484 of RSV F protein (SEQ ID NOS: 1 and 2).

[051] As used herein, domain I (DI) is formed by approximately residues 26 - 50 and 309 - 401 of RSV F protein (SEQ ID NOS: 1 and 2).

[052] As used herein, domain II (DII) is formed by approximately residues 400 - 460 of RSV F protein (SEQ ID NOS: 1 and 2).

[053] As used herein, domain III (Dili) is formed by approximately residues 51-98 and 206 - 308, or residues 51 - 308 of RSV F protein (SEQ ID NOS: 1 and 2).

[054] As used herein, a "purified" protein or polypeptide is a protein or polypeptide which is recombinantly or synthetically produced, or produced by its natural host, and has been isolated from other components of the recombinant or synthetic production system or natural host such that the amount of the protein relative to other macromolecular components present in a composition is substantially higher than that present in a crude preparation. In general, a purified protein will be at least about 50% homogeneous and more preferably at least about 75%, at least about 80%, at least about 85%, at least about 90%, at least about 95% or substantially homogeneous.

[055] As used herein, "substantially free of lipids and lipoproteins" refers to compositions, proteins and polypeptides that are at least about 95% free of lipids and lipoproteins on a mass basis when protein and/or polypeptide (e.g., RSV F polypeptide) purity is observed on an SDS PAGE gel and total protein content is measured using either UV280 absorption or BCA analysis, and lipid and lipoprotein content is determined using the Phospholipase C assay (Wako, code no. 433-36201).

[056] As used herein, "close proximity" refers to a distance of not more than about 10Å, not more than about 8Å, not more than about 6Å, not more than about 4Å, or not more than about 2Å. When two or more amino acid residues are in close proximity, the distance between the alpha carbons of the amino acid residues are is more than about 10Å, not more than about 8Å, not more than about 6Å, not more than about 4Å, or not more than about 2Å.

[057] Features of RSV F protein suitable for use in this invention are described herein with reference to particular amino acids that are identified by the position of the amino acid in the sequence of RSV F protein from the A2 strain (SEQ ID NO: 1). RSV F proteins can have the amino acid sequence of the F protein from the A2 strain or any other desired strain. When the F protein from a strain other than the A2 strain is used, the amino acids of

the F protein are to be numbered with reference to the numbering of the F protein from the A2 strain, with the insertion of gaps as needed. This can be achieved by aligning the sequence of any desired RSV F protein with the F protein of the strain A2. Sequence alignments are preferably produced using the algorithm disclosed by Corpet, Nucleic Acids Research, 1998, 16(22):10881-10890, using default parameters (Blossum 62 symbol comparison table, gap open penalty: 12, gap extension penalty: 2).

[058] As described and exemplified herein, the 3.2 Å x-ray crystal structure of a post-fusion form of RSV F protein has been determined. A model of the pre-fusion form of RSV F protein was made by comparing the RSV F post-fusion x-ray crystal structure to the known structures of the pre- and post-fusion parainfluenza virus F proteins. This model of the pre-fusion form of RSV F reveals structural features that differ from those of prior models of pre-fusion RSV F and allows for rational structure-based design of stabilized pre-fusion forms of RSV F.

[059] Accordingly, the invention relates to pre-fusion respiratory syncytial virus F (RSV F) polypeptides and/or proteins, and immunogenic compositions comprising pre-fusion RSV F polypeptides and/or proteins. The invention also relates to methods and use of pre-fusion RSV F polypeptides and/or proteins for inducing an immune response, and or by protective immunity against RSV. The invention also relates to nucleic acids that encode pre-fusion RSV F polypeptides and/or proteins.

[060] Generally, the immunogenic compositions comprise pre-fusion RSV F polypeptides and/or proteins that elicit neutralizing antibodies. For example, antibodies that bind to the same epitopes as Palivizumab, Motavizumab and 101F.

[061] Pre-fusion and post-fusion PIV F structures reveal *en bloc* shifts of domains and large rearrangements of HRA and HRB. In domain III of the pre-fusion PIV5 structure, HRA folds into three a-helices and two β-strands rather than the long post-fusion HRA helix (Yin et al, 2006). However, when pre-fusion and post-fusion conformations of individual PIV F domains are compared, the non-rearranging parts superimpose well. Superimposing post-fusion RSV F domains on their pre-fusion PIV5 F counterparts did not result in major clashes and positioned all the pairs of cysteines that form interdomain disulfide bonds in proximity to each other. The pre-fusion RSV F model obtained by thus combining information from the post-fusion RSV F x-ray crystal structure and the pre-fusion PIV5 F structure revealed a feature not apparent from prior homology models of pre-fusion RSV F based solely on the PIV5 pre-fusion structure (McLellan et al *NSMB* 2010 (141)). The

helices of the Palivizumab/Motivizumab epitope are exposed on the surface of the pre-fusion RSV F trimer model, as they are on post-fusion RSV F trimer x-ray crystal structure (Figure 9). In our pre-fusion RSV F model, the loop connecting β4 and HRC (part of domain III) could hinder access of Palivizumab or Motavizumab to their epitope. However, it is likely that the loop has sufficient flexibility to adopt an alternative conformation that permits antibody binding (Figure 9B).

[062] The pre-fusion model disclosed herein, which is based on the RSV F post-fusion x-ray crystal structure and the PIV5 prefusion structure (Yin et al, 2006 (145)), shows that the elongated HRA helix of the post-fusion RSV F (residues 137-212) folds into strands and helices similar to the PIV5 pre-fusion crystal structure. The fusion peptide of RSV F, residues 137-154, forms a coil and helix that is packed into the RSV F pre-fusion head. Four helices are formed; helix a1 is approximately residues 145-157, helix a2 is approximately residues 158-167, helix a3 is approximately residues 168-176 and helix a4 is approximately residues 194-212. Two strands are formed; strand b1 is approximately residues 177-184, strand b2 is approximately residues 185-193 (Figure 9).

Pre-fusion Conformation

[055] The invention includes pre-fusion RSV F polypeptides and proteins and immunogenic compositions that contain pre-fusion RSV F polypeptides and proteins. The RSV F protein and polypeptides can contain 1 or more amino acid replacements, deletions and/or additions that stabilize the pre-fusion conformation or destabilize the post-fusion conformation, for example, a pre-fusion RSV F stabilized with disulfide bonds, or a pre-fusion RSV F formed by destabilizing the post-fusion conformation.

Stabilization through disulfide bonds

[056] The RSV F pre-fusion model may be used as a guide to select amino acid residues that are in close proximity to each other in the pre-fusion conformation and that are no longer in close proximity in the post-fusion conformation. Such amino acids may be mutated to cysteine residues to allow disulfide formation that stabilizes the prefusion conformation, for example by preventing the HRB helix from associating with the HRA helix, thus preventing refolding to the post-fusion conformation.

[057] A stabilized pre-fusion RSV F protein of the invention may comprise a disulfide bond between any two structural elements, or between one structural element and

the remainder of the RSV F protein, or between a structural element of one subunit of a trimer and a structural element of another subunit of the same trimer. Generally, a first amino acid in one structural element and a second amino acid that is in a different structural element, or the same structural element on a separate monomer, and that is also in close proximity to the first amino acid in the prefusion model are selected for replacement with cysteine. The distance between the residues (e.g., the alpha carbons) can be less than about 10Å, less than about 8Å, less than about 6Å, less than about 5Å, less than about 4Å, or less than about 3Å. The cysteine replacements of the first amino acid and the second amino acid, and a disulfide bond between them can be modeled. The length of the modeled disulfide bond, in some embodiments, does not exactly match the ~2Å length considered to be optimal for disulfide bonds. Preferably, the modeled disulfide bond length (distance between sulfur nuclei) is about 0.5Å-3.5Å, about 1.0Å-3.0Å, or about 1.5Å-2.5Å, which, due to structural flexibility, are expected to form disulfide bonds in the protein.

[058] In one embodiment, pre-fusion RSV F protein may be stabilized in the pre-fusion conformation through the introduction of at least one cysteine mutation in a first structural element in close proximity to at least one other cysteine (natural or introduced) in a second structural element or the remaining RSV F head region. Disulfide bonds form between the introduced cysteine that prevent the post-fusion HRA-HRB six-helix bundle from forming. For example, pre-fusion RSV F protein may be stabilized in the pre-fusion conformation through the introduction of at least one cysteine mutation in the HRA helix region, HRB helix region, the fusion peptide, helix al, helix a2, helix a3, helix a4, strand βï, strand β2, DI, DII, or Dili in close proximity to at least one other cysteine (natural or introduced) in a different structural region (e.g., selected from the HRA helix region, HRB helix region, the fusion peptide, helix al, helix a2, helix a3, helix a4, strand βï, strand β2, DI, DII, or Dili), thereby forming one or more disulfide bridges that would prevent the post-fusion HRA-HRB six-helix bundle from forming.

[059] The cysteines may be introduced to the HRB or the HRB linker to create disulfide bonds between the cysteines. In one embodiment, one or more cysteines may be introduced to the HRB linker and helix region (approximately residues 452 to 515) to form disulfides with portions of the RSV F head region. In another embodiment, a disulfide bond between the HRB linker or helix and the remainder of the RSV F protein may be used to stabilize the protein in the pre-fusion conformation. In a preferred embodiment, a disulfide bridge is formed between the HRB pre-fusion stalk and the DI or DII region at the "top" of the head (e.g., M396C + F483C).

[060] In a preferred embodiment, the pre-fusion RSV F protein comprises two cysteine mutations, M396C and F483C, thereby comprising a disulfide bond between the HRB pre-fusion stalk and the DI region.

[061] In other preferred embodiments, a disulfide bridge is formed between the HRA region and Dili region. For example, the RSV F protein can contain amino acid replacements selected from the group consisting of V56C + V164C, I57C + S190C, T58C + V164C, N165C + V296C, K168C + V296C, and combinations thereof.

[062] In one embodiment, the pre-fusion RSV F protein comprises a first cysteine mutation in the HRA region, and a second cysteine (natural or introduced) in the fusion peptide, helix al, helix a2, helix a3, helix a4, strand βï , strand β2 of the pre-fusion HRA region, or Dili. In this embodiment, the protein comprises a disulfide bond between the first and second cysteine that prevents the post fusion HRA-HRB six-helix bundle from forming.

[063] In one embodiment, the pre-fusion RSV F protein comprises a first cysteine mutation in the HRB helix region, and a second cysteine (natural or introduced) in DI or DII. In this embodiment, the protein comprises a disulfide bond between the first and second cysteine that prevents the post-fusion HRA-HRB six-helix bundle from forming.

[064] In one embodiment, the pre-fusion RSV F protein comprises a first cysteine mutation in the fusion peptide, and a second cysteine (natural or introduced) in the HRA region, helix al, helix a2, helix a3, helix a4, strand βï , strand β2 or Dili. In this embodiment, the protein comprises a disulfide bond between the first and second cysteine that prevents the post-fusion HRA elongated helix from forming.

[065] In one embodiment, the pre-fusion RSV F protein comprises a first cysteine mutation in the helix al, and a second cysteine (natural or introduced) in the HRA region, the fusion peptide, helix a2, helix a3, helix a4, strand βï , strand β2, or Dili. In this embodiment, the protein comprises a disulfide bond between the first and second cysteine that prevents the post-fusion HRA-HRB six-helix bundle from forming.

[066] In one embodiment, the pre-fusion RSV F protein comprises a first cysteine mutation in the helix a2, and a second cysteine (natural or introduced) in the HRA region, the fusion peptide, helix al, helix a3, helix a4, strand βï , strand β2, or Dili. In this embodiment, the protein comprises a disulfide bond between the first and second cysteine that prevents the post-fusion HRA-HRB six-helix bundle from forming.

[067] In one embodiment, the pre-fusion RSV F protein comprises a first cysteine mutation in the helix a3, and a second cysteine (natural or introduced) in the HRA region, the fusion peptide, helix al, helix a2, helix a4, strand βï , strand β2, or Dili. In this embodiment,

the protein comprises a disulfide bond between the first and second cysteine that prevents the post-fusion HRA-HRB six-helix bundle from forming.

[068] In one embodiment, the pre-fusion RSV F protein comprises a first cysteine mutation in the helix a4, and a second cysteine (natural or introduced) in the HRA region, the fusion peptide, helix al, helix a2, helix a3, strand βï , strand β2, or Dili. In this embodiment, the protein comprises a disulfide bond between the first and second cysteine that prevents the post-fusion HRA-HRB six-helix bundle from forming.

[069] In one embodiment, the pre-fusion RSV F protein comprises a first cysteine mutation in the strand βï , and a second cysteine (natural or introduced) in the HRA region, the fusion peptide, helix al, helix a2, helix a3, helix a4, strand β2, or Dili. In this embodiment, the protein comprises a disulfide bond between the first and second cysteine that prevents the post-fusion HRA-HRB six-helix bundle from forming.

[070] In one embodiment, the pre-fusion RSV F protein comprises a first cysteine mutation in the strand β2, and a cysteine (natural or introduced) in the HRA helix region, the fusion peptide, helix al, helix a2, helix a3, helix a4, strand βï , DI, DII, or Dili. In this embodiment, the protein comprises a disulfide bond between the first and second cysteine that prevents the post-fusion HRA-HRB six-helix bundle from forming.

[071] In one embodiment, the pre-fusion RSV F protein comprises a first cysteine mutation in the DI region, and a second cysteine (natural or introduced) in the HRB helix region. In this embodiment, the protein comprises a disulfide bond between the first and second cysteine that prevents the post-fusion HRA-HRB six-helix bundle from forming.

[072] In one embodiment, the pre-fusion RSV F protein comprises a first cysteine mutation in the DII region, and a second cysteine (natural or introduced) in the HRB helix region. In this embodiment, the protein comprises a disulfide bond between the first and second cysteine that prevents the post-fusion HRA-HRB six-helix bundle from forming.

[073] In one embodiment, the pre-fusion RSV F protein comprises a first cysteine mutation in the Dili region, and a second cysteine (natural or introduced) in the HRA helix region. In this embodiment, the protein comprises a disulfide bond between the first and second cysteine that prevents the post-fusion HRA-HRB six-helix bundle from forming.

[074] In another embodiment, the pre-fusion RSV F protein comprises a first introduced cysteine in the HRA helix region, HRB helix region, the fusion peptide, helix al, helix a2, helix a3, helix a4, strand βï , strand β2, DI, DII, or Dili region and a second cysteine (natural or introduced) in any other region of the RSV F protein that is in close proximity to the introduced cysteine. In this embodiment, the protein comprises a disulfide

bond between the first and second cysteine that prevents the post-fusion HRA-HRB six-helix bundle from forming.

[075] In a specific embodiment, the pre-fusion RSV F protein comprises two cysteine mutations selected from the group consisting of V56C + V164C, I57C + S190C, T58C+V164C, N165C+V296C, and K168C + V296C, and combinations thereof, thereby comprising a disulfide bridge between the HRA region and the Dili region.

[076] In one embodiment, the pre-fusion RSV F protein comprises two cysteine mutations, V56C and V164C, thereby comprising a disulfide bridge between the HRA region and the Dili region.

[077] In one embodiment, the pre-fusion RSV F protein comprises two cysteine mutations, I57C and S190C, thereby comprising a disulfide bridge between the HRA region and the Dili region.

[078] In one embodiment, the pre-fusion RSV F protein comprises two cysteine mutations, T58C and V164C, thereby comprising a disulfide bridge between the HRA region and the Dili region.

[079] In one embodiment, the pre-fusion RSV F protein comprises two cysteine mutations, N165C and T296C, thereby comprising a disulfide bridge between the HRA region and the Dili region.

[080] In one embodiment, the pre-fusion RSV F protein comprises two cysteine mutations, K168C and T296C, thereby comprising a disulfide bridge between the HRA region and the Dili region.

[081] In one embodiment, the pre-fusion RSV F protein comprises two cysteine mutations, M396C + F483C, thereby comprising a disulfide bridge between the HRB region and the DII region.

[082] The RSV F pre-fusion protein of the present invention is stabilized in the pre-fusion conformation by mutations that stabilize the pre-fusion subunit, which forms trimers.

[083] In some embodiments, the RSV F pre-fusion protein of the present invention is a trimer of RSV F monomers, and pre-fusion conformation is stabilized by one or more disulfide bonds between cysteine residues that are introduced into different monomers.

[084] Exemplary amino acid sequences of RSV F monomers that contain introduced cysteine residues that stabilize the pre-fusion conformation are presented below (SEQ ID NOS: 4-9). The presented sequences contain a signal peptide and a HIS tag (GGSAGSGHHHHHH; SEQ ID NO:3). The pre-fusion RSV F protein of the invention can

contain any of the amino acid sequences shown below, with or without the signal peptide and/or HIS tag.

>RSV F HRA disulfidel (V56C + V164C) (SEQ ID NO: 4)
MELLILKANAITTILTAVTFCFASGQNITEEFYQSTCSAVSKGYLSALRTGWYTSCITIELSNIKEN
KCNGTDAKVKLIKQELDKYKNAVTELQLLMQSTPATNNRARRELPRFMNYTLNNAKKTNVTLSKKRK
RRFLGFLLGVGSAIASGVAVSKVLHLEGECNKIKSALLSTNKAVVSLSNGVSVLTSKVLDLKNYIDK
QLLPIVNKQSCSISNIETVIEFQQKNNRLLEITREFSVNAGVTTPVSTYMLTNSELLSLINDMPITN
DQKKLMSNNVQIVRQQSYSIMSIIKEEVLAYWQLPLYGVIDTPCWKLHTSPLCTTNTKEGSNICLT
RTDRGWYCDNAGSVSFFPQAETCKVQSNRVFCDTMNSLTLPSEVNLCNVDIFNPKYDCKIMTSKTDV
SSSVITSLGAIVSCYGKTKCTASNKNRGIIKTFSNGCDYVSNKGVDTVSVGNTLYYVNKQEGKSLYV
KGEPIINFYDPLVFPSDEFDASISQVNEKINQSLAFIRKSDELLHNVNAGKSTTNGGSAGSGHHHHH
H

>RSV F HRA disulfide2 (I57C + S190C) (SEQ ID NO: 5)
MELLILKANAITTILTAVTFCFASGQNITEEFYQSTCSAVSKGYLSALRTGWYTSVCTIELSNIKEN
KCNGTDAKVKLIKQELDKYKNAVTELQLLMQSTPATNNRARRELPRFMNYTLNNAKKTNVTLSKKRK
RRFLGFLLGVGSAIASGVAVSBCVLHLEGEVNKIKSALLSTNKAWSLSNGVSVLTCBCVLDLKNYIDK
QLLPIVNKQSCSISNIETVIEFQQKNNRLLEITREFSVNAGVTTPVSTYMLTNSELLSLINDMPITN
DQKKLMSNNVQIVRQQSYSIMSIIKEEVLAYWQLPLYGVIDTPCWKLHTSPLCTTNTKEGSNICLT
RTDRGWYCDNAGSVSFFPQAETCKVQSNRVFCDTMNSLTLPSEVNLCNVDIFNPKYDCKIMTSKTDV
SSSVITSLGAIVSCYGKTKCTASNKNRGIIKTFSNGCDYVSNKGVDTVSVGNTLYYVNKQEGKSLYV
KGEPIINFYDPLVFPSDEFDASISQVNEKINQSLAFIRKSDELLHNVNAGKSTTNGGSAGSGHHHHH
H

>RSV F HRA disulfide3 (T58C + V164C) (SEQ ID NO: 6)
MELLILKANAITTILTAVTFCFASGQNITEEFYQSTCSAVSKGYLSALRTGWYTSVICIELSNIKEN
KCNGTDAKVKLIKQELDKYKNAVTELQLLMQSTPATNNRARRELPRFMNYTLNNAKKTNVTLSKKRK
RRFLGFLLGVGSAIASGVAVSKVLHLEGECNKIKSALLSTNKAVVSLSNGVSVLTSKVLDLKNYIDK
QLLPIVNKQSCSISNIETVIEFQQKNNRLLEITREFSVNAGVTTPVSTYMLTNSELLSLINDMPITN
DQKKLMSNNVQIVRQQSYSIMSIIKEEVLAYWQLPLYGVIDTPCWKLHTSPLCTTNTKEGSNICLT
RTDRGWYCDNAGSVSFFPQAETCKVQSNRVFCDTMNSLTLPSEVNLCNVDIFNPKYDCKIMTSKTDV
SSSVITSLGAIVSCYGKTKCTASNKNRGIIKTFSNGCDYVSNKGVDTVSVGNTLYYVNKQEGKSLYV
KGEPIINFYDPLVFPSDEFDASISQVNEKINQSLAFIRKSDELLHNVNAGKSTTNGGSAGSGHHHHH
H

>RSV F HRA disulfide4 (N165C + V296C) (SEQ ID NO: 7)
MELLILKANAITTILTAVTFCFASGQNITEEFYQSTCSAVSKGYLSALRTGWYTSVITIELSNIKEN
KCNGTDAKVKLIKQELDKYKNAVTELQLLMQSTPATNNRARRELPRFMNYTLNNAKKTNVTLSKKRK
RRFLGFLLGVGSAIASGVAVSBCVLHLEGEVCKIKSALLSTNKAWSLSNGVSVLTSBCVLDLKNYIDK
QLLPIVNKQSCSISNIETVIEFQQKNNRLLEITREFSVNAGVTTPVSTYMLTNSELLSLINDMPITN
DQKKLMSNNVQIVRQQSYSIMSIIKEECLAYWQLPLYGVIDTPCWKLHTSPLCTTNTKEGSNICLT
RTDRGWYCDNAGSVSFFPQAETCKVQSNRVFCDTMNSLTLPSEVNLCNVDIFNPKYDCKIMTSKTDV
SSSVITSLGAIVSCYGKTKCTASNKNRGIIKTFSNGCDYVSNKGVDTVSVGNTLYYVNKQEGKSLYV
KGEPIINFYDPLVFPSDEFDASISQVNEKINQSLAFIRKSDELLHNVNAGKSTTNGGSAGSGHHHHH
H

>RSV F HRA disulfides (K168C + V296C) (SEQ ID NO: 8)
MELLILKANAITTILTAVTFCFASGQNITEEFYQSTCSAVSKGYLSALRTGWYTSVITIELSNIKEN

**KCNGTDAKVKLIKQELDKYKNAVTELQLLMQSTPATIWRARRELPRFMNYTLNNAKKTNVTLSKKRK
RRFLGFLLGVGSAIASGVAVSBCVLHLEGEVNKICSALLSTNKAWSLSNGVSVLTSBCVLDLKNYIDK
QLLPIVNKQSCSISNIETVIEFQQKNNRLLEITREFSVNAGVTTPVSTYMLTNSELLSLINDMPITN
DQKKLMSNNVQIVRQQSYSIMSIIKEECLAYWQLPLYGVIDTPCWKLHTSPLCTTNTKEGSNICLT
RTDRGWYCDNAGSVSFFPQAETCKVQSNRVFCDTMNSLTLPSEVNLCNVDIFNPKYDCKIMTSKTDV
SSSVITSLGAIVSCYGKTKCTASNKNRGIIKTFSNGCDYVSNKGVDTVSVGNTLYYVNKQEGKSLYV
KGEPIINFYDPLVFPSDEFDASISQVNEKINQSLAFIRKSDELLHNVNAGKSTTNGGSAGSGHHHHH
H**

>RSV F HRB disulfide (M396C + F483C) (SEQ ID NO: 9)
**MELLILKANAITTILTAVTFCFASGQNITEEFYQSTCSAVSKGYLSALRTGWYTSVITIELSNIKEN
KCNGTDAKVKLIKQELDKYKNAVTELQLLMQSTPATNNRARRELPRFMNYTLNNAKKTNVTLSKKRK
RRFLGFLLGVGSAIASGVAVSKVLHLEGEVNKIKSALLSTNKAVVSLSNGVSVLTSKVLDLKNYIDK
QLLPIVNKQSCSISNIETVIEFQQKNNRLLEITREFSVNAGVTTPVSTYMLTNSELLSLINDMPITN
DQKKLMSNNVQIVRQQSYSIMSIIKEEVLAYWQLPLYGVIDTPCWKLHTSPLCTTNTKEGSNICLT
RTDRGWYCDNAGSVSFFPQAETCKVQSNRVFCDTMNSLTLPSEVNLCNVDIFNPKYDCKICTSKTDV
SSSVITSLGAIVSCYGKTKCTASNKNRGIIKTFSNGCDYVSNKGVDTVSVGNTLYYVNKQEGKSLYV
KGEPIINFYDPLVCPSDEFDASISQVNEKINQSLAFIRKSDELLHNVNAGKSTTNGGSAGSGHHHHH
H**

Destabilization of post-fusion RSV F

[055] A major feature of the RSV F post-fusion structure is the 6-helix bundle in the stalk region. In the post-fusion conformation, the three HRA helices and the three HRB helices form a very stable 6-helix bundle. An alternative strategy for producing a stabilized pre-fusion RSV F protein of the invention, is by destabilizing the post-fusion 6-helix bundle, and/or preventing the 6-helix bundle formation (e.g., through deletion of the HRB helix, introduction of point mutations, addition of glycosylation or other modification sites).

[056] The 6-helix bundle formation may be prevented by deleting the HRA helix or the HRB helix.

[057] Preferably, the HRB helical region is deleted or mutated to prevent formation of the post-fusion conformation. The HRB region forms the stalk of the RSV F pre-fusion conformation, is in close proximity to the viral membrane and likely does not contain important neutralizing epitopes. Deletion of the HRB helix (residues 484 and C-terminal) may prevent the refolding of the RSV F protein from the pre-fusion state to the post-fusion state.

[058] A stabilized pre-fusion RSV F protein of the invention may comprise the RSV ectodomain sequence with the HRB region deleted or mutated, and preferably further comprises an additional mutation or deletion to the remaining ectodomain sequence. For example, the RSV ectodomain may comprise one or more introduced cysteines to create disulfide bridges that stabilize the prefusion structure as described herein, mutated or deleted

furin cleavage sites, mutated or deleted fusion peptide sequence, or other mutations previously described in WO 201 1/008974, incorporated herein in its entirety. The RSV ectodomain may be the ectodomain of a naturally occurring RSV F protein, or it may contain mutations in addition to the deletions and/or mutations of the HRA or HRB region.

[059] In one embodiment, the stabilized pre-fusion RSV F protein comprises an ectodomain of a naturally occurring RSV F protein in which the HRB region is deleted and one or more mutations that prevent cleavage at one or both of the furin cleavage sites (i.e, amino acids 109 and 136 of SEQ ID NOS:l and 2) are present.

[060] In one embodiment, the stabilized pre-fusion RSV F protein comprises an ectodomain of a naturally occurring RSV F protein in which the HRB region is deleted and the fusion peptide is mutated (amino acids 137 and 153 of SEQ ID NOS: 1 or 2). For example, this region can be deleted in whole or in part.

[061] In another embodiment, the stabilized pre-fusion RSV F protein comprises a wild-type RSV ectodomain in which the HRB region and the fusion peptide is deleted, in whole or in part.

[062] In another embodiment, the stabilized pre-fusion RSV F protein comprises a wild-type RSV ectodomain in which the HRB region is deleted and an oligomerization sequence has been added. When an oligomerization sequence is present, it is preferably a trimerization sequence. Suitable oligomerization sequences are well known in the art and include, for example, the coiled coil of the yeast GCN4 leucine zipper protein, trimerizing sequence from bacteriophage T4 fibritin ("foldon"), and the trimer domain of influenza HA.

[063] In another embodiment, the stabilized pre-fusion RSV F protein comprises a wild-type RSV ectodomain in which the HRB region is deleted and the p27 region is mutated (amino acids 110-136 of SEQ ID NOS: 1 or 2), including deletion of the p27 region in whole or in part. For example, lysine and/or arginine residues in the p27 region (about amino acids 110-136 of SEQ ID NOS: 1 or 2) can be substituted or deleted.

[064] In another embodiment, the stabilized pre-fusion RSV F protein comprises a wild-type RSV ectodomain in which the HRB region is deleted and an amino acid sequence that provides a protease cleavage site is added. Generally, the amino acid sequence that provides a protease cleavage site will be located within about 60 amino acids, about 50 amino acids, about 40 amino acids, about 30 amino acids, about 20 amino acids, about 10 amino acids, or substantially adjacent to the amino terminus of the transmembrane domain (amino acid 525 of SEQ ID NO:l or 2).

[065] An exemplary amino acid sequence of an RSV F monomer in which the fusion peptide and HRB are deleted to stabilize the pre-fusion conformation is presented below (SEQ ID NO: 10). The presented sequence contains a signal peptide and a HIS tag (GGSAGSGHHHHHH; SEQ ID NO:3). The pre-fusion RSV F protein of the invention can contain the amino acid sequences shown below, with or without the signal peptide and/or HIS tag.

>RSV F delHRB fusion peptide deletion HIS (SEQ ID NO: 10)
MELLILKANAITTILTAVTFCFASGQNITEEFYQSTCSAVSKGYLSALRTGWYTSVITIELS NIKENKCNGTDAKVKLIKQELDKYKNAVTELQLLMQSTPATNNRARRELPRFMNYTLNNAKK TNVTLSKKRKRRSAIASGVAVSBCVLHLEGEVNKIKSALLSTNKAWSLSNGVSVLTSBCVLDL KNYIDKQLLPIVNKQSCSISNIETVIEFQQKNNRLLEITREFSVNAGVTTPVSTYMLTNSEL LSLINDMPITNDQKKLMSNNVQIVRQQSYSIMSIIKEEVLAYWQLPLYGVIDTPCWKLHTS PLCTTNTKEGSNICLTRTDRGWYCDNAGSVSFFPQAETCBCVQSNRVFCDTMNSLTLPSEVNL CNVDIFNPKYDCKIMTSKTDVSSSVITSLGAIVSCYGKTKCTASNKNRGIIKTFSNGCDYVS NKGVDTVSVGNTLYYVNKQEGKSLYVKGEPIINFYDPLVFPSGGSAGSGHHHHHH

[066] The stabilized pre-fusion RSV F protein of the invention may also be formed by hindering 6-helix bundle formation in the HRA or HRB regions (approximately residues 154-212 and 484 to 513, respectively) through engineered point mutations or introduction of glycosylation sites (e.g., AsnXaaSer/Thr; SEQ ID NO:l 1) or other modification sites (e.g., lipidation, phosphorylation). Glycosylation sites, or other post-translational modification sites or point mutations which interfere with 6-helix bundle formation through electrostatic or steric hindrance, can be introduced through the HRA or HRB helical regions. Glycosylation can interfere with 6-helix bundle formation and prevent flipping of the RSV F construct to the post-fusion conformation.

[067] A stabilized pre-fusion RSV F protein of the invention may comprise one or more mutations that form one or more glycosylation sites in the HRA or HRB helical regions. The RSV F protein may contain mutations or deletions in addition to those that introduce the glycosylation sites in the HRA or HRB helical regions.

[068] In one embodiment, the RSV F protein comprises S173N and N175T mutations and the pre-fusion RSV F protein has a glycosylation site on current serine residue 173.

[069] In another embodiment, the RSV F protein comprises a mutation A177T, so that the pre-fusion RSV F protein has a glycosylation site on current residue N175.

[070] In another embodiment, the RSV F protein comprises G184N and S186T mutations and the pre-fusion RSV F protein has a glycosylation site on current residue G184.

Chimeric pre-fusion F structures with relevant RSV F epitopes

[071] The invention also relates to chimeric pre-fusion F proteins that contain neutralizing epitopes from RSV F protein. Generally, the chimeric pre-fusion F proteins comprise a stabilized F protein from a different virus, such as the Parainfluenza Virus (PIV1, PIV2, PIV3, PIV4, PIV5), Newcastle Disease Virus (NDV), Sendai virus (SeV), Hendra Virus, Nipah Virus (NiV), human metapneumovirus or avian metapneumovirus, in which portions that are exposed on the surface of the protein are replaced with corresponding portions of RSV F. Preferably, the portions contain neutralizing epitopes of RSV F.

[072] For example, any non-RSV (e.g., parainfluenza virus or metapneumovirus) F protein that is stabilized in the pre-fusion conformation (e.g., by virtue of a GCN trimer domain fused C-terminally to the HRB region), may be used as a template for the protein (i.e., an uncleaved NDV F-GCN fusion protein). For example, the SV5 of PIV5 pre-fusion F protein, described by Yin et al., 2006 (145) or the NDV pre-fusion F described by Swanson et al, 2010 (146) may be used in the chimeric F protein construct. The template may then be mutated to introduce known or suspected neutralizing epitopes of RSV F. Thus, the protein may have a pre-fusion F structure exhibiting the neutralizing epitopes, but not non-neutralizing epitopes, of RSV F. A clear benefit to this construct is that it would not raise non-neutralizing RSV F antibodies.

[073] A pre-fusion chimera protein of the invention may comprise a parainfluenza virus F protein, stabilized in the pre-fusion conformation that is mutated to introduce neutralizing epitopes of RSV F. The parainfluenza virus F protein may be any parainfluenza virus F protein, preferably the SV5 of PIV5 pre-fusion F protein, described by Yin et al., 2006 (147) or the NDV pre-fusion F described by Swanson et al, 2010 (146). Exemplary neutralizing epitopes that may be introduced by mutation include the epitopes disclosed in Table 1. For example, the amino acids that form the epitopes recognized by the antibodies listed in Table 1 can be introduced into the corresponding positions (e.g., identified by structural comparison, such as structure based alignment) of a non RSV-F protein (e.g., parainfluenza virus F protein or metapneumovirus F protein) that is stabilized in the pre-fusion conformation. For example, the chimeric F protein can contain the RSV F site A epitope or site C epitope. In particular example, the chimeric F protein contains one or more RSV F residues selected from the amino acid residues at positions 262 - 276 of RSV F. In another particular example, the chimeric F protein contains one or more RSV F residues selected from the amino acid residues at positions 429 - 447 of RSV F.

Table 1. Neutralizing epitopes of RSV F[a]

Site"	mAb	Residues	Method	Reference
A	11	N268I	Escape[c]	(149)
A	151	K272N	Escape	(150)
A	1129	S275F	Escape	(150)
A	1153	N262S	Escape	(150)
A	1200	K272N	Escape	(150)
A	1214	N276Y	Escape	(150)
A	1237	N276Y	Escape	(150)
A	47F	N262Y, N268I	Escape	(151)
A	7C2	K272E, K272T	Escape	(149)
A	B4	K272T	Escape	(149)
A	Fab 19[d]	I266M	Escape	(149)
A	AK13A2	N262Y	Escape	(149)
A	PVZ[e]	K272M, K272Q, N268I	Escape	(152)
A	PVZ[e]	K272M, K272T, S275F	Engineered[f]	(153)
A	MVZ[g]	N262, N268, D269, K272, S275	Structure[h]	(141)
C	7.936	I432T, K433T, V447A	Escape	(154)
C	9.432	S436F	Escape	(154)
C	19[d]	R429S	Escape	(149)
C	19[d]	R429K, R429S, G430A	Engineered	(153)
C	20	R429S	Escape	(149)
C	101F	K433T	Escape	(155)
C	101F	K433D, K433L, K433N, K433Q, K433R	Engineered	(153)
C	101F	R429, 1431, 1432, K433, T434, F435, S436, N437	Structure	(148)

[a] Results of studies using peptide binding or peptide inhibition are not included in this table.
[b] Sites are based on the competition and cross-neutralization analysis of Beeler et al., 1989 (156).
[c] An escape mutation is included if it is the sole mutation in an antibody-resistant strain.
[d] Fabl9 and 19 are unrelated antibodies. The similar names are coincidental.
[e] Palivizumab
[f] Engineered mutations in intact recombinant RSV F that allowed intact processing, full fusion activity and reduced monoclonal antibody binding to less than 15% of wild type are included.
[g] Motavizumab
[h] Residues from peptides in peptide-Fab complex structures are included if either their side chain or backbone atoms make significant contact with the antibody. The biological significance of the peptide-antibody interactions observed in these structural studies has been confirmed by other techniques.

[074] In one embodiment, the chimeric F protein of the invention comprises the HRA region of RSV F (residues 137-212) in place of the equivalent HRA residues of NDV-GCN pre-fusion F. Thus, prefusion F protein (NDV-GCN) is expressed with potential neutralizing epitope sites (HRA region of RSV F) on the top of the pre-fusion F head, permitting neutralizing RSV F antibodies to be elicited. Additional neutralizing epitopes may be added if desired, for example the motavizumab epitope or the 10 IF epitope.

[075] An exemplary amino acid sequence of a chimeric protein containing prefusion NDV F mutated to include RSV F HRA amino acid sequences is presented below (SEQ ID NO: 13). The presented sequences contain a signal peptide, a GCN-trimerization domain and a HIS tag. The chimeric pre-fusion F protein of the invention can contain the amino acid sequence shown below, with or without the signal peptide and/or GCN-trimerization domain and/or HIS tag.

NDV RSV HRA prefusion (underlined portion is RSV HRA, italicized portion is C-terminal GCN trimeric domain and HIS6 (SEQ ID NO: 12) affinity purification tag) (SEQ ID NO: 13).

MGSRSSTRIPVPLMLTVRVMLALSCVCPTSALDGRPLAAAGIVVTGDKAVNIYTSSQTGSIII
KLLPNMPKDKEACAKAPLEAYNRTLTTLLTPLGDSIRRIQESVTTSGGGKQGRLIGAIIGFLG
FLLGVGSAIASGVAVSKVLHLEGEVNKIKSALLSTNKAVVSLSNGVSVLTSKVLDLKNYIDK
QLLPIVNKQSC IKITQQVGVELNLYLTELTTVFGPQITSPALTQLTIQALYNLAGGNMDYLLT
KLGVGNNQLSSLISSGLITGNPILYDSQTQLLGIQVTLPSVGNLNNMRATYLETLSVSTTKGF
ASALVPKVVTQVGSVIEELDTSYCIETDLDLYCTRIVTFPMSPGIYSCLSGNTSACMYSKTEG
ALTTPYMTLKGSVIANCKMTTCRCADPPGIISQNYGEAVSLIDRQSCNILSLDGITLRLSGEFD
ATYQKNISIQDSQVIVTGNLDISTELGNVNNSISNALDKLEESNSKLDKVED^ffiE/L *SKIHffiN*
EIARIKKLIGEAGGPLVPRGSHHHHHH

The RSV F glycoprotein

[076] The F glycoprotein of RSV directs viral penetration by fusion between the virion envelope and the host cell plasma membrane. It is a type I single-pass integral membrane protein having four general domains: N-terminal ER-translocating signal sequence (SS), ectodomain (ED), transmembrane domain (TM), and a cytoplasmic tail (CT). CT contains a single palmitoylated cysteine residue. The sequence of F protein is highly conserved among RSV isolates, but is constantly evolving (7). Unlike most paramyxoviruses, the F protein in RSV can mediate entry and syncytium formation independent of the other viral proteins (HN is usually necessary in addition to F in other paramyxoviruses).

[077] The hRSV F mRNA is translated into a 574 amino acid precursor protein designated F_0, which contains a signal peptide sequence at the N-terminus that is removed by a signal peptidase in the endoplasmic reticulum. Fo is cleaved at two sites (a.a. 109/1 10 and 136/137) by cellular proteases (in particular furin) in the trans-Golgi, removing a short glycosylated intervening sequence and generating two subunits designated Fi (-50 kDa; C-terminus; residues 137-574) and F_2 (-20 kDa; N- terminus; residues 1-109) (See, *e.g.*, FIG. 4A). Fi contains a hydrophobic fusion peptide at its N-terminus and also two hydrophobic

heptad-repeat regions (HRA and HRB). HRA is near the fusion peptide and HRB is near to the transmembrane domain (See, *e.g.,* FIG. 4A). The Fi-F_2 heterodimers are assembled as homotrimers in the virion.

[078] RSV exists as a single serotype but has two antigenic subgroups: A and B. The F glycoproteins of the two groups are about 90% identical. The A subgroup, the B subgroup, or a combination or hybrid of both can be used in the invention. An example sequence for the A subgroup is SEQ ID NO: 1 (A2 strain; GenBank GI: 138251; Swiss Prot P03420), and for the B subgroup is SEQ ID NO: 2 (18537 strain; GI: 138250; Swiss Prot P13843). SEQ ID NO:l and SEQ ID NO:2 are both 574 amino acid sequences. The signal peptide in A2 strain is a.a. 1-21, but in 18537 strain it is 1-22. In both sequences the TM domain is from about a.a. 530-550, but has alternatively been reported as 525-548.

SEQ ID NO: 1

```
  1  MELLILKANAITTILTAVTFCFASGQNITEEFYQSTCSAVSKGYLSALRTGWYTSVITIE   60
 61  LSNIKENKCNGTDAKVKLIKQELDKYKNAVTELQLLMQSTPPTNNRARRELPRFMNYTLN   120
121  NAKKTNVTLSKKRKRRFLGFLLGVGSAIASGVAVSKVLHLEGEVNKIKSALLSTNKAWS    180
181  LSNGVSVLTSKVLDLKNYIDKQLLPIVNKQSCS ISNIETVIEFQQKNNRLLEITREFSVN   240
241  AGVTTPVSTYMLTNSELLSLINDMPITNDQKKLMSNNVQIVRQQSYS IMSIIKEEVLAYV   300
301  VQLPLYGVIDTPCWKLHTSPLCTTNTKEGSNICLTRTDRGWYCDNAGSVSFFPQAETCKV   360
361  QSNRVFCDTMNSLTLPSEINLCNVDIFNPKYDCKIMTSKTDVSSSVITSLGAIVSCYGKT   420
421  KCTASNKNRGI IKTFSNGCDYVSNKGMDTVSVGNTLYYVNKQEGKSLYVKGEP IINFYDP   480
481  LVFPSDEFDAS ISQVNEKINQSLAF IRKSDELLHNVNAGKSTTNIMITTI IIVI IVILLS   540
541  LIAVGLLLYCKARSTPVTLSKDQLSGINNIAFSN   574
```

SEQ ID NO: 2

```
  1  MELLIHRSSAIFLTLAVNALYLTSSQNITEEFYQSTCSAVSRGYFSALRTGWYTSVITIE   60
 61  LSNIKETKCNGTDTKVKLIKQELDKYKNAVTELQLLMQNTPAANNRARREAPQYMNYTIN   120
121  TTKNLNVSISKKRKRRFLGFLLGVGSAIASGIAVSKVLHLEGEVNKIKNALLSTNKAWS    180
181  LSNGVSVLTSKVLDLKNYINNRLLPIVNQQSCRISNIETVIEFQQMNSRLLEITREFSVN   240
241  AGVTTPLSTYMLTNSELLSLINDMPITNDQKKLMSSNVQIVRQQSYS IMSIIKEEVLAYV   300
301  VQLPI YGVIDTPCWKLHTSPLCTTNIKEGSNICLTRTDRGWYCDNAGSVSFFPQADTCKV   360
361  QSNRVFCDTMNSLTLPSEVSLCNTDIFNSKYDCKIMTSKTDISSSVITSLGAIVSCYGKT   420
421  KCTASNKNRGI IKTFSNGCDYVSNKGVDTVSVGNTLYYVNKLEGKNLYVKGEP IINYYDP   480
481  LVFPSDEFDAS ISQVNEKINQSLAF IRRSDELLHNVNTGKSTTNIMITT IIIVI IWLLS   540
541  LIAIGLLLYCKAKNTPVTLSKDQLSGINNIAFSK   574
```

[079] The invention may use any desired RSV F amino acid sequence, such as the amino acid sequence of SEQ ID NO: 1 or 2, or a sequence having identity to SEQ ID NO: 1 or 2. Typically it will have at least 75% identity to SEQ ID NO: 1 or 2 *e.g.,* at least 80%, at least 85%, at least 90%, at least 95%, at least 97%, at least 98%, at least 99%,identity to SEQ ID NO:l or 2. The sequence may be found naturally in RSV.

[080] Where the invention uses an ectodomain of F protein, in whole or in part, it may comprise:

(i) a polypeptide comprising about amino acid 22-525 of SEQ ID NO: 1.

(ii) a polypeptide comprising about amino acids 23-525 of SEQ ID NO: 2.

(iii) a polypeptide comprising an amino acid sequence having at least 75% identity *(e.g.,* at least 80%, at least 85%, at least 90%, at least 95%, at least 97%, at least 98%, at least 99% identity) to (i) or (ii).

(iv) a polypeptide comprising a fragment of (i), (ii) or (iii), wherein the fragment comprises at least one **F** protein epitope. The fragment will usually be at least about 100 amino acids long, *e.g.* , at least about 150, at least about 200, at least about 250, at least about 300, at least about 350, at least about 400, at least about 450 amino acids long.

[081] The ectodomain can be an **Fo** form with or without the signal peptide, or can comprise two separate peptide chains *(e.g.,* an **Fi** subunit and a $\mathbf{F_2}$ subunit) that are associated with each other, for example, the subunits may be linked by a disulfide bridge. Accordingly, all or a portion of about amino acid 101 to about 161, such as amino acids 110-136, may be absent from the ectodomain. Thus the ectodomain, in whole or in part, can comprise:

(v) a first peptide chain and a second peptide chain that is associated with the first polypeptide chain, where the first peptide chain comprises an amino acid sequence having at least 75% identity *(e.g.,* at least 80%, at least 85%, at least 90%, at least 95%, at least 97%, at least 98%, at least 99%, or even 100% identity) to about amino acid 22 to about amino acid 101 of SEQ ID NO: 1 or to about amino acid 23 to about amino acid 101 of SEQ ID NO: 2, and the second peptide chain comprises an amino acid sequence having at least 75% identity *(e.g.* , at least 80%, at least 85%, at least 90%, at least 95%, at least 97%, at least 98%, at least 99%, or even 100% identity) to about amino acid 162 to about 525 of SEQ ID NO: 1 or to about amino acid 162 to 525 of SEQ ID NO: 2.

(vi) a first peptide chain and a second peptide chain that is associated with the first polypeptide chain, where the first peptide chain comprises an amino acid sequence comprising a fragment of about amino acid 22 to about amino acid 101 of SEQ ID NO: 1 or of about amino acid 23 to about amino acid 109 of SEQ ID NO: 2, and the second peptide chain comprises a fragment of about amino acid 162 to about amino acid 525 of SEQ ID NO: 1 or of about amino acid 161 to about amino acid 525 of SEQ ID NO: 2. One or both of the fragments will comprise at least one **F** protein epitope. The fragment in the first peptide chain will usually be at least 20 amino acids long, *e.g.* , at least 30, at least 40, at least 50, at least 60, at least 70, at least 80 amino acids long. The fragment in the second peptide chain will usually be at least 100 amino acids long, *e.g.* , at least 150, at least 200, at least 250, at least 300, at least 350, at least 400, at least 450 amino acids long.

(vii) a molecule obtainable by furin digestion of (i), (ii), (iii) or (iv).

[082] Thus an amino acid sequence used with the invention may be found naturally within RSV F protein (e.g., a soluble RSV F protein lacking TM and CT, about amino acids 522-574 of SEQ ID NOS: 1 or 2), and/or it may have one or more *(e.g.,* 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21, 22, 23, 24, 25, 26, 27, 28, 29, 30) single amino acid mutations (insertions, deletions or substitutions) relative to a natural RSV sequence. For instance, it is known to mutate F proteins to eliminate their furin cleavage sequences, thereby preventing intracellular processing. In certain embodiments, the RSV F protein lacks TM and CT (about amino acids 522-574 of SEQ ID NOS: 1 or 2) and contains one or more (e.g., 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21, 22, 23, 24, 25, 26, 27, 28, 29, 30) single amino acid mutations (insertions, deletions or substitutions) relative to a natural RSV sequence.

Furin-cleavage, Trypsin-cleavage and Fusion Peptide Mutations

[083] If desired, post-fusion RSV F polypeptides or proteins may contain one or more mutations, for example, mutations that prevent cleavage at one or both of the furin cleavage sites *(i.e.,* amino acids 109 and 136 of SEQ ID NOS: 1 and 2), that prevent cleavage of or introduce trypsin cleavage sites, mutations in the p27 region, and/or mutation in the fusion peptide. Such mutations can prevent aggregation of the soluble polypeptides or proteins and thereby facilitate purifications, can prevent cell-cell fusion if the RSV F protein is expressed on the surface of a cell, such as by expression from a viral replicon (e.g., alphavirus replicon particles), or if the RSV F protein is a component of a virus-like particle.

[084] Examples of suitable furin cleavage mutations include replacement of amino acid residues 106 - 109 of SEQ ID NO: 1 or 2 with RARK (SEQ ID NO: 14), RARQ (SEQ ID NO:15), QAQN (SEQ ID NO:16), or IEGR (SEQ ID NO:17). Alternatively, or in addition, amino acid residues 133 - 136 of SEQ ID NO: 1 or 2 can be replaced with RKKK (SEQ ID NO: 18), AAAR, QNQN (SEQ ID NO: 19), QQQR (SEQ ID NO:20) or IEGR (SEQ ID NO: 17). (Δ indicates that the amino acid residue has been deleted.) These furin cleavage mutations can be combined, if desired, with other mutations described herein, such as trypsin cleavage mutations and fusion peptide mutations.

[085] Examples of suitable trypsin cleavage mutations include deletion of any lysine or arginine residue between about position 101 and position 161 of SEQ ID NO:l or 2, or replacement of any such lysine or arginine residue with an amino acid other than lysine or arginine. For example, lysine and/or arginine residues in the p27 region (about amino acids

110-136 of SEQ ID NOS: 1 or 2) can be substituted or deleted, including deletion of the p27 region in whole or in part.

[086] The mutations described herein can be combined, if desired, in any combination. For example, furin mutations can be combined with partial or complete deletion of the fusion peptide region and/or deletion of the HRA or HRB helical region.

[087] In addition to the mutations described above, e.g., furin-cleavage and fusion peptide mutations, or alternatively, soluble RSV F polypeptides or proteins, such as those that lack the transmembrane region and cytoplasmic tail, or HRA and HRB deletions, or cysteine mutations, may contain one or more oligomerization sequences. When an oligomerization sequence is present, it is preferably a trimerization sequence. Suitable oligomerization sequences are well known in the art and include, for example, the coiled coil of the yeast GCN4 leucine zipper protein, trimerizing sequence from bacteriophage T4 fibritin ("foldon"), and the trimer domain of influenza HA. These and other suitable oligomerization sequences are described in greater detail herein.

[088] In particular embodiments, the sequence of the carboxy terminus of the RSV F polypeptide or protein, starting from position 480, is

(GCN) PLVFPSDEFDAS ISQVNEKINQSLAF IRKSDELLHNVNDKIEEILSKI YHIENE IARIKKLIGE (SEQ ID NO: 21)

(HA) PLVFP SDEF DAS ISQVNEKINQSLAF IRKSDELLHNVNEKF HQ IEKEFSEVEGRIQDLEK (SEQ ID NO :22)

(Idealized helix) PLVFPSDEFDASISQINEKINQILAFIRKIDELLHNIN (SEQ ID NO:23)

(foldon short)
PLVFPSDEFDAS ISQVNEKINQSLAF IRKSDELLHNVNGSGYIPEAPRDGQAYVRKDGEWVLLSTFL (SEQ ID NO :24); or

(foldon long)
PLVFPSDEFDAS ISQVNEKINQSLAF IRKSDELLHNVNNKNDDKGSGYIPEAPRDGQAYVRKDGEWVLLSTFL
(SEQ ID NO:25)

[089] If desired, RSV F polypeptides or proteins that contain a transmembrane region may contain an added amino acid sequence that provides a protease cleavage site. This type of RSV F polypeptide or protein can be produced by expression on the surface of a cell, and recovered in soluble form after cleavage from the cell surface using an appropriate protease. Generally, the amino acid sequence that provides a protease cleavage site will be

located within about 60 amino acids, about 50 amino acids, about 40 amino acids, about 30 amino acids, about 20 amino acids, about 10 amino acids, or substantially adjacent to the amino terminus of the transmembrane domain (amino acid 525 of SEQ ID NO:1 or 2). Many suitable amino acid sequences that are cleaved by commercially available proteases are well-known in the art. For example, thrombin cleaves the sequence LVPR (SEQ ID NO:26), factor Xa cleaves the sequence IEGR (SEQ ID NO: 17) and enterokinase cleaves the sequence DDDDK (SEQ ID NO:27). These amino acid sequences can be introduced into an RSV F polypeptide.

[090] Immunogenic polypeptides used according to the invention will usually be isolated or purified. Thus, they will not be associated with molecules with which they are normally, if applicable, found in nature. For example, an F protein used with the invention will not be in the form of a RSV virion (although it may be in the form of an artificial virion, such as a virosome or VLP).

[091] Polypeptides will usually be prepared by expression in a recombinant host system. Generally, they (e.g., RSV ecto-domains) are produced by expression of recombinant constructs that encode the ecto-domains in suitable recombinant host cells, although any suitable methods can be used. Suitable recombinant host cells include, for example, insect cells (e.g., *Aedes aegypti, Autographa californica, Bombyx mori, Drosophila melanogaster, Spodoptera frugiperda,* and *Trichoplusia ni),* mammalian cells (e.g., human, non-human primate, horse, cow, sheep, dog, cat, and rodent *(e.g.,* hamster), avian cells (e.g., chicken, duck, and geese), bacteria (e.g., E. coli, Bacillus subtilis, and Streptococcus spp.), yeast cells (e.g., *Saccharomyces cerevisiae, Candida albicans, Candida maltosa, Hansenual polymorpha, Kluyveromyces fragilis, Kluyveromyces lactis, Pichia guillerimondii, Pichia pastoris, Schizosaccharomyces pombe* and *Yarrowia lipolytica),* Tetrahymena cells *(e.g., Tetrahymena thermophila)* or combinations thereof. Many suitable insect cells and mammalian cells are well-known in the art. Suitable insect cells include, for example, Sf9 cells, Sf21 cells, Tn5 cells, Schneider S2 cells, and High Five cells (a clonal isolate derived from the parental Trichoplusia ni BTI-TN-5B1-4 cell line (Invitrogen)). Suitable mammalian cells include, for example, Chinese hamster ovary (CHO) cells, human embryonic kidney cells (HEK293 cells, typically transformed by sheared adenovirus type 5 DNA), NIH-3T3 cells, 293-T cells, Vero cells, HeLa cells, PERC.6 cells (ECACC deposit number 96022940), Hep G2 cells, MRC-5 (ATCC CCL-171), WI-38 (ATCC CCL-75), fetal rhesus lung cells (ATCC CL-160), Madin-Darby bovine kidney ("MDBK") cells, Madin-Darby canine kidney ("MDCK") cells (e.g., MDCK (NBL2), ATCC CCL34; or MDCK 33016, DSM ACC 2219),

baby hamster kidney (BHK) cells, such as BHK21-F, HKCC cells, and the like. Suitable avian cells include, for example, chicken embryonic stem cells (e.g., EBx® cells), chicken embryonic fibroblasts, chicken embryonic germ cells, duck cells (e.g., AGE1.CR and AGEl.CR.pIX cell lines (ProBioGen) which are described, for example, in *Vaccine* 27:4975-4982 (2009) and WO2005/042728), EB66 cells, and the like.

[092] Suitable insect cell expression systems, such as baculovirus systems, are known to those of skill in the art and described in, *e.g.*, Summers and Smith, *Texas Agricultural Experiment Station Bulletin* No. 1555 (1987). Materials and methods for baculovirus/insert cell expression systems are commercially available in kit form from, *inter alia,* Invitrogen, San Diego CA. Avian cell expression systems are also known to those of skill in the art and described in, *e.g.*, U.S. Patent Nos. 5,340,740; 5,656,479; 5,830,510; 6,1 14,168; and 6,500,668; European Patent No. EP 0787180B; European Patent Application No. EP03291813.8 ;WO 03/043415; and WO 03/076601. Similarly, bacterial and mammalian cell expression systems are also known in the art and described in, *e.g., Yeast Genetic Engineering* (Barr *et al,* eds., 1989) Butterworths, London.

[093] Recombinant constructs encoding pre-fusion RSV F protein can be prepared in suitable vectors using conventional methods. A number of suitable vectors for expression of recombinant proteins in insect or mammalian cells are well-known and conventional in the art. Suitable vectors can contain a number of components, including, but not limited to one or more of the following: an origin of replication; a selectable marker gene; one or more expression control elements, such as a transcriptional control element (e.g., a promoter, an enhancer, a terminator), and/or one or more translation signals; and a signal sequence or leader sequence for targeting to the secretory pathway in a selected host cell (e.g., of mammalian origin or from a heterologous mammalian or non-mammalian species). For example, for expression in insect cells a suitable baculovirus expression vector, such as pFastBac (Invitrogen), is used to produce recombinant baculovirus particles. The baculovirus particles are amplified and used to infect insect cells to express recombinant protein. For expression in mammalian cells, a vector that will drive expression of the construct in the desired mammalian host cell (e.g., Chinese hamster ovary cells) is used.

[094] Pre-fusion RSV F protein polypeptides can be purified using any suitable methods. For example, methods for purifying pre-fusion RSV F polypeptides by immunoaffinity chromatography are known in the art. *Ruiz-Arguello et al, J. Gen. Virol,* §5:3677-3687 (2004). Suitable methods for purifying desired proteins including precipitation and various types of chromatography, such as hydrophobic interaction, ion exchange,

affinity, chelating and size exclusion are well-known in the art. Suitable purification schemes can be created using two or more of these or other suitable methods. If desired, the pre-cision RSV F protein polypeptides can include a "tag" that facilitates purification, such as an epitope tag or a HIS tag. Such tagged polypeptides can conveniently be purified, for example from conditioned media, by chelating chromatography or affinity chromatography.

[095] The pre-fusion RSV F polypeptides may also be produced *in situ* by expression of nucleic acids that encode them in the cells of a subject. For example, by expression of a self-replicating RNA described herein.

[096] Polypeptides may include additional sequences in addition to the pre-fusion RSV sequences. For example, a polypeptide may include a sequence to facilitate purification *{e.g.,* a poly-His sequence). Similarly, for expression purposes, the natural leader peptide of F protein may be substituted for a different one. For example, reference 6 used a honeybee melittin leader peptide in place of the natural one.

Self-Replicating RNA

[097] The pre-fusion RSV-F polypeptides described herein can be produced by expression of recombinant nucleic acids that encode the polypeptides in the cells of a subject. Preferred nucleic acids that can be administered to a subject to cause the production of pre-fusion RSV-F polypeptides are self-replicating RNA molecules. The self-replicating RNA molecules of the invention are based on the genomic RNA of RNA viruses, but lack the genes encoding one or more structural proteins. The self-replicating RNA molecules are capable of being translated to produce non-structural proteins of the RNA virus and heterologous proteins encoded by the self-replicating RNA.

[098] The self-replicating RNA generally contains at least one or more genes selected from the group consisting of viral replicase, viral proteases, viral helicases and other nonstructural viral proteins, and also comprise 5'- and 3'-end cis-active replication sequences, and if desired, a heterologous sequences that encode a desired amino acid sequences (e.g., a protein, an antigen). A subgenomic promoter that directs expression of the heterologous sequence can be included in the self-replicating RNA. If desired, the heterologous sequence may be fused in frame to other coding regions in the self-replicating RNA and/or may be under the control of an internal ribosome entry site (IRES).

[099] Self-replicating RNA molecules of the invention can be designed so that the self-replicating RNA molecule cannot induce production of infectious viral particles. This can be achieved, for example, by omitting one or more viral genes encoding structural

proteins that are necessary for the production of viral particles in the self-replicating RNA. For example, when the self-replicating RNA molecule is based on an alpha virus, such as Sinebis virus (SIN), Semliki forest virus and Venezuelan equine encephalitis virus (VEE), one or more genes encoding viral structural proteins, such as capsid and/or envelope glycoproteins, can be omitted. If desired, self-replicating RNA molecules of the invention can be designed to induce production of infectious viral particles that are attenuated or virulent, or to produce viral particles that are capable of a single round of subsequent infection.

[0100] A self-replicating RNA molecule can, when delivered to a vertebrate cell even without any proteins, lead to the production of multiple daughter RNAs by transcription from itself (or from an antisense copy of itself). The self-replicating RNA can be directly translated after delivery to a cell, and this translation provides a RNA-dependent RNA polymerase which then produces transcripts from the delivered RNA. Thus the delivered RNA leads to the production of multiple daughter RNAs. These transcripts are antisense relative to the delivered RNA and may be translated themselves to provide in situ expression of a gene product, or may be transcribed to provide further transcripts with the same sense as the delivered RNA which are translated to provide in situ expression of the encoded RSV-F polypeptide.

[0101] One suitable system for achieving self-replication is to use an alphavirus-based RNA replicon. These + stranded replicons are translated after delivery to a cell to give of a replicase (or replicase-transcriptase). The replicase is translated as a polyprotein which auto cleaves to provide a replication complex which creates genomic - strand copies of the + strand delivered RNA. These - strand transcripts can themselves be transcribed to give further copies of the + stranded parent RNA and also to give a subgenomic transcript which encodes the RSV-F polypeptide. Translation of the subgenomic transcript thus leads to in situ expression of the RSV-F polypeptide by the infected cell. Suitable alphavirus replicons can use a replicase from a sindbis virus, a semliki forest virus, an eastern equine encephalitis virus, a Venezuelan equine encephalitis virus, etc.

[0102] A preferred self-replicating RNA molecule thus encodes (i) a RNA-dependent RNA polymerase which can transcribe RNA from the self-replicating RNA molecule and (ii) an RSV-F polypeptide. The polymerase can be an alphavirus replicase e.g. comprising alphavirus protein nsP4.

[0103] Whereas natural alphavirus genomes encode structural virion proteins in addition to the non structural replicase polyprotein, it is preferred that an alphavirus based

self-replicating RNA molecule of the invention does not encode alphavirus structural proteins. Thus the self replicating RNA can lead to the production of genomic RNA copies of itself in a cell, but not to the production of RNA-containing alphavirus virions. The inability to produce these virions means that, unlike a wild-type alphavirus, the self-replicating RNA molecule cannot perpetuate itself in infectious form. The alphavirus structural proteins which are necessary for perpetuation in wild-type viruses are absent from self replicating RNAs of the invention and their place is taken by gene(s) encoding the desired gene product, such that the subgenomic transcript encodes the desired gene product rather than the structural alphavirus virion proteins.

[0104] Thus a self-replicating RNA molecule useful with the invention may have two open reading frames. The first (5') open reading frame encodes a replicase; the second (3') open reading frame encodes an RSV-F polypeptide. In some embodiments the RNA may have additional (downstream) open reading frames e.g. that encode further desired gene products. A self-replicating RNA molecule can have a 5' sequence which is compatible with the encoded replicase.

[0105] In one aspect, the self-replicating RNA molecule is derived from or based on an alphavirus. In other aspects, the self-replicating RNA molecule is derived from or based on a virus other than an alphavirus, preferably, a positive-stranded RNA viruses, and more preferably a picornavirus, flavivirus, rubivirus, pestivirus, hepacivirus, calicivirus, or coronavirus. Suitable wild-type alphavirus sequences are well-known and are available from sequence depositories, such as the American Type Culture Collection, Rockville, Md. Representative examples of suitable alphaviruses include Aura (ATCC VR-368), Bebaru virus (ATCC VR-600, ATCC VR-1240), Cabassou (ATCC VR-922), Chikungunya virus (ATCC VR-64, ATCC VR-1241), Eastern equine encephalomyelitis virus (ATCC VR-65, ATCC VR-1242), Fort Morgan (ATCC VR-924), Getah virus (ATCC VR-369, ATCC VR-1243), Kyzylagach (ATCC VR-927), Mayaro (ATCC VR-66), Mayaro virus (ATCC VR-1277), Middleburg (ATCC VR-370), Mucambo virus (ATCC VR-580, ATCC VR-1244), Ndumu (ATCC VR-371), Pixuna virus (ATCC VR-372, ATCC VR-1245), Ross River virus (ATCC VR-373, ATCC VR-1246), Semliki Forest (ATCC VR-67, ATCC VR-1247), Sindbis virus (ATCC VR-68, ATCC VR-1248), Tonate (ATCC VR-925), Triniti (ATCC VR-469), Una (ATCC VR-374), Venezuelan equine encephalomyelitis (ATCC VR-69, ATCC VR-923, ATCC VR-1250 ATCC VR-1249, ATCC VR-532), Western equine encephalomyelitis (ATCC VR-70, ATCC VR-1251, ATCC VR-622, ATCC VR-1252), Whataroa (ATCC VR-926), and Y-62-33 (ATCC VR-375).

[0106] The self-replicating RNA may be associated with a delivery system. The self-replicating RNA may be administered with or without an adjuvant.

RNA DELIVERY SYSTEMS

[0107] The self-replicating RNA of the invention are suitable for delivery in a variety of modalities, such as naked RNA delivery or in combination with lipids, polymers or other compounds that facilitate entry into the cells. Self-replicating RNA molecules of the present invention can be introduced into target cells or subjects using any suitable technique, *e.g.,* by direct injection, microinjection, electroporation, lipofection, biolystics, and the like. The self-replicating RNA molecule may also be introduced into cells by way of receptor-mediated endocytosis. See *e.g.,* U.S. Pat. No. 6,090,619; Wu and Wu, J. Biol. Chem., 263:14621 (1988); and Curiel *et al.,* Proc. Natl. Acad. Sci. USA, 88:8850 (1991). For example, U.S. Pat. No. 6,083,741 discloses introducing an exogenous nucleic acid into mammalian cells by associating the nucleic acid to apolycation moiety *(e.g.,* poly-L-lysine having 3-100 lysine residues), which is itself coupled to an integrin receptor-binding moiety *(e.g.,* a cyclic peptide having the sequence Arg-Gly-Asp).

[0108] The self-replicating RNA molecule of the present invention can be delivered into cells via amphiphiles. See *e.g.,* U.S. Pat. No. 6,071,890. Typically, a nucleic acid molecule may form a complex with the cationic amphiphile. Mammalian cells contacted with the complex can readily take it up.

[0109] The self-replicating RNA can be delivered as naked RNA *(e.g.* merely as an aqueous solution of RNA) but, to enhance entry into cells and also subsequent intercellular effects, the self-replicating RNA is preferably administered in combination with a delivery system, such as a particulate or emulsion delivery system. A large number of delivery systems are well known to those of skill in the art. Such delivery systems include, for example liposome-based delivery (Debs and Zhu (1993) WO 93/24640; Mannino and Gould-Fogerite (1988) BioTechniques 6(7): 682-691; Rose U.S. Pat. No. 5,279,833; Brigham (1991) WO 91/06309; and Feigner *et al.* (1987) Proc. Natl. Acad. Sci. USA 84: 7413-7414), as well as use of viral vectors *(e.g.,* adenoviral (see, *e.g.,* Berns *et al.* (1995) Ann. NY Acad. Sci. 772: 95-104; Ali *et al.* (1994) Gene Ther. 1: 367-384; and Haddada *et al.* (1995) Curr. Top. Microbiol. Immunol. 199 (Pt 3): 297-306 for review), papillomaviral, retroviral (see, *e.g.,* Buchscher *et al.* (1992) J. Virol. 66(5) 2731-2739; Johann *et al.* (1992) J. Virol. 66 (5): 1635-1640 (1992); Sommerfelt *et al.,* (1990) Virol. 176:58-59; Wilson *et al.* (1989) J. Virol. 63:2374-2378; Miller *et al.,* J. Virol. 65:2220-2224 (1991); Wong-Staal *etal,*

PCT/US94/05700, and Rosenburg and Fauci (1993) in Fundamental Immunology, Third Edition Paul (ed) Raven Press, Ltd., New York and the references therein, and Yu *et al.*, Gene Therapy (1994) supra.), and adeno-associated viral vectors (see, West *et al.* (1987) Virology 160:38-47; Carter *et al.* (1989) U.S. Pat. No. 4,797,368; Carter *et al.* WO 93/24641 (1993); Kotin (1994) Human Gene Therapy 5:793-801; Muzyczka (1994) J. Clin. Invst. 94:1351 and Samulski (supra) for an overview of AAV vectors; see also, Lebkowski, U.S. Pat. No. 5,173,414; Tratschin *etal.* (1985) Mol. Cell. Biol. 5(1 1):3251-3260; Tratschin, *et al.* (1984) Mol. Cell. Biol., 4:2072-2081; Hermonat and Muzyczka (1984) Proc. Natl. Acad. Sci. USA, 81:6466-6470; McLaughlin *et al.* (1988) and Samulski *et al.* (1989) J. Virol., 63:03822-3828), and the like.

[0110] Three particularly useful delivery systems are (i) liposomes (ii) non-toxic and biodegradable polymer microparticles (iii) cationic submicron oil-in-water emulsions.

Liposomes

[0111] Various amphiphilic lipids can form bilayers in an aqueous environment to encapsulate a RNA-containing aqueous core as a liposome. These lipids can have an anionic, cationic or zwitterionic hydrophilic head group. Formation of liposomes from anionic phospholipids dates back to the 1960s, and cationic liposome-forming lipids have been studied since the 1990s. Some phospholipids are anionic whereas other are zwitterionic. Suitable classes of phospholipid include, but are not limited to, phosphatidylethanolamines, phosphatidylcholines, phosphatidylserines, and phosphatidylglycerols, and some useful phospholipids are listed in Table 2. Useful cationic lipids include, but are not limited to, dioleoyl trimethylammonium propane (DOTAP), l,2-distearyloxy-N,N-dimethyl-3-aminopropane (DSDMA), l,2-dioleyloxy-N,Ndimethyl-3-aminopropane (DODMA), 1,2-dilinoleyloxy-N,N-dimethyl-3-aminopropane (DLinDMA), 1,2-dilinolenyloxy-N,N-dimethyl-3-aminopropane (DLenDMA). Zwitterionic lipids include, but are not limited to, acyl zwitterionic lipids and ether zwitterionic lipids. Examples of useful zwitterionic lipids are DPPC, DOPC and dodecylphosphocholine. The lipids can be saturated or unsaturated.

[0112] Liposomes can be formed from a single lipid or from a mixture of lipids. A mixture may comprise (i) a mixture of anionic lipids (ii) a mixture of cationic lipids (iii) a mixture of zwitterionic lipids (iv) a mixture of anionic lipids and cationic lipids (v) a mixture of anionic lipids and zwitterionic lipids (vi) a mixture of zwitterionic lipids and cationic lipids or (vii) a mixture of anionic lipids, cationic lipids and zwitterionic lipids. Similarly, a mixture may comprise both saturated and unsaturated lipids. For example, a mixture may comprise

DSPC (zwitterionic, saturated), DlinDMA (cationic, unsaturated), and/or DMPG (anionic, saturated). Where a mixture of lipids is used, not all of the component lipids in the mixture need to be amphiphilic *e.g.* one or more amphiphilic lipids can be mixed with cholesterol.

[0113] The hydrophilic portion of a lipid can be PEGylated *(i.e.* modified by covalent attachment of a polyethylene glycol). This modification can increase stability and prevent non-specific adsorption of the liposomes. For instance, lipids can be conjugated to PEG using techniques such as those disclosed in Heyes *etal.* (2005) *J Controlled Release* 107:276-287.

[0114] A mixture of DSPC, DlinDMA, PEG-DMPG and cholesterol is used in the examples. A separate aspect of the invention is a liposome comprising DSPC, DlinDMA, PEG-DMG and cholesterol. This liposome preferably encapsulates RNA, such as a self-replicating RNA *e.g.* encoding an immunogen.

[0115] Liposomes are usually divided into three groups: multilamellar vesicles (MLV); small unilamellar vesicles (SUV); and large unilamellar vesicles (LUV). MLVs have multiple bilayers in each vesicle, forming several separate aqueous compartments. SUVs and LUVs have a single bilayer encapsulating an aqueous core; SUVs typically have a diameter <50nm, and LUVs have a diameter >50nm. Liposomes useful with of the invention are ideally LUVs with a diameter in the range of 50-220nm. For a composition comprising a population of LUVs with different diameters: (i) at least 80% by number should have diameters in the range of 20-220nm, (ii) the average diameter (Zav, by intensity) of the population is ideally in the range of 40-200nm, and/or (iii) the diameters should have a polydispersity index <0.2.

[0116] Techniques for preparing suitable liposomes are well known in the art *e.g.* see Liposomes: Methods and Protocols, Volume 1: Pharmaceutical Nanocarriers: Methods and Protocols. (ed. Weissig). Humana Press, 2009. ISBN 160327359X; Liposome Technology, volumes I, II & III. (ed. Gregoriadis). Informa Healthcare, 2006; and Functional Polymer Colloids and Microparticles volume 4 (Microspheres, microcapsules & liposomes). (eds. Arshady & Guyot). Citus Books, 2002. One useful method involves mixing (i) an ethanolic solution of the lipids (ii) an aqueous solution of the nucleic acid and (iii) buffer, followed by mixing, equilibration, dilution and purification (Heyes *et al.* (2005) *J Controlled Release* 107:276-87.).

[0117] RNA is preferably encapsulated within the liposomes, and so the liposome forms a outer layer around an aqueous RNA-containing core. This encapsulation has been found to protect RNA from RNase digestion.. The liposomes can include some external RNA

(e.g. on the surface of the liposomes), but at least half of the RNA (and ideally all of it) is encapsulated.

Polymeric microparticles

[0118] Various polymers can form microparticles to encapsulate or adsorb RNA. The use of a substantially non-toxic polymer means that a recipient can safely receive the particles, and the use of a biodegradable polymer means that the particles can be metabolised after delivery to avoid long-term persistence. Useful polymers are also sterilisable, to assist in preparing pharmaceutical grade formulations.

[0119] Suitable non-toxic and biodegradable polymers include, but are not limited to, poly(a-hydroxy acids), polyhydroxy butyric acids, polylactones (including polycaprolactones), polydioxanones, polyvalerolactone, polyorthoesters, polyanhydrides, polycyanoacrylates, tyrosine-derived polycarbonates, polyvinyl-pyrrolidinones or polyester-amides, and combinations thereof.

[0120] In some embodiments, the microparticles are formed from poly(a-hydroxy acids), such as a poly(lactides) ("PLA"), copolymers of lactide and glycolide such as a poly(D,L-lactide-co-glycolide) ("PLG"), and copolymers of D,L-lactide and caprolactone. Useful PLG polymers include those having a lactide/glycolide molar ratio ranging, for example, from 20:80 to 80:20 *e.g.* 25:75, 40:60, 45:55, 55:45, 60:40, 75:25. Useful PLG polymers include those having a molecular weight between, for example, 5,000-200,000 Da *e.g.* between 10,000-100,000, 20,000-70,000, 40,000-50,000 Da.

[0121] The microparticles ideally have a diameter in the range of 0.02 μιη to 8μιη. For a composition comprising a population of microparticles with different diameters at least 80% by number should have diameters in the range of 0.03-7μιη.

[0122] Techniques for preparing suitable microparticles are well known in the art *e.g.* see Functional Polymer Colloids and Microparticles volume 4 (Microspheres, microcapsules & liposomes). (eds. Arshady & Guyot). Citus Books, 2002; *Polymers in Drug Delivery*. (eds. Uchegbu & Schatzlein). CRC Press, 2006. (in particular chapter 7) and *Microparticulate Systems for the Delivery of Proteins and Vaccines*. (eds. Cohen & Bernstein). CRC Press, 1996. To facilitate adsorption of RNA, a microparticle may include a cationic surfactant and/or lipid *e.g.* as disclosed in O'Hagan *et al.* (2001) *J Virologyl5:* 9037-9043; and Singh *et al.* (2003) *Pharmaceutical Research* 20: 247-251. An alternative way of making polymeric microparticles is by molding and curing *e.g.* as disclosed in WO2009/1 32206.

[0123] Microparticles of the invention can have a zeta potential of between 40-100 mV.

[0124] RNA can be adsorbed to the microparticles, and adsorption is facilitated by including cationic materials *(e.g.* cationic lipids) in the microparticle.

Oil-in-water cationic emulsions

[0125] Oil-in-water emulsions are known for adjuvanting influenza vaccines *e.g.* the MF59™ adjuvant in the FLUAD™ product, and the AS03 adjuvant in the PREPANDRIX™ product. RNA delivery according to the present invention can utilise an oil-in-water emulsion, provided that the emulsion includes one or more cationic molecules. For instance, a cationic lipid can be included in the emulsion to provide a positive droplet surface to which negatively-charged RNA can attach.

[0126] The emulsion comprises one or more oils. Suitable oil(s) include those from, for example, an animal (such as fish) or a vegetable source. The oil is ideally biodegradable (metabolisable) and biocompatible. Sources for vegetable oils include nuts, seeds and grains. Peanut oil, soybean oil, coconut oil, and olive oil, the most commonly available, exemplify the nut oils. Jojoba oil can be used *e.g.* obtained from the jojoba bean. Seed oils include safflower oil, cottonseed oil, sunflower seed oil, sesame seed oil and the like. In the grain group, corn oil is the most readily available, but the oil of other cereal grains such as wheat, oats, rye, rice, teff, triticale and the like may also be used. 6-10 carbon fatty acid esters of glycerol and 1,2-propanediol, while not occurring naturally in seed oils, may be prepared by hydrolysis, separation and esterification of the appropriate materials starting from the nut and seed oils. Fats and oils from mammalian milk are metabolizable and so may be used. The procedures for separation, purification, saponification and other means necessary for obtaining pure oils from animal sources are well known in the art.

[0127] Most fish contain metabolizable oils which may be readily recovered. For example, cod liver oil, shark liver oils, and whale oil such as spermaceti exemplify several of the fish oils which may be used herein. A number of branched chain oils are synthesized biochemically in 5-carbon isoprene units and are generally referred to as terpenoids. Squalane, the saturated analog to squalene, can also be used. Fish oils, including squalene and squalane, are readily available from commercial sources or may be obtained by methods known in the art.

[0128] Other useful oils are the tocopherols, particularly in combination with squalene. Where the oil phase of an emulsion includes a tocopherol, any of the α, β, γ, δ, ε or

ξ tocopherols can be used, but a-tocopherols are preferred. D-a-tocopherol and DL-a-tocopherol can both be used. A preferred a-tocopherol is DL-a-tocopherol. An oil combination comprising squalene and a tocopherol *(e.g.* DL-a-tocopherol) can be used.

[0129] Preferred emulsions comprise squalene, a shark liver oil which is a branched, unsaturated terpenoid ($C_{30}H_{50}$; $[(CH_3)_2C[=CHCH_2CH_2C(CH_3)]_2=CHCH_2-]_2$; 2,6,10,15,19,23-hexamethyl-2,6,10,14,18,22-tetracosahexaene; CAS RN 7683-64-9).

[0130] The oil in the emulsion may comprise a combination of oils *e.g.* squalene and at least one further oil.

[0131] The aqueous component of the emulsion can be plain water *(e.g.* w.f.i.) or can include further components *e.g.* solutes. For instance, it may include salts to form a buffer *e.g.* citrate or phosphate salts, such as sodium salts. Typical buffers include: a phosphate buffer; a Tris buffer; a borate buffer; a succinate buffer; a histidine buffer; or a citrate buffer. A buffered aqueous phase is preferred, and buffers will typically be included in the 5-20mM range.

[0132] The emulsion also includes a cationic lipid. Preferably this lipid is a surfactant so that it can facilitate formation and stabilisation of the emulsion. Useful cationic lipids generally contains a nitrogen atom that is positively charged under physiological conditions *e.g.* as a tertiary or quaternary amine. This nitrogen can be in the hydrophilic head group of an amphiphilic surfactant. Useful cationic lipids include, but are not limited to: 1,2-dioleoyloxy-3 -(trimethylammonio)propane (DOTAP), 3'-[N-(N',N'-Dimethylaminoethane)-carbamoyl] Cholesterol (DC Cholesterol), dimethyldioctadecyl-ammonium (DDA *e.g.* the bromide), l,2-Dimyristoyl-3-Trimethyl-AmmoniumPropane (DMTAP), dipalmitoyl(C16:0)trimethyl ammonium propane (DPTAP), distearoyltrimethylammonium propane (DSTAP). Other useful cationic lipids are: benzalkonium chloride (BAK), benzethonium chloride, cetramide (which contains tetradecyltrimethylammonium bromide and possibly small amounts of dedecyltrimethylammonium bromide and hexadecyltrimethyl ammonium bromide), cetylpyridinium chloride (CPC), cetyl trimethylammonium chloride (CTAC), N,N',N'-polyoxyethylene (10)-N-tallow-l,3 -diaminopropane, dodecyltrimethylammonium bromide, hexadecyltrimethyl-ammonium bromide, mixed alkyl-trimethyl- ammonium bromide, benzyldimethyldodecylammonium chloride, benzyldimethylhexadecyl-ammonium chloride, benzyltrimethylammonium methoxide, cetyldimethylethylammonium bromide, dimethyldioctadecyl ammonium bromide (DDAB), methylbenzethonium chloride, decamethonium chloride, methyl mixed trialkyl ammonium chloride, methyl trioctylammonium chloride), N,N-dimethyl-N-[2 (2-methyl-4-

(1,1,3,3tetramethylbutyl)- phenoxy]-ethoxy)ethyl]-benzenemetha-naminium chloride (DEBDA), dialkyldimetylammonium salts, [l-(2,3-dioleyloxy)-propyl]-N,N,N,trimethylammonium chloride, l,2-diacyl-3-(trimethylammonio) propane (acyl group=dimyristoyl, dipalmitoyl, distearoyl, dioleoyl), l,2-diacyl-3 (dimethylammonio)propane (acyl group=dimyristoyl, dipalmitoyl, distearoyl, dioleoyl), 1,2-dioleoyl-3-(4'-trimethyl- ammonio)butanoyl-sn-glycerol, 1,2-dioleoyl 3-succinyl-sn-glycerol choline ester, cholesteryl (4'-trimethylammonio) butanoate), N-alkyl pyridinium salts (e.g. cetylpyridinium bromide and cetylpyridinium chloride), N-alkylpiperidinium salts, dicationic bolaform electrolytes (C12Me6; C12BU6), dialkylglycetylphosphorylcholine, lysolecithin, L-α dioleoylphosphatidylethanolamine, cholesterol hemisuccinate choline ester, lipopolyamines, including but not limited to dioctadecylamidoglycylspermine (DOGS), dipalmitoyl phosphatidylethanol-amidospermine (DPPES), lipopoly-L (or D)- lysine (LPLL, LPDL), poly (L (or D)-lysine conjugated to N- glutarylphosphatidylethanolamine, didodecyl glutamate ester with pendant amino group (C^GluPhCnN), ditetradecyl glutamate ester with pendant amino group (C14GIuCnN+), cationic derivatives of cholesterol, including but not limited to cholesteryl-3 β-oxysuccinamidoethylenetrimethylammonium salt, cholesteryl-3 β-oxysuccinamidoethylene-dimethylamine, cholesteryl-3 β-carboxyamidoethylenetrimethylammonium salt, and cholesteryl-3 β-carboxyamidoethylenedimethylamine. Other useful cationic lipids are described in US 2008/0085870 and US 2008/0057080, which are incorporated herein by reference.

[0133] The cationic lipid is preferably biodegradable (metabolisable) and biocompatible.

[0134] In addition to the oil and cationic lipid, an emulsion can include a non-ionic surfactant and/or a zwitterionic surfactant. Such surfactants include, but are not limited to: the polyoxyethylene sorbitan esters surfactants (commonly referred to as the Tweens), especially polysorbate 20 and polysorbate 80; copolymers of ethylene oxide (EO), propylene oxide (PO), and/or butylene oxide (BO), sold under the DOWFAX™ tradename, such as linear EO/PO block copolymers; octoxynols, which can vary in the number of repeating ethoxy (oxy-l,2-ethanediyl) groups, with octoxynol-9 (Triton X-100, or t-octylphenoxypolyethoxyethanol) being of particular interest; (octylphenoxy)polyethoxyethanol (IGEPAL CA-630/NP-40); phospholipids such as phosphatidylcholine (lecithin); polyoxyethylene fatty ethers derived from lauryl, cetyl, stearyl and oleyl alcohols (known as Brij surfactants), such as triethyleneglycol monolauryl ether (Brij 30); polyoxyethylene-9-lauryl ether; and sorbitan esters (commonly known as the

Spans), such as sorbitan trioleate (Span 85) and sorbitan monolaurate. Preferred surfactants for including in the emulsion are polysorbate 80 (Tween 80; polyoxyethylene sorbitan monooleate), Span 85 (sorbitan trioleate), lecithin and Triton X-100.

[0135] Mixtures of these surfactants can be included in the emulsion *e.g.* Tween 80/Span 85 mixtures, or Tween 80/Triton-X100 mixtures. A combination of a polyoxyethylene sorbitan ester such as polyoxyethylene sorbitan monooleate (Tween 80) and an octoxynol such as t-octylphenoxy-polyethoxyethanol (Triton X-100) is also suitable. Another useful combination comprises laureth 9 plus a polyoxyethylene sorbitan ester and/or an octoxynol. Useful mixtures can comprise a surfactant with a HLB value in the range of 10-20 *(e.g.* polysorbate 80, with a HLB of 15.0) and a surfactant with a HLB value in the range of 1-10 *(e.g.* sorbitan trioleate, with a HLB of 1.8).

[0136] Preferred amounts of oil (% by volume) in the final emulsion are between 2-20% *e.g.* 5-15%, 6-14%, 7-13%, 8-12%. A squalene content of about 4-6% or about 9-11% is particularly useful.

[0137] Preferred amounts of surfactants (% by weight) in the final emulsion are between 0.001% and 8%. For example: polyoxyethylene sorbitan esters (such as polysorbate 80) 0.2 to 4%, in particular between 0.4-0.6%, between 0.45-0.55%, about 0.5% or between 1.5-2%, between 1.8-2.2%, between 1.9-2.1%, about 2%, or 0.85-0.95%, or about 1%; sorbitan esters (such as sorbitan trioleate) 0.02 to 2%, in particular about 0.5% or about 1%; octyl- or nonylphenoxy polyoxyethanols (such as Triton X-100) 0.001 to 0.1%, in particular 0.005 to 0.02%; polyoxyethylene ethers (such as laureth 9) 0.1 to 8%, preferably 0.1 to 10% and in particular 0.1 to 1% or about 0.5%.

[0138] The absolute amounts of oil and surfactant, and their ratio, can be varied within wide limits while still forming an emulsion. A skilled person can easily vary the relative proportions of the components to obtain a desired emulsion, but a weight ratio of between 4:1 and 5:1 for oil and surfactant is typical (excess oil).

[0139] An important parameter for ensuring immunostimulatory activity of an emulsion, particularly in large animals, is the oil droplet size (diameter). The most effective emulsions have a droplet size in the submicron range. Suitably the droplet sizes will be in the range 50-750nm. Most usefully the average droplet size is less than 250nm *e.g.* less than 200nm, less than 150nm. The average droplet size is usefully in the range of 80-180nm. Ideally, at least 80% (by number) of the emulsion's oil droplets are less than 250 nm in diameter, and preferably at least 90%. Apparatuses for determining the average droplet size in an emulsion, and the size distribution, are commercially available. These typically use the

techniques of dynamic light scattering and/or single-particle optical sensing *e.g.* the Accusizer™ and Nicomp™ series of instruments available from Particle Sizing Systems (Santa Barbara, USA), or the Zetasizer™ instruments from Malvern Instruments (UK), or the Particle Size Distribution Analyzer instruments from Horiba (Kyoto, Japan).

[0140] Ideally, the distribution of droplet sizes (by number) has only one maximum *i.e.* there is a single population of droplets distributed around an average (mode), rather than having two maxima. Preferred emulsions have a polydispersity of <0.4 *e.g.* 0.3, 0.2, or less.

[0141] Suitable emulsions with submicron droplets and a narrow size distribution can be obtained by the use of microfluidisation. This technique reduces average oil droplet size by propelling streams of input components through geometrically fixed channels at high pressure and high velocity. These streams contact channel walls, chamber walls and each other. The results shear, impact and cavitation forces cause a reduction in droplet size. Repeated steps of microfluidisation can be performed until an emulsion with a desired droplet size average and distribution are achieved.

[0142] As an alternative to microfluidisation, thermal methods can be used to cause phase inversion. These methods can also provide a submicron emulsion with a tight particle size distribution.

[0143] Preferred emulsions can be filter sterilized *i.e.* their droplets can pass through a 220nm filter. As well as providing a sterilization, this procedure also removes any large droplets in the emulsion.

[0144] In certain embodiments, the cationic lipid in the emulsion is DOTAP. The cationic oil-in-water emulsion may comprise from about 0.5 mg/ml to about 25 mg/ml DOTAP. For example, the cationic oil-in-water emulsion may comprise DOTAP at from about 0.5 mg/ml to about 25 mg/ml, from about 0.6 mg/ml to about 25 mg/ml, from about 0.7 mg/ml to about 25 mg/ml, from about 0.8 mg/ml to about 25 mg/ml, from about 0.9 mg/ml to about 25 mg/ml, from about 1.0 mg/ml to about 25 mg/ml, from about 1.1 mg/ml to about 25 mg/ml, from about 1.2 mg/ml to about 25 mg/ml, from about 1.3 mg/ml to about 25 mg/ml, from about 1.4 mg/ml to about 25 mg/ml, from about 1.5 mg/ml to about 25 mg/ml, from about 1.6 mg/ml to about 25 mg/ml, from about 1.7 mg/ml to about 25 mg/ml, from about 0.5 mg/ml to about 24 mg/ml, from about 0.5 mg/ml to about 22 mg/ml, from about 0.5 mg/ml to about 20 mg/ml, from about 0.5 mg/ml to about 18 mg/ml, from about 0.5 mg/ml to about 15 mg/ml, from about 0.5 mg/ml to about 12 mg/ml, from about 0.5 mg/ml to about 10 mg/ml, from about 0.5 mg/ml to about 5 mg/ml, from about 0.5 mg/ml to about 2 mg/ml, from about 0.5 mg/ml to about 1.9 mg/ml, from about 0.5 mg/ml to about 1.8 mg/ml, from about 0.5

mg/ml to about 1.7 mg/ml, from about 0.5 mg/ml to about 1.6 mg/ml, from about 0.6 mg/ml to about 1.6 mg/ml, from about 0.7 mg/ml to about 1.6 mg/ml, from about 0.8 mg/ml to about 1.6 mg/ml, about 0.5 mg/ml, about 0.6 mg/ml, about 0.7 mg/ml, about 0.8 mg/ml, about 0.9 mg/ml, about 1.0 mg/ml, about 1.1 mg/ml, about 1.2 mg/ml, about 1.3 mg/ml, about 1.4 mg/ml, about 1.5 mg/ml, about 1.6 mg/ml, about 12 mg/ml, about 18 mg/ml, about 20 mg/ml, about 21.8 mg/ml, about 24 mg/ml, *etc*. In an exemplary embodiment, the cationic oil-in-water emulsion comprises from about 0.8 mg/ml to about 1.6 mg/ml DOTAP, such as 0.8 mg/ml, 1.2 mg/ml, 1.4 mg/ml or 1.6 mg/ml.

[0145] In certain embodiments, the cationic lipid is DC Cholesterol. The cationic oil-in-water emulsion may comprise DC Cholesterol at from about 0.1 mg/ml to about 5 mg/ml DC Cholesterol. For example, the cationic oil-in-water emulsion may comprise DC Cholesterol from about 0.1 mg/ml to about 5 mg/ml, from about 0.2 mg/ml to about 5 mg/ml, from about 0.3 mg/ml to about 5 mg/ml, from about 0.4 mg/ml to about 5 mg/ml, from about 0.5 mg/ml to about 5 mg/ml, from about 0.62 mg/ml to about 5 mg/ml, from about 1 mg/ml to about 5 mg/ml, from about 1.5 mg/ml to about 5 mg/ml, from about 2 mg/ml to about 5 mg/ml, from about 2.46 mg/ml to about 5 mg/ml, from about 3 mg/ml to about 5 mg/ml, from about 3.5 mg/ml to about 5 mg/ml, from about 4 mg/ml to about 5 mg/ml, from about 4.5 mg/ml to about 5 mg/ml, from about 0.1 mg/ml to about 4.92 mg/ml, from about 0.1 mg/ml to about 4.5 mg/ml, from about 0.1 mg/ml to about 4 mg/ml, from about 0.1 mg/ml to about 3.5 mg/ml, from about 0.1 mg/ml to about 3 mg/ml, from about 0.1 mg/ml to about 2.46 mg/ml, from about 0.1 mg/ml to about 2 mg/ml, from about 0.1 mg/ml to about 1.5 mg/ml, from about 0.1 mg/ml to about 1 mg/ml, from about 0.1 mg/ml to about 0.62 mg/ml, about 0.15 mg/ml, about 0.3 mg/ml, about 0.6 mg/ml, about 0.62 mg/ml, about 0.9 mg/ml, about 1.2 mg/ml, about 2.46 mg/ml, about 4.92 mg/ml, *etc*. In an exemplary embodiment, the cationic oil-in-water emulsion comprises from about 0.62 mg/ml to about 4.92 mg/ml DC Cholesterol, such as 2.46 mg/ml.

[0146] In certain embodiments, the cationic lipid is DDA. The cationic oil-in-water emulsion may comprise from about 0.1 mg/ml to about 5 mg/ml DDA. For example, the cationic oil-in-water emulsion may comprise DDA at from about 0.1 mg/ml to about 5 mg/ml, from about 0.1 mg/ml to about 4.5 mg/ml, from about 0.1 mg/ml to about 4 mg/ml, from about 0.1 mg/ml to about 3.5 mg/ml, from about 0.1 mg/ml to about 3 mg/ml, from about 0.1 mg/ml to about 2.5 mg/ml, from about 0.1 mg/ml to about 2 mg/ml, from about 0.1 mg/ml to about 1.5 mg/ml, from about 0.1 mg/ml to about 1.45 mg/ml, from about 0.2 mg/ml to about 5 mg/ml, from about 0.3 mg/ml to about 5 mg/ml, from about 0.4 mg/ml to about 5

mg/ml, from about 0.5 mg/ml to about 5 mg/ml, from about 0.6 mg/ml to about 5 mg/ml, from about 0.73 mg/ml to about 5 mg/ml, from about 0.8 mg/ml to about 5 mg/ml, from about 0.9 mg/ml to about 5 mg/ml, from about 1.0 mg/ml to about 5 mg/ml, from about 1.2 mg/ml to about 5 mg/ml, from about 1.45 mg/ml to about 5 mg/ml, from about 2 mg/ml to about 5 mg/ml, from about 2.5 mg/ml to about 5 mg/ml, from about 3 mg/ml to about 5 mg/ml, from about 3.5 mg/ml to about 5 mg/ml, from about 4 mg/ml to about 5 mg/ml, from about 4.5 mg/ml to about 5 mg/ml, about 1.2 mg/ml, about 1.45 mg/ml, etc. Alternatively, the cationic oil-in-water emulsion may comprise DDA at about 20 mg/ml, about 21 mg/ml, about 21.5 mg/ml, about 21.6 mg/ml, about 25 mg/ml. In an exemplary embodiment, the cationic oil-in-water emulsion comprises from about 0.73 mg/ml to about 1.45 mg/ml DDA, such as 1.45 mg/ml.

[0147] Catheters or like devices may be used to deliver the self-replicating RNA molecules of the invention, as naked RNA or in combination with a delivery system, into a target organ or tissue. Suitable catheters are disclosed in, *e.g.,* U.S. Pat. Nos. 4,186,745; 5,397,307; 5,547,472; 5,674,192; and 6,129,705, all of which are incorporated herein by reference.

[0148] The present invention includes the use of suitable delivery systems, such as liposomes, polymer microparticles or submicron emulsion microparticles with encapsulated or adsorbed self-replicating RNA, to deliver a self-replicating RNA molecule that encodes an RSV-F polypeptide, for example, to elicit an immune response alone, or in combination with another macromolecule. The invention includes liposomes, microparticles and submicron emulsions with adsorbed and/or encapsulated self-replicating RNA molecules, and combinations thereof.

[0149] As demonstrated further in the Examples, the self-replicating RNA molecules associated with liposomes and submicron emulsion microparticles can be effectively delivered to the host cell, and can induce an immune response to the protein encoded by the self-replicating RNA.

Immunogenic compositions

[0150] The invention provides immunogenic compositions. The immunogenic compositions may include a single active immunogenic agent, or several immunogenic agents. For example, the immunogenic composition can comprise pre-fusion RSV F polypeptides or a combination of pre-fusion chimeric RSV F polypeptides. The immunogenic composition can comprise a self-replicating RNA encoding a pre-fusion RSV-

F polypeptide, and preferably also comprises a suitable delivery system, such as liposomes, polymeric microparticles, an oil-in-water emulsion and combinations thereof.

[0151] Immunogenic compositions of the invention may also comprise one or more immunoregulatory agents. Preferably, one or more of the immunoregulatory agents include one or more adjuvants, for example two, three, four or more adjuvants. The adjuvants may include a TH1 adjuvant and/or a TH2 adjuvant, further discussed below.

[0152] In another embodiment, an immunogenic composition of the invention comprises a polypeptide that displays an epitope present in a pre-fusion conformation of RSV-F glycoprotein.

[0153] In another embodiment, an immunogenic composition of the invention comprises one or more pre-fusion chimera proteins based on two different pre-fusion non-RSV (F proteins (e.g, metapneumovirus, parainfluenza, such asPIV5, NDV), in which both have the same RSV F neutralizing epitopes mutated on the protein surface.

[0154] The compositions of the invention are preferably suitable for administration to a mammalian subject, such as a human, and include one or more pharmaceutically acceptable carrier(s) and/or excipient(s), including adjuvants. A thorough discussion of such components is available in reference 29. Compositions will generally be in aqueous form. When the composition is an immunogenic composition, it will elicit an immune response when administered to a mammal, such as a human. The immunogenic composition can be used to prepare a vaccine formulation for immunizing a mammal.

[0155] The immunogenic compositions may include a single active immunogenic agent, or several immunogenic agents. For example, the pre-fusion RSV F protein can be full length or a ecto-domain polypeptide and can be in a single form (e.g., uncleaved monomer, cleaved monomer, uncleaved trimer, cleaved trimer) or in two or more forms (e.g., a mixture of uncleaved monomer and uncleaved trimer or a dynamic equilibrium between uncleaved monomer and uncleaved trimer). In addition, the compositions can contain a pre-fusion RSV F protein and one or more other RSV proteins *(e.g.,* a G protein and/or an M protein) and/or it may be combined with immunogens from other pathogens.

[0156] The composition may include preservatives such as thiomersal or 2-phenoxyethanol. It is preferred, however, that the vaccine should be substantially free from *(i.e.,* less than 5μg/ml) mercurial material, *e.g.,* thiomersal-free. Immunogenic compositions containing no mercury are more preferred. Preservative-free immunogenic compositions are particularly preferred.

[0157] To control tonicity, it is preferred to include a physiological salt, such as a sodium salt. Sodium chloride (NaCl) is preferred, which may be present at between 1 and 20 mg/ml. Other salts that may be present include potassium chloride, potassium dihydrogen phosphate, disodium phosphate dehydrate, magnesium chloride, calcium chloride, and the like.

[0158] Compositions will generally have an osmolality of between 200 mOsm/kg and 400 mOsm/kg, preferably between 240-360 mOsm/kg, and will more preferably fall within the range of 290-310 mOsm/kg.

[0159] Compositions may include one or more buffers. Typical buffers include: a phosphate buffer; a Tris buffer; a borate buffer; a succinate buffer; a histidine buffer (particularly with an aluminum hydroxide adjuvant); or a citrate buffer. Buffers will typically be included in the 5-20mM range. The pH of a composition will generally be between 5.0 and 8.1, and more typically between 6.0 and 8.0, *e.g.*, between 6.5 and 7.5, or between 7.0 and 7.8. A process of the invention may therefore include a step of adjusting the pH of the bulk vaccine prior to packaging.

[0160] The composition is preferably sterile. The composition is preferably non-pyrogenic, *e.g.*, containing < 1 EU (endotoxin unit, a standard measure) per dose, and preferably <0.1 EU per dose. The composition is preferably gluten free. Human vaccines are typically administered in a dosage volume of about 0.5ml, although a half dose *(i.e.,* about 0.25ml) may be administered to children.

Adjuvants

[0161] Compositions of the invention, that contain RSV-F polypeptides, or nucleic acids that encode RSV-F polypeptides, may also include one or more adjuvants, for example two, three, four or more adjuvants, which can function to enhance the immune responses (humoral and/or cellular) elicited in a patient who receives the composition. The adjuvants may include a TH1 adjuvant and/or a TH2 adjuvant. Adjuvants which may be used in compositions of the invention include, but are not limited to:

- Mineral-containing compositions. Mineral-containing compositions suitable for use as adjuvants in the invention include mineral salts, such as calcium salts and aluminum salts (or mixtures thereof). The invention includes mineral salts such as hydroxides *(e.g.* oxyhydroxides), phosphates *(e.g.* hydroxyphosphates, orthophosphates), sulphates, *etc.,* or mixtures of different mineral compounds, with the compounds taking any suitable form *(e.g.* gel, crystalline, amorphous, *etc.),* and

with adsorption being preferred. Calcium salts include calcium phosphate *(e.g.,* the "CAP" particles disclosed in ref. 38). Aluminum salts include hydroxides, phosphates, sulfates, and the like. The mineral containing compositions may also be formulated as a particle of metal salt (39). Aluminum salt adjuvants are described in more detail below.

- Oil emulsion compositions (see in more detail below). Oil emulsion compositions suitable for use as adjuvants in the invention include squalene-water emulsions, such as MF59 (5% Squalene, 0.5% Tween 80 and 0.5% Span, formulated into submicron particles using a microfluidizer).
- Cytokine-inducing agents (see in more detail below). Cytokine-inducing agents suitable for use in the invention include toll-like receptor 7 (TLR7) agonists *(e.g.* benzonaphthyridine compounds disclosed in WO 2009/1 11337.
- Saponins (chapter 22 of ref. 74), which are a heterologous group of sterol glycosides and triterpenoid glycosides that are found in the bark, leaves, stems, roots and even flowers of a wide range of plant species. Saponin from the bark of the *Quillaia saponaria* Molina tree have been widely studied as adjuvants. Saponin can also be commercially obtained from *Smilax ornata* (sarsaprilla), *Gypsophilla paniculata* (brides veil), and *Saponaria officianalis* (soap root). Saponin adjuvant formulations include purified formulations, such as QS21, as well as lipid formulations, such as ISCOMs. QS21 is marketed as STIMULON (TM). Saponin compositions have been purified using HPLC and RP-HPLC. Specific purified fractions using these techniques have been identified, including QS7, QS17, QS18, QS21, QH-A, QH-B and QH-C. Preferably, the saponin is QS21. A method of production of QS21 is disclosed in ref. 40. Saponin formulations may also comprise a sterol, such as cholesterol (41). Combinations of saponins and cholesterols can be used to form unique particles called immunostimulating complexes (ISCOMs) (chapter 23 of ref. 74). ISCOMs typically also include a phospholipid such as phosphatidylethanolamine or phosphatidylcholine. Any known saponin can be used in ISCOMs. Preferably, the ISCOM includes one or more of QuilA, QHA & QHC. ISCOMs are further described in refs. 41-43. Optionally, the ISCOMS may be devoid of additional detergent (44). A review of the development of saponin based adjuvants can be found in refs. 45 & 46.
- Fatty adjuvants (see in more detail below), including oil-in-water emulsions, modified natural lipid As derived from enterobacterial lipopolysaccharides, phospholipid compounds (such as the synthetic phospholipid dimer, E6020) and the like.

- Bacterial ADP-ribosylating toxins *(e.g.,* the *E. coli* heat labile enterotoxin "LT", cholera toxin "CT", or pertussis toxin "PT") and detoxified derivatives thereof, such as the mutant toxins known as LT-K63 and LT-R72 (47). The use of detoxified ADP-ribosylating toxins as mucosal adjuvants is described in ref. 48 and as parenteral adjuvants in ref. 49.
- Bioadhesives and mucoadhesives, such as esterified hyaluronic acid microspheres (50) or chitosan and its derivatives (51).
- Microparticles *(i.e.,* a particle of -100 nm to -150 μιη in diameter, more preferably -200 nm to -30 μιη in diameter, or -500 nm to -10 μιη in diameter) formed from materials that are biodegradable and non-toxic *(e.g.,* a poly(a-hydroxy acid), a polyhydroxybutyric acid, a polyorthoester, a polyanhydride, a polycaprolactone, and the like), with poly(lactide-co-glycolide) being preferred, optionally treated to have a negatively-charged surface *(e.g.,* with SDS) or a positively-charged surface *(e.g.,* with a cationic detergent, such as CTAB).
- Liposomes (Chapters 13 & 14 of ref. 74). Examples of liposome formulations suitable for use as adjuvants are described in refs. 52-54.
- Polyoxyethylene ethers and polyoxyethylene esters (55). Such formulations further include polyoxyethylene sorbitan ester surfactants in combination with an octoxynol (56) as well as polyoxyethylene alkyl ethers or ester surfactants in combination with at least one additional non-ionic surfactant such as an octoxynol (57). Preferred polyoxyethylene ethers are selected from the following group: polyoxyethylene-9-lauryl ether (laureth 9), polyoxyethylene-9-steoryl ether, polyoxytheylene-8-steoryl ether, polyoxyethylene-4-lauryl ether, polyoxyethylene-35-lauryl ether, and polyoxyethylene-23-lauryl ether.
- Muramyl peptides, such as N-acetylmuramyl-L-threonyl-D-isoglutamine ("thr-MDP"), N-acetyl-normuramyl-L-alanyl-D-isoglutamine (nor-MDP), N-acetylglucsaminyl-N-acetylmuramyl-L-Al-D-isoglu-L-Ala-dipalmitoxy propylamide ("DTP-DPP", or "Theramide™), N-acetylmuramyl-L-alanyl-D-isoglutaminyl-L-alanine-2-(l'-2'dipalmitoyl-sn-glycero-3-hydroxyphosphoryloxy)-ethylamine ("MTP-PE").
- An outer membrane protein proteosome preparation prepared from a first Gram-negative bacterium in combination with a liposaccharide preparation derived from a second Gram-negative bacterium, wherein the outer membrane protein proteosome and liposaccharide preparations form a stable non-covalent adjuvant complex. Such

complexes include "IVX-908", a complex comprised of *Neisseria meningitidis* outer membrane and lipopolysaccharides.

- A polyoxidonium polymer (58, 59) or other N-oxidized polyethylene-piperazine derivative.
- Methyl inosine 5'-monophosphate ("MIMP") (60).
- A polyhydroxlated pyrrolizidine compound (61), such as one having formula:

  where R is selected from the group comprising hydrogen, straight or branched, unsubstituted or substituted, saturated or unsaturated acyl, alkyl *{e.g.,* cycloalkyl), alkenyl, alkynyl and aryl groups, or a pharmaceutically acceptable salt or derivative thereof. Examples include, but are not limited to: casuarine, casuarine-6-a-D-glucopyranose, 3-*epi*-casuarine, 7-ep/-casuarine, 3,7-die/?/-casuarine, and the like
- A CDId ligand, such as an a-glycosylceramide (62-69) *{e.g.,* a-galactosylceramide), phytosphingosine-containing a-glycosylceramides, OCH, KRN7000 [(2S,3S,4R)-1-0-(a-D-galactopyranosyl)-2-(N-hexacosanoylamino)-l,3,4-octadecanetriol], CRONY-101, 3"-0-sulfo-galactosylceramide, *etc.*
- A gamma inulin (70) or derivative thereof, such as algammulin.
- Virosomes and virus-like particles (VLPs). These structures generally contain one or more proteins from a virus optionally combined or formulated with a phospholipid. They are generally non-pathogenic, non-replicating and generally do not contain any of the native viral genome. The viral proteins may be recombinantly produced or isolated from whole viruses. These viral proteins suitable for use in virosomes or VLPs include proteins derived from influenza virus (such as HA or NA), Hepatitis B virus (such as core or capsid proteins), Hepatitis E virus, measles virus, Sindbis virus, Rotavirus, Foot-and-Mouth Disease virus, Retrovirus, Norwalk virus, human Papilloma virus, HIV, RNA-phages, Q6-phage (such as coat proteins), GA-phage, fr-phage, AP205 phage, and Ty (such as retrotransposon Ty protein pi).

[0162] These and other adjuvant-active substances are discussed in more detail in references 74 & 75.

[0163] Compositions may include two, three, four or more adjuvants. For example, compositions of the invention may advantageously include both an oil-in-water emulsion and a cytokine-inducing agent, or both a mineral-containing composition and a cytokine-inducing agent, or two oil-in-water emulsion adjuvants, or two benzonaphthyridine compounds, etc.

[0164] Antigens and adjuvants in a composition will typically be in admixture.

Oil emulsion adjuvants

[0165] Oil emulsion compositions suitable for use as adjuvants in the invention include squalene-water emulsions, such as MF59 (5% Squalene, 0.5% Tween 80, and 0.5% Span 85, formulated into submicron particles using a microfluidizer). Complete Freund's adjuvant (CFA) and incomplete Freund's adjuvant (IFA) may also be used.

[0166] Various oil-in-water emulsions are known, and they typically include at least one oil and at least one surfactant, with the oil(s) and surfactant(s) being biodegradable (metabolizable) and biocompatible. The oil droplets in the emulsion are generally less than 5 μιη in diameter, and may even have a sub-micron diameter, with these small sizes being achieved with a microfluidizer to provide stable emulsions. Droplets with a size less than 220 nm are preferred as they can be subjected to filter sterilization.

[0167] The invention can be used with oils such as those from an animal (such as fish) or vegetable source. Sources for vegetable oils include nuts, seeds and grains. Peanut oil, soybean oil, coconut oil, and olive oil, the most commonly available, exemplify the nut oils. Jojoba oil can be used, *e.g.,* obtained from the jojoba bean. Seed oils include safflower oil, cottonseed oil, sunflower seed oil, sesame seed oil and the like. In the grain group, corn oil is the most readily available, but the oil of other cereal grains such as wheat, oats, rye, rice, teff, triticale and the like may also be used. 6-10 carbon fatty acid esters of glycerol and 1,2-propanediol, while not occurring naturally in seed oils, may be prepared by hydrolysis, separation and esterification of the appropriate materials starting from the nut and seed oils. Fats and oils from mammalian milk are metabolizable and may therefore be used in the practice of this invention. The procedures for separation, purification, saponification and other means necessary for obtaining pure oils from animal sources are well known in the art. Most fish contain metabolizable oils which may be readily recovered. For example, cod liver oil, shark liver oils, and whale oil such as spermaceti exemplify several of the fish oils which may be used herein. A number of branched chain oils are synthesized biochemically in 5-carbon isoprene units and are generally referred to as terpenoids. Shark liver oil contains a branched, unsaturated terpenoid known as squalene, 2,6,10,15, 19,23-hexamethyl-2,6,10,14,18,22-tetracosahexaene, which is particularly preferred herein. Squalane, the saturated analog to squalene, is also preferred oil. Fish oils, including squalene and squalane, are readily available from commercial sources or may be obtained by methods known in the art. Other preferred oils are the tocopherols (see below). Mixtures of oils can be used.

[0168] Surfactants can be classified by their 'HLB' (hydrophile/lipophile balance). Preferred surfactants of the invention have a HLB of at least 10, preferably at least 15, and more preferably at least 16. The invention can be used with surfactants including, but not limited to: the polyoxyethylene sorbitan esters surfactants (commonly referred to as the Tweens), especially polysorbate 20 and polysorbate 80; copolymers of ethylene oxide (EO), propylene oxide (PO), and/or butylene oxide (BO), sold under the DOWFAX (TM) tradename, such as linear EO/PO block copolymers; octoxynols, which can vary in the number of repeating ethoxy (oxy-l,2-ethanediyl) groups, with octoxynol-9 (Triton X-100, or t-octylphenoxypolyethoxyethanol) being of particular interest; (octylphenoxy)polyethoxyethanol (IGEPAL CA-630/NP-40); phospholipids such as phosphatidylcholine (lecithin); nonylphenol ethoxylates, such as the TERGITOL (TM) NP series; polyoxyethylene fatty ethers derived from lauryl, cetyl, stearyl and oleyl alcohols (known as Brij surfactants), such as triethyleneglycol monolauryl ether (Brij 30); and sorbitan esters (commonly known as the SPANs), such as sorbitan trioleate (Span 85) and sorbitan monolaurate. Non-ionic surfactants are preferred. Preferred surfactants for including in the emulsion are TWEEN 80 (TM) (polyoxyethylene sorbitan monooleate), Span 85 (sorbitan trioleate), lecithin and Triton X-100.

[0169] Mixtures of surfactants can be used *e.g.,* TWEEN 80 (TM)/Span 85 mixtures. A combination of a polyoxyethylene sorbitan ester such as polyoxyethylene sorbitan monooleate (TWEEN 80 (TM)) and an octoxynol such as t-octylphenoxypolyethoxyethanol (Triton X-100) is also suitable. Another useful combination comprises laureth 9 plus a polyoxyethylene sorbitan ester and/or an octoxynol.

[0170] Preferred amounts of surfactants (% by weight) are: polyoxyethylene sorbitan esters (such as TWEEN 80 (TM)) 0.01 to 1%, in particular about 0.1 %; octyl- or nonylphenoxy polyoxyethanols (such as Triton X-100, or other detergents in the Triton series) 0.001 to 0.1 %, in particular 0.005 to 0.02%; polyoxyethylene ethers (such as laureth 9) 0.1 to 20 %, preferably 0.1 to 10 % and in particular 0.1 to 1 % or about 0.5%.

[0171] Specific oil-in-water emulsion adjuvants useful with the invention include, but are not limited to:

- A submicron emulsion of squalene, TWEEN 80 (TM), and Span 85. The composition of the emulsion by volume can be about 5% squalene, about 0.5% polysorbate 80 and about 0.5% Span 85. In weight terms, these ratios become 4.3% squalene, 0.5% polysorbate 80 and 0.48% Span 85. This adjuvant is known as 'MF59' (71-73), as

described in more detail in Chapter 10 of ref. 74 and chapter 12 of ref. 75. The MF59 emulsion advantageously includes citrate ions, *e.g.,* lOmM sodium citrate buffer.

- An emulsion of squalene, a tocopherol, and TWEEN 80 (TM). The emulsion may include phosphate buffered saline. It may also include Span 85 *(e.g.,* at 1%) and/or lecithin. These emulsions may have from 2 to 10% squalene, from 2 to 10% tocopherol and from 0.3 to 3% TWEEN 80 (TM), and the weight ratio of squalene tocopherol is preferably < 1 as this provides a more stable emulsion. Squalene and TWEEN 80 (TM) may be present volume ratio of about 5:2. One such emulsion can be made by dissolving TWEEN 80 (TM) in PBS to give a 2% solution, then mixing 90ml of this solution with a mixture of (5g of DL-a-tocopherol and 5ml squalene), then microfluidizing the mixture. The resulting emulsion may have submicron oil droplets, *e.g.,* with an average diameter of between 100 and 250nm, preferably about 180nm.
- An emulsion of squalene, a tocopherol, and a Triton detergent *(e.g.,* Triton X-100). The emulsion may also include a 3d-MPL (see below). The emulsion may contain a phosphate buffer.
- An emulsion comprising a polysorbate *(e.g.,* polysorbate 80), a Triton detergent *(e.g.,* Triton X-100) and a tocopherol *(e.g.,* an a-tocopherol succinate). The emulsion may include these three components at a mass ratio of about 75:11:10 *(e.g.,* 750 μg/ml polysorbate 80, 110 μg/ml Triton X-100 and 100 μg/ml α-tocopherol succinate), and these concentrations should include any contribution of these components from antigens. The emulsion may also include squalene. The emulsion may also include a 3d-MPL (see below). The aqueous phase may contain a phosphate buffer.
- An emulsion of squalane, polysorbate 80 and poloxamer 401 ("PLURONIC (TM) L121"). The emulsion can be formulated in phosphate buffered saline, pH 7.4. This emulsion is a useful delivery vehicle for muramyl dipeptides, and has been used with threonyl-MDP in the "SAF-1" adjuvant (76) (0.05-1% Thr-MDP, 5% squalane, 2.5% Pluronic L121 and 0.2% polysorbate 80). It can also be used without the Thr-MDP, as in the "AF" adjuvant (77) (5% squalane, 1.25% Pluronic L121 and 0.2% polysorbate 80). Microfluidization is preferred.
- An emulsion comprising squalene, an aqueous solvent, a polyoxyethylene alkyl ether hydrophilic nonionic surfactant *(e.g.* polyoxyethylene (12) cetostearyl ether) and a hydrophobic nonionic surfactant *(e.g.* a sorbitan ester or mannide ester, such as sorbitan monoleate or 'Span 80')· The emulsion is preferably thermoreversible and/or has at least 90% of the oil droplets (by volume) with a size less than 200 nm. The emulsion may also include one or more of: alditol; a cryoprotective agent *(e.g.* a sugar, such as

dodecylmaltoside and/or sucrose); and/or an alkylpolyglycoside. Such emulsions may be lyophilized.

- An emulsion having from 0.5-50% of an oil, 0.1-10% of a phospholipid, and 0.05-5% of a non-ionic surfactant. As described in reference 78, preferred phospholipid components are phosphatidylcholine, phosphatidylethanolamine, phosphatidylserine, phosphatidylinositol, phosphatidylglycerol, phosphatidic acid, sphingomyelin and cardiolipin. Submicron droplet sizes are advantageous.
- A submicron oil-in-water emulsion of a non-metabolizable oil (such as light mineral oil) and at least one surfactant (such as lecithin, TWEEN 80 (TM) or Span 80). Additives may be included, such as QuilA saponin, cholesterol, a saponin-lipophile conjugate (such as GPI-0100, described in reference 79, produced by addition of aliphatic amine to desacylsaponin via the carboxyl group of glucuronic acid), dimethyidioctadecylammonium bromide and/or N,N-dioctadecyl-N,N-bis (2-hydroxyethyl)propanediamine.
- An emulsion comprising a mineral oil, a non-ionic lipophilic ethoxylated fatty alcohol, and a non-ionic hydrophilic surfactant *(e.g.* an ethoxylated fatty alcohol and/or polyoxyethylene-polyoxypropylene block copolymer).
- An emulsion comprising a mineral oil, a non-ionic hydrophilic ethoxylated fatty alcohol, and a non-ionic lipophilic surfactant *(e.g.* an ethoxylated fatty alcohol and/or polyoxyethylene-polyoxypropylene block copolymer).
- An emulsion in which a saponin *(e.g.,* QuilA or QS21) and a sterol *(e.g.,* a cholesterol) are associated as helical micelles (80).

[0172] The emulsions may be mixed with antigen extemporaneously, at the time of delivery. Thus the adjuvant and antigen may be kept separately in a packaged or distributed vaccine, ready for final formulation at the time of use. The antigen will generally be in an aqueous form, such that the vaccine is finally prepared by mixing two liquids. The volume ratio of the two liquids for mixing can vary *(e.g.,* between 5:1 and 1:5) but is generally about 1:1.

Cytokine-inducing agents

[0173] Cytokine-inducing agents for inclusion in compositions of the invention are able, when administered to a patient, to elicit the immune system to release cytokines, including interferons and interleukins. Preferred agents can elicit the release of one or more of: interferon-γ; interleukin-1; interleukin-2; interleukin-12; TNF-a; TNF-β; and GM-CSF.

Preferred agents elicit the release of cytokines associated with a Thl-type immune response, *e.g.,* interferon-γ, TNF-a, interleukin-2. Stimulation of both interferon-γ and interleukin-2 is preferred.

[0174] As a result of receiving a composition of the invention, therefore, a patient will have T cells that, when stimulated with a RSV F protein, will release the desired cytokine(s) in an antigen-specific manner. For example, T cells purified from their blood will release γ-interferon when exposed *in vitro* to F protein. Methods for measuring such responses in peripheral blood mononuclear cells (PBMC) are known in the art, and include ELISA, ELISPOT, flow-cytometry and real-time PCR. For example, reference 81 reports a study in which antigen-specific T cell-mediated immune responses against tetanus toxoid, specifically γ-interferon responses, were monitored, and found that ELISPOT was the most sensitive method to discriminate antigen-specific TT-induced responses from spontaneous responses, but that intracytoplasmic cytokine detection by flow cytometry was the most efficient method to detect re-stimulating effects.

[0175] Suitable cytokine-inducing agents include, but are not limited to:

- An immunostimulatory oligonucleotide, such as one containing a CpG motif (a dinucleotide sequence containing an unmethylated cytosine linked by a phosphate bond to a guanosine), or a double-stranded RNA, or an oligonucleotide containing a palindromic sequence, or an oligonucleotide containing a poly(dG) sequence.
- 3-O-deacylated monophosphoryl lipid A ('3dMPL', also known as 'MPL (TM)') (82-85).
- An imidazoquinoline compound, such as IMIQUIMOD (TM) ("R-837") (86, 87), RESIQUIMOD (TM) ("R-848") (88), and their analogs; and salts thereof *{e.g.,* the hydrochloride salts). Further details about immunostimulatory imidazoquinolines can be found in references 89 to 93.
- A benzonaphthyridine compound, such as: (a) a compound having the formula:

wherein:

R^4 is selected from H, halogen, $-C(0)OR^7$, $-C(0)R^7$, $-C(0)N(R^{11}R^{12})$, $-N(R^{11}R^{12})$, $-N(R^9)_2$, $-NHN(R^9)_2$, $-SR^7$, $-(CH_2)_nOR^7$, $-(CH_2)_nR^7$, $-LR^8$, $-LR^{10}$, $-OLR^8$, $-OLR^{10}$, Ci-C_6alkyl, Ci-C_6heteroalkyl, Ci-C_6haloalkyl, C_2-Csalkene, C_2-Csalkyne, Ci-C_6alkoxy, Ci-Cehaloalkoxy, aryl, heteroaryl, C_3-Cscycloalkyl, and

C_3-C_8heterocycloalkyl, wherein the Ci-C6alkyl, Ci-C6heteroalkyl, C_1-C_6haloalkyl, C2-Csalkene, C2-Csalkyne, Ci-C_6alkoxy, Ci-C6haloalkoxy, aryl, heteroaryl, C_3-Cscycloalkyl, and C_3-Csheterocycloalkyl groups of R^4 are each optionally substituted with 1 to 3 substituents independently selected from halogen, -CN, -$N0_2$, -R^7, -OR^8, -$C(0)R^8$, -$OC(0)R^8$, -$C(0)OR^8$, -$N(R^9)_2$, -$P(0)(OR^8)_2$, -$OP(0)(OR^8)_2$, -$P(O)(OR^{10})_2$, -$OP(O)(OR^{10})_2$, -$C(0)N(R^9)_2$, -$S(0)_2R^8$, -$S(0)R^8$, -$S(0)_2N(R^9)_2$, and -$NR^9S(0)_2R^8$;

each L is independently selected from a bond, -$(0(CH2)_m)_t$-, Ci-C6alkyl, C2-C6alkenylene and C2-C6alkynylene, wherein the Ci-C6alkyl, C2-C6alkenylene and C2-C6alkynylene of L are each optionally substituted with 1 to 4 substituents independently selected from halogen, -R^8, -OR^8, -$N(R^9)_2$, -$P(0)(OR^8)_2$, -$OP(0)(OR^8)_2$, -$P(O)(OR^{10})_2$, and -$OP(O)(OR^{10})_2$;

R^7 is selected from H, Ci-C_6alkyl, aryl, heteroaryl, C_3-Cscycloalkyl, Ci-C6heteroalkyl, Ci-C6haloalkyl, C2-Csalkene, C2-Csalkyne, Ci-C6alkoxy, Ci-C6haloalkoxy, and C_3-Csheterocycloalkyl, wherein the Ci-C6alkyl, aryl, heteroaryl, C_3-Cscycloalkyl, Ci-C6heteroalkyl, Ci-C6haloalkyl, C2-Csalkene, C2-Csalkyne, Ci-C6alkoxy, Ci-C6haloalkoxy, and C_3-Csheterocycloalkyl groups of R^7 are each optionally substituted with 1 to 3 R^{13} groups;

each R^8 is independently selected from H, -$CH(R^{10})2$, Ci-Csalkyl, C2-C_8alkene, C2-Csalkyne, Ci-C6haloalkyl, Ci-C6alkoxy, Ci-C6heteroalkyl, C_3-Cscycloalkyl, C2-Csheterocycloalkyl, Ci-C6hydroxyalkyl and Ci-C6haloalkoxy, wherein the Ci-Csalkyl, C2-Csalkene, C2-Csalkyne, Ci-C6heteroalkyl, Ci-C6haloalkyl, Ci-C6alkoxy, C_3-Cscycloalkyl, C2-C_8heterocycloalkyl, Ci-C6hydroxyalkyl and Ci-C6haloalkoxy groups of R^8 are each optionally substituted with 1 to 3 substituents independently selected from -CN, R^{11}, -OR^{11}, -SR^{11}, -$C(0)R^{11}$, -$OC(0)R^{11}$, -$C(0)N(R^9)_2$, -$C(0)OR^{11}$, -$NR^9C(0)R^{11}$, -NR^9R^{10}, -$NR^{11}R^{12}$, -$N(R^9)_2$, -OR^9, -OR^{10}, -$C(0)NR^{11}R^{12}$, -$C(0)NR^{11}OH$, -$S(0)_2R^{11}$, -$S(0)R^{11}$, -$S(0)_2NR^{11}R^{12}$, -$NR^{11}S(0)2R^{11}$, -$P(0)(OR^{11})_2$, and

$-OP(0)(OR^{11})_2$;

each R^9 is independently selected from H, $-C(0)R^8$, $-C(0)OR^8$, $-C(0)R^{10}$, $-C(0)OR^{10}$, $-S(0)_2R^{10}$, $-Ci-C_6$ alkyl, $Ci-C_6$ heteroalkyl and C_3-C_6 cycloalkyl, or each R^9 is independently a Ci-C6alkyl that together with N they are attached to form a C_3-Csheterocycloalkyl, wherein the C_3-Csheterocycloalkyl ring optionally contains an additional heteroatom selected from N, O and S, and wherein the $Ci-C_6$ alkyl, $Ci-C_6$ heteroalkyl, C_{3-C6} cycloalkyl, or C_3-Csheterocycloalkyl groups of R^9 are each optionally substituted with 1 to 3 substituents independently selected from -CN, R^{11}, $-OR^{11}$, $-SR^{11}$, $-C(0)R^{11}$, $-OC(0)R^{11}$, $-C(0)OR^{11}$, $-NR^{11}R^{12}$, $-C(0)NR^{11}R^{12}$, $-C(0)NR^{11}OH$, $-S(0)_2R^{11}$, $-S(0)R^{11}$, $-S(0)_2NR^{11}R^{12}$, $-NR^{11}S(0)_2R^{11}$, $-P(0)(OR^{11})_2$, and $-OP(0)(OR^{11})_2$;

each R^{10} is independently selected from aryl, C_3-Cscycloalkyl, C_3-Csheterocycloalkyl and heteroaryl, wherein the aryl, C_3-C_8cycloalkyl, C_3-Csheterocycloalkyl and heteroaryl groups are optionally substituted with 1 to 3 substituents selected from halogen, $-R^8$, $-OR^8$, $-LR^9$, $-LOR^9$, $-N(R^9)_2$, $-NR^9C(0)R^8$, $-NR^9C0_2R^8$, $-C0_2R^8$, $-C(0)R^8$ and $-C(0)N(R^9)_2$;

R^{11} and R^{12} are independently selected from H, Ci-C6alkyl, Ci-C6heteroalkyl, Ci-C6haloalkyl, aryl, heteroaryl, C_3-C_8cycloalkyl, and C_3-Csheterocycloalkyl, wherein the Ci-C6alkyl, Ci-C6heteroalkyl, Ci-C6haloalkyl, aryl, heteroaryl, C_3-Cscycloalkyl, and C_3-Csheterocycloalkyl groups of R^{11} and R^{12} are each optionally substituted with 1 to 3 substituents independently selected from halogen, -CN, R^8, $-OR^8$, $-C(0)R^8$, $OC(0)R^8$, $-C(0)OR^8$, $-N(R^9)_2$, $-NR^8C(0)R^8$, $-NR^8C(0)OR^8$, $-C(0)N(R^9)_2$, Cs-Csheterocycloalkyl, $-S(0)_2R^8$, $-S(0)_2N(R^9)_2$, $-NR^9S(0)_2R^8$, $Ci-C_6$haloalkyl and $Ci-C_6$haloalkoxy;

or R^{11} and R^{12} are each independently Ci-C6alkyl and taken together with the N atom to which they are attached form an optionally substituted C_3-Csheterocycloalkyl ring optionally containing an additional heteroatom selected from N, O and S;

each R^{13} is independently selected from halogen, -CN, -LR^9, -LOR^9, -OLR^9, -LR^{10}, -LOR^{10}, -OLR^{10}, -LR^8, -LOR^8, -OLR^8, -LSR^8, -LSR^{10}, -$LC(0)R^8$, -$OLC(0)R^8$, -$LC(0)OR^8$, -$LC(0)R^{10}$, -$LOC(0)OR^8$, -$LC(0)NR^9R^{11}$, -$LC(0)NR^9R^8$, -$LN(R^9)_2$, -LNR^9R^8, -LNR^9R^{10}, -$LC(0)N(R^9)_2$, -$LS(0)_2R^8$, -$LS(0)R^8$, -$LC(0)NR^8OH$, -$LNR^9C(0)R^8$, -$LNR^9C(0)OR^8$, -$LS(0)_2N(R^9)_2$, -$OLS(0)_2N(R^9)_2$, -$LNR^9S(0)_2R^8$, -$LC(0)NR^9LN(R^9)_2$, -$LP(0)(OR^8)_2$, -$LOP(0)(OR^8)_2$, -$LP(O)(OR^{10})_2$ and -$OLP(O)(OR^{10})_2$;

each R^A is independently selected from -R^8, -R^7, -OR^7, -OR^8, -R^{10}, -OR^{10}, -SR^8, -**NO2**, -CN, -$N(R^9)_2$, -$NR^9C(0)R^8$, -$NR^9C(S)R^8$, -$NR^9C(0)N(R^9)_2$, -$NR^9C(S)N(R^9)_2$, -$NR^9C0_2R^8$, -$NR^9NR^9C(0)R^8$, -$NR^9NR^9C(0)N(R^9)_2$, -$NR^9NR^9C0_2R^8$, -$C(0)C(0)R^8$, -$C(0)CH_2C(0)R^8$, -$C0_2R^8$, -$(CH_2)_nC0_2R^8$, -$C(0)R^8$, -$C(S)R^8$, -$C(0)N(R^9)_2$, -$C(S)N(R^9)_2$, -$OC(0)N(R^9)_2$, -$OC(0)R^8$, -$C(0)N(OR^8)R^8$, -$C(NOR^8)R^8$, -$S(0)_2R^8$, -$S(0)_3R^8$, -$S0_2N(R^9)_2$, -$S(0)R^8$, -$NR^9S0_2N(R^9)_2$, -$NR^9S0_2R^8$, -$P(0)(OR^8)_2$, -$OP(0)(OR^8)_2$, -$P(O)(OR^{10})_2$, -$OP(O)(OR^{10})_2$, -$N(OR^8)R^8$, -CH=CHC0_2R^8, -$C(=NH)-N(R^9)_2$, and -$(CH_2)_nNHC(0)R^8$; or two adjacent R^A substituents on Ring A form a 5-6 membered ring that contains up to two heteroatoms as ring members;

n is, independently at each occurrence, 0, 1, 2, 3, 4, 5, 6, 7 or 8;

each m is independently selected from 1, 2, 3, 4, 5 and 6, and

t is 1, 2, 3, 4, 5, 6, 7 or 8; (b) a compound having the formula:

wherein:

R^4 is selected from H, halogen, -$C(0)OR^7$, -$C(0)R^7$, -$C(0)N(R^{11}R^{12})$, -$N(R^{11}R^{12})$, -$N(R^9)_2$, -$NHN(R^9)_2$, -SR^7, -$(CH_2)_nOR^7$, -$(CH_2)_nR^7$, -LR^8, -LR^{10}, -OLR^8, -OLR^{10}, Ci-C_6alkyl, Ci-C_6heteroalkyl, Ci-Cehaloalkyl, C_2-Csalkene, C_2-Csalkyne, Ci-C_6alkoxy,

Ci-C6haloalkoxy, aryl, heteroaryl, $_{C\ 3}$-Cscycloalkyl, and $_{C3}$-Csheterocycloalkyl, wherein the Ci-C_6alkyl, Ci-C6heteroalkyl, C_1-Cehaloalkyl, C_2-Csalkene, C_2-Csalkyne, Ci-C6alkoxy, Ci-C6haloalkoxy, aryl, heteroaryl, $_{C\ 3}$-Cscycloalkyl, and $_{C\ 3}$-Csheterocycloalkyl groups of R^4 are each optionally substituted with 1 to 3 substituents independently selected from halogen, -CN, -N0 $_2$, -R^7, -OR^8, -C(0)R ^{8}, -OC(0)R ^{8}, -C(0)OR ^{8}, -$N(R^9)_2$, -P(0)(OR ^{8})$_2$, -OP(0)(OR ^{8})$_2$, -P(O)(OR^{10})$_2$, -OP(O)(OR^{10})$_2$, -C(0)N(R ^{9})$_2$, -S(0) $_2$R^8, -S(0)R ^{8}, -S(0) $_2$N(R^9)$_2$, and -NR^{9}S(0) $_2$R^8;

each L is independently selected from a bond, -(0(CH $_2$)$_m$)$_t$-, Ci-C6alkyl, C_2-C_6alkenylene and C_2-C6alkynylene, wherein the Ci-C6alkyl, C_2-C_6alkenylene and C_2-C_6alkynylene of L are each optionally substituted with 1 to 4 substituents independently selected from halogen, -R^8, -OR^8, -$N(R^9)_2$, -P(0)(OR ^{8})$_2$, -OP(0)(OR ^{8})$_2$, -P(O)(OR^{10})$_2$, and -OP(O)(OR^{10})$_2$;

R^7 is selected from H, Ci-C6alkyl, aryl, heteroaryl, $_{C\ 3}$-Cscycloalkyl, Ci-C6heteroalkyl, Ci-C6haloalkyl, C_2-Csalkene, C_2-Csalkyne, Ci-C6alkoxy, Ci-C6haloalkoxy, and $_{C\ 3}$-Csheterocycloalkyl, wherein the Ci-C6alkyl, aryl, heteroaryl, $_{C\ 3}$-Cscycloalkyl, Ci-C6heteroalkyl, Ci-C6haloalkyl, C_2-Csalkene, C_2-Csalkyne, Ci-C6alkoxy, Ci-C6haloalkoxy, and $_{C\ 3}$-Csheterocycloalkyl groups of R^7 are each optionally substituted with 1 to 3 R^{13} groups;

each R^8 is independently selected from H, -CH(R^{10})$_2$, Ci-Csalkyl, C_2-C_8alkene, C_2-Csalkyne, Ci-C6haloalkyl, Ci-C6alkoxy, Ci-C6heteroalkyl, $_{C\ 3}$-Cscycloalkyl, C_2-Csheterocycloalkyl, Ci-C6hydroxyalkyl and Ci-C6haloalkoxy, wherein the Ci-Csalkyl, C_2-Csalkene, C_2-Csalkyne, Ci-C6heteroalkyl, Ci-C6haloalkyl, Ci-C6alkoxy, $_{C\ 3}$-Cscycloalkyl, C_2-C_8heterocycloalkyl, Ci-C6hydroxyalkyl and Ci-C6haloalkoxy groups of R^8 are each optionally substituted with 1 to 3 substituents independently selected from -CN, R^{11}, -OR^{11}, -SR^{11}, -C(0)R ^{11}, -OC(0)R ^{11}, -C(0)N(R ^{9})$_2$, -C(0)OR ^{11}, -NR^{9}C(0)R ^{11}, -NR^{9}R^{10}, -NR^{11}R^{12},

$-N(R^9)_2$, $-OR^9$, $-OR^{10}$, $-C(0)NR^{11}R^{12}$, $-C(0)NR^{11}OH$, $-S(0)_2R^{11}$, $-S(0)R^{11}$, $-S(0)_2NR^{11}R^{12}$, $-NR^{11}S(O)_2R^{11}$, $-P(0)(OR^{11})_2$, and $-OP(0)(OR^{11})_2$;

each R^9 is independently selected from H, $-C(0)R^8$, $-C(0)OR^8$, $-C(0)R^{10}$, $-C(0)OR^{10}$, $-S(0)_2R^{10}$, $-Ci-C_6$ alkyl, $Ci-C_6$ heteroalkyl and C_3-C_6 cycloalkyl, or each R^9 is independently a Ci-C6alkyl that together with N they are attached to form a C_3-Csheterocycloalkyl, wherein the C_3-Csheterocycloalkyl ring optionally contains an additional heteroatom selected from N, O and S, and wherein the $Ci-C_6$ alkyl, $Ci-C_6$ heteroalkyl, C_{3-C6} cycloalkyl, or C_3-Csheterocycloalkyl groups of R^9 are each optionally substituted with 1 to 3 substituents independently selected from -CN, R^{11}, $-OR^{11}$, $-SR^{11}$, $-C(0)R^{11}$, $-OC(0)R^{11}$, $-C(0)OR^{11}$, $-NR^{11}R^{12}$, $-C(0)NR^{11}R^{12}$, $-C(0)NR^{11}OH$, $-S(0)_2R^{11}$, $-S(0)R^{11}$, $-S(0)_2NR^{11}R^{12}$, $-NR^{11}S(0)_2R^{11}$, $-P(0)(OR^{11})_2$, and $-OP(0)(OR^{11})_2$;

each R^{10} is independently selected from aryl, C_3-Cscycloalkyl, C_3-Csheterocycloalkyl and heteroaryl, wherein the aryl, C_3-C_8cycloalkyl, C_3-Csheterocycloalkyl and heteroaryl groups are optionally substituted with 1 to 3 substituents selected from halogen, $-R^8$, $-OR^8$, $-LR^9$, $-LOR^9$, $-N(R^9)_2$, $-NR^9C(0)R^8$, $-NR^9C0_2R^8$, $-C0_2R^8$, $-C(0)R^8$ and $-C(0)N(R^9)_2$;

R^{11} and R^{12} are independently selected from H, Ci-C6alkyl, Ci-C6heteroalkyl, Ci-C6haloalkyl, aryl, heteroaryl, C_3-C_8cycloalkyl, and C_3-Csheterocycloalkyl, wherein the Ci-C6alkyl, Ci-C6heteroalkyl, Ci-C6haloalkyl, aryl, heteroaryl, C_3-Cscycloalkyl, and C_3-Csheterocycloalkyl groups of R^{11} and R^{12} are each optionally substituted with 1 to 3 substituents independently selected from halogen, -CN, R^8, $-OR^8$, $-C(0)R^8$, $OC(0)R^8$, $-C(0)OR^8$, $-N(R^9)_2$, $-NR^8C(0)R^8$, $-NR^8C(0)OR^8$, $-C(0)N(R^9)_2$, C_3-C_8heterocycloalkyl, $-S(0)_2R^8$, $-S(0)_2N(R^9)_2$, $-NR^9S(0)_2R^8$, $Ci-C_6$haloalkyl and $Ci-C_6$haloalkoxy;

or R^{11} and R^{12} are each independently Ci-C6alkyl and taken together with the N atom to which they are attached form an optionally substituted C_3-

Csheterocycloalkyl ring optionally containing an additional heteroatom selected from N, O and S;

each R^{13} is independently selected from halogen, -CN, -LR^9, -LOR^9, -OLR^9, -LR^{10}, -LOR^{10}, -OLR^{10}, -LR^8, -LOR^8, -OLR^8, -LSR^8, -LSR^{10}, -$LC(0)R^8$, -$OLC(0)R^8$, -$LC(0)OR^8$, -$LC(0)R^{10}$, -$LOC(0)OR^8$, -$LC(0)NR^9R^{11}$, -$LC(0)NR^9R^8$, -$LN(R^9)_2$, -LNR^9R^8, -LNR^9R^{10}, -$LC(0)N(R^9)_2$, -$LS(0)_2R^8$, -$LS(0)R^8$, -$LC(0)NR^8OH$, -$LNR^9C(0)R^8$, -$LNR^9C(0)OR^8$, –$LS(0)_2N(R^9)_2$, -$OLS(0)_2N(R^9)_2$, -$LNR^9S(0)_2R^8$, -$LC(0)NR^9LN(R^9)_2$, -$LP(0)(OR^8)_2$, -$LOP(0)(OR^8)_2$, -$LP(O)(OR^{10})_2$ and -$OLP(O)(OR^{10})_2$;

each R^A is independently selected from -R^8, -R^7, -OR^7, -OR^8, -R^{10}, -OR^{10}, -SR^8, -$N0_2$, -CN, -$N(R^9)_2$, -$NR^9C(0)R^8$, -$NR^9C(S)R^8$, -$NR^9C(0)N(R^9)_2$, -$NR^9C(S)N(R^9)_2$, -$NR^9C0_2R^8$, -$NR^9NR^9C(0)R^8$, -$NR^9NR^9C(0)N(R^9)_2$, -$NR^9NR^9C0_2R^8$, -$C(0)C(0)R^8$, -$C(0)CH_2C(0)R^8$, -$C0_2R^8$, -$(CH_2)_nC0_2R^8$, -$C(0)R^8$, -$C(S)R^8$, -$C(0)N(R^9)_2$, -$C(S)N(R^9)_2$, -$OC(0)N(R^9)_2$, -$OC(0)R^8$, -$C(0)N(OR^8)R^8$, -$C(NOR^8)R^8$, -$S(0)_2R^8$, -$S(0)_3R^8$, -$S0_2N(R^9)_2$, -$S(0)R^8$, -$NR^9S0_2N(R^9)_2$, -$NR^9S0_2R^8$, -$P(0)(OR^8)_2$, -$OP(0)(OR^8)_2$, -$P(O)(OR^{10})_2$, -$OP(O)(OR^{10})_2$, -$N(OR^8)R^8$, -$CH=CHC0_2R^8$, -$C(=NH)-N(R^9)_2$, and -$(CH_2)_nNHC(0)R^8$;

n is, independently at each occurrence, 0, 1, 2, 3, 4, 5, 6, 7 or 8;

each m is independently selected from 1, 2, 3, 4, 5 and 6, and

t is 1, 2, 3, 4, 5, 6, 7 or 8; or (c) a pharmaceutically acceptable salt of any of (a) or (b).

[0176] Other benzonaphthyridine compounds, and methods of making benzonaphthyridine compounds, are described in WO 2009/1 11337. A benzonaphthyridine compound, or a salt thereof, can be used on its own, or in combination with one or more further compounds. For example, a benzonaphthyridine compound can be used in combination with an oil-in-water emulsion or a mineral-containing composition. In a particular embodiment, a benzonaphthyridine compound is used in combination with an oil-in-water emulsion (e.g. a squalene-water emulsion, such as MF59) or a mineral-containing composition (e.g., a mineral said such as an aluminum salt or a calcium salt).

- A thiosemicarbazone compound, such as those disclosed in reference 94. Methods of formulating, manufacturing, and screening for active compounds are also described in

reference 94. The thiosemicarbazones are particularly effective in the stimulation of human peripheral blood mononuclear cells for the production of cytokines, such as TNF-a.

- A tryptanthrin compound, such as those disclosed in reference 95. Methods of formulating, manufacturing, and screening for active compounds are also described in reference 95. The thiosemicarbazones are particularly effective in the stimulation of human peripheral blood mononuclear cells for the production of cytokines, such as TNF-a.
- A nucleoside analog, such as: (a) Isatorabine (ANA-245; 7-thia-8-oxoguanosine):

and prodrugs thereof; (b) ANA975; (c) ANA-025-1; (d) ANA380; (e) the compounds disclosed in references 96 to 98; (f) a compound having the formula:

wherein:

R_i and R_2 are each independently H, halo, $-NR_aRb$, -OH, Ci_6 alkoxy, substituted Ci_6 alkoxy, heterocyclyl, substituted heterocyclyl, C_6-io aryl, substituted C_6-io aryl, Ci_6 alkyl, or substituted Ci_6 alkyl;

R_3 is absent, H, Ci_6 alkyl, substituted Ci_6 alkyl, C_6-io aryl, substituted C_6-io aryl, heterocyclyl, or substituted heterocyclyl;

R_4 and R_5 are each independently H, halo, heterocyclyl, substituted heterocyclyl, -C(0)-Rd, Ci_6 alkyl, substituted Ci_6 alkyl, or bound together to form a 5 membered ring as in R_{4-5}:

R_{4-5}

the binding being achieved at the bonds indicated by a

X_i and X_2 are each independently N, C, O, or S;

R_8 is H, halo, -OH, Ci_6 alkyl, C_{2-6} alkenyl, C_{2-6} alkynyl, -OH, $-NR_aR_b$, $-(CH_2)_n$-0-R_c, -0-(d_ 6 alkyl), $-S(0)_pR_e$, or -C(0)-R_d;

R_9 is H, Ci-6 alkyl, substituted Ci_6 alkyl, heterocyclyl, substituted heterocyclyl or R_{9a}, wherein Rg_a is:

R_{9a}

the binding being achieved at the bond indicated by a

Rio and R_{11} are each independently H, halo, Ci_6 alkoxy, substituted Ci_6 alkoxy, $-NR_aR_b$, or -OH;

each R_a and R_b is independently H, Ci_6 alkyl, substituted Ci_6 alkyl, -C(0)Ra, C6-10 aryl;

each R_c is independently H, phosphate, diphosphate, triphosphate, Ci_6 alkyl, or substituted Ci_6 alkyl;

each R_d is independently H, halo, Ci_6 alkyl, substituted Ci_6 alkyl, Ci_6 alkoxy, substituted Ci_6 alkoxy, -NH_2, -NH(Ci_6 alkyl), -NH(substituted Ci_6 alkyl), -N(Ci_6 alkyl)$_2$, -N(substituted Ci_6 alkyl)$_2$, C_6-io aryl, or heterocyclyl;

each R_e is independently H, Ci_6 alkyl, substituted Ci_6 alkyl, C_6-io aryl, substituted C_6-io aryl, heterocyclyl, or substituted heterocyclyl;

each Rf is independently H, Ci_6 alkyl, substituted Ci_6 alkyl, -C(0)R_d, phosphate, diphosphate, or triphosphate;

each n is independently 0, 1, 2, or 3;

each p is independently 0, 1, or 2; or

or (g) a pharmaceutically acceptable salt of any of (a) to (f), a tautomer of any of (a) to (f), or a pharmaceutically acceptable salt of the tautomer.

- Loxoribine (7-allyl-8-oxoguanosine) (99).
- Compounds disclosed in reference 100, including: Acylpiperazine compounds, Indoledione compounds, Tetrahydraisoquinoline (THIQ) compounds, Benzocyclodione compounds, Aminoazavinyl compounds, Aminobenzimidazole quinolinone (ABIQ) compounds (101, 102), Hydrapthalamide compounds, Benzophenone compounds, Isoxazole compounds, Sterol compounds, Quinazilinone compounds, Pyrrole compounds (103), Anthraquinone compounds, Quinoxaline compounds, Triazine compounds, Pyrazalopyrimidine compounds, and Benzazole compounds (104).
- Compounds disclosed in reference 105.
- An aminoalkyl glucosaminide phosphate derivative, such as RC-529 (106, 107).
- A phosphazene, such as poly[di(carboxylatophenoxy)phosphazene] ("PCPP") as described, for example, in references 108 and 109.
- Small molecule immunopotentiators (SMIPs) such as:

  N2-methyl-l-(2-methylpropyl)-lH-imidazo[4,5-c]quinoline-2,4-diamine

  N2,N2-dimethyl-l-(2-methylpropyl)-lH-imidazo[4,5-c]quinoline-2,4-diamine

  N2-ethyl-N2-methyl-1-(2-methylpropyl)-lH-imidazo[4,5-c]quinoline-2,4-diamine

N2-methyl-l-(2-methylpropyl)-N2-propyl-lH-imidazo[4,5-c]quinoline-2,4-diamine

l-(2-methylpropyl)-N2-propyl-lH-imidazo[4,5-c]quinoline-2,4-diamine

N2-butyl-l-(2-methylpropyl)-lH-imidazo[4,5-c]quinoline-2,4-diamine

N2-butyl-N2-methyl-l-(2-methylpropyl)-lH-imidazo[4,5-c]quinoline-2,4-diamine

N2-methyl-l-(2-methylpropyl)-N2-pentyl-lH-imidazo[4,5-c]quinoline-2,4-diamine

N2-methyl-l-(2-methylpropyl)-N2-prop-2-enyl-lH-imidazo[4,5-c]quinoline-2,4-diamine

l-(2-methylpropyl)-2-[(phenylmethyl)thio]-lH-imidazo[4,5-c]quinolin-4-amine

1-(2-methylpropyl)-2-(propylthio)-lH-imidazo[4,5-c]quinolin-4-amine

2-[[4-amino-l-(2-methylpropyl)-lH-imidazo[4,5-c]quinolin-2-yl](methyl)amino]ethanol

2-[[4-amino-l-(2-methylpropyl)-lH-imidazo[4,5-c]quinolin-2-yl](methyl)amino]ethyl acetate

4-amino- 1-(2-methylpropyl)- 1,3-dihydro-2H-imidazo[4,5-c]quinolin-2-one

N2-butyl-l-(2-methylpropyl)-N4,N4-bis(phenylmethyl)-lH-imidazo[4,5-c]quinoline-2,4-diamine

N2-butyl-N2-methyl-l-(2-methylpropyl)-N4,N4-bis(phenylmethyl)-lH-imidazo[4,5-c]quinoline-2,4-diamine

N2-methyl-l-(2-methylpropyl)-N4,N4-bis(phenylmethyl)-lH-imidazo[4,5-c]quinoline-2,4-diamine

N2,N2-dimethyl-l-(2-methylpropyl)-N4,N4-bis(phenylmethyl)4H-imidazo[4,5-c]quinoline-2,4-diamine

1-[4-amino-2-[methyl(propyl)amino]-1H-imidazo[4,5-cjquinolin- 1-yl]-2-methylpropan-2-ol

l-[4-amino-2-(propylamino)-lH-imidazo[4,5-c]quinolin-l-yl]-2-methylpropan-2-ol

N4,N4-dibenzyl-l-(2-methoxy-2-methylpropyl)-N2-propyl-lH-imidazo[4,5-c]quinoline-2,4-diamine.

[0177] The cytokine-inducing agents for use in the present invention may be modulators and/or agonists of Toll-Like Receptors (TLR). For example, they may be

agonists of one or more of the human TLR1, TLR2, TLR3, TLR4, TLR7, TLR8, and/or TLR9 proteins. Preferred agents are agonists of TLR4 *(e.g.* , modified natural lipid As derived from enterobacterial lipopolysaccharides, phospholipid compounds, such as the synthetic phospholipid dimer, E6020), TLR7 *(e.g.,* benzonaphthyridines, imidazoquinolines) and/or TLR9 *(e.g.,* CpG oligonucleotides). These agents are useful for activating innate immunity pathways.

[0178] The cytokine-inducing agent can be added to the composition at various stages during its production. For example, it may be within an antigen composition, and this mixture can then be added to an oil-in-water emulsion. As an alternative, it may be within an oil-in-water emulsion, in which case the agent can either be added to the emulsion components before emulsification, or it can be added to the emulsion after emulsification. Similarly, the agent may be coacervated within the emulsion droplets. The location and distribution of the cytokine-inducing agent within the final composition will depend on its hydrophilic/lipophilic properties, *e.g.,* the agent can be located in the aqueous phase, in the oil phase, and/or at the oil-water interface.

[0179] The cytokine-inducing agent can be conjugated to a separate agent, such as an antigen *(e.g.,* CRM197). A general review of conjugation techniques for small molecules is provided in ref. 110. As an alternative, the adjuvants may be non-covalently associated with additional agents, such as by way of hydrophobic or ionic interactions.

[0180] Preferred cytokine-inducing agents are (a) benzonapthridine compounds; (b) immunostimulatory oligonucleotides and (c) 3dMPL.

[0181] Immunostimulatory oligonucleotides can include nucleotide modifications/analogs such as phosphorothioate modifications and can be double-stranded or (except for RNA) single-stranded. References 111, 112, and 113disclose possible analog substitutions, *e.g.,* replacement of guanosine with 2'-deoxy-7-deazaguanosine. The adjuvant effect of CpG oligonucleotides is further discussed in refs. 114 to 119. A CpG sequence may be directed to TLR9, such as the motif GTCGTT or TTCGTT (120). The CpG sequence may be specific for inducing a Thl immune response, such as a CpG-A ODN (oligodeoxynucleotide), or it may be more specific for inducing a B cell response, such a CpG-B ODN. CpG-A and CpG-B ODNs are discussed in refs. 121-123. Preferably, the CpG is a CpG-A ODN. Preferably, the CpG oligonucleotide is constructed so that the 5' end is accessible for receptor recognition. Optionally, two CpG oligonucleotide sequences may be attached at their 3' ends to form "immunomers". See, for example, references 120 & 124-

126. A useful CpG adjuvant is CpG7909, also known as PROMUNE (TM) (Coley Pharmaceutical Group, Inc.).

[0182] As an alternative, or in addition, to using CpG sequences, TpG sequences can be used (127). These oligonucleotides may be free from unmethylated CpG motifs.

[0183] The immunostimulatory oligonucleotide may be pyrimidine-rich. For example, it may comprise more than one consecutive thymidine nucleotide *(e.g.,* TTTT, as disclosed in ref. 127), and/or it may have a nucleotide composition with >25% thymidine *(e.g.,* >35%, >40%, >50%, >60%, >80%, *etc.).* For example, it may comprise more than one consecutive cytosine nucleotide *(e.g.,* CCCC, as disclosed in ref. 127), and/or it may have a nucleotide composition with >25% cytosine *(e.g., >35%,* >40%, >50%, >60%, >80%, *etc.).* These oligonucleotides may be free from unmethylated CpG motifs.

[0184] Immunostimulatory oligonucleotides will typically comprise at least 20 nucleotides. They may comprise fewer than 100 nucleotides.

[0185] 3dMPL (also known as 3 de-O-acylated monophosphoryl lipid A or 3-0-desacyl-4'-monophosphoryl lipid A) is an adjuvant in which position 3 of the reducing end glucosamine in monophosphoryl lipid A has been de-acylated. 3dMPL has been prepared from a heptoseless mutant of *Salmonella minnesota,* and is chemically similar to lipid A but lacks an acid-labile phosphoryl group and a base-labile acyl group. It activates cells of the monocyte/macrophage lineage and stimulates release of several cytokines, including IL-1, IL-12, TNF-a and GM-CSF (see also ref. 128). Preparation of 3dMPL was originally described in reference 129.

[0186] 3dMPL can take the form of a mixture of related molecules, varying by their acylation *(e.g.,* having 3, 4, 5 or 6 acyl chains, which may be of different lengths). The two glucosamine (also known as 2-deoxy-2-amino-glucose) monosaccharides are N-acylated at their 2-position carbons *(i.e.,* at positions 2 and 2'), and there is also O-acylation at the 3' position. The group attached to carbon 2 has formula -NH-CO-CH_2-$CR^1R^{1'}$. The group attached to carbon 2' has formula -NH-CO-CH_2-$CR^2R^{2'}$. The group attached to carbon 3' has formula -0-CO-CH_2-$CR^3R^{3'}$. A representative structure is:

[0187] Groups R^1, R^2 and R^3 are each independently -$(CH_2)_n$-CH_3. The value of *n* is preferably between 8 and 16, more preferably between 9 and 12, and is most preferably 10.

[0188] Groups $R^{1'}$, $R^{2'}$ and $R^{3'}$ can each independently be: (a) -H; (b) -OH; or (c) -0-CO-R^4,where R^4 is either - H or -$(CH_2)_m$-CH_3, wherein the value of *m* is preferably between 8 and 16, and is more preferably 10, 12 or 14. At the 2 position, *m* is preferably 14.

At the 2' position, *m* is preferably 10. At the 3' position, *m* is preferably 12. Groups $R^{1'}$, $R^{2'}$ and $R^{3'}$ are thus preferably -O-acyl groups from dodecanoic acid, tetradecanoic acid or hexadecanoic acid.

[0189] When all of $R^{1'}$, $R^{2'}$ and $R^{3'}$ are -H then the 3dMPL has only 3 acyl chains (one on each of positions 2, 2' and 3')· When only two of $R^{1'}$, $R^{2'}$ and $R^{3'}$ are -H then the 3dMPL can have 4 acyl chains. When only one of $R^{1'}$, $R^{2'}$ and $R^{3'}$ is -H then the 3dMPL can have 5 acyl chains. When none of $R^{1'}$, $R^{2'}$ and $R^{3'}$ is -H then the 3dMPL can have 6 acyl chains. The 3dMPL adjuvant used according to the invention can be a mixture of these forms, with from 3 to 6 acyl chains, but it is preferred to include 3dMPL with 6 acyl chains in the mixture, and in particular to ensure that the hexaacyl chain form makes up at least 10% by weight of the total 3dMPL *e.g.*, >20%, >30%, >40%, >50% or more. 3dMPL with 6 acyl chains has been found to be the most adjuvant-active form.

[0190] Thus the most preferred form of 3dMPL for inclusion in compositions of the invention has formula (IV), shown below.

[0191] Where 3dMPL is used in the form of a mixture then references to amounts or concentrations of 3dMPL in compositions of the invention refer to the combined 3dMPL species in the mixture.

[0192] In aqueous conditions, 3dMPL can form micellar aggregates or particles with different sizes *e.g.*, with a diameter <150nm or >500nm. Either or both of these can be used with the invention, and the better particles can be selected by routine assay. Smaller particles *{e.g.*, small enough to give a clear aqueous suspension of 3dMPL) are preferred for use according to the invention because of their superior activity (130). Preferred particles have a mean diameter less than 220nm, more preferably less than 200nm or less than 150nm or less than 120nm, and can even have a mean diameter less than lOOnm. In most cases, however, the mean diameter will not be lower than 50nm. These particles are small enough to be suitable for filter sterilization. Particle diameter can be assessed by the routine technique of dynamic light scattering, which reveals a mean particle diameter. Where a particle is said to have a diameter of *x* nm, there will generally be a distribution of particles about this mean, but at least 50% by number *(e.g.*, >60%, >70%, >80%, >90%, or more) of the particles will have a diameter within the range x+25%.

[0193] 3dMPL can advantageously be used in combination with an oil-in-water emulsion. Substantially all of the 3dMPL may be located in the aqueous phase of the emulsion.

[0194] The 3dMPL can be used on its own, or in combination with one or more further compounds. For example, it is known to use 3dMPL in combination with the QS21 saponin (131) (including in an oil-in-water emulsion (132)), with an immunostimulatory oligonucleotide, with both QS21 and an immunostimulatory oligonucleotide, with aluminum phosphate (133), with aluminum hydroxide (134), or with both aluminum phosphate and aluminum hydroxide.

Formula (IV)

Fatty adjuvants

[0195] Fatty adjuvants that can be used with the invention include the oil-in-water emulsions described above, and also include, for example:

- A phospholipid compound of formula I, II or III, or a salt thereof:

I II III

as defined in reference 135, such as 'ER 803058', 'ER 803732', 'ER 804053', ER 804058', 'ER 804059', 'ER 804442', 'ER 804680', 'ER 804764', ER 803022 or 'ER 804057' *e.g.:*

ER804057

ER-803022.

ER804057 is also called E6020. A phospholipid compound of formula I, II or III, or a salt thereof, can be used on its own, or in combination with one or more further compounds. For example, a compound of formula I, II or III, can be used in combination with an oil-in-water emulsion or a mineral-containing composition. In a

particular embodiment, E6020 is used in combination with an oil-in-water emulsion (e.g. a squalene-water emulsion, such as MF59) or a mineral-containing composition (e.g., a mineral said such as an aluminum salt or a calcium salt).

- Derivatives of lipid A from *Escherichia coli* such as OM-174 (described in refs. 136 & 137).
- A formulation of a cationic lipid and a (usually neutral) co-lipid, such as aminopropyl-dimethyl-myristoleyloxy-propanaminium bromide-diphytanoylphosphatidyl-ethanolamine ("VAXFECTIN (TM)") or aminopropyl-dimethyl-bis-dodecyloxy-propanaminium bromide-dioleoylphosphatidyl-ethanolamine ("GAP-DLRIE:DOPE"). Formulations containing (+)-N-(3-aminopropyl)-N,N-dimethyl-2,3-bis(syn-9-tetradeceneyloxy)-l-propanaminium salts are preferred (138).
- 3-O-deacylated monophosphoryl lipid A (see above).
- Compounds containing lipids linked to a phosphate-containing acyclic backbone, such as the TLR4 antagonist E5564 (139, 140):

    - Lipopeptides (i.e., compounds comprising one or more fatty acid residues and two or more amino acid residues), such as lipopeptides based on glycerylcysteine. Specific examples of such peptides include compounds of the following formula

in which each of R^1 and R^2 represents a saturated or unsaturated, aliphatic or mixed aliphatic-cycloaliphatic hydrocarbon radical having from 8 to 30, preferably 11 to 21, carbon atoms that is optionally also substituted by oxygen functions, R^3 represents hydrogen or the radical R1-CO-O-CH2- in which R^1 has the same meaning as above, and X represents an amino acid bonded by a peptide linkage and having a free, esterified or amidated carboxy group, or an amino acid sequence of from 2 to 10 amino acids of which the terminal carboxy group is in free, esterified or amidated form. In certain embodiments, the amino acid sequence comprises a D-amino acid, for example, D-glutamic acid (D-Glu) or D-gamma-carboxy-glutamic acid (D-Gla).

[0196] Bacterial lipopeptides generally recognize TLR2, without requiring TLR6 to participate. (TLRs operate cooperatively to provide specific recognition of various triggers, and TLR2 plus TLR6 together recognize peptidoglycans, while TLR2 recognizes lipopeptides without TLR6.) These are sometimes classified as natural lipopeptides and

synthetic lipopeptides. Synthetic lipopeptides tend to behave similarly, and are primarily recognized by TLR2.

[0197] Lipopeptides suitable for use as adjuvants include compounds have the formula:

where the chiral center labeled * and the one labeled *** are both in the R configuration; the chiral center labeled ** is either in the R or S configuration;

each R^{1a} and R^{1b} is independently an aliphatic or cycloaliphatic-aliphatic hydrocarbon group having 7-21 carbon atoms, optionally substituted by oxygen functions, or one of R^{1a} and R^{1b}, but not both, is H;

R^2 is an aliphatic or cycloaliphatic hydrocarbon group having 1-21 carbon atoms and optionally substituted by oxygen functions;

n is 0 or 1;

As represents either -O-Kw-CO- or -NH-Kw-CO- , where Kw is an aliphatic hydrocarbon group having 1-12 carbon atoms;

As^1 is a D- or L-alpha-amino acid;

Z^1 and Z^2 each independently represent -OH or the N-terminal radical of a D- or L-alpha amino acid of an amino-(lower alkane)-sulfonic acid or of a peptide having up to 6 amino acids selected from the D- and L-alpha aminocarboxylic acids and amino-lower alkyl-sulfonic acids; and

Z^3 is H or -CO-Z^4, wher Z^4 is -OH or the N-terminal radical of a D- or L-alpha amino acid of an amino-(lower alkane)- sulfonic acid or of a peptide having up to 6 amino acids selected from the D and L-alpha aminocarboxylic acids and amino-lower alkyl-sulfonic acids; or an ester or amide formed from the carboxylic acid of such compounds. Suitable amides include -N¾ and NH(lower alkyl), and suitable esters include C1-C4 alkyl esters. (lower alkyl or lower alkane, as used herein, refers to Ci-C_6 straight chain or branched alkyls).

[0198] Such compounds are described in more detail in US 4,666,886. In one particular embodiment, the lipopeptide has the formula:

[0199] Another example of a lipopeptide species is called LP40, and is an agonist of TLR2. Akdis, et al., *Eur. J. Immunology,* 33: 2717-26 (2003).

[0200] These are related to a known class of lipopeptides from *E. coli,* referred to as murein lipoproteins. Certain partial degradation products of those proteins called murein lipopetides are described in Hantke, et al., *Eur. J. Biochem.,* 34: 284-296 (1973). These comprise a peptide linked to N-acetyl muramic acid and are thus related to Muramyl peptides, which are described in Baschang, et al., *Tetrahedron,* 45(20): 6331-6360 (1989).

Aluminum salt adjuvants

[0201] The adjuvants known as "aluminum hydroxide" and "aluminum phosphate" may be used. These names are conventional, but are used for convenience only, as neither is a precise description of the actual chemical compound which is present *(e.g.,* see chapter 9 of reference 74). The invention can use any of the "hydroxide" or "phosphate" adjuvants that are in general use as adjuvants.

[0202] The adjuvants known as "aluminum hydroxide" are typically aluminum oxyhydroxide salts, which are usually at least partially crystalline. Aluminum oxyhydroxide, which can be represented by the formula AIO(OH), can be distinguished from other aluminum compounds, such as aluminum hydroxide Al(OH)3, by infrared (IR) spectroscopy, in particular by the presence of an adsorption band at 1070cm^{-1} and a strong shoulder at 3090-3 100cm^{-1} (chapter 9 of ref. 74). The degree of crystallinity of an aluminum hydroxide adjuvant is reflected by the width of the diffraction band at half height (WHH), with poorly-crystalline particles showing greater line broadening due to smaller crystallite sizes. The surface area increases as WHH increases, and adjuvants with higher WHH values have been seen to have greater capacity for antigen adsorption. A fibrous morphology *(e.g.,* as seen in transmission electron micrographs) is typical for aluminum hydroxide adjuvants. The pi of aluminum hydroxide adjuvants is typically about \ \, *i.e.,* the adjuvant itself has a positive surface charge at physiological pH. Adsorptive capacities of between 1.8-2.6 mg protein per mg Al^{+++} at pH 7.4 have been reported for aluminum hydroxide adjuvants.

[0203] The adjuvants known as "aluminum phosphate" are typically aluminum hydroxyphosphates, often also containing a small amount of sulfate *(i.e.,* aluminum hydroxyphosphate sulfate). They may be obtained by precipitation, and the reaction conditions and concentrations during precipitation influence the degree of substitution of phosphate for hydroxyl in the salt. Hydroxyphosphates generally have a PO_4/AI molar ratio

between 0.3 and 1.2. Hydroxyphosphates can be distinguished from strict $A1P0_4$ by the presence of hydroxyl groups. For example, an IR spectrum band at $3164cm^{-1}$ *(e.g.,* when heated to 200°C) indicates the presence of structural hydroxyls (ch.9 of ref. 74).

[0204] The PO_4/AI^{3+} molar ratio of an aluminum phosphate adjuvant will generally be between 0.3 and 1.2, preferably between 0.8 and 1.2, and more preferably 0.95+0.1. The aluminum phosphate will generally be amorphous, particularly for hydroxyphosphate salts. A typical adjuvant is amorphous aluminum hydroxyphosphate with PO_4/AI molar ratio between 0.84 and 0.92, included at 0.6mg Al^{3+}/ml. The aluminum phosphate will generally be particulate *(e.g.,* plate-like morphology as seen in transmission electron micrographs). Typical diameters of the particles are in the range 0.5-20μιη *(e.g.,* about 5-10μιη) after any antigen adsorption. Adsorptive capacities of between 0.7-1.5 mg protein per mg Al^{+++} at pH 7.4 have been reported for aluminum phosphate adjuvants.

[0205] The point of zero charge (PZC) of aluminum phosphate is inversely related to the degree of substitution of phosphate for hydroxyl, and this degree of substitution can vary depending on reaction conditions and concentration of reactants used for preparing the salt by precipitation. PZC is also altered by changing the concentration of free phosphate ions in solution (more phosphate = more acidic PZC) or by adding a buffer such as a histidine buffer (makes PZC more basic). Aluminum phosphates used according to the invention will generally have a PZC of between 4.0 and 7.0, more preferably between 5.0 and 6.5, *e.g.,* about 5.7.

[0206] Suspensions of aluminum salts used to prepare compositions of the invention may contain a buffer *(e.g.,* a phosphate or a histidine or a Tris buffer), but this is not always necessary. The suspensions are preferably sterile and pyrogen-free. A suspension may include free aqueous phosphate ions *e.g.,* present at a concentration between 1.0 and 20 mM, preferably between 5 and 15 mM, and more preferably about 10 mM. The suspensions may also comprise sodium chloride.

[0207] The invention can use a mixture of both an aluminum hydroxide and an aluminum phosphate. In this case there may be more aluminum phosphate than hydroxide *e.g.,* a weight ratio of at least 2:1 *e.g.,* >5:1, >6:1, >7:1, >8:1, >9:1, *etc.*

[0208] The concentration of Al^{+++} in a composition for administration to a patient is preferably less than lOmg/ml *e.g.,* <5 mg/ml, <4 mg/ml, <3 mg/ml, <2 mg/ml, <1 mg/ml, *etc.* A preferred range is between 0.3 and lmg/ml. A maximum of 0.85mg/dose is preferred.

[0209] As well as including one or more aluminum salt adjuvants, the adjuvant component may include one or more further adjuvant or immunostimulating agents. Such

additional components include, but are not limited to: a benzonaphthyridine compound, a 3-O-deacylated monophosphoryl lipid A adjuvant ('3d-MPL'); and/or an oil-in-water emulsion. 3d-MPL has also been referred to as 3 de-O-acylated monophosphoryl lipid A or as 3-0-desacyl-4'-monophosphoryl lipid A. The name indicates that position 3 of the reducing end glucosamine in monophosphoryl lipid A is de-acylated. It has been prepared from a heptoseless mutant of *S.minnesota*, and is chemically similar to lipid A but lacks an acid-labile phosphoryl group and a base-labile acyl group. It activates cells of the monocyte/macrophage lineage and stimulates release of several cytokines, including IL-1, IL-12, TNF-a and GM-CSF. Preparation of 3d-MPL was originally described in reference 129, and the product has been manufactured and sold by Corixa Corporation under the name MPL (TM). Further details can be found in refs 82 to 85.

[0210] The use of an aluminum hydroxide and/or aluminum phosphate adjuvant is useful, particularly in children, and antigens are generally adsorbed to these salts. Squalene-in-water emulsions are also preferred, particularly in the elderly. Useful adjuvant combinations include combinations of Thl and Th2 adjuvants such as CpG and alum, or resiquimod and alum. A combination of aluminum phosphate and 3dMPL may be used. Other combinations that may be used include: alum and a benzonapthridine compound or a SMIP, a squalene-in-water emulsion (such as MF59) and a benzonapthridine compound or a SMIP, and E6020 and a squalene-in-water emulsion, such as MF59) or alum.

[0211] The compositions of the invention may elicit both a cell mediated immune response as well as a humoral immune response.

[0212] Two types of T cells, CD4 and CD8 cells, are generally thought necessary to initiate and/or enhance cell mediated immunity and humoral immunity. CD8 T cells can express a CD8 co-receptor and are commonly referred to as Cytotoxic T lymphocytes (CTLs). CD8 T cells are able to recognized or interact with antigens displayed on MHC Class I molecules.

[0213] CD4 T cells can express a CD4 co-receptor and are commonly referred to as T helper cells. CD4 T cells are able to recognize antigenic peptides bound to MHC class II molecules. Upon interaction with a MHC class II molecule, the CD4 cells can secrete factors such as cytokines. These secreted cytokines can activate B cells, cytotoxic T cells, macrophages, and other cells that participate in an immune response. Helper T cells or CD4+ cells can be further divided into two functionally distinct subsets: TH1 phenotype and TH2 phenotypes which differ in their cytokine and effector function.

[0214] Activated TH1 cells enhance cellular immunity (including an increase in antigen-specific CTL production) and are therefore of particular value in responding to intracellular infections. Activated TH1 cells may secrete one or more of IL-2, IFN-γ, and TNF-β. A TH1 immune response may result in local inflammatory reactions by activating macrophages, NK (natural killer) cells, and CD8 cytotoxic T cells (CTLs). A TH1 immune response may also act to expand the immune response by stimulating growth of B and T cells with IL-12. TH1 stimulated B cells may secrete IgG2a.

[0215] Activated TH2 cells enhance antibody production and are therefore of value in responding to extracellular infections. Activated TH2 cells may secrete one or more of IL-4, IL-5, IL-6, and IL-10. A TH2 immune response may result in the production of IgGl, IgE, IgA and memory B cells for future protection.

[0216] An enhanced immune response may include one or more of an enhanced TH1 immune response and a TH2 immune response.

[0217] A TH1 immune response may include one or more of an increase in CTLs, an increase in one or more of the cytokines associated with a TH1 immune response (such as IL-2, IFN-γ, and TNF-β), an increase in activated macrophages, an increase in NK activity, or an increase in the production of IgG2a. Preferably, the enhanced TH1 immune response will include an increase in IgG2a production.

[0218] A TH1 immune response may be elicited using a TH1 adjuvant. A TH1 adjuvant will generally elicit increased levels of IgG2a production relative to immunization of the antigen without adjuvant. TH1 adjuvants suitable for use in the invention may include for example saponin formulations, virosomes and virus like particles, non-toxic derivatives of enterobacterial lipopolysaccharide (LPS), immunostimulatory oligonucleotides. Immunostimulatory oligonucleotides, such as oligonucleotides containing a CpG motif, are preferred TH1 adjuvants for use in the invention.

[0219] A TH2 immune response may include one or more of an increase in one or more of the cytokines associated with a TH2 immune response (such as IL-4, IL-5, IL-6 and IL-10), or an increase in the production of IgGl, IgE, IgA and memory B cells. Preferably, the enhanced TH2 immune response will include an increase in IgGl production.

[0220] A TH2 immune response may be elicited using a TH2 adjuvant. A TH2 adjuvant will generally elicit increased levels of IgGl production relative to immunization of the antigen without adjuvant. TH2 adjuvants suitable for use in the invention include, for example, mineral containing compositions, oil-emulsions, and ADP-ribosylating toxins and

detoxified derivatives thereof. Mineral containing compositions, such as aluminium salts are preferred TH2 adjuvants for use in the invention.

[0221] A composition may include a combination of a THl adjuvant and a TH2 adjuvant. Preferably, such a composition elicits an enhanced THl and an enhanced TH2 response, i.e., an increase in the production of both IgGl and IgG2a production relative to immunization without an adjuvant. Still more preferably, the composition comprising a combination of a THl and a TH2 adjuvant elicits an increased THl and/or an increased TH2 immune response relative to immunization with a single adjuvant *(i.e.,* relative to immunization with a THl adjuvant alone or immunization with a TH2 adjuvant alone).

[0222] The immune response may be one or both of a THl immune response and a TH2 response. Preferably, immune response provides for one or both of an enhanced THl response and an enhanced TH2 response.

[0223] The enhanced immune response may be one or both of a systemic and a mucosal immune response. Preferably, the immune response provides for one or both of an enhanced systemic and an enhanced mucosal immune response. Preferably the mucosal immune response is a TH2 immune response. Preferably, the mucosal immune response includes an increase in the production of IgA.

Methods of treatment, and administration

[0224] Compositions of the invention are suitable for administration to mammals, and the invention provides a method of inducing an immune response in a mammal, comprising the step of administering a composition (e.g., an immunogenic composition) of the invention to the mammal. The compositions (e.g., an immunogenic composition) can be used to produce a vaccine formulation for immunizing a mammal. The mammal is typically a human, and the RSV F protein is typically a human RSV F protein. However, the mammal can be any other mammal that is susceptible to infection with RSV, such as a cow that can be infected with bovine RSV. For example, the immune response may be raised following administration of a purified RSV F protein, an alphavirus particle, or self-replicating RNA.

[0225] The invention also provides the use of two or more pre-fusion chimerid proteins based on two or more different non-RSV (e.g., parainfluenza virus, metapneumovirus) F pre-fusion proteins (i.e., PIV5 and NDV) that each have the same RSV F neutralizing epitopes mutated on the protein surface. Thus, inoculation with one chimeric pre-fusion F, and a second inoculation with the second pre-fusion F may prime several

antibodies, some to RSV and some to the template protein backbone. The second inoculation may bias boosting of only the shared RSV F neutralizing epitopes.

[0226] The invention also provides a composition of the invention for use as a medicament, *e.g.,* for use in immunizing a patient against RSV infection.

[0227] The invention also provides the use of a polypeptide as described above in the manufacture of a medicament for raising an immune response in a patient.

[0228] The immune response raised by these methods and uses will generally include an antibody response, preferably a protective antibody response. Methods for assessing antibody responses after RSV vaccination are well known in the art.

[0229] Compositions of the invention can be administered in a number of suitable ways, such as intramuscular injection *(e.g.,* into the arm or leg), subcutaneous injection, intranasal administration, oral administration, intradermal administration, transcutaneous administration, transdermal administration, and the like. The appropriate route of administration will be dependent upon the age, health and other characteristics of the mammal. A clinician will be able to determine an appropriate route of administration based on these and other factors.

[0230] Immunogenic compositions, and vaccine formulations, may be used to treat both children and adults, including pregnant women. Thus a subject may be less than 1 year old, 1-5 years old, 5-15 years old, 15-55 years old, or at least 55 years old. Preferred subjects for receiving the vaccines are the elderly *(e.g.,* >50 years old, >60 years old, and preferably >65 years), the young *(e.g.,* <6 years old, such as 4 - 6 years old, <5 years old), and pregnant women. The vaccines are not suitable solely for these groups, however, and may be used more generally in a population.

[0231] Treatment can be by a single dose schedule or a multiple dose schedule. Multiple doses may be used in a primary immunization schedule and/or in a booster immunization schedule. In a multiple dose schedule the various doses may be given by the same or different routes, *e.g.,* a parenteral prime and mucosal boost, a mucosal prime and parenteral boost, *etc.* Administration of more than one dose (typically two doses) is particularly useful in immunologically naïve patients. Multiple doses will typically be administered at least 1 week apart *(e.g.,* about 2 weeks, about 3 weeks, about 4 weeks, about 6 weeks, about 8 weeks, about 10 weeks, about 12 weeks, about 16 weeks, and the like.).

[0232] Vaccine formulations produced using a composition of the invention may be administered to patients at substantially the same time as *(e.g.,* during the same medical consultation or visit to a healthcare professional or vaccination centre) other vaccines.

General

[0233] The term "comprising" encompasses "including" as well as "consisting" and "consisting essentially of" *e.g.,* a composition "comprising" X may consist exclusively of X or may include something additional e.g., X + Y.

[0234] The word "substantially" does not exclude "completely" *e.g., a* composition which is "substantially free" from Y may be completely free from Y. Where necessary, the word "substantially" may be omitted from the definition of the invention.

[0235] The term "about" in relation to a numerical value x means, for example, x+10%.

[0236] Unless specifically stated, a process comprising a step of mixing two or more components does not require any specific order of mixing. Thus components can be mixed in any order. Where there are three components then two components can be combined with each other, and then the combination may be combined with the third component, etc.

[0237] Where animal (and particularly bovine) materials are used in the culture of cells, they should be obtained from sources that are free from transmissible spongiform encaphalopathies (TSEs), and in particular free from bovine spongiform encephalopathy (BSE). Overall, it is preferred to culture cells in the total absence of animal-derived materials.

[0238] Where a compound is administered to the body as part of a composition then that compound may alternatively be replaced by a suitable prodrug.

[0239] Where a cell substrate is used for reassortment or reverse genetics procedures, it is preferably one that has been approved for use in human vaccine production *e.g.,* as in Ph Eur general chapter 5.2.3.

[0240] Identity between polypeptide sequences is preferably determined by the Smith-Waterman homology search algorithm as implemented in the MPSRCH program (Oxford Molecular), using an affine gap search with parameters gap open penalty=12 and gap extension penalty=l .

Table 2. Phospholipids

DDPC	1,2-Didecanoyl-sn-Glycero-3-phosphatidylcholine
DEPA	1,2-Dierucoyl-sn-Glycero-3-Phosphate
DEPC	1,2-Erucoyl-sn-Glycero-3-phosphatidylcholine

DEPE	l,2-Dierucoyl-sn-Glycero-3-phosphatidylethanolamine
DEPG	l,2-Dierucoyl-sn-Glycero-3[Phosphatidyl-rac-(l -glycerol...)
DLOPC	l,2-Linoleoyl-sn-Glycero-3-phosphatidylcholine
DLPA	l,2-Dilauroyl-sn-Glycero-3-Phosphate
DLPC	l,2-Dilauroyl-sn-Glycero-3-phosphatidylcholine
DLPE	l,2-Dilauroyl-sn-Glycero-3-phosphatidylethanolamine
DLPG	l,2-Dilauroyl-sn-Glycero-3[Phosphatidyl-rac-(l -glycerol...)
DLPS	l,2-Dilauroyl-sn-Glycero-3-phosphatidylserine
DMG	l,2-Dimyristoyl-sn-glycero-3-phosphoethanolamine
DMPA	l,2-Dimyristoyl-sn-Glycero-3-Phosphate
DMPC	l,2-Dimyristoyl-sn-Glycero-3-phosphatidylcholine
DMPE	l,2-Dimyristoyl-sn-Glycero-3-phosphatidylethanolamine
DMPG	l,2-Myristoyl-sn-Glycero-3[Phosphatidyl-rac-(l -glycerol...)
DMPS	l,2-Dimyristoyl-sn-Glycero-3-phosphatidylserine
DOPA	l,2-Dioleoyl-sn-Glycero-3-Phosphate
DOPC	l,2-Dioleoyl-sn-Glycero-3-phosphatidylcholine
DOPE	l,2-Dioleoyl-sn-Glycero-3-phosphatidylethanolamine
DOPG	l,2-Dioleoyl-sn-Glycero-3[Phosphatidyl-rac-(l-glycerol...)
DOPS	l,2-Dioleoyl-sn-Glycero-3-phosphatidylserine
DPPA	l,2-Dipalmitoyl-sn-Glycero-3-Phosphate
DPPC	l,2-Dipalmitoyl-sn-Glycero-3-phosphatidylcholine
DPPE	l,2-Dipalmitoyl-sn-Glycero-3-phosphatidylethanolamine
DPPG	l,2-Dipalmitoyl-sn-Glycero-3[Phosphatidyl-rac-(l-glycerol...)
DPPS	l,2-Dipalmitoyl-sn-Glycero-3-phosphatidylserine
DPyPE	l,2-diphytanoyl-sn-glycero-3-phosphoethanolamine
DSPA	l,2-Distearoyl-sn-Glycero-3-Phosphate
DSPC	l,2-Distearoyl-sn-Glycero-3-phosphatidylcholine
DSPE	l,2-Diostearpyl-sn-Glycero-3-phosphatidylethanolamine
DSPG	l,2-Distearoyl-sn-Glycero-3[Phosphatidyl-rac-(l -glycerol...)
DSPS	l,2-Distearoyl-sn-Glycero-3-phosphatidylserine
EPC	Egg-PC
HEPC	Hydrogenated Egg PC
HSPC	High purity Hydrogenated Soy PC
HSPC	Hydrogenated Soy PC
LYSOPC MYRISTIC	l-Myristoyl-sn-Glycero-3-phosphatidylcholine
LYSOPC PALMITIC	l-Palmitoyl-sn-Glycero-3-phosphatidylcholine
LYSOPC STEARIC	l-Stearoyl-sn-Glycero-3-phosphatidylcholine

Milk Sphingomyelin MPPC l-Myristoyl,2-palmitoyl-sn-Glycero 3-phosphatidylcholine
MSPC l-Myristoyl,2-stearoyl-sn-Glycero-3-phosphatidylcholine
PMPC 1-Palmitoyl,2-myristoyl-sn-Glycero-3-phosphatidylcholine
POPC 1-Palmitoyl, 2-oleoyl- sn- Glycero- 3-phosphatidylcholine
POPE l-Palmitoyl-2-oleoyl-sn-Glycero-3-phosphatidylethanolamine
POPG l,2-Dioleoyl-sn-Glycero-3[Phosphatidyl-rac-(l-glycerol)...]
PSPC 1-Palmitoyl, 2-stearoyl- sn- Glycero- 3-phosphatidylcholine
SMPC l-Stearoyl,2-myristoyl-sn-Glycero-3-phosphatidylcholine
SOPC l-Stearoyl,2-oleoyl-sn-Glycero-3-phosphatidylcholine
SPPC l-Stearoyl,2-palmitoyl-sn-Glycero-3-phosphatidylcholine

EXEMPLIFICATION

1. Post-fusion structure and pre-fusion model

Post-Fusion RSV F Structure

[0241] A stable, non-aggregating soluble RSV F subunit antigen was prepared by deletion of the fusion peptide, transmembrane region, and cytoplasmic domain (FIG. 1). This engineered F was expressed efficiently and was readily purified. Electron microscopy of negatively stained specimens showed that it formed non-aggregated, homogeneous crutch-shaped molecules, consistent with post-fusion F trimers (FIG. 2A). This engineered F trimer was stable, and circular dichroism spectroscopy revealed no significant melting at temperatures up to 95°C (FIGS. 2B and 2C).

[0242] This RSV F protein was crystallized and its structure was determined by molecular replacement and three-fold non-crystallographic symmetry (NCS) averaging (Table 3 and FIG. 3). The structure does not include the p27 fragment (the peptide between the two furin sites that is lost upon cleavage), the fusion peptide, the transmembrane region, or the cytoplasmic domain (FIG. 4).

Table 3. **Crystallographic data**

Data collection statistics

Space Group	P 2i 2i 2i
Cell dimensions (Å)	*a* = 87.930
	b = 113.160
	c = 311.370

	$\alpha = \beta = \gamma = 90.00^{\circ}$
Resolution limit (Å)	50-3.2
Unique reflections	51,911
Unique reflections †	40,398
Redundancy	3.9 (3.7)¥
Overall completeness (%)	99.4 (99.4)
Overall completeness (%)†	77.0 (26.7)
<I/σ>	12.2 (2.2)
R_{sym} (%)	7.7 (71.0)

Refinement Statistics^

Polypeptide chains	3
Protein atoms	10,398
Residues in allowed regions of the Ramachandran plot (%)	98.5
Residues in most favored regions of Ramachandran plot (%)	83.5
RMSD bond lengths (Å)	0.021
RMSD bond angles (deg)	2.053
Mean B values (A^2)	15.71
Resolution range (Å)	30-3.2
R_{work} (%)	23.1 (34.9)
R_{free} (%)	26.6 (40.2)

¥ Values in parentheses refer to data in the highest resolution shell
† Statistics for the data after anisotropic correction.
†† Refinement values for the data after anisotropic correction.

[0243] The overall architecture of post-fusion RSV F is shared with other post-fusion parainfluenza fusion proteins. The protein is composed of three tightly intertwined subunits, forming a globular head and an elongated stalk. Each subunit contains three domains, designated I, II, and III (FIGS. 4A-C). Domains I and II are at the top of the trimeric head and form a triangular crown. Domain III forms the base of the head. A long helix, HRA, extends from domain III and forms the trimeric coiled-coil in the center of the stalk. The HRB helix is tethered to domain II and reaches down to the head-distal end of the stalk, where it forms the outer coils of a six-helix bundle with the HRA interior coiled-coil. In full-length F, the hydrophobic fusion peptide (N-terminal to HRA) and the transmembrane region (C-terminal to HRB), would be juxtaposed at the bottom of the stalk and inserted into the target cell membrane.

[0244] Domains I and II of RSV, parainfluenza virus 3 (PIV3), and parainfluenza virus 5 (PIV5) F proteins are structurally conserved (FIGS. 5A and 5B). The only significant difference is in the orientation of the sole helix of domain I (η3 of RSV F and α6 of PIV3 and PIV5 Fs) relative to their common β-sheets. In contrast, RSV F domain III has features

that were not predicted from parainfluenza-based modeling (FIG. 6). When the four-stranded β-sheets of RSV F domain III and PIV3 F domain III are superimposed, key differences in the domains' helical regions are apparent. Helix HRA kinks at a more N-terminal position in RSV F than in PIV3 F, causing an approximately 60° difference in the rotation of the heads relative to the stalks (FIGS. 6A, 6B, 6D). Influenza hemagglutinins also vary in the orientations of their heads relative to their stalks, with 30°-50° differences in rotation between subtypes. (Ha, Y. et al., *Embo Journal* **21,** 865-875 (2002)).

[0245] The RSV F domain III helical bundle region contains an extra helix (ot6), changing the orientation of the bundled helices relative to those in parainfluenza Fs (FIGS. 6A-C and FIG. 1). RSV F helices αζ5 and αζ6 are almost parallel and are exposed on the trimer surface; the equivalent to RSV F αζ6 helix in the PIV3 helical bundle (α5, FIG. 6C) is buried in the inter-subunit interface of the trimer. RSV F helices αζ5 and αζ6 form the epitope bound by the related neutralizing antibodies Palivizumab and Motavizumab. The structure of a complex between the Motavizumab Fab and a 24-residue RSV F peptide that includes αζ5 and α6 has been reported (McLellan, J. S. *et al. Nat Struct Mol Biol* 17, 248-250 (2010)). Comparison between this structure and the post-fusion RSV F structure revealed a close match between the α5-α6 helices (r.m.s.d. = 0.52 Å; FIG. 7A). Superposition of the two structures based on these helices models a complex between Motavizumab and post-fusion RSV F (FIG. 7B). This model reveals no steric hindrance that would prevent Motavizumab (or, presumably, Palivizumab) from binding to post-fusion RSV F. Binding of Palivizumab to the post-fusion F ectodomain in solution using surface plasmon resonance (K_D of 4.2 x 10^{-10} M) was confirmed.

[0246] Pre-fusion and post-fusion parainfluenza F structures reveal *en bloc* shifts of domains and large rearrangements of HRA and HRB. In domain III of the pre-fusion PIV5 F structure (the only reported pre-fusion parainfluenza F structure), HRA folds into three α-helices and two β-strands rather than the long post-fusion HRA helix (Yin, H. S., et al. *Nature* 439, 38-44 (2006)). However, when pre-fusion and post-fusion conformations of individual parainfluenza F protein domains are compared, the non-rearranging parts superimpose well. Superimposing post-fusion RSV F domains on their pre-fusion PIV5 F counterparts did not result in major clashes and positions all the pairs of cysteines that form interdomain disulfide bonds in proximity (FIG. 8B).

[0247] The resulting pre-fusion RSV F model reveals a feature not apparent from modeling pre-fusion RSV F domains based on the PIV5 pre-fusion domain structures

(McLellan, J. S. *et al. Nat Struct Mol Biol* 17, 248-250 (2010)). The helices of the Motavizumab epitope are exposed on the surface of the pre-fusion RSV F trimer, as they are on post-fusion RSV F trimer (FIG. 9). In the current pre-fusion RSV F model, the loop connecting β4 and HRC (part of domain III) would hinder access of Palivizumab or Motavizumab to the epitope. However, the loop may have sufficient flexibility to adopt an alternative conformation that permits antibody binding (FIG. 9B).

[0248] The antigenic structure of RSV F has been mapped by a variety of techniques (FIG. 1). The best documented epitope clusters are designated A and C (Beeler, J. A. & van Wyke Coelingh, K. *J Virol* 63, 2941-2950 (1989)), and others have been proposed. The Motavizumab-peptide structure corroborated the location of site A, although it called into question the site's exposure on the RSF F trimer (McLellan, J. S. *et al.* Structural basis of respiratory syncytial virus neutralization by motavizumab. *Nat Struct Mol Biol* 17, 248-250 (2010)); a crystal structure of an RSV F peptide (residues 422-436) bound to the 101F neutralizing antibody corroborated the location of site C (McLellan, J. S. *et al. J Virol* 84, 12236-12244 (2010)). The post-fusion structure of RSV F and the pre-fusion RSV F model indicate that sites A and C remain exposed and structurally similar in both conformations (FIGS. 8A and 8B). Superposition of the lOlF-peptide complex on the RSV F pre-fusion model and post-fusion structure confirmed that 101F would not clash with F in either conformation (FIG. 10).

[0249] Provided in the Appendix is the PDB file of the RSV F pre-fusion model based on the RSV F post-fusion structure and sequence/domain alignments to the PIV5 pre-fusion structure. The PDB file contains the atomic coordinates for the pre-fusion model, and can be used with suitable software for molecular visualization and analysis (e.g., Roger Sayle and E. James Milner-White. "RasMol: Biomolecular graphics for all", *Trends in Biochemical Sciences (TIBS)*, September 1995, Vol. 20, No. 9, p. 374.) to display the model. Included in the model are the three subunit chains with the fusion peptide and HRA region folded as in PIV5, making significant contacts with DHL HRB regions of the three subunits trimerize into the pre-fusion stalk and are associated with D1 and DII.

2. Destablizing the post-fusion 6-helix bundle through deletion of the HRB helix

[0250] An HRB deletion construct was designed to prevent formation of the post-fusion conformation. Two constructs have been designed to address this strategy. The first is a wild-type ectodomain lacking the HRB region (RSV F residues 1-483) call Del HRB:

[0251] The sequence presented below contain a signal peptide and a HIS tag (GGSAGSGHHHHHH; SEQ ID NO:3). The pre-fusion RSV F protein of the invention can contain the amino acid sequences shown below, with or without the signal peptide and/or HIS tag.

>RSV F delHRB HIS (SEQ ID NO: 28)
MELLILKANAITTILTAVTFCFASGQNITEEFYQSTCSAVSKGYLSALRTGWYTSVITIE
LSNIKENKCNGTDAKVKLIKQELDKYKNAVTELQLLMQSTPATNNRARRELPRFMN
YTLNNAKKTNVTLSKKRKRRFLGFLLGVGSAIASGVAVSKVLHLEGEVNKIKSALLS
TNKAVVSLSNGVSVLTSKVLDLKNYIDKQLLPIVNKQSCSISNIETVIEFQQKNNRLLE
ITREFSVNAGVTTPVSTYMLTNSELLSLINDMPITNDQKKLMSNNVQIVRQQSYSIMSI
IKEEVLAYVVQLPLYGVIDTPCWKLHTSPLCTTNTKEGSNICLTRTDRGWYCDNAGS
VSFFPQAETCKVQSNRVFCDTMNSLTLPSEVNLCNVDIFNPKYDCKIMTSKTDVSSSV
ITSLGAIVSCYGKTKCTASNKNRGIIKTFSNGCDYVSNKGVDTVSVGNTLYYVNKQE
GKSLYVKGEPIINFYDPLVFPSGGSAGSGHHHHHH

[0252] The above sequence has both furin cleavage sites unaltered, and was expected to be processed by the cell. In addition, the above sequence has the wild-type fusion peptide sequence. In previous experiments, when the RSV F ectodomain-based proteins were cleaved by the cell and contained fusion peptides, they formed soluble aggregates with cellular debris in the form of RSV F rosettes. If this construct remained in the pre-fusion conformation (due to the lack of the HRB helix thought to be required for post-fusion conformation) than the fusion peptide should be burried in the RSV F head domain and should not form rosette aggreagates. This construct was expressed, purified by affinity purification and evaluated by EM analysis (FIG. 12).

[0253] It is clear both by its migration on an SEC column in the void volume, as well as from the EM micrograph that the construct formed rosettes similar to the rosettes formed by post-fusion RSV F proteins. This result was a surprise as it was hypothesized that the HRB is required to stabilize the HRA in its elongated helix formation (as it is observed that HRA peptides do not form trimers). Thus, we hypothesized that the fusion peptides, binding

with one another or with cellular debris, are stabilizing the HRA helixes in their elongated, post-fusion formation.

[0254] We have hypothesized that the post-fusion like phenotype of the DelHRB construct was due to stabilization of the HRA into elongated helices by binding of the fusion peptides to one another or cellular debris. To test this hypothesis we are generating the following construct (DelHRB fusion peptide deletion: below) which is similar to the DelHRB but has the fusion peptide deletion consistent with our post-fusion trimer. We will test by EM microscopy the phenotype of the contract to see if it forms crutch-like structures similar to that of the post-fusion like phenotype observed in the DelHRB rosettes of if the construct forms pre-fusion head shapes, which are similar to the spherical shape of the lollipop phenotype published in the literature.

[0255] The sequence presented below contain a signal peptide and a HIS tag (GGSAGSGHHHHHH; SEQ ID NO:3). The pre-fusion RSV F protein of the invention can contain the amino acid sequences shown below, with or without the signal peptide and/or HIS tag.

>RSV F delHRB fusion peptide deletion HIS (SEQ ID NO: 10)
MELLILKANAITTILTAVTFCFASGQNITEEFYQSTCSAVSKGYLSALRTGWYT
SVITIELSNIKENKCNGTDAKVKLIKQELDKYKNAVTELQLLMQSTPATNNRA
RRELPRFMNYTLNNAKKTNVTLSKKRKRRSAIASGVAVSKVLHLEGEVNKIK
SALLSTNKAVVSLSNGVSVLTSKVLDLKNYIDKQLLPIVNKQSCSISNIETVIEF
QQKNNRLLEITREFSVNAGVTTPVSTYMLTNSELLSLINDMPITNDQKKLMSN
NVQIVRQQSYSIMSIIKEEVLAYVVQLPLYGVIDTPCWKLHTSPLCTTNTKEGS
NICLTRTDRGWYCDNAGSVSFFPQAETCKVQSNRVFCDTMNSLTLPSEVNLC
NVDIFNPKYDCKIMTSKTDVSSSVITSLGAIVSCYGKTKCTASNKNRGIIKTFS
NGCDYVSNKGVDTVSVGNTLYYVNKQEGKSLYVKGEPIINFYDPLVFPSGGS
AGSGHHHHHH

3. Prefusion Stabilization with Intrachain Disulfide Bond Formation

[0256] The RSV F model, based on the RSV F post-fusion structure and PIV5 pre-fusion structure, was used to engineer cysteine mutations intended to form disulfide bonds that stabilize RSV F in the pre-fusion conformation (Figure 11). The intrachain disulfide bond constructs were expressed, and were secreted from the cell into the media and then cleaved from F0 to F1/F2 to various degrees (Figure 14). RSV F T58C/V164C (expressed in

mammalian cells) was found to express as a cleaved species which is secreted into the media. The material was purified by chelating purification and evaluated by the rosette/trimer HPLC-SEC assay using the Bio-Sil 250 SEC column with 2x PBS as mobile phase (Figure 15). As this is a cleaved F containing a fusion peptide, it was expected that would be in the postfusion form and would form rosettes and migrate in the void volume similar to postfusion RSV F rosettes (Figure 15A). If the cleaved F protein harboring a fusion peptide was folded in the prefusion form, one would expect the fusion peptide to be buried in the prefusion head region preventing rosette formation. Prefusion trimers should migrate in the included volume with a retention time similar to the RSV F postfusion trimer lacking the fusion peptide (Figure 15B). RSV F HRA Disulfide T58C V164C was run on HPLC-SEC, and the majority of material migrated in the column void volume, indicating the material was aggregating or forming rosettes of postfusion F. A smaller portion of the protein migrated in the included volume with a retention time consistent with an F trimer, suggesting some material formed the desired stabilized prefusion F.

[0257] The disulfide constructs were subsequently cloned into baculovirus expression vectors and three constructs (HRA disulfides N165C/V296C and K168C/V296C and HRB M396C/F483C) were expressed. K168C/V296C and M396C/F483C, which were cleaved when expressed in mammalian cells, were secreted by insect cells predominantly as an uncleaved species (as shown by anti-HIS western blot). Both constructs migrated in the void fraction, which was inconsistent with previous observations that uncleaved species run as monomers. The proteins may have aggregated by virtue of incorrect disulfide formation. Gel shift analysis using anti-HIS western (Figure 16) suggested that intra-chain disulfide bonds were not formed. The pure material taken from the void fraction of the SEC was analyzed with SDS-PAGE and coomassie staining, and each protein was found to be approximately 50% cleaved (Figure 16). A third disulfide construct was expressed and N165C/V296C was secreted predominantly as the desired cleaved product as judged by western blot (Figure 16A).

4. NDV F prefusion structure for further development of the RSV-NDV chimera subunit

A strategy for rescuing the RSV HRA prefusion epitopes was developed to generate an NDV F prefusion construct and mutate select residues of the HRA to those of RSV F. Initial attempts to replace the HRA of NDV with the HRA of RSV generated a construct which was not expressed/secreted from the cell. This indicated that the protein was

misfolded. Further refinement of the residues of NDV F available for mutagenisis (i.e. those located on the protein surface) was required. A new construct, NDV F stabilized with a GCN trimerization domain (uncleaved) migrated as a trimer by SEC analysis. This was expected as this construct was shown to be a pre-fusion trimer by electron microscopy (Swanson et al, 2010).

5. EM analysis of RSV F with HRB and fusion peptide deletion related to NDV pre-fusion construct

[0258] The HRB-deleted RSV F harboring the fusion-peptide was generated, and the protein was purified. The construct migrated in the void volume of the SEC column consistent with RSV F rosettes. The construct was evaluated by EM and shown to form rosettes similar to the postfusion RSV F (Figure 18A). An RSV F protein with both the HRB and fusion peptide deleted (Del-HRB Del-FP) was generated, expressed and purified. RSV F with the HRB and fusion peptide deleted ran partially as a trimer on SEC (Figure 18B). Gel analysis showed that RSV F del-HRB and Del-FP migrated both in the aggregation/rosette peak and trimer peak (Figure 18C). For comparison, the uncleaved NDV pre-fusion construct had very little material in the void fraction (Figure 18C). The RSV F Del-HRB Del-FP was collected from the trimer volume and evaluated by EM.

[0259] Electron micrographs of the NDV pre-fusion construct showed predominately the spherical heads expected for pre-fusion F (Figure 18D). A portion of the material seemed to be associated in rosette-like aggregates, which should not be permitted as the construct is uncleaved and pre-fusion. This amount of association may be due to aggregation by the HIS-tag, and may explain why the RSV Del-HRB Del-FP contained some aggregate/rosette even when the fusion peptide was not present. EM analysis of RSV F Del-HRB Del-FP showed that the material was heterogeneous (Figure 18E). RSV F Del-HRB Del-FP formed rosette-like structures similar to NDV F, as well as post-fusion like "crutches" and pre-fusion like "spheres".

R057 delHRB delFP trunc 6H (fusion peptide deleted)
MELLILKANAITTILTAVTFCFASGQNITEEFYQSTCSAVSKGYLSALRT
GWYTSVITIELSNIKENKCNGTDAKVKLIKQELDKYKNAVTELQLLMQ
STPATNNRARRELPRFMNYTLNNAKKTNVTLSKKRKRRSAIASGVAV
SKVLHLEGEVNKIKSALLSTNKAVVSLSNGVSVLTSKVLDLKNYIDKQ
LLPIVNKQSCSISNIETVIEFQQKNNRLLEITREFSVNAGVTTPVSTYML
TNSELLSLINDMPITNDQKKLMSNNVQIVRQQSYSIMSIIKEEVLAYVV
QLPLYGVIDTPCWKLHTSPLCTTNTKEGSNICLTRTDRGWYCDNAGSV

SFFPQAETCKVQSNRVFCDTMNSLTLPSEVNLCNVDIFNPKYDCKIMT
SKTDVSSSVITSLGAIVSCYGKTKCTASNKNRGIIKTFSNGCDYVSNKG
VDTVSVGNTLYYVNKQEGKSLYVKGEPIINFYDPLVFPSGGSAGSGHH
HHHH** (SEQ ID NO: 10)

R105 delHRB delFP+linker trunk 6H (fusion peptide and linker deleted)
MELLILKANAITTILTAVTFCFASGQNITEEFYQSTCSAVSKGYLSALRT
GWYTSVITIELSNIKENKCNGTDAKVKLIKQELDKYKNAVTELQLLMQ
STPATNNRARRELPRFMNYTLNNAKKTNVTLSKKRKRRSAIASGVAV
SKVLHLEGEVNKIKSALLSTNKAVVSLSNGVSVLTSKVLDLKNYIDKQ
LLPIVNKQSCSISNIETVIEFQQKNNRLLEITREFSVNAGVTTPVSTYML
TNSELLSLINDMPITNDQKKLMSNNVQIVRQQSYSIMSIIKEEVLAYVV
QLPLYGVIDTPCWKLHTSPLCTTNTKEGSNICLTRTDRGWYCDNAGSV
SFFPQAETCKVQSNRVFCDTMNSLTLPSEVNLCNVDIFNPKYDCKIMT
SKTDVSSSVITSLGAIVSCYGKTKCTASNKNRGIIKTFSNGCDYVSNKG
VDTVSVGNTLYYVNKQEGGGSAGSGHHHHHH** (SEQ ID NO:38)

6. Design of RSV F non-native HRB constructs

[0260] A stable RSV prefusion F was generated by replacing the HRB region with either the HRB region of NDV (with or without an additional glycine linker: HRB2) or PIV5. Mammalian expression of the non-native HRB constructs showed that each of the constructs were expressed and secreted well (Figure 19). Additionally, the band observed migrated consistent with the cleaved F1 species, suggesting that the proteins were properly processed. The constructs existed with or without fusion peptide (as indicated in Figure 19).

ADDITIONAL REFERENCES

[0261] The following references are hereby incorporated by reference for all that they teach.

1. *Fields Virology*. 4th edition, 2001.

2. Snell *et al.* (1997) *Virus Genes* 14:63-72.

3. Bembridge *et al.* (1999) *J Virol* 73: 10086-10094.

4. Li *et al.* (1998) *J Exp Med* 188:681-688

5. US Patent No. 6,060,308.

6. Yin *et al.* (2006) *Nature* 439:38-45.

7. Kim *et al.* (2007) *J Med Virol* 79: 820-828.

8. Yin *et al.* (2005) *Proc Natl Acad Sci USA.* 102(26):9288-93.

9. Chen *et al.* (2004) *J Virol* 78:4508-16.

10. Yang et at. (2002) *J Virol* 76:4634-42.

11. Harbury *et al.* (1993) *Science* 262:1401-1407.

12. Stevens *et al.* (2004) *Science* 303:1866-70.

13. Burkhard *et al.* (2001) *Trends Cell Biol* 11:82-88.

14. Section 5.5.2 of Proteins by Creighton (ISBN 0-7167-2317-4).

15. Yu (2002) *Adv Drug Deliv Rev* 54:1 113-1 129.

16. Muller *et al.* (2000) *Methods Enzymol* 328:261-282.

17. Beck & Brodsky (1998) *J Struct Biol* 122:17-29.

18. Lupas (1996) *Trends Biochem Sci* 21:375-382.

19. Adamson *et al.* (1993) *Curr Opin Biotechnol* 4:428-347.

20. Kammerer (1997) *Matrix Biol* 15:555-568.

21. Chao *et al.* (1998) *J Chromatog B Biomed Sci Appl* 715:307-329.

22. Arndt *et* fl/. (2002) *Structure* 10:1235-1248.

23. Liu & Lu (2002) *J Biol Chem* 277:48708-48713.

24. WO2006/011060.

25. Section 5.5.3 of Proteins by Creighton (ISBN 0-7167-2317-4).

26. Zhang & Chen (1999) *J Biol Chem* 274:22409-22413.

27. Slovic ***et*** *al.* (2003) *Protein Sci* 12:337-348

28. Gardner & Dutch (2007) *J Virol* 8 1:8303-14.

29. Gennaro (2000) *Remington: The Science and Practice of Pharmacy*. 20th edition, ISBN: 0683306472.

30. Nony *et al.* (2001) *Vaccine* 27:3645-51.

31. Greenbaum *et al.* (2004) *Vaccine* 22:2566-77.

32. Zurbriggen *et al.* (2003) *Expert Rev Vaccines* 2:295-304.

33. Piascik (2003) *J Am Pharm Assoc (Wash DC).* 43:728-30.

34. Mann *et al.* (2004) *Vaccine* 22:2425-9.

35. Halperin *et al.* (1979) *Am J Public Health* 69:1247-50.

36. Herbert *et al.* (1979) *J Infect Dis* 140:234-8.

37. Chen *et al.* (2003) *Vaccine* 21:2830-6.

38. US Patent No.6355271.

39. WO00/23105.

40. US Patent No. 5,057,540.

41. W096/33739.

42. EP-A-0109942.

43. W096/11711.

44. WO00/07621.

45. Barr *et al.* (1998) *Advanced Drug Delivery Reviews* 32:247-271.

46. Sjolanderet *et al.* (1998) *Advanced Drug Delivery Reviews* 32:321-338.

47. Pizza *et al.* (2000) *Int J Med Microbiol* 290:455-461.

48. W095/17211.

49. W098/42375.

50. Singh *et al* (2001) *J Cont Release* 70:267-276.

51. WO99/27960.

52. US Patent No. 6,090,406.

53. US Patent No. 5,916,588.

54. EP-A-0626169.

55. W099/52549.

56. WO01/21207.

57. WO01/21152.

58. Dyakonova *et al.* (2004) Int Immunopharmacol 4(13): 1615-23.

59. FR-2859633.

60. Signorelli & Hadden (2003) *Int Immunopharmacol* 3(8): 1177-86.

61. WO2004/064715.

62. De Libera *et al,* (2005) *Nature Reviews Immunology* 5:485-496

63. US Patent No.5,936,076.

64. Old *et al. , J Clin Investig,* 113:1631-1640

65. US2005/0 192248

66. Yang *et al.* (2004) *Angew Chem Int Ed* 43:3818-3822

67. WO2005/102049.

68. Goffet *et al* (2004) *Am Chem Soc* 126:13602-13603

69. WO03/105769.

70. Cooper (1995) *Pharm Biotechnol* 6:559-80.

71. WO90/14837.

72. Podda & Del Giudice (2003) *Expert Rev Vaccines* 2:197-203.

73. Podda (2001) *Vaccine* 19: 2673-2680.

74. *Vaccine Design: The Subunit and Adjuvant Approach* (eds. Powell & Newman) Plenum Press 1995 (ISBN 0-306-44867-X).

75. *Vaccine Adjuvants: Preparation Methods and Research Protocols* (Volume 42 of *Methods in Molecular Medicine* series). ISBN: 1-59259-083-7. Ed. O'Hagan.

76. Allison & Byars (1992) *Res Immunol* 143:519-25.

77. Hariharan *et al.* (1995) *Cancer Res* 55:3486-9.

78. W095/1 1700.

79. US Patent No.6,080,725.

80. WO2005/0971 81.

81. Tassignon *et al.* (2005) *J Immunol Meth* 305:188-98.

82. Myers *et al.* (1990) pages 145-156 of *Cellular and molecular aspects of endotoxin reactions.*

83. Ulrich (2000) Chapter 16 (pages 273-282) of reference 75.

84. Johnson *et al.* (1999) *J Med Chem* 42:4640-9.

85. Baldrick *et al.* (2002) *Regulatory Toxicol Pharmacol* 35:398-413.

86. US Patent No. 4,680,338.

87. US Patent No. 4,988,815.

88. W092/15582.

89. Stanley (2002) *Clin Exp Dermatol* 27:57 1-577.

90. Wu *etal.* (2004) *Antiviral Res.* 64(2):79-83.

91. Vasilakos *et al.* (2000) *Cell Immunol.* 204(l):64-74.

92. US Patent Nos. 4689338, 4929624, 5238944, 5266575, 5268376, 5346905, 5352784, 5389640, 5395937, 5482936, 5494916, 5525612, 6083505, 6440992, 6627640, 6664264, 6664265, 6667312, 6677347, 6677348, 6677349, 6683088, 6703402, 6743920, 6800624, 6809203, 6888000, and 6924293.

93. Jones (2003) *Curr Opin Investig Drugs* 4:214-218.

94. WO2004/060308.

95. WO2004/064759.

96. US Patent No. 6,924,271.

97. US2005/0070556.

98. US Patent No. 5,658,731.

99. US Patent No. 5,011,828.

100. WO2004/87 153.

101. US Patent No. 6,605,617.

102. WO02/18383.

103. WO2004/018455.

104. WO03/082272.

105. WO2006/002422.

106. Johnson *et al.* (1999) *Bioorg Med Chem Lett* 9:2273-2278.

107. Evans *et al.* (2003) *Expert Rev Vaccines* 2:219-229.

108. Andrianov ***et*** *al.* (1998) *Biomaterials* 19:109-1 15.

109. Payne *et al.* (1998) *Adv Drug Delivery Review* 31:185-196.

110. Thompson *et al.* (2003) *Methods in Molecular Medicine* 94:255-266.

111. Kandimalla *et al.* (2003) *Nucleic Acids Research* 31:2393-2400.

112. WO02/26757.

113. W099/62923.

114. Krieg (2003) *Nature Medicine* 9:831-835.

115. McCluskie *et al.* (2002) *FEMS Immunology and Medical Microbiology* 32:179-185.

116. WO98/40100.

117. US Patent No. 6,207,646.

118. US Patent No. 6,239,116.

119. US Patent No. 6,429,199.

120. Kandimalla *et al.* (2003) *Biochemical Society Transactions* 31 (part 3): 654-658.

121. Blackwell *et al.* (2003) *J Immunol* 170:4061-4068.

122. Krieg (2002) *Trends Immunol* 23:64-65.

123. WO01/95935.

124. Kandimalla *et al.* (2003) *BBRC* 306:948-953.

125. Bhagat *et al.* (2003) *BBRC* 300:853-861.

126. WO03/035836.

127. WO01/22972.

128. Thompson *et al.* (2005) *J Leukoc Biol* 78: 'The low-toxicity versions of LPS, MPL® adjuvant and RC529, are efficient adjuvants for CD4+ T cells'.

129. UK patent application GB-A-22202 11.

130. W094/21292.

131. WO94/00153.

132. WO95/17210.

133. W096/26741.

134. WO93/19780.

135. WO03/011223.

136. Meraldi *et al.* (2003) *Vaccine* 21:2485-249 1.

137. Pajak *et al.* (2003) *Vaccine* 21:836-842.

138. US Patent No. 6,586,409.

139. Wong *et al.* (2003) *J Clin Pharmacol* 43(7):735-42.

140. US2005/0215517.

141. McLellan JS, *et al.* (2010) Structural basis of respiratory syncytial virus neutralization by motavizumab. *Nat Struct Mol Biol* 17(2):248-250.

142. Ruiz-Arguello MB, *et al.* (2004) Thermostability of the human respiratory syncytial virus fusion protein before and after activation: implications for the membrane-fusion mechanism. *J Gen Virol* 85(Pt 12):3677-3687.

143. Calder LJ, *et al.* (2000) Electron microscopy of the human respiratory syncytial virus fusion protein and complexes that it forms with monoclonal antibodies. *Virology* 271(1):122-131 .

144. Connolly SA, Leser GP, Yin HS, Jardetzky TS, & Lamb RA (2006) Refolding of a paramyxovirus F protein from prefusion to postfusion conformations observed by liposome binding and electron microscopy, *Proc Natl Acad Sci USA* 103(47): 17903-17908.

145. Yin HS, Wen XL, Paterson RG, Lamb RA, & Jardetzky TS (2006) Structure of the parainfluenza virus 5 F protein in its metastable, prefusion conformation, *Nature* 439(7072):38-44.

146. Swanson K, *et al.* (2010) Structure of the Newcastle disease virus F protein in the post-fusion conformation, *Virology* 402(2):372-379.

147. Yin HS, Wen X, Paterson RG, Lamb RA, & Jardetzky TS (2006) Structure of the parainfluenza virus 5 F protein in its metastable, prefusion conformation, *Nature* 439(7072):38-44.

148. McLellan JS, *et al.* (2010) Structure of a Major Antigenic Site on the Respiratory Syncytial Virus Fusion Glycoprotein in Complex with Neutralizing Antibody 10 IF. *J Virol* 84:12236-12244.

149. Arbiza J, *et al.* (1992) Characterization of two antigenic sites recognized by neutralizing monoclonal antibodies directed against the fusion glycoprotein of human respiratory syncytial virus. *J Gen Virol* 73:2225-2234.

150. Crowe JE, *et al.* (1998) Monoclonal antibody-resistant mutants selected with a respiratory syncytial virus-neutralizing human antibody fab fragment (Fab 19) define a unique epitope on the fusion (F) glycoprotein. *Virology* 252:373-375.

151. Lopez JA, Penas C, Garcia-Barreno B, Melero JA, & Portela A (1990) Location of a highly conserved neutralizing epitope in the F glycoprotein of human respiratory syncytial virus. *J Virol* 64:927-930.

152. Zhao X, Chen FP, & Sullender WM (2004) Respiratory syncytial virus escape mutant derived in vitro resists palivizumab prophylaxis in cotton rats. *Virology* 318:608-612.

153. Liu C, *et al.* (2007) Relationship between the loss of neutralizing antibody binding and fusion activity of the F protein of human respiratory syncytial virus. *Virol J* 4:71.

154. Lopez JA, *et al.* (1998) Antigenic structure of human respiratory syncytial virus fusion glycoprotein. *J Virol* 72:6922-6928.

155. Wu SJ, *et al.* (2007) Characterization of the epitope for anti-human respiratory syncytial virus F protein monoclonal antibody 101F using synthetic peptides and genetic approaches. *J Gen Virol* 88:2719-2723.

156. Beeler JA & van Wyke Coelingh K (1989) Neutralization epitopes of the F glycoprotein of respiratory syncytial virus: effect of mutation upon fusion function. *J Virol* 63:2941-2950.

The entire teachings of all documents cited herein are hereby incorporated herein by reference.

APPENDIX

(APPENDIX discloses SEQ ID NOS 29-32, 29-32 and 29-32, respectively, in order of appearance)

```
HEADER    —                          XX-XXX-9-   xxxx
COMPND    ---
SSBOND   1 CYS G   69    CYS G  212
SSBOND   2 CYS G  313    CYS G  343
SSBOND   3 CYS G  322    CYS G  333
SSBOND   4 CYS G  358    CYS G  367
SSBOND   5 CYS G  382    CYS G  393
SSBOND   6 CYS G  416    CYS G  422
LINKR        CI  NAG J1535            ND2 ASN G  70            NAG-ASN
LINKR        CI  NAG J1545            ND2 ASN G 500            NAG-ASN
LINKR        CI  NAG J1525            ND2 ASN G  27            NAG-ASN
SSBOND   7 CYS H   69    CYS H  212
SSBOND   8 CYS H  313    CYS H  343
SSBOND   9 CYS H  322    CYS H  333
SSBOND  10 CYS H  358    CYS H  367
SSBOND  11 CYS H  382    CYS H  393
SSBOND  12 CYS H  416    CYS H  422
LINKR        CI  NAG K1535            ND2 ASN H  70            NAG-ASN
LINKR        OD1 ASN H 500            C7  NAG K1545            ASN-NAG
LINKR        CI  NAG K1545            ND2 ASN H 500            NAG-ASN
LINKR        OD1 ASN H  27            0 7  NAG K1525           ASN-NAG1
LINKR        CI  NAG K1525            ND2 ASN H  27            NAG-ASN
SSBOND  13 CYS I   69    CYS I  212
SSBOND  14 CYS I  313    CYS I  343
SSBOND  15 CYS I  322    CYS I  333
SSBOND  16 CYS I  358    CYS I  367
SSBOND  17 CYS I  382    CYS I  393
SSBOND  18 CYS I  416    CYS I  422
LINKR        CI  NAG L1535            ND2 ASN I  70            NAG-ASN
LINKR        CI  NAG L1545            ND2 ASN I 500            NAG-ASN
LINKR        CI  NAG L1525            ND2 ASN I  27            NAG-ASN
LINKR          GLN G  98              PHE G 137              gap
LINKR          ASN G 325              SER G 330              gap
LINKR          LYS G 465              GLU G 472              gap
LINKR          NAG J1535              NAG J1536              BETA 1-4
LINKR          NAG J1545              NAG J1546              BETA 1-4
LINKR          NAG J1525              NAG J1526              BETA 1-4
LINKR          PRO G 304              TYR G 306              gap
LINKR          THR G  50              ILE G 309              gap
LINKR          GLN H  98              PHE H 137              gap
LINKR          ASN H 325              SER H 330              gap
LINKR          LYS H 465              GLU H 472              gap
LINKR          PRO H 304              TYR H 306              gap
LINKR          THR H  50              ILE H 309              gap
LINKR          GLN I  98              PHE 1 137              gap
LINKR          ASN I 325              SER I 330              gap
LINKR          LYS 1465               GLU 1472               gap
LINKR          PRO I 304              TYR I 306              gap
LINKR          THR I  50              ILE I 309              gap
LINKR          NAG K1535                NAG K1536              BETA 1-4
LINKR          NAG L1535                NAG L1536              BETA 1-4
LINKR          NAG K1545                NAG K1546              BETA 1-4
LINKR          NAG L1545                NAG L1546              BETA 1-4
```

```
LINKR         NAG K1525              NAG K1526            BETA 1-4
LINKR         NAG L1525              NAG L1526            BETA 1-4
MODRES     NAG J 1535  NAG-b-D                           RENAME
MODRES     NAG J 1536  NAG-b-D                           RENAME
MODRES     NAG J 1545  NAG-b-D                           RENAME
MODRES     NAG J 1546  NAG-b-D                           RENAME
MODRES     NAG J 1525  NAG-b-D                           RENAME
MODRES     NAG J 1526  NAG-b-D                           RENAME
MODRES     NAG K 1535  NAG-b-D                           RENAME
MODRES     NAG K 1536  NAG-b-D                           RENAME
MODRES     NAG K 1545  NAG-b-D                           RENAME
MODRES     NAG K 1546  NAG-b-D                           RENAME
MODRES     NAG K 1525  NAG-b-D                           RENAME
MODRES     NAG K 1526  NAG-b-D                           RENAME
MODRES     NAG L 1535  NAG-b-D                           RENAME
MODRES     NAG L 1536  NAG-b-D                           RENAME
MODRES     NAG L 1545  NAG-b-D                           RENAME
MODRES     NAG L 1546  NAG-b-D                           RENAME
MODRES     NAG L 1525  NAG-b-D                           RENAME
MODRES     NAG L 1526  NAG-b-D                           RENAME
CRYSTl   160.206  259.864   154.012  90.00  90.00  90.00 C 2 2 21
SCALE1     0.006242  0.000000  0.000000        0.00000
SCALE2     0.000000  0.003848  0.000000        0.00000
SCALE3     0.000000  0.000000  0.006493        0.00000
ATOM      1 N   GLN G  26      24.299  30.940  -8.771   1.00 23.62          N
ATOM      2 CA  GLN G  26      22.913  30.470  -9.055   1.00 23.82          C
ATOM      3 CB  GLN G  26      22.260  29.923  -7.783   1.00 23.94          C
ATOM      4 CG  GLN G  26      23.103  28.894  -7.043   1.00 28.83          C
ATOM      5 CD  GLN G  26      24.309  29.508  -6.355   1.00 36.36          C
ATOM      6 OE1 GLN G  26      25.367  29.671  -6.963   1.00 39.09          O
ATOM      7 NE2 GLN G  26      24.176  29.785  -5.063   1.00 37.86          N
ATOM      8 C   GLN G  26      22.064  31.593  -9.645   1.00 23.09          C
ATOM      9 O   GLN G  26      22.368  32.772  -9.466   1.00 24.21          O
ATOM     10 N   ASN G  27      21.079  31.214 -10.452   1.00 20.98          N
ATOM     11 CA  ASN G  27      20.182  32.172 -11.089   1.00 19.70          C
ATOM     12 CB  ASN G  27      20.879  32.850 -12.269   1.00 20.41          C
ATOM     13 CG  ASN G  27      19.973  33.815 -13.014   1.00 23.56          C
ATOM     14 0D1 ASN G  27      19.456  34.775 -12.440   1.00 24.42          O
ATOM     15 ND2 ASN G  27      19.784  33.561 -14.310   1.00 27.70          N
ATOM     16 C   ASN G  27      18.931  31.465 -11.578   1.00 18.42          C
ATOM     17 O   ASN G  27      18.705  31.356 -12.783   1.00 18.47          O
ATOM     18 N   ILE G  28      18.240  30.807 -10.655   1.00 16.54          N
ATOM     19 CA  ILE G  28      17.060  30.044 -11.018   1.00 14.59          C
ATOM     20 CB  ILE G  28      16.771  28.910 -10.025   1.00 14.01          C
ATOM     21 CGI ILE G  28      17.176  29.324  -8.610   1.00 15.60          C
ATOM     22 CD1 ILE G  28      16.159  30.199  -7.917   1.00 16.26          C
ATOM     23 CG2 ILE G  28      17.501  27.642 -10.441   1.00 12.57          C
ATOM     24 C   ILE G  28      15.843  30.942 -11.157   1.00 13.86          C
ATOM     25 O   ILE G  28      15.699  31.935 -10.443   1.00 13.70          O
ATOM     26 N   THR G  29      15.098  30.702 -12.227   1.00 13.23          N
ATOM     27 CA  THR G  29      13.968  31.532 -12.592   1.00 12.65          C
ATOM     28 CB  THR G  29      14.306  32.435 -13.790   1.00 12.69          C
ATOM     29 0G1 THR G  29      15.728  32.530 -13.936   1.00 12.62          O
ATOM     30 CG2 THR G  29      13.723  33.825 -13.594   1.00 12.92          C
ATOM     31 C   THR G  29      12.854  30.597 -13.010   1.00 12.47          C
ATOM     32 O   THR G  29      13.106  29.526 -13.560   1.00 12.53          O
ATOM     33 N   GLU G  30      11.622  31.050 -12.847   1.00 11.98          N
ATOM     34 CA  GLU G  30      10.500  30.392 -13.480   1.00 11.68          C
ATOM     35 CB  GLU G  30       9.587  29.781 -12.416   1.00 11.98          C
ATOM     36 CG  GLU G  30       8.848  28.524 -12.856   1.00 13.38          C
```

ATOM 37 CD GLU G 30 8.295 27.732 -11.682 1.00 16.03 C
ATOM 38 OE1 GLU G 30 7.552 28.313 -10.863 1.00 16.65 O
ATOM 39 OE2 GLU G 30 8.577 26.519 -11.596 1.00 17.06 O
ATOM 40 C GLU G 30 9.743 31.433 -14.281 1.00 11.39 C
ATOM 41 O GLU G 30 9.521 32.547 -13.806 1.00 11.50 O
ATOM 42 N GLU G 31 9.449 31.119 -15.535 1.00 11.11 N
ATOM 43 CA GLU G 31 8.573 31.975 -16.305 1.00 11.06 C
ATOM 44 CB GLU G 31 9.345 32.716 -17.394 1.00 11.48 C
ATOM 45 CG GLU G 31 9.026 32.268 -18.803 1.00 13.90 C
ATOM 46 CD GLU G 31 9.622 33.190 -19.843 1.00 17.27 C
ATOM 47 OE1 GLU G 31 8.852 33.749 -20.653 1.00 17.55 O
ATOM 48 OE2 GLU G 31 10.849 33.418 -19.804 1.00 18.73 O
ATOM 49 C GLU G 31 7.370 31.240 -16.871 1.00 10.47 C
ATOM 50 O GLU G 31 7.459 30.080 -17.274 1.00 10.12 O
ATOM 51 N PHE G 32 6.220 31.890 -16.753 1.00 10.15 N
ATOM 52 CA PHE G 32 4.932 31.235 -16.887 1.00 9.62 C
ATOM 53 CB PHE G 32 3.967 31.777 -15.832 1.00 9.42 C
ATOM 54 CG PHE G 32 2.524 31.512 -16.141 1.00 9.27 C
ATOM 55 CD1 PHE G 32 2.021 30.222 -16.085 1.00 9.37 C
ATOM 56 CE1 PHE G 32 0.701 29.960 -16.407 1.00 9.52 C
ATOM 57 CZ PHE G 32 -0.132 30.993 -16.800 1.00 9.82 C
ATOM 58 CE2 PHE G 32 0.362 32.285 -16.877 1.00 10.13 C
ATOM 59 CD2 PHE G 32 1.681 32.541 -16.536 1.00 10.06 C
ATOM 60 C PHE G 32 4.386 31.524 -18.276 1.00 9.64 C
ATOM 61 O PHE G 32 4.479 32.650 -18.763 1.00 9.84 O
ATOM 62 N TYR G 33 3.846 30.501 -18.926 1.00 9.59 N
ATOM 63 CA TYR G 33 3.342 30.662 -20.281 1.00 9.67 C
ATOM 64 CB TYR G 33 3.951 29.617 -21.212 1.00 9.52 C
ATOM 65 CG TYR G 33 5.422 29.834 -21.467 1.00 10.94 C
ATOM 66 CD1 TYR G 33 6.379 29.220 -20.670 1.00 12.23 C
ATOM 67 CE1 TYR G 33 7.726 29.448 -20.870 1.00 12.93 C
ATOM 68 CZ TYR G 33 8.128 30.348 -21.833 1.00 13.47 C
ATOM 69 OH TYR G 33 9.469 30.588 -22.028 1.00 14.54 O
ATOM 70 CE2 TYR G 33 7.195 31.019 -22.594 1.00 13.56 C
ATOM 71 CD2 TYR G 33 5.850 30.781 -22.388 1.00 12.96 C
ATOM 72 C TYR G 33 1.824 30.604 -20.327 1.00 9.94 C
ATOM 73 O TYR G 33 1.234 29.530 -20.446 1.00 10.16 O
ATOM 74 N GLN G 34 1.199 31.769 -20.211 1.00 10.06 N
ATOM 75 CA GLN G 34 -0.225 31.846 -19.927 1.00 10.01 C
ATOM 76 CB GLN G 34 -0.649 33.302 -19.751 1.00 10.22 C
ATOM 77 CG GLN G 34 -2.138 33.486 -19.551 1.00 11.12 C
ATOM 78 CD GLN G 34 -2.485 34.867 -19.039 1.00 13.13 C
ATOM 79 OE1 GLN G 34 -2.668 35.804 -19.819 1.00 14.24 O
ATOM 80 NE2 GLN G 34 -2.553 35.007 -17.719 1.00 13.79 N
ATOM 81 C GLN G 34 -1.039 31.198 -21.039 1.00 9.94 C
ATOM 82 O GLN G 34 -2.165 30.752 -20.819 1.00 10.08 O
ATOM 83 N SER G 35 -0.468 31.167 -22.238 1.00 9.87 N
ATOM 84 CA SER G 35 -1.185 30.690 -23.415 1.00 9.91 C
ATOM 85 CB SER G 35 -0.619 31.337 -24.684 1.00 10.03 C
ATOM 86 OG SER G 35 0.776 31.572 -24.564 1.00 10.81 O
ATOM 87 C SER G 35 -1.119 29.167 -23.518 1.00 9.56 C
ATOM 88 O SER G 35 -1.688 28.566 -24.431 1.00 9.59 O
ATOM 89 N THR G 36 -0.417 28.553 -22.572 1.00 9.21 N
ATOM 90 CA THR G 36 -0.209 27.113 -22.573 1.00 9.06 C
ATOM 91 CB THR G 36 1.230 26.755 -23.010 1.00 9.49 C
ATOM 92 OG1 THR G 36 1.493 27.310 -24.305 1.00 10.82 O
ATOM 93 CG2 THR G 36 1.410 25.245 -23.074 1.00 9.45 C
ATOM 94 C THR G 36 -0.455 26.599 -21.162 1.00 8.77 C
ATOM 95 O THR G 36 -0.171 25.445 -20.845 1.00 8.60 O
ATOM 96 N CYS G 37 -0.982 27.478 -20.315 1.00 8.69 N

```
ATOM     97  CA  CYS G  37     -1.097  27.201 -18.890   1.00  8.69           C
ATOM     98  CB  CYS G  37     -2.468  26.605 -18.571   1.00  8.81           C
ATOM     99  SG  CYS G  37     -3.003  26.848 -16.864   1.00 10.80           S
ATOM    100  C   CYS G  37      0.005  26.263 -18.414   1.00  8.27           C
ATOM    101  O   CYS G  37     -0.268  25.166 -17.926   1.00  8.27           O
ATOM    102  N   SER G  38      1.251  26.687 -18.586   1.00  7.92           N
ATOM    103  CA  SER G  38      2.386  25.886 -18.157   1.00  7.51           C
ATOM    104  CB  SER G  38      2.817  24.924 -19.264   1.00  7.63           C
ATOM    105  OG  SER G  38      3.392  25.627 -20.351   1.00  8.54           O
ATOM    106  C   SER G  38      3.558  26.757 -17.735   1.00  7.02           C
ATOM    107  O   SER G  38      3.663  27.917 -18.132   1.00  6.83           O
ATOM    108  N   ALA G  39      4.407  26.198 -16.882   1.00  6.64           N
ATOM    109  CA  ALA G  39      5.466  26.961 -16.245   1.00  6.58           C
ATOM    110  CB  ALA G  39      5.136  27.195 -14.782   1.00  6.67           C
ATOM    111  C   ALA G  39      6.789  26.222 -16.382   1.00  6.93           C
ATOM    112  O   ALA G  39      6.842  24.998 -16.261   1.00  7.38           O
ATOM    113  N   VAL G  40      7.843  26.966 -16.698   1.00  6.87           N
ATOM    114  CA  VAL G  40      9.175  26.388 -16.797   1.00  6.55           C
ATOM    115  CB  VAL G  40      9.741  26.507 -18.222   1.00  6.22           C
ATOM    116  CGI VAL G  40     11.237  26.233 -18.223   1.00  6.52           C
ATOM    117  CG2 VAL G  40      9.018  25.553 -19.160   1.00  6.62           C
ATOM    118  C   VAL G  40     10.140  27.033 -15.813   1.00  6.73           C
ATOM    119  O   VAL G  40     10.302  28.253 -15.789   1.00  6.83           O
ATOM    120  N   SER G  41     10.772  26.198 -14.997   1.00  6.86           N
ATOM    121  CA  SER G  41     11.897  26.625 -14.181   1.00  6.75           C
ATOM    122  CB  SER G  41     11.974  25.785 -12.905   1.00  7.06           C
ATOM    123  OG  SER G  41     10.751  25.110 -12.666   1.00  7.50           O
ATOM    124  C   SER G  41     13.206  26.525 -14.958   1.00  6.56           C
ATOM    125  O   SER G  41     13.526  25.482 -15.529   1.00  6.08           O
ATOM    126  N   LYS G  42     13.972  27.612 -14.946   1.00  7.02           N
ATOM    127  CA  LYS G  42     15.140  27.757 -15.809   1.00  7.83           C
ATOM    128  CB  LYS G  42     14.949  28.933 -16.769   1.00  8.15           C
ATOM    129  CG  LYS G  42     13.666  28.888 -17.578   1.00  9.75           C
ATOM    130  CD  LYS G  42     13.510  30.148 -18.414   1.00 12.62           C
ATOM    131  CE  LYS G  42     12.360  30.022 -19.398   1.00 14.04           C
ATOM    132  NZ  LYS G  42     12.643  30.734 -20.675   1.00 14.96           N
ATOM    133  C   LYS G  42     16.394  27.988 -14.971   1.00  7.80           C
ATOM    134  O   LYS G  42     16.323  28.557 -13.882   1.00  8.15           O
ATOM    135  N   GLY G  43     17.550  27.717 -15.566   1.00  7.59           N
ATOM    136  CA  GLY G  43     18.820  28.160 -15.002   1.00  7.35           C
ATOM    137  C   GLY G  43     19.529  27.058 -14.240   1.00  7.10           C
ATOM    138  O   GLY G  43     20.294  27.323 -13.313   1.00  7.13           O
ATOM    139  N   TYR G  44     19.309  25.819 -14.668   1.00  7.01           N
ATOM    140  CA  TYR G  44     19.922  24.656 -14.033   1.00  6.89           C
ATOM    141  CB  TYR G  44     18.878  23.561 -13.815   1.00  6.88           C
ATOM    142  CG  TYR G  44     17.809  23.928 -12.816   1.00  6.41           C
ATOM    143  CD1 TYR G  44     16.553  24.343 -13.236   1.00  6.62           C
ATOM    144  CE1 TYR G  44     15.580  24.703 -12.325   1.00  6.48           C
ATOM    145  CZ  TYR G  44     15.862  24.662 -10.976   1.00  6.88           C
ATOM    146  OH  TYR G  44     14.897  25.025 -10.065   1.00  7.50           O
ATOM    147  CE2 TYR G  44     17.110  24.279 -10.536   1.00  6.68           C
ATOM    148  CD2 TYR G  44     18.077  23.922 -11.454   1.00  5.91           C
ATOM    149  C   TYR G  44     21.060  24.106 -14.886   1.00  6.86           C
ATOM    150  O   TYR G  44     21.012  24.190 -16.113   1.00  7.14           O
ATOM    151  N   LEU G  45     21.979  23.385 -14.249   1.00  6.44           N
ATOM    152  CA  LEU G  45     23.146  22.842 -14.946   1.00  6.12           C
ATOM    153  CB  LEU G  45     24.425  23.552 -14.482   1.00  6.31           C
ATOM    154  CG  LEU G  45     24.534  25.052 -14.775   1.00  6.38           C
ATOM    155  CD1 LEU G  45     25.624  25.690 -13.928   1.00  7.05           C
ATOM    156  CD2 LEU G  45     24.787  25.299 -16.255   1.00  7.05           C
```

```
ATOM    157  C   LEU G  45     23.279  21.312 -14.800   1.00  5.84        C
ATOM    158  O   LEU G  45     23.333  20.797 -13.683   1.00  5.94        O
ATOM    159  N   SER G  46     23.470  20.620 -15.929   1.00  5.43        N
ATOM    160  CA  SER G  46     23.249  19.157 -16.047   1.00  5.26        C
ATOM    161  CB  SER G  46     22.913  18.795 -17.498   1.00  5.21        C
ATOM    162  OG  SER G  46     24.090  18.532 -18.243   1.00  4.95        O
ATOM    163  C   SER G  46     24.481  18.355 -15.585   1.00  5.51        C
ATOM    164  O   SER G  46     25.480  18.961 -15.200   1.00  6.03        O
ATOM    165  N   ALA G  47     24.453  17.015 -15.656   1.00  5.24        N
ATOM    166  CA  ALA G  47     25.584  16.224 -15.104   1.00  4.83        C
ATOM    167  CB  ALA G  47     25.690  16.412 -13.599   1.00  5.01        C
ATOM    168  C   ALA G  47     25.854  14.751 -15.494   1.00  4.35        C
ATOM    169  O   ALA G  47     24.926  13.972 -15.719   1.00  4.45        O
ATOM    170  N   LEU G  48     27.119  14.348 -15.323   1.00  3.67        N
ATOM    171  CA  LEU G  48     27.564  12.948 -15.451   1.00  3.15        C
ATOM    172  CB  LEU G  48     28.365  12.755 -16.750   1.00  2.78        C
ATOM    173  CG  LEU G  48     27.659  12.681 -18.108   1.00  2.18        C
ATOM    174  CD1 LEU G  48     28.223  11.532 -18.935   1.00  2.00        C
ATOM    175  CD2 LEU G  48     26.156  12.531 -17.934   1.00  3.94        C
ATOM    176  C   LEU G  48     28.443  12.517 -14.259   1.00  3.06        C
ATOM    177  O   LEU G  48     29.670  12.486 -14.373   1.00  3.27        O
ATOM    178  N   ARG G  49     27.810  12.061 -13.177   1.00  2.91        N
ATOM    179  CA  ARG G  49     28.509  11.788 -11.915   1.00  2.88        C
ATOM    180  CB  ARG G  49     27.538  11.277 -10.847   1.00  2.69        C
ATOM    181  CG  ARG G  49     28.117  11.273  -9.440   1.00  2.15        C
ATOM    182  CD  ARG G  49     28.015   9.897  -8.806   1.00  2.00        C
ATOM    183  NE  ARG G  49     29.322   9.271  -8.623   1.00  5.18        N
ATOM    184  CZ  ARG G  49     29.526   7.956  -8.629   1.00  7.68        C
ATOM    185  NH1 ARG G  49     28.518   7.129  -8.866   1.00  8.32        N
ATOM    186  NH2 ARG G  49     30.748   7.469  -8.455   1.00  8.12        N
ATOM    187  C   ARG G  49     29.678  10.816 -12.065   1.00  3.09        C
ATOM    188  O   ARG G  49     29.570   9.796 -12.747   1.00  3.08        O
ATOM    189  N   THR G  50     30.820  11.189 -11.489   1.00  3.37        N
ATOM    190  CA  THR G  50     32.099  10.564 -11.823   1.00  3.55        C
ATOM    191  CB  THR G  50     32.487  10.773 -13.299   1.00  3.25        C
ATOM    192  OG1 THR G  50     32.842  12.144 -13.519   1.00  2.66        O
ATOM    193  CG2 THR G  50     31.328  10.401 -14.212   1.00  3.46        C
ATOM    194  C   THR G  50     33.259  10.968 -10.908   1.00  4.07        C
ATOM    195  O   THR G  50     33.768  10.130 -10.165   1.00  4.35        O
ATOM    196  N   GLY G  51     33.818  12.158 -11.108   1.00  4.24        N
ATOM    197  CA  GLY G  51     34.942  12.544 -10.272   1.00  4.78        C
ATOM    198  C   GLY G  51     34.692  11.849  -8.951   1.00  4.98        C
ATOM    199  O   GLY G  51     33.618  12.018  -8.375   1.00  5.00        O
ATOM    200  N   TRP G  52     35.476  10.816  -8.667   1.00  5.34        N
ATOM    201  CA  TRP G  52     35.123   9.926  -7.569   1.00  5.42        C
ATOM    202  CB  TRP G  52     34.864   8.497  -8.049   1.00  5.75        C
ATOM    203  CG  TRP G  52     33.714   8.373  -9.001   1.00  6.38        C
ATOM    204  CD1 TRP G  52     33.776   7.964 -10.300   1.00  7.27        C
ATOM    205  NE1 TRP G  52     32.533   8.031 -10.878   1.00  7.46        N
ATOM    206  CE2 TRP G  52     31.627   8.449  -9.938   1.00  7.15        C
ATOM    207  CD2 TRP G  52     32.331   8.658  -8.735   1.00  7.02        C
ATOM    208  CE3 TRP G  52     31.627   9.102  -7.608   1.00  6.83        C
ATOM    209  CZ3 TRP G  52     30.261   9.289  -7.711   1.00  6.73        C
ATOM    210  CH2 TRP G  52     29.589   9.062  -8.922   1.00  7.13        C
ATOM    211  CZ2 TRP G  52     30.252   8.637 -10.041   1.00  6.82        C
ATOM    212  C   TRP G  52     36.148   9.926  -6.456   1.00  5.34        C
ATOM    213  O   TRP G  52     37.349  10.027  -6.698   1.00  5.47        O
ATOM    214  N   TYR G  53     35.670   9.629  -5.256   1.00  5.29        N
ATOM    215  CA  TYR G  53     36.528   9.560  -4.093   1.00  5.58        C
ATOM    216  CB  TYR G  53     36.260  10.754  -3.176   1.00  5.51        C
```

ATOM 217 CG TYR G 53 37.079 10.756 -1.910 1.00 6.59 C
ATOM 218 CD1 TYR G 53 38.312 11.391 -1.858 1.00 8.25 c
ATOM 219 CE1 TYR G 53 39.043 11.436 -0.685 1.00 9.40 c
ATOM 220 CZ TYR G 53 38.524 10.875 0.462 1.00 9.24 c
ATOM 221 OH TYR G 53 39.246 10.915 1.633 1.00 9.61 o
ATOM 222 CE2 TYR G 53 37.287 10.272 0.443 1.00 8.78 c
ATOM 223 CD2 TYR G 53 36.559 10.247 -0.730 1.00 7.93 c
ATOM 224 C TYR G 53 36.286 8.245 -3.364 1.00 5.74 c
ATOM 225 O TYR G 53 35.186 7.996 -2.870 1.00 6.19 o
ATOM 226 N THR G 54 37.221 7.317 -3.532 1.00 6.04 N
ATOM 227 CA THR G 54 37.132 6.013 -2.888 1.00 6.67 c
ATOM 228 CB THR G 54 38.232 5.060 -3.396 1.00 6.97 c
ATOM 229 OG1 THR G 54 37.876 4.562 -4.691 1.00 7.51 o
ATOM 230 CG2 THR G 54 38.409 3.889 -2.442 1.00 7.98 c
ATOM 231 C THR G 54 37.254 6.158 -1.376 1.00 6.97 c
ATOM 232 O THR G 54 37.900 7.083 -0.884 1.00 7.32 o
ATOM 233 N SER G 55 36.616 5.254 -0.639 1.00 7.24 N
ATOM 234 CA SER G 55 37.025 4.966 0.732 1.00 7.65 c
ATOM 235 CB SER G 55 36.459 6.009 1.705 1.00 7.69 c
ATOM 236 OG SER G 55 36.690 5.632 3.053 1.00 7.51 o
ATOM 237 C SER G 55 36.629 3.561 1.171 1.00 8.03 c
ATOM 238 O SER G 55 35.510 3.109 0.924 1.00 8.43 o
ATOM 239 N VAL G 56 37.522 2.919 1.915 1.00 8.14 N
ATOM 240 CA VAL G 56 37.401 1.500 2.215 1.00 8.41 c
ATOM 241 CB VAL G 56 38.732 0.763 1.967 1.00 8.72 c
ATOM 242 CGI VAL G 56 38.479 -0.703 1.654 1.00 9.29 c
ATOM 243 CG2 VAL G 56 39.509 1.433 0.843 1.00 9.51 c
ATOM 244 C VAL G 56 37.005 1.312 3.673 1.00 8.19 c
ATOM 245 O VAL G 56 37.760 1.658 4.578 1.00 8.54 o
ATOM 246 N ILE G 57 35.784 0.845 3.898 1.00 7.91 N
ATOM 247 CA ILE G 57 35.255 0.779 5.249 1.00 7.64 c
ATOM 248 CB ILE G 57 33.912 1.510 5.372 1.00 7.35 c
ATOM 249 CGI ILE G 57 34.063 2.964 4.918 1.00 7.25 c
ATOM 250 CD1 ILE G 57 32.922 3.860 5.343 1.00 8.42 c
ATOM 251 CG2 ILE G 57 33.404 1.449 6.804 1.00 7.52 c
ATOM 252 C ILE G 57 35.125 -0.655 5.739 1.00 7.69 c
ATOM 253 O ILE G 57 34.629 -1.527 5.025 1.00 7.79 o
ATOM 254 N THR G 58 35.726 -0.917 6.894 1.00 7.85 N
ATOM 255 CA THR G 58 35.912 -2.275 7.379 1.00 8.15 c
ATOM 256 CB THR G 58 37.405 -2.631 7.469 1.00 8.14 c
ATOM 257 OG1 THR G 58 38.159 -1.761 6.615 1.00 8.62 o
ATOM 258 CG2 THR G 58 37.634 -4.075 7.053 1.00 7.94 c
ATOM 259 C THR G 58 35.291 -2.414 8.763 1.00 8.20 c
ATOM 260 O THR G 58 35.589 -1.633 9.664 1.00 8.18 o
ATOM 261 N ILE G 59 34.396 -3.384 8.915 1.00 8.54 N
ATOM 262 CA ILE G 59 33.617 -3.525 10.143 1.00 9.23 c
ATOM 263 CB ILE G 59 32.144 -3.139 9.912 1.00 8.92 c
ATOM 264 CGI ILE G 59 32.031 -1.688 9.443 1.00 9.27 c
ATOM 265 CD1 ILE G 59 30.626 -1.285 9.045 1.00 10.89 c
ATOM 266 CG2 ILE G 59 31.326 -3.377 11.170 1.00 8.74 c
ATOM 267 C ILE G 59 33.648 -4.973 10.621 1.00 10.02 c
ATOM 268 O ILE G 59 33.170 -5.865 9.921 1.00 10.20 o
ATOM 269 N GLU G 60 34.251 -5.221 11.779 1.00 10.95 N
ATOM 270 CA GLU G 60 34.630 -6.586 12.133 1.00 12.13 c
ATOM 271 CB GLU G 60 35.311 -6.605 13.510 1.00 12.44 c
ATOM 272 CG GLU G 60 36.583 -5.750 13.558 1.00 15.04 c
ATOM 273 CD GLU G 60 37.500 -6.089 14.724 1.00 19.34 c
ATOM 274 OE1 GLU G 60 37.163 -5.716 15.869 1.00 20.63 o
ATOM 275 OE2 GLU G 60 38.625 -6.578 14.476 1.00 21.19 o
ATOM 276 C GLU G 60 33.397 -7.503 12.086 1.00 12.46 c

ATOM 277 O GLU G 60 32.369 -7.164 12.677 1.00 12.68 O
ATOM 278 N LEU G 61 33.448 -8.627 11.361 1.00 12.80 N
ATOM 279 CA LEU G 61 32.635 -9.731 11.843 1.00 12.71 C
ATOM 280 CB LEU G 61 32.816 -11.079 11.148 1.00 12.55 C
ATOM 281 CG LEU G 61 31.902 -12.059 11.912 1.00 12.39 C
ATOM 282 CD1 LEU G 61 30.438 -11.897 11.514 1.00 13.14 C
ATOM 283 CD2 LEU G 61 32.335 -13.513 11.814 1.00 12.50 C
ATOM 284 C LEU G 61 33.223 -9.800 13.207 1.00 12.94 C
ATOM 285 O LEU G 61 34.388 -10.187 13.351 1.00 12.78 O
ATOM 286 N SER G 62 32.676 -8.895 13.997 1.00 13.61 N
ATOM 287 CA SER G 62 32.941 -8.871 15.409 1.00 14.70 C
ATOM 288 CB SER G 62 32.339 -7.611 16.023 1.00 14.52 C
ATOM 289 OG SER G 62 32.798 -6.455 15.345 1.00 14.80 O
ATOM 290 C SER G 62 32.342 -10.111 16.051 1.00 15.48 C
ATOM 291 O SER G 62 31.132 -10.187 16.263 1.00 15.50 O
ATOM 292 N ASN G 63 33.164 -11.141 16.199 1.00 16.61 N
ATOM 293 CA ASN G 63 32.650 -12.422 16.635 1.00 17.77 C
ATOM 294 CB ASN G 63 33.597 -13.559 16.266 1.00 17.73 C
ATOM 295 CG ASN G 63 32.857 -14.834 15.934 1.00 18.52 C
ATOM 296 OD1 ASN G 63 31.848 -15.156 16.561 1.00 18.29 O
ATOM 297 ND2 ASN G 63 33.295 -15.516 14.883 1.00 19.40 N
ATOM 298 C ASN G 63 32.325 -12.448 18.119 1.00 18.53 C
ATOM 299 O ASN G 63 32.967 -11.768 18.919 1.00 18.82 O
ATOM 300 N ILE G 64 31.240 -13.135 18.457 1.00 19.60 N
ATOM 301 CA ILE G 64 30.912 -13.413 19.848 1.00 21.04 C
ATOM 302 CB ILE G 64 29.403 -13.648 20.038 1.00 20.60 C
ATOM 303 CGI ILE G 64 28.593 -12.612 19.259 1.00 20.13 C
ATOM 304 CD1 ILE G 64 27.150 -12.497 19.722 1.00 20.19 C
ATOM 305 CG2 ILE G 64 29.040 -13.615 21.514 1.00 20.74 C
ATOM 306 C ILE G 64 31.660 -14.643 20.347 1.00 22.58 C
ATOM 307 O ILE G 64 31.672 -15.682 19.687 1.00 23.07 O
ATOM 308 N LYS G 65 32.173 -14.559 21.570 1.00 24.21 N
ATOM 309 CA LYS G 65 32.425 -15.751 22.374 1.00 25.86 C
ATOM 310 CB LYS G 65 33.801 -15.682 23.043 1.00 25.90 C
ATOM 311 CG LYS G 65 34.437 -14.301 23.031 1.00 26.69 C
ATOM 312 CD LYS G 65 33.621 -13.312 23.847 1.00 28.26 C
ATOM 313 CE LYS G 65 34.477 -12.614 24.890 1.00 28.67 C
ATOM 314 NZ LYS G 65 33.661 -12.120 26.034 1.00 28.95 N
ATOM 315 C LYS G 65 31.329 -15.991 23.413 1.00 26.81 C
ATOM 316 O LYS G 65 31.299 -15.345 24.461 1.00 26.72 O
ATOM 317 N GLU G 66 30.491 -16.990 23.149 1.00 27.90 N
ATOM 318 CA GLU G 66 29.237 -17.188 23.879 1.00 28.82 C
ATOM 319 CB GLU G 66 28.305 -18.104 23.076 1.00 28.88 C
ATOM 320 CG GLU G 66 27.621 -19.192 23.895 1.00 30.33 C
ATOM 321 CD GLU G 66 27.188 -20.381 23.052 1.00 33.17 C
ATOM 322 OE1 GLU G 66 26.253 -21.098 23.468 1.00 35.05 O
ATOM 323 OE2 GLU G 66 27.824 -20.634 22.007 1.00 33.14 O
ATOM 324 C GLU G 66 29.494 -17.783 25.263 1.00 29.12 C
ATOM 325 O GLU G 66 30.348 -18.655 25.418 1.00 29.28 O
ATOM 326 N ASN G 67 28.773 -17.301 26.272 1.00 29.32 N
ATOM 327 CA ASN G 67 29.094 -17.661 27.650 1.00 29.39 C
ATOM 328 CB ASN G 67 29.462 -16.429 28.477 1.00 29.62 C
ATOM 329 CG ASN G 67 30.963 -16.231 28.580 1.00 29.84 C
ATOM 330 OD1 ASN G 67 31.651 -17.000 29.252 1.00 29.93 O
ATOM 331 ND2 ASN G 67 31.494 -15.324 27.768 1.00 29.22 N
ATOM 332 C ASN G 67 28.069 -18.540 28.367 1.00 29.15 C
ATOM 333 O ASN G 67 27.324 -18.070 29.227 1.00 29.06 O
ATOM 334 N LYS G 68 27.964 -19.788 27.921 1.00 28.87 N
ATOM 335 CA LYS G 68 27.848 -20.936 28.819 1.00 28.78 C
ATOM 336 CB LYS G 68 29.127 -21.783 28.771 1.00 28.89 C

```
ATOM    337  CG  LYS G  68      29.681 -22.003  27.364  1.00 29.26           C
ATOM    338  CD  LYS G  68      31.070 -22.631  27.392  1.00 29.68           C
ATOM    339  CE  LYS G  68      31.200 -23.648  28.514  1.00 29.46           C
ATOM    340  NZ  LYS G  68      32.473 -24.417  28.425  1.00 29.58           N
ATOM    341  C   LYS G  68      27.492 -20.555  30.268  1.00 28.60           C
ATOM    342  O   LYS G  68      28.346 -20.603  31.154  1.00 28.64           O
ATOM    343  N   CYS G  69      26.261 -20.069  30.468  1.00 28.09           N
ATOM    344  CA  CYS G  69      25.535 -20.153  31.759  1.00 27.63           C
ATOM    345  CB  CYS G  69      25.056 -18.753  32.214  1.00 27.07           C
ATOM    346  SG  CYS G  69      23.368 -18.230  31.662  1.00 28.01           S
ATOM    347  C   CYS G  69      24.339 -21.120  31.667  1.00 27.69           C
ATOM    348  O   CYS G  69      23.967 -21.533  30.570  1.00 27.41           O
ATOM    349  N   ASN G  70      23.718 -21.458  32.800  1.00 28.06           N
ATOM    350  CA  ASN G  70      22.359 -22.029  32.778  1.00 28.87           C
ATOM    351  CB  ASN G  70      22.332 -23.517  33.167  1.00 30.52           C
ATOM    352  CG  ASN G  70      23.711 -24.156  33.213  1.00 39.60           C
ATOM    353  OD1 ASN G  70      24.336 -24.404  32.180  1.00 44.97           O
ATOM    354  ND2 ASN G  70      24.204 -24.392  34.429  1.00 51.04           N
ATOM    355  C   ASN G  70      21.297 -21.261  33.577  1.00 26.97           C
ATOM    356  O   ASN G  70      21.275 -21.320  34.807  1.00 26.50           O
ATOM    357  N   GLY G  71      20.320 -20.703  32.866  1.00 25.46           N
ATOM    358  CA  GLY G  71      19.231 -19.956  33.496  1.00 23.67           C
ATOM    359  C   GLY G  71      17.990 -20.807  33.709  1.00 22.81           C
ATOM    360  O   GLY G  71      18.004 -22.008  33.436  1.00 22.79           O
ATOM    361  N   THR G  72      16.924 -20.195  34.225  1.00 21.93           N
ATOM    362  CA  THR G  72      15.666 -20.910  34.453  1.00 21.30           C
ATOM    363  CB  THR G  72      14.737 -20.162  35.441  1.00 21.12           C
ATOM    364  OG1 THR G  72      14.073 -19.090  34.761  1.00 19.87           O
ATOM    365  CG2 THR G  72      15.532 -19.609  36.619  1.00 20.76           C
ATOM    366  C   THR G  72      14.923 -21.169  33.139  1.00 21.50           C
ATOM    367  O   THR G  72      14.471 -20.236  32.474  1.00 21.85           O
ATOM    368  N   ASP G  73      14.797 -22.445  32.781  1.00 21.43           N
ATOM    369  CA  ASP G  73      14.514 -22.861  31.404  1.00 21.46           C
ATOM    370  CB  ASP G  73      13.109 -22.427  30.971  1.00 21.69           C
ATOM    371  CG  ASP G  73      12.794 -22.806  29.529  1.00 22.46           C
ATOM    372  0D1 ASP G  73      13.730 -22.837  28.701  1.00 23.01           O
ATOM    373  OD2 ASP G  73      11.611 -23.068  29.224  1.00 23.09           O
ATOM    374  C   ASP G  73      15.561 -22.365  30.406  1.00 20.96           C
ATOM    375  O   ASP G  73      15.703 -21.161  30.188  1.00 20.61           O
ATOM    376  N   ALA G  74      16.237 -23.305  29.748  1.00 20.42           N
ATOM    377  CA  ALA G  74      17.299 -22.967  28.802  1.00 20.38           C
ATOM    378  CB  ALA G  74      18.658 -23.365  29.363  1.00 20.11           C
ATOM    379  C   ALA G  74      17.092 -23.586  27.421  1.00 20.45           C
ATOM    380  O   ALA G  74      18.059 -23.849  26.707  1.00 20.46           O
ATOM    381  N   LYS G  75      15.839 -23.747  27.010  1.00 20.67           N
ATOM    382  CA  LYS G  75      15.550 -24.031  25.610  1.00 20.99           C
ATOM    383  CB  LYS G  75      14.110 -24.512  25.445  1.00 21.20           C
ATOM    384  CG  LYS G  75      13.808 -25.810  26.181  1.00 22.02           C
ATOM    385  CD  LYS G  75      12.692 -25.624  27.198  1.00 23.66           C
ATOM    386  CE  LYS G  75      13.000 -26.348  28.498  1.00 24.93           C
ATOM    387  NZ  LYS G  75      12.517 -25.588  29.683  1.00 25.55           N
ATOM    388  C   LYS G  75      15.798 -22.788  24.765  1.00 20.92           C
ATOM    389  O   LYS G  75      16.187 -22.880  23.600  1.00 20.92           O
ATOM    390  N   VAL G  76      15.659 -21.629  25.399  1.00 20.63           N
ATOM    391  CA  VAL G  76      16.187 -20.379  24.872  1.00 20.36           C
ATOM    392  CB  VAL G  76      15.654 -19.174  25.673  1.00 20.25           C
ATOM    393  CGI VAL G  76      16.330 -17.891  25.215  1.00 20.82           C
ATOM    394  CG2 VAL G  76      14.139 -19.068  25.530  1.00 20.09           C
ATOM    395  C   VAL G  76      17.717 -20.356  24.872  1.00 20.29           C
ATOM    396  O   VAL G  76      18.353 -20.568  25.905  1.00 20.21           O
```

```
ATOM    397  N   LYS G  77      18.294 -20.039  23.716  1.00 20.17           N
ATOM    398  CA  LYS G  77      19.745 -20.018  23.547  1.00 20.17           C
ATOM    399  CB  LYS G  77      20.267 -21.419  23.194  1.00 20.62           C
ATOM    400  CG  LYS G  77      20.894 -22. 180  24.367  1.00 23.31           C
ATOM    401  CD  LYS G  77      20.940 -23.684  24.105  1.00 26.74           C
ATOM    402  CE  LYS G  77      21.242 -24.468  25.376  1.00 28.32           C
ATOM    403  NZ  LYS G  77      21.041 -25.932  25.189  1.00 29.66           N
ATOM    404  C   LYS G  77      20.159 -19.010  22.468  1.00 19.45           C
ATOM    405  O   LYS G  77      20.754 -19.378  21.453  1.00 19.36           O
ATOM    406  N   LEU G  78      19.862 -17.736  22.710  1.00 18.70           N
ATOM    407  CA  LEU G  78      19.857 -16.728  21.656  1.00 17.98           C
ATOM    408  CB  LEU G  78      19.534 -15.357  22.246  1.00 17.72           C
ATOM    409  CG  LEU G  78      18.293 -15.357  23.142  1.00 17.51           C
ATOM    410  CD1 LEU G  78      18.1 17 -14.023  23.860  1.00 17.41           C
ATOM    4 11 CD2 LEU G  78      17.045 -15.734  22.349  1.00 17.62           C
ATOM    412  C   LEU G  78      2 1.181 -16.680  20.908  1.00 17.77           C
ATOM    413  O   LEU G  78      21.209 -16.672  19.678  1.00 17.89           O
ATOM    414  N   ILE G  79      22.273 -16.585  21.657  1.00 17.29           N
ATOM    415  CA  ILE G  79      23.592 -16.438  21.058  1.00 17.00           C
ATOM    416  CB  ILE G  79      24.691 -16.295  22.126  1.00 16.96           C
ATOM    417  CGI ILE G  79      24.486 -15.01 1  22.932  1.00 17.21           C
ATOM    418  CD1 ILE G  79      25.529 -14.794  24.009  1.00 17.51           C
ATOM    419  CG2 ILE G  79      26.066 -16.303  21.477  1.00 17.30           C
ATOM    420  C   ILE G  79      23.923 -17.616  20. 147  1.00 16.83           C
ATOM    421  O   ILE G  79      24.307 -17.428  18.992  1.00 17.02           O
ATOM    422  N   LYS G  80      23.678 -18.870  20.478  1.00 16.55           N
ATOM    423  CA  LYS G  80      24.058 -19.851  19.437  1.00 16.38           C
ATOM    424  CB  LYS G  80      23.872 -21.278  19.959  1.00 16.73           C
ATOM    425  CG  LYS G  80      24.274 -22.360  18.971  1.00 17.99           C
ATOM    426  CD  LYS G  80      25.741 -22.245  18.590  1.00 20.71           C
ATOM    427  CE  LYS G  80      26.170 -23.396  17.697  1.00 22.92           C
ATOM    428  NZ  LYS G  80      25.352 -23.472  16.454  1.00 24.75           N
ATOM    429  C   LYS G  80      23.334 -19.690  18.060  1.00 15.79           C
ATOM    430  O   LYS G  80      23.970 -19.700  16.969  1.00 15.32           O
ATOM    431  N   GLN G  8 1     22.019 -19.489  18. 112  1.00 15.48           N
ATOM    432  CA  GLN G  8 1      21.192 -19.385  16.905  1.00 15.33           C
ATOM    433  CB  GLN G  8 1      19.71 1 -19.320  17.287  1.00 15.70           C
ATOM    434  CG  GLN G  8 1      19.269 -20.415  18.242  1.00 17.88           C
ATOM    435  CD  GLN G  8 1      17.848 -20.225  18.734  1.00 20.46           C
ATOM    436  OE1 GLN G  8 1       17.1 16 -19.367  18.241  1.00 2 1.59           O
ATOM    437  NE2 GLN G  8 1       17.451 -21.028  19.716  1.00 20.26           N
ATOM    438  C   GLN G  8 1      21.546 -18. 192  16.019  1.00 14.63           C
ATOM    439  O   GLN G  8 1      21.582 -18.295  14.780  1.00 14.60           O
ATOM    440  N   GLU G  82      21.808 -17.057  16.658  1.00 13.81           N
ATOM    441  CA  GLU G  82       22.159 -15.854  15.925  1.00 13.37           C
ATOM    442  CB  GLU G  82       22.317 -14.664  16.873  1.00 13.20           C
ATOM    443  CG  GLU G  82       21.010 -13.984  17.235  1.00 15.04           C
ATOM    444  CD  GLU G  82       20.314 -13.388  16.026  1.00 17.51           C
ATOM    445  OE1 GLU G  82        19.726 -12.293  16. 154  1.00 18.22           O
ATOM    446  OE2 GLU G  82        20.355 -14.015  14.946  1.00 17.87           O
ATOM    447  C   GLU G  82      23.450 -16. 101  15. 169  1.00 12.99           C
ATOM    448  O   GLU G  82      23.584 -15.705  14.014  1.00 12.89           O
ATOM    449  N   LEU G  83      24.393 -16.778  15.815  1.00 12.89           N
ATOM    450  CA  LEU G  83       25.665 -17.066  15.174  1.00 13.08           C
ATOM    451  CB  LEU G  83       26.613 -17.761  16.151  1.00 13.26           C
ATOM    452  CG  LEU G  83       26.970 -16.978  17.415  1.00 14.18           C
ATOM    453  CD1 LEU G  83        27.933 -17.774  18.282  1.00 15. 11           C
ATOM    454  CD2 LEU G  83        27.557 -15.620  17.059  1.00 14.79           C
ATOM    455  C   LEU G  83      25.444 -17.940  13.949  1.00 13.18           C
ATOM    456  O   LEU G  83      26.007 -17.673  12.876  1.00 13.05           O
```

```
ATOM    457  N   ASP G  84     24.588 -18.953  14.074  1.00 13.56           N
ATOM    458  CA  ASP G  84     24.346 -19.788  12.891  1.00 14.15           C
ATOM    459  CB  ASP G  84     23.439 -20.973  13.232  1.00 14.80           C
ATOM    460  CG  ASP G  84     24.004 -21.841  14.338  1.00 18.26           C
ATOM    461  0D1 ASP G  84     24.605 -22.891  14.026  1.00 21. 11          O
ATOM    462  OD2 ASP G  84     23.837 -21 .480  15.520  1.00 22. 12          O
ATOM    463  C   ASP G  84     23.737 -18.979  11.731  1.00 13.56           C
ATOM    464  O   ASP G  84     24.147 -19.1 11  10.549  1.00 13.70           O
ATOM    465  N   LYS G  85     22.780 -18.1 15  12.068  1.00 12.87           N
ATOM    466  CA  LYS G  85     22.128 -17.318  11.033  1.00 12.31           C
ATOM    467  CB  LYS G  85     20.987 -16.487  11.619  1.00 12.41           C
ATOM    468  CG  LYS G  85     20.087 -15.857  10.568  1.00 12.26           C
ATOM    469  CD  LYS G  85     19.083 -14.900  11.189  1.00 12.72           C
ATOM    470  CE  LYS G  85     19.772 -13.667  11.750  1.00 14.40           C
ATOM    471  NZ  LYS G  85     18.789 -12.676  12.268  1.00 16.45           N
ATOM    472  C   LYS G  85     23.147 -16.409  10.353  1.00 11.85           C
ATOM    473  O   LYS G  85     23.143 -16.238   9.125  1.00 11.66           O
ATOM    474  N   TYR G  86     24.031 -15.839  11.165  1.00 11.32           N
ATOM    475  CA  TYR G  86     25.051 -14.936  10.665  1.00 11.07           C
ATOM    476  CB  TYR G  86     25.863 -14.349  11.820  1.00 11.12           C
ATOM    477  CG  TYR G  86     27.216 -13.824  11.399  1.00 11.30           C
ATOM    478  CD1 TYR G  86     27.349 -12.561  10.838  1.00 12.16           C
ATOM    479  CE1 TYR G  86     28.584 -12.080  10.449  1.00 12.39           C
ATOM    480  CZ  TYR G  86     29.705 -12.864  10.619  1.00 12.62           C
ATOM    481  OH  TYR G  86     30.938 -12.388  10.233  1.00 12.72           O
ATOM    482  CE2 TYR G  86     29.599 -14.121  11.172  1.00 11.38           C
ATOM    483  CD2 TYR G  86     28.360 -14.595  11.558  1.00 11.05           C
ATOM    484  C   TYR G  86     25.971 -15.667   9.708  1.00 10.75           C
ATOM    485  O   TYR G  86     26.320 -15. 140   8.656  1.00 10.45           O
ATOM    486  N   LYS G  87     26.343 -16.894  10.053  1.00 10.66           N
ATOM    487  CA  LYS G  87     27.220 -17.656   9.174  1.00 11.03           C
ATOM    488  CB  LYS G  87     27.588 -18.996   9.813  1.00 11.36           C
ATOM    489  CG  LYS G  87     28.300 -18.874  11.149  1.00 12.79           C
ATOM    490  CD  LYS G  87     28.627 -20.242  11.722  1.00 14.76           C
ATOM    491  CE  LYS G  87     29.336 -20.123  13.060  1.00 15.29           C
ATOM    492  NZ  LYS G  87     29.664 -21.460  13.626  1.00 16.27           N
ATOM    493  C   LYS G  87     26.541 -17.891   7.826  1.00 10.83           C
ATOM    494  O   LYS G  87     27.163 -17.715   6.758  1.00 11.1 1          O
ATOM    495  N   ASN G  88     25.256 -18.243   7.858  1.00 10.52           N
ATOM    496  CA  ASN G  88     24.567 -18.464   6.584  1.00 10.21           C
ATOM    497  CB  ASN G  88     23.149 -18.989   6.821  1.00 10.61           C
ATOM    498  CG  ASN G  88     22.406 -19.271   5.529  1.00 11.81           C
ATOM    499  OD1 ASN G  88     22.998 -19.285   4.450  1.00 12.97           O
ATOM    500  ND2 ASN G  88     21.101 -19.496   5.633  1.00 13.82           N
ATOM    501  C   ASN G  88     24.528 -17.187   5.730  1.00  9.42           C
ATOM    502  O   ASN G  88     24.780 -17.206   4.500  1.00  8.94           O
ATOM    503  N   ALA G  89     24.251 -16.068   6.395  1.00  8.77           N
ATOM    504  CA  ALA G  89     24.164 -14.796   5.693  1.00  8.21           C
ATOM    505  CB  ALA G  89     23.734 -13.693   6.647  1.00  7.99           C
ATOM    506  C   ALA G  89     25.510 -14.465   5.063  1.00  7.78           C
ATOM    507  O   ALA G  89     25.586 -13.988   3.927  1.00  7.88           O
ATOM    508  N   VAL G  90     26.574 -14.738   5.809  1.00  7.01           N
ATOM    509  CA  VAL G  90     27.921 -14.464   5.344  1.00  6.26           C
ATOM    510  CB  VAL G  90     28.965 -14.771   6.433  1.00  5.91           C
ATOM    5 11 CGI VAL G  90     30.361 -14.414   5.945  1.00  5.92           C
ATOM    512  CG2 VAL G  90     28.631 -14.020   7.714  1.00  5.26           C
ATOM    513  C   VAL G  90     28.240 -15.284   4.104  1.00  6.25           C
ATOM    514  O   VAL G  90     28.798 -14.758   3.144  1.00  6.32           O
ATOM    515  N   THR G  91     27.858 -16.558   4.098  1.00  6.24           N
ATOM    516  CA  THR G  91     28. 129 -17.376   2.915  1.00  6.68           C
```

```
ATOM    517  CB  THR G  91      27.705 -18.840   3.129  1.00  6.62           C
ATOM    518  OG1 THR G  91      28.438 -19.397   4.227  1.00  7.19           O
ATOM    519  CG2 THR G  91      27.971 -19.661   1.876  1.00  7.27           C
ATOM    520  C   THR G  91      27.392 -16.808   1.698  1.00  7.02           C
ATOM    521  O   THR G  91      27.953 -16.709   0.569  1.00  7.16           O
ATOM    522  N   GLU G  92      26.143 -16.402   1.925  1.00  7.31           N
ATOM    523  CA  GLU G  92      25.382 -15.849   0.812  1.00  7.81           C
ATOM    524  CB  GLU G  92      23.942 -15.547   1.231  1.00  8.23           C
ATOM    525  CG  GLU G  92      23.030 -16.761   1.222  1.00 10.91           C
ATOM    526  CD  GLU G  92      22.895 -17.372  -0.161  1.00 14.95           C
ATOM    527  OEl GLU G  92      21.801 -17.878  -0.489  1.00 16.14           O
ATOM    528  OE2 GLU G  92      23.884 -17.346  -0.923  1.00 16.53           O
ATOM    529  C   GLU G  92      26.053 -14.587   0.267  1.00  7.47           C
ATOM    530  O   GLU G  92      26.210 -14.432  -0.947  1.00  7.32           O
ATOM    531  N   LEU G  93      26.501 -13.717   1.167  1.00  7.30           N
ATOM    532  CA  LEU G  93      27.140 -12.467   0.759  1.00  7.47           C
ATOM    533  CB  LEU G  93      27.442 -11.589   1.973  1.00  7.15           C
ATOM    534  CG  LEU G  93      26.217 -11.021   2.692  1.00  7.20           C
ATOM    535  CD1 LEU G  93      26.638 -10.123   3.845  1.00  7.93           C
ATOM    536  CD2 LEU G  93      25.325 -10.266   1.716  1.00  6.91           C
ATOM    537  C   LEU G  93      28.414 -12.761  -0.020  1.00  7.89           C
ATOM    538  O   LEU G  93      28.746 -12.083  -0.991  1.00  7.94           O
ATOM    539  N   GLN G  94      29.116 -13.789   0.434  1.00  8.31           N
ATOM    540  CA  GLN G  94      30.361 -14.248  -0.160  1.00  9.05           C
ATOM    541  CB  GLN G  94      30.985 -15.349   0.701  1.00  9.18           C
ATOM    542  CG  GLN G  94      31.324 -14.908   2.114  1.00 10.79           C
ATOM    543  CD  GLN G  94      31.993 -16.003   2.920  1.00 13.82           C
ATOM    544  OEl GLN G  94      32.210 -17.109   2.427  1.00 14.98           O
ATOM    545  NE2 GLN G  94      32.324 -15.698   4.170  1.00 15.25           N
ATOM    546  C   GLN G  94      30.220 -14.731  -1.603  1.00  9.25           C
ATOM    547  O   GLN G  94      31.124 -14.514  -2.410  1.00  9.43           O
ATOM    548  N   LEU G  95      29.114 -15.393  -1.941  1.00  9.55           N
ATOM    549  CA  LEU G  95      29.003 -15.935  -3.318  1.00 10.17           C
ATOM    550  CB  LEU G  95      27.752 -16.811  -3.437  1.00  9.79           C
ATOM    551  CG  LEU G  95      27.700 -18.053  -2.545  1.00  8.86           C
ATOM    552  CD1 LEU G  95      26.403 -18.817  -2.764  1.00  8.31           C
ATOM    553  CD2 LEU G  95      28.904 -18.947  -2.798  1.00  7.62           C
ATOM    554  C   LEU G  95      29.057 -14.945  -4.528  1.00 11.22           C
ATOM    555  O   LEU G  95      29.643 -15.248  -5.567  1.00 11.55           O
ATOM    556  N   LEU G  96      28.430 -13.786  -4.361  1.00 12.40           N
ATOM    557  CA  LEU G  96      28.142 -12.747  -5.335  1.00 13.66           C
ATOM    558  CB  LEU G  96      27.471 -11.548  -4.668  1.00 13.38           C
ATOM    559  CG  LEU G  96      26.008 -11.779  -4.288  1.00 13.32           C
ATOM    560  CD1 LEU G  96      25.321 -10.462  -3.975  1.00 12.84           C
ATOM    561  CD2 LEU G  96      25.278 -12.519  -5.397  1.00 13.38           C
ATOM    562  C   LEU G  96      29.392 -12.314  -6.094  1.00 14.97           C
ATOM    563  O   LEU G  96      29.293 -11.741  -7.178  1.00 15.21           O
ATOM    564  N   MET G  97      30.564 -12.678  -5.576  1.00 16.74           N
ATOM    565  CA  MET G  97      31.799 -11.956  -5.894  1.00 18.96           C
ATOM    566  CB  MET G  97      32.828 -12.102  -4.766  1.00 19.12           C
ATOM    567  CG  MET G  97      32.353 -11.577  -3.413  1.00 21.87           C
ATOM    568  SD  MET G  97      32.586  -9.794  -3.210  1.00 27.46           S
ATOM    569  CE  MET G  97      32.408  -9.214  -4.899  1.00 24.25           C
ATOM    570  C   MET G  97      32.408 -12.377  -7.233  1.00 20.09           C
ATOM    571  O   MET G  97      33.064 -11.581  -7.905  1.00 20.58           O
ATOM    572  N   GLN G  98      32.151 -13.618  -7.634  1.00 21.33           N
ATOM    573  CA  GLN G  98      32.735 -14.171  -8.853  1.00 22.21           C
ATOM    574  CB  GLN G  98      33.777 -15.243  -8.513  1.00 22.53           C
ATOM    575  CG  GLN G  98      34.695 -14.883  -7.347  1.00 23.85           C
ATOM    576  CD  GLN G  98      34.172 -15.376  -6.008  1.00 25.21           C
```

```
ATOM    577  OE1 GLN G  98      33.109 -14.957  -5.549  1.00 24.47           O
ATOM    578  NE2 GLN G  98      34.939 -16.243  -5.358  1.00 24.85           N
ATOM    579  C   GLN G  98      31.660 -14.756  -9.766  1.00 22.15           C
ATOM    580  O   GLN G  98      30.475 -14.451  -9.624  1.00 21.77           O
ATOM    581  N   PHE G 137      36.645 -13.585 -16.969  1.00 33.25           N
ATOM    582  CA  PHE G 137      35.365 -12.919 -16.764  1.00 36.79           C
ATOM    583  CB  PHE G 137      35.255 -11.672 -17.642  1.00 20.00           C
ATOM    584  CG  PHE G 137      36.265 -10.611 -17.319  1.00 20.00           C
ATOM    585  CD1 PHE G 137      36.015  -9.677 -16.331  1.00 20.00           C
ATOM    586  CE1 PHE G 137      36.932  -8.682 -16.050  1.00 20.00           C
ATOM    587  CZ  PHE G 137      38.108  -8.607 -16.766  1.00 20.00           C
ATOM    588  CE2 PHE G 137      38.362  -9.523 -17.764  1.00 20.00           C
ATOM    589  CD2 PHE G 137      37.439 -10.510 -18.045  1.00 20.00           C
ATOM    590  C   PHE G 137      34.195 -13.850 -17.063  1.00 48.73           C
ATOM    591  O   PHE G 137      33.039 -13.434 -16.993  1.00 49.28           O
ATOM    592  N   LEU G 138      34.498 -15.040 -17.571  1.00 42.04           N
ATOM    593  CA  LEU G 138      33.471 -16.059 -17.783  1.00 44.26           C
ATOM    594  CB  LEU G 138      34.037 -17.258 -18.553  1.00 20.00           C
ATOM    595  CG  LEU G 138      34.341 -17.114 -20.050  1.00 20.00           C
ATOM    596  CD1 LEU G 138      34.975 -18.387 -20.605  1.00 20.00           C
ATOM    597  CD2 LEU G 138      33.095 -16.756 -20.843  1.00 20.00           C
ATOM    598  C   LEU G 138      32.896 -16.527 -16.451  1.00 43.68           C
ATOM    599  O   LEU G 138      31.839 -17.157 -16.406  1.00 50.27           O
ATOM    600  N   GLY G 139      33.614 -16.234 -15.370  1.00 38.56           N
ATOM    601  CA  GLY G 139      33.145 -16.544 -14.022  1.00 47.99           C
ATOM    602  C   GLY G 139      31.826 -15.881 -13.662  1.00 44.53           C
ATOM    603  O   GLY G 139      31.082 -16.383 -12.819  1.00 32.21           O
ATOM    604  N   PHE G 140      31.510 -14.778 -14.337  1.00 46.33           N
ATOM    605  CA  PHE G 140      30.319 -13.992 -14.021  1.00 42.95           C
ATOM    606  CB  PHE G 140      30.530 -12.516 -14.386  1.00 20.00           C
ATOM    607  CG  PHE G 140      31.590 -11.827 -13.564  1.00 20.00           C
ATOM    608  CD1 PHE G 140      31.295 -11.318 -12.310  1.00 20.00           C
ATOM    609  CE1 PHE G 140      32.272 -10.683 -11.553  1.00 20.00           C
ATOM    610  CZ  PHE G 140      33.540 -10.511 -12.066  1.00 20.00           C
ATOM    611  CE2 PHE G 140      33.832 -10.970 -13.334  1.00 20.00           C
ATOM    612  CD2 PHE G 140      32.851 -11.591 -14.090  1.00 20.00           C
ATOM    613  C   PHE G 140      29.077 -14.525 -14.731  1.00 38.13           C
ATOM    614  O   PHE G 140      27.970 -14.040 -14.504  1.00 57.33           O
ATOM    615  N   LEU G 141      29.271 -15.480 -15.634  1.00 35.20           N
ATOM    616  CA  LEU G 141      28.173 -15.996 -16.446  1.00 27.01           C
ATOM    617  CB  LEU G 141      26.983 -16.392 -15.560  1.00 20.00           C
ATOM    618  CG  LEU G 141      27.185 -17.555 -14.580  1.00 20.00           C
ATOM    619  CD1 LEU G 141      25.930 -17.779 -13.747  1.00 20.00           C
ATOM    620  CD2 LEU G 141      27.588 -18.835 -15.306  1.00 20.00           C
ATOM    621  C   LEU G 141      27.750 -14.978 -17.504  1.00 35.79           C
ATOM    622  O   LEU G 141      28.543 -14.613 -18.370  1.00 46.92           O
ATOM    623  N   LEU G 142      26.509 -14.508 -17.424  1.00 38.67           N
ATOM    624  CA  LEU G 142      26.075 -13.372 -18.231  1.00 33.84           C
ATOM    625  CB  LEU G 142      24.737 -13.667 -18.914  1.00 20.00           C
ATOM    626  CG  LEU G 142      24.720 -14.676 -20.063  1.00 20.00           C
ATOM    627  CD1 LEU G 142      23.339 -14.707 -20.705  1.00 20.00           C
ATOM    628  CD2 LEU G 142      25.773 -14.324 -21.101  1.00 20.00           C
ATOM    629  C   LEU G 142      25.959 -12.123 -17.368  1.00 36.89           C
ATOM    630  O   LEU G 142      25.257 -12.119 -16.358  1.00 45.42           O
ATOM    631  N   GLY G 143      26.763 -11.115 -17.688  1.00 26.84           N
ATOM    632  CA  GLY G 143      26.817  -9.895 -16.892  1.00 27.41           C
ATOM    633  C   GLY G 143      26.590  -8.645 -17.722  1.00 29.08           C
ATOM    634  O   GLY G 143      26.918  -8.603 -18.908  1.00 40.24           O
ATOM    635  N   VAL G 144      26.026  -7.622 -17.092  1.00 30.17           N
ATOM    636  CA  VAL G 144      25.849  -6.331 -17.739  1.00 34.15           C
```

ATOM 637 CB VAL G 144 24.768 -5.496 -17.035 1.00 20.00 C
ATOM 638 CGI VAL G 144 24.730 -4.081 -17.599 1.00 20.00 C
ATOM 639 CG2 VAL G 144 23.414 -6.166 -17.170 1.00 20.00 C
ATOM 640 C VAL G 144 27.152 -5.543 -17.760 1.00 36.67 C
ATOM 641 O VAL G 144 28.104 -5.880 -17.054 1.00 42.49 O
ATOM 642 N GLY G 145 27.185 -4.487 -18.567 1.00 47.09 N
ATOM 643 CA GLY G 145 28.309 -3.563 -18.568 1.00 44.51 C
ATOM 644 C GLY G 145 28.683 -3.184 -17.151 1.00 44.94 C
ATOM 645 O GLY G 145 29.809 -3.424 -16.714 1.00 40.58 O
ATOM 646 N SER G 146 27.732 -2.662 -16.387 1.00 42.06 N
ATOM 647 CA SER G 146 28.033 -2.190 -15.035 1.00 47.39 C
ATOM 648 CB SER G 146 26.797 -1.534 -14.414 1.00 20.00 C
ATOM 649 OG SER G 146 25.719 -2.450 -14.333 1.00 20.00 O
ATOM 650 C SER G 146 28.570 -3.280 -14.101 1.00 51.48 C
ATOM 651 O SER G 146 29.491 -3.034 -13.317 1.00 47.45 O
ATOM 652 N ALA G 147 28.004 -4.480 -14.183 1.00 39.51 N
ATOM 653 CA ALA G 147 28.430 -5.576 -13.316 1.00 43.38 C
ATOM 654 CB ALA G 147 27.531 -6.788 -13.513 1.00 20.00 C
ATOM 655 C ALA G 147 29.894 -5.954 -13.541 1.00 47.39 C
ATOM 656 O ALA G 147 30.635 -6.211 -12.587 1.00 50.18 O
ATOM 657 N ILE G 148 30.309 -5.983 -14.804 1.00 44.67 N
ATOM 658 CA ILE G 148 31.690 -6.311 -15.140 1.00 43.56 C
ATOM 659 CB ILE G 148 31.898 -6.390 -16.663 1.00 20.00 C
ATOM 660 CGI ILE G 148 30.998 -7.469 -17.269 1.00 20.00 C
ATOM 661 CD1 ILE G 148 31.142 -7.612 -18.768 1.00 20.00 C
ATOM 662 CG2 ILE G 148 33.358 -6.663 -16.987 1.00 20.00 C
ATOM 663 C ILE G 148 32.633 -5.265 -14.558 1.00 51.18 C
ATOM 664 O ILE G 148 33.699 -5.592 -14.031 1.00 39.17 O
ATOM 665 N ALA G 149 32.226 -4.003 -14.651 1.00 42.17 N
ATOM 666 CA ALA G 149 33.020 -2.906 -14.116 1.00 36.76 C
ATOM 667 CB ALA G 149 32.386 -1.571 -14.466 1.00 20.00 C
ATOM 668 C ALA G 149 33.150 -3.058 -12.607 1.00 45.19 C
ATOM 669 O ALA G 149 34.222 -2.843 -12.041 1.00 47.83 O
ATOM 670 N SER G 150 32.054 -3.443 -11.961 1.00 43.64 N
ATOM 671 CA SER G 150 32.062 -3.643 -10.518 1.00 43.46 C
ATOM 672 CB SER G 150 30.657 -3.968 -10.010 1.00 20.00 C
ATOM 673 OG SER G 150 30.165 -5.160 -10.596 1.00 20.00 O
ATOM 674 C SER G 150 33.030 -4.762 -10.146 1.00 44.80 C
ATOM 675 O SER G 150 33.774 -4.653 -9.170 1.00 41.55 O
ATOM 676 N GLY G 151 33.025 -5.833 -10.935 1.00 27.01 N
ATOM 677 CA GLY G 151 33.927 -6.946 -10.697 1.00 35.21 C
ATOM 678 C GLY G 151 35.376 -6.519 -10.839 1.00 42.40 C
ATOM 679 O GLY G 151 36.246 -6.924 -10.055 1.00 45.11 O
ATOM 680 N VAL G 152 35.638 -5.691 -11.846 1.00 40.20 N
ATOM 681 CA VAL G 152 36.983 -5.185 -12.076 1.00 46.73 C
ATOM 682 CB VAL G 152 37.056 -4.330 -13.354 1.00 20.00 C
ATOM 683 CGI VAL G 152 38.472 -3.816 -13.568 1.00 20.00 C
ATOM 684 CG2 VAL G 152 36.587 -5.134 -14.557 1.00 20.00 C
ATOM 685 C VAL G 152 37.424 -4.345 -10.885 1.00 48.62 C
ATOM 686 O VAL G 152 38.565 -4.438 -10.432 1.00 49.32 O
ATOM 687 N ALA G 153 36.502 -3.537 -10.370 1.00 35.09 N
ATOM 688 CA ALA G 153 36.788 -2.690 -9.220 1.00 42.37 C
ATOM 689 CB ALA G 153 35.604 -1.787 -8.918 1.00 20.00 C
ATOM 690 C ALA G 153 37.120 -3.557 -8.014 1.00 37.79 C
ATOM 691 O ALA G 153 38.029 -3.247 -7.243 1.00 39.25 O
ATOM 692 N VAL G 154 36.378 -4.648 -7.859 1.00 38.88 N
ATOM 693 CA VAL G 154 36.610 -5.579 -6.763 1.00 35.53 C
ATOM 694 CB VAL G 154 35.549 -6.695 -6.737 1.00 20.00 C
ATOM 695 CGI VAL G 154 35.814 -7.651 -5.584 1.00 20.00 C
ATOM 696 CG2 VAL G 154 34.154 -6.098 -6.634 1.00 20.00 C

```
ATOM    697  C   VAL G 154      37.996  -6.209  -6.863  1.00 41.00           C
ATOM    698  O   VAL G 154      38.690  -6.353  -5.856  1.00 50.08           O
ATOM    699  N   SER G 155      38.403  -6.579  -8.075  1.00 37.82           N
ATOM    700  CA  SER G 155      39.733  -7.158  -8.271  1.00 44.68           C
ATOM    701  CB  SER G 155      39.906  -7.630  -9.715  1.00 20.00           C
ATOM    702  OG  SER G 155      39.757  -6.554 -10.625  1.00 20.00           O
ATOM    703  C   SER G 155      40.817  -6.140  -7.914  1.00 41.82           C
ATOM    704  O   SER G 155      41.834  -6.468  -7.304  1.00 49.37           O
ATOM    705  N   LYS G 156      40.566  -4.900  -8.314  1.00 36.99           N
ATOM    706  CA  LYS G 156      41.440  -3.756  -8.097  1.00 35.11           C
ATOM    707  CB  LYS G 156      40.989  -2.562  -8.943  1.00 20.00           C
ATOM    708  CG  LYS G 156      41.146  -2.767 -10.443  1.00 20.00           C
ATOM    709  CD  LYS G 156      40.541  -1.606 -11.227  1.00 20.00           C
ATOM    710  CE  LYS G 156      40.906  -1.679 -12.708  1.00 20.00           C
ATOM    711  NZ  LYS G 156      40.298  -0.569 -13.497  1.00 20.00           N
ATOM    712  C   LYS G 156      41.489  -3.378  -6.620  1.00 35.98           C
ATOM    713  O   LYS G 156      42.501  -2.874  -6.136  1.00 42.31           O
ATOM    714  N   VAL G 157      40.433  -3.719  -5.886  1.00 37.88           N
ATOM    715  CA  VAL G 157      40.341  -3.361  -4.475  1.00 50.94           C
ATOM    716  CB  VAL G 157      38.894  -3.057  -4.061  1.00 20.00           C
ATOM    717  CGI VAL G 157      38.799  -2.928  -2.551  1.00 20.00           C
ATOM    718  CG2 VAL G 157      38.403  -1.790  -4.745  1.00 20.00           C
ATOM    719  C   VAL G 157      40.882  -4.474  -3.591  1.00 47.82           C
ATOM    720  O   VAL G 157      41.021  -4.309  -2.379  1.00 56.87           O
ATOM    721  N   LEU G 158      41.279  -5.588  -4.192  1.00 39.52           N
ATOM    722  CA  LEU G 158      41.557  -6.817  -3.448  1.00 50.27           C
ATOM    723  CB  LEU G 158      41.899  -7.952  -4.419  1.00 20.00           C
ATOM    724  CG  LEU G 158      40.817  -8.321  -5.435  1.00 20.00           C
ATOM    725  CD1 LEU G 158      41.287  -9.458  -6.330  1.00 20.00           C
ATOM    726  CD2 LEU G 158      39.521  -8.689  -4.729  1.00 20.00           C
ATOM    727  C   LEU G 158      42.627  -6.743  -2.351  1.00 54.47           C
ATOM    728  O   LEU G 158      42.456  -7.343  -1.285  1.00 49.26           O
ATOM    729  N   HIS G 159      43.716  -6.021  -2.585  1.00 59.45           N
ATOM    730  CA  HIS G 159      44.772  -5.947  -1.579  1.00 49.11           C
ATOM    731  CB  HIS G 159      45.963  -5.146  -2.108  1.00 20.00           C
ATOM    732  CG  HIS G 159      46.583  -5.728  -3.340  1.00 20.00           C
ATOM    733  ND1 HIS G 159      47.606  -6.651  -3.293  1.00 20.00           N
ATOM    734  CE1 HIS G 159      47.951  -6.984  -4.524  1.00 20.00           C
ATOM    735  NE2 HIS G 159      47.189  -6.311  -5.368  1.00 20.00           N
ATOM    736  CD2 HIS G 159      46.325  -5.518  -4.652  1.00 20.00           C
ATOM    737  C   HIS G 159      44.256  -5.325  -0.280  1.00 44.09           C
ATOM    738  O   HIS G 159      44.572  -5.797   0.819  1.00 42.13           O
ATOM    739  N   LEU G 160      43.449  -4.277  -0.410  1.00 37.55           N
ATOM    740  CA  LEU G 160      42.876  -3.609   0.751  1.00 43.52           C
ATOM    741  CB  LEU G 160      42.095  -2.365   0.323  1.00 20.00           C
ATOM    742  CG  LEU G 160      42.891  -1.283  -0.409  1.00 20.00           C
ATOM    743  CD1 LEU G 160      41.996  -0.107  -0.769  1.00 20.00           C
ATOM    744  CD2 LEU G 160      44.073  -0.825   0.432  1.00 20.00           C
ATOM    745  C   LEU G 160      41.966  -4.559   1.523  1.00 47.22           C
ATOM    746  O   LEU G 160      41.969  -4.578   2.756  1.00 43.25           O
ATOM    747  N   GLU G 161      41.190  -5.350   0.788  1.00 40.88           N
ATOM    748  CA  GLU G 161      40.292  -6.318   1.402  1.00 40.61           C
ATOM    749  CB  GLU G 161      39.434  -7.005   0.338  1.00 20.00           C
ATOM    750  CG  GLU G 161      38.558  -6.055  -0.462  1.00 20.00           C
ATOM    751  CD  GLU G 161      37.719  -6.773  -1.501  1.00 20.00           C
ATOM    752  OE1 GLU G 161      36.959  -6.094  -2.224  1.00 20.00           O
ATOM    753  OE2 GLU G 161      37.819  -8.014  -1.596  1.00 20.00           O
ATOM    754  C   GLU G 161      41.097  -7.352   2.179  1.00 39.76           C
ATOM    755  O   GLU G 161      40.720  -7.747   3.284  1.00 44.02           O
ATOM    756  N   GLY G 162      42.213  -7.781   1.599  1.00 34.18           N
```

```
ATOM    757  CA  GLY G 162      43.079  -8.742   2.256  1.00 35.01           C
ATOM    758  C   GLY G 162      43.637  -8.163   3.542  1.00 34.86           C
ATOM    759  O   GLY G 162      43.706  -8.844   4.570  1.00 47.81           O
ATOM    760  N   GLU G 163      44.019  -6.890   3.489  1.00 40.78           N
ATOM    761  CA  GLU G 163      44.546  -6.213   4.669  1.00 37.20           C
ATOM    762  CB  GLU G 163      45.016  -4.801   4.315  1.00 20.00           C
ATOM    763  CG  GLU G 163      46.112  -4.758   3.264  1.00 20.00           C
ATOM    764  CD  GLU G 163      46.555  -3.345   2.942  1.00 20.00           C
ATOM    765  OE1 GLU G 163      47.454  -3.181   2.090  1.00 20.00           O
ATOM    766  OE2 GLU G 163      46.003  -2.399   3.540  1.00 20.00           O
ATOM    767  C   GLU G 163      43.480  -6.158   5.758  1.00 46.12           C
ATOM    768  O   GLU G 163      43.770  -6.363   6.939  1.00 58.66           O
ATOM    769  N   VAL G 164      42.243  -5.885   5.354  1.00 42.23           N
ATOM    770  CA  VAL G 164      41.129  -5.833   6.292  1.00 35.45           C
ATOM    771  CB  VAL G 164      39.827  -5.387   5.602  1.00 20.00           C
ATOM    772  CGI VAL G 164      38.684  -5.343   6.604  1.00 20.00           C
ATOM    773  CG2 VAL G 164      40.015  -4.032   4.937  1.00 20.00           C
ATOM    774  C   VAL G 164      40.908  -7.195   6.947  1.00 46.32           C
ATOM    775  O   VAL G 164      40.656  -7.284   8.153  1.00 45.08           O
ATOM    776  N   ASN G 165      41.011  -8.257   6.151  1.00 40.82           N
ATOM    777  CA  ASN G 165      40.854  -9.603   6.687  1.00 46.48           C
ATOM    778  CB  ASN G 165      40.897 -10.652   5.573  1.00 20.00           C
ATOM    779  CG  ASN G 165      39.710 -10.560   4.634  1.00 20.00           C
ATOM    780  OD1 ASN G 165      38.643 -11.108   4.909  1.00 20.00           O
ATOM    781  ND2 ASN G 165      39.896  -9.881   3.509  1.00 20.00           N
ATOM    782  C   ASN G 165      41.947  -9.884   7.708  1.00 50.90           C
ATOM    783  O   ASN G 165      41.694 -10.455   8.769  1.00 47.11           O
ATOM    784  N   LYS G 166      43.161  -9.451   7.385  1.00 48.36           N
ATOM    785  CA  LYS G 166      44.305  -9.640   8.269  1.00 38.71           C
ATOM    786  CB  LYS G 166      45.591  -9.154   7.595  1.00 20.00           C
ATOM    787  CG  LYS G 166      45.907  -9.850   6.277  1.00 20.00           C
ATOM    788  CD  LYS G 166      47.180  -9.298   5.649  1.00 20.00           C
ATOM    789  CE  LYS G 166      47.495  -9.990   4.331  1.00 20.00           C
ATOM    790  NZ  LYS G 166      48.735  -9.455   3.701  1.00 20.00           N
ATOM    791  C   LYS G 166      44.090  -8.907   9.591  1.00 45.07           C
ATOM    792  O   LYS G 166      44.459  -9.402  10.657  1.00 56.09           O
ATOM    793  N   ILE G 167      43.491  -7.725   9.508  1.00 42.02           N
ATOM    794  CA  ILE G 167      43.256  -6.876  10.673  1.00 43.86           C
ATOM    795  CB  ILE G 167      43.338  -5.380  10.304  1.00 20.00           C
ATOM    796  CGI ILE G 167      44.721  -5.042   9.743  1.00 20.00           C
ATOM    797  CD1 ILE G 167      44.884  -3.589   9.349  1.00 20.00           C
ATOM    798  CG2 ILE G 167      43.025  -4.514  11.516  1.00 20.00           C
ATOM    799  C   ILE G 167      41.921  -7.143  11.377  1.00 49.02           C
ATOM    800  O   ILE G 167      41.570  -6.443  12.327  1.00 37.71           O
ATOM    801  N   LYS G 168      41.175  -8.142  10.911  1.00 33.87           N
ATOM    802  CA  LYS G 168      39.851  -8.426  11.471  1.00 35.11           C
ATOM    803  CB  LYS G 168      39.163  -9.533  10.667  1.00 20.00           C
ATOM    804  CG  LYS G 168      38.874  -9.175   9.219  1.00 20.00           C
ATOM    805  CD  LYS G 168      38.101 -10.286   8.524  1.00 20.00           C
ATOM    806  CE  LYS G 168      37.755  -9.909   7.092  1.00 20.00           C
ATOM    807  NZ  LYS G 168      36.921 -10.950   6.427  1.00 20.00           N
ATOM    808  C   LYS G 168      39.820  -8.790  12.966  1.00 39.27           C
ATOM    809  O   LYS G 168      38.932  -8.339  13.690  1.00 32.39           O
ATOM    810  N   SER G 169      40.770  -9.599  13.428  1.00 41.30           N
ATOM    811  CA  SER G 169      40.805 -10.008  14.827  1.00 43.23           C
ATOM    812  CB  SER G 169      42.030 -10.884  15.100  1.00 20.00           C
ATOM    813  OG  SER G 169      43.231 -10.175  14.847  1.00 20.00           O
ATOM    814  C   SER G 169      40.796  -8.806  15.767  1.00 41.44           C
ATOM    815  O   SER G 169      40.016  -8.759  16.718  1.00 44.82           O
ATOM    816  N   ALA G 170      41.695  -7.857  15.522  1.00 39.78           N
```

```
ATOM    817  CA  ALA G 170      41.753  -6.638  16.319  1.00 41.01           C
ATOM    818  CB  ALA G 170      42.928  -5.775  15.887  1.00 20.00           C
ATOM    819  C   ALA G 170      40.448  -5.857  16.211  1.00 46.04           C
ATOM    820  O   ALA G 170      39.912  -5.381  17.211  1.00 46.67           O
ATOM    821  N   LEU G 171      39.921  -5.766  14.995  1.00 34.26           N
ATOM    822  CA  LEU G 171      38.642  -5.108  14.762  1.00 37.69           C
ATOM    823  CB  LEU G 171      38.269  -5.179  13.280  1.00 20.00           C
ATOM    824  CG  LEU G 171      39.239  -4.485  12.323  1.00 20.00           C
ATOM    825  CD1 LEU G 171      38.764  -4.625  10.881  1.00 20.00           C
ATOM    826  CD2 LEU G 171      39.417  -3.022  12.711  1.00 20.00           C
ATOM    827  C   LEU G 171      37.534  -5.723  15.616  1.00 44.67           C
ATOM    828  O   LEU G 171      36.683  -5.010  16.151  1.00 34.27           O
ATOM    829  N   LEU G 172      37.577  -7.043  15.776  1.00 34.80           N
ATOM    830  CA  LEU G 172      36.536  -7.765  16.498  1.00 28.87           C
ATOM    831  CB  LEU G 172      36.606  -9.258  16.179  1.00 20.00           C
ATOM    832  CG  LEU G 172      36.254  -9.646  14.744  1.00 20.00           C
ATOM    833  CD1 LEU G 172      36.412 -11.143  14.539  1.00 20.00           C
ATOM    834  CD2 LEU G 172      34.842  -9.201  14.414  1.00 20.00           C
ATOM    835  C   LEU G 172      36.655  -7.547  18.001  1.00 29.90           C
ATOM    836  O   LEU G 172      35.650  -7.435  18.704  1.00 41.09           O
ATOM    837  N   SER G 173      37.889  -7.498  18.490  1.00 35.08           N
ATOM    838  CA  SER G 173      38.139  -7.406  19.923  1.00 35.53           C
ATOM    839  CB  SER G 173      39.578  -7.823  20.245  1.00 20.00           C
ATOM    840  OG  SER G 173      40.515  -7.012  19.556  1.00 20.00           O
ATOM    841  C   SER G 173      37.860  -5.999  20.450  1.00 35.07           C
ATOM    842  O   SER G 173      37.581  -5.815  21.636  1.00 51.28           O
ATOM    843  N   THR G 174      37.893  -5.021  19.550  1.00 46.35           N
ATOM    844  CA  THR G 174      37.721  -3.621  19.922  1.00 43.83           C
ATOM    845  CB  THR G 174      38.341  -2.681  18.860  1.00 20.00           C
ATOM    846  OG1 THR G 174      37.702  -2.897  17.595  1.00 20.00           O
ATOM    847  CG2 THR G 174      39.839  -2.940  18.719  1.00 20.00           C
ATOM    848  C   THR G 174      36.236  -3.300  20.083  1.00 52.54           C
ATOM    849  O   THR G 174      35.448  -3.528  19.165  1.00 64.10           O
ATOM    850  N   ASN G 175      35.839  -2.919  21.295  1.00 55.57           N
ATOM    851  CA  ASN G 175      34.501  -2.371  21.528  1.00 40.58           C
ATOM    852  CB  ASN G 175      34.109  -2.499  23.005  1.00 20.00           C
ATOM    853  CG  ASN G 175      33.819  -3.933  23.416  1.00 20.00           C
ATOM    854  OD1 ASN G 175      33.530  -4.786  22.578  1.00 20.00           O
ATOM    855  ND2 ASN G 175      33.845  -4.190  24.720  1.00 20.00           N
ATOM    856  C   ASN G 175      34.404  -0.909  21.089  1.00 43.65           C
ATOM    857  O   ASN G 175      35.035  -0.032  21.682  1.00 53.11           O
ATOM    858  N   LYS G 176      33.694  -0.671  19.990  1.00 44.89           N
ATOM    859  CA  LYS G 176      33.519   0.680  19.463  1.00 46.42           C
ATOM    860  CB  LYS G 176      34.847   1.244  18.945  1.00 20.00           C
ATOM    861  CG  LYS G 176      35.789   1.756  20.031  1.00 20.00           C
ATOM    862  CD  LYS G 176      37.220   1.872  19.511  1.00 20.00           C
ATOM    863  CE  LYS G 176      38.243   1.433  20.560  1.00 20.00           C
ATOM    864  NZ  LYS G 176      39.542   1.012  19.953  1.00 20.00           N
ATOM    865  C   LYS G 176      32.478   0.701  18.352  1.00 45.00           C
ATOM    866  O   LYS G 176      32.405  -0.217  17.534  1.00 60.64           O
ATOM    867  N   ALA G 177      31.674   1.756  18.330  1.00 46.01           N
ATOM    868  CA  ALA G 177      30.717   1.962  17.257  1.00 43.65           C
ATOM    869  CB  ALA G 177      29.708   3.027  17.652  1.00 20.00           C
ATOM    870  C   ALA G 177      31.437   2.359  15.977  1.00 41.42           C
ATOM    871  O   ALA G 177      31.168   1.813  14.907  1.00 45.37           O
ATOM    872  N   VAL G 178      32.360   3.308  16.097  1.00 35.70           N
ATOM    873  CA  VAL G 178      33.228   3.683  14.987  1.00 43.93           C
ATOM    874  CB  VAL G 178      32.876   5.083  14.432  1.00 20.00           C
ATOM    875  CGI VAL G 178      33.896   5.516  13.379  1.00 20.00           C
ATOM    876  CG2 VAL G 178      31.463   5.090  13.860  1.00 20.00           C
```

ATOM 877 C VAL G 178 34.685 3.676 15.427 1.00 34.16 C
ATOM 878 O VAL G 178 35.005 4.063 16.550 1.00 44.45 O
ATOM 879 N VAL G 179 35.560 3.200 14.550 1.00 44.87 N
ATOM 880 CA VAL G 179 36.972 3.080 14.884 1.00 38.47 C
ATOM 881 CB VAL G 179 37.255 1.806 15.696 1.00 20.00 C
ATOM 882 CGI VAL G 179 38.742 1.679 15.986 1.00 20.00 C
ATOM 883 CG2 VAL G 179 36.457 1.817 16.984 1.00 20.00 C
ATOM 884 C VAL G 179 37.855 3.091 13.643 1.00 44.79 C
ATOM 885 O VAL G 179 37.560 2.423 12.650 1.00 51.88 O
ATOM 886 N SER G 180 38.955 3.835 13.719 1.00 45.23 N
ATOM 887 CA SER G 180 39.937 3.871 12.643 1.00 48.99 C
ATOM 888 CB SER G 180 40.875 5.069 12.812 1.00 20.00 C
ATOM 889 OG SER G 180 41.649 4.948 13.993 1.00 20.00 O
ATOM 890 C SER G 180 40.740 2.577 12.610 1.00 48.15 C
ATOM 891 O SER G 180 41.386 2.212 13.594 1.00 60.42 O
ATOM 892 N LEU G 181 40.594 1.827 11.521 1.00 42.42 N
ATOM 893 CA LEU G 181 41.389 0.622 11.302 1.00 43.22 C
ATOM 894 CB LEU G 181 40.818 -0.190 10.139 1.00 20.00 C
ATOM 895 CG LEU G 181 39.415 -0.753 10.350 1.00 20.00 C
ATOM 896 CD1 LEU G 181 38.958 -1.514 9.118 1.00 20.00 C
ATOM 897 CD2 LEU G 181 39.394 -1.643 11.577 1.00 20.00 C
ATOM 898 C LEU G 181 42.838 0.984 11.011 1.00 29.14 C
ATOM 899 O LEU G 181 43.144 1.559 9.967 1.00 43.42 O
ATOM 900 N SER G 182 43.721 0.695 11.960 1.00 41.83 N
ATOM 901 CA SER G 182 45.089 1.186 11.883 1.00 53.52 C
ATOM 902 CB SER G 182 45.421 2.069 13.086 1.00 20.00 C
ATOM 903 OG SER G 182 45.500 1.303 14.275 1.00 20.00 O
ATOM 904 C SER G 182 46.110 0.063 11.741 1.00 44.76 C
ATOM 905 O SER G 182 45.995 -0.984 12.379 1.00 37.73 O
ATOM 906 N ASN G 183 47.028 0.245 10.799 1.00 47.84 N
ATOM 907 CA ASN G 183 48.262 -0.525 10.744 1.00 59.45 C
ATOM 908 CB ASN G 183 48.350 -1.276 9.412 1.00 20.00 C
ATOM 909 CG ASN G 183 47.312 -2.375 9.290 1.00 20.00 C
ATOM 910 OD1 ASN G 183 46.897 -2.964 10.287 1.00 20.00 O
ATOM 911 ND2 ASN G 183 46.954 -2.715 8.057 1.00 20.00 N
ATOM 912 C ASN G 183 49.445 0.428 10.872 1.00 75.41 C
ATOM 913 O ASN G 183 49.386 1.559 10.391 1.00102.31 O
ATOM 914 N GLY G 184 50.463 0.021 11.624 1.00 79.30 N
ATOM 915 CA GLY G 184 51.584 0.906 11.931 1.00 88.92 C
ATOM 916 C GLY G 184 51.464 2.278 11.287 1.00101.85 C
ATOM 917 O GLY G 184 51.911 2.485 10.158 1.001 13.48 O
ATOM 918 N VAL G 185 50.833 3.209 11.999 1.00 86.84 N
ATOM 919 CA VAL G 185 50.888 4.635 11.665 1.00 81.80 C
ATOM 920 CB VAL G 185 52.336 5.149 11.526 1.00 20.00 C
ATOM 921 CGI VAL G 185 52.340 6.607 11.085 1.00 20.00 C
ATOM 922 CG2 VAL G 185 53.086 4.984 12.838 1.00 20.00 C
ATOM 923 C VAL G 185 50.097 5.027 10.417 1.00 81.69 C
ATOM 924 O VAL G 185 50.205 6.157 9.942 1.00 99.84 O
ATOM 925 N SER G 186 49.286 4.109 9.902 1.00 70.63 N
ATOM 926 CA SER G 186 48.501 4.392 8.705 1.00 72.29 C
ATOM 927 CB SER G 186 49.173 3.803 7.463 1.00 20.00 C
ATOM 928 OG SER G 186 49.228 2.389 7.534 1.00 20.00 O
ATOM 929 C SER G 186 47.066 3.893 8.820 1.00 62.99 C
ATOM 930 O SER G 186 46.820 2.769 9.258 1.00 58.35 O
ATOM 931 N VAL G 187 46.122 4.736 8.415 1.00 66.49 N
ATOM 932 CA VAL G 187 44.709 4.389 8.471 1.00 57.36 C
ATOM 933 CB VAL G 187 43.834 5.635 8.704 1.00 20.00 C
ATOM 934 CGI VAL G 187 42.371 5.248 8.769 1.00 20.00 C
ATOM 935 CG2 VAL G 187 44.254 6.346 9.982 1.00 20.00 C
ATOM 936 C VAL G 187 44.266 3.684 7.191 1.00 53.67 C

```
ATOM    937  O   VAL G 187      44.408   4.222   6.093  1.00 50.10           O
ATOM    938  N   LEU G 188      43.768   2.460   7.338  1.00 43.20           N
ATOM    939  CA  LEU G 188      43.289   1.678   6.201  1.00 41.76           C
ATOM    940  CB  LEU G 188      43.404   0.183   6.495  1.00 20.00           C
ATOM    941  CG  LEU G 188      44.821  -0.375   6.633  1.00 20.00           C
ATOM    942  CD1 LEU G 188      44.777  -1.845   7.014  1.00 20.00           C
ATOM    943  CD2 LEU G 188      45.605  -0.174   5.345  1.00 20.00           C
ATOM    944  C   LEU G 188      41.843   2.021   5.862  1.00 44.75           C
ATOM    945  O   LEU G 188      41.384   1.777   4.746  1.00 45.28           O
ATOM    946  N   THR G 189      41.111   2.500   6.863  1.00 39.28           N
ATOM    947  CA  THR G 189      39.710   2.863   6.694  1.00 36.51           C
ATOM    948  CB  THR G 189      38.985   1.880   5.760  1.00 20.00           C
ATOM    949  OG1 THR G 189      38.871   0.604   6.400  1.00 20.00           O
ATOM    950  CG2 THR G 189      39.759   1.715   4.458  1.00 20.00           C
ATOM    951  C   THR G 189      39.006   2.891   8.046  1.00 45.83           C
ATOM    952  O   THR G 189      39.637   3.112   9.079  1.00 42.57           O
ATOM    953  N   SER G 190      37.692   2.695   8.033  1.00 40.44           N
ATOM    954  CA  SER G 190      36.902   2.779   9.255  1.00 41.82           C
ATOM    955  CB  SER G 190      35.919   3.953   9.188  1.00 20.00           C
ATOM    956  OG  SER G 190      34.930   3.737   8.196  1.00 20.00           O
ATOM    957  C   SER G 190      36.153   1.479   9.527  1.00 33.81           C
ATOM    958  O   SER G 190      35.609   0.860   8.611  1.00 49.61           O
ATOM    959  N   LYS G 191      36.134   1.069  10.791  1.00 37.37           N
ATOM    960  CA  LYS G 191      35.365  -0.097  11.208  1.00 41.23           C
ATOM    961  CB  LYS G 191      36.239  -1.047  12.027  1.00 20.00           C
ATOM    962  CG  LYS G 191      37.323  -1.731  11.216  1.00 20.00           C
ATOM    963  CD  LYS G 191      38.193  -2.623  12.085  1.00 20.00           C
ATOM    964  CE  LYS G 191      39.313  -3.257  11.267  1.00 20.00           C
ATOM    965  NZ  LYS G 191      40.316  -3.959  12.119  1.00 20.00           N
ATOM    966  C   LYS G 191      34.143   0.315  12.018  1.00 35.03           C
ATOM    967  O   LYS G 191      34.267   0.958  13.059  1.00 40.06           O
ATOM    968  N   VAL G 192      32.966  -0.093  11.555  1.00 33.70           N
ATOM    969  CA  VAL G 192      31.712   0.327  12.171  1.00 27.61           C
ATOM    970  CB  VAL G 192      30.816   1.081  11.173  1.00 20.00           C
ATOM    971  CGI VAL G 192      29.505   1.481  11.832  1.00 20.00           C
ATOM    972  CG2 VAL G 192      31.540   2.293  10.617  1.00 20.00           C
ATOM    973  C   VAL G 192      30.929  -0.857  12.723  1.00 31.74           C
ATOM    974  O   VAL G 192      30.965  -1.954  12.167  1.00 25.58           O
ATOM    975  N   LEU G 193      30.177  -0.610  13.790  1.00 28.88           N
ATOM    976  CA  LEU G 193      29.272  -1.609  14.342  1.00 34.36           C
ATOM    977  CB  LEU G 193      29.940  -2.349  15.504  1.00 20.00           C
ATOM    978  CG  LEU G 193      31.127  -3.249  15.156  1.00 20.00           C
ATOM    979  CD1 LEU G 193      31.818  -3.743  16.418  1.00 20.00           C
ATOM    980  CD2 LEU G 193      30.677  -4.419  14.295  1.00 20.00           C
ATOM    981  C   LEU G 193      27.982  -0.950  14.818  1.00 33.03           C
ATOM    982  O   LEU G 193      27.963  -0.290  15.856  1.00 44.93           O
ATOM    983  N   ASP G 194      26.896  -1.170  14.081  1.00 35.09           N
ATOM    984  CA  ASP G 194      25.724  -0.298  14.150  1.00 41.39           C
ATOM    985  CB  ASP G 194      24.766  -0.589  12.995  1.00 20.00           C
ATOM    986  CG  ASP G 194      25.292  -0.090  11.667  1.00 20.00           C
ATOM    987  OD1 ASP G 194      26.173   0.795  11.668  1.00 20.00           O
ATOM    988  OD2 ASP G 194      24.863  -0.620  10.621  1.00 20.00           O
ATOM    989  C   ASP G 194      24.976  -0.377  15.479  1.00 38.04           C
ATOM    990  O   ASP G 194      24.097   0.442  15.752  1.00 48.03           O
ATOM    991  N   LEU G 195      25.259  -1.410  16.263  1.00 43.64           N
ATOM    992  CA  LEU G 195      24.463  -1.682  17.449  1.00 35.97           C
ATOM    993  CB  LEU G 195      23.832  -3.071  17.366  1.00 20.00           C
ATOM    994  CG  LEU G 195      22.988  -3.340  16.117  1.00 20.00           C
ATOM    995  CD1 LEU G 195      22.479  -4.773  16.112  1.00 20.00           C
ATOM    996  CD2 LEU G 195      21.847  -2.340  15.969  1.00 20.00           C
```

```
ATOM    997  C   LEU G 195      25.254  -1.525  18.744  1.00 43.63           C
ATOM    998  O   LEU G 195      24.675  -1.495  19.830  1.00 34.71           O
ATOM    999  N   ASN G 196      26.558  -1.299  18.617  1.00 44.30           N
ATOM   1000  CA  ASN G 196      27.458  -1.365  19.765  1.00 42.38           C
ATOM   1001  CB  ASN G 196      28.900  -1.082  19.342  1.00 20.00           C
ATOM   1002  CG  ASN G 196      29.508  -2.223  18.551  1.00 20.00           C
ATOM   1003  OD1 ASN G 196      29.101  -3.377  18.688  1.00 20.00           O
ATOM   1004  ND2 ASN G 196      30.503  -1.908  17.731  1.00 20.00           N
ATOM   1005  C   ASN G 196      27.041  -0.434  20.900  1.00 43.66           C
ATOM   1006  O   ASN G 196      26.944  -0.855  22.053  1.00 33.62           O
ATOM   1007  N   ASN G 197      26.706   0.806  20.560  1.00 34.31           N
ATOM   1008  CA  ASN G 197      26.346   1.793  21.570  1.00 38.83           C
ATOM   1009  CB  ASN G 197      26.089   3.153  20.926  1.00 20.00           C
ATOM   1010  CG  ASN G 197      27.362   3.819  20.456  1.00 20.00           C
ATOM   1011  OD1 ASN G 197      28.459   3.458  20.880  1.00 20.00           O
ATOM   1012  ND2 ASN G 197      27.228   4.768  19.541  1.00 20.00           N
ATOM   1013  C   ASN G 197      25.139   1.365  22.392  1.00 39.90           C
ATOM   1014  O   ASN G 197      25.185   1.357  23.621  1.00 39.04           O
ATOM   1015  N   TYR G 198      24.065   0.992  21.705  1.00 35.09           N
ATOM   1016  CA  TYR G 198      22.875   0.482  22.373  1.00 41.03           C
ATOM   1017  CB  TYR G 198      21.804   0.093  21.352  1.00 20.00           C
ATOM   1018  CG  TYR G 198      21.274   1.257  20.549  1.00 20.00           C
ATOM   1019  CD1 TYR G 198      20.238   2.041  21.031  1.00 20.00           C
ATOM   1020  CE1 TYR G 198      19.753   3.105  20.299  1.00 20.00           C
ATOM   1021  CZ  TYR G 198      20.310   3.398  19.069  1.00 20.00           C
ATOM   1022  OH  TYR G 198      19.829   4.450  18.325  1.00 20.00           O
ATOM   1023  CE2 TYR G 198      21.321   2.616  18.559  1.00 20.00           C
ATOM   1024  CD2 TYR G 198      21.799   1.557  19.299  1.00 20.00           C
ATOM   1025  C   TYR G 198      23.219  -0.712  23.252  1.00 43.65           C
ATOM   1026  O   TYR G 198      22.800  -0.783  24.406  1.00 52.37           O
ATOM   1027  N   ILE G 199      24.079  -1.587  22.744  1.00 35.86           N
ATOM   1028  CA  ILE G 199      24.490  -2.772  23.486  1.00 45.39           C
ATOM   1029  CB  ILE G 199      25.380  -3.704  22.627  1.00 20.00           C
ATOM   1030  CGI ILE G 199      24.556  -4.357  21.512  1.00 20.00           C
ATOM   1031  CD1 ILE G 199      25.365  -5.260  20.598  1.00 20.00           C
ATOM   1032  CG2 ILE G 199      26.037  -4.775  23.487  1.00 20.00           C
ATOM   1033  C   ILE G 199      25.210  -2.392  24.779  1.00 37.89           C
ATOM   1034  O   ILE G 199      24.808  -2.808  25.865  1.00 45.28           O
ATOM   1035  N   ASP G 200      26.185  -1.495  24.669  1.00 37.36           N
ATOM   1036  CA  ASP G 200      26.988  -1.098  25.821  1.00 46.66           C
ATOM   1037  CB  ASP G 200      28.069  -0.096  25.405  1.00 20.00           C
ATOM   1038  CG  ASP G 200      29.216  -0.751  24.660  1.00 20.00           C
ATOM   1039  OD1 ASP G 200      29.360  -1.989  24.751  1.00 20.00           O
ATOM   1040  OD2 ASP G 200      29.996  -0.025  24.009  1.00 20.00           O
ATOM   1041  C   ASP G 200      26.109  -0.506  26.916  1.00 51.05           C
ATOM   1042  O   ASP G 200      26.370  -0.693  28.105  1.00 57.39           O
ATOM   1043  N   LYS G 201      25.004   0.108  26.507  1.00 57.68           N
ATOM   1044  CA  LYS G 201      24.104   0.766  27.443  1.00 44.02           C
ATOM   1045  CB  LYS G 201      23.138   1.687  26.698  1.00 20.00           C
ATOM   1046  CG  LYS G 201      23.815   2.816  25.941  1.00 20.00           C
ATOM   1047  CD  LYS G 201      22.797   3.680  25.223  1.00 20.00           C
ATOM   1048  CE  LYS G 201      23.464   4.802  24.446  1.00 20.00           C
ATOM   1049  NZ  LYS G 201      22.489   5.542  23.596  1.00 20.00           N
ATOM   1050  C   LYS G 201      23.325  -0.250  28.274  1.00 43.56           C
ATOM   1051  O   LYS G 201      22.868   0.060  29.374  1.00 51.34           O
ATOM   1052  N   GLN G 202      23.218  -1.475  27.764  1.00 46.06           N
ATOM   1053  CA  GLN G 202      22.308  -2.472  28.333  1.00 44.95           C
ATOM   1054  CB  GLN G 202      21.324  -2.975  27.277  1.00 20.00           C
ATOM   1055  CG  GLN G 202      20.207  -1.997  26.966  1.00 20.00           C
ATOM   1056  CD  GLN G 202      19.339  -2.450  25.809  1.00 20.00           C
```

```
ATOM   1057  OE1 GLN G 202      19.694  -3.372  25.074   1.00 20.00           O
ATOM   1058  NE2 GLN G 202      18.171  -1.835  25.672   1.00 20.00           N
ATOM   1059  C   GLN G 202      23.029  -3.657  28.974   1.00 42.35           C
ATOM   1060  O   GLN G 202      22.446  -4.374  29.787   1.00 47.00           O
ATOM   1061  N   LEU G 203      24.253  -3.922  28.530   1.00 49.55           N
ATOM   1062  CA  LEU G 203      25.003  -5.081  29.008   1.00 50.77           C
ATOM   1063  CB  LEU G 203      26.244  -5.322  28.140   1.00 20.00           C
ATOM   1064  CG  LEU G 203      26.031  -5.802  26.698   1.00 20.00           C
ATOM   1065  CD1 LEU G 203      27.361  -5.942  25.970   1.00 20.00           C
ATOM   1066  CD2 LEU G 203      25.263  -7.115  26.661   1.00 20.00           C
ATOM   1067  C   LEU G 203      25.397  -4.938  30.479   1.00 52.51           C
ATOM   1068  O   LEU G 203      25.830  -3.873  30.918   1.00 46.02           O
ATOM   1069  N   LEU G 204      25.226  -6.017  31.238   1.00 51.45           N
ATOM   1070  CA  LEU G 204      25.644  -6.053  32.635   1.00 58.44           C
ATOM   1071  CB  LEU G 204      24.863  -7.127  33.399   1.00 20.00           C
ATOM   1072  CG  LEU G 204      23.352  -6.918  33.522   1.00 20.00           C
ATOM   1073  CD1 LEU G 204      22.691  -8.136  34.147   1.00 20.00           C
ATOM   1074  CD2 LEU G 204      23.044  -5.665  34.328   1.00 20.00           C
ATOM   1075  C   LEU G 204      27.146  -6.307  32.759   1.00 54.99           C
ATOM   1076  O   LEU G 204      27.710  -7.096  31.998   1.00 55.13           O
ATOM   1077  N   PRO G 205      27.783  -5.693  33.770   1.00 58.64           N
ATOM   1078  CA  PRO G 205      29.236  -5.775  33.842   1.00 52.19           C
ATOM   1079  CB  PRO G 205      29.551  -5.040  35.142   1.00 20.00           C
ATOM   1080  CG  PRO G 205      28.379  -5.337  36.014   1.00 20.00           C
ATOM   1081  CD  PRO G 205      27.182  -5.464  35.099   1.00 20.00           C
ATOM   1082  C   PRO G 205      29.647  -7.230  33.970   1.00 54.30           C
ATOM   1083  O   PRO G 205      30.783  -7.593  33.663   1.00 70.22           O
ATOM   1084  N   ILE G 206      28.709  -8.050  34.430   1.00 62.70           N
ATOM   1085  CA  ILE G 206      28.925  -9.480  34.557   1.00 68.19           C
ATOM   1086  CB  ILE G 206      29.450  -9.843  35.957   1.00 20.00           C
ATOM   1087  CGI ILE G 206      30.853  -9.269  36.164   1.00 20.00           C
ATOM   1088  CD1 ILE G 206      31.328  -9.317  37.600   1.00 20.00           C
ATOM   1089  CG2 ILE G 206      29.454  -11.352  36.151   1.00 20.00           C
ATOM   1090  C   ILE G 206      27.618 -10.223  34.304   1.00 62.35           C
ATOM   1091  O   ILE G 206      26.548  -9.772  34.715   1.00 67.16           O
ATOM   1092  N   VAL G 207      27.702 -11.314  33.552   1.00 52.22           N
ATOM   1093  CA  VAL G 207      26.527 -12.112  33.234   1.00 51.31           C
ATOM   1094  CB  VAL G 207      26.414 -12.378  31.722   1.00 20.00           C
ATOM   1095  CGI VAL G 207      25.235 -13.293  31.430   1.00 20.00           C
ATOM   1096  CG2 VAL G 207      26.279 -11.066  30.963   1.00 20.00           C
ATOM   1097  C   VAL G 207      26.546 -13.438  33.985   1.00 62.09           C
ATOM   1098  O   VAL G 207      27.257 -14.369  33.605   1.00 58.88           O
ATOM   1099  N   ASN G 208      25.828 -13.484  35.102   1.00 71.72           N
ATOM   1100  CA  ASN G 208      25.723 -14.698  35.900   1.00 70.92           C
ATOM   1101  CB  ASN G 208      25.837 -14.370  37.390   1.00 20.00           C
ATOM   1102  CG  ASN G 208      27.235 -13.938  37.787   1.00 20.00           C
ATOM   1103  OD1 ASN G 208      28.216 -14.286  37.129   1.00 20.00           O
ATOM   1104  ND2 ASN G 208      27.335 -13.190  38.880   1.00 20.00           N
ATOM   1105  C   ASN G 208      24.423 -15.446  35.628   1.00 63.05           C
ATOM   1106  O   ASN G 208      23.637 -15.050  34.767   1.00 61.34           O
ATOM   1107  N   LYS G 209      24.168 -16.485  36.418   1.00 68.91           N
ATOM   1108  CA  LYS G 209      23.006 -17.341  36.212   1.00 59.11           C
ATOM   1109  CB  LYS G 209      23.129 -18.620  37.043   1.00 20.00           C
ATOM   1110  CG  LYS G 209      24.239 -19.552  36.588   1.00 20.00           C
ATOM   1111  CD  LYS G 209      24.335 -20.774  37.486   1.00 20.00           C
ATOM   1112  CE  LYS G 209      25.423 -21.724  37.012   1.00 20.00           C
ATOM   1113  NZ  LYS G 209      25.548 -22.912  37.901   1.00 20.00           N
ATOM   1114  C   LYS G 209      21.696 -16.628  36.539   1.00 50.69           C
ATOM   1115  O   LYS G 209      20.616 -17.121  36.212   1.00 51.01           O
ATOM   1116  N   GLN G 210      21.792 -15.499  37.235   1.00 44.68           N
```

```
ATOM   1117  CA  GLN G 210      20.621 -14.676  37.518  1.00 49.52           C
ATOM   1118  CB  GLN G 210      20.828 -13.874  38.806  1.00 20.00           C
ATOM   1119  CG  GLN G 210      20.877 -14.719  40.070  1.00 20.00           C
ATOM   1120  CD  GLN G 210      21.149 -13.893  41.313  1.00 20.00           C
ATOM   1121  OE1 GLN G 210      21.709 -12.800  41.237  1.00 20.00           O
ATOM   1122  NE2 GLN G 210      20.755 -14.417  42.469  1.00 20.00           N
ATOM   1123  C   GLN G 210      20.336 -13.730  36.356  1.00 62.08           C
ATOM   1124  O   GLN G 210      19.271 -13.785  35.741  1.00 80.43           O
ATOM   1125  N   SER G 211      21.324 -12.905  36.028  1.00 58.92           N
ATOM   1126  CA  SER G 211      21.231 -11.987  34.898  1.00 47.88           C
ATOM   1127  CB  SER G 211      22.594 -11.350  34.621  1.00 20.00           C
ATOM   1128  OG  SER G 211      23.553 -12.334  34.274  1.00 20.00           O
ATOM   1129  C   SER G 211      20.722 -12.689  33.642  1.00 57.32           C
ATOM   1130  O   SER G 211      19.919 -12.133  32.893  1.00 50.74           O
ATOM   1131  N   CYS G 212      21.149 -13.934  33.451  1.00 44.34           N
ATOM   1132  CA  CYS G 212      20.890 -14.659  32.210  1.00 57.52           C
ATOM   1133  CB  CYS G 212      21.127 -16.180  32.363  1.00 20.00           C
ATOM   1134  SG  CYS G 212      22.836 -16.682  32.889  1.00 20.00           S
ATOM   1135  C   CYS G 212      19.541 -14.314  31.540  1.00 60.91           C
ATOM   1136  O   CYS G 212      19.536 -13.729  30.460  1.00 52.17           O
ATOM   1137  N   SER G 213      18.465 -14.813  32.151  1.00 21.55           N
ATOM   1138  CA  SER G 213      17.107 -14.631  31.656  1.00 21.67           C
ATOM   1139  CB  SER G 213      16.133 -15.512  32.444  1.00 21.81           C
ATOM   1140  OG  SER G 213      16.471 -16.882  32.323  1.00 23.00           O
ATOM   1141  C   SER G 213      16.633 -13.188  31.682  1.00 21.45           C
ATOM   1142  O   SER G 213      16.026 -12.728  30.722  1.00 21.98           O
ATOM   1143  N   ILE G 214      16.856 -12.475  32.783  1.00 20.90           N
ATOM   1144  CA  ILE G 214      16.585 -11.050  32.758  1.00 20.45           C
ATOM   1145  CB  ILE G 214      16.587 -10.444  34.170  1.00 20.53           C
ATOM   1146  CGI ILE G 214      15.498 -11.091  35.029  1.00 20.46           C
ATOM   1147  CD1 ILE G 214      15.418 -10.535  36.434  1.00 21.75           C
ATOM   1148  CG2 ILE G 214      16.393  -8.937  34.103  1.00 20.34           C
ATOM   1149  C   ILE G 214      17.686 -10.409  31.926  1.00 20.15           C
ATOM   1150  O   ILE G 214      17.435  -9.671  30.968  1.00 19.91           O
ATOM   1151  N   SER G 215      18.918 -10.770  32.280  1.00 19.84           N
ATOM   1152  CA  SER G 215      20.109 -10.297  31.594  1.00 19.58           C
ATOM   1153  CB  SER G 215      21.369 -10.722  32.349  1.00 19.76           C
ATOM   1154  OG  SER G 215      22.538 -10.269  31.688  1.00 19.97           O
ATOM   1155  C   SER G 215      20.132 -10.852  30.189  1.00 19.34           C
ATOM   1156  O   SER G 215      20.448 -10.152  29.230  1.00 19.54           O
ATOM   1157  N   ASN G 216      19.774 -12.125  30.082  1.00 18.80           N
ATOM   1158  CA  ASN G 216      19.738 -12.791  28.798  1.00 18.36           C
ATOM   1159  CB  ASN G 216      19.394 -14.271  28.966  1.00 18.41           C
ATOM   1160  CG  ASN G 216      20.426 -15.020  29.786  1.00 19.55           C
ATOM   1161  OD1 ASN G 216      20.308 -16.227  30.000  1.00 20.52           O
ATOM   1162  ND2 ASN G 216      21.445 -14.306  30.250  1.00 20.43           N
ATOM   1163  C   ASN G 216      18.708 -12.107  27.927  1.00 17.78           C
ATOM   1164  O   ASN G 216      18.930 -11.905  26.744  1.00 17.91           O
ATOM   1165  N   ILE G 217      17.578 -11.750  28.527  1.00 17.02           N
ATOM   1166  CA  ILE G 217      16.502 -11.089  27.804  1.00 16.60           C
ATOM   1167  CB  ILE G 217      15.247 -10.916  28.680  1.00 16.46           C
ATOM   1168  CGI ILE G 217      14.608 -12.275  28.969  1.00 16.26           C
ATOM   1169  CD1 ILE G 217      13.360 -12.195  29.822  1.00 16.44           C
ATOM   1170  CG2 ILE G 217      14.251  -9.987  28.005  1.00 16.70           C
ATOM   1171  C   ILE G 217      16.953  -9.731  27.297  1.00 16.73           C
ATOM   1172  O   ILE G 217      16.658  -9.355  26.166  1.00 16.80           O
ATOM   1173  N   GLU G 218      17.679  -9.000  28.137  1.00 17.02           N
ATOM   1174  CA  GLU G 218      18.177  -7.692  27.741  1.00 17.70           C
ATOM   1175  CB  GLU G 218      18.867  -6.998  28.916  1.00 18.20           C
ATOM   1176  CG  GLU G 218      17.955  -6.748  30.106  1.00 21.31           C
```

```
ATOM   1177  CD  GLU G 218      18.652  -6.004  31.228  1.00 25.72           C
ATOM   1178  OE1 GLU G 218      18.016  -5.781  32.279  1.00 26.96           O
ATOM   1179  OE2 GLU G 218      19.834  -5.640  31.058  1.00 27.07           O
ATOM   1180  C   GLU G 218      19.144  -7.855  26.578  1.00 17.29           C
ATOM   1181  O   GLU G 218      19.123  -7.081  25.617  1.00 17.62           O
ATOM   1182  N   THR G 219      19.983  -8.882  26.667  1.00 16.62           N
ATOM   1183  CA  THR G 219      20.964  -9.150  25.630  1.00 15.95           C
ATOM   1184  CB  THR G 219      21.879 -10.328  26.007  1.00 15.95           C
ATOM   1185  OG1 THR G 219      22.582 -10.021  27.218  1.00 15.63           O
ATOM   1186  CG2 THR G 219      22.884 -10.597  24.897  1.00 15.97           C
ATOM   1187  C   THR G 219      20.250  -9.470  24.330  1.00 15.64           C
ATOM   1188  O   THR G 219      20.656  -9.022  23.267  1.00 15.93           O
ATOM   1189  N   VAL G 220      19.179 -10.248  24.431  1.00 14.98           N
ATOM   1190  CA  VAL G 220      18.390 -10.644  23.278  1.00 14.51           C
ATOM   1191  CB  VAL G 220      17.285 -11.644  23.665  1.00 14.29           C
ATOM   1192  CGI VAL G 220      16.474 -12.037  22.440  1.00 14.24           C
ATOM   1193  CG2 VAL G 220      17.890 -12.871  24.329  1.00 14.10           C
ATOM   1194  C   VAL G 220      17.759  -9.424  22.636  1.00 14.64           C
ATOM   1195  O   VAL G 220      17.718  -9.315  21.420  1.00 14.79           O
ATOM   1196  N   ILE G 221      17.264  -8.510  23.463  1.00 14.43           N
ATOM   1197  CA  ILE G 221      16.658  -7.287  22.959  1.00 14.36           C
ATOM   1198  CB  ILE G 221      16.046  -6.448  24.095  1.00 14.03           C
ATOM   1199  CGI ILE G 221      14.955  -7.243  24.816  1.00 13.72           C
ATOM   1200  CD1 ILE G 221      13.820  -7.679  23.914  1.00 14.17           C
ATOM   1201  CG2 ILE G 221      15.487  -5.142  23.550  1.00 13.91           C
ATOM   1202  C   ILE G 221      17.700  -6.459  22.222  1.00 14.82           C
ATOM   1203  O   ILE G 221      17.427  -5.902  21.158  1.00 14.82           O
ATOM   1204  N   GLU G 222      18.901  -6.390  22.788  1.00 15.51           N
ATOM   1205  CA  GLU G 222      19.983  -5.640  22.165  1.00 16.52           C
ATOM   1206  CB  GLU G 222      21.211  -5.601  23.076  1.00 16.80           C
ATOM   1207  CG  GLU G 222      20.971  -4.899  24.403  1.00 19.14           C
ATOM   1208  CD  GLU G 222      22.231  -4.780  25.236  1.00 22.62           C
ATOM   1209  OE1 GLU G 222      22.152  -4.246  26.362  1.00 24.35           O
ATOM   1210  OE2 GLU G 222      23.301  -5.219  24.765  1.00 23.98           O
ATOM   1211  C   GLU G 222      20.335  -6.269  20.825  1.00 16.65           C
ATOM   1212  O   GLU G 222      20.599  -5.574  19.842  1.00 16.95           O
ATOM   1213  N   PHE G 223      20.339  -7.597  20.802  1.00 16.70           N
ATOM   1214  CA  PHE G 223      20.652  -8.350  19.603  1.00 16.95           C
ATOM   1215  CB  PHE G 223      20.705  -9.848  19.904  1.00 16.85           C
ATOM   1216  CG  PHE G 223      21.104 -10.689  18.724  1.00 17.23           C
ATOM   1217  CD1 PHE G 223      22.438 -10.954  18.465  1.00 17.98           C
ATOM   1218  CE1 PHE G 223      22.808 -11.727  17.381  1.00 18.28           C
ATOM   1219  CZ  PHE G 223      21.842 -12.243  16.541  1.00 18.19           C
ATOM   1220  CE2 PHE G 223      20.508 -11.986  16.788  1.00 18.14           C
ATOM   1221  CD2 PHE G 223      20.144 -11.213  17.874  1.00 17.75           C
ATOM   1222  C   PHE G 223      19.610  -8.066  18.540  1.00 17.28           C
ATOM   1223  O   PHE G 223      19.945  -7.907  17.382  1.00 17.17           O
ATOM   1224  N   GLN G 224      18.348  -8.003  18.948  1.00 17.62           N
ATOM   1225  CA  GLN G 224      17.243  -7.712  18.044  1.00 18.16           C
ATOM   1226  CB  GLN G 224      15.898  -7.868  18.757  1.00 18.51           C
ATOM   1227  CG  GLN G 224      15.586  -9.296  19.178  1.00 20.06           C
ATOM   1228  CD  GLN G 224      14.158  -9.465  19.658  1.00 22.03           C
ATOM   1229  OE1 GLN G 224      13.769 -10.539  20.117  1.00 22.15           O
ATOM   1230  NE2 GLN G 224      13.368  -8.403  19.552  1.00 22.11           N
ATOM   1231  C   GLN G 224      17.387  -6.309  17.475  1.00 18.04           C
ATOM   1232  O   GLN G 224      17.090  -6.068  16.306  1.00 18.17           O
ATOM   1233  N   GLN G 225      17.819  -5.382  18.323  1.00 17.90           N
ATOM   1234  CA  GLN G 225      18.051  -4.012  17.894  1.00 17.95           C
ATOM   1235  CB  GLN G 225      18.389  -3.120  19.090  1.00 18.13           C
ATOM   1236  CG  GLN G 225      17.267  -3.006  20.109  1.00 19.04           C
```

ATOM 1237 CD GLN G 225 17.588 -2.034 21.227 1.00 21.22 C
ATOM 1238 OE1 GLN G 225 18.661 -1.431 21.252 1.00 22.55 O
ATOM 1239 NE2 GLN G 225 16.656 -1.876 22.159 1.00 22.48 N
ATOM 1240 C GLN G 225 19.168 -3.958 16.855 1.00 17.84 C
ATOM 1241 O GLN G 225 19.061 -3.239 15.861 1.00 17.71 O
ATOM 1242 N LYS G 226 20.235 -4.724 17.077 1.00 17.95 N
ATOM 1243 CA LYS G 226 21.328 -4.762 16.112 1.00 18.00 C
ATOM 1244 CB LYS G 226 22.486 -5.613 16.634 1.00 18.21 C
ATOM 1245 CG LYS G 226 23.157 -5.048 17.875 1.00 18.50 C
ATOM 1246 CD LYS G 226 24.365 -5.878 18.279 1.00 19.87 C
ATOM 1247 CE LYS G 226 25.066 -5.278 19.487 1.00 21.36 C
ATOM 1248 NZ LYS G 226 26.270 -6.061 19.878 1.00 21.83 N
ATOM 1249 C LYS G 226 20.772 -5.345 14.826 1.00 17.84 C
ATOM 1250 O LYS G 226 21.062 -4.880 13.723 1.00 17.94 O
ATOM 1251 N ASN G 227 19.954 -6.374 15.002 1.00 17.70 N
ATOM 1252 CA ASN G 227 19.238 -7.032 13.932 1.00 17.66 C
ATOM 1253 CB ASN G 227 18.471 -8.244 14.459 1.00 17.36 C
ATOM 1254 CG ASN G 227 19.384 -9.296 15.057 1.00 17.40 C
ATOM 1255 OD1 ASN G 227 18.929 -10.350 15.502 1.00 17.84 O
ATOM 1256 ND2 ASN G 227 20.682 -9.015 15.070 1.00 17.22 N
ATOM 1257 C ASN G 227 18.287 -6.028 13.328 1.00 17.76 C
ATOM 1258 O ASN G 227 18.159 -5.956 12.106 1.00 17.92 O
ATOM 1259 N ASN G 228 17.627 -5.226 14.164 1.00 17.78 N
ATOM 1260 CA ASN G 228 16.800 -4.172 13.548 1.00 17.59 C
ATOM 1261 CB ASN G 228 15.958 -3.344 14.528 1.00 17.89 C
ATOM 1262 CG ASN G 228 15.101 -2.277 13.809 1.00 18.43 C
ATOM 1263 OD1 ASN G 228 15.506 -1.119 13.688 1.00 18.74 O
ATOM 1264 ND2 ASN G 228 13.998 -2.715 13.205 1.00 18.61 N
ATOM 1265 C ASN G 228 17.603 -3.255 12.662 1.00 17.09 C
ATOM 1266 O ASN G 228 17.657 -3.466 11.456 1.00 17.17 O
ATOM 1267 N ARG G 229 18.197 -2.211 13.224 1.00 16.33 N
ATOM 1268 CA ARG G 229 19.046 -1.400 12.381 1.00 15.76 C
ATOM 1269 CB ARG G 229 19.957 -0.486 13.184 1.00 15.70 C
ATOM 1270 CG ARG G 229 20.207 0.822 12.468 1.00 14.99 C
ATOM 1271 CD ARG G 229 21.391 1.555 13.041 1.00 15.33 C
ATOM 1272 NE ARG G 229 22.116 2.303 12.021 1.00 15.59 N
ATOM 1273 CZ ARG G 229 23.182 3.053 12.276 1.00 15.85 C
ATOM 1274 NH1 ARG G 229 23.593 3.214 13.525 1.00 16.20 N
ATOM 1275 NH2 ARG G 229 23.859 3.614 11.285 1.00 16.63 N
ATOM 1276 C ARG G 229 19.863 -2.343 11.516 1.00 15.62 C
ATOM 1277 O ARG G 229 19.671 -2.402 10.304 1.00 15.73 O
ATOM 1278 N LEU G 230 20.612 -3.225 12.168 1.00 15.46 N
ATOM 1279 CA LEU G 230 21.409 -4.212 11.454 1.00 15.22 C
ATOM 1280 CB LEU G 230 22.161 -5.113 12.432 1.00 15.08 C
ATOM 1281 CG LEU G 230 23.055 -6.187 11.808 1.00 14.70 C
ATOM 1282 CD1 LEU G 230 24.375 -5.579 11.364 1.00 15.19 C
ATOM 1283 CD2 LEU G 230 23.300 -7.324 12.791 1.00 15.46 C
ATOM 1284 C LEU G 230 20.565 -5.055 10.501 1.00 15.31 C
ATOM 1285 O LEU G 230 20.963 -5.294 9.362 1.00 15.46 O
ATOM 1286 N LEU G 231 19.444 -5.573 10.997 1.00 15.48 N
ATOM 1287 CA LEU G 231 18.581 -6.442 10.197 1.00 15.75 C
ATOM 1288 CB LEU G 231 17.308 -6.793 10.967 1.00 15.90 C
ATOM 1289 CG LEU G 231 17.482 -7.640 12.226 1.00 16.63 C
ATOM 1290 CD1 LEU G 231 16.128 -8.049 12.772 1.00 18.45 C
ATOM 1291 CD2 LEU G 231 18.348 -8.858 11.954 1.00 16.67 C
ATOM 1292 C LEU G 231 18.210 -5.785 8.872 1.00 15.76 C
ATOM 1293 O LEU G 231 18.203 -6.432 7.824 1.00 15.84 O
ATOM 1294 N GLU G 232 17.824 -4.516 8.943 1.00 15.71 N
ATOM 1295 CA GLU G 232 17.298 -3.811 7.786 1.00 15.93 C
ATOM 1296 CB GLU G 232 16.537 -2.565 8.229 1.00 16.15 C

ATOM 1297 CG GLU G 232 15.461 -2.846 9.254 1.00 18.59 C
ATOM 1298 CD GLU G 232 14.077 -2.874 8.644 1.00 21.47 C
ATOM 1299 OE1 GLU G 232 13.964 -3.077 7.415 1.00 22.14 O
ATOM 1300 OE2 GLU G 232 13.100 -2.664 9.393 1.00 23.34 O
ATOM 1301 C GLU G 232 18.399 -3.431 6.806 1.00 15.45 C
ATOM 1302 O GLU G 232 18.169 -3.373 5.601 1.00 15.95 O
ATOM 1303 N ILE G 233 19.594 -3.169 7.323 1.00 14.54 N
ATOM 1304 CA ILE G 233 20.774 -3.128 6.476 1.00 13.69 C
ATOM 1305 CB ILE G 233 22.049 -2.830 7.281 1.00 13.63 C
ATOM 1306 CGI ILE G 233 21.823 -1.640 8.211 1.00 13.58 C
ATOM 1307 CD1 ILE G 233 23.101 -0.917 8.578 1.00 13.55 C
ATOM 1308 CG2 ILE G 233 23.215 -2.543 6.348 1.00 13.88 C
ATOM 1309 C ILE G 233 20.927 -4.450 5.736 1.00 13.28 C
ATOM 1310 O ILE G 233 20.979 -4.473 4.508 1.00 13.04 O
ATOM 1311 N THR G 234 20.758 -5.546 6.469 1.00 13.18 N
ATOM 1312 CA THR G 234 21.038 -6.878 5.940 1.00 13.39 C
ATOM 1313 CB THR G 234 20.839 -7.965 7.015 1.00 13.21 C
ATOM 1314 OGl THR G 234 21.845 -7.836 8.028 1.00 13.15 O
ATOM 1315 CG2 THR G 234 20.916 -9.351 6.394 1.00 13.22 C
ATOM 1316 C THR G 234 20.146 -7.204 4.748 1.00 13.76 C
ATOM 1317 O THR G 234 20.606 -7.766 3.753 1.00 13.95 O
ATOM 1318 N ARG G 235 18.849 -6.966 4.911 1.00 14.26 N
ATOM 1319 CA ARG G 235 17.891 -7.151 3.826 1.00 14.92 C
ATOM 1320 CB ARG G 235 16.463 -6.925 4.328 1.00 15.30 C
ATOM 1321 CG ARG G 235 15.771 -5.712 3.722 1.00 16.27 C
ATOM 1322 CD ARG G 235 14.867 -5.020 4.735 1.00 18.52 C
ATOM 1323 NE ARG G 235 14.345 -5.948 5.734 1.00 17.86 N
ATOM 1324 CZ ARG G 235 13.438 -6.884 5.478 1.00 16.91 C
ATOM 1325 NHl ARG G 235 12.970 -7.035 4.248 1.00 16.59 N
ATOM 1326 NH2 ARG G 235 13.018 -7.687 6.444 1.00 16.86 N
ATOM 1327 C ARG G 235 18.192 -6.211 2.665 1.00 15.05 C
ATOM 1328 O ARG G 235 18.292 -6.640 1.517 1.00 15.15 O
ATOM 1329 N GLU G 236 18.386 -4.935 2.984 1.00 15.18 N
ATOM 1330 CA GLU G 236 18.751 -3.930 1.992 1.00 15.24 C
ATOM 1331 CB GLU G 236 19.179 -2.636 2.687 1.00 15.69 C
ATOM 1332 CG GLU G 236 18.875 -1.369 1.904 1.00 18.22 C
ATOM 1333 CD GLU G 236 19.004 -0.115 2.750 1.00 21.59 C
ATOM 1334 OE1 GLU G 236 19.395 0.937 2.199 1.00 24.41 O
ATOM 1335 OE2 GLU G 236 18.660 -0.168 3.953 1.00 21.59 O
ATOM 1336 C GLU G 236 19.870 -4.421 1.077 1.00 14.61 C
ATOM 1337 O GLU G 236 19.746 -4.377 -0.147 1.00 14.82 O
ATOM 1338 N PHE G 237 20.963 -4.883 1.675 1.00 14.05 N
ATOM 1339 CA PHE G 237 22.110 -5.358 0.907 1.00 13.84 C
ATOM 1340 CB PHE G 237 23.285 -5.682 1.836 1.00 14.04 C
ATOM 1341 CG PHE G 237 24.161 -4.500 2.143 1.00 14.84 C
ATOM 1342 CD1 PHE G 237 24.412 -4.131 3.454 1.00 15.30 C
ATOM 1343 CE1 PHE G 237 25.268 -3.087 3.743 1.00 15.15 C
ATOM 1344 CZ PHE G 237 25.871 -2.389 2.717 1.00 15.19 C
ATOM 1345 CE2 PHE G 237 25.645 -2.760 1.407 1.00 15.02 C
ATOM 1346 CD2 PHE G 237 24.796 -3.809 1.125 1.00 15.03 C
ATOM 1347 C PHE G 237 21.741 -6.586 0.078 1.00 13.51 C
ATOM 1348 O PHE G 237 22.027 -6.652 -1.117 1.00 13.43 O
ATOM 1349 N SER G 238 21.092 -7.551 0.721 1.00 13.11 N
ATOM 1350 CA SER G 238 20.669 -8.772 0.049 1.00 12.82 C
ATOM 1351 CB SER G 238 19.929 -9.688 1.021 1.00 12.86 C
ATOM 1352 OG SER G 238 20.730 -9.975 2.151 1.00 12.76 O
ATOM 1353 C SER G 238 19.770 -8.444 -1.131 1.00 12.69 C
ATOM 1354 O SER G 238 19.749 -9.165 -2.128 1.00 12.63 O
ATOM 1355 N VAL G 239 19.024 -7.352 -1.010 1.00 12.59 N
ATOM 1356 CA VAL G 239 18.143 -6.916 -2.082 1.00 12.80 C

ATOM 1357 CB VAL G 239 17.045 -5.961 -1.578 1.00 12.71 C
ATOM 1358 CGI VAL G 239 16.215 -5.451 -2.747 1.00 13.63 C
ATOM 1359 CG2 VAL G 239 16.157 -6.658 -0.562 1.00 13.57 C
ATOM 1360 C VAL G 239 18.906 -6.242 -3.214 1.00 12.94 C
ATOM 1361 O VAL G 239 18.337 -5.980 -4.273 1.00 13.10 O
ATOM 1362 N ASN G 240 20.173 -5.913 -2.981 1.00 4.15 N
ATOM 1363 CA ASN G 240 20.892 -5.047 -3.909 1.00 4.33 C
ATOM 1364 CB ASN G 240 21.377 -3.779 -3.214 1.00 4.59 C
ATOM 1365 CG ASN G 240 20.260 -2.790 -2.978 1.00 5.36 C
ATOM 1366 ODl ASN G 240 19.681 -2.263 -3.926 1.00 6.27 O
ATOM 1367 ND2 ASN G 240 19.828 -2.683 -1.727 1.00 7.15 N
ATOM 1368 C ASN G 240 22.025 -5.707 -4.689 1.00 4.19 C
ATOM 1369 O ASN G 240 22.565 -5.115 -5.625 1.00 4.19 O
ATOM 1370 N ALA G 241 22.299 -6.970 -4.382 1.00 3.93 N
ATOM 1371 CA ALA G 241 23.459 -7.657 -4.941 1.00 3.90 C
ATOM 1372 CB ALA G 241 23.179 -8.102 -6.368 1.00 3.86 C
ATOM 1373 C ALA G 241 24.702 -6.772 -4.887 1.00 4.22 C
ATOM 1374 O ALA G 241 25.347 -6.532 -5.907 1.00 4.47 O
ATOM 1375 N GLY G 242 24.955 -6.190 -3.719 1.00 4.53 N
ATOM 1376 CA GLY G 242 26.289 -5.717 -3.368 1.00 4.65 C
ATOM 1377 C GLY G 242 26.609 -4.323 -3.872 1.00 4.67 C
ATOM 1378 O GLY G 242 27.770 -3.913 -3.869 1.00 5.27 O
ATOM 1379 N VAL G 243 25.577 -3.570 -4.246 1.00 4.37 N
ATOM 1380 CA VAL G 243 25.750 -2.172 -4.646 1.00 4.32 C
ATOM 1381 CB VAL G 243 26.048 -2.039 -6.153 1.00 3.99 C
ATOM 1382 CGI VAL G 243 26.962 -0.845 -6.414 1.00 4.22 C
ATOM 1383 CG2 VAL G 243 26.649 -3.327 -6.699 1.00 3.85 C
ATOM 1384 C VAL G 243 24.510 -1.342 -4.335 1.00 4.61 C
ATOM 1385 O VAL G 243 23.394 -1.734 -4.673 1.00 4.89 O
ATOM 1386 N THR G 244 24.722 -0.145 -3.801 1.00 4.95 N
ATOM 1387 CA THR G 244 23.615 0.714 -3.408 1.00 5.71 C
ATOM 1388 CB THR G 244 23.475 0.801 -1.879 1.00 6.11 C
ATOM 1389 OGl THR G 244 24.257 -0.228 -1.260 1.00 7.17 O
ATOM 1390 CG2 THR G 244 22.028 0.651 -1.475 1.00 7.55 C
ATOM 1391 C THR G 244 23.802 2.114 -3.967 1.00 5.61 C
ATOM 1392 O THR G 244 24.927 2.590 -4.117 1.00 5.85 O
ATOM 1393 N THR G 245 22.695 2.794 -4.223 1.00 5.53 N
ATOM 1394 CA THR G 245 22.677 4.241 -4.120 1.00 5.81 C
ATOM 1395 CB THR G 245 22.461 4.903 -5.490 1.00 6.13 C
ATOM 1396 OGl THR G 245 23.555 4.575 -6.355 1.00 8.11 O
ATOM 1397 CG2 THR G 245 22.394 6.408 -5.336 1.00 6.63 C
ATOM 1398 C THR G 245 21.609 4.679 -3.126 1.00 5.73 C
ATOM 1399 O THR G 245 20.778 3.869 -2.718 1.00 5.86 O
ATOM 1400 N PRO G 246 21.521 5.993 -2.867 1.00 5.68 N
ATOM 1401 CA PRO G 246 21.893 6.537 -1.574 1.00 5.11 C
ATOM 1402 CB PRO G 246 20.537 6.719 -0.893 1.00 5.19 C
ATOM 1403 CG PRO G 246 19.582 7.023 -2.060 1.00 5.90 C
ATOM 1404 CD PRO G 246 20.305 6.660 -3.353 1.00 6.36 C
ATOM 1405 C PRO G 246 22.831 5.666 -0.743 1.00 4.85 C
ATOM 1406 O PRO G 246 22.663 4.447 -0.677 1.00 5.25 O
ATOM 1407 N VAL G 247 23.900 6.281 -0.249 1.00 4.35 N
ATOM 1408 CA VAL G 247 24.742 5.647 0.749 1.00 3.82 C
ATOM 1409 CB VAL G 247 26.177 6.196 0.717 1.00 3.52 C
ATOM 1410 CGI VAL G 247 27.082 5.352 1.597 1.00 3.62 C
ATOM 1411 CG2 VAL G 247 26.697 6.207 -0.707 1.00 3.60 C
ATOM 1412 C VAL G 247 24.134 5.824 2.131 1.00 3.69 C
ATOM 1413 O VAL G 247 24.038 6.942 2.637 1.00 3.36 O
ATOM 1414 N SER G 248 23.471 4.769 2.588 1.00 3.72 N
ATOM 1415 CA SER G 248 22.676 4.824 3.803 1.00 3.96 C
ATOM 1416 CB SER G 248 22.187 3.427 4.172 1.00 4.07 C

ATOM 1417 OG SER G 248 23.188 2.722 4.884 1.00 4.13 O
ATOM 1418 C SER G 248 23.484 5.392 4.959 1.00 4.35 C
ATOM 1419 O SER G 248 24.697 5.201 5.026 1.00 4.36 O
ATOM 1420 N THR G 249 22.776 5.880 5.972 1.00 4.53 N
ATOM 1421 CA THR G 249 23.405 6.259 7.226 1.00 4.61 C
ATOM 1422 CB THR G 249 22.408 6.945 8.175 1.00 4.70 C
ATOM 1423 OG1 THR G 249 21.562 5.959 8.778 1.00 5.42 O
ATOM 1424 CG2 THR G 249 21.553 7.945 7.412 1.00 4.88 C
ATOM 1425 C THR G 249 24.026 5.054 7.925 1.00 4.47 C
ATOM 1426 O THR G 249 24.830 5.210 8.844 1.00 4.74 O
ATOM 1427 N TYR G 250 23.694 3.855 7.454 1.00 4.32 N
ATOM 1428 CA TYR G 250 24.325 2.641 7.968 1.00 4.42 C
ATOM 1429 CB TYR G 250 23.393 1.435 7.845 1.00 4.91 C
ATOM 1430 CG TYR G 250 22.028 1.638 8.462 1.00 6.81 C
ATOM 1431 CD1 TYR G 250 20.881 1.242 7.790 1.00 8.89 C
ATOM 1432 CE1 TYR G 250 19.631 1.390 8.359 1.00 10.73 C
ATOM 1433 CZ TYR G 250 19.513 1.941 9.622 1.00 12.28 C
ATOM 1434 OH TYR G 250 18.265 2.135 10.172 1.00 12.24 O
ATOM 1435 CE2 TYR G 250 20.640 2.325 10.320 1.00 12.15 C
ATOM 1436 CD2 TYR G 250 21.890 2.148 9.749 1.00 9.81 C
ATOM 1437 C TYR G 250 25.656 2.342 7.285 1.00 4.21 C
ATOM 1438 O TYR G 250 26.539 1.730 7.886 1.00 4.20 O
ATOM 1439 N MET G 251 25.766 2.697 6.007 1.00 4.14 N
ATOM 1440 CA MET G 251 27.045 2.616 5.300 1.00 4.15 C
ATOM 1441 CB MET G 251 26.852 2.798 3.790 1.00 4.14 C
ATOM 1442 CG MET G 251 26.019 1.722 3.123 1.00 4.51 C
ATOM 1443 SD MET G 251 26.772 0.087 3.219 1.00 3.81 S
ATOM 1444 CE MET G 251 25.773 -0.814 2.036 1.00 4.55 C
ATOM 1445 C MET G 251 27.996 3.686 5.816 1.00 4.13 C
ATOM 1446 O MET G 251 29.178 3.427 6.043 1.00 4.24 O
ATOM 1447 N LEU G 252 27.495 4.913 5.886 1.00 4.23 N
ATOM 1448 CA LEU G 252 28.283 6.032 6.369 1.00 4.22 C
ATOM 1449 CB LEU G 252 28.645 6.965 5.215 1.00 4.14 C
ATOM 1450 CG LEU G 252 30.017 6.731 4.581 1.00 4.05 C
ATOM 1451 CD1 LEU G 252 30.513 7.997 3.891 1.00 5.22 C
ATOM 1452 CD2 LEU G 252 31.023 6.242 5.617 1.00 6.20 C
ATOM 1453 C LEU G 252 27.515 6.799 7.432 1.00 4.62 C
ATOM 1454 O LEU G 252 26.389 7.238 7.203 1.00 4.97 O
ATOM 1455 N THR G 253 28.127 6.949 8.600 1.00 4.90 N
ATOM 1456 CA THR G 253 27.659 7.913 9.583 1.00 5.57 C
ATOM 1457 CB THR G 253 28.420 7.769 10.903 1.00 5.55 C
ATOM 1458 OG1 THR G 253 28.440 6.390 11.293 1.00 6.43 O
ATOM 1459 CG2 THR G 253 27.757 8.598 11.988 1.00 6.28 C
ATOM 1460 C THR G 253 27.865 9.329 9.069 1.00 6.03 C
ATOM 1461 O THR G 253 28.888 9.629 8.453 1.00 6.68 O
ATOM 1462 N ASN G 254 26.974 10.230 9.460 1.00 6.39 N
ATOM 1463 CA ASN G 254 27.257 11.649 9.342 1.00 6.79 C
ATOM 1464 CB ASN G 254 26.292 12.459 10.198 1.00 6.85 C
ATOM 1465 CG ASN G 254 26.317 13.927 9.853 1.00 6.81 C
ATOM 1466 OD1 ASN G 254 25.991 14.303 8.728 1.00 7.67 O
ATOM 1467 ND2 ASN G 254 26.919 14.726 10.726 1.00 6.19 N
ATOM 1468 C ASN G 254 28.685 11.958 9.760 1.00 7.08 C
ATOM 1469 O ASN G 254 29.495 12.426 8.961 1.00 6.90 O
ATOM 1470 N SER G 255 28.974 11.718 11.034 1.00 7.21 N
ATOM 1471 CA SER G 255 30.320 11.869 11.561 1.00 7.37 C
ATOM 1472 CB SER G 255 30.477 11.067 12.859 1.00 8.09 C
ATOM 1473 OG SER G 255 29.239 10.928 13.536 1.00 10.47 O
ATOM 1474 C SER G 255 31.365 11.429 10.538 1.00 6.82 C
ATOM 1475 O SER G 255 32.237 12.207 10.150 1.00 6.99 O
ATOM 1476 N GLU G 256 31.240 10.192 10.068 1.00 6.17 N

ATOM 1477 CA GLU G 256 32.218 9.629 9.152 1.00 6.13 C
ATOM 1478 CB GLU G 256 31.913 8.158 8.883 1.00 6.22 C
ATOM 1479 CG GLU G 256 32.296 7.240 10.026 1.00 8.41 C
ATOM 1480 CD GLU G 256 31.422 6.006 10.099 1.00 10.26 C
ATOM 1481 OE1 GLU G 256 30.637 5.776 9.156 1.00 11.90 O
ATOM 1482 OE2 GLU G 256 31.532 5.255 11.090 1.00 9.55 O
ATOM 1483 C GLU G 256 32.231 10.401 7.845 1.00 5.76 C
ATOM 1484 O GLU G 256 33.275 10.892 7.418 1.00 5.93 O
ATOM 1485 N LEU G 257 31.075 10.476 7.194 1.00 5.67 N
ATOM 1486 CA LEU G 257 30.972 11.191 5.930 1.00 5.37 C
ATOM 1487 CB LEU G 257 29.512 11.334 5.486 1.00 5.03 C
ATOM 1488 CG LEU G 257 29.282 12.309 4.325 1.00 3.65 C
ATOM 1489 CD1 LEU G 257 29.846 11.755 3.024 1.00 2.00 C
ATOM 1490 CD2 LEU G 257 27.810 12.657 4.172 1.00 2.14 C
ATOM 1491 C LEU G 257 31.623 12.563 6.048 1.00 5.64 C
ATOM 1492 O LEU G 257 32.401 12.970 5.185 1.00 5.81 O
ATOM 1493 N LEU G 258 31.353 13.249 7.153 1.00 5.75 N
ATOM 1494 CA LEU G 258 31.792 14.629 7.301 1.00 5.91 C
ATOM 1495 CB LEU G 258 31. 162 15.276 8.535 1.00 6.10 C
ATOM 1496 CG LEU G 258 29.897 16.091 8.256 1.00 5.75 C
ATOM 1497 CD1 LEU G 258 29.230 16.525 9.552 1.00 6.33 C
ATOM 1498 CD2 LEU G 258 30.219 17.294 7.385 1.00 7.33 C
ATOM 1499 C LEU G 258 33.315 14.758 7.331 1.00 6.03 C
ATOM 1500 O LEU G 258 33.874 15.664 6.713 1.00 5.73 O
ATOM 1501 N SER G 259 33.983 13.867 8.061 1.00 6.47 N
ATOM 1502 CA SER G 259 35.442 13.887 8.139 1.00 6.95 C
ATOM 1503 CB SER G 259 35.929 13.137 9.381 1.00 7.05 C
ATOM 1504 OG SER G 259 36.284 11.802 9.064 1.00 6.86 O
ATOM 1505 C SER G 259 36.060 13.284 6.883 1.00 6.74 C
ATOM 1506 O SER G 259 37.173 13.638 6.493 1.00 6.86 O
ATOM 1507 N LEU G 260 35.31 1 12.400 6.234 1.00 6.31 N
ATOM 1508 CA LEU G 260 35.715 11.854 4.946 1.00 6.09 C
ATOM 1509 CB LEU G 260 34.747 10.756 4.507 1.00 6.09 C
ATOM 1510 CG LEU G 260 35.306 9.334 4.473 1.00 6.24 C
ATOM 151 1 CD1 LEU G 260 34.338 8.388 3.779 1.00 6.53 C
ATOM 1512 CD2 LEU G 260 36.663 9.309 3.790 1.00 5.98 C
ATOM 1513 C LEU G 260 35.775 12.947 3.887 1.00 6.25 C
ATOM 1514 O LEU G 260 36.696 12.982 3.072 1.00 6.37 O
ATOM 1515 N ILE G 261 34.724 13.760 3.826 1.00 6.63 N
ATOM 1516 CA ILE G 261 34.729 14.952 2.987 1.00 7.19 C
ATOM 1517 CB ILE G 261 33.504 15.840 3.262 1.00 7.09 C
ATOM 1518 CG1 ILE G 261 32.292 15.350 2.474 1.00 7.46 C
ATOM 1519 CD1 ILE G 261 30.991 15.952 2.951 1.00 8.38 C
ATOM 1520 CG2 ILE G 261 33.809 17.290 2.916 1.00 6.61 C
ATOM 1521 C ILE G 261 35.966 15.768 3.307 1.00 8.01 C
ATOM 1522 O ILE G 261 36.716 16.162 2.414 1.00 8.26 O
ATOM 1523 N ASN G 262 36.157 16.040 4.592 1.00 9.05 N
ATOM 1524 CA ASN G 262 37.337 16.748 5.049 1.00 9.88 C
ATOM 1525 CB ASN G 262 37.517 16.575 6.555 1.00 9.99 C
ATOM 1526 CG ASN G 262 38.185 17.770 7.197 1.00 11.16 C
ATOM 1527 OD1 ASN G 262 38.493 18.756 6.526 1.00 12.70 O
ATOM 1528 ND2 ASN G 262 38.391 17.701 8.506 1.00 13.20 N
ATOM 1529 C ASN G 262 38.585 16.282 4.316 1.00 10.17 C
ATOM 1530 O ASN G 262 39.426 17.093 3.928 1.00 10.52 O
ATOM 1531 N ASP G 263 38.684 14.976 4.094 1.00 10.62 N
ATOM 1532 CA ASP G 263 39.925 14.380 3.621 1.00 11.02 C
ATOM 1533 CB ASP G 263 40.022 12.917 4.055 1.00 11.49 C
ATOM 1534 CG ASP G 263 41.297 12.251 3.577 1.00 12.80 C
ATOM 1535 OD1 ASP G 263 42.377 12.863 3.715 1.00 14.72 O
ATOM 1536 OD2 ASP G 263 41.220 11.113 3.068 1.00 13.88 O

```
ATOM   1537  C   ASP G 263      40.067   14.491    2.107   1.00 10.92          C
ATOM   1538  O   ASP G 263      41.135   14.224    1.556   1.00 10.96          O
ATOM   1539  N   MET G 264      39.003   14.931    1.442   1.00 10.91          N
ATOM   1540  CA  MET G 264      38.989   14.992   -0.015   1.00 10.78          C
ATOM   1541  CB  MET G 264      37.557   15.121   -0.534   1.00 10.51          C
ATOM   1542  CG  MET G 264      36.669   13.937   -0.194   1.00 11.26          C
ATOM   1543  SD  MET G 264      35.025   14.078   -0.916   1.00 12.70          S
ATOM   1544  CE  MET G 264      34.634   15.778   -0.513   1.00 13.92          C
ATOM   1545  C   MET G 264      39.851   16.135   -0.543   1.00 10.85          C
ATOM   1546  O   MET G 264      39.830   17.238    0.002   1.00 11.03          O
ATOM   1547  N   PRO G 265      40.626   15.863   -1.604   1.00 10.88          N
ATOM   1548  CA  PRO G 265      41.558   16.827   -2.184   1.00 11.09          C
ATOM   1549  CB  PRO G 265      42.357   15.986   -3.188   1.00 11.28          C
ATOM   1550  CG  PRO G 265      41.513   14.787   -3.453   1.00 11.24          C
ATOM   1551  CD  PRO G 265      40.807   14.515   -2.167   1.00 11.03          C
ATOM   1552  C   PRO G 265      40.845   17.965   -2.908   1.00 11.19          C
ATOM   1553  O   PRO G 265      41.070   18.175   -4.100   1.00 11.47          O
ATOM   1554  N   ILE G 266      40.053   18.739   -2.173   1.00 11.54          N
ATOM   1555  CA  ILE G 266      39.282   19.820   -2.777   1.00 12.15          C
ATOM   1556  CB  ILE G 266      37.792   19.454   -2.914   1.00 12.22          C
ATOM   1557  CGI ILE G 266      37.245   18.928   -1.585   1.00 12.53          C
ATOM   1558  CD1 ILE G 266      35.733   18.918   -1.510   1.00 12.40          C
ATOM   1559  CG2 ILE G 266      37.594   18.431   -4.023   1.00 12.74          C
ATOM   1560  C   ILE G 266      39.413   21.132   -2.013   1.00 12.29          C
ATOM   1561  O   ILE G 266      39.853   21.156   -0.863   1.00 12.36          O
ATOM   1562  N   THR G 267      39.034   22.223   -2.670   1.00 12.29          N
ATOM   1563  CA  THR G 267      39.039   23.541   -2.050   1.00 12.43          C
ATOM   1564  CB  THR G 267      38.564   24.627   -3.034   1.00 12.40          C
ATOM   1565  OGl THR G 267      37.340   25.204   -2.562   1.00 13.21          O
ATOM   1566  CG2 THR G 267      38.341   24.033   -4.417   1.00 12.21          C
ATOM   1567  C   THR G 267      38.141   23.560   -0.819   1.00 12.37          C
ATOM   1568  O   THR G 267      37.440   22.589   -0.537   1.00 12.29          O
ATOM   1569  N   ASN G 268      38.174   24.664   -0.081   1.00 12.47          N
ATOM   1570  CA  ASN G 268      37.523   24.720    1.219   1.00 12.57          C
ATOM   1571  CB  ASN G 268      38.199   25.751    2.121   1.00 12.69          C
ATOM   1572  CG  ASN G 268      39.221   25.127    3.048   1.00 13.65          C
ATOM   1573  ODl ASN G 268      39.463   23.921    3.000   1.00 14.37          O
ATOM   1574  ND2 ASN G 268      39.843   25.949    3.884   1.00 15.74          N
ATOM   1575  C   ASN G 268      36.028   24.995    1.123   1.00 12.43          C
ATOM   1576  O   ASN G 268      35.232   24.403    1.853   1.00 12.51          O
ATOM   1577  N   ASP G 269      35.655   25.926    0.252   1.00 12.34          N
ATOM   1578  CA  ASP G 269      34.248   26.218    0.008   1.00 12.33          C
ATOM   1579  CB  ASP G 269      34.106   27.359   -0.999   1.00 12.89          C
ATOM   1580  CG  ASP G 269      34.761   28.639   -0.525   1.00 14.84          C
ATOM   1581  ODl ASP G 269      34.594   28.989    0.663   1.00 16.90          O
ATOM   1582  OD2 ASP G 269      35.473   29.277   -1.328   1.00 17.65          O
ATOM   1583  C   ASP G 269      33.532   24.978   -0.506   1.00 11.60          C
ATOM   1584  O   ASP G 269      32.411   24.679   -0.095   1.00 11.65          O
ATOM   1585  N   GLN G 270      34.189   24.260   -1.410   1.00 10.62          N
ATOM   1586  CA  GLN G 270      33.728   22.943   -1.816   1.00 10.01          C
ATOM   1587  CB  GLN G 270      34.795   22.236   -2.647   1.00 10.18          C
ATOM   1588  CG  GLN G 270      34.248   21.533   -3.870   1.00 11.49          C
ATOM   1589  CD  GLN G 270      35.200   21.598   -5.043   1.00 14.38          C
ATOM   1590  OE1 GLN G 270      35.516   20.579   -5.655   1.00 16.38          O
ATOM   1591  NE2 GLN G 270      35.718   22.789   -5.318   1.00 15.41          N
ATOM   1592  C   GLN G 270      33.366   22.094   -0.606   1.00  9.48          C
ATOM   1593  O   GLN G 270      32.213   21.698   -0.437   1.00  9.12          O
ATOM   1594  N   LYS G 271      34.358   21.809    0.231   1.00  9.19          N
ATOM   1595  CA  LYS G 271      34.126   21.040    1.445   1.00  8.89          C
ATOM   1596  CB  LYS G 271      35.362   21.070    2.345   1.00  8.52          C
```

ATOM 1597 CG LYS G 271 36.541 20.285 1.797 1.00 9.14 C
ATOM 1598 CD LYS G 271 37.643 20.147 2.832 1.00 10.72 C
ATOM 1599 CE LYS G 271 39.013 20.137 2.176 1.00 10.79 C
ATOM 1600 NZ LYS G 271 40.035 19.472 3.030 1.00 9.77 N
ATOM 1601 C LYS G 271 32.907 21.563 2.199 1.00 8.83 C
ATOM 1602 O LYS G 271 31.959 20.820 2.452 1.00 9.05 O
ATOM 1603 N LYS G 272 32.899 22.863 2.474 1.00 8.65 N
ATOM 1604 CA LYS G 272 31.789 23.482 3.187 1.00 8.50 C
ATOM 1605 CB LYS G 272 31.997 24.992 3.304 1.00 9.14 C
ATOM 1606 CG LYS G 272 30.762 25.748 3.766 1.00 11.58 C
ATOM 1607 CD LYS G 272 30.925 27.246 3.575 1.00 15.78 C
ATOM 1608 CE LYS G 272 29.995 28.021 4.492 1.00 17.65 C
ATOM 1609 NZ LYS G 272 30.462 29.418 4.703 1.00 19.68 N
ATOM 1610 C LYS G 272 30.458 23.191 2.503 1.00 7.88 C
ATOM 1611 O LYS G 272 29.486 22.808 3.154 1.00 8.12 O
ATOM 1612 N LEU G 273 30.408 23.416 1.194 1.00 6.95 N
ATOM 1613 CA LEU G 273 29.217 23.104 0.413 1.00 5.70 C
ATOM 1614 CB LEU G 273 29.469 23.344 -1.077 1.00 5.85 C
ATOM 1615 CG LEU G 273 28.313 23.000 -2.020 1.00 4.65 C
ATOM 1616 CD1 LEU G 273 27.277 24.114 -2.032 1.00 4.57 C
ATOM 1617 CD2 LEU G 273 28.829 22.729 -3.425 1.00 3.69 C
ATOM 1618 C LEU G 273 28.781 21.663 0.644 1.00 5.14 C
ATOM 1619 O LEU G 273 27.678 21.409 1.128 1.00 5.25 O
ATOM 1620 N MET G 274 29.665 20.724 0.327 1.00 4.52 N
ATOM 1621 CA MET G 274 29.354 19.312 0.482 1.00 4.59 C
ATOM 1622 CB MET G 274 30.573 18.454 0.152 1.00 4.35 C
ATOM 1623 CG MET G 274 30.938 18.457 -1.319 1.00 4.50 C
ATOM 1624 SD MET G 274 32.305 17.344 -1.679 1.00 5.51 S
ATOM 1625 CE MET G 274 31.469 15.758 -1.633 1.00 5.26 C
ATOM 1626 C MET G 274 28.864 19.014 1.893 1.00 5.18 C
ATOM 1627 O MET G 274 27.893 18.280 2.075 1.00 5.61 O
ATOM 1628 N SER G 275 29.457 19.689 2.875 1.00 5.89 N
ATOM 1629 CA SER G 275 29.118 19.465 4.278 1.00 6.18 C
ATOM 1630 CB SER G 275 30.161 20.108 5.194 1.00 6.33 C
ATOM 1631 OG SER G 275 31.457 19.601 4.925 1.00 5.91 O
ATOM 1632 C SER G 275 27.726 19.989 4.619 1.00 6.58 C
ATOM 1633 O SER G 275 27.031 19.425 5.464 1.00 7.03 O
ATOM 1634 N ASN G 276 27.313 21.054 3.940 1.00 7.07 N
ATOM 1635 CA ASN G 276 25.979 21.606 4.140 1.00 7.86 C
ATOM 1636 CB ASN G 276 25.987 23.126 3.942 1.00 8.34 C
ATOM 1637 CG ASN G 276 26.343 23.881 5.214 1.00 9.77 C
ATOM 1638 ODl ASN G 276 26.033 23.439 6.320 1.00 11.84 O
ATOM 1639 ND2 ASN G 276 26.964 25.044 5.057 1.00 11.15 N
ATOM 1640 C ASN G 276 24.908 20.954 3.262 1.00 7.71 C
ATOM 1641 O ASN G 276 23.780 21.442 3.191 1.00 7.84 O
ATOM 1642 N ASN G 277 25.239 19.819 2.649 1.00 7.77 N
ATOM 1643 CA ASN G 277 24.372 19.220 1.631 1.00 7.85 C
ATOM 1644 CB ASN G 277 24.704 19.777 0.246 1.00 7.58 C
ATOM 1645 CG ASN G 277 24.023 21.099 -0.027 1.00 8.29 C
ATOM 1646 ODl ASN G 277 22.818 21.152 -0.272 1.00 9.04 O
ATOM 1647 ND2 ASN G 277 24.798 22.176 -0.008 1.00 9.57 N
ATOM 1648 C ASN G 277 24.410 17.693 1.590 1.00 7.86 C
ATOM 1649 O ASN G 277 24.154 17.089 0.549 1.00 7.85 O
ATOM 1650 N VAL G 278 24.886 17.093 2.674 1.00 7.67 N
ATOM 1651 CA VAL G 278 24.839 15.645 2.879 1.00 7.77 C
ATOM 1652 CB VAL G 278 24.594 15.309 4.352 1.00 7.98 C
ATOM 1653 CGI VAL G 278 25.915 15.261 5.100 1.00 7.21 C
ATOM 1654 CG2 VAL G 278 23.655 16.332 4.977 1.00 8.99 C
ATOM 1655 C VAL G 278 23.843 14.865 2.019 1.00 7.76 C
ATOM 1656 O VAL G 278 24.183 13.811 1.483 1.00 7.84 O

```
ATOM   1657  N   GLN G 279      22.569   15.228    2.118  1.00  7.47           N
ATOM   1658  CA  GLN G 279      21.510   14.444    1.492  1.00  7.07           C
ATOM   1659  CB  GLN G 279      20.187   15.204    1.550  1.00  7.62           C
ATOM   1660  CG  GLN G 279      19.021   14.376    2.044  1.00 10.35           C
ATOM   1661  CD  GLN G 279      17.682   14.997    1.702  1.00 13.70           C
ATOM   1662  OE1 GLN G 279      17.612   16.002    0.996  1.00 15.06           O
ATOM   1663  NE2 GLN G 279      16.607   14.383    2.179  1.00 13.97           N
ATOM   1664  C   GLN G 279      21.852   14.121    0.042  1.00  6.02           C
ATOM   1665  O   GLN G 279      22.032   12.958   -0.323  1.00  5.45           O
ATOM   1666  N   ILE G 280      21.863   15.154   -0.792  1.00  5.25           N
ATOM   1667  CA  ILE G 280      22.325   15.034   -2.169  1.00  4.74           C
ATOM   1668  CB  ILE G 280      22.650   16.408   -2.771  1.00  4.58           C
ATOM   1669  CGI ILE G 280      21.527   17.396   -2.461  1.00  4.16           C
ATOM   1670  CD1 ILE G 280      20.235   17.078   -3.177  1.00  3.88           C
ATOM   1671  CG2 ILE G 280      22.835   16.293   -4.271  1.00  3.92           C
ATOM   1672  C   ILE G 280      23.550   14.135   -2.286  1.00  4.43           C
ATOM   1673  O   ILE G 280      23.493   13.081   -2.917  1.00  4.39           O
ATOM   1674  N   VAL G 281      24.676   14.596   -1.749  1.00  4.05           N
ATOM   1675  CA  VAL G 281      25.906   13.816   -1.795  1.00  3.58           C
ATOM   1676  CB  VAL G 281      26.918   14.251   -0.714  1.00  3.13           C
ATOM   1677  CGI VAL G 281      28.296   13.684   -1.026  1.00  2.34           C
ATOM   1678  CG2 VAL G 281      26.978   15.768   -0.616  1.00  2.21           C
ATOM   1679  C   VAL G 281      25.593   12.335   -1.626  1.00  3.96           C
ATOM   1680  O   VAL G 281      25.875   11.534   -2.515  1.00  4.15           O
ATOM   1681  N   ARG G 282      24.908   11.994   -0.539  1.00  4.23           N
ATOM   1682  CA  ARG G 282      24.500   10.615   -0.296  1.00  4.45           C
ATOM   1683  CB  ARG G 282      23.570   10.540    0.911  1.00  3.96           C
ATOM   1684  CG  ARG G 282      24.225   10.953    2.203  1.00  2.99           C
ATOM   1685  CD  ARG G 282      23.924    9.962    3.303  1.00  2.28           C
ATOM   1686  NE  ARG G 282      24.332   10.474    4.605  1.00  2.00           N
ATOM   1687  CZ  ARG G 282      25.026    9.777    5.498  1.00  2.44           C
ATOM   1688  NHl  ARG G 282     25.359    8.517    5.251  1.00  2.04           N
ATOM   1689  NH2 ARG G 282      25.369   10.333    6.650  1.00  3.44           N
ATOM   1690  C   ARG G 282      23.798   10.039   -1.516  1.00  5.32           C
ATOM   1691  O   ARG G 282      24.143    8.958   -1.997  1.00  5.95           O
ATOM   1692  N   GLN G 283      22.800   10.765   -2.006  1.00  5.50           N
ATOM   1693  CA  GLN G 283      22.045   10.327   -3.169  1.00  5.80           C
ATOM   1694  CB  GLN G 283      20.910   11.303   -3.471  1.00  6.19           C
ATOM   1695  CG  GLN G 283      19.768   11.219   -2.480  1.00  9.68           C
ATOM   1696  CD  GLN G 283      18.840   12.406   -2.561  1.00 13.92           C
ATOM   1697  OE1 GLN G 283      18.991   13.269   -3.426  1.00 16.20           O
ATOM   1698  NE2 GLN G 283      17.833   12.428   -1.696  1.00 14.17           N
ATOM   1699  C   GLN G 283      22.953   10.175   -4.379  1.00  5.44           C
ATOM   1700  O   GLN G 283      22.687    9.364   -5.264  1.00  5.43           O
ATOM   1701  N   GLN G 284      24.067   10.896   -4.371  1.00  5.26           N
ATOM   1702  CA  GLN G 284      24.957   10.920   -5.521  1.00  5.18           C
ATOM   1703  CB  GLN G 284      25.568   12.307   -5.702  1.00  5.32           C
ATOM   1704  CG  GLN G 284      24.813   13.189   -6.673  1.00  6.85           C
ATOM   1705  CD  GLN G 284      25.434   14.560   -6.804  1.00  9.21           C
ATOM   1706  OE1 GLN G 284      25.863   15.160   -5.819  1.00  9.74           O
ATOM   1707  NE2 GLN G 284      25.492   15.064   -8.027  1.00  9.79           N
ATOM   1708  C   GLN G 284      26.060    9.882   -5.400  1.00  4.67           C
ATOM   1709  O   GLN G 284      26.884    9.736   -6.302  1.00  4.19           O
ATOM   1710  N   SER G 285      26.109    9.199   -4.262  1.00  4.51           N
ATOM   1711  CA  SER G 285      27.204    8.281   -3.990  1.00  4.39           C
ATOM   1712  CB  SER G 285      27.767    8.510   -2.587  1.00  4.13           C
ATOM   1713  OG  SER G 285      28.180    9.856   -2.421  1.00  4.40           O
ATOM   1714  C   SER G 285      26.767    6.834   -4.166  1.00  4.44           C
ATOM   1715  O   SER G 285      25.587    6.555   -4.382  1.00  4.82           O
ATOM   1716  N   TYR G 286      27.751    5.949   -4.271  1.00  4.53           N
```

ATOM 1717 CA TYR G 286 27.500 4.517 -4.291 1.00 4.80 C
ATOM 1718 CB TYR G 286 27.978 3.915 -5.612 1.00 4.88 C
ATOM 1719 CG TYR G 286 27.168 4.354 -6.809 1.00 5.68 C
ATOM 1720 CDl TYR G 286 27.156 5.681 -7.218 1.00 7.34 C
ATOM 1721 CE1 TYR G 286 26.429 6.081 -8.322 1.00 9.02 C
ATOM 1722 CZ TYR G 286 25.720 5.145 -9.044 1.00 9.40 C
ATOM 1723 OH TYR G 286 24.998 5.538 -10.146 1.00 10.44 O
ATOM 1724 CE2 TYR G 286 25.730 3.820 -8.668 1.00 9.38 C
ATOM 1725 CD2 TYR G 286 26.444 3.433 -7.553 1.00 7.39 C
ATOM 1726 C TYR G 286 28.208 3.845 -3.124 1.00 4.76 C
ATOM 1727 O TYR G 286 29.130 4.41 1 -2.541 1.00 5.25 O
ATOM 1728 N SER G 287 27.765 2.642 -2.779 1.00 4.52 N
ATOM 1729 CA SER G 287 28.528 1.786 -1.884 1.00 4.45 C
ATOM 1730 CB SER G 287 27.888 1.743 -0.496 1.00 4.57 C
ATOM 1731 OG SER G 287 28.421 0.681 0.275 1.00 4.38 O
ATOM 1732 C SER G 287 28.670 0.381 -2.454 1.00 4.61 C
ATOM 1733 O SER G 287 27.683 -0.253 -2.820 1.00 4.40 O
ATOM 1734 N ILE G 288 29.914 -0.002 -2.717 1.00 5.11 N
ATOM 1735 CA ILE G 288 30.227 -1.318 -3.258 1.00 5.81 C
ATOM 1736 CB ILE G 288 31.376 -1.250 -4.288 1.00 5.52 C
ATOM 1737 CGI ILE G 288 31.377 0.095 -5.021 1.00 5.47 C
ATOM 1738 CDl ILE G 288 31.007 0.002 -6.487 1.00 6.23 C
ATOM 1739 CG2 ILE G 288 31.298 -2.421 -5.256 1.00 6.22 C
ATOM 1740 C ILE G 288 30.664 -2.245 -2. 138 1.00 6.71 C
ATOM 1741 O ILE G 288 31.615 -1.948 -1.414 1.00 7.30 O
ATOM 1742 N MET G 289 30.085 -3.438 -2. 118 1.00 7.71 N
ATOM 1743 CA MET G 289 30.585 -4.515 -1.277 1.00 8.57 C
ATOM 1744 CB MET G 289 29.605 -5.692 -1.306 1.00 8.71 C
ATOM 1745 CG MET G 289 29.648 -6.584 -0.077 1.00 9.70 C
ATOM 1746 SD MET G 289 28.615 -8.046 -0.280 1.00 12.59 S
ATOM 1747 CE MET G 289 29.227 -8.678 -1.839 1.00 12.41 C
ATOM 1748 C MET G 289 31.975 -4.963 -1.736 1.00 9.12 C
ATOM 1749 O MET G 289 32.231 -5.086 -2.935 1.00 9.31 O
ATOM 1750 N SER G 290 32.891 -5.122 -0.784 1.00 9.80 N
ATOM 1751 CA SER G 290 34.272 -5.469 -1.098 1.00 10.49 C
ATOM 1752 CB SER G 290 35.242 -4.513 -0.401 1.00 10.64 C
ATOM 1753 OG SER G 290 36.498 -4.486 -1.058 1.00 11.99 O
ATOM 1754 C SER G 290 34.592 -6.918 -0.742 1.00 10.75 C
ATOM 1755 O SER G 290 34.631 -7.778 -1.621 1.00 10.89 O
ATOM 1756 N ILE G 291 34.760 -7.206 0.544 1.00 11.04 N
ATOM 1757 CA ILE G 291 34.884 -8.596 0.965 1.00 11.41 C
ATOM 1758 CB ILE G 291 36.329 -9.120 0.900 1.00 11.80 C
ATOM 1759 CGI ILE G 291 37.332 -7.977 1.061 1.00 11.81 C
ATOM 1760 CDl ILE G 291 38.227 -8.1 13 2.277 1.00 11.76 C
ATOM 1761 CG2 ILE G 291 36.561 -9.846 -0.416 1.00 12.39 C
ATOM 1762 C ILE G 291 34.214 -8.982 2.277 1.00 11.13 C
ATOM 1763 O ILE G 291 34.299 -8.268 3.277 1.00 10.55 O
ATOM 1764 N ILE G 292 33.536 -10. 124 2.246 1.00 11.36 N
ATOM 1765 CA ILE G 292 32.802 -10.620 3.398 1.00 11.82 C
ATOM 1766 CB ILE G 292 31.359 -11.016 3.029 1.00 11.86 C
ATOM 1767 CGI ILE G 292 31.087 -10.734 1.550 1.00 13.42 C
ATOM 1768 CDl ILE G 292 31.289 -9.282 1.158 1.00 15.86 C
ATOM 1769 CG2 ILE G 292 30.358 -10.287 3.923 1.00 10.85 C
ATOM 1770 C ILE G 292 33.505 -11.826 3.992 1.00 11.72 C
ATOM 1771 O ILE G 292 33.683 -12.849 3.330 1.00 11.28 O
ATOM 1772 N LYS G 293 33.946 -11.679 5.234 1.00 12.1 1 N
ATOM 1773 CA LYS G 293 34.275 -12.823 6.058 1.00 12.92 C
ATOM 1774 CB LYS G 293 35.715 -12.720 6.553 1.00 13.15 C
ATOM 1775 CG LYS G 293 36.674 -12.179 5.512 1.00 14.17 C
ATOM 1776 CD LYS G 293 38.000 -12.910 5.561 1.00 15.37 C

```
ATOM   1777  CE  LYS G 293      38.720 -12.826   4.229  1.00 16.68           C
ATOM   1778  NZ  LYS G 293      39.984 -13.607   4.242  1.00 18.18           N
ATOM   1779  C   LYS G 293      33.310 -12.923   7.232  1.00 13.32           C
ATOM   1780  O   LYS G 293      32.633 -11.952   7.578  1.00 13.17           O
ATOM   1781  N   GLU G 294      33.140 -14.141   7.735  1.00 14.07           N
ATOM   1782  CA  GLU G 294      32.217 -14.398   8.831  1.00 15.07           C
ATOM   1783  CB  GLU G 294      32.474 -15.786   9.425  1.00 15.94           C
ATOM   1784  CG  GLU G 294      32.183 -16.935   8.471  1.00 19.87           C
ATOM   1785  CD  GLU G 294      32.165 -18.282   9.169  1.00 23.88           C
ATOM   1786  OE1 GLU G 294      31.348 -18.465  10.097  1.00 23.75           O
ATOM   1787  OE2 GLU G 294      32.950 -19.168   8.766  1.00 25.81           O
ATOM   1788  C   GLU G 294      32.301 -13.320   9.917  1.00 14.40           C
ATOM   1789  O   GLU G 294      31.281 -12.936  10.491  1.00 14.33           O
ATOM   1790  N   GLU G 295      33.502 -12.779  10.132  1.00 13.97           N
ATOM   1791  CA  GLU G 295      33.765 -11.861  11.251  1.00 13.84           C
ATOM   1792  CB  GLU G 295      34.681 -12.508  12.299  1.00 14.67           C
ATOM   1793  CG  GLU G 295      35.496 -13.688  11.794  1.00 17.56           C
ATOM   1794  CD  GLU G 295      36.393 -13.328  10.626  1.00 21.41           C
ATOM   1795  OE1 GLU G 295      36.085 -13.752   9.493  1.00 22.35           O
ATOM   1796  OE2 GLU G 295      37.472 -12.745  10.861  1.00 23.20           O
ATOM   1797  C   GLU G 295      34.340 -10.502  10.827  1.00 12.77           C
ATOM   1798  O   GLU G 295      34.771  -9.712  11.670  1.00 12.58           O
ATOM   1799  N   VAL G 296      34.389 -10.256   9.522  1.00 11.72           N
ATOM   1800  CA  VAL G 296      34.634  -8.911   9.011  1.00 10.65           C
ATOM   1801  CB  VAL G 296      36.143  -8.604   8.894  1.00 10.47           C
ATOM   1802  CGI VAL G 296      36.369  -7.112   8.687  1.00  9.77           C
ATOM   1803  CG2 VAL G 296      36.879  -9.090  10.133  1.00 11.31           C
ATOM   1804  C   VAL G 296      33.949  -8.664   7.669  1.00 10.26           C
ATOM   1805  O   VAL G 296      33.931  -9.530   6.793  1.00 10.09           O
ATOM   1806  N   LEU G 297      33.379  -7.473   7.525  1.00  9.77           N
ATOM   1807  CA  LEU G 297      32.842  -7.027   6.250  1.00  8.97           C
ATOM   1808  CB  LEU G 297      31.332  -6.796   6.367  1.00  8.64           C
ATOM   1809  CG  LEU G 297      30.643  -6.020   5.243  1.00  9.01           C
ATOM   1810  CD1 LEU G 297      30.733  -6.773   3.927  1.00  9.79           C
ATOM   1811  CD2 LEU G 297      29.194  -5.752   5.606  1.00  9.43           C
ATOM   1812  C   LEU G 297      33.544  -5.745   5.821  1.00  8.34           C
ATOM   1813  O   LEU G 297      33.645  -4.793   6.595  1.00  8.64           O
ATOM   1814  N   ALA G 298      34.131  -5.767   4.631  1.00  7.21           N
ATOM   1815  CA  ALA G 298      34.751  -4.573   4.079  1.00  6.33           C
ATOM   1816  CB  ALA G 298      36.231  -4.800   3.860  1.00  6.68           C
ATOM   1817  C   ALA G 298      34.074  -4.177   2.778  1.00  5.85           C
ATOM   1818  O   ALA G 298      33.727  -5.033   1.965  1.00  5.96           O
ATOM   1819  N   TYR G 299      33.820  -2.883   2.620  1.00  5.28           N
ATOM   1820  CA  TYR G 299      33.178  -2.376   1.417  1.00  4.63           C
ATOM   1821  CB  TYR G 299      31.660  -2.340   1.595  1.00  4.36           C
ATOM   1822  CG  TYR G 299      31.204  -1.517   2.776  1.00  4.34           C
ATOM   1823  CD1 TYR G 299      30.967  -0.156   2.648  1.00  4.48           C
ATOM   1824  CE1 TYR G 299      30.505   0.592   3.717  1.00  4.55           C
ATOM   1825  CZ  TYR G 299      30.292  -0.019   4.937  1.00  3.72           C
ATOM   1826  OH  TYR G 299      29.847   0.720   6.009  1.00  2.38           O
ATOM   1827  CE2 TYR G 299      30.540  -1.366   5.092  1.00  4.13           C
ATOM   1828  CD2 TYR G 299      31.007  -2.102   4.020  1.00  4.38           C
ATOM   1829  C   TYR G 299      33.692  -0.988   1.063  1.00  4.32           C
ATOM   1830  O   TYR G 299      34.067  -0.214   1.944  1.00  4.67           O
ATOM   1831  N   VAL G 300      33.609  -0.641  -0.217  1.00  3.87           N
ATOM   1832  CA  VAL G 300      34.121   0.636  -0.696  1.00  3.57           C
ATOM   1833  CB  VAL G 300      34.892   0.481  -2.020  1.00  3.52           C
ATOM   1834  CGI VAL G 300      35.278   1.843  -2.576  1.00  3.44           C
ATOM   1835  CG2 VAL G 300      36.127  -0.374  -1.808  1.00  3.90           C
ATOM   1836  C   VAL G 300      32.999   1.654  -0.861  1.00  3.53           C
```

```
ATOM   1837  O   VAL G 300     31.959   1.360  -1.451  1.00  3.68          O
ATOM   1838  N   VAL G 301     33.163   2.795  -0.205  1.00  3.41          N
ATOM   1839  CA  VAL G 301     32.321   3.950  -0.451  1.00  3.36          C
ATOM   1840  CB  VAL G 301     32.264   4.847   0.789  1.00  3.24          C
ATOM   1841  CGI VAL G 301     31.738   6.229   0.428  1.00  3.76          C
ATOM   1842  CG2 VAL G 301     31.431   4.190   1.884  1.00  3.10          C
ATOM   1843  C   VAL G 301     32.854   4.766  -1.619  1.00  3.48          C
ATOM   1844  O   VAL G 301     34.065   4.911  -1.786  1.00  3.92          O
ATOM   1845  N   GLN G 302     31.943   5.410  -2.339  1.00  3.21          N
ATOM   1846  CA  GLN G 302     32.285   6.084  -3.578  1.00  3.01          C
ATOM   1847  CB  GLN G 302     31.901   5.213  -4.775  1.00  3.24          C
ATOM   1848  CG  GLN G 302     31.990   5.924  -6.113  1.00  5.21          C
ATOM   1849  CD  GLN G 302     32.153   4.963  -7.271  1.00  7.54          C
ATOM   1850  OE1 GLN G 302     32.555   3.814  -7.086  1.00  7.28          O
ATOM   1851  NE2 GLN G 302     31.793   5.412  -8.467  1.00  9.27          N
ATOM   1852  C   GLN G 302     31.571   7.424  -3.652  1.00  2.42          C
ATOM   1853  O   GLN G 302     30.344   7.479  -3.737  1.00  2.40          O
ATOM   1854  N   LEU G 303     32.323   8.492  -3.426  1.00  2.00          N
ATOM   1855  CA  LEU G 303     31.729   9.802  -3.232  1.00  2.00          C
ATOM   1856  CB  LEU G 303     32.303  10.471  -1.979  1.00  2.00          C
ATOM   1857  CG  LEU G 303     32.332   9.619  -0.706  1.00  2.00          C
ATOM   1858  CD1 LEU G 303     32.849  10.428   0.474  1.00  2.00          C
ATOM   1859  CD2 LEU G 303     30.960   9.033  -0.400  1.00  2.00          C
ATOM   1860  C   LEU G 303     31.955  10.674  -4.460  1.00  2.00          C
ATOM   1861  O   LEU G 303     32.835  10.391  -5.273  1.00  2.45          O
ATOM   1862  N   PRO G 304     31.136  11.723  -4.614  1.00  2.00          N
ATOM   1863  CA  PRO G 304     31.230  12.520  -5.827  1.00  2.07          C
ATOM   1864  CB  PRO G 304     29.999  13.432  -5.754  1.00  2.00          C
ATOM   1865  CG  PRO G 304     29.497  13.323  -4.348  1.00  2.00          C
ATOM   1866  CD  PRO G 304     29.880  11.966  -3.888  1.00  2.06          C
ATOM   1867  C   PRO G 304     32.513  13.340  -5.854  1.00  2.11          C
ATOM   1868  O   PRO G 304     32.814  14.030  -4.878  1.00  2.13          O
ATOM   1869  N   ALA G 305     33.407  12.935  -6.752  1.00 30.00          N
ATOM   1870  CA  ALA G 305     33.971  13.839  -7.760  1.00 30.00          C
ATOM   1871  CB  ALA G 305     35.427  13.480  -8.043  1.00 30.00          C
ATOM   1872  C   ALA G 305     33.151  13.838  -9.059  1.00 30.00          C
ATOM   1873  O   ALA G 305     32.743  12.775  -9.530  1.00 30.00          O
ATOM   1874  N   TYR G 306     32.752  15.032  -9.522  1.00 13.49          N
ATOM   1875  CA  TYR G 306     31.656  15.131 -10.505  1.00 13.70          C
ATOM   1876  CB  TYR G 306     30.892  16.462 -10.539  1.00 13.93          C
ATOM   1877  CG  TYR G 306     31.430  17.687  -9.879  1.00 14.08          C
ATOM   1878  CD1 TYR G 306     32.339  18.519 -10.551  1.00 14.59          C
ATOM   1879  CE1 TYR G 306     32.383  19.885 -10.286  1.00 14.82          C
ATOM   1880  CZ  TYR G 306     31.470  20.425  -9.404  1.00 14.52          C
ATOM   1881  OH  TYR G 306     31.626  21.709  -8.943  1.00 13.02          O
ATOM   1882  CE2 TYR G 306     30.465  19.645  -8.899  1.00 15.22          C
ATOM   1883  CD2 TYR G 306     30.596  18.296  -8.957  1.00 14.61          C
ATOM   1884  C   TYR G 306     32.048  14.998 -11.938  1.00 13.68          C
ATOM   1885  O   TYR G 306     33.051  14.374 -12.273  1.00 13.95          O
ATOM   1886  N   GLY G 307     31.521  16.002 -12.645  1.00 13.54          N
ATOM   1887  CA  GLY G 307     31.871  16.332 -14.033  1.00 13.37          C
ATOM   1888  C   GLY G 307     30.772  16.073 -15.065  1.00 13.47          C
ATOM   1889  O   GLY G 307     30.263  14.955 -15.138  1.00 13.90          O
ATOM   1890  N   VAL G 308     30.591  16.991 -16.021  1.00 13.31          N
ATOM   1891  CA  VAL G 308     29.883  16.654 -17.276  1.00 13.30          C
ATOM   1892  CB  VAL G 308     28.555  15.924 -16.985  1.00 13.03          C
ATOM   1893  CGI VAL G 308     28.183  15.008 -18.138  1.00 13.62          C
ATOM   1894  CG2 VAL G 308     28.619  15.178 -15.665  1.00 12.86          C
ATOM   1895  C   VAL G 308     29.425  17.870 -18.046  1.00 13.58          C
ATOM   1896  O   VAL G 308     30.236  18.677 -18.508  1.00 13.71          O
```

```
ATOM   1897  N   ILE G 309     28.221  18.219 -17.643  1.00  4.08           N
ATOM   1898  CA  ILE G 309     28.140  19.052 -16.487  1.00  4.84           C
ATOM   1899  CB  ILE G 309     29.493  19.031 -15.728  1.00  4.89           C
ATOM   1900  CGI ILE G 309     29.924  17.598 -15.412  1.00  5.85           C
ATOM   1901  CD1 ILE G 309     29.235  17.007 -14.197  1.00  8.12           C
ATOM   1902  CG2 ILE G 309     29.423  19.879 -14.473  1.00  4.44           C
ATOM   1903  C   ILE G 309     28.075  20.346 -17.222  1.00  5.23           C
ATOM   1904  O   ILE G 309     28.803  20.526 -18.199  1.00  5.92           O
ATOM   1905  N   ASP G 310     26.984  21.057 -17.020  1.00  5.33           N
ATOM   1906  CA  ASP G 310     26.985  22.446 -17.403  1.00  5.83           C
ATOM   1907  CB  ASP G 310     28.432  22.938 -17.554  1.00  6.21           C
ATOM   1908  CG  ASP G 310     29.280  22.660 -16.321  1.00  7.19           C
ATOM   1909  OD1 ASP G 310     30.432  22.200 -16.480  1.00  7.74           O
ATOM   1910  OD2 ASP G 310     28.844  23.021 -15.209  1.00  7.58           O
ATOM   1911  C   ASP G 310     26.233  22.676 -18.712  1.00  6.02           C
ATOM   1912  O   ASP G 310     26.323  23.760 -19.287  1.00  6.05           O
ATOM   1913  N   THR G 311     25.448  21.696 -19.157  1.00  6.24           N
ATOM   1914  CA  THR G 311     24.352  21.982 -20.088  1.00  6.14           C
ATOM   1915  CB  THR G 311     23.883  20.720 -20.852  1.00  5.69           C
ATOM   1916  OG1 THR G 311     24.925  19.737 -20.850  1.00  5.34           O
ATOM   1917  CG2 THR G 311     23.526  21.069 -22.291  1.00  7.10           C
ATOM   1918  C   THR G 311     23.160  22.578 -19.339  1.00  6.78           C
ATOM   1919  O   THR G 311     22.863  22.163 -18.218  1.00  7.33           O
ATOM   1920  N   PRO G 312     22.414  23.483 -19.992  1.00  7.00           N
ATOM   1921  CA  PRO G 312     21.205  23.982 -19.341  1.00  7.23           C
ATOM   1922  CB  PRO G 312     20.748  25.113 -20.267  1.00  7.00           C
ATOM   1923  CG  PRO G 312     21.341  24.786 -21.593  1.00  6.59           C
ATOM   1924  CD  PRO G 312     22.649  24.119 -21.300  1.00  6.99           C
ATOM   1925  C   PRO G 312     20.138  22.895 -19.263  1.00  7.69           C
ATOM   1926  O   PRO G 312     19.973  22.130 -20.213  1.00  7.55           O
ATOM   1927  N   CYS G 313     19.469  22.781 -18.120  1.00  8.10           N
ATOM   1928  CA  CYS G 313     18.164  22.128 -18.088  1.00  8.54           C
ATOM   1929  CB  CYS G 313     18.165  20.883 -17.192  1.00  8.77           C
ATOM   1930  SG  CYS G 313     19.762  20.065 -16.969  1.00 10.74           S
ATOM   1931  C   CYS G 313     17.029  23.057 -17.686  1.00  8.19           C
ATOM   1932  O   CYS G 313     17.246  24.212 -17.319  1.00  8.07           O
ATOM   1933  N   TRP G 314     15.832  22.485 -17.634  1.00  7.93           N
ATOM   1934  CA  TRP G 314     14.663  23.177 -17.125  1.00  7.80           C
ATOM   1935  CB  TRP G 314     14.110  24.131 -18.184  1.00  8.13           C
ATOM   1936  CG  TRP G 314     13.856  23.474 -19.505  1.00  9.09           C
ATOM   1937  CD1 TRP G 314     12.657  23.036 -19.985  1.00 10.26           C
ATOM   1938  NE1 TRP G 314     12.807  22.540 -21.257  1.00 10.86           N
ATOM   1939  CE2 TRP G 314     14.121  22.661 -21.628  1.00 10.68           C
ATOM   1940  CD2 TRP G 314     14.813  23.243 -20.547  1.00 10.49           C
ATOM   1941  CE3 TRP G 314     16.185  23.483 -20.675  1.00 11.67           C
ATOM   1942  CZ3 TRP G 314     16.814  23.119 -21.850  1.00 12.98           C
ATOM   1943  CH2 TRP G 314     16.104  22.513 -22.894  1.00 12.74           C
ATOM   1944  CZ2 TRP G 314     14.758  22.286 -22.807  1.00 11.73           C
ATOM   1945  C   TRP G 314     13.603  22.153 -16.742  1.00  7.34           C
ATOM   1946  O   TRP G 314     13.578  21.044 -17.275  1.00  7.47           O
ATOM   1947  N   LYS G 315     12.783  22.500 -15.757  1.00  6.75           N
ATOM   1948  CA  LYS G 315     11.667  21.654 -15.363  1.00  6.37           C
ATOM   1949  CB  LYS G 315     11.631  21.475 -13.844  1.00  6.38           C
ATOM   1950  CG  LYS G 315     10.746  20.331 -13.374  1.00  6.55           C
ATOM   1951  CD  LYS G 315     10.695  20.252 -11.854  1.00  8.01           C
ATOM   1952  CE  LYS G 315      9.848  19.077 -11.383  1.00  8.78           C
ATOM   1953  NZ  LYS G 315      9.177  19.368 -10.085  1.00 10.21           N
ATOM   1954  C   LYS G 315     10.348  22.231 -15.855  1.00  6.32           C
ATOM   1955  O   LYS G 315     10.123  23.441 -15.798  1.00  6.21           O
ATOM   1956  N   LEU G 316      9.529  21.370 -16.443  1.00  6.58           N
```

```
ATOM   1957  CA  LEU G 316      8.273  21.796 -17.027   1.00  7.02           C
ATOM   1958  CB  LEU G 316      8.140  21.253 -18.448   1.00  6.64           C
ATOM   1959  CG  LEU G 316      6.756  21.379 -19.086   1.00  6.21           C
ATOM   1960  CD1 LEU G 316      6.358  22.841 -19.221   1.00  5.94           C
ATOM   1961  CD2 LEU G 316      6.730  20.687 -20.439   1.00  6.57           C
ATOM   1962  C   LEU G 316      7.116  21.308 -16.172   1.00  7.77           C
ATOM   1963  O   LEU G 316      6.942  20.105 -15.976   1.00  8.47           O
ATOM   1964  N   HIS G 317      6.363  22.247 -15.613   1.00  8.05           N
ATOM   1965  CA  HIS G 317      5.073  21.923 -15.031   1.00  8.21           C
ATOM   1966  CB  HIS G 317      4.956  22.485 -13.614   1.00  9.04           C
ATOM   1967  CG  HIS G 317      6.260  22.565 -12.886   1.00 11.41           C
ATOM   1968  ND1 HIS G 317      6.606  21.691 -11.877   1.00 13.62           N
ATOM   1969  CE1 HIS G 317      7.781  22.035 -11.383   1.00 14.91           C
ATOM   1970  NE2 HIS G 317      8.208  23.105 -12.029   1.00 14.25           N
ATOM   1971  CD2 HIS G 317      7.271  23.462 -12.969   1.00 12.67           C
ATOM   1972  C   HIS G 317      3.943  22.453 -15.894   1.00  7.39           C
ATOM   1973  O   HIS G 317      4.132  23.381 -16.680   1.00  7.23           O
ATOM   1974  N   THR G 318      2.736  22.006 -15.580   1.00  7.11           N
ATOM   1975  CA  THR G 318      1.704  21.826 -16.583   1.00  6.56           C
ATOM   1976  CB  THR G 318      1.869  20.474 -17.309   1.00  6.28           C
ATOM   1977  OG1 THR G 318      2.413  20.694 -18.616   1.00  6.33           O
ATOM   1978  CG2 THR G 318      0.534  19.761 -17.435   1.00  6.52           C
ATOM   1979  C   THR G 318      0.349  21.865 -15.893   1.00  6.58           C
ATOM   1980  O   THR G 318      0.104  21.105 -14.958   1.00  6.67           O
ATOM   1981  N   SER G 319     -0.501  22.802 -16.301   1.00  6.81           N
ATOM   1982  CA  SER G 319     -1.840  22.911 -15.730   1.00  7.31           C
ATOM   1983  CB  SER G 319     -1.929  24.106 -14.779   1.00  7.14           C
ATOM   1984  OG  SER G 319     -3.255  24.292 -14.314   1.00  6.84           O
ATOM   1985  C   SER G 319     -2.922  23.006 -16.800   1.00  7.93           C
ATOM   1986  O   SER G 319     -2.717  23.624 -17.845   1.00  8.65           O
ATOM   1987  N   PRO G 320     -4.104  22.440 -16.514   1.00  8.08           N
ATOM   1988  CA  PRO G 320     -5.172  22.399 -17.500   1.00  8.34           C
ATOM   1989  CB  PRO G 320     -6.336  21.738 -16.743   1.00  7.99           C
ATOM   1990  CG  PRO G 320     -5.908  21.662 -15.304   1.00  8.01           C
ATOM   1991  CD  PRO G 320     -4.422  21.635 -15.324   1.00  8.10           C
ATOM   1992  C   PRO G 320     -5.564  23.793 -17.984   1.00  9.03           C
ATOM   1993  O   PRO G 320     -5.261  24.788 -17.325   1.00  8.74           O
ATOM   1994  N   LEU G 321     -6.134  23.854 -19.184   1.00 10.31           N
ATOM   1995  CA  LEU G 321     -6.366  25.113 -19.885   1.00 11.63           C
ATOM   1996  CB  LEU G 321     -5.207  25.402 -20.848   1.00 11.31           C
ATOM   1997  CG  LEU G 321     -4.949  26.848 -21.291   1.00 10.97           C
ATOM   1998  CD1 LEU G 321     -4.174  26.884 -22.600   1.00 10.04           C
ATOM   1999  CD2 LEU G 321     -6.241  27.639 -21.416   1.00 10.69           C
ATOM   2000  C   LEU G 321     -7.683  25.027 -20.662   1.00 12.92           C
ATOM   2001  O   LEU G 321     -7.890  24.095 -21.439   1.00 13.29           O
ATOM   2002  N   CYS G 322     -8.593  25.964 -20.400   1.00 13.39           N
ATOM   2003  CA  CYS G 322     -9.923  25.955 -21.017   1.00 14.16           C
ATOM   2004  CB  CYS G 322    -10.994  25.588 -19.990   1.00 13.72           C
ATOM   2005  SG  CYS G 322    -10.587  24.180 -18.943   1.00 13.42           S
ATOM   2006  C   CYS G 322    -10.274  27.299 -21.650   1.00 15.46           C
ATOM   2007  O   CYS G 322    -10.048  28.352 -21.054   1.00 15.94           O
ATOM   2008  N   THR G 323    -10.985  27.241 -22.773   1.00 16.70           N
ATOM   2009  CA  THR G 323    -11.694  28.395 -23.326   1.00 17.84           C
ATOM   2010  CB  THR G 323    -12.389  28.017 -24.647   1.00 17.50           C
ATOM   2011  OG1 THR G 323    -12.703  26.618 -24.638   1.00 15.70           O
ATOM   2012  CG2 THR G 323    -11.486  28.322 -25.831   1.00 18.05           C
ATOM   2013  C   THR G 323    -12.756  28.915 -22.359   1.00 19.54           C
ATOM   2014  O   THR G 323    -13.178  28.188 -21.461   1.00 19.84           O
ATOM   2015  N   THR G 324    -13.354  30.061 -22.684   1.00 21.17           N
ATOM   2016  CA  THR G 324    -14.592  30.460 -22.017   1.00 22.89           C
```

ATOM 2017 CB THR G 324 -14.343 31.388 -20.821 1.00 22.69 C
ATOM 2018 OG1 THR G 324 -12.937 31.469 -20.560 1.00 22.10 O
ATOM 2019 CG2 THR G 324 -15.061 30.857 -19.587 1.00 22.03 C
ATOM 2020 C THR G 324 -15.712 31.033 -22.885 1.00 24.39 C
ATOM 2021 O THR G 324 -16.838 31.194 -22.414 1.00 24.53 O
ATOM 2022 N ASN G 325 -15.427 31.299 -24.155 1.00 25.72 N
ATOM 2023 CA ASN G 325 -16.490 31.473 -25.144 1.00 27.01 C
ATOM 2024 CB ASN G 325 -16.986 32.922 -25.170 1.00 27.37 C
ATOM 2025 CG ASN G 325 -18.079 33.184 -24.148 1.00 28.46 C
ATOM 2026 OD1 ASN G 325 -19.267 33.164 -24.471 1.00 30.37 O
ATOM 2027 ND2 ASN G 325 -17.678 33.444 -22.909 1.00 28.78 N
ATOM 2028 C ASN G 325 -16.075 31.032 -26.543 1.00 27.36 C
ATOM 2029 O ASN G 325 -14.887 30.902 -26.837 1.00 27.94 O
ATOM 2030 N SER G 330 -15.165 27.730 -23.322 1.00 35.76 N
ATOM 2031 CA SER G 330 -16.301 26.817 -23.281 1.00 35.01 C
ATOM 2032 CB SER G 330 -17.459 27.366 -24.117 1.00 35.47 C
ATOM 2033 OG SER G 330 -17.137 27.368 -25.497 1.00 33.31 O
ATOM 2034 C SER G 330 -15.906 25.431 -23.779 1.00 34.35 C
ATOM 2035 O SER G 330 -15.111 25.299 -24.709 1.00 34.33 O
ATOM 2036 N ASN G 331 -16.430 24.399 -23.128 1.00 32.48 N
ATOM 2037 CA ASN G 331 -16.609 23.102 -23.770 1.00 30.72 C
ATOM 2038 CB ASN G 331 -17.432 23.247 -25.060 1.00 31.31 C
ATOM 2039 CG ASN G 331 -18.924 23.445 -24.801 1.00 32.11 C
ATOM 2040 OD1 ASN G 331 -19.426 23.149 -23.716 1.00 32.54 O
ATOM 2041 ND2 ASN G 331 -19.651 23.849 -25.838 1.00 31.30 N
ATOM 2042 C ASN G 331 -15.298 22.357 -24.074 1.00 28.71 C
ATOM 2043 O ASN G 331 -15.322 21.324 -24.741 1.00 29.07 O
ATOM 2044 N ILE G 332 -14.155 22.896 -23.649 1.00 25.44 N
ATOM 2045 CA ILE G 332 -12.868 22.313 -24.053 1.00 21.83 C
ATOM 2046 CB ILE G 332 -12.546 22.613 -25.536 1.00 21.42 C
ATOM 2047 CGI ILE G 332 -11.286 21.867 -25.981 1.00 19.89 C
ATOM 2048 CD1 ILE G 332 -11.573 20.576 -26.724 1.00 17.67 C
ATOM 2049 CG2 ILE G 332 -12.428 24.111 -25.776 1.00 20.61 C
ATOM 2050 C ILE G 332 -11.667 22.657 -23.162 1.00 20.37 C
ATOM 2051 O ILE G 332 -11.388 23.829 -22.903 1.00 19.95 O
ATOM 2052 N CYS G 333 -10.896 21.634 -22.794 1.00 18.27 N
ATOM 2053 CA CYS G 333 -9.666 21.842 -22.031 1.00 16.47 C
ATOM 2054 CB CYS G 333 -9.923 21.703 -20.529 1.00 16.14 C
ATOM 2055 SG CYS G 333 -11.374 22.595 -19.936 1.00 17.09 S
ATOM 2056 C CYS G 333 -8.480 20.967 -22.450 1.00 15.73 C
ATOM 2057 O CYS G 333 -8.652 19.820 -22.871 1.00 15.43 O
ATOM 2058 N LEU G 334 -7.298 21.425 -22.047 1.00 15.06 N
ATOM 2059 CA LEU G 334 -6.022 20.883 -22.498 1.00 13.79 C
ATOM 2060 CB LEU G 334 -5.346 21.857 -23.472 1.00 13.39 C
ATOM 2061 CG LEU G 334 -5.891 21.998 -24.895 1.00 13.93 C
ATOM 2062 CD1 LEU G 334 -4.764 22.327 -25.858 1.00 14.20 C
ATOM 2063 CD2 LEU G 334 -6.617 20.739 -25.331 1.00 14.52 C
ATOM 2064 C LEU G 334 -5.142 20.748 -21.263 1.00 13.22 C
ATOM 2065 O LEU G 334 -5.033 21.685 -20.472 1.00 13.31 O
ATOM 2066 N THR G 335 -4.417 19.640 -21.169 1.00 12.58 N
ATOM 2067 CA THR G 335 -3.277 19.561 -20.268 1.00 12.17 C
ATOM 2068 CB THR G 335 -3.612 18.748 -19.001 1.00 12.02 C
ATOM 2069 OG1 THR G 335 -5.021 18.815 -18.744 1.00 12.64 O
ATOM 2070 CG2 THR G 335 -2.858 19.295 -17.803 1.00 11.47 C
ATOM 2071 C THR G 335 -2.093 18.930 -20.986 1.00 11.97 C
ATOM 2072 O THR G 335 -2.258 17.980 -21.751 1.00 11.93 O
ATOM 2073 N ARG G 336 -0.942 19.586 -20.892 1.00 11.60 N
ATOM 2074 CA ARG G 336 0.254 19.122 -21.578 1.00 12.15 C
ATOM 2075 CB ARG G 336 1.293 20.239 -21.640 1.00 12.16 C
ATOM 2076 CG ARG G 336 2.162 20.208 -22.879 1.00 12.67 C

ATOM 2077 CD ARG G 336 2.261 21.590 -23.500 1.00 12.52 C
ATOM 2078 NE ARG G 336 3.341 22.374 -22.912 1.00 12.35 N
ATOM 2079 CZ ARG G 336 4.632 22.136 -23.117 1.00 12.54 C
ATOM 2080 NH1 ARG G 336 5.006 21.109 -23.867 1.00 12.38 N
ATOM 2081 NH2 ARG G 336 5.549 22.904 -22.545 1.00 12.48 N
ATOM 2082 C ARG G 336 0.841 17.907 -20.872 1.00 12.71 C
ATOM 2083 O ARG G 336 1.185 17.974 -19.693 1.00 12.62 O
ATOM 2084 N THR G 337 0.885 16.779 -21.574 1.00 13.70 N
ATOM 2085 CA THR G 337 1.284 15.514 -20.964 1.00 14.91 C
ATOM 2086 CB THR G 337 1.084 14.331 -21.931 1.00 15.27 C
ATOM 2087 OG1 THR G 337 -0.264 14.329 -22.421 1.00 16.65 O
ATOM 2088 CG2 THR G 337 1.370 13.015 -21.226 1.00 15.94 C
ATOM 2089 C THR G 337 2.744 15.546 -20.519 1.00 15.16 C
ATOM 2090 O THR G 337 3.069 15.159 -19.396 1.00 15.60 O
ATOM 2091 N ASP G 338 3.623 15.968 -21.424 1.00 15.15 N
ATOM 2092 CA ASP G 338 5.055 15.721 -21.283 1.00 15.52 C
ATOM 2093 CB ASP G 338 5.781 15.935 -22.613 1.00 16.81 C
ATOM 2094 CG ASP G 338 5.051 16.899 -23.529 1.00 20.57 C
ATOM 2095 OD1 ASP G 338 5.160 16.744 -24.763 1.00 23.00 O
ATOM 2096 OD2 ASP G 338 4.290 17.747 -23.017 1.00 22.92 O
ATOM 2097 C ASP G 338 5.674 16.595 -20.201 1.00 14.21 C
ATOM 2098 O ASP G 338 6.235 17.654 -20.486 1.00 14.00 O
ATOM 2099 N ARG G 339 5.617 16.113 -18.965 1.00 12.79 N
ATOM 2100 CA ARG G 339 6.087 16.877 -17.822 1.00 11.71 C
ATOM 2101 CB ARG G 339 5.108 16.747 -16.665 1.00 11.73 C
ATOM 2102 CG ARG G 339 3.773 17.383 -16.931 1.00 12.49 C
ATOM 2103 CD ARG G 339 3.116 17.761 -15.633 1.00 13.24 C
ATOM 2104 NE ARG G 339 1.712 17.370 -15.607 1.00 12.04 N
ATOM 2105 CZ ARG G 339 0.844 17.804 -14.703 1.00 11.74 C
ATOM 2106 NH1 ARG G 339 1.259 18.579 -13.710 1.00 13.43 N
ATOM 2107 NH2 ARG G 339 -0.427 17.428 -14.759 1.00 9.80 N
ATOM 2108 C ARG G 339 7.443 16.388 -17.365 1.00 11.16 C
ATOM 2109 O ARG G 339 7.703 15.185 -17.376 1.00 11.37 O
ATOM 2110 N GLY G 340 8.141 17.269 -16.660 1.00 10.43 N
ATOM 2111 CA GLY G 340 9.340 16.886 -15.933 1.00 9.52 C
ATOM 2112 C GLY G 340 10.559 17.608 -16.465 1.00 8.80 C
ATOM 2113 O GLY G 340 10.475 18.759 -16.903 1.00 8.56 O
ATOM 2114 N TRP G 341 11.700 16.935 -16.411 1.00 8.25 N
ATOM 2115 CA TRP G 341 12.965 17.581 -16.704 1.00 7.98 C
ATOM 2116 CB TRP G 341 14.089 16.966 -15.879 1.00 7.79 C
ATOM 2117 CG TRP G 341 14.110 17.460 -14.478 1.00 7.67 C
ATOM 2118 CD1 TRP G 341 13.519 16.869 -13.399 1.00 8.12 C
ATOM 2119 NE1 TRP G 341 13.686 17.648 -12.283 1.00 8.60 N
ATOM 2120 CE2 TRP G 341 14.304 18.815 -12.649 1.00 7.57 C
ATOM 2121 CD2 TRP G 341 14.536 18.754 -14.037 1.00 7.52 C
ATOM 2122 CE3 TRP G 341 15.176 19.830 -14.663 1.00 7.86 C
ATOM 2123 CZ3 TRP G 341 15.535 20.925 -13.898 1.00 7.14 C
ATOM 2124 CH2 TRP G 341 15.279 20.962 -12.521 1.00 6.39 C
ATOM 2125 CZ2 TRP G 341 14.663 19.919 -11.880 1.00 7.30 C
ATOM 2126 C TRP G 341 13.286 17.490 -18.180 1.00 8.26 C
ATOM 2127 O TRP G 341 13.320 16.402 -18.755 1.00 8.35 O
ATOM 2128 N TYR G 342 13.400 18.649 -18.811 1.00 8.44 N
ATOM 2129 CA TYR G 342 14.197 18.777 -20.012 1.00 8.53 C
ATOM 2130 CB TYR G 342 13.486 19.670 -21.015 1.00 8.43 C
ATOM 2131 CG TYR G 342 12.099 19.192 -21.318 1.00 9.17 C
ATOM 2132 CD1 TYR G 342 11.097 19.299 -20.363 1.00 10.32 C
ATOM 2133 CE1 TYR G 342 9.849 18.765 -20.582 1.00 10.99 C
ATOM 2134 CZ TYR G 342 9.618 18.033 -21.724 1.00 11.00 C
ATOM 2135 OH TYR G 342 8.365 17.521 -21.964 1.00 12.82 O
ATOM 2136 CE2 TYR G 342 10.626 17.838 -22.643 1.00 10.67 C

ATOM 2137 CD2 TYR G 342 11.871 18.365 -22.403 1.00 10.41 C
ATOM 2138 C TYR G 342 15.550 19.359 -19.680 1.00 8.64 C
ATOM 2139 O TYR G 342 15.754 19.906 -18.596 1.00 8.40 O
ATOM 2140 N CYS G 343 16.460 19.284 -20.641 1.00 8.87 N
ATOM 2141 CA CYS G 343 17.875 19.346 -20.332 1.00 9.35 C
ATOM 2142 CB CYS G 343 18.190 18.501 -19.092 1.00 9.17 C
ATOM 2143 SG CYS G 343 19.879 18.684 -18.466 1.00 11.88 S
ATOM 2144 C CYS G 343 18.722 18.920 -21.524 1.00 9.42 C
ATOM 2145 O CYS G 343 18.505 17.856 -22.103 1.00 9.96 O
ATOM 2146 N ASP G 344 19.534 19.857 -22.005 1.00 9.36 N
ATOM 2147 CA ASP G 344 20.127 19.778 -23.338 1.00 9.24 C
ATOM 2148 CB ASP G 344 20.797 21.108 -23.703 1.00 9.34 C
ATOM 2149 CG ASP G 344 19.874 22.037 -24.474 1.00 10.72 C
ATOM 2150 OD1 ASP G 344 19.475 21.677 -25.602 1.00 13.93 O
ATOM 2151 OD2 ASP G 344 19.548 23.127 -23.954 1.00 11.87 O
ATOM 2152 C ASP G 344 21.148 18.651 -23.425 1.00 9.09 C
ATOM 2153 O ASP G 344 22.100 18.605 -22.646 1.00 9.39 O
ATOM 2154 N ASN G 345 21.038 17.843 -24.474 1.00 9.13 N
ATOM 2155 CA ASN G 345 22.114 16.939 -24.849 1.00 9.52 C
ATOM 2156 CB ASN G 345 21.589 15.509 -24.978 1.00 9.61 C
ATOM 2157 CG ASN G 345 22.640 14.472 -24.643 1.00 9.21 C
ATOM 2158 OD1 ASN G 345 23.121 14.400 -23.512 1.00 6.21 O
ATOM 2159 ND2 ASN G 345 23.032 13.685 -25.638 1.00 11.05 N
ATOM 2160 C ASN G 345 22.772 17.381 -26.149 1.00 10.06 C
ATOM 2161 O ASN G 345 22.506 18.476 -26.644 1.00 11.10 O
ATOM 2162 N ALA G 346 23.644 16.539 -26.692 1.00 9.74 N
ATOM 2163 CA ALA G 346 24.410 16.904 -27.877 1.00 9.58 C
ATOM 2164 CB ALA G 346 25.241 15.723 -28.356 1.00 9.60 C
ATOM 2165 C ALA G 346 23.498 17.406 -28.994 1.00 9.66 C
ATOM 2166 O ALA G 346 22.977 16.618 -29.782 1.00 9.39 O
ATOM 2167 N GLY G 347 23.290 18.720 -29.038 1.00 10.04 N
ATOM 2168 CA GLY G 347 22.598 19.358 -30.157 1.00 10.68 C
ATOM 2169 C GLY G 347 21.105 19.098 -30.137 1.00 10.90 C
ATOM 2170 O GLY G 347 20.366 19.569 -31.002 1.00 11.46 O
ATOM 2171 N SER G 348 20.691 18.235 -29.219 1.00 10.30 N
ATOM 2172 CA SER G 348 19.301 17.838 -29.098 1.00 9.94 C
ATOM 2173 CB SER G 348 19.103 16.421 -29.639 1.00 9.88 C
ATOM 2174 OG SER G 348 19.440 16.352 -31.013 1.00 10.09 O
ATOM 2175 C SER G 348 18.950 17.883 -27.624 1.00 9.60 C
ATOM 2176 O SER G 348 19.775 18.267 -26.796 1.00 9.59 O
ATOM 2177 N VAL G 349 17.723 17.505 -27.292 1.00 9.54 N
ATOM 2178 CA VAL G 349 17.254 17.643 -25.925 1.00 9.56 C
ATOM 2179 CB VAL G 349 16.091 18.639 -25.823 1.00 9.28 C
ATOM 2180 CGI VAL G 349 15.814 18.985 -24.360 1.00 9.24 C
ATOM 2181 CG2 VAL G 349 16.391 19.892 -26.641 1.00 9.94 C
ATOM 2182 C VAL G 349 16.824 16.309 -25.341 1.00 9.59 C
ATOM 2183 O VAL G 349 16.029 15.585 -25.939 1.00 9.69 O
ATOM 2184 N SER G 350 17.288 16.029 -24.130 1.00 9.93 N
ATOM 2185 CA SER G 350 16.915 14.800 -23.451 1.00 10.44 C
ATOM 2186 CB SER G 350 18.146 14.108 -22.858 1.00 10.04 C
ATOM 2187 OG SER G 350 18.768 13.261 -23.812 1.00 8.41 O
ATOM 2188 C SER G 350 15.854 15.039 -22.381 1.00 11.45 C
ATOM 2189 O SER G 350 15.882 16.041 -21.665 1.00 11.58 O
ATOM 2190 N PHE G 351 14.893 14.126 -22.318 1.00 12.28 N
ATOM 2191 CA PHE G 351 13.722 14.291 -21.469 1.00 13.04 C
ATOM 2192 CB PHE G 351 12.468 14.485 -22.321 1.00 12.87 C
ATOM 2193 CG PHE G 351 11.192 14.388 -21.539 1.00 13.52 C
ATOM 2194 CD1 PHE G 351 11.026 15.127 -20.378 1.00 13.76 C
ATOM 2195 CE1 PHE G 351 9.857 15.044 -19.648 1.00 14.10 C
ATOM 2196 CZ PHE G 351 8.855 14.175 -20.045 1.00 14.07 C

```
ATOM   2197  CE2 PHE G 351      9.028  13.395 -21.172  1.00 14.14           C
ATOM   2198  CD2 PHE G 351     10.202  13.489 -21.903  1.00 13.92           C
ATOM   2199  C   PHE G 351     13.526  13.082 -20.563  1.00 13.84           C
ATOM   2200  O   PHE G 351     13.246  11.979 -21.038  1.00 13.96           O
ATOM   2201  N   PHE G 352     13.463  13.340 -19.263  1.00 14.72           N
ATOM   2202  CA  PHE G 352     13.315  12.275 -18.286  1.00 15.98           C
ATOM   2203  CB  PHE G 352     14.429  12.360 -17.243  1.00 15.75           C
ATOM   2204  CG  PHE G 352     15.720  12.912 -17.780  1.00 15.51           C
ATOM   2205  CD1 PHE G 352     15.899  14.279 -17.924  1.00 15.05           C
ATOM   2206  CE1 PHE G 352     17.098  14.793 -18.375  1.00 14.05           C
ATOM   2207  CZ  PHE G 352     18.126  13.938 -18.719  1.00 13.28           C
ATOM   2208  CE2 PHE G 352     17.948  12.570 -18.615  1.00 13.71           C
ATOM   2209  CD2 PHE G 352     16.745  12.064 -18.163  1.00 14.94           C
ATOM   2210  C   PHE G 352     11.952  12.360 -17.612  1.00 17.56           C
ATOM   2211  O   PHE G 352     11.591  13.401 -17.066  1.00 17.74           O
ATOM   2212  N   PRO G 353     11.165  11.280 -17.705  1.00 19.05           N
ATOM   2213  CA  PRO G 353      9.719  11.355 -17.537  1.00 20.40           C
ATOM   2214  CB  PRO G 353      9.220  10.060 -18.189  1.00 20.26           C
ATOM   2215  CG  PRO G 353     10.352   9.587 -19.046  1.00 19.71           C
ATOM   2216  CD  PRO G 353     11.580  10.012 -18.325  1.00 18.97           C
ATOM   2217  C   PRO G 353      9.291  11.404 -16.072  1.00 21.94           C
ATOM   2218  O   PRO G 353      8.222  11.935 -15.768  1.00 22.29           O
ATOM   2219  N   GLN G 354     10.105  10.851 -15.175  1.00 23.38           N
ATOM   2220  CA  GLN G 354      9.731  10.792 -13.761  1.00 24.64           C
ATOM   2221  CB  GLN G 354      9.107   9.440 -13.400  1.00 24.93           C
ATOM   2222  CG  GLN G 354      9.407   8.322 -14.376  1.00 26.00           C
ATOM   2223  CD  GLN G 354     10.859   7.909 -14.354  1.00 25.92           C
ATOM   2224  OE1 GLN G 354     11.380   7.473 -13.327  1.00 25.67           O
ATOM   2225  NE2 GLN G 354     11.521   8.030 -15.498  1.00 24.27           N
ATOM   2226  C   GLN G 354     10.823  11.177 -12.759  1.00 24.85           C
ATOM   2227  O   GLN G 354     12.009  10.943 -12.989  1.00 24.51           O
ATOM   2228  N   ALA G 355     10.392  11.709 -11.618  1.00 25.22           N
ATOM   2229  CA  ALA G 355     11.296  12.264 -10.619  1.00 25.34           C
ATOM   2230  CB  ALA G 355     10.565  12.449  -9.296  1.00 25.09           C
ATOM   2231  C   ALA G 355     12.531  11.390 -10.427  1.00 24.92           C
ATOM   2232  O   ALA G 355     13.646  11.791 -10.766  1.00 25.23           O
ATOM   2233  N   GLU G 356     12.339  10.258  -9.755  1.00 23.93           N
ATOM   2234  CA  GLU G 356     13.282   9.141  -9.803  1.00 22.77           C
ATOM   2235  CB  GLU G 356     12.642   7.925 -10.474  1.00 23.22           C
ATOM   2236  CG  GLU G 356     11.489   7.338  -9.681  1.00 26.33           C
ATOM   2237  CD  GLU G 356     11.607   7.632  -8.199  1.00 30.93           C
ATOM   2238  OE1 GLU G 356     11.148   8.711  -7.764  1.00 31.97           O
ATOM   2239  OE2 GLU G 356     12.276   6.846  -7.494  1.00 32.21           O
ATOM   2240  C   GLU G 356     14.591   9.493 -10.492  1.00 21.31           C
ATOM   2241  O   GLU G 356     15.656   9.462  -9.876  1.00 21.01           O
ATOM   2242  N   THR G 357     14.511  9.752 -11.791  1.00 19.51           N
ATOM   2243  CA  THR G 357     15.690   9.787 -12.639  1.00 17.55           C
ATOM   2244  CB  THR G 357     15.305   9.928 -14.114  1.00 17.30           C
ATOM   2245  OG1 THR G 357     13.908   9.660 -14.273  1.00 17.32           O
ATOM   2246  CG2 THR G 357     16.099   8.958 -14.957  1.00 17.72           C
ATOM   2247  C   THR G 357     16.596  10.949 -12.262  1.00 16.62           C
ATOM   2248  O   THR G 357     17.761  10.991 -12.655  1.00 17.29           O
ATOM   2249  N   CYS G 358     16.028  11.935 -11.579  1.00 14.88           N
ATOM   2250  CA  CYS G 358     16.684  13.225 -11.440  1.00 13.15           C
ATOM   2251  CB  CYS G 358     16.025  14.262 -12.349  1.00 13.04           C
ATOM   2252  SG  CYS G 358     16.175  13.900 -14.114  1.00 14.02           S
ATOM   2253  C   CYS G 358     16.711  13.714  -9.997  1.00 12.08           C
ATOM   2254  O   CYS G 358     15.705  13.661  -9.289  1.00 12.15           O
ATOM   2255  N   LYS G 359     17.890  14.140  -9.554  1.00 11.35           N
ATOM   2256  CA  LYS G 359     18.024  14.888  -8.311  1.00 11.01           C
```

ATOM 2257 CB LYS G 359 18.968 14.165 -7.353 1.00 11.16 C
ATOM 2258 CG LYS G 359 19.450 12.824 -7.857 1.00 13.28 C
ATOM 2259 CD LYS G 359 19.029 11.720 -6.912 1.00 16.1 1 C
ATOM 2260 CE LYS G 359 19.561 10.378 -7.366 1.00 17.91 C
ATOM 2261 NZ LYS G 359 18.972 9.264 -6.575 1.00 20.99 N
ATOM 2262 C LYS G 359 18.561 16.282 -8.584 1.00 10.46 C
ATOM 2263 O LYS G 359 19.145 16.533 -9.637 1.00 10.70 O
ATOM 2264 N VAL G 360 18.526 17.128 -7.564 1.00 9.99 N
ATOM 2265 CA VAL G 360 18.797 18.538 -7.763 1.00 9.84 C
ATOM 2266 CB VAL G 360 17.573 19.270 -8.346 1.00 9.42 C
ATOM 2267 CGI VAL G 360 16.360 19.095 -7.442 1.00 10.07 C
ATOM 2268 CG2 VAL G 360 17.886 20.740 -8.572 1.00 9.56 C
ATOM 2269 C VAL G 360 19.259 19.21 1 -6.478 1.00 9.98 C
ATOM 2270 O VAL G 360 18.707 18.970 -5.405 1.00 9.96 O
ATOM 2271 N GLN G 361 20.372 19.931 -6.578 1.00 10.39 N
ATOM 2272 CA GLN G 361 20.979 20.583 -5.427 1.00 11.53 C
ATOM 2273 CB GLN G 361 22.220 19.809 -4.971 1.00 12.03 C
ATOM 2274 CG GLN G 361 22.907 20.381 -3.737 1.00 16.44 C
ATOM 2275 CD GLN G 361 23.241 19.314 -2.714 1.00 25. 16 C
ATOM 2276 OE1 GLN G 361 24.398 18.921 -2.564 1.00 29.01 O
ATOM 2277 NE2 GLN G 361 22.220 18.812 -2.029 1.00 27.20 N
ATOM 2278 C GLN G 361 21.373 22.005 -5.794 1.00 11.15 C
ATOM 2279 O GLN G 361 22.354 22.221 -6.506 1.00 11.80 O
ATOM 2280 N SER G 362 20.61 1 22.976 -5.308 1.00 10.90 N
ATOM 2281 CA SER G 362 20.759 24.332 -5.798 1.00 10.30 C
ATOM 2282 CB SER G 362 22.208 24.792 -5.625 1.00 10.47 C
ATOM 2283 OG SER G 362 22.406 26.082 -6.179 1.00 11.17 O
ATOM 2284 C SER G 362 20.385 24.348 -7.272 1.00 9.58 C
ATOM 2285 O SER G 362 19.409 23.717 -7.677 1.00 9.48 O
ATOM 2286 N ASN G 363 21.256 24.926 -8.089 1.00 9.12 N
ATOM 2287 CA ASN G 363 21.023 24.985 -9.525 1.00 8.73 C
ATOM 2288 CB ASN G 363 21.537 26.308 -10.085 1.00 9.01 C
ATOM 2289 CG ASN G 363 23.018 26.497 -9.849 1.00 9.29 C
ATOM 2290 OD1 ASN G 363 23.681 25.636 -9.270 1.00 9.82 O
ATOM 2291 ND2 ASN G 363 23.555 27.615 -10.323 1.00 10.08 N
ATOM 2292 C ASN G 363 21.701 23.822 -10.237 1.00 8.12 C
ATOM 2293 O ASN G 363 21.961 23.881 -11.439 1.00 8.10 O
ATOM 2294 N ARG G 364 22.103 22.828 -9.453 1.00 7.20 N
ATOM 2295 CA ARG G 364 22.733 21.628 -9.984 1.00 6.82 C
ATOM 2296 CB ARG G 364 23.843 21.154 -9.044 1.00 6.91 C
ATOM 2297 CG ARG G 364 25.1 10 20.721 -9.754 1.00 7.92 C
ATOM 2298 CD ARG G 364 25.588 21.797 -10.709 1.00 8.20 C
ATOM 2299 NE ARG G 364 25.809 21.275 -12.053 1.00 8.70 N
ATOM 2300 CZ ARG G 364 26.690 21.777 -12.910 1.00 8.88 C
ATOM 2301 NHl ARG G 364 27.407 22.843 -12.578 1.00 8.57 N
ATOM 2302 NH2 ARG G 364 26.840 21.228 -14. 107 1.00 10.59 N
ATOM 2303 C ARG G 364 21.703 20.519 -10.166 1.00 6.58 C
ATOM 2304 O ARG G 364 20.980 20.173 -9.233 1.00 6.65 O
ATOM 2305 N VAL G 365 21.719 19.897 -11.341 1.00 6.64 N
ATOM 2306 CA VAL G 365 20.802 18.805 -11.658 1.00 6.54 C
ATOM 2307 CB VAL G 365 19.823 19.208 -12.782 1.00 5.95 C
ATOM 2308 CGI VAL G 365 19.069 17.993 -13.302 1.00 5.48 C
ATOM 2309 CG2 VAL G 365 18.861 20.277 -12.291 1.00 6.22 C
ATOM 2310 C VAL G 365 21.569 17.549 -12.089 1.00 7.35 C
ATOM 231 1 O VAL G 365 22.61 1 17.641 -12.740 1.00 8.33 O
ATOM 2312 N PHE G 366 21.009 16.380 -11.781 1.00 7.37 N
ATOM 2313 CA PHE G 366 21.654 15.097 -12.072 1.00 7.44 C
ATOM 2314 CB PHE G 366 22.371 14.567 -10.822 1.00 7.30 C
ATOM 2315 CG PHE G 366 23.464 15.468 -10.314 1.00 6.70 C
ATOM 2316 CD1 PHE G 366 23.160 16.576 -9.538 1.00 6.70 C

```
ATOM   2317  CE1 PHE G 366      24.162  17.406  -9.068  1.00  5.94           C
ATOM   2318  CZ  PHE G 366      25.487  17.053  -9.244  1.00  5.71           C
ATOM   2319  CE2 PHE G 366      25.804  15.897  -9.935  1.00  5.96           C
ATOM   2320  CD2 PHE G 366      24.793  15.094 -10.437  1.00  6.52           C
ATOM   2321  C   PHE G 366      20.626  14.059 -12.546  1.00  7.45           C
ATOM   2322  O   PHE G 366      19.770  13.635 -11.769  1.00  7.45           O
ATOM   2323  N   CYS G 367      20.783  13.569 -13.777  1.00  8.00           N
ATOM   2324  CA  CYS G 367      19.838  12.602 -14.369  1.00  8.90           C
ATOM   2325  CB  CYS G 367      18.879  13.313 -15.335  1.00  9.46           C
ATOM   2326  SG  CYS G 367      17.966  14.707 -14.624  1.00 10.79           S
ATOM   2327  C   CYS G 367      20.563  11.445 -15.089  1.00  9.09           C
ATOM   2328  O   CYS G 367      21.751  11.556 -15.396  1.00  9.24           O
ATOM   2329  N   ASP G 368      19.864  10.330 -15.323  1.00  9.54           N
ATOM   2330  CA  ASP G 368      20.480   9.110 -15.890  1.00 10.55           C
ATOM   2331  CB  ASP G 368      20.253   7.906 -14.962  1.00 10.53           C
ATOM   2332  CG  ASP G 368      21.043   6.674 -15.386  1.00 11.11           C
ATOM   2333  OD1 ASP G 368      21.241   6.475 -16.603  1.00 11.42           O
ATOM   2334  OD2 ASP G 368      21.441   5.892 -14.497  1.00 11.35           O
ATOM   2335  C   ASP G 368      19.947   8.774 -17.285  1.00 11.45           C
ATOM   2336  O   ASP G 368      19.035   7.958 -17.422  1.00 12.05           O
ATOM   2337  N   THR G 369      20.606   9.281 -18.321  1.00 12.41           N
ATOM   2338  CA  THR G 369      20.367   8.772 -19.666  1.00 13.00           C
ATOM   2339  CB  THR G 369      21.685   8.338 -20.361  1.00 12.69           C
ATOM   2340  OG1 THR G 369      22.580   9.456 -20.444  1.00 11.72           O
ATOM   2341  CG2 THR G 369      21.409   7.813 -21.765  1.00 13.33           C
ATOM   2342  C   THR G 369      19.406   7.585 -19.574  1.00 14.13           C
ATOM   2343  O   THR G 369      18.260   7.681 -20.008  1.00 14.72           O
ATOM   2344  N   MET G 370      19.790   6.577 -18.795  1.00 15.25           N
ATOM   2345  CA  MET G 370      19.286   5.221 -18.993  1.00 16.60           C
ATOM   2346  CB  MET G 370      19.132   4.486 -17.664  1.00 17.42           C
ATOM   2347  CG  MET G 370      19.948   3.204 -17.580  1.00 20.31           C
ATOM   2348  SD  MET G 370      19.542   1.991 -18.855  1.00 26.43           S
ATOM   2349  CE  MET G 370      20.369   2.694 -20.281  1.00 24.07           C
ATOM   2350  C   MET G 370      17.997   5.144 -19.811  1.00 16.54           C
ATOM   2351  O   MET G 370      17.975   4.516 -20.870  1.00 16.74           O
ATOM   2352  N   ASN G 371      16.923   5.762 -19.327  1.00 16.35           N
ATOM   2353  CA  ASN G 371      15.648   5.694 -20.042  1.00 16.07           C
ATOM   2354  CB  ASN G 371      14.554   5.050 -19.184  1.00 16.41           C
ATOM   2355  CG  ASN G 371      14.652   3.531 -19.153  1.00 16.71           C
ATOM   2356  OD1 ASN G 371      14.117   2.843 -20.025  1.00 15.75           O
ATOM   2357  ND2 ASN G 371      15.228   3.003 -18.080  1.00 17.76           N
ATOM   2358  C   ASN G 371      15.160   7.004 -20.661  1.00 15.55           C
ATOM   2359  O   ASN G 371      14.132   7.023 -21.334  1.00 15.84           O
ATOM   2360  N   SER G 372      16.006   8.030 -20.612  1.00 14.76           N
ATOM   2361  CA  SER G 372      15.784   9.270 -21.364  1.00 13.91           C
ATOM   2362  CB  SER G 372      17.101  10.025 -21.561  1.00 14.04           C
ATOM   2363  OG  SER G 372      17.984   9.303 -22.405  1.00 15.09           O
ATOM   2364  C   SER G 372      15.111   9.064 -22.717  1.00 13.07           C
ATOM   2365  O   SER G 372      15.417   8.111 -23.437  1.00 13.02           O
ATOM   2366  N   LEU G 373      14.347  10.072 -23.130  1.00 12.23           N
ATOM   2367  CA  LEU G 373      13.882  10.192 -24.508  1.00 11.45           C
ATOM   2368  CB  LEU G 373      12.358  10.365 -24.534  1.00 11.43           C
ATOM   2369  CG  LEU G 373      11.464   9.123 -24.683  1.00 11.04           C
ATOM   2370  CD1 LEU G 373      11.965   7.948 -23.852  1.00 11.76           C
ATOM   2371  CD2 LEU G 373      10.020   9.434 -24.330  1.00 10.49           C
ATOM   2372  C   LEU G 373      14.550  11.392 -25.176  1.00 11.17           C
ATOM   2373  O   LEU G 373      14.658  12.460 -24.574  1.00 11.27           O
ATOM   2374  N   THR G 374      15.011  11.208 -26.411  1.00 10.70           N
ATOM   2375  CA  THR G 374      15.791  12.235 -27.102  1.00 10.23           C
ATOM   2376  CB  THR G 374      16.998  11.634 -27.863  1.00 10.24           C
```

ATOM 2377 OG1 THR G 374 17.406 10.410 -27.239 1.00 11.25 O
ATOM 2378 CG2 THR G 374 18.168 12.612 -27.872 1.00 10.52 C
ATOM 2379 C THR G 374 14.934 13.032 -28.079 1.00 9.54 C
ATOM 2380 O THR G 374 14.316 12.468 -28.983 1.00 9.70 O
ATOM 2381 N LEU G 375 14.965 14.352 -27.935 1.00 8.83 N
ATOM 2382 CA LEU G 375 14.013 15.221 -28.61 1 1.00 7.83 C
ATOM 2383 CB LEU G 375 12.949 15.719 -27.631 1.00 7.38 C
ATOM 2384 CG LEU G 375 12.160 14.689 -26.824 1.00 5.06 C
ATOM 2385 CD1 LEU G 375 11.352 15.385 -25.741 1.00 2.41 C
ATOM 2386 CD2 LEU G 375 11.246 13.885 -27.734 1.00 4.31 C
ATOM 2387 C LEU G 375 14.728 16.416 -29.222 1.00 7.79 C
ATOM 2388 O LEU G 375 15.743 16.872 -28.696 1.00 7.92 O
ATOM 2389 N PRO G 376 14. 102 17.026 -30.234 1.00 7.51 N
ATOM 2390 CA PRO G 376 14.606 18.224 -30.892 1.00 7.90 C
ATOM 2391 CB PRO G 376 13.837 18.238 -32.21 1 1.00 7.90 C
ATOM 2392 CG PRO G 376 12.558 17.556 -31 .891 1.00 7.97 C
ATOM 2393 CD PRO G 376 12.913 16.481 -30.912 1.00 7.40 C
ATOM 2394 C PRO G 376 14.294 19.486 -30.095 1.00 8.35 C
ATOM 2395 O PRO G 376 13.205 19.61 1 -29.533 1.00 8.71 O
ATOM 2396 N SER G 377 15.206 20.451 -30.137 1.00 9.1 1 N
ATOM 2397 CA SER G 377 14.990 21.743 -29.494 1.00 9.91 C
ATOM 2398 CB SER G 377 16.155 22.691 -29.792 1.00 10.23 C
ATOM 2399 OG SER G 377 17.300 2 1.973 -30.222 1.00 10.90 O
ATOM 2400 C SER G 377 13.673 22.377 -29.937 1.00 10.14 C
ATOM 2401 O SER G 377 13.295 23.444 -29.450 1.00 10.08 O
ATOM 2402 N GLU G 378 13.01 1 21.749 -30.906 1.00 10.71 N
ATOM 2403 CA GLU G 378 11.714 22.222 -31.382 1.00 11.40 C
ATOM 2404 CB GLU G 378 11.357 21.569 -32.721 1.00 11.65 C
ATOM 2405 CG GLU G 378 11.978 22.250 -33.933 1.00 13.46 C
ATOM 2406 CD GLU G 378 13.490 22.160 -33.938 1.00 16.20 C
ATOM 2407 OE1 GLU G 378 14.046 21.522 -33.021 1.00 15.73 O
ATOM 2408 OE2 GLU G 378 14.121 22.732 -34.852 1.00 18.38 O
ATOM 2409 C GLU G 378 10.623 21.944 -30.353 1.00 11.27 C
ATOM 2410 O GLU G 378 9.561 22.565 -30.377 1.00 11.28 O
ATOM 241 1 N VAL G 379 10.909 21.031 -29.430 1.00 11.31 N
ATOM 2412 CA VAL G 379 10.053 20.819 -28.269 1.00 11.59 C
ATOM 2413 CB VAL G 379 10.737 19.926 -27.216 1.00 11.27 C
ATOM 2414 CGI VAL G 379 10.100 20.131 -25.850 1.00 11.60 C
ATOM 2415 CG2 VAL G 379 10.667 18.465 -27.631 1.00 11.54 C
ATOM 2416 C VAL G 379 9.665 22.144 -27.620 1.00 12.16 C
ATOM 2417 O VAL G 379 8.541 22.307 -27.146 1.00 12.51 O
ATOM 2418 N ASN G 380 10.587 23.100 -27.634 1.00 12.98 N
ATOM 2419 CA ASN G 380 10.415 24.335 -26.878 1.00 14.00 C
ATOM 2420 CB ASN G 380 11.703 25.156 -26.884 1.00 14.59 C
ATOM 2421 CG ASN G 380 12.829 24.474 -26.138 1.00 17.09 C
ATOM 2422 OD1 ASN G 380 13.073 24.764 -24.966 1.00 20.41 O
ATOM 2423 ND2 ASN G 380 13.432 23.471 -26.767 1.00 18.86 N
ATOM 2424 C ASN G 380 9.242 25.192 -27.349 1.00 13.96 C
ATOM 2425 O ASN G 380 8.640 25.915 -26.555 1.00 14.38 O
ATOM 2426 N LEU G 381 8.994 25.197 -28.655 1.00 13.61 N
ATOM 2427 CA LEU G 381 7.918 26.006 -29.220 1.00 13.72 C
ATOM 2428 CB LEU G 381 7.854 25.829 -30.737 1.00 13.79 C
ATOM 2429 CG LEU G 381 9.183 25.514 -31.424 1.00 14.92 C
ATOM 2430 CD1 LEU G 381 8.969 25.231 -32.902 1.00 15.56 C
ATOM 2431 CD2 LEU G 381 10.171 26.655 -31.230 1.00 15.78 C
ATOM 2432 C LEU G 381 6.590 25.603 -28.600 1.00 13.62 C
ATOM 2433 O LEU G 381 5.600 26.331 -28.682 1.00 13.57 O
ATOM 2434 N CYS G 382 6.590 24.440 -27.963 1.00 13.47 N
ATOM 2435 CA CYS G 382 5.383 23.876 -27.392 1.00 13.57 C
ATOM 2436 CB CYS G 382 5.572 22.380 -27.161 1.00 13.62 C

```
ATOM   2437  SG  CYS G 382      4.877  21.350 -28.457   1.00 15.64           S
ATOM   2438  C   CYS G 382      5.019  24.572 -26.085   1.00 13.33           C
ATOM   2439  O   CYS G 382      3.861  24.561 -25.669   1.00 13.57           O
ATOM   2440  N   ASN G 383      5.999  25.236 -25.480   1.00 13.21           N
ATOM   2441  CA  ASN G 383      5.736  26.114 -24.345   1.00 13.22           C
ATOM   2442  CB  ASN G 383      7.046  26.621 -23.742   1.00 13.18           C
ATOM   2443  CG  ASN G 383      7.979  25.498 -23.349   1.00 13.42           C
ATOM   2444  OD1 ASN G 383      7.560  24.505 -22.755   1.00 13.68           O
ATOM   2445  ND2 ASN G 383      9.255  25.648 -23.682   1.00 14.32           N
ATOM   2446  C   ASN G 383      4.872  27.298 -24.747   1.00 13.28           C
ATOM   2447  O   ASN G 383      4.229  27.925 -23.906   1.00 13.50           O
ATOM   2448  N   VAL G 384      5.000  27.699 -26.005   1.00 13.24           N
ATOM   2449  CA  VAL G 384      4.313  28.878 -26.496   1.00 13.29           C
ATOM   2450  CB  VAL G 384      5.234  29.751 -27.370   1.00 13.28           C
ATOM   2451  CGI VAL G 384      4.414  30.627 -28.302   1.00 13.73           C
ATOM   2452  CG2 VAL G 384      6.145  30.599 -26.495   1.00 12.76           C
ATOM   2453  C   VAL G 384      3.045  28.514 -27.261   1.00 13.57           C
ATOM   2454  O   VAL G 384      2.050  29.233 -27.188   1.00 13.31           O
ATOM   2455  N   ASP G 385      3.056  27.383 -27.960   1.00 14.07           N
ATOM   2456  CA  ASP G 385      1.999  27.121 -28.932   1.00 14.61           C
ATOM   2457  CB  ASP G 385      2.452  27.379 -30.366   1.00 14.71           C
ATOM   2458  CG  ASP G 385      1.436  28.182 -31.154   1.00 16.69           C
ATOM   2459  OD1 ASP G 385      0.270  28.259 -30.713   1.00 18.63           O
ATOM   2460  OD2 ASP G 385      1.807  28.759 -32.197   1.00 19.10           O
ATOM   2461  C   ASP G 385      1.170  25.841 -28.816   1.00 14.63           C
ATOM   2462  O   ASP G 385     -0.043  25.880 -29.017   1.00 14.34           O
ATOM   2463  N   ILE G 386      1.820  24.697 -28.624   1.00 14.54           N
ATOM   2464  CA  ILE G 386      1.116  23.413 -28.688   1.00 14.46           C
ATOM   2465  CB  ILE G 386     -0.230  23.466 -27.928   1.00 13.83           C
ATOM   2466  CGI ILE G 386     -0.004  23.458 -26.415   1.00 13.44           C
ATOM   2467  CD1 ILE G 386     -1.184  23.970 -25.612   1.00 12.39           C
ATOM   2468  CG2 ILE G 386     -1.119  22.301 -28.341   1.00 13.51           C
ATOM   2469  C   ILE G 386      0.791  23.079 -30.134   1.00 14.73           C
ATOM   2470  O   ILE G 386      1.282  22.092 -30.683   1.00 14.68           O
ATOM   2471  N   PHE G 387     -0.191  23.797 -30.667   1.00 14.71           N
ATOM   2472  CA  PHE G 387     -0.462  23.794 -32.092   1.00 14.78           C
ATOM   2473  CB  PHE G 387     -1.889  24.254 -32.366   1.00 14.77           C
ATOM   2474  CG  PHE G 387     -2.906  23.607 -31.479   1.00 14.75           C
ATOM   2475  CD1 PHE G 387     -3.418  24.287 -30.390   1.00 15.03           C
ATOM   2476  CE1 PHE G 387     -4.333  23.684 -29.549   1.00 14.62           C
ATOM   2477  CZ  PHE G 387     -4.683  22.364 -29.747   1.00 14.55           C
ATOM   2478  CE2 PHE G 387     -4.113  21.651 -30.780   1.00 14.68           C
ATOM   2479  CD2 PHE G 387     -3.206  22.265 -31.621   1.00 14.61           C
ATOM   2480  C   PHE G 387      0.526  24.670 -32.837   1.00 14.91           C
ATOM   2481  O   PHE G 387      0.658  25.862 -32.559   1.00 14.86           O
ATOM   2482  N   ASN G 388      1.361  24.007 -33.621   1.00 15.11           N
ATOM   2483  CA  ASN G 388      2.352  24.663 -34.443   1.00 15.38           C
ATOM   2484  CB  ASN G 388      3.362  25.405 -33.570   1.00 14.86           C
ATOM   2485  CG  ASN G 388      4.097  24.480 -32.625   1.00 14.86           C
ATOM   2486  OD1 ASN G 388      5.078  23.840 -33.004   1.00 12.80           O
ATOM   2487  ND2 ASN G 388      3.575  24.338 -31.413   1.00 15.97           N
ATOM   2488  C   ASN G 388      3.057  23.576 -35.229   1.00 16.11           C
ATOM   2489  O   ASN G 388      3.416  22.537 -34.670   1.00 15.92           O
ATOM   2490  N   PRO G 389      3.071  23.722 -36.557   1.00 16.99           N
ATOM   2491  CA  PRO G 389      4.005  22.905 -37.315   1.00 17.40           C
ATOM   2492  CB  PRO G 389      4.169  23.689 -38.618   1.00 17.72           C
ATOM   2493  CG  PRO G 389      3.905  25.099 -38.236   1.00 17.47           C
ATOM   2494  CD  PRO G 389      2.825  25.023 -37.203   1.00 17.05           C
ATOM   2495  C   PRO G 389      5.338  22.827 -36.583   1.00 17.86           C
ATOM   2496  O   PRO G 389      5.638  23.687 -35.755   1.00 18.45           O
```

```
ATOM   2497  N   LYS G 390      6.139  21.817 -36.902  1.00 17.97           N
ATOM   2498  CA  LYS G 390      7.443  21.658 -36.273  1.00 18.06           C
ATOM   2499  CB  LYS G 390      7.947  22.997 -35.730  1.00 17.92           C
ATOM   2500  CG  LYS G 390      8.466  23.945 -36.798  1.00 18.58           C
ATOM   2501  CD  LYS G 390      9.962  23.777 -37.006  1.00 20.61           C
ATOM   2502  CE  LYS G 390     10.562  24.985 -37.707  1.00 2 1.48          C
ATOM   2503  NZ  LYS G 390     10. 191  25.032 -39. 148  1.00 23.16          N
ATOM   2504  C   LYS G 390      7.398  20.623 -35. 156  1.00 18.01           C
ATOM   2505  O   LYS G 390      8.177  19.670 -35. 152  1.00 18.43           O
ATOM   2506  N   TYR G 391      6.481  20.805 -34.213  1.00 17.68           N
ATOM   2507  CA  TYR G 391      6.234  19.780 -33.21 1  1.00 17.33           C
ATOM   2508  CB  TYR G 391      6.862  20. 158 -31.872  1.00 17.42           C
ATOM   2509  CG  TYR G 391      7.485  18.979 -31 .173  1.00 17.27           C
ATOM   2510  CD1 TYR G 391      8.188  18.028 -31 .898  1.00 17.29           C
ATOM   251 1  CE1 TYR G 391      8.672  16.885 -31.297  1.00 17.32           C
ATOM   2512  CZ  TYR G 391      8.408  16.653 -29.965  1.00 16.51           C
ATOM   2513  OH  TYR G 391      8.940  15.541 -29.354  1.00 16.65           O
ATOM   2514  CE2 TYR G 391      7.656  17.552 -29.237  1.00 16.52           C
ATOM   2515  CD2 TYR G 391      7.167  18.687 -29.853  1.00 17.24           C
ATOM   2516  C   TYR G 391      4.757  19.471 -33.034  1.00 17.43           C
ATOM   2517  O   TYR G 391      3.984  20.332 -32.614  1.00 17.70           O
ATOM   2518  N   ASP G 392      4.398  18.202 -33. 196  1.00 17.56           N
ATOM   2519  CA  ASP G 392      3.191  17.693 -32.565  1.00 17.69           C
ATOM   2520  CB  ASP G 392      2.610  16.498 -33.322  1.00 17.89           C
ATOM   2521  CG  ASP G 392      3.494  16.038 -34.456  1.00 18.86           C
ATOM   2522  OD1 ASP G 392      4.636  15.613 -34. 185  1.00 20.34          O
ATOM   2523  OD2 ASP G 392      3.008  15.998 -35.604  1.00 18.51           O
ATOM   2524  C   ASP G 392      3.428  17.344 -31. 107  1.00 17.1 1          C
ATOM   2525  O   ASP G 392      4.495  16.860 -30.731  1.00 17.04           O
ATOM   2526  N   CYS G 393      2.452  17.684 -30.280  1.00 16.33           N
ATOM   2527  CA  CYS G 393      2.723  18. 199 -28.957  1.00 16. 17          C
ATOM   2528  CB  CYS G 393      2.419  19.693 -28.910  1.00 16.1 1          C
ATOM   2529  SG  CYS G 393      3.237  20.556 -27.570  1.00 20.23           S
ATOM   2530  C   CYS G 393      1.812  17.471 -27.995  1.00 15.37           C
ATOM   2531  O   CYS G 393      0.592  17.525 -28. 139  1.00 15.15           O
ATOM   2532  N   LYS G 394      2.399  16.618 -27. 168  1.00 14.91           N
ATOM   2533  CA  LYS G 394      1.608  15.678 -26.398  1.00 14.50           C
ATOM   2534  CB  LYS G 394      2.495  14.607 -25.771  1.00 14.60           C
ATOM   2535  CG  LYS G 394      3.531  14.052 -26.730  1.00 16.44           C
ATOM   2536  CD  LYS G 394      4.034  12.699 -26.272  1.00 20.45           C
ATOM   2537  CE  LYS G 394      4.868  12.823 -25.009  1.00 23.05           C
ATOM   2538  NZ  LYS G 394      4.057  13.264 -23.841  1.00 24.13           N
ATOM   2539  C   LYS G 394      0.767  16.388 -25.344  1.00 14.00           C
ATOM   2540  O   LYS G 394      1.249  17.268 -24.630  1.00 14.14           O
ATOM   2541  N   ILE G 395     -0.486  15.955 -25.236  1.00 13.28           N
ATOM   2542  CA  ILE G 395     -1.587  16.768 -24.725  1.00 12.89           C
ATOM   2543  CB  ILE G 395     -2.234  17.626 -25.843  1.00 12.75           C
ATOM   2544  CGI ILE G 395     -1.418  18.897 -26.097  1.00 13.58           C
ATOM   2545  CD1 ILE G 395     -1.635  19.507 -27.466  1.00 15.33           C
ATOM   2546  CG2 ILE G 395     -3.669  17.980 -25.477  1.00 12.16           C
ATOM   2547  C   ILE G 395     -2.631  15.761 -24.284  1.00 13.15           C
ATOM   2548  O   ILE G 395     -2.826  14.746 -24.951  1.00 13.45           O
ATOM   2549  N   MET G 396     -3.440  16.127 -23.303  1.00 13.06           N
ATOM   2550  CA  MET G 396     -4.668  15.392 -23.085  1.00 13.00           C
ATOM   2551  CB  MET G 396     -4.579  14.539 -21.824  1.00 13.34           C
ATOM   2552  CG  MET G 396     -5.208  15.167 -20.600  1.00 14.30           C
ATOM   2553  SD  MET G 396     -5.006  14.087 -19. 179  1.00 18.50          S
ATOM   2554  CE  MET G 396     -3.465  13.282 -19.61 1  1.00 17.80          C
ATOM   2555  C   MET G 396     -5.889  16.288 -23.050  1.00 12.96           C
ATOM   2556  O   MET G 396     -5.81 1  17.453 -22.663  1.00 13.04           O
```

```
ATOM   2557  N   THR G 397      -7.037  15.686 -23.336  1.00 12.78           N
ATOM   2558  CA  THR G 397      -8.200  16.415 -23.815  1.00 12.51           C
ATOM   2559  CB  THR G 397      -8.653  15.898 -25.193  1.00 12.39           C
ATOM   2560  OG1 THR G 397      -7.837  16.481 -26.216  1.00 12.50           O
ATOM   2561  CG2 THR G 397     -10.114  16.250 -25.447  1.00 12.55           C
ATOM   2562  C   THR G 397      -9.343  16.223 -22.834  1.00 12.58           C
ATOM   2563  O   THR G 397      -9.563  15.117 -22.340  1.00 12.88           O
ATOM   2564  N   SER G 398     -10.157  17.255 -22.663  1.00 12.55           N
ATOM   2565  CA  SER G 398     -11.452  17.049 -22.049  1.00 12.76           C
ATOM   2566  CB  SER G 398     -11.323  16.949 -20.527  1.00 12.52           C
ATOM   2567  OG  SER G 398     -12.592  16.781 -19.919  1.00 12.72           O
ATOM   2568  C   SER G 398     -12.478  18.103 -22.410  1.00 12.99           C
ATOM   2569  O   SER G 398     -12.269  18.917 -23.311  1.00 13.13           O
ATOM   2570  N   LYS G 399     -13.435  18.245 -21.504  1.00 13.01           N
ATOM   2571  CA  LYS G 399     -14.399  19.325 -21.544  1.00 13.29           C
ATOM   2572  CB  LYS G 399     -15.777  18.777 -21.908  1.00 13.79           C
ATOM   2573  CG  LYS G 399     -16.044  18.714 -23.399  1.00 14.34           C
ATOM   2574  CD  LYS G 399     -16.965  19.840 -23.833  1.00 16.43           C
ATOM   2575  CE  LYS G 399     -17.285  19.750 -25.315  1.00 17.37           C
ATOM   2576  NZ  LYS G 399     -17.904  21.003 -25.828  1.00 16.62           N
ATOM   2577  C   LYS G 399     -14.460  19.996 -20.179  1.00 13.09           C
ATOM   2578  O   LYS G 399     -14.619  21.213 -20.084  1.00 12.87           O
ATOM   2579  N   THR G 400     -14.348  19.198 -19.123  1.00 13.04           N
ATOM   2580  CA  THR G 400     -14.535  19.715 -17.776  1.00 13.38           C
ATOM   2581  CB  THR G 400     -15.257  18.709 -16.861  1.00 13.74           C
ATOM   2582  OG1 THR G 400     -15.856  17.678 -17.655  1.00 14.38           O
ATOM   2583  CG2 THR G 400     -16.337  19.409 -16.051  1.00 14.32           C
ATOM   2584  C   THR G 400     -13.226  20.134 -17.120  1.00 13.20           C
ATOM   2585  O   THR G 400     -12.169  19.594 -17.445  1.00 13.12           O
ATOM   2586  N   ASP G 401     -13.378  20.770 -15.963  1.00 12.97           N
ATOM   2587  CA  ASP G 401     -12.358  21.654 -15.396  1.00 12.50           C
ATOM   2588  CB  ASP G 401     -13.014  22.766 -14.590  1.00 12.73           C
ATOM   2589  CG  ASP G 401     -12.765  24.122 -15.183  1.00 13.98           C
ATOM   2590  OD1 ASP G 401     -13.073  24.301 -16.380  1.00 16.55           O
ATOM   2591  OD2 ASP G 401     -12.168  24.973 -14.492  1.00 14.80           O
ATOM   2592  C   ASP G 401     -11.269  21.029 -14.529  1.00 12.13           C
ATOM   2593  O   ASP G 401     -11.547  20.130 -13.729  1.00 12.31           O
ATOM   2594  N   VAL G 402     -10.200  21.822 -14.390  1.00 11.49           N
ATOM   2595  CA  VAL G 402      -9.667  22.261 -13.080  1.00 10.74           C
ATOM   2596  CB  VAL G 402      -8.369  21.519 -12.744  1.00 10.60           C
ATOM   2597  CGI VAL G 402      -7.449  22.413 -11.914  1.00 11.26           C
ATOM   2598  CG2 VAL G 402      -8.672  20.211 -12.019  1.00 10.99           C
ATOM   2599  C   VAL G 402      -9.360  23.769 -12.883  1.00 10.24           C
ATOM   2600  O   VAL G 402      -9.387  24.539 -13.845  1.00 10.30           O
ATOM   2601  N   SER G 403      -8.762  24.081 -11.719  1.00  9.76           N
ATOM   2602  CA  SER G 403      -8.493  25.474 -11.271  1.00  9.18           C
ATOM   2603  CB  SER G 403      -9.790  26.197 -10.893  1.00  9.41           C
ATOM   2604  OG  SER G 403     -10.714  25.319 -10.274  1.00 10.82           O
ATOM   2605  C   SER G 403      -7.394  25.745 -10.199  1.00  8.51           C
ATOM   2606  O   SER G 403      -7.465  25.236  -9.076  1.00  8.30           O
ATOM   2607  N   SER G 404      -6.524  26.720 -10.502  1.00  8.35           N
ATOM   2608  CA  SER G 404      -5.785  27.535  -9.507  1.00  8.18           C
ATOM   2609  CB  SER G 404      -4.851  26.657  -8.669  1.00  8.18           C
ATOM   2610  OG  SER G 404      -3.507  26.782  -9.100  1.00  8.83           O
ATOM   2611  C   SER G 404      -4.979  28.665 -10.187  1.00  7.62           C
ATOM   2612  O   SER G 404      -5.183  28.942 -11.369  1.00  7.57           O
ATOM   2613  N   SER G 405      -4.041  29.282  -9.462  1.00  7.08           N
ATOM   2614  CA  SER G 405      -3.258  30.409 -10.003  1.00  6.53           C
ATOM   2615  CB  SER G 405      -3.844  31.752  -9.555  1.00  6.42           C
ATOM   2616  OG  SER G 405      -2.883  32.790  -9.662  1.00  5.66           O
```

```
ATOM   2617  C   SER G 405     -1.756  30.364  -9.693   1.00  6.28           C
ATOM   2618  O   SER G 405     -1.338  29.830  -8.666   1.00  5.98           O
ATOM   2619  N   VAL G 406     -0.980  31.079 -10.506   1.00  6.22           N
ATOM   2620  CA  VAL G 406      0.479  31.053 -10.436   1.00  6.50           C
ATOM   2621  CB  VAL G 406      1.068  30.055 -11.453   1.00  6.45           C
ATOM   2622  CGI VAL G 406      2.518  29.743 -11.116   1.00  7.66           C
ATOM   2623  CG2 VAL G 406      0.236  28.783 -11.495   1.00  7.38           C
ATOM   2624  C   VAL G 406      1.029  32.438 -10.760   1.00  6.24           C
ATOM   2625  O   VAL G 406      0.763  32.981 -11.832   1.00  6.14           O
ATOM   2626  N   ILE G 407      1.803  33.001  -9.840   1.00  6.32           N
ATOM   2627  CA  ILE G 407      2.315  34.354 -10.014   1.00  6.60           C
ATOM   2628  CB  ILE G 407      2.445  35.097  -8.674   1.00  6.27           C
ATOM   2629  CG1 ILE G 407      1.070  35.564  -8.194   1.00  6.19           C
ATOM   2630  CD1 ILE G 407      1.086  36.200  -6.824   1.00  8.34           C
ATOM   2631  CG2 ILE G 407      3.391  36.282  -8.813   1.00  6.42           C
ATOM   2632  C   ILE G 407      3.657  34.361 -10.728   1.00  7.20           C
ATOM   2633  O   ILE G 407      4.576  33.631 -10.356   1.00  7.42           O
ATOM   2634  N   THR G 408      3.797  35.273 -11.682   1.00  7.57           N
ATOM   2635  CA  THR G 408      4.983  35.324 -12.517   1.00  8.19           C
ATOM   2636  CB  THR G 408      4.622  35.305 -14.011   1.00  8.15           C
ATOM   2637  OG1 THR G 408      3.785  36.426 -14.318   1.00  8.88           O
ATOM   2638  CG2 THR G 408      3.891  34.020 -14.364   1.00  7.93           C
ATOM   2639  C   THR G 408      5.804  36.569 -12.225   1.00  8.55           C
ATOM   2640  O   THR G 408      5.418  37.408 -11.410   1.00  9.07           O
ATOM   2641  N   SER G 409      6.918  36.698 -12.935   1.00  8.70           N
ATOM   2642  CA  SER G 409      7.843  37.799 -12.723   1.00  9.20           C
ATOM   2643  CB  SER G 409      9.067  37.643 -13.628   1.00  9.72           C
ATOM   2644  OG  SER G 409      9.571  36.320 -13.581   1.00 10.75           O
ATOM   2645  C   SER G 409      7.153  39.125 -13.007   1.00  9.01           C
ATOM   2646  O   SER G 409      7.433  40.135 -12.359   1.00  9.02           O
ATOM   2647  N   LEU G 410      6.259  39.118 -13.990   1.00  8.91           N
ATOM   2648  CA  LEU G 410      5.790  40.352 -14.604   1.00  9.29           C
ATOM   2649  CB  LEU G 410      6.438  40.546 -15.976   1.00  9.61           C
ATOM   2650  CG  LEU G 410      7.245  41.834 -16.150   1.00  9.70           C
ATOM   2651  CD1 LEU G 410      8.433  41.858 -15.200   1.00 11.11           C
ATOM   2652  CD2 LEU G 410      7.705  41.994 -17.591   1.00  9.16           C
ATOM   2653  C   LEU G 410      4.272  40.351 -14.729   1.00  9.12           C
ATOM   2654  O   LEU G 410      3.683  41.248 -15.332   1.00  9.08           O
ATOM   2655  N   GLY G 411      3.646  39.332 -14.154   1.00  9.03           N
ATOM   2656  CA  GLY G 411      2.203  39.315 -13.982   1.00  8.44           C
ATOM   2657  C   GLY G 411      1.765  38.048 -13.284   1.00  7.91           C
ATOM   2658  O   GLY G 411      2.435  37.568 -12.369   1.00  7.85           O
ATOM   2659  N   ALA G 412      0.674  37.465 -13.763   1.00  7.30           N
ATOM   2660  CA  ALA G 412      0.129  36.264 -13.153   1.00  6.92           C
ATOM   2661  CB  ALA G 412     -0.742  36.623 -11.960   1.00  6.90           C
ATOM   2662  C   ALA G 412     -0.661  35.453 -14.166   1.00  6.99           C
ATOM   2663  O   ALA G 412     -1.257  36.002 -15.093   1.00  6.94           O
ATOM   2664  N   ILE G 413     -0.621  34.137 -14.006   1.00  7.29           N
ATOM   2665  CA  ILE G 413     -1.478  33.244 -14.766   1.00  7.49           C
ATOM   2666  CB  ILE G 413     -0.711  31.990 -15.201   1.00  7.24           C
ATOM   2667  CG1 ILE G 413      0.314  32.350 -16.278   1.00  7.18           C
ATOM   2668  CD1 ILE G 413      0.927  31.150 -16.973   1.00  7.70           C
ATOM   2669  CG2 ILE G 413     -1.674  30.916 -15.688   1.00  7.70           C
ATOM   2670  C   ILE G 413     -2.657  32.822 -13.908   1.00  7.94           C
ATOM   2671  O   ILE G 413     -2.544  32.749 -12.685   1.00  8.39           O
ATOM   2672  N   VAL G 414     -3.782  32.521 -14.544   1.00  8.22           N
ATOM   2673  CA  VAL G 414     -4.909  31.961 -13.816   1.00  8.77           C
ATOM   2674  CB  VAL G 414     -5.865  33.050 -13.296   1.00  8.57           C
ATOM   2675  CGI VAL G 414     -6.133  34.085 -14.376   1.00  9.12           C
ATOM   2676  CG2 VAL G 414     -7.162  32.427 -12.803   1.00  8.90           C
```

```
ATOM   2677  C   VAL G 414      -5.674  30.901 -14.594  1.00  8.92           C
ATOM   2678  O   VAL G 414      -6.114  31.129 -15.722  1.00  9.00           O
ATOM   2679  N   SER G 415      -5.750  29.714 -14.004  1.00  8.97           N
ATOM   2680  CA  SER G 415      -6.472  28.598 -14.592  1.00  9.02           C
ATOM   2681  CB  SER G 415      -5.625  27.328 -14.520  1.00  8.98           C
ATOM   2682  OG  SER G 415      -4.353  27.532 -15.108  1.00  9.54           O
ATOM   2683  C   SER G 415      -7.791  28.390 -13.864  1.00  9.36           C
ATOM   2684  O   SER G 415      -7.818  27.884 -12.742  1.00  9.61           O
ATOM   2685  N   CYS G 416      -8.854  28.950 -14.430  1.00  9.57           N
ATOM   2686  CA  CYS G 416     -10.175  28.857 -13.831  1.00  9.61           C
ATOM   2687  CB  CYS G 416     -10.895  30.201 -13.912  1.00  9.62           C
ATOM   2688  SG  CYS G 416     -12.025  30.497 -12.543  1.00 11.33           S
ATOM   2689  C   CYS G 416     -11.000  27.796 -14.534  1.00  9.61           C
ATOM   2690  O   CYS G 416     -11.361  27.950 -15.700  1.00  9.80           O
ATOM   2691  N   TYR G 417     -11.298  26.717 -13.821  1.00  9.48           N
ATOM   2692  CA  TYR G 417     -11.930  25.566 -14.438  1.00  9.28           C
ATOM   2693  CB  TYR G 417     -10.888  24.501 -14.782  1.00  9.17           C
ATOM   2694  CG  TYR G 417     -10.011  24.860 -15.962  1.00  8.71           C
ATOM   2695  CD1 TYR G 417      -8.661  24.543 -15.968  1.00  8.54           C
ATOM   2696  CE1 TYR G 417      -7.857  24.869 -17.043  1.00  9.56           C
ATOM   2697  CZ  TYR G 417      -8.407  25.480 -18.149  1.00  9.83           C
ATOM   2698  OH  TYR G 417      -7.602  25.828 -19.207  1.00 10.51           O
ATOM   2699  CE2 TYR G 417      -9.738  25.830 -18.159  1.00  9.36           C
ATOM   2700  CD2 TYR G 417     -10.532  25.522 -17.068  1.00  8.95           C
ATOM   2701  C   TYR G 417     -13.034  24.978 -13.566  1.00  9.35           C
ATOM   2702  O   TYR G 417     -13.171  25.332 -12.395  1.00  9.11           O
ATOM   2703  N   GLY G 418     -13.848  24.115 -14.165  1.00  9.71           N
ATOM   2704  CA  GLY G 418     -14.993  23.534 -13.481  1.00  9.95           C
ATOM   2705  C   GLY G 418     -15.925  24.594 -12.936  1.00 10.09           C
ATOM   2706  O   GLY G 418     -16.170  25.611 -13.585  1.00 10.17           O
ATOM   2707  N   LYS G 419     -16.323  24.426 -11.681  1.00 10.17           N
ATOM   2708  CA  LYS G 419     -17.328  25.289 -11.075  1.00 10.50           C
ATOM   2709  CB  LYS G 419     -18.123  24.523 -10.015  1.00 11.09           C
ATOM   2710  CG  LYS G 419     -19.389  23.867 -10.538  1.00 12.94           C
ATOM   2711  CD  LYS G 419     -20.304  23.450  -9.397  1.00 15.52           C
ATOM   2712  CE  LYS G 419     -21.702  23.127  -9.899  1.00 17.07           C
ATOM   2713  NZ  LYS G 419     -21.688  22.058 -10.936  1.00 19.30           N
ATOM   2714  C   LYS G 419     -16.737  26.560 -10.464  1.00 10.23           C
ATOM   2715  O   LYS G 419     -17.451  27.325  -9.817  1.00 10.58           O
ATOM   2716  N   THR G 420     -15.429  26.755 -10.607  1.00 10.10           N
ATOM   2717  CA  THR G 420     -14.730  27.754  -9.801  1.00  9.74           C
ATOM   2718  CB  THR G 420     -13.232  27.432  -9.651  1.00  9.28           C
ATOM   2719  OG1 THR G 420     -12.992  26.073 -10.034  1.00  9.21           O
ATOM   2720  CG2 THR G 420     -12.788  27.635  -8.209  1.00  9.03           C
ATOM   2721  C   THR G 420     -14.900  29.178 -10.329  1.00  9.95           C
ATOM   2722  O   THR G 420     -15.143  29.387 -11.518  1.00 10.35           O
ATOM   2723  N   LYS G 421     -14.816  30.149  -9.424  1.00 10.07           N
ATOM   2724  CA  LYS G 421     -14.950  31.559  -9.780  1.00 10.21           C
ATOM   2725  CB  LYS G 421     -15.973  32.239  -8.867  1.00 10.30           C
ATOM   2726  CG  LYS G 421     -17.368  32.341  -9.457  1.00 12.43           C
ATOM   2727  CD  LYS G 421     -18.345  32.931  -8.452  1.00 15.12           C
ATOM   2728  CE  LYS G 421     -19.766  32.470  -8.727  1.00 15.21           C
ATOM   2729  NZ  LYS G 421     -20.617  32.544  -7.508  1.00 15.98           N
ATOM   2730  C   LYS G 421     -13.608  32.271  -9.658  1.00 10.09           C
ATOM   2731  O   LYS G 421     -12.911  32.125  -8.653  1.00 10.36           O
ATOM   2732  N   CYS G 422     -13.271  33.085 -10.653  1.00  9.81           N
ATOM   2733  CA  CYS G 422     -12.006  33.808 -10.631  1.00  9.56           C
ATOM   2734  CB  CYS G 422     -10.953  33.092 -11.475  1.00  9.72           C
ATOM   2735  SG  CYS G 422     -10.831  31.329 -11.131  1.00 11.42           S
ATOM   2736  C   CYS G 422     -12.126  35.268 -11.044  1.00  9.18           C
```

```
ATOM   2737  O   CYS G 422     -12.927  35.624 -11.909   1.00  9.27           O
ATOM   2738  N   THR G 423     -11.232  36.084 -10.497   1.00  8.93           N
ATOM   2739  CA  THR G 423     -11.422  37.525 -10.427   1.00  8.64           C
ATOM   2740  CB  THR G 423     -12.062  37.938  -9.088   1.00  8.32           C
ATOM   2741  OG1 THR G 423     -13.201  37.111  -8.821   1.00  7.97           O
ATOM   2742  CG2 THR G 423     -12.494  39.396  -9.130   1.00  8.36           C
ATOM   2743  C   THR G 423     -10.059  38.190 -10.513   1.00  8.86           C
ATOM   2744  O   THR G 423      -9.183  37.928  -9.688   1.00  9.26           O
ATOM   2745  N   ALA G 424      -9.913  39.124 -11.444   1.00  8.74           N
ATOM   2746  CA  ALA G 424      -8.792  40.052 -11.408   1.00  8.79           C
ATOM   2747  CB  ALA G 424      -8.164  40.180 -12.786   1.00  8.94           C
ATOM   2748  C   ALA G 424      -9.240  41.414 -10.894   1.00  8.84           C
ATOM   2749  O   ALA G 424     -10.084  42.070 -11.504   1.00  9.24           O
ATOM   2750  N   SER G 425      -8.669  41.836  -9.771   1.00  8.81           N
ATOM   2751  CA  SER G 425      -9.007  43.124  -9.180   1.00  8.85           C
ATOM   2752  CB  SER G 425      -9.483  42.942  -7.737   1.00  8.94           C
ATOM   2753  OG  SER G 425      -9.918  41.613  -7.507   1.00  7.69           O
ATOM   2754  C   SER G 425      -7.815  44.072  -9.222   1.00  9.01           C
ATOM   2755  O   SER G 425      -6.669  43.651  -9.059   1.00  8.63           O
ATOM   2756  N   ASN G 426      -8.089  45.354  -9.441   1.00  9.54           N
ATOM   2757  CA  ASN G 426      -7.033  46.328  -9.686   1.00 10.19           C
ATOM   2758  CB  ASN G 426      -7.537  47.462 -10.583   1.00  9.77           C
ATOM   2759  CG  ASN G 426      -8.273  48.540  -9.808   1.00  9.43           C
ATOM   2760  OD1 ASN G 426      -8.253  48.561  -8.578   1.00  9.01           O
ATOM   2761  ND2 ASN G 426      -8.938  49.436 -10.528   1.00  9.01           N
ATOM   2762  C   ASN G 426      -6.434  46.891  -8.400   1.00 11.16           C
ATOM   2763  O   ASN G 426      -6.629  46.340  -7.316   1.00 11.06           O
ATOM   2764  N   LYS G 427      -5.658  47.961  -8.543   1.00 12.38           N
ATOM   2765  CA  LYS G 427      -5.016  48.627  -7.413   1.00 13.52           C
ATOM   2766  CB  LYS G 427      -4.455  49.981  -7.851   1.00 14.00           C
ATOM   2767  CG  LYS G 427      -2.987  49.956  -8.233   1.00 16.18           C
ATOM   2768  CD  LYS G 427      -2.434  51.366  -8.365   1.00 18.24           C
ATOM   2769  CE  LYS G 427      -0.955  51.413  -8.022   1.00 19.72           C
ATOM   2770  NZ  LYS G 427      -0.707  51.116  -6.584   1.00 21.43           N
ATOM   2771  C   LYS G 427      -5.976  48.829  -6.245   1.00 13.71           C
ATOM   2772  O   LYS G 427      -5.630  48.562  -5.093   1.00 13.63           O
ATOM   2773  N   ASN G 428      -7.119  49.443  -6.535   1.00 14.28           N
ATOM   2774  CA  ASN G 428      -8.080  49.830  -5.505   1.00 14.60           C
ATOM   2775  CB  ASN G 428      -9.009  50.934  -6.020   1.00 14.57           C
ATOM   2776  CG  ASN G 428      -8.353  51.808  -7.071   1.00 13.24           C
ATOM   2777  OD1 ASN G 428      -7.314  52.420  -6.823   1.00  9.74           O
ATOM   2778  ND2 ASN G 428      -9.009  51.946  -8.217   1.00 12.83           N
ATOM   2779  C   ASN G 428      -8.914  48.658  -4.994   1.00 14.83           C
ATOM   2780  O   ASN G 428      -9.645  48.793  -4.013   1.00 15.25           O
ATOM   2781  N   ARG G 429      -8.920  47.564  -5.750   1.00 14.78           N
ATOM   2782  CA  ARG G 429      -9.725  46.395  -5.407   1.00 14.74           C
ATOM   2783  CB  ARG G 429     -10.088  46.405  -3.920   1.00 14.93           C
ATOM   2784  CG  ARG G 429      -8.949  45.999  -2.999   1.00 16.26           C
ATOM   2785  CD  ARG G 429      -8.954  44.502  -2.732   1.00 19.79           C
ATOM   2786  NE  ARG G 429      -7.694  44.046  -2.152   1.00 22.68           N
ATOM   2787  CZ  ARG G 429      -7.270  44.369  -0.935   1.00 23.54           C
ATOM   2788  NH1 ARG G 429      -7.998  45.170  -0.168   1.00 22.87           N
ATOM   2789  NH2 ARG G 429      -6.107  43.912  -0.492   1.00 23.53           N
ATOM   2790  C   ARG G 429     -10.989  46.304  -6.256   1.00 14.35           C
ATOM   2791  O   ARG G 429     -11.653  45.268  -6.287   1.00 14.62           O
ATOM   2792  N   GLY G 430     -11.306  47.386  -6.961   1.00 13.67           N
ATOM   2793  CA  GLY G 430     -12.201  47.311  -8.110   1.00 12.80           C
ATOM   2794  C   GLY G 430     -11.870  46.136  -9.009   1.00 12.11           C
ATOM   2795  O   GLY G 430     -10.707  45.903  -9.338   1.00 12.18           O
ATOM   2796  N   ILE G 431     -12.892  45.374  -9.380   1.00 11.58           N
```

ATOM 2797 CA ILE G 431 -12.700 44.155 -10.157 1.00 10.76 C
ATOM 2798 CB ILE G 431 -13.777 43.106 -9.812 1.00 10.43 C
ATOM 2799 CGI ILE G 431 -13.615 42.625 -8.368 1.00 10.95 C
ATOM 2800 CD1 ILE G 431 -14.920 42.259 -7.695 1.00 12.08 C
ATOM 2801 CG2 ILE G 431 -13.720 41.940 -10.785 1.00 10.07 C
ATOM 2802 C ILE G 431 -12.770 44.465 -11.651 1.00 10.68 C
ATOM 2803 O ILE G 431 -13.790 44.954 -12.136 1.00 10.40 O
ATOM 2804 N ILE G 432 -11.677 44.225 -12.373 1.00 10.90 N
ATOM 2805 CA ILE G 432 -11.658 44.482 -13.815 1.00 11.42 C
ATOM 2806 CB ILE G 432 -10.276 44.936 -14.327 1.00 11.63 C
ATOM 2807 CGI ILE G 432 -9.411 45.460 -13.180 1.00 12.68 C
ATOM 2808 CD1 ILE G 432 -7.977 45.738 -13.579 1.00 13.89 C
ATOM 2809 CG2 ILE G 432 -10.432 45.992 -15.412 1.00 12.24 C
ATOM 2810 C ILE G 432 -12.118 43.290 -14.648 1.00 11.41 C
ATOM 2811 O ILE G 432 -12.834 43.463 -15.635 1.00 11.63 O
ATOM 2812 N LYS G 433 -11.505 42.136 -14.405 1.00 11.52 N
ATOM 2813 CA LYS G 433 -11.792 40.950 -15.203 1.00 11.96 C
ATOM 2814 CB LYS G 433 -10.516 40.392 -15.837 1.00 12.31 C
ATOM 2815 CG LYS G 433 -10.770 39.317 -16.885 1.00 14.42 C
ATOM 2816 CD LYS G 433 -9.723 39.348 -17.987 1.00 16.74 C
ATOM 2817 CE LYS G 433 -9.997 38.283 -19.038 1.00 17.08 C
ATOM 2818 NZ LYS G 433 -9.612 38.735 -20.404 1.00 17.30 N
ATOM 2819 C LYS G 433 -12.496 39.873 -14.387 1.00 11.65 C
ATOM 2820 O LYS G 433 -12.479 39.899 -13.156 1.00 11.48 O
ATOM 2821 N THR G 434 -13.143 38.946 -15.086 1.00 11.28 N
ATOM 2822 CA THR G 434 -13.816 37.821 -14.445 1.00 11.21 C
ATOM 2823 CB THR G 434 -15.222 38.216 -13.955 1.00 11.30 C
ATOM 2824 OG1 THR G 434 -15.963 37.037 -13.619 1.00 11.83 O
ATOM 2825 CG2 THR G 434 -15.966 38.988 -15.035 1.00 11.84 C
ATOM 2826 C THR G 434 -13.939 36.646 -15.415 1.00 10.94 C
ATOM 2827 O THR G 434 -14.257 36.836 -16.589 1.00 10.93 O
ATOM 2828 N PHE G 435 -13.628 35.442 -14.939 1.00 11.10 N
ATOM 2829 CA PHE G 435 -12.871 34.486 -15.744 1.00 11.96 C
ATOM 2830 CB PHE G 435 -11.673 33.929 -14.977 1.00 11.51 C
ATOM 2831 CG PHE G 435 -10.437 34.772 -15.100 1.00 11.19 C
ATOM 2832 CD1 PHE G 435 -9.910 35.409 -13.989 1.00 10.86 C
ATOM 2833 CE1 PHE G 435 -8.824 36.254 -14.107 1.00 10.24 C
ATOM 2834 CZ PHE G 435 -8.286 36.516 -15.352 1.00 9.89 C
ATOM 2835 CE2 PHE G 435 -8.834 35.927 -16.474 1.00 10.78 C
ATOM 2836 CD2 PHE G 435 -9.920 35.082 -16.348 1.00 11.14 C
ATOM 2837 C PHE G 435 -13.678 33.371 -16.403 1.00 13.00 C
ATOM 2838 O PHE G 435 -14.218 32.494 -15.726 1.00 13.03 O
ATOM 2839 N SER G 436 -13.506 33.272 -17.717 1.00 13.89 N
ATOM 2840 CA SER G 436 -14.276 32.356 -18.546 1.00 14.67 C
ATOM 2841 CB SER G 436 -14.391 32.910 -19.969 1.00 15.04 C
ATOM 2842 OG SER G 436 -15.702 33.377 -20.235 1.00 16.58 O
ATOM 2843 C SER G 436 -13.627 30.975 -18.578 1.00 14.75 C
ATOM 2844 O SER G 436 -13.081 30.559 -19.601 1.00 14.75 O
ATOM 2845 N ASN G 437 -13.713 30.256 -17.465 1.00 14.44 N
ATOM 2846 CA ASN G 437 -13.595 28.805 -17.496 1.00 14.35 C
ATOM 2847 CB ASN G 437 -14.935 28.179 -17.896 1.00 14.75 C
ATOM 2848 CG ASN G 437 -14.999 26.690 -17.610 1.00 15.51 C
ATOM 2849 OD1 ASN G 437 -15.013 26.275 -16.450 1.00 16.85 O
ATOM 2850 ND2 ASN G 437 -15.246 25.906 -18.652 1.00 16.10 N
ATOM 2851 C ASN G 437 -12.497 28.371 -18.464 1.00 13.69 C
ATOM 2852 O ASN G 437 -12.754 27.652 -19.430 1.00 13.40 O
ATOM 2853 N GLY G 438 -11.290 28.880 -18.237 1.00 13.39 N
ATOM 2854 CA GLY G 438 -10.183 28.701 -19.170 1.00 12.92 C
ATOM 2855 C GLY G 438 -8.839 28.941 -18.510 1.00 12.72 C
ATOM 2856 O GLY G 438 -8.620 28.538 -17.367 1.00 12.83 O

```
ATOM   2857  N   CYS G 439     -7.971  29.677 -19.195  1.00 12.17           N
ATOM   2858  CA  CYS G 439     -6.654  29.999 -18.658  1.00 11.52           C
ATOM   2859  CB  CYS G 439     -5.696  28.822 -18.844  1.00 11.68           C
ATOM   2860  SG  CYS G 439     -3.974  29.301 -19.104  1.00 12.89           S
ATOM   2861  C   CYS G 439     -6.077  31.258 -19.297  1.00 10.95           C
ATOM   2862  O   CYS G 439     -5.762  31.275 -20.488  1.00 10.77           O
ATOM   2863  N   ASP G 440     -5.921  32.303 -18.490  1.00 10.41           N
ATOM   2864  CA  ASP G 440     -5.546  33.619 -18.993  1.00 10.06           C
ATOM   2865  CB  ASP G 440     -6.685  34.620 -18.778  1.00 10.85           C
ATOM   2866  CG  ASP G 440     -7.418  34.956 -20.062  1.00 13.11           C
ATOM   2867  OD1 ASP G 440     -6.891  35.765 -20.854  1.00 14.97           O
ATOM   2868  OD2 ASP G 440     -8.559  34.479 -20.237  1.00 15.27           O
ATOM   2869  C   ASP G 440     -4.276  34.131 -18.318  1.00  9.01           C
ATOM   2870  O   ASP G 440     -3.793  33.542 -17.350  1.00  9.09           O
ATOM   2871  N   TYR G 441     -3.806  35.287 -18.778  1.00  7.92           N
ATOM   2872  CA  TYR G 441     -2.645  35.959 -18.199  1.00  7.24           C
ATOM   2873  CB  TYR G 441     -1.457  35.871 -19.165  1.00  7.04           C
ATOM   2874  CG  TYR G 441     -0.227  36.631 -18.724  1.00  6.77           C
ATOM   2875  CD1 TYR G 441      0.762  36.008 -17.974  1.00  7.41           C
ATOM   2876  CE1 TYR G 441      1.902  36.688 -17.593  1.00  6.79           C
ATOM   2877  CZ  TYR G 441      2.106  37.980 -18.034  1.00  6.49           C
ATOM   2878  OH  TYR G 441      3.230  38.670 -17.635  1.00  5.09           O
ATOM   2879  CE2 TYR G 441      1.157  38.606 -18.817  1.00  7.52           C
ATOM   2880  CD2 TYR G 441      0.017  37.918 -19.186  1.00  7.12           C
ATOM   2881  C   TYR G 441     -3.005  37.421 -17.946  1.00  6.89           C
ATOM   2882  O   TYR G 441     -3.809  38.000 -18.677  1.00  7.12           O
ATOM   2883  N   VAL G 442     -2.452  37.999 -16.886  1.00  6.73           N
ATOM   2884  CA  VAL G 442     -2.612  39.427 -16.615  1.00  6.78           C
ATOM   2885  CB  VAL G 442     -3.614  39.671 -15.472  1.00  6.51           C
ATOM   2886  CGI VAL G 442     -5.041  39.483 -15.967  1.00  7.38           C
ATOM   2887  CG2 VAL G 442     -3.322  38.742 -14.303  1.00  6.00           C
ATOM   2888  C   VAL G 442     -1.262  40.025 -16.234  1.00  7.13           C
ATOM   2889  O   VAL G 442     -0.272  39.301 -16.134  1.00  7.77           O
ATOM   2890  N   SER G 443     -1.210  41.335 -16.022  1.00  7.12           N
ATOM   2891  CA  SER G 443      0.062  41.970 -15.700  1.00  7.64           C
ATOM   2892  CB  SER G 443      0.770  42.447 -16.969  1.00  7.83           C
ATOM   2893  OG  SER G 443      0.637  43.847 -17.131  1.00  7.99           O
ATOM   2894  C   SER G 443     -0.051  43.104 -14.690  1.00  8.16           C
ATOM   2895  O   SER G 443     -1.142  43.607 -14.420  1.00  8.69           O
ATOM   2896  N   ASN G 444      1.086  43.484 -14.117  1.00  8.73           N
ATOM   2897  CA  ASN G 444      1.139  44.600 -13.184  1.00  9.50           C
ATOM   2898  CB  ASN G 444      2.521  44.684 -12.538  1.00  9.65           C
ATOM   2899  CG  ASN G 444      3.256  43.357 -12.565  1.00 10.64           C
ATOM   2900  OD1 ASN G 444      2.641  42.291 -12.498  1.00 12.28           O
ATOM   2901  ND2 ASN G 444      4.578  43.416 -12.685  1.00 11.75           N
ATOM   2902  C   ASN G 444      0.791  45.922 -13.857  1.00 10.24           C
ATOM   2903  O   ASN G 444      1.086  46.126 -15.034  1.00  9.89           O
ATOM   2904  N   LYS G 445      0.266  46.855 -13.069  1.00 11.63           N
ATOM   2905  CA  LYS G 445     -0.752  47.787 -13.545  1.00 13.07           C
ATOM   2906  CB  LYS G 445     -0.107  49.048 -14.123  1.00 13.70           C
ATOM   2907  CG  LYS G 445     -1.068  50.216 -14.307  1.00 15.80           C
ATOM   2908  CD  LYS G 445     -2.384  49.986 -13.575  1.00 18.31           C
ATOM   2909  CE  LYS G 445     -2.166  49.766 -12.086  1.00 19.03           C
ATOM   2910  NZ  LYS G 445     -1.048  50.592 -11.554  1.00 20.02           N
ATOM   2911  C   LYS G 445     -1.681  47.147 -14.572  1.00 12.96           C
ATOM   2912  O   LYS G 445     -1.258  46.313 -15.372  1.00 13.24           O
ATOM   2913  N   GLY G 446     -2.943  47.559 -14.558  1.00 13.08           N
ATOM   2914  CA  GLY G 446     -4.051  46.616 -14.597  1.00 12.42           C
ATOM   2915  C   GLY G 446     -4.212  45.900 -13.272  1.00 11.83           C
ATOM   2916  O   GLY G 446     -4.832  46.426 -12.347  1.00 12.44           O
```

ATOM 2917 N VAL G 447 -3.517 44.777 -13.126 1.00 10.63 N
ATOM 2918 CA VAL G 447 -3.875 43.795 -12.114 1.00 10.01 C
ATOM 2919 CB VAL G 447 -3.898 42.365 -12.681 1.00 9.97 C
ATOM 2920 CGI VAL G 447 -4.591 41.422 -11.708 1.00 10.51 C
ATOM 2921 CG2 VAL G 447 -4.594 42.345 -14.033 1.00 10.50 C
ATOM 2922 C VAL G 447 -2.978 43.851 -10.882 1.00 9.53 C
ATOM 2923 O VAL G 447 -1.761 44.008 -10.985 1.00 9.61 O
ATOM 2924 N ASP G 448 -3.586 43.575 -9.735 1.00 9.16 N
ATOM 2925 CA ASP G 448 -2.956 43.763 -8.437 1.00 8.75 C
ATOM 2926 CB ASP G 448 -3.515 45.022 -7.771 1.00 9.22 C
ATOM 2927 CG ASP G 448 -2.579 45.599 -6.729 1.00 11.44 C
ATOM 2928 ODl ASP G 448 -1.725 44.849 -6.212 1.00 13.83 O
ATOM 2929 OD2 ASP G 448 -2.713 46.799 -6.409 1.00 14.13 O
ATOM 2930 C ASP G 448 -3.313 42.546 -7.598 1.00 8.18 C
ATOM 2931 O ASP G 448 -2.555 42.122 -6.725 1.00 8.06 O
ATOM 2932 N THR G 449 -4.451 41.949 -7.933 1.00 7.63 N
ATOM 2933 CA THR G 449 -4.991 40.823 -7.192 1.00 6.80 C
ATOM 2934 CB THR G 449 -5.988 41.293 -6.116 1.00 6.89 C
ATOM 2935 OG1 THR G 449 -5.284 41.584 -4.902 1.00 6.16 O
ATOM 2936 CG2 THR G 449 -7.032 40.219 -5.848 1.00 7.55 C
ATOM 2937 C THR G 449 -5.717 39.906 -8.164 1.00 6.53 C
ATOM 2938 O THR G 449 -6.385 40.370 -9.087 1.00 6.59 O
ATOM 2939 N VAL G 450 -5.536 38.603 -7.989 1.00 6.07 N
ATOM 2940 CA VAL G 450 -6.531 37.646 -8.434 1.00 6.02 C
ATOM 2941 CB VAL G 450 -5.981 36.723 -9.535 1.00 5.61 C
ATOM 2942 CGI VAL G 450 -5.377 37.545 -10.663 1.00 5.32 C
ATOM 2943 CG2 VAL G 450 -4.954 35.761 -8.958 1.00 5.55 C
ATOM 2944 C VAL G 450 -7.021 36.811 -7.263 1.00 6.37 C
ATOM 2945 O VAL G 450 -6.299 36.609 -6.287 1.00 6.54 O
ATOM 2946 N SER G 451 -8.307 36.486 -7.288 1.00 6.41 N
ATOM 2947 CA SER G 451 -8.857 35.507 -6.370 1.00 6.70 C
ATOM 2948 CB SER G 451 -9.995 36.120 -5.553 1.00 7.13 C
ATOM 2949 OG SER G 451 -10.537 37.254 -6.207 1.00 9.26 O
ATOM 2950 C SER G 451 -9.354 34.292 -7.139 1.00 6.47 C
ATOM 2951 O SER G 451 -9.896 34.423 -8.238 1.00 6.54 O
ATOM 2952 N VAL G 452 -8.962 33.116 -6.664 1.00 6.56 N
ATOM 2953 CA VAL G 452 -9.578 31.868 -7.091 1.00 6.31 C
ATOM 2954 CB VAL G 452 -8.516 30.849 -7.542 1.00 5.74 C
ATOM 2955 CGI VAL G 452 -9.170 29.688 -8.275 1.00 5.06 C
ATOM 2956 CG2 VAL G 452 -7.471 31.523 -8.419 1.00 5.56 C
ATOM 2957 C VAL G 452 -10.381 31.264 -5.944 1.00 6.60 C
ATOM 2958 O VAL G 452 -9.861 31.079 -4.844 1.00 7.04 O
ATOM 2959 N GLY G 453 -11.652 30.975 -6.198 1.00 6.54 N
ATOM 2960 CA GLY G 453 -12.581 30.650 -5.124 1.00 6.43 C
ATOM 2961 C GLY G 453 -12.375 31.548 -3.920 1.00 6.09 C
ATOM 2962 O GLY G 453 -12.581 32.759 -3.999 1.00 5.90 O
ATOM 2963 N ASN G 454 -11.872 30.971 -2.833 1.00 6.02 N
ATOM 2964 CA ASN G 454 -11.672 31.727 -1.603 1.00 6.39 C
ATOM 2965 CB ASN G 454 -12.335 31.027 -0.420 1.00 6.81 C
ATOM 2966 CG ASN G 454 -13.717 31.567 -0.135 1.00 8.99 C
ATOM 2967 OD1 ASN G 454 -13.867 32.523 0.625 1.00 11.67 O
ATOM 2968 ND2 ASN G 454 -14.693 31.112 -0.911 1.00 10.25 N
ATOM 2969 C ASN G 454 -10.211 32.020 -1.296 1.00 6.15 C
ATOM 2970 O ASN G 454 -9.900 32.765 -0.367 1.00 6.47 O
ATOM 2971 N THR G 455 -9.322 31.491 -2.128 1.00 5.40 N
ATOM 2972 CA THR G 455 -7.912 31.841 -2.053 1.00 4.53 C
ATOM 2973 CB THR G 455 -7.033 30.774 -2.724 1.00 4.70 C
ATOM 2974 OG1 THR G 455 -7.344 29.486 -2.180 1.00 5.28 O
ATOM 2975 CG2 THR G 455 -5.560 31.074 -2.491 1.00 5.57 C
ATOM 2976 C THR G 455 -7.659 33.187 -2.717 1.00 4.01 C

```
ATOM   2977  O   THR G 455     -8.312  33.540  -3.698  1.00  3.78           O
ATOM   2978  N   LEU G 456     -6.716  33.943  -2.165  1.00  3.87           N
ATOM   2979  CA  LEU G 456     -6.355  35.237  -2.726  1.00  4.05           C
ATOM   2980  CB  LEU G 456     -6.684  36.360  -1.742  1.00  3.95           C
ATOM   2981  CG  LEU G 456     -6.595  37.779  -2.306  1.00  3.76           c
ATOM   2982  CD1 LEU G 456     -7.572  37.962  -3.457  1.00  5.35           c
ATOM   2983  CD2 LEU G 456     -6.845  38.809  -1.216  1.00  4.10           c
ATOM   2984  C   LEU G 456     -4.879  35.288  -3.105  1.00  4.47           c
ATOM   2985  O   LEU G 456     -4.006  35.028  -2.276  1.00  4.94           o
ATOM   2986  N   TYR G 457     -4.609  35.652  -4.355  1.00  4.59           N
ATOM   2987  CA  TYR G 457     -3.242  35.786  -4.849  1.00  4.60           c
ATOM   2988  CB  TYR G 457     -3.056  34.938  -6.113  1.00  4.71           c
ATOM   2989  CG  TYR G 457     -3.201  33.447  -5.888  1.00  5.62           c
ATOM   2990  CD1 TYR G 457     -4.451  32.838  -5.896  1.00  7.09           c
ATOM   2991  CE1 TYR G 457     -4.582  31.473  -5.712  1.00  8.22           c
ATOM   2992  CZ  TYR G 457     -3.456  30.699  -5.533  1.00  8.06           c
ATOM   2993  OH  TYR G 457     -3.580  29.341  -5.349  1.00  8.80           o
ATOM   2994  CE2 TYR G 457     -2.204  31.276  -5.547  1.00  7.18           c
ATOM   2995  CD2 TYR G 457     -2.083  32.639  -5.735  1.00  6.66           c
ATOM   2996  C   TYR G 457     -2.924  37.256  -5.152  1.00  4.46           c
ATOM   2997  O   TYR G 457     -3.742  37.959  -5.745  1.00  4.92           o
ATOM   2998  N   TYR G 458     -1.727  37.706  -4.772  1.00  3.90           N
ATOM   2999  CA  TYR G 458     -1.312  39.118  -4.919  1.00  3.26           c
ATOM   3000  CB  TYR G 458     -0.740  39.635  -3.582  1.00  3.16           c
ATOM   3001  CG  TYR G 458     -1.716  39.659  -2.411  1.00  3.29           c
ATOM   3002  CD1 TYR G 458     -1.782  38.602  -1.509  1.00  3.93           c
ATOM   3003  CE1 TYR G 458     -2.632  38.646  -0.412  1.00  4.90           c
ATOM   3004  CZ  TYR G 458     -3.395  39.773  -0.185  1.00  5.12           c
ATOM   3005  OH  TYR G 458     -4.250  39.817   0.893  1.00  5.42           o
ATOM   3006  CE2 TYR G 458     -3.311  40.852  -1.039  1.00  4.72           c
ATOM   3007  CD2 TYR G 458     -2.457  40.801  -2.128  1.00  3.89           c
ATOM   3008  C   TYR G 458     -0.248  39.290  -6.043  1.00  3.04           c
ATOM   3009  O   TYR G 458      0.749  38.569  -6.041  1.00  3.37           o
ATOM   3010  N   VAL G 459     -0.351  40.348  -6.866  1.00  2.71           N
ATOM   3011  CA  VAL G 459      0.376  40.435  -8.177  1.00  2.61           c
ATOM   3012  CB  VAL G 459     -0.589  40.554  -9.380  1.00  2.22           c
ATOM   3013  CGI VAL G 459      0.154  40.287 -10.682  1.00  2.62           c
ATOM   3014  CG2 VAL G 459     -1.756  39.589  -9.224  1.00  2.61           c
ATOM   3015  C   VAL G 459      1.609  41.392  -8.360  1.00  3.03           c
ATOM   3016  O   VAL G 459      2.575  41.281  -7.604  1.00  3.21           o
ATOM   3017  N   ASN G 460      1.708  42.037  -9.537  1.00106.93           N
ATOM   3018  CA  ASN G 460      2.714  43.111  -9.870  1.00 95.54           c
ATOM   3019  CB  ASN G 460      3.598  43.589  -8.700  1.00 20.00           c
ATOM   3020  CG  ASN G 460      4.310  44.931  -9.000  1.00 20.00           c
ATOM   3021  OD1 ASN G 460      3.713  45.851  -9.563  1.00 20.00           o
ATOM   3022  ND2 ASN G 460      5.548  45.065  -8.532  1.00 20.00           N
ATOM   3023  C   ASN G 460      3.403  43.322 -11.247  1.00 99.41           c
ATOM   3024  O   ASN G 460      3.869  44.430 -11.523  1.00108.91           o
ATOM   3025  N   LYS G 461      3.568  42.271 -12.055  1.00 97.04           N
ATOM   3026  CA  LYS G 461      4.464  42.327 -13.236  1.00105.93           c
ATOM   3027  CB  LYS G 461      5.335  41.068 -13.312  1.00 20.00           c
ATOM   3028  CG  LYS G 461      6.382  40.951 -12.209  1.00 20.00           c
ATOM   3029  CD  LYS G 461      7.131  39.623 -12.296  1.00 20.00           c
ATOM   3030  CE  LYS G 461      8.255  39.536 -11.268  1.00 20.00           c
ATOM   3031  NZ  LYS G 461      8.886  38.184 -11.223  1.00 20.00           N
ATOM   3032  C   LYS G 461      3.727  42.546 -14.573  1.00102.28           c
ATOM   3033  O   LYS G 461      2.507  42.702 -14.590  1.00105.02           o
ATOM   3034  N   GLN G 462      4.464  42.556 -15.685  1.00 96.68           N
ATOM   3035  CA  GLN G 462      3.854  42.633 -17.020  1.00105.71           c
ATOM   3036  CB  GLN G 462      3.988  44.047 -17.593  1.00 20.00           c
```

```
ATOM   3037  CG  GLN G 462       3.237  45.115 -16.814  1.00 20.00           C
ATOM   3038  CD  GLN G 462       3.484  46.512 -17.353  1.00 20.00           C
ATOM   3039  OE1 GLN G 462       4.527  46.786 -17.947  1.00 20.00           O
ATOM   3040  NE2 GLN G 462       2.529  47.408 -17.135  1.00 20.00           N
ATOM   3041  C   GLN G 462       4.479  41.626 -17.986  1.00101.50           C
ATOM   3042  O   GLN G 462       5.701  41.501 -18.051  1.00105.94           O
ATOM   3043  N   GLU G 463       3.646  40.946 -18.769  1.00 98.92           N
ATOM   3044  CA  GLU G 463       4.140  39.928 -19.693  1.00108.59           C
ATOM   3045  CB  GLU G 463       3.380  38.612 -19.512  1.00 20.00           C
ATOM   3046  CG  GLU G 463       3.682  37.900 -18.201  1.00 20.00           C
ATOM   3047  CD  GLU G 463       2.842  36.650 -18.005  1.00 20.00           C
ATOM   3048  OE1 GLU G 463       2.003  36.350 -18.881  1.00 20.00           O
ATOM   3049  OE2 GLU G 463       3.075  35.929 -17.011  1.00 20.00           O
ATOM   3050  C   GLU G 463       4.074  40.384 -21.146  1.001 16.39           C
ATOM   3051  O   GLU G 463       3.025  40.814 -21.627  1.001 18.70           O
ATOM   3052  N   GLY G 464       5.200  40.272 -21.845  1.00127.70           N
ATOM   3053  CA  GLY G 464       5.261  40.610 -23.261  1.00143.17           C
ATOM   3054  C   GLY G 464       4.710  39.509 -24.146  1.00149.77           C
ATOM   3055  O   GLY G 464       4.443  38.400 -23.681  1.00155.06           O
ATOM   3056  N   LYS G 465       4.544  39.816 -25.428  1.00153.73           N
ATOM   3057  CA  LYS G 465       3.994  38.862 -26.384  1.00153.69           C
ATOM   3058  CB  LYS G 465       4.816  37.571 -26.389  1.00 20.00           C
ATOM   3059  CG  LYS G 465       6.228  37.735 -26.927  1.00 20.00           C
ATOM   3060  CD  LYS G 465       6.996  36.424 -26.873  1.00 20.00           C
ATOM   3061  CE  LYS G 465       8.402  36.585 -27.426  1.00 20.00           C
ATOM   3062  NZ  LYS G 465       9.172  35.312 -27.363  1.00 20.00           N
ATOM   3063  C   LYS G 465       2.532  38.552 -26.080  1.00155.37           C
ATOM   3064  O   LYS G 465       1.710  38.437 -26.988  1.00155.20           O
ATOM   3065  N   GLU G 472      -0.074  35.733 -32.259  1.00145.47           N
ATOM   3066  CA  GLU G 472      -0.706  34.866 -33.247  1.00151.12           C
ATOM   3067  CB  GLU G 472       0.178  34.736 -34.490  1.00 20.00           C
ATOM   3068  CG  GLU G 472       0.339  36.028 -35.276  1.00 20.00           C
ATOM   3069  CD  GLU G 472       1.271  35.876 -36.463  1.00 20.00           C
ATOM   3070  OE1 GLU G 472       1.954  34.835 -36.556  1.00 20.00           O
ATOM   3071  OE2 GLU G 472       1.325  36.803 -37.299  1.00 20.00           O
ATOM   3072  C   GLU G 472      -0.993  33.486 -32.663  1.00153.35           C
ATOM   3073  O   GLU G 472      -0.069  32.755 -32.306  1.00159.41           O
ATOM   3074  N   PRO G 473      -2.282  33.131 -32.557  1.00150.51           N
ATOM   3075  CA  PRO G 473      -2.668  31.819 -32.081  1.00141.97           C
ATOM   3076  CB  PRO G 473      -3.684  32.152 -30.990  1.00 20.00           C
ATOM   3077  CG  PRO G 473      -4.311  33.467 -31.446  1.00 20.00           C
ATOM   3078  CD  PRO G 473      -3.423  34.059 -32.523  1.00 20.00           C
ATOM   3079  C   PRO G 473      -3.357  31.051 -33.200  1.00135.14           C
ATOM   3080  O   PRO G 473      -3.883  31.662 -34.131  1.00144.93           O
ATOM   3081  N   ILE G 474      -3.379  29.727 -33.098  1.001 18.07           N
ATOM   3082  CA  ILE G 474      -3.969  28.899 -34.142  1.00105.14           C
ATOM   3083  CB  ILE G 474      -3.193  29.027 -35.469  1.00 20.00           C
ATOM   3084  CGI ILE G 474      -3.315  30.446 -36.028  1.00 20.00           C
ATOM   3085  CD1 ILE G 474      -2.352  30.745 -37.156  1.00 20.00           C
ATOM   3086  CG2 ILE G 474      -3.696  28.008 -36.481  1.00 20.00           C
ATOM   3087  C   ILE G 474      -4.007  27.432 -33.730  1.00104.75           C
ATOM   3088  O   ILE G 474      -3.033  26.702 -33.915  1.001 11.83           O
ATOM   3089  N   ILE G 475      -5.149  26.992 -33.213  1.00 94.65           N
ATOM   3090  CA  ILE G 475      -5.249  25.667 -32.611  1.00 79.88           C
ATOM   3091  CB  ILE G 475      -5.443  25.753 -31.087  1.00 20.00           C
ATOM   3092  CGI ILE G 475      -4.165  26.260 -30.413  1.00 20.00           C
ATOM   3093  CD1 ILE G 475      -4.414  27.012 -29.122  1.00 20.00           C
ATOM   3094  CG2 ILE G 475      -5.873  24.406 -30.525  1.00 20.00           C
ATOM   3095  C   ILE G 475      -6.374  24.834 -33.223  1.00 79.52           C
ATOM   3096  O   ILE G 475      -7.554  25.117 -33.016  1.00 82.70           O
```

```
ATOM   3097  N   ASN G 476      -5.996  23.761 -33.912   1.00 69.64           N
ATOM   3098  CA  ASN G 476      -6.962  22.821 -34.472   1.00 68.88           C
ATOM   3099  CB  ASN G 476      -6.365  22.100 -35.683   1.00 20.00           C
ATOM   3100  CG  ASN G 476      -6.170  23.019 -36.872   1.00 20.00           C
ATOM   3101  OD1 ASN G 476      -6.855  24.032 -37.009   1.00 20.00           O
ATOM   3102  ND2 ASN G 476      -5.251  22.651 -37.756   1.00 20.00           N
ATOM   3103  C   ASN G 476      -7.434  21.799 -33.443   1.00 67.13           C
ATOM   3104  O   ASN G 476      -6.628  21.229 -32.707   1.00 73.10           O
ATOM   3105  N   PHE G 477      -8.735  21.527 -33.438   1.00 64.95           N
ATOM   3106  CA  PHE G 477      -9.327  20.624 -32.455   1.00 68.13           C
ATOM   3107  CB  PHE G 477     -10.854  20.711 -32.493   1.00 20.00           C
ATOM   3108  CG  PHE G 477     -11.397  22.047 -32.079   1.00 20.00           C
ATOM   3109  CD1 PHE G 477     -11.580  22.352 -30.740   1.00 20.00           C
ATOM   3110  CE1 PHE G 477     -12.086  23.580 -30.357   1.00 20.00           C
ATOM   3111  CZ  PHE G 477     -12.426  24.514 -31.316   1.00 20.00           C
ATOM   3112  CE2 PHE G 477     -12.257  24.219 -32.654   1.00 20.00           C
ATOM   3113  CD2 PHE G 477     -11.750  22.989 -33.030   1.00 20.00           C
ATOM   3114  C   PHE G 477      -8.890  19.180 -32.672   1.00 65.57           C
ATOM   3115  O   PHE G 477      -9.270  18.290 -31.911   1.00 49.83           O
ATOM   3116  N   TYR G 478      -8.204  18.931 -33.782   1.00 51.97           N
ATOM   3117  CA  TYR G 478      -7.618  17.619 -34.036   1.00 52.01           C
ATOM   3118  CB  TYR G 478      -7.356  17.428 -35.530   1.00 20.00           C
ATOM   3119  CG  TYR G 478      -8.609  17.426 -36.372   1.00 20.00           C
ATOM   3120  CD1 TYR G 478      -9.337  16.259 -36.567   1.00 20.00           C
ATOM   3121  CE1 TYR G 478     -10.489  16.255 -37.329   1.00 20.00           C
ATOM   3122  CZ  TYR G 478     -10.930  17.429 -37.902   1.00 20.00           C
ATOM   3123  OH  TYR G 478     -12.078  17.432 -38.658   1.00 20.00           O
ATOM   3124  CE2 TYR G 478     -10.230  18.602 -37.717   1.00 20.00           C
ATOM   3125  CD2 TYR G 478      -9.079  18.596 -36.954   1.00 20.00           C
ATOM   3126  C   TYR G 478      -6.325  17.459 -33.251   1.00 66.63           C
ATOM   3127  O   TYR G 478      -5.548  16.535 -33.492   1.00 63.45           O
ATOM   3128  N   ASP G 479      -6.062  18.423 -32.375   1.00 65.34           N
ATOM   3129  CA  ASP G 479      -4.928  18.351 -31.469   1.00 65.32           C
ATOM   3130  CB  ASP G 479      -4.205  19.698 -31.413   1.00 20.00           C
ATOM   3131  CG  ASP G 479      -3.509  20.038 -32.717   1.00 20.00           C
ATOM   3132  OD1 ASP G 479      -3.293  19.119 -33.534   1.00 20.00           O
ATOM   3133  OD2 ASP G 479      -3.184  21.225 -32.930   1.00 20.00           O
ATOM   3134  C   ASP G 479      -5.383  17.937 -30.076   1.00 64.83           C
ATOM   3135  O   ASP G 479      -4.561  17.574 -29.236   1.00 60.42           O
ATOM   3136  N   PRO G 480      -6.707  17.893 -29.861   1.00 47.60           N
ATOM   3137  CA  PRO G 480      -7.262  17.523 -28.572   1.00 46.52           C
ATOM   3138  CB  PRO G 480      -8.509  18.400 -28.480   1.00 20.00           C
ATOM   3139  CG  PRO G 480      -8.954  18.565 -29.904   1.00 20.00           C
ATOM   3140  CD  PRO G 480      -7.755  18.332 -30.799   1.00 20.00           C
ATOM   3141  C   PRO G 480      -7.662  16.056 -28.548   1.00 52.36           C
ATOM   3142  O   PRO G 480      -8.804  15.721 -28.860   1.00 64.15           O
ATOM   3143  N   LEU G 481      -6.698  15.183 -28.281   1.00 62.90           N
ATOM   3144  CA  LEU G 481      -6.977  13.759 -28.138   1.00 54.24           C
ATOM   3145  CB  LEU G 481      -6.143  12.944 -29.128   1.00 20.00           C
ATOM   3146  CG  LEU G 481      -6.449  13.142 -30.613   1.00 20.00           C
ATOM   3147  CD1 LEU G 481      -5.475  12.348 -31.471   1.00 20.00           C
ATOM   3148  CD2 LEU G 481      -7.884  12.747 -30.922   1.00 20.00           C
ATOM   3149  C   LEU G 481      -6.700  13.285 -26.717   1.00 59.81           C
ATOM   3150  O   LEU G 481      -6.199  14.041 -25.884   1.00 64.98           O
ATOM   3151  N   VAL G 482      -6.956  12.008 -26.470   1.00 59.66           N
ATOM   3152  CA  VAL G 482      -6.588  11.404 -25.203   1.00 49.67           C
ATOM   3153  CB  VAL G 482      -7.741  10.579 -24.619   1.00 20.00           C
ATOM   3154  CGI VAL G 482      -7.390  10.116 -23.220   1.00 20.00           C
ATOM   3155  CG2 VAL G 482      -9.021  11.398 -24.607   1.00 20.00           C
ATOM   3156  C   VAL G 482      -5.357  10.525 -25.372   1.00 53.03           C
```

ATOM 3157 O VAL G 482 -5.147 9.945 -26.437 1.00 46.27 O
ATOM 3158 N PHE G 483 -4.464 10.579 -24.387 1.00 61.61 N
ATOM 3159 CA PHE G 483 -3.282 9.723 -24.370 1.00 65.03 C
ATOM 3160 CB PHE G 483 -2.011 10.562 -24.235 1.00 20.00 C
ATOM 3161 CG PHE G 483 -1.788 11.500 -25.385 1.00 20.00 C
ATOM 3162 CD1 PHE G 483 -1.173 11.059 -26.546 1.00 20.00 C
ATOM 3163 CE1 PHE G 483 -1.039 11.897 -27.632 1.00 20.00 C
ATOM 3164 CZ PHE G 483 -1.577 13.170 -27.589 1.00 20.00 C
ATOM 3165 CE2 PHE G 483 -2.199 13.618 -26.442 1.00 20.00 C
ATOM 3166 CD2 PHE G 483 -2.315 12.781 -25.355 1.00 20.00 C
ATOM 3167 C PHE G 483 -3.358 8.663 -23.275 1.00 71.00 C
ATOM 3168 O PHE G 483 -2.688 8.776 -22.248 1.00100.44 O
ATOM 3169 N PRO G 484 -4.338 7.759 -23.403 1.00 54.44 N
ATOM 3170 CA PRO G 484 -4.502 6.677 -22.459 1.00 47.46 C
ATOM 3171 CB PRO G 484 -5.761 7.096 -21.701 1.00 20.00 C
ATOM 3172 CG PRO G 484 -6.554 7.922 -22.714 1.00 20.00 C
ATOM 3173 CD PRO G 484 -5.649 8.206 -23.894 1.00 20.00 C
ATOM 3174 C PRO G 484 -4.778 5.378 -23.204 1.00 41.56 C
ATOM 3175 O PRO G 484 -5.689 5.321 -24.029 1.00 46.53 O
ATOM 3176 N SER G 485 -3.961 4.363 -22.958 1.00 46.30 N
ATOM 3177 CA SER G 485 -4.081 3.108 -23.686 1.00 49.30 C
ATOM 3178 CB SER G 485 -3.559 1.943 -22.841 1.00 20.00 C
ATOM 3179 OG SER G 485 -4.215 1.884 -21.588 1.00 20.00 O
ATOM 3180 C SER G 485 -5.521 2.856 -24.147 1.00 41.24 C
ATOM 3181 O SER G 485 -5.809 2.890 -25.345 1.00 46.93 O
ATOM 3182 N ASP G 486 -6.437 2.720 -23.190 1.00 49.48 N
ATOM 3183 CA ASP G 486 -7.816 2.321 -23.485 1.00 37.44 C
ATOM 3184 CB ASP G 486 -8.659 2.287 -22.205 1.00 20.00 C
ATOM 3185 CG ASP G 486 -8.296 1.125 -21.289 1.00 20.00 C
ATOM 3186 OD1 ASP G 486 -7.611 0.188 -21.746 1.00 20.00 O
ATOM 3187 OD2 ASP G 486 -8.637 1.184 -20.089 1.00 20.00 O
ATOM 3188 C ASP G 486 -8.447 3.271 -24.491 1.00 45.66 C
ATOM 3189 O ASP G 486 -9.005 2.844 -25.501 1.00 39.86 O
ATOM 3190 N GLU G 487 -8.317 4.566 -24.225 1.00 49.20 N
ATOM 3191 CA GLU G 487 -8.853 5.585 -25.116 1.00 45.70 C
ATOM 3192 CB GLU G 487 -8.656 6.982 -24.525 1.00 20.00 C
ATOM 3193 CG GLU G 487 -9.449 7.237 -23.251 1.00 20.00 C
ATOM 3194 CD GLU G 487 -9.144 8.590 -22.635 1.00 20.00 C
ATOM 3195 OE1 GLU G 487 -8.175 9.245 -23.078 1.00 20.00 O
ATOM 3196 OE2 GLU G 487 -9.865 8.988 -21.695 1.00 20.00 O
ATOM 3197 C GLU G 487 -8.222 5.504 -26.501 1.00 41.48 C
ATOM 3198 O GLU G 487 -8.914 5.623 -27.512 1.00 48.92 O
ATOM 3199 N PHE G 488 -6.910 5.306 -26.545 1.00 42.16 N
ATOM 3200 CA PHE G 488 -6.206 5.215 -27.815 1.00 39.33 C
ATOM 3201 CB PHE G 488 -4.701 5.086 -27.590 1.00 20.00 C
ATOM 3202 CG PHE G 488 -4.074 6.308 -26.992 1.00 20.00 C
ATOM 3203 CD1 PHE G 488 -3.910 7.454 -27.747 1.00 20.00 C
ATOM 3204 CE1 PHE G 488 -3.320 8.574 -27.202 1.00 20.00 C
ATOM 3205 CZ PHE G 488 -2.847 8.542 -25.898 1.00 20.00 C
ATOM 3206 CE2 PHE G 488 -3.006 7.404 -25.136 1.00 20.00 C
ATOM 3207 CD2 PHE G 488 -3.630 6.302 -25.678 1.00 20.00 C
ATOM 3208 C PHE G 488 -6.724 4.040 -28.634 1.00 43.06 C
ATOM 3209 O PHE G 488 -7.101 4.203 -29.794 1.00 61.71 O
ATOM 3210 N ASP G 489 -6.910 2.906 -27.972 1.00 41.95 N
ATOM 3211 CA ASP G 489 -7.330 1.695 -28.658 1.00 42.75 C
ATOM 3212 CB ASP G 489 -7.257 0.499 -27.717 1.00 20.00 C
ATOM 3213 CG ASP G 489 -5.838 0.116 -27.389 1.00 20.00 C
ATOM 3214 OD1 ASP G 489 -4.920 0.637 -28.056 1.00 20.00 O
ATOM 3215 OD2 ASP G 489 -5.636 -0.633 -26.411 1.00 20.00 O
ATOM 3216 C ASP G 489 -8.733 1.825 -29.233 1.00 45.61 C

```
ATOM   3217  O   ASP G 489      -9.066   1.181 -30.226   1.00 54.39          O
ATOM   3218  N   ALA G 490      -9.568   2.622 -28.575   1.00 42.89          N
ATOM   3219  CA  ALA G 490     -10.929   2.848 -29.044   1.00 38.40          C
ATOM   3220  CB  ALA G 490     -11.760   3.516 -27.963   1.00 20.00          C
ATOM   3221  C   ALA G 490     -10.932   3.687 -30.315   1.00 39.67          C
ATOM   3222  O   ALA G 490     -11.651   3.386 -31.267   1.00 56.80          O
ATOM   3223  N   SER G 491     -10.138   4.752 -30.315   1.00 40.38          N
ATOM   3224  CA  SER G 491      -9.984   5.586 -31.499   1.00 41.77          C
ATOM   3225  CB  SER G 491      -9.155   6.831 -31.176   1.00 20.00          C
ATOM   3226  OG  SER G 491      -7.806   6.490 -30.912   1.00 20.00          O
ATOM   3227  C   SER G 491      -9.333   4.801 -32.631   1.00 39.01          C
ATOM   3228  O   SER G 491      -9.688   4.967 -33.798   1.00 36.91          O
ATOM   3229  N   ILE G 492      -8.387   3.938 -32.278   1.00 38.11          N
ATOM   3230  CA  ILE G 492      -7.741   3.077 -33.259   1.00 41.21          C
ATOM   3231  CB  ILE G 492      -6.630   2.211 -32.620   1.00 20.00          C
ATOM   3232  CGI ILE G 492      -5.507   3.092 -32.061   1.00 20.00          C
ATOM   3233  CD1 ILE G 492      -4.533   2.346 -31.163   1.00 20.00          C
ATOM   3234  CG2 ILE G 492      -6.067   1.219 -33.634   1.00 20.00          C
ATOM   3235  C   ILE G 492      -8.773   2.170 -33.916   1.00 39.22          C
ATOM   3236  O   ILE G 492      -8.778   2.008 -35.135   1.00 47.54          O
ATOM   3237  N   SER G 493      -9.703   1.662 -33.111   1.00 41.64          N
ATOM   3238  CA  SER G 493     -10.786   0.819 -33.612   1.00 35.15          C
ATOM   3239  CB  SER G 493     -11.579   0.202 -32.454   1.00 20.00          C
ATOM   3240  OG  SER G 493     -12.267   1.196 -31.716   1.00 20.00          O
ATOM   3241  C   SER G 493     -11.716   1.614 -34.523   1.00 47.90          C
ATOM   3242  O   SER G 493     -12.169   1.115 -35.555   1.00 50.94          O
ATOM   3243  N   GLN G 494     -11.936   2.877 -34.169   1.00 42.51          N
ATOM   3244  CA  GLN G 494     -12.789   3.766 -34.955   1.00 41.96          C
ATOM   3245  CB  GLN G 494     -13.107   5.036 -34.167   1.00 20.00          C
ATOM   3246  CG  GLN G 494     -13.991   4.813 -32.955   1.00 20.00          C
ATOM   3247  CD  GLN G 494     -14.211   6.084 -32.163   1.00 20.00          C
ATOM   3248  OE1 GLN G 494     -13.406   7.013 -32.223   1.00 20.00          O
ATOM   3249  NE2 GLN G 494     -15.317   6.140 -31.430   1.00 20.00          N
ATOM   3250  C   GLN G 494     -12.151   4.137 -36.291   1.00 33.86          C
ATOM   3251  O   GLN G 494     -12.829   4.195 -37.318   1.00 54.89          O
ATOM   3252  N   VAL G 495     -10.881   4.523 -36.241   1.00 34.99          N
ATOM   3253  CA  VAL G 495     -10.108   4.772 -37.451   1.00 38.42          C
ATOM   3254  CB  VAL G 495      -8.642   5.097 -37.120   1.00 20.00          C
ATOM   3255  CGI VAL G 495      -7.840   5.297 -38.394   1.00 20.00          C
ATOM   3256  CG2 VAL G 495      -8.562   6.327 -36.231   1.00 20.00          C
ATOM   3257  C   VAL G 495     -10.152   3.573 -38.393   1.00 42.74          C
ATOM   3258  O   VAL G 495     -10.424   3.720 -39.584   1.00 44.00          O
ATOM   3259  N   ASN G 496      -9.947   2.383 -37.838   1.00 42.45          N
ATOM   3260  CA  ASN G 496      -9.967   1.147 -38.617   1.00 43.01          C
ATOM   3261  CB  ASN G 496      -9.572  -0.046 -37.743   1.00 20.00          C
ATOM   3262  CG  ASN G 496      -8.118   0.000 -37.319   1.00 20.00          C
ATOM   3263  OD1 ASN G 496      -7.293   0.648 -37.965   1.00 20.00          O
ATOM   3264  ND2 ASN G 496      -7.796  -0.684 -36.226   1.00 20.00          N
ATOM   3265  C   ASN G 496     -11.305   0.875 -39.310   1.00 43.13          C
ATOM   3266  O   ASN G 496     -11.334   0.405 -40.448   1.00 54.76          O
ATOM   3267  N   GLU G 497     -12.407   1.099 -38.598   1.00 42.08          N
ATOM   3268  CA  GLU G 497     -13.738   0.938 -39.183   1.00 43.13          C
ATOM   3269  CB  GLU G 497     -14.827   1.144 -38.127   1.00 20.00          C
ATOM   3270  CG  GLU G 497     -14.937   0.018 -37.110   1.00 20.00          C
ATOM   3271  CD  GLU G 497     -15.946   0.316 -36.017   1.00 20.00          C
ATOM   3272  OE1 GLU G 497     -16.552   1.408 -36.049   1.00 20.00          O
ATOM   3273  OE2 GLU G 497     -16.177  -0.566 -35.164   1.00 20.00          O
ATOM   3274  C   GLU G 497     -13.937   1.915 -40.337   1.00 49.77          C
ATOM   3275  O   GLU G 497     -14.552   1.580 -41.349   1.00 42.88          O
ATOM   3276  N   LYS G 498     -13.367   3.108 -40.195   1.00 41.82          N
```

```
ATOM   3277  CA  LYS G 498     -13.435   4.123 -41.240  1.00 53.60           C
ATOM   3278  CB  LYS G 498     -12.968   5.479 -40.705  1.00 20.00           C
ATOM   3279  CG  LYS G 498     -13.937   6.125 -39.728  1.00 20.00           C
ATOM   3280  CD  LYS G 498     -13.439   7.484 -39.269  1.00 20.00           C
ATOM   3281  CE  LYS G 498     -14.393   8.108 -38.265  1.00 20.00           C
ATOM   3282  NZ  LYS G 498     -13.896   9.421 -37.768  1.00 20.00           N
ATOM   3283  C   LYS G 498     -12.61 1   3.724 -42.458  1.00 55.29           C
ATOM   3284  O   LYS G 498     -13.033   3.926 -43.594  1.00 61.06           O
ATOM   3285  N   ILE G 499     -11.430   3.165 -42.214  1.00 52.22           N
ATOM   3286  CA  ILE G 499     -10.609   2.604 -43.284  1.00 48.26           C
ATOM   3287  CB  ILE G 499      -9.296   2.009 -42.729  1.00 20.00           C
ATOM   3288  CGI ILE G 499      -8.446   3.101 -42.072  1.00 20.00           C
ATOM   3289  CD1 ILE G 499      -7.506   2.582 -41.002  1.00 20.00           C
ATOM   3290  CG2 ILE G 499      -8.516   1.288 -43.825  1.00 20.00           C
ATOM   3291  C   ILE G 499     -11.376   1.515 -44.031  1.00 49.07           C
ATOM   3292  O   ILE G 499     -11.282   1.398 -45.253  1.00 58.45           O
ATOM   3293  N   ASN G 500     -12.183   0.764 -43.288  1.00 51.02           N
ATOM   3294  CA  ASN G 500     -12.992  -0.307 -43.857  1.00 52.06           C
ATOM   3295  CB  ASN G 500     -13.500  -1.238 -42.748  1.00 20.00           C
ATOM   3296  CG  ASN G 500     -14.173  -2.487 -43.292  1.00 20.00           C
ATOM   3297  OD1 ASN G 500     -13.795  -3.005 -44.342  1.00 20.00           O
ATOM   3298  ND2 ASN G 500     -15.127  -3.019 -42.536  1.00 20.00           N
ATOM   3299  C   ASN G 500     -14.161   0.250 -44.659  1.00 48.31           C
ATOM   3300  O   ASN G 500     -14.645  -0.386 -45.596  1.00 56.89           O
ATOM   3301  N   GLN G 501     -14.582   1.461 -44.312  1.00 55.87           N
ATOM   3302  CA  GLN G 501     -15.607   2.160 -45.074  1.00 53.55           C
ATOM   3303  CB  GLN G 501     -16.243   3.258 -44.222  1.00 20.00           C
ATOM   3304  CG  GLN G 501     -17.012   2.741 -43.015  1.00 20.00           C
ATOM   3305  CD  GLN G 501     -17.674   3.857 -42.226  1.00 20.00           C
ATOM   3306  OE1 GLN G 501     -17.178   4.985 -42.189  1.00 20.00           O
ATOM   3307  NE2 GLN G 501     -18.772   3.536 -41.553  1.00 20.00           N
ATOM   3308  C   GLN G 501     -15.030   2.751 -46.357  1.00 45.67           C
ATOM   3309  O   GLN G 501     -15.627   2.633 -47.429  1.00 58.31           O
ATOM   3310  N   SER G 502     -13.824   3.303 -46.258  1.00 43.44           N
ATOM   3311  CA  SER G 502     -13.117   3.801 -47.432  1.00 45.40           C
ATOM   3312  CB  SER G 502     -11.789   4.468 -47.045  1.00 20.00           C
ATOM   3313  OG  SER G 502     -10.928   3.572 -46.361  1.00 20.00           O
ATOM   3314  C   SER G 502     -12.891   2.677 -48.436  1.00 55.15           C
ATOM   3315  O   SER G 502     -13.234   2.819 -49.610  1.00 52.57           O
ATOM   3316  N   LEU G 503     -12.552   1.495 -47.922  1.00 55.35           N
ATOM   3317  CA  LEU G 503     -12.227   0.349 -48.768  1.00 52.12           C
ATOM   3318  CB  LEU G 503     -11.591  -0.778 -47.943  1.00 20.00           C
ATOM   3319  CG  LEU G 503     -10.187  -0.535 -47.373  1.00 20.00           C
ATOM   3320  CD1 LEU G 503      -9.810  -1.609 -46.357  1.00 20.00           C
ATOM   3321  CD2 LEU G 503      -9.144  -0.458 -48.481  1.00 20.00           C
ATOM   3322  C   LEU G 503     -13.471  -0.159 -49.489  1.00 55.74           C
ATOM   3323  O   LEU G 503     -13.402  -0.586 -50.642  1.00 57.75           O
ATOM   3324  N   ALA G 504     -14.618  -0.046 -48.826  1.00 57.22           N
ATOM   3325  CA  ALA G 504     -15.893  -0.410 -49.436  1.00 59.12           C
ATOM   3326  CB  ALA G 504     -16.981  -0.532 -48.377  1.00 20.00           C
ATOM   3327  C   ALA G 504     -16.293   0.605 -50.499  1.00 58.10           C
ATOM   3328  O   ALA G 504     -16.773   0.241 -51.573  1.00 63.64           O
ATOM   3329  N   PHE G 505     -16.075   1.881 -50.198  1.00 58.17           N
ATOM   3330  CA  PHE G 505     -16.303   2.940 -51.171  1.00 56.56           C
ATOM   3331  CB  PHE G 505     -15.991   4.309 -50.564  1.00 20.00           C
ATOM   3332  CG  PHE G 505     -16.870   4.665 -49.405  1.00 20.00           C
ATOM   3333  CD1 PHE G 505     -18.185   5.035 -49.615  1.00 20.00           C
ATOM   3334  CE1 PHE G 505     -19.045   5.205 -48.555  1.00 20.00           C
ATOM   3335  CZ  PHE G 505     -18.617   4.934 -47.269  1.00 20.00           C
ATOM   3336  CE2 PHE G 505     -17.314   4.545 -47.047  1.00 20.00           C
```

ATOM 3337 CD2 PHE G 505 -16.446 4.423 -48.109 1.00 20.00 C
ATOM 3338 C PHE G 505 -15.462 2.715 -52.416 1.00 60.12 C
ATOM 3339 O PHE G 505 -15.922 2.939 -53.535 1.00 65.46 O
ATOM 3340 N ILE G 506 -14.235 2.242 -52.213 1.00 56.10 N
ATOM 3341 CA ILE G 506 -13.325 1.960 -53.320 1.00 57.32 C
ATOM 3342 CB ILE G 506 -11.911 1.590 -52.825 1.00 20.00 C
ATOM 3343 CGI ILE G 506 -11.167 2.839 -52.352 1.00 20.00 C
ATOM 3344 CD1 ILE G 506 -10.010 2.533 -51.425 1.00 20.00 C
ATOM 3345 CG2 ILE G 506 -11.126 0.882 -53.925 1.00 20.00 C
ATOM 3346 C ILE G 506 -13.845 0.812 -54.170 1.00 67.33 C
ATOM 3347 O ILE G 506 -13.674 0.803 -55.390 1.00 76.99 O
ATOM 3348 N ARG G 507 -14.325 -0.230 -53.503 1.00 67.87 N
ATOM 3349 CA ARG G 507 -14.920 -1.360 -54.195 1.00 62.11 C
ATOM 3350 CB ARG G 507 -15.328 -2.440 -53.196 1.00 20.00 C
ATOM 3351 CG ARG G 507 -14.151 -3.082 -52.491 1.00 20.00 C
ATOM 3352 CD ARG G 507 -14.592 -4.218 -51.585 1.00 20.00 C
ATOM 3353 NE ARG G 507 -13.453 -4.836 -50.911 1.00 20.00 N
ATOM 3354 CZ ARG G 507 -13.555 -5.749 -49.950 1.00 20.00 C
ATOM 3355 NH1 ARG G 507 -14.748 -6.221 -49.609 1.00 20.00 N
ATOM 3356 NH2 ARG G 507 -12.459 -6.278 -49.422 1.00 20.00 N
ATOM 3357 C ARG G 507 -16.119 -0.920 -55.026 1.00 67.30 C
ATOM 3358 O ARG G 507 -16.131 -1.079 -56.247 1.00 67.02 O
ATOM 3359 N LYS G 508 -17.080 -0.274 -54.375 1.00 66.83 N
ATOM 3360 CA LYS G 508 -18.220 0.295 -55.078 1.00 68.12 C
ATOM 3361 CB LYS G 508 -19.052 1.156 -54.133 1.00 20.00 C
ATOM 3362 CG LYS G 508 -19.813 0.362 -53.096 1.00 20.00 C
ATOM 3363 CD LYS G 508 -20.707 1.269 -52.270 1.00 20.00 C
ATOM 3364 CE LYS G 508 -21.508 0.479 -51.248 1.00 20.00 C
ATOM 3365 NZ LYS G 508 -22.370 1.366 -50.421 1.00 20.00 N
ATOM 3366 C LYS G 508 -17.758 1.131 -56.261 1.00 65.22 C
ATOM 3367 O LYS G 508 -18.149 0.880 -57.402 1.00 72.34 O
ATOM 3368 N SER G 509 -16.859 2.071 -55.990 1.00 64.87 N
ATOM 3369 CA SER G 509 -16.316 2.939 -57.028 1.00 56.47 C
ATOM 3370 CB SER G 509 -15.268 3.896 -56.442 1.00 20.00 C
ATOM 3371 OG SER G 509 -14.170 3.190 -55.888 1.00 20.00 O
ATOM 3372 C SER G 509 -15.736 2.147 -58.205 1.00 56.96 C
ATOM 3373 O SER G 509 -16.064 2.412 -59.363 1.00 65.57 O
ATOM 3374 N ASP G 510 -14.906 1.154 -57.902 1.00 64.34 N
ATOM 3375 CA ASP G 510 -14.282 0.340 -58.939 1.00 64.83 C
ATOM 3376 CB ASP G 510 -13.338 -0.690 -58.316 1.00 20.00 C
ATOM 3377 CG ASP G 510 -12.073 -0.063 -57.768 1.00 20.00 C
ATOM 3378 OD1 ASP G 510 -11.789 1.104 -58.112 1.00 20.00 O
ATOM 3379 OD2 ASP G 510 -11.361 -0.735 -56.993 1.00 20.00 O
ATOM 3380 C ASP G 510 -15.339 -0.362 -59.782 1.00 62.11 C
ATOM 3381 O ASP G 510 -15.346 -0.251 -61.008 1.00 67.61 O
ATOM 3382 N GLU G 511 -16.244 -1.067 -59.112 1.00 64.95 N
ATOM 3383 CA GLU G 511 -17.319 -1.774 -59.791 1.00 60.64 C
ATOM 3384 CB GLU G 511 -18.359 -2.259 -58.780 1.00 20.00 C
ATOM 3385 CG GLU G 511 -17.818 -3.293 -57.801 1.00 20.00 C
ATOM 3386 CD GLU G 511 -18.840 -3.723 -56.760 1.00 20.00 C
ATOM 3387 OE1 GLU G 511 -19.857 -3.017 -56.585 1.00 20.00 O
ATOM 3388 OE2 GLU G 511 -18.603 -4.746 -56.083 1.00 20.00 O
ATOM 3389 C GLU G 511 -17.970 -0.888 -60.842 1.00 59.91 C
ATOM 3390 O GLU G 511 -18.090 -1.278 -62.003 1.00 55.45 O
ATOM 3391 N LEU G 512 -18.270 0.349 -60.460 1.00 44.35 N
ATOM 3392 CA LEU G 512 -18.978 1.259 -61.346 1.00 49.60 C
ATOM 3393 CB LEU G 512 -19.424 2.511 -60.590 1.00 20.00 C
ATOM 3394 CG LEU G 512 -20.377 2.256 -59.416 1.00 20.00 C
ATOM 3395 CD1 LEU G 512 -20.747 3.550 -58.696 1.00 20.00 C
ATOM 3396 CD2 LEU G 512 -21.624 1.499 -59.858 1.00 20.00 C

ATOM 3397 C LEU G 512 -18.128 1.626 -62.557 1.00 58.00 C
ATOM 3398 O LEU G 512 -18.542 1.415 -63.696 1.00 55.11 O
ATOM 3399 N LEU G 513 -16.883 2.015 -62.305 1.00 57.91 N
ATOM 3400 CA LEU G 513 -15.963 2.384 -63.378 1.00 57.49 C
ATOM 3401 CB LEU G 513 -14.609 2.810 -62.801 1.00 20.00 C
ATOM 3402 CG LEU G 513 -14.558 4.136 -62.038 1.00 20.00 C
ATOM 3403 CD1 LEU G 513 -13.242 4.263 -61.282 1.00 20.00 C
ATOM 3404 CD2 LEU G 513 -14.743 5.302 -62.996 1.00 20.00 C
ATOM 3405 C LEU G 513 -15.775 1.231 -64.362 1.00 58.78 C
ATOM 3406 O LEU G 513 -15.707 1.437 -65.574 1.00 59.88 O
ATOM 3407 N HIS G 514 -15.708 0.015 -63.829 1.00 60.07 N
ATOM 3408 CA HIS G 514 -15.540 -1.175 -64.652 1.00 62.82 C
ATOM 3409 CB HIS G 514 -15.189 -2.383 -63.782 1.00 20.00 C
ATOM 3410 CG HIS G 514 -13.924 -2.217 -63.001 1.00 20.00 C
ATOM 3411 ND1 HIS G 514 -12.683 -2.154 -63.598 1.00 20.00 N
ATOM 3412 CE1 HIS G 514 -11.757 -2.005 -62.668 1.00 20.00 C
ATOM 3413 NE2 HIS G 514 -12.351 -1.975 -61.489 1.00 20.00 N
ATOM 3414 CD2 HIS G 514 -13.706 -2.113 -61.669 1.00 20.00 C
ATOM 3415 C HIS G 514 -16.796 -1.465 -65.463 1.00 65.10 C
ATOM 3416 O HIS G 514 -16.745 -2.170 -66.470 1.00 66.73 O
ATOM 3417 N ASN G 515 -17.926 -0.941 -65.000 1.00 63.45 N
ATOM 3418 CA ASN G 515 -19.179 -1.062 -65.732 1.00 56.53 C
ATOM 3419 CB ASN G 515 -20.370 -0.925 -64.783 1.00 20.00 C
ATOM 3420 CG ASN G 515 -20.503 -2.107 -63.845 1.00 20.00 C
ATOM 3421 OD1 ASN G 515 -19.979 -3.190 -64.113 1.00 20.00 O
ATOM 3422 ND2 ASN G 515 -21.206 -1.906 -62.734 1.00 20.00 N
ATOM 3423 C ASN G 515 -19.289 -0.043 -66.860 1.00 60.06 C
ATOM 3424 O ASN G 515 -19.825 -0.335 -67.928 1.00 66.48 O
ATOM 3425 N VAL G 516 -18.818 1.168 -66.598 1.00 54.29 N
ATOM 3426 CA VAL G 516 -18.783 2.200 -67.620 1.00 52.70 C
ATOM 3427 CB VAL G 516 -18.233 3.518 -67.056 1.00 20.00 C
ATOM 3428 CGI VAL G 516 -18.151 4.566 -68.153 1.00 20.00 C
ATOM 3429 CG2 VAL G 516 -19.098 4.003 -65.904 1.00 20.00 C
ATOM 3430 C VAL G 516 -17.910 1.753 -68.784 1.00 60.10 C
ATOM 3431 O VAL G 516 -18.340 1.765 -69.937 1.00 61.55 O
ATOM 3432 N ASN G 517 -16.733 1.232 -68.455 1.00 69.10 N
ATOM 3433 CA ASN G 517 -15.793 0.770 -69.466 1.00 67.75 C
ATOM 3434 CB ASN G 517 -14.564 0.137 -68.807 1.00 20.00 C
ATOM 3435 CG ASN G 517 -13.665 1.163 -68.146 1.00 20.00 C
ATOM 3436 OD1 ASN G 517 -13.646 2.330 -68.534 1.00 20.00 O
ATOM 3437 ND2 ASN G 517 -12.873 0.718 -67.177 1.00 20.00 N
ATOM 3438 C ASN G 517 -16.439 -0.209 -70.444 1.00 71.17 C
ATOM 3439 O ASN G 517 -16.188 -0.154 -71.649 1.00 66.42 O
ATOM 3440 N ALA G 518 -17.351 -1.033 -69.935 1.00 72.11 N
ATOM 3441 CA ALA G 518 -18.026 -2.024 -70.764 1.00 74.82 C
ATOM 3442 CB ALA G 518 -18.558 -3.164 -69.912 1.00 20.00 C
ATOM 3443 C ALA G 518 -19.145 -1.399 -71.593 1.00 70.11 C
ATOM 3444 O ALA G 518 -19.363 -1.789 -72.739 1.00 65.18 O
ATOM 3445 N GLY G 519 -19.865 -0.448 -71.006 1.00 56.07 N
ATOM 3446 CA GLY G 519 -20.825 0.357 -71.760 1.00 53.01 C
ATOM 3447 C GLY G 519 -20.156 1.166 -72.856 1.00 63.58 C
ATOM 3448 O GLY G 519 -20.684 1.295 -73.962 1.00 69.35 O
ATOM 3449 N LYS G 520 -18.950 1.647 -72.561 1.00 58.33 N
ATOM 3450 CA LYS G 520 -18.122 2.361 -73.533 1.00 53.44 C
ATOM 3451 CB LYS G 520 -16.848 2.877 -72.865 1.00 20.00 C
ATOM 3452 CG LYS G 520 -17.081 3.958 -71.831 1.00 20.00 C
ATOM 3453 CD LYS G 520 -15.781 4.341 -71.152 1.00 20.00 C
ATOM 3454 CE LYS G 520 -15.984 5.482 -70.173 1.00 20.00 C
ATOM 3455 NZ LYS G 520 -14.753 5.730 -69.376 1.00 20.00 N
ATOM 3456 C LYS G 520 -17.746 1.492 -74.731 1.00 58.24 C

ATOM 3457 O LYS G 520 -17.445 2.006 -75.810 1.00 48.60 O
ATOM 3458 N SER G 521 -17.583 0.198 -74.478 1.00 67.19 N
ATOM 3459 CA SER G 521 -17.366 -0.776 -75.542 1.00 60.42 C
ATOM 3460 CB SER G 521 -16.953 -2.131 -74.959 1.00 20.00 C
ATOM 3461 OG SER G 521 -18.028 -2.751 -74.272 1.00 20.00 O
ATOM 3462 C SER G 521 -18.588 -0.942 -76.444 1.00 54.19 C
ATOM 3463 O SER G 521 -18.456 -1.004 -77.664 1.00 65.36 O
ATOM 3464 N THR G 522 -19.761 -1.120 -75.840 1.00 50.09 N
ATOM 3465 CA THR G 522 -21.001 -1.210 -76.608 1.00 57.59 C
ATOM 3466 CB THR G 522 -22.235 -1.431 -75.705 1.00 20.00 C
ATOM 3467 OG1 THR G 522 -22.276 -0.422 -74.689 1.00 20.00 O
ATOM 3468 CG2 THR G 522 -22.196 -2.805 -75.058 1.00 20.00 C
ATOM 3469 C THR G 522 -21.206 0.063 -77.423 1.00 59.16 C
ATOM 3470 O THR G 522 -21.384 0.010 -78.640 1.00 65.90 O
ATOM 3471 N THR G 523 -21.024 1.205 -76.768 1.00 52.59 N
ATOM 3472 CA THR G 523 -21.234 2.498 -77.404 1.00 42.19 C
ATOM 3473 CB THR G 523 -20.961 3.638 -76.423 1.00 20.00 C
ATOM 3474 OG1 THR G 523 -19.578 3.622 -76.049 1.00 20.00 O
ATOM 3475 CG2 THR G 523 -21.819 3.467 -75.180 1.00 20.00 C
ATOM 3476 C THR G 523 -20.352 2.676 -78.636 1.00 48.90 C
ATOM 3477 O THR G 523 -20.786 3.238 -79.641 1.00 63.19 O
ATOM 3478 N ASN G 524 -19.113 2.197 -78.553 1.00 52.51 N
ATOM 3479 CA ASN G 524 -18.206 2.200 -79.701 1.00 57.54 C
ATOM 3480 CB ASN G 524 -16.783 1.822 -79.276 1.00 20.00 C
ATOM 3481 CG ASN G 524 -16.110 2.908 -78.457 1.00 20.00 C
ATOM 3482 OD1 ASN G 524 -16.515 4.069 -78.492 1.00 20.00 O
ATOM 3483 ND2 ASN G 524 -15.087 2.529 -77.699 1.00 20.00 N
ATOM 3484 C ASN G 524 -18.669 1.296 -80.843 1.00 54.12 C
ATOM 3485 O ASN G 524 -18.530 1.652 -82.013 1.00 61.31 O
ATOM 3486 N SER G 525 -19.149 0.102 -80.502 1.00 48.97 N
ATOM 3487 CA SER G 525 -19.658 -0.841 -81.499 1.00 64.81 C
ATOM 3488 CB SER G 525 -20.077 -2.157 -80.838 1.00 61.22 C
ATOM 3489 OG SER G 525 -18.947 -2.929 -80.475 1.00 85.90 O
ATOM 3490 C SER G 525 -20.840 -0.249 -82.254 1.00 69.67 C
ATOM 3491 O SER G 525 -21.093 -0.600 -83.406 1.00 72.60 O
ATOM 3492 N LYS G 526 -21.592 0.610 -81.577 1.00 66.06 N
ATOM 3493 CA LYS G 526 -22.723 1.280 -82.197 1.00 63.67 C
ATOM 3494 CB LYS G 526 -23.675 1.815 -81.127 1.00 70.55 C
ATOM 3495 CG LYS G 526 -24.473 0.741 -80.407 1.00 75.29 C
ATOM 3496 CD LYS G 526 -25.171 1.313 -79.183 1.00 85.03 C
ATOM 3497 CE LYS G 526 -25.776 0.219 -78.325 1.00 82.65 C
ATOM 3498 NZ LYS G 526 -26.303 0.770 -77.048 1.00 73.89 N
ATOM 3499 C LYS G 526 -22.259 2.417 -83.103 1.00 55.36 C
ATOM 3500 O LYS G 526 -22.797 2.611 -84.191 1.00 70.69 O
ATOM 3501 N ILE G 527 -21.275 3.181 -82.638 1.00 57.52 N
ATOM 3502 CA ILE G 527 -20.718 4.273 -83.431 1.00 58.48 C
ATOM 3503 CB ILE G 527 -19.545 4.966 -82.712 1.00 57.00 C
ATOM 3504 CGI ILE G 527 -20.021 5.620 -81.415 1.00 49.07 C
ATOM 3505 CD1 ILE G 527 -20.228 7.116 -81.534 1.00 46.18 C
ATOM 3506 CG2 ILE G 527 -18.902 6.004 -83.621 1.00 52.63 C
ATOM 3507 C ILE G 527 -20.224 3.758 -84.774 1.00 65.20 C
ATOM 3508 O ILE G 527 -20.455 4.380 -85.810 1.00 66.48 O
ATOM 3509 N TYR G 528 -19.487 2.652 -84.740 1.00 69.78 N
ATOM 3510 CA TYR G 528 -18.985 2.034 -85.961 1.00 72.52 C
ATOM 3511 CB TYR G 528 -18.268 0.712 -85.657 1.00 73.16 C
ATOM 3512 CG TYR G 528 -17.130 0.810 -84.658 1.00 76.94 C
ATOM 3513 CD1 TYR G 528 -16.667 -0.323 -83.994 1.00 70.95 C
ATOM 3514 CE1 TYR G 528 -15.628 -0.245 -83.077 1.00 67.73 C
ATOM 3515 CZ TYR G 528 -15.064 0.981 -82.789 1.00 71.89 C
ATOM 3516 OH TYR G 528 -14.046 1.065 -81.866 1.00 75.44 O

ATOM 3517 CE2 TYR G 528 -15.505 2.121 -83.433 1.00 77.03 C
ATOM 3518 CD2 TYR G 528 -16.523 2.029 -84.373 1.00 77.84 C
ATOM 3519 C TYR G 528 -20.130 1.796 -86.949 1.00 71.63 C
ATOM 3520 O TYR G 528 -20.150 2.377 -88.036 1.00 84.20 O
ATOM 3521 N HIS G 529 -21.116 1.002 -86.534 1.00 67.69 N
ATOM 3522 CA HIS G 529 -22.239 0.633 -87.398 1.00 60.28 C
ATOM 3523 CB HIS G 529 -23.215 -0.283 -86.659 1.00 67.84 C
ATOM 3524 CG HIS G 529 -22.668 -1.645 -86.376 1.00 88.54 C
ATOM 3525 ND1 HIS G 529 -23.472 -2.756 -86.236 1.00 93.34 N
ATOM 3526 CE1 HIS G 529 -22.725 -3.802 -85.933 1.00 86.23 C
ATOM 3527 NE2 HIS G 529 -21.465 -3.410 -85.871 1.00 91.95 N
ATOM 3528 CD2 HIS G 529 -21.401 -2.067 -86.151 1.00 93.77 C
ATOM 3529 C HIS G 529 -22.987 1.845 -87.944 1.00 63.30 C
ATOM 3530 O HIS G 529 -23.453 1.828 -89.083 1.00 61.02 O
ATOM 3531 N ILE G 530 -23.209 2.842 -87.091 1.00 59.79 N
ATOM 3532 CA ILE G 530 -23.752 4.121 -87.543 1.00 45.70 C
ATOM 3533 CB ILE G 530 -23.965 5.095 -86.374 1.00 40.57 C
ATOM 3534 CG1 ILE G 530 -25.130 4.627 -85.499 1.00 42.86 C
ATOM 3535 CD1 ILE G 530 -25.537 5.624 -84.437 1.00 51.01 C
ATOM 3536 CG2 ILE G 530 -24.224 6.501 -86.901 1.00 35.31 C
ATOM 3537 C ILE G 530 -22.822 4.775 -88.557 1.00 57.52 C
ATOM 3538 O ILE G 530 -23.260 5.253 -89.604 1.00 71.18 O
ATOM 3539 N GLU G 531 -21.534 4.787 -88.234 1.00 67.55 N
ATOM 3540 CA GLU G 531 -20.508 5.305 -89.129 1.00 69.79 C
ATOM 3541 CB GLU G 531 -19.126 5.105 -88.505 1.00 84.02 C
ATOM 3542 CG GLU G 531 -18.143 6.228 -88.780 1.00104.22 C
ATOM 3543 CD GLU G 531 -16.823 6.033 -88.058 1.00116.08 C
ATOM 3544 OE1 GLU G 531 -16.849 5.706 -86.853 1.00118.71 O
ATOM 3545 OE2 GLU G 531 -15.762 6.211 -88.693 1.00119.69 O
ATOM 3546 C GLU G 531 -20.567 4.624 -90.495 1.00 64.87 C
ATOM 3547 O GLU G 531 -20.720 5.285 -91.522 1.00 55.58 O
ATOM 3548 N ASN G 532 -20.409 3.304 -90.499 1.00 65.70 N
ATOM 3549 CA ASN G 532 -20.502 2.516 -91.724 1.00 64.16 C
ATOM 3550 CB ASN G 532 -20.351 1.026 -91.402 1.00 60.58 C
ATOM 3551 CG ASN G 532 -20.304 0.165 -92.642 1.00 67.75 C
ATOM 3552 OD1 ASN G 532 -19.416 0.312 -93.481 1.00 53.59 O
ATOM 3553 ND2 ASN G 532 -21.285 -0.716 -92.786 1.00 61.81 N
ATOM 3554 C ASN G 532 -21.809 2.759 -92.472 1.00 72.17 C
ATOM 3555 O ASN G 532 -21.823 2.885 -93.696 1.00 85.75 O
ATOM 3556 N GLU G 533 -22.907 2.812 -91.726 1.00 79.68 N
ATOM 3557 CA GLU G 533 -24.220 3.041 -92.307 1.00 71.96 C
ATOM 3558 CB GLU G 533 -25.300 2.936 -91.234 1.00 67.87 C
ATOM 3559 CG GLU G 533 -26.680 2.653 -91.788 1.00 81.94 C
ATOM 3560 CD GLU G 533 -26.710 1.397 -92.632 1.00 92.79 C
ATOM 3561 OE1 GLU G 533 -26.313 0.331 -92.119 1.00 95.90 O
ATOM 3562 OE2 GLU G 533 -26.989 1.501 -93.843 1.00 93.14 O
ATOM 3563 C GLU G 533 -24.296 4.406 -92.974 1.00 68.54 C
ATOM 3564 O GLU G 533 -25.101 4.616 -93.879 1.00 79.29 O
ATOM 3565 N ILE G 534 -23.542 5.359 -92.440 1.00 69.50 N
ATOM 3566 CA ILE G 534 -23.498 6.702 -93.003 1.00 72.55 C
ATOM 3567 CB ILE G 534 -23.070 7.737 -91.956 1.00 79.55 C
ATOM 3568 CG1 ILE G 534 -24.053 7.740 -90.784 1.00 80.41 C
ATOM 3569 CD1 ILE G 534 -25.321 6.951 -91.049 1.00 89.38 C
ATOM 3570 CG2 ILE G 534 -22.981 9.118 -92.588 1.00 78.63 C
ATOM 3571 C ILE G 534 -22.538 6.766 -94.180 1.00 74.92 C
ATOM 3572 O ILE G 534 -22.589 7.693 -94.987 1.00 81.01 O
ATOM 3573 N ALA G 535 -21.648 5.786 -94.255 1.00 79.52 N
ATOM 3574 CA ALA G 535 -20.721 5.683 -95.368 1.00 82.64 C
ATOM 3575 CB ALA G 535 -19.529 4.824 -94.974 1.00 75.39 C
ATOM 3576 C ALA G 535 -21.416 5.115 -96.604 1.00 81.39 C

ATOM 3577 O ALA G 535 -21.170 5.557 -97.727 1.00 85.54 O
ATOM 3578 N ARG G 536 -22.325 4.171 -96.380 1.00 78.41 N
ATOM 3579 CA ARG G 536 -23.115 3.581 -97.457 1.00 83.27 C
ATOM 3580 CB ARG G 536 -23.781 2.287 -96.984 1.00 84.58 C
ATOM 3581 CG ARG G 536 -22.808 1.180 -96.618 1.00103.24 C
ATOM 3582 CD ARG G 536 -23.316 -0.171 -97.085 1.001 14.72 C
ATOM 3583 NE ARG G 536 -24.587 -0.515 -96.457 1.001 17.80 N
ATOM 3584 CZ ARG G 536 -25.297 -1.600 -96.750 1.001 16.66 C
ATOM 3585 NH1 ARG G 536 -24.875 -2.439 -97.685 1.001 14.57 N
ATOM 3586 NH2 ARG G 536 -26.417 -1.862 -96.089 1.001 16.38 N
ATOM 3587 C ARG G 536 -24.172 4.552 -97.973 1.00 82.20 C
ATOM 3588 O ARG G 536 -24.315 4.737 -99.182 1.00 86.28 O
ATOM 3589 N ILE G 537 -24.941 5.135 -97.058 1.00 77.08 N
ATOM 3590 CA ILE G 537 -25.917 6.156 -97.430 1.00 66.79 C
ATOM 3591 CB ILE G 537 -26.719 6.680 -96.216 1.00 64.76 C
ATOM 3592 CGI ILE G 537 -27.614 5.583 -95.640 1.00 66.92 C
ATOM 3593 CD1 ILE G 537 -28.487 6.055 -94.493 1.00 70.83 C
ATOM 3594 CG2 ILE G 537 -27.593 7.848 -96.631 1.00 51.02 C
ATOM 3595 C ILE G 537 -25.221 7.330 -98.108 1.00 74.94 C
ATOM 3596 O ILE G 537 -25.824 8.043 -98.907 1.00 97.16 O
ATOM 3597 N LYS G 538 -23.941 7.514 -97.804 1.00 75.09 N
ATOM 3598 CA LYS G 538 -23.162 8.575 -98.427 1.00 90.28 C
ATOM 3599 CB LYS G 538 -22.051 9.054 -97.491 1.00 93.73 C
ATOM 3600 CG LYS G 538 -21.584 10.479 -97.760 1.00 96.60 C
ATOM 3601 CD LYS G 538 -20.446 10.876 -96.830 1.00 95.37 C
ATOM 3602 CE LYS G 538 -20.008 12.313 -97.067 1.00100.63 C
ATOM 3603 NZ LYS G 538 -18.989 12.750 -96.074 1.00 99.58 N
ATOM 3604 C LYS G 538 -22.574 8.114 -99.754 1.00102.20 C
ATOM 3605 O LYS G 538 -21.940 8.891-100.466 1.001 12.11 O
ATOM 3606 N LYS G 539 -22.870 6.874-100.126 1.00105.15 N
ATOM 3607 CA LYS G 539 -22.411 6.328-101.396 1.00105.65 C
ATOM 3608 CB LYS G 539 -21.904 4.897-101.211 1.001 10.12 C
ATOM 3609 CG LYS G 539 -21.426 4.246-102.498 1.001 13.31 C
ATOM 3610 CD LYS G 539 -21.023 2.794-102.284 1.001 14.26 C
ATOM 3611 CE LYS G 539 -20.414 2.201-103.550 1.001 18.39 C
ATOM 3612 NZ LYS G 539 -19.511 1.047-103.263 1.00121.77 N
ATOM 3613 C LYS G 539 -23.517 6.364-102.444 1.00108.88 C
ATOM 3614 O LYS G 539 -23.375 5.808-103.532 1.001 10.77 O
ATOM 3615 N LEU G 540 -24.625 7.011-102.102 1.001 11.50 N
ATOM 3616 CA LEU G 540 -25.722 7.201-103.038 1.001 10.31 C
ATOM 3617 CB LEU G 540 -27.025 6.656-102.451 1.00101.19 C
ATOM 3618 CG LEU G 540 -26.983 5.200-101.978 1.00 94.26 C
ATOM 3619 CD1 LEU G 540 -28.376 4.691-101.683 1.00 86.40 C
ATOM 3620 CD2 LEU G 540 -26.307 4.311-103.004 1.00 84.54 C
ATOM 3621 C LEU G 540 -25.865 8.679-103.374 1.001 18.37 C
ATOM 3622 O LEU G 540 -26.802 9.081-104.064 1.001 16.71 O
ATOM 3623 N ILE G 541 -24.894 9.474-102.934 1.00130.80 N
ATOM 3624 CA ILE G 541 -24.844 10.896-103.267 1.00140.48 C
ATOM 3625 CB ILE G 541 -25.701 11.746-102.294 1.00138.99 C
ATOM 3626 CGI ILE G 541 -27.145 11.234-102.257 1.00133.30 C
ATOM 3627 CD1 ILE G 541 -28.050 11.879-103.291 1.00136.26 C
ATOM 3628 CG2 ILE G 541 -25.680 13.218-102.707 1.00136.12 C
ATOM 3629 C ILE G 541 -23.407 11.410-103.250 1.00144.97 C
ATOM 3630 O ILE G 541 -23.116 12.480-103.783 1.00145.83 O
ATOM 3631 N GLY G 542 -22.519 10.663-102.602 1.00148.77 N
ATOM 3632 CA GLY G 542 -21.119 11.060-102.505 1.00153.58 C
ATOM 3633 C GLY G 542 -20.209 10.194-103.357 1.00160.45 C
ATOM 3634 O GLY G 542 -20.636 9.643-104.372 1.00163.41 O
ATOM 3635 N GLU G 543 -18.962 10.042-102.921 1.00163.83 N
ATOM 3636 CA GLU G 543 -17.983 9.236-103.649 1.00165.52 C

ATOM 3637 CB GLU G 543 -16.557 9.674-103.305 1.00158.94 C
ATOM 3642 C GLU G 543 -18.156 7.742-103.381 1.00168.27 C
ATOM 3643 O GLU G 543 -19.1 16 7.322-102.736 1.00167.37 O
ATOM 3644 N GLN H 26 -24.590 4.282 7.491 1.00 23.62 B N
ATOM 3645 CA GLN H 26 -23.869 3.499 6.449 1.00 23.82 B C
ATOM 3646 CB GLN H 26 -22.633 2.827 7.055 1.00 23.94 B C
ATOM 3647 CG GLN H 26 -21.724 3.775 7.833 1.00 28.83 B C
ATOM 3648 CD GLN H 26 -22.314 4.205 9.165 1.00 36.36 B C
ATOM 3649 OE1 GLN H 26 -23.057 5.183 9.238 1.00 39.09 B O
ATOM 3650 NE2 GLN H 26 -21.891 3.545 10.238 1.00 37.86 B N
ATOM 3651 C GLN H 26 -24.797 2.460 5.813 1.00 23.09 B C
ATOM 3652 O GLN H 26 -25.818 2.096 6.397 1.00 24.21 B O
ATOM 3653 N ASN H 27 -24.543 2.146 4.544 1.00 20.98 B N
ATOM 3654 CA ASN H 27 -25.343 1.173 3.786 1.00 19.70 B C
ATOM 3655 CB ASN H 27 -26.642 1.832 3.269 1.00 20.41 B C
ATOM 3656 CG ASN H 27 -27.524 0.887 2.423 1.00 23.56 B C
ATOM 3657 OD1 ASN H 27 -27.835 -0.233 2.837 1.00 24.42 B O
ATOM 3658 ND2 ASN H 27 -27.836 1.322 1.182 1.00 27.70 B N
ATOM 3659 C ASN H 27 -24.507 0.652 2.619 1.00 18.42 B C
ATOM 3660 O ASN H 27 -24.904 0.783 1.462 1.00 18.47 B O
ATOM 3661 N ILE H 28 -23.291 0.196 2.907 1.00 16.54 B N
ATOM 3662 CA ILE H 28 -22.439 -0.335 1.849 1.00 14.59 B C
ATOM 3663 CB ILE H 28 -20.939 -0.378 2.223 1.00 14.01 B C
ATOM 3664 CGI ILE H 28 -20.746 -0.823 3.674 1.00 15.60 B C
ATOM 3665 CD1 ILE H 28 -20.221 -2.240 3.815 1.00 16.26 B C
ATOM 3666 CG2 ILE H 28 -20.276 0.964 1.942 1.00 12.57 B C
ATOM 3667 C ILE H 28 -22.898 -1.700 1.360 1.00 13.86 B C
ATOM 3668 O ILE H 28 -23.458 -2.494 2.1 19 1.00 13.70 B O
ATOM 3669 N THR H 29 -22.868 -1.850 0.044 1.00 13.23 B N
ATOM 3670 CA THR H 29 -23.353 -3.045 -0.612 1.00 12.65 B C
ATOM 3671 CB THR H 29 -24.751 -2.816 -1.206 1.00 12.69 B C
ATOM 3672 OG1 THR H 29 -25.331 -1.643 -0.623 1.00 12.62 B O
ATOM 3673 CG2 THR H 29 -25.650 -4.012 -0.934 1.00 12.92 B C
ATOM 3674 C THR H 29 -22.392 -3.355 -1.741 1.00 12.47 B C
ATOM 3675 O THR H 29 -21.760 -2.457 -2.297 1.00 12.53 B O
ATOM 3676 N GLU H 30 -22.300 -4.626 -2.095 1.00 11.98 B N
ATOM 3677 CA GLU H 30 -21.668 -5.007 -3.338 1.00 11.68 B C
ATOM 3678 CB GLU H 30 -20.393 -5.803 -3.049 1.00 11.98 B C
ATOM 3679 CG GLU H 30 -19.274 -5.593 -4.058 1.00 13.38 B C
ATOM 3680 CD GLU H 30 -17.927 -6.054 -3.533 1.00 16.03 B C
ATOM 3681 OE1 GLU H 30 -17.846 -7.190 -3.019 1.00 16.65 B O
ATOM 3682 OE2 GLU H 30 -16.968 -5.253 -3.563 1.00 17.06 B O
ATOM 3683 C GLU H 30 -22.655 -5.860 -4.1 14 1.00 11.39 B C
ATOM 3684 O GLU H 30 -23.316 -6.727 -3.542 1.00 11.50 B O
ATOM 3685 N GLU H 31 -22.850 -5.534 -5.384 1.00 11.1 1 B N
ATOM 3686 CA GLU H 31 -23.602 -6.419 -6.248 1.00 11.06 B C
ATOM 3687 CB GLU H 31 -24.955 -5.813 -6.61 1 1.00 11.48 B C
ATOM 3688 CG GLU H 31 -25.093 -5.417 -8.063 1.00 13.90 B C
ATOM 3689 CD GLU H 31 -26.500 -4.981 -8.404 1.00 17.27 B C
ATOM 3690 OE1 GLU H 31 -27.092 -5.567 -9.335 1.00 17.55 B O
ATOM 3691 OE2 GLU H 31 -27.053 -4.130 -7.676 1.00 18.73 B O
ATOM 3692 C GLU H 31 -22.828 -6.839 -7.485 1.00 10.47 B C
ATOM 3693 O GLU H 31 -22.042 -6.071 -8.040 1.00 10.12 B O
ATOM 3694 N PHE H 32 -22.962 -8.1 16 -7.818 1.00 10.15 B N
ATOM 3695 CA PHE H 32 -22.042 -8.788 -8.716 1.00 9.62 B C
ATOM 3696 CB PHE H 32 -21.692 -10.167 -8. 158 1.00 9.42 B C
ATOM 3697 CG PHE H 32 -21 .130 - 11.106 -9. 179 1.00 9.27 B C
ATOM 3698 CD1 PHE H 32 -19.865 -10.896 -9.702 1.00 9.37 B C
ATOM 3699 CE1 PHE H 32 -19.315 - 11.784 -10.605 1.00 9.52 B C
ATOM 3700 CZ PHE H 32 -20.027 -12.905 -10.989 1.00 9.82 B C

ATOM 3701 CE2 PHE H 32 -21.294 -13.127 -10.472 1.00 10.13 B C
ATOM 3702 CD2 PHE H 32 -21.822 -12.250 -9.544 1.00 10.06 B C
ATOM 3703 C PHE H 32 -22.707 -8.941 -10.074 1.00 9.64 B C
ATOM 3704 O PHE H 32 -23.887 -9.282 -10.159 1.00 9.84 B O
ATOM 3705 N TYR H 33 -21.965 -8.638 -11.132 1.00 9.59 B N
ATOM 3706 CA TYR H 33 -22.526 -8.672 -12.474 1.00 9.67 B C
ATOM 3707 CB TYR H 33 -22.259 -7.360 -13.207 1.00 9.52 B C
ATOM 3708 CG TYR H 33 -23.038 -6.196 -12.645 1.00 10.94 B C
ATOM 3709 CD1 TYR H 33 -22.482 -5.372 -11.677 1.00 12.23 B C
ATOM 3710 CE1 TYR H 33 -23.198 -4.323 -11.137 1.00 12.93 B C
ATOM 3711 CZ TYR H 33 -24.510 -4.129 -11.510 1.00 13.47 B C
ATOM 3712 OH TYR H 33 -25.231 -3.093 -10.963 1.00 14.54 B O
ATOM 3713 CE2 TYR H 33 -25.100 -4.963 -12.436 1.00 13.56 B C
ATOM 3714 CD2 TYR H 33 -24.373 -6.006 -12.976 1.00 12.96 B C
ATOM 3715 C TYR H 33 -22.001 -9.853 -13.273 1.00 9.94 B C
ATOM 3716 O TYR H 33 -20.998 -9.747 -13.978 1.00 10.16 B O
ATOM 3717 N GLN H 34 -22.714 -10.969 -13.184 1.00 10.06 B N
ATOM 3718 CA GLN H 34 -22.191 -12.249 -13.632 1.00 10.01 B C
ATOM 3719 CB GLN H 34 -23.190 -13.361 -13.327 1.00 10.22 B C
ATOM 3720 CG GLN H 34 -22.760 -14.720 -13.829 1.00 11.12 B C
ATOM 3721 CD GLN H 34 -23.604 -15.836 -13.257 1.00 13.13 B C
ATOM 3722 OE1 GLN H 34 -24.746 -16.042 -13.673 1.00 14.24 B O
ATOM 3723 NE2 GLN H 34 -23.057 -16.550 -12.278 1.00 13.79 B N
ATOM 3724 C GLN H 34 -21.889 -12.220 -15.123 1.00 9.94 B C
ATOM 3725 O GLN H 34 -21.096 -13.018 -15.622 1.00 10.08 B O
ATOM 3726 N SER H 35 -22.564 -11.324 -15.836 1.00 9.87 B N
ATOM 3727 CA SER H 35 -22.458 -11.253 -17.290 1.00 9.91 B C
ATOM 3728 CB SER H 35 -23.743 -10.676 -17.889 1.00 10.03 B C
ATOM 3729 OG SER H 35 -24.034 -9.401 -17.343 1.00 10.81 B O
ATOM 3730 C SER H 35 -21.256 -10.410 -17.713 1.00 9.56 B C
ATOM 3731 O SER H 35 -21.002 -10.214 -18.903 1.00 9.59 B O
ATOM 3732 N THR H 36 -20.539 -9.892 -16.724 1.00 9.21 B N
ATOM 3733 CA THR H 36 -19.420 -8.996 -16.964 1.00 9.06 B C
ATOM 3734 CB THR H 36 -19.817 -7.536 -16.686 1.00 9.49 B C
ATOM 3735 OG1 THR H 36 -20.874 -7.149 -17.573 1.00 10.82 B O
ATOM 3736 CG2 THR H 36 -18.629 -6.609 -16.883 1.00 9.45 B C
ATOM 3737 C THR H 36 -18.292 -9.403 -16.029 1.00 8.77 B C
ATOM 3738 O THR H 36 -17.298 -8.693 -15.882 1.00 8.60 B o
ATOM 3739 N CYS H 37 -18.457 -10.572 -15.415 1.00 8.69 B N
ATOM 3740 CA CYS H 37 -17.594 -11.011 -14.327 1.00 8.69 B C
ATOM 3741 CB CYS H 37 -16.509 -11.955 -14.846 1.00 8.81 B c
ATOM 3742 SG CYS H 37 -15.737 -12.977 -13.569 1.00 10.80 B s
ATOM 3743 C CYS H 37 -16.958 -9.820 -13.631 1.00 8.27 B c
ATOM 3744 O CYS H 37 -15.735 -9.671 -13.628 1.00 8.27 B o
ATOM 3745 N SER H 38 -17.796 -8.950 -13.080 1.00 7.92 B N
ATOM 3746 CA SER H 38 -17.309 -7.784 -12.360 1.00 7.51 B c
ATOM 3747 CB SER H 38 -17.130 -6.595 -13.308 1.00 7.63 B c
ATOM 3748 OG SER H 38 -18.369 -6.193 -13.864 1.00 8.54 B o
ATOM 3749 C SER H 38 -18.227 -7.411 -11.207 1.00 7.02 B c
ATOM 3750 O SER H 38 -19.404 -7.771 -11.192 1.00 6.83 B o
ATOM 3751 N ALA H 39 -17.647 -6.784 -10.191 1.00 6.64 B N
ATOM 3752 CA ALA H 39 -18.371 -6.478 -8.969 1.00 6.58 B c
ATOM 3753 CB ALA H 39 -17.843 -7.320 -7.817 1.00 6.67 B c
ATOM 3754 C ALA H 39 -18.242 -4.995 -8.651 1.00 6.93 B c
ATOM 3755 O ALA H 39 -17.217 -4.378 -8.944 1.00 7.38 B o
ATOM 3756 N VAL H 40 -19.333 -4.401 -8.179 1.00 6.87 B N
ATOM 3757 CA VAL H 40 -19.316 -3.008 -7.746 1.00 6.55 B c
ATOM 3758 CB VAL H 40 -20.208 -2.122 -8.635 1.00 6.22 B c
ATOM 3759 CGI VAL H 40 -20.465 -0.783 -7.959 1.00 6.52 B C
ATOM 3760 CG2 VAL H 40 -19.564 -1.921 -9.998 1.00 6.62 B C

ATOM 3761 C VAL H 40 -19.743 -2.862 -6.290 1.00 6.73 B C
ATOM 3762 O VAL H 40 -20.805 -3.340 -5.891 1.00 6.83 B o
ATOM 3763 N SER H 41 -18.883 -2.240 -5.492 1.00 6.86 B N
ATOM 3764 CA SER H 41 -19.251 -1.825 -4.148 1.00 6.75 B C
ATOM 3765 CB SER H 41 -18.020 -1.779 -3.242 1.00 7.06 B c
ATOM 3766 OG SER H 41 -16.905 -2.388 -3.866 1.00 7.50 B o
ATOM 3767 C SER H 41 -19.922 -0.461 -4.180 1.00 6.56 B c
ATOM 3768 O SER H 41 -19.392 0.490 -4.756 1.00 6.08 B o
ATOM 3769 N LYS H 42 -21.097 -0.378 -3.565 1.00 7.02 B N
ATOM 3770 CA LYS H 42 -21.938 0.810 -3.662 1.00 7.83 B c
ATOM 3771 CB LYS H 42 -23.296 0.459 -4.269 1.00 8.15 B c
ATOM 3772 CG LYS H 42 -23.226 -0.171 -5.641 1.00 9.75 B c
ATOM 3773 CD LYS H 42 -24.621 -0.473 -6.153 1.00 12.62 B c
ATOM 3774 CE LYS H 42 -24.579 -1.069 -7.548 1.00 14.04 B c
ATOM 3775 NZ LYS H 42 -25.858 -0.856 -8.279 1.00 14.96 B N
ATOM 3776 C LYS H 42 -22.143 1.444 -2.290 1.00 7.80 B c
ATOM 3777 O LYS H 42 -21.947 0.798 -1.258 1.00 8.15 B o
ATOM 3778 N GLY H 43 -22.594 2.696 -2.290 1.00 7.59 B N
ATOM 3779 CA GLY H 43 -23.140 3.321 -1.090 1.00 7.35 B c
ATOM 3780 C GLY H 43 -22.131 4.200 -0.378 1.00 7.10 B c
ATOM 3781 O GLY H 43 -22.239 4.439 0.824 1.00 7.13 B o
ATOM 3782 N TYR H 44 -21.173 4.723 -1.136 1.00 7.01 B N
ATOM 3783 CA TYR H 44 -20.106 5.549 -0.577 1.00 6.89 B c
ATOM 3784 CB TYR H 44 -18.755 5.125 -1.160 1.00 6.88 B c
ATOM 3785 CG TYR H 44 -18.296 3.748 -0.732 1.00 6.41 B c
ATOM 3786 CD1 TYR H 44 -18.340 2.676 -1.615 1.00 6.62 B c
ATOM 3787 CE1 TYR H 44 -17.871 1.427 -1.245 1.00 6.48 B c
ATOM 3788 CZ TYR H 44 -17.312 1.253 0.005 1.00 6.88 B c
ATOM 3789 OH TYR H 44 -16.834 0.020 0.386 1.00 7.50 B o
ATOM 3790 CE2 TYR H 44 -17.197 2.318 0.870 1.00 6.68 B c
ATOM 3791 CD2 TYR H 44 -17.670 3.559 0.492 1.00 5.91 B c
ATOM 3792 C TYR H 44 -20.357 7.026 -0.886 1.00 6.86 B c
ATOM 3793 O TYR H 44 -20.912 7.354 -1.933 1.00 7.14 B o
ATOM 3794 N LEU H 45 -19.834 7.916 -0.045 1.00 6.44 B N
ATOM 3795 CA LEU H 45 -20.073 9.356 -0.205 1.00 6.12 B c
ATOM 3796 CB LEU H 45 -20.896 9.917 0.966 1.00 6.31 B c
ATOM 3797 CG LEU H 45 -22.355 9.463 1.108 1.00 6.38 B c
ATOM 3798 CD1 LEU H 45 -22.859 9.699 2.524 1.00 7.05 B c
ATOM 3799 CD2 LEU H 45 -23.256 10.158 0.096 1.00 7.05 B c
ATOM 3800 C LEU H 45 -18.791 10.173 -0.413 1.00 5.84 B c
ATOM 3801 O LEU H 45 -17.966 10.289 0.493 1.00 5.94 B o
ATOM 3802 N SER H 46 -18.764 10.924 -1.512 1.00 5.43 B N
ATOM 3803 CA SER H 46 -17.528 11.442 -2.112 1.00 5.26 B c
ATOM 3804 CB SER H 46 -17.801 11.821 -3.568 1.00 5.21 B c
ATOM 3805 OG SER H 46 -18.827 12.800 -3.647 1.00 4.95 B o
ATOM 3806 C SER H 46 -17.113 12.696 -1.355 1.00 5.51 B c
ATOM 3807 O SER H 46 -17.968 13.359 -0.771 1.00 6.03 B o
ATOM 3808 N ALA H 47 -15.850 13.103 -1.424 1.00 5.24 B N
ATOM 3809 CA ALA H 47 -15.530 14.323 -0.704 1.00 4.83 B c
ATOM 3810 CB ALA H 47 -16.269 14.344 0.622 1.00 5.01 B c
ATOM 3811 C ALA H 47 -14.089 14.763 -0.512 1.00 4.35 B c
ATOM 3812 O ALA H 47 -13.178 13.936 -0.449 1.00 4.45 B o
ATOM 3813 N LEU H 48 -13.989 15.994 -0.016 1.00 3.67 B N
ATOM 3814 CA LEU H 48 -12.719 16.625 0.308 1.00 3.15 B c
ATOM 3815 CB LEU H 48 -12.390 17.712 -0.720 1.00 2.78 B c
ATOM 3816 CG LEU H 48 -12.856 17.464 -2.159 1.00 2.18 B c
ATOM 3817 CD1 LEU H 48 -12.396 18.583 -3.082 1.00 2.00 B c
ATOM 3818 CD2 LEU H 48 -12.378 16.109 -2.666 1.00 3.94 B c
ATOM 3819 C LEU H 48 -12.768 17.232 1.707 1.00 3.06 B c
ATOM 3820 O LEU H 48 -13.519 18.174 1.961 1.00 3.27 B o

ATOM 3821 N ARG H 49 -11.879 16.758 2.571 1.00 2.91 B N
ATOM 3822 CA ARG H 49 -11.733 17.305 3.912 1.00 2.88 B C
ATOM 3823 CB ARG H 49 -10.649 16.538 4.668 1.00 2.69 B C
ATOM 3824 CG ARG H 49 -11.032 16.140 6.075 1.00 2.15 B c
ATOM 3825 CD ARG H 49 -9.882 16.395 7.026 1.00 2.00 B c
ATOM 3826 NE ARG H 49 -9.728 17.816 7.320 1.00 5.18 B N
ATOM 3827 CZ ARG H 49 -8.580 18.478 7.231 1.00 7.68 B c
ATOM 3828 NH1 ARG H 49 -7.481 17.849 6.838 1.00 8.32 B N
ATOM 3829 NH2 ARG H 49 -8.521 19.756 7.575 1.00 8.12 B N
ATOM 3830 C ARG H 49 -11.364 18.780 3.843 1.00 3.09 B C
ATOM 3831 O ARG H 49 -10.497 19.175 3.064 1.00 3.08 B o
ATOM 3832 N THR H 50 -12.022 19.593 4.661 1.00 3.37 B N
ATOM 3833 CA THR H 50 -11.594 20.970 4.855 1.00 3.55 B C
ATOM 3834 CB THR H 50 -12.413 21.946 3.998 1.00 3.25 B c
ATOM 3835 OG1 THR H 50 -13.807 21.633 4.109 1.00 2.66 B o
ATOM 3836 CG2 THR H 50 -11.992 21.844 2.543 1.00 3.46 B c
ATOM 3837 C THR H 50 -11.665 21.395 6.313 1.00 4.07 B c
ATOM 3838 O THR H 50 -11.171 22.462 6.678 1.00 4.35 B o
ATOM 3840 CA GLY H 51 -13.255 22.675 6.821 1.00 4.78 B c
ATOM 3841 C GLY H 51 -11.930 22.228 7.407 1.00 4.98 B c
ATOM 3842 O GLY H 51 -11.589 21.046 7.365 1.00 5.00 B o
ATOM 3843 N TRP H 52 -11.162 23.180 7.925 1.00 5.34 B N
ATOM 3844 CA TRP H 52 -9.845 22.878 8.465 1.00 5.42 B c
ATOM 3845 CB TRP H 52 -8.754 23.540 7.632 1.00 5.75 B c
ATOM 3846 CG TRP H 52 -8.691 23.029 6.243 1.00 6.38 B c
ATOM 3847 CD1 TRP H 52 -9.100 23.678 5.117 1.00 7.27 B c
ATOM 3848 NE1 TRP H 52 -8.926 22.875 4.019 1.00 7.46 B N
ATOM 3849 CE2 TRP H 52 -8.445 21.660 4.430 1.00 7.15 B c
ATOM 3850 CD2 TRP H 52 -8.315 21.710 5.832 1.00 7.02 B c
ATOM 3851 CE3 TRP H 52 -7.799 20.595 6.500 1.00 6.83 B c
ATOM 3852 CZ3 TRP H 52 -7.466 19.473 5.761 1.00 6.73 B c
ATOM 3853 CH2 TRP H 52 -7.634 19.445 4.372 1.00 7.13 B c
ATOM 3854 CZ2 TRP H 52 -8.111 20.529 3.689 1.00 6.82 B c
ATOM 3855 C TRP H 52 -9.723 23.329 9.905 1.00 5.34 B C
ATOM 3856 O TRP H 52 -10.279 24.359 10.289 1.00 5.47 B o
ATOM 3857 N TYR H 53 -8.800 22.695 10.615 1.00 5.29 B N
ATOM 3858 CA TYR H 53 -8.531 23.038 11.997 1.00 5.58 B c
ATOM 3859 CB TYR H 53 -9.040 21.934 12.919 1.00 5.51 B c
ATOM 3860 CG TYR H 53 -8.759 22.187 14.377 1.00 6.59 B c
ATOM 3861 CD1 TYR H 53 -9.668 22.879 15.169 1.00 8.25 B c
ATOM 3862 CE1 TYR H 53 -9.440 23.068 16.521 1.00 9.40 B c
ATOM 3863 CZ TYR H 53 -8.293 22.555 17.096 1.00 9.24 B c
ATOM 3864 OH TYR H 53 -8.053 22.750 18.439 1.00 9.61 B o
ATOM 3865 CE2 TYR H 53 -7.360 21.893 16.321 1.00 8.78 B c
ATOM 3866 CD2 TYR H 53 -7.600 21.709 14.971 1.00 7.93 B c
ATOM 3867 C TYR H 53 -7.042 23.256 12.214 1.00 5.74 B c
ATOM 3868 O TYR H 53 -6.259 22.306 12.223 1.00 6.19 B o
ATOM 3869 N THR H 54 -6.645 24.521 12.296 1.00 6.04 B N
ATOM 3870 CA THR H 54 -5.249 24.869 12.519 1.00 6.67 B c
ATOM 3871 CB THR H 54 -5.032 26.391 12.438 1.00 6.97 B c
ATOM 3872 OG1 THR H 54 -4.958 26.793 11.064 1.00 7.51 B o
ATOM 3873 CG2 THR H 54 -3.747 26.788 13.147 1.00 7.98 B c
ATOM 3874 C THR H 54 -4.775 24.360 13.877 1.00 6.97 B c
ATOM 3875 O THR H 54 -5.576 24.173 14.792 1.00 7.32 B o
ATOM 3876 N SER H 55 -3.479 24.086 13.987 1.00 7.24 B N
ATOM 3877 CA SER H 55 -2.811 24.106 15.282 1.00 7.65 B c
ATOM 3878 CB SER H 55 -3.110 22.830 16.072 1.00 7.69 B c
ATOM 3879 OG SER H 55 -2.308 22.754 17.238 1.00 7.51 B o
ATOM 3880 C SER H 55 -1.308 24.309 15.154 1.00 8.03 B c
ATOM 3881 O SER H 55 -0.654 23.695 14.311 1.00 8.43 B o

ATOM 3882 N VAL H 56 -0.760 25.106 16.063 1.00 8.14 B N
ATOM 3883 CA VAL H 56 0.600 25.601 15.930 1.00 8.41 B C
ATOM 3884 CB VAL H 56 0.672 27.116 16.193 1.00 8.72 B C
ATOM 3885 CGI VAL H 56 1.868 27.723 15.477 1.00 9.29 B C
ATOM 3886 CG2 VAL H 56 -0.619 27.792 15.756 1.00 9.51 B C
ATOM 3887 C VAL H 56 1.509 24.884 16.917 1.00 8.19 B C
ATOM 3888 O VAL H 56 1.348 25.011 18.129 1.00 8.54 B O
ATOM 3889 N ILE H 57 2.428 24.086 16.389 1.00 7.91 B N
ATOM 3890 CA ILE H 57 3.224 23.192 17.214 1.00 7.64 B C
ATOM 3891 CB ILE H 57 3.175 21.749 16.674 1.00 7.35 B C
ATOM 3892 CGI ILE H 57 1.726 21.302 16.462 1.00 7.25 B C
ATOM 3893 CD1 ILE H 57 1.593 19.930 15.834 1.00 8.42 B C
ATOM 3894 CG2 ILE H 57 3.915 20.799 17.603 1.00 7.52 B C
ATOM 3895 C ILE H 57 4.670 23.670 17.258 1.00 7.69 B C
ATOM 3896 O ILE H 57 5.272 23.936 16.219 1.00 7.79 B O
ATOM 3897 N THR H 58 5.175 23.897 18.467 1.00 7.85 B N
ATOM 3898 CA THR H 58 6.465 24.554 18.659 1.00 8.15 B C
ATOM 3899 CB THR H 58 6.297 25.903 19.383 1.00 8.14 B C
ATOM 3900 OG1 THR H 58 4.946 26.360 19.239 1.00 8.62 B O
ATOM 3901 CG2 THR H 58 7.246 26.943 18.806 1.00 7.94 B C
ATOM 3902 C THR H 58 7.393 23.666 19.485 1.00 8.20 B C
ATOM 3903 O THR H 58 7.051 23.281 20.600 1.00 8.18 B O
ATOM 3904 N ILE H 59 8.565 23.351 18.941 1.00 8.54 B N
ATOM 3905 CA ILE H 59 9.482 22.397 19.572 1.00 9.23 B C
ATOM 3906 CB ILE H 59 9.604 21.112 18.729 1.00 8.92 B C
ATOM 3907 CGI ILE H 59 8.231 20.482 18.496 1.00 9.27 B C
ATOM 3908 CD1 ILE H 59 8.253 19.315 17.533 1.00 10.89 B C
ATOM 3909 CG2 ILE H 59 10.559 20.130 19.387 1.00 8.74 B C
ATOM 3910 C ILE H 59 10.880 23.004 19.691 1.00 10.02 B C
ATOM 3911 O ILE H 59 11.474 23.380 18.684 1.00 10.20 B O
ATOM 3912 N GLU H 60 11.434 23.059 20.898 1.00 10.95 B N
ATOM 3913 CA GLU H 60 12.592 23.923 21.138 1.00 12.13 B C
ATOM 3914 CB GLU H 60 12.914 23.976 22.634 1.00 12.44 B C
ATOM 3915 CG GLU H 60 11.854 24.705 23.444 1.00 15.04 B C
ATOM 3916 CD GLU H 60 12.365 25.173 24.793 1.00 19.34 B C
ATOM 3917 OE1 GLU H 60 12.659 24.309 25.647 1.00 20.63 B O
ATOM 3918 OE2 GLU H 60 12.495 26.401 24.990 1.00 21.19 B O
ATOM 3919 C GLU H 60 13.816 23.509 20.301 1.00 12.46 B C
ATOM 3920 O GLU H 60 14.196 22.336 20.316 1.00 12.68 B O
ATOM 3921 N LEU H 61 14.390 24.428 19.510 1.00 12.80 B N
ATOM 3922 CA LEU H 61 15.786 24.207 19.132 1.00 12.71 B C
ATOM 3923 CB LEU H 61 16.470 25.295 18.316 1.00 12.55 B C
ATOM 3924 CG LEU H 61 17.932 24.803 18.355 1.00 12.39 B C
ATOM 3925 CD1 LEU H 61 18.053 23.370 17.848 1.00 13.14 B C
ATOM 3926 CD2 LEU H 61 18.944 25.717 17.683 1.00 12.50 B C
ATOM 3927 C LEU H 61 16.459 24.114 20.455 1.00 12.94 B C
ATOM 3928 O LEU H 61 16.827 25.135 21.048 1.00 12.78 B O
ATOM 3929 N SER H 62 16.080 23.014 21.081 1.00 13.61 B N
ATOM 3930 CA SER H 62 16.441 22.760 22.447 1.00 14.70 B C
ATOM 3931 CB SER H 62 15.805 21.454 22.924 1.00 14.52 B C
ATOM 3932 OG SER H 62 14.398 21.584 23.034 1.00 14.80 B O
ATOM 3933 C SER H 62 17.947 22.650 22.469 1.00 15.48 B C
ATOM 3934 O SER H 62 18.498 21.677 21.961 1.00 15.50 B O
ATOM 3935 N ASN H 63 18.597 23.777 22.721 1.00 16.61 B N
ATOM 3936 CA ASN H 63 20.030 23.839 22.523 1.00 17.77 B C
ATOM 3937 CB ASN H 63 20.519 25.279 22.439 1.00 17.73 B C
ATOM 3938 CG ASN H 63 21.686 25.433 21.493 1.00 18.52 B C
ATOM 3939 OD1 ASN H 63 22.559 24.567 21.428 1.00 18.29 B O
ATOM 3940 ND2 ASN H 63 21.641 26.467 20.665 1.00 19.40 B N
ATOM 3941 C ASN H 63 20.795 23.070 23.587 1.00 18.53 B C

ATOM 3942 O ASN H 63 20.356 22.967 24.732 1.00 18.82 B O
ATOM 3943 N ILE H 64 21.887 22.440 23.169 1.00 19.60 B N
ATOM 3944 CA ILE H 64 22.830 21.832 24.096 1.00 21.04 B C
ATOM 3945 CB ILE H 64 23.599 20.680 23.429 1.00 20.60 B C
ATOM 3946 CGI ILE H 64 22.650 19.824 22.590 1.00 20.13 B C
ATOM 3947 CD1 ILE H 64 23.355 18.820 21.712 1.00 20.19 B C
ATOM 3948 CG2 ILE H 64 24.321 19.843 24.474 1.00 20.74 B C
ATOM 3949 C ILE H 64 23.837 22.859 24.601 1.00 22.58 B C
ATOM 3950 O ILE H 64 24.450 23.577 23.811 1.00 23.07 B O
ATOM 3951 N LYS H 65 24.104 22.827 25.903 1.00 24.21 B N
ATOM 3952 CA LYS H 65 25.356 23.354 26.435 1.00 25.86 B C
ATOM 3953 CB LYS H 65 25.109 24.202 27.686 1.00 25.90 B C
ATOM 3954 CG LYS H 65 23.736 24.015 28.312 1.00 26.69 B c
ATOM 3955 CD LYS H 65 23.556 22.597 28.830 1.00 28.26 B c
ATOM 3956 CE LYS H 65 23.104 22.591 30.281 1.00 28.67 B c
ATOM 3957 NZ LYS H 65 23.397 21.291 30.946 1.00 28.95 B N
ATOM 3958 C LYS H 65 26.377 22.252 26.719 1.00 26.81 B c
ATOM 3959 O LYS H 65 26.297 21.561 27.736 1.00 26.72 B o
ATOM 3960 N GLU H 66 27.382 22.159 25.852 1.00 27.90 B N
ATOM 3961 CA GLU H 66 28.276 21.001 25.793 1.00 28.82 B c
ATOM 3962 CB GLU H 66 29.031 20.991 24.457 1.00 28.88 B c
ATOM 3963 CG GLU H 66 30.531 20.737 24.572 1.00 30.33 B c
ATOM 3964 CD GLU H 66 31.320 21.283 23.391 1.00 33.17 B c
ATOM 3965 OE1 GLU H 66 32.446 20.796 23.151 1.00 35.05 B o
ATOM 3966 OE2 GLU H 66 30.864 22.268 22.775 1.00 33.14 B o
ATOM 3967 C GLU H 66 29.267 21.029 26.954 1.00 29.12 B c
ATOM 3968 O GLU H 66 29.751 22.097 27.329 1.00 29.28 B o
ATOM 3969 N ASN H 67 29.545 19.871 27.547 1.00 29.32 B N
ATOM 3970 CA ASN H 67 30.326 19.847 28.783 1.00 29.39 B c
ATOM 3971 CB ASN H 67 29.525 19.250 29.941 1.00 29.62 B c
ATOM 3972 CG ASN H 67 28.892 20.317 30.814 1.00 29.84 B c
ATOM 3973 OD1 ASN H 67 29.589 21.032 31.534 1.00 29.93 B o
ATOM 3974 ND2 ASN H 67 27.597 20.540 30.625 1.00 29.22 B N
ATOM 3975 C ASN H 67 31.745 19.271 28.698 1.00 29.15 B c
ATOM 3976 O ASN H 67 31.977 18.111 29.044 1.00 29.06 B o
ATOM 3977 N LYS H 68 32.625 20.020 28.036 1.00 28.87 B N
ATOM 3978 CA LYS H 68 34.033 20.170 28.428 1.00 28.78 B c
ATOM 3979 CB LYS H 68 34.334 21.625 28.806 1.00 28.89 B c
ATOM 3980 CG LYS H 68 33.742 22.653 27.846 1.00 29.26 B c
ATOM 3981 CD LYS H 68 33.794 24.057 28.427 1.00 29.68 B c
ATOM 3982 CE LYS H 68 35.058 24.267 29.243 1.00 29.46 B c
ATOM 3983 NZ LYS H 68 35.195 25.675 29.705 1.00 29.58 B N
ATOM 3984 C LYS H 68 34.543 19.202 29.509 1.00 28.60 B c
ATOM 3985 O LYS H 68 34.879 19.622 30.618 1.00 28.64 B o
ATOM 3986 N CYS H 69 34.618 17.912 29.162 1.00 28.09 B N
ATOM 3987 CA CYS H 69 35.404 16.889 29.895 1.00 27.63 B c
ATOM 3988 CB CYS H 69 34.502 15.694 30.287 1.00 27.07 B c
ATOM 3989 SG CYS H 69 34.515 14.237 29.134 1.00 28.01 B s
ATOM 3990 C CYS H 69 36.550 16.388 29.003 1.00 27.69 B c
ATOM 3991 O CYS H 69 36.474 16.529 27.785 1.00 27.41 B o
ATOM 3992 N ASN H 70 37.563 15.732 29.576 1.00 28.06 B N
ATOM 3993 CA ASN H 70 38.498 14.929 28.760 1.00 28.87 B c
ATOM 3994 CB ASN H 70 39.930 15.507 28.746 1.00 30.52 B c
ATOM 3995 CG ASN H 70 40.024 16.921 29.323 1.00 39.60 B c
ATOM 3996 OD1 ASN H 70 39.691 17.905 28.661 1.00 44.97 B o
ATOM 3997 ND2 ASN H 70 40.562 17.019 30.542 1.00 51.04 B N
ATOM 3998 C ASN H 70 38.528 13.423 29.067 1.00 26.97 B c
ATOM 3999 O ASN H 70 39.060 13.009 30.096 1.00 26.50 B o
ATOM 4000 N GLY H 71 38.111 12.611 28.096 1.00 25.46 B N
ATOM 4001 CA GLY H 71 38.117 11.148 28.237 1.00 23.67 B c

```
ATOM   4002  C   GLY H  71     39.357  10.485  27.657   1.00 22.81      B    C
ATOM   4003  O   GLY H  71     40.279  11.169  27.211   1.00 22.79      B    o
ATOM   4004  N   THR H  72     39.400   9.155  27.687   1.00 21.93      B    N
ATOM   4005  CA  THR H  72     40.517   8.418  27.100   1.00 21.30      B    C
ATOM   4006  CB  THR H  72     40.594   6.975  27.644   1.00 21.12      B    c
ATOM   4007  OG1 THR H  72     39.700   6.131  26.909   1.00 19.87      B    o
ATOM   4008  CG2 THR H  72     40.210   6.947  29.115   1.00 20.76      B    c
ATOM   4009  C   THR H  72     40.436   8.407  25.571   1.00 21.50      B    c
ATOM   4010  O   THR H  72     39.458   7.924  24.999   1.00 21.85      B    o
ATOM   4011  N   ASP H  73     41.391   9.077  24.927   1.00 21.43      B    N
ATOM   4012  CA  ASP H  73     41.246   9.509  23.534   1.00 21.46      B    c
ATOM   4013  CB  ASP H  73     41.137   8.304  22.598   1.00 21.69      B    c
ATOM   4014  CG  ASP H  73     40.965   8.708  21.150   1.00 22.46      B    c
ATOM   4015  OD1 ASP H  73     40.678   9.896  20.894   1.00 23.01      B    o
ATOM   4016  OD2 ASP H  73     41.102   7.835  20.269   1.00 23.09      B    o
ATOM   4017  C   ASP H  73     40.060  10.451  23.324   1.00 20.96      B    c
ATOM   4018  O   ASP H  73     38.909  10.066  23.530   1.00 20.61      B    o
ATOM   4019  N   ALA H  74     40.342  11.642  22.802   1.00 20.42      B    N
ATOM   4020  CA  ALA H  74     39.342  12.698  22.730   1.00 20.38      B    c
ATOM   4021  CB  ALA H  74     39.707  13.839  23.670   1.00 20.11      B    c
ATOM   4022  C   ALA H  74     39.133  13.223  21.310   1.00 20.45      B    c
ATOM   4023  O   ALA H  74     38.545  14.286  21.121   1.00 20.46      B    o
ATOM   4024  N   LYS H  75     39.659  12.513  20.318   1.00 20.67      B    N
ATOM   4025  CA  LYS H  75     39.416  12.887  18.929   1.00 20.99      B    c
ATOM   4026  CB  LYS H  75     40.195  11.977  17.978   1.00 21.20      B    c
ATOM   4027  CG  LYS H  75     41.704  12.110  18.091   1.00 22.02      B    c
ATOM   4028  CD  LYS H  75     42.349  10.782  18.451   1.00 23.66      B    c
ATOM   4029  CE  LYS H  75     43.483  10.971  19.447   1.00 24.93      B    c
ATOM   4030  NZ  LYS H  75     43.559   9.859  20.434   1.00 25.55      B    N
ATOM   4031  C   LYS H  75     37.925  12.790  18.645   1.00 20.92      B    c
ATOM   4032  O   LYS H  75     37.397  13.474  17.768   1.00 20.92      B    o
ATOM   4033  N   VAL H  76     37.265  11.904  19.382   1.00 20.63      B    N
ATOM   4034  CA  VAL H  76     35.813  11.844  19.414   1.00 20.36      B    c
ATOM   4035  CB  VAL H  76     35.326  10.521  20.029   1.00 20.25      B    c
ATOM   4036  CGI VAL H  76     33.817  10.537  20.157   1.00 20.82      B    c
ATOM   4037  CG2 VAL H  76     35.769   9.341  19.175   1.00 20.09      B    c
ATOM   4038  C   VAL H  76     35.234  13.006  20.213   1.00 20.29      B    c
ATOM   4039  O   VAL H  76     35.629  13.244  21.356   1.00 20.21      B    o
ATOM   4040  N   LYS H  77     34.284  13.715  19.613   1.00 20.17      B    N
ATOM   4041  CA  LYS H  77     33.726  14.916  20.224   1.00 20.17      B    c
ATOM   4042  CB  LYS H  77     34.593  16.136  19.904   1.00 20.62      B    c
ATOM   4043  CG  LYS H  77     35.797  16.307  20.825   1.00 23.31      B    c
ATOM   4044  CD  LYS H  77     36.952  16.989  20.103   1.00 26.74      B    c
ATOM   4045  CE  LYS H  77     38.196  17.046  20.971   1.00 28.32      B    c
ATOM   4046  NZ  LYS H  77     39.203  18.004  20.436   1.00 29.66      B    N
ATOM   4047  C   LYS H  77     32.294  15.141  19.759   1.00 19.45      B    c
ATOM   4048  O   LYS H  77     31.971  16.170  19.165   1.00 19.36      B    o
ATOM   4049  N   LEU H  78     31.441  14.162  20.033   1.00 18.70      B    N
ATOM   4050  CA  LEU H  78     30.155  14.056  19.365   1.00 17.98      B    c
ATOM   4051  CB  LEU H  78     29.356  12.892  19.945   1.00 17.72      B    c
ATOM   4052  CG  LEU H  78     30.168  11.596  20.034   1.00 17.51      B    c
ATOM   4053  CD1 LEU H  78     29.321  10.446  20.554   1.00 17.41      B    c
ATOM   4054  CD2 LEU H  78     30.802  11.249  18.690   1.00 17.62      B    c
ATOM   4055  C   LEU H  78     29.354  15.355  19.422   1.00 17.77      B    c
ATOM   4056  O   LEU H  78     28.996  15.911  18.384   1.00 17.89      B    o
ATOM   4057  N   ILE H  79     29.145  15.882  20.624   1.00 17.29      B    N
ATOM   4058  CA  ILE H  79     28.336  17.086  20.778   1.00 17.00      B    c
ATOM   4059  CB  ILE H  79     28.194  17.527  22.256   1.00 16.96      B    c
ATOM   4060  CGI ILE H  79     27.588  16.401  23.098   1.00 17.21      B    c
ATOM   4061  CD1 ILE H  79     27.086  16.855  24.459   1.00 17.51      B    c
```

ATOM 4062 CG2 ILE H 79 27.307 18.762 22.359 1.00 17.30 B C
ATOM 4063 C ILE H 79 28.854 18.238 19.911 1.00 16.83 B C
ATOM 4064 O ILE H 79 28.119 18.753 19.065 1.00 17.02 B O
ATOM 4065 N LYS H 80 30.124 18.571 19.800 1.00 16.55 B N
ATOM 4066 CA LYS H 80 30.366 19.684 18.841 1.00 16.38 B C
ATOM 4067 CB LYS H 80 31.861 20.021 18.833 1.00 16.73 B C
ATOM 4068 CG LYS H 80 32.255 21.150 17.895 1.00 17.99 B C
ATOM 4069 CD LYS H 80 32.343 22.475 18.640 1.00 20.71 B C
ATOM 4070 CE LYS H 80 32.566 23.632 17.681 1.00 22.92 B C
ATOM 4071 NZ LYS H 80 31.339 23.929 16.886 1.00 24.75 B N
ATOM 4072 C LYS H 80 29.884 19.466 17.349 1.00 15.79 B C
ATOM 4073 O LYS H 80 29.216 20.348 16.717 1.00 15.32 B O
ATOM 4074 N GLN H 81 30.177 18.286 16.806 1.00 15.48 B N
ATOM 4075 CA GLN H 81 29.878 17.961 15.401 1.00 15.33 B C
ATOM 4076 CB GLN H 81 30.465 16.593 15.049 1.00 15.70 B C
ATOM 4077 CG GLN H 81 31.870 16.364 15.565 1.00 17.88 B C
ATOM 4078 CD GLN H 81 32.301 14.917 15.435 1.00 20.46 B C
ATOM 4079 OE1 GLN H 81 31.670 14.133 14.730 1.00 21.59 B O
ATOM 4080 NE2 GLN H 81 33.378 14.554 16.123 1.00 20.26 B N
ATOM 4081 C GLN H 81 28.388 17.966 15.047 1.00 14.63 B C
ATOM 4082 O GLN H 81 27.972 18.429 13.962 1.00 14.60 B O
ATOM 4083 N GLU H 82 27.589 17.434 15.964 1.00 13.81 B N
ATOM 4084 CA GLU H 82 26.157 17.373 15.759 1.00 13.37 B C
ATOM 4085 CB GLU H 82 25.479 16.677 16.938 1.00 13.20 B C
ATOM 4086 CG GLU H 82 25.315 15.176 16.781 1.00 15.04 B C
ATOM 4087 CD GLU H 82 24.344 14.824 15.669 1.00 17.51 B C
ATOM 4088 OE1 GLU H 82 23.130 15.074 15.841 1.00 18.22 B O
ATOM 4089 OE2 GLU H 82 24.789 14.286 14.632 1.00 17.87 B O
ATOM 4090 C GLU H 82 25.650 18.794 15.638 1.00 12.99 B C
ATOM 4091 O GLU H 82 24.834 19.102 14.767 1.00 12.89 B O
ATOM 4092 N LEU H 83 26.174 19.677 16.482 1.00 12.89 B N
ATOM 4093 CA LEU H 83 25.727 21.057 16.454 1.00 13.08 B C
ATOM 4094 CB LEU H 83 26.419 21.865 17.552 1.00 13.26 B C
ATOM 4095 CG LEU H 83 26.057 21.498 18.994 1.00 14.18 B C
ATOM 4096 CD1 LEU H 83 26.535 22.566 19.968 1.00 15.11 B C
ATOM 4097 CD2 LEU H 83 24.558 21.282 19.117 1.00 14.79 B C
ATOM 4098 C LEU H 83 26.032 21.656 15.092 1.00 13.18 B C
ATOM 4099 O LEU H 83 25.150 22.261 14.459 1.00 13.05 B O
ATOM 4100 N ASP H 84 27.239 21.416 14.581 1.00 13.56 B N
ATOM 4101 CA ASP H 84 27.527 21.999 13.258 1.00 14.15 B C
ATOM 4102 CB ASP H 84 28.982 21.729 12.856 1.00 14.80 B C
ATOM 4103 CG ASP H 84 29.949 21.873 14.018 1.00 18.26 B C
ATOM 4104 OD1 ASP H 84 30.237 23.025 14.417 1.00 21.11 B O
ATOM 4105 OD2 ASP H 84 30.439 20.837 14.522 1.00 22.12 B O
ATOM 4106 C ASP H 84 26.572 21.490 12.150 1.00 13.56 B C
ATOM 4107 O ASP H 84 26.023 22.286 11.326 1.00 13.70 B O
ATOM 4108 N LYS H 85 26.328 20.180 12.146 1.00 12.87 B N
ATOM 4109 CA LYS H 85 25.458 19.616 11.106 1.00 12.31 B C
ATOM 4110 CB LYS H 85 25.412 18.090 11.210 1.00 12.41 B C
ATOM 4111 CG LYS H 85 24.611 17.417 10.110 1.00 12.26 B C
ATOM 4112 CD LYS H 85 24.213 16.002 10.506 1.00 12.72 B C
ATOM 4113 CE LYS H 85 23.359 16.018 11.762 1.00 14.40 B C
ATOM 4114 NZ LYS H 85 22.929 14.654 12.180 1.00 16.45 B N
ATOM 4115 C LYS H 85 24.038 20.192 11.202 1.00 11.85 B C
ATOM 4116 O LYS H 85 23.384 20.522 10.179 1.00 11.66 B O
ATOM 4117 N TYR H 86 23.571 20.318 12.442 1.00 11.32 B N
ATOM 4118 CA TYR H 86 22.232 20.825 12.683 1.00 11.07 B C
ATOM 4119 CB TYR H 86 21.875 20.784 14.167 1.00 11.12 B C
ATOM 4120 CG TYR H 86 20.899 21.871 14.551 1.00 11.30 B C
ATOM 4121 CD1 TYR H 86 19.564 21.805 14.169 1.00 12.16 B C

ATOM 4122 CE1 TYR H 86 18.672 22.804 14.514 1.00 12.39 B C
ATOM 4123 CZ TYR H 86 19.106 23.886 15.243 1.00 12.62 B C
ATOM 4124 OH TYR H 86 18.218 24.880 15.587 1.00 12.72 B o
ATOM 4125 CE2 TYR H 86 20.428 23.980 15.632 1.00 11.38 B c
ATOM 4126 CD2 TYR H 86 21.315 22.979 15.284 1.00 11.05 B c
ATOM 4127 C TYR H 86 22.120 22.247 12.181 1.00 10.75 B c
ATOM 4128 O TYR H 86 21.114 22.622 11.573 1.00 10.45 B o
ATOM 4129 N LYS H 87 23.155 23.046 12.419 1.00 10.66 B N
ATOM 4130 CA LYS H 87 23.093 24.423 11.971 1.00 11.03 B c
ATOM 4131 CB LYS H 87 24.333 25.191 12.407 1.00 11.36 B c
ATOM 4132 CG LYS H 87 24.600 25.106 13.890 1.00 12.79 B c
ATOM 4133 CD LYS H 87 25.805 25.931 14.269 1.00 14.76 B c
ATOM 4134 CE LYS H 87 25.989 25.979 15.771 1.00 15.29 B c
ATOM 4135 NZ LYS H 87 27.137 26.849 16.138 1.00 16.27 B N
ATOM 4136 C LYS H 87 22.961 24.455 10.457 1.00 10.83 B c
ATOM 4137 O LYS H 87 22.122 25.189 9.920 1.00 11.11 B o
ATOM 4138 N ASN H 88 23.724 23.621 9.755 1.00 10.52 B N
ATOM 4139 CA ASN H 88 23.568 23.646 8.297 1.00 10.21 B c
ATOM 4140 CB ASN H 88 24.586 22.715 7.640 1.00 10.61 B c
ATOM 4141 CG ASN H 88 24.426 22.646 6.134 1.00 11.81 B c
ATOM 4142 OD1 ASN H 88 24.215 23.664 5.474 1.00 12.97 B o
ATOM 4143 ND2 ASN H 88 24.515 21.443 5.585 1.00 13.82 B N
ATOM 4144 C ASN H 88 22.142 23.279 7.825 1.00 9.42 B C
ATOM 4145 o ASN H 88 21.538 23.959 6.939 1.00 8.94 B o
ATOM 4146 N ALA H 89 21.576 22.237 8.435 1.00 8.77 B N
ATOM 4147 CA ALA H 89 20.225 21.834 8.022 1.00 8.21 B C
ATOM 4148 CB ALA H 89 19.811 20.551 8.725 1.00 7.99 B c
ATOM 4149 C ALA H 89 19.208 22.951 8.293 1.00 7.78 B c
ATOM 4150 o ALA H 89 18.307 23.249 7.472 1.00 7.88 B o
ATOM 4151 N VAL H 90 19.383 23.581 9.449 1.00 7.01 B N
ATOM 4152 CA VAL H 90 18.493 24.639 9.880 1.00 6.26 B c
ATOM 4153 CB VAL H 90 18.866 25.140 11.289 1.00 5.91 B c
ATOM 4154 CGI VAL H 90 18.089 26.401 11.626 1.00 5.92 B C
ATOM 4155 CG2 VAL H 90 18.608 24.054 12.318 1.00 5.26 B C
ATOM 4156 C VAL H 90 18.565 25.785 8.894 1.00 6.25 B C
ATOM 4157 O VAL H 90 17.547 26.368 8.538 1.00 6.32 B O
ATOM 4158 N THR H 91 19.771 26.092 8.434 1.00 6.24 B N
ATOM 4159 CA THR H 91 19.956 27.171 7.478 1.00 6.68 B C
ATOM 4160 CB THR H 91 21.444 27.375 7.139 1.00 6.62 B C
ATOM 4161 OG1 THR H 91 22.183 27.602 8.345 1.00 7.19 B O
ATOM 4162 CG2 THR H 91 21.619 28.565 6.210 1.00 7.27 B C
ATOM 4163 C THR H 91 19.203 26.886 6.180 1.00 7.02 B C
ATOM 4164 O THR H 91 18.505 27.767 5.661 1.00 7.16 B O
ATOM 4165 N GLU H 92 19.285 25.654 5.679 1.00 7.31 B N
ATOM 4166 CA GLU H 92 18.529 25.358 4.446 1.00 7.81 B C
ATOM 4167 CB GLU H 92 18.838 23.939 3.965 1.00 8.23 B C
ATOM 4168 CG GLU H 92 20.139 23.800 3.192 1.00 10.91 B C
ATOM 4169 CD GLU H 92 20.104 24.541 1.870 1.00 14.95 B C
ATOM 4170 OE1 GLU H 92 19.434 24.052 0.934 1.00 16.14 B O
ATOM 4171 OE2 GLU H 92 20.751 25.605 1.762 1.00 16.53 B O
ATOM 4172 C GLU H 92 17.003 25.530 4.644 1.00 7.47 B C
ATOM 4173 O GLU H 92 16.248 26.099 3.776 1.00 7.32 B O
ATOM 4174 N LEU H 93 16.541 25.053 5.800 1.00 7.30 B N
ATOM 4175 CA LEU H 93 15.117 25.171 6.098 1.00 7.47 B C
ATOM 4176 CB LEU H 93 14.760 24.426 7.385 1.00 7.15 B C
ATOM 4177 CG LEU H 93 14.797 22.898 7.297 1.00 7.20 B C
ATOM 4178 CD1 LEU H 93 14.346 22.282 8.610 1.00 7.93 B C
ATOM 4179 CD2 LEU H 93 13.941 22.397 6.141 1.00 6.91 B C
ATOM 4180 C LEU H 93 14.686 26.639 6.179 1.00 7.89 B C
ATOM 4181 O LEU H 93 13.626 27.012 5.675 1.00 7.94 B O

ATOM 4182 N GLN H 94 15.527 27.464 6.797 1.00 8.31 B N
ATOM 4183 CA GLN H 94 15.259 28.893 6.952 1.00 9.05 B C
ATOM 4184 CB GLN H 94 16.325 29.554 7.831 1.00 9.18 B C
ATOM 4185 CG GLN H 94 16.331 29.049 9.271 1.00 10.79 B C
ATOM 4186 CD GLN H 94 17.231 29.868 10.179 1.00 13.82 B C
ATOM 4187 OE1 GLN H 94 17.866 30.828 9.741 1.00 14.98 B O
ATOM 4188 NE2 GLN H 94 17.289 29.493 11.452 1.00 15.25 B N
ATOM 4189 C GLN H 94 15.190 29.545 5.576 1.00 9.25 B C
ATOM 4190 O GLN H 94 14.389 30.446 5.329 1.00 9.43 B o
ATOM 4191 N LEU H 95 16.050 29.058 4.691 1.00 9.55 B N
ATOM 4192 CA LEU H 95 16.140 29.479 3.294 1.00 10.17 B C
ATOM 4193 CB LEU H 95 17.327 28.800 2.605 1.00 9.79 B c
ATOM 4194 CG LEU H 95 18.721 29.321 2.958 1.00 8.86 B c
ATOM 4195 CDl LEU H 95 19.789 28.548 2.198 1.00 8.31 B c
ATOM 4196 CD2 LEU H 95 18.823 30.809 2.667 1.00 7.62 B c
ATOM 4197 C LEU H 95 14.865 29.250 2.467 1.00 11.22 B c
ATOM 4198 O LEU H 95 14.579 30.030 1.560 1.00 11.55 B o
ATOM 4199 N LEU H 96 14.105 28.190 2.748 1.00 12.40 B N
ATOM 4200 CA LEU H 96 12.870 27.931 1.929 1.00 13.66 B c
ATOM 4201 CB LEU H 96 12.338 26.527 2.247 1.00 13.38 B c
ATOM 4202 CG LEU H 96 13.163 25.359 1.709 1.00 13.32 B c
ATOM 4203 CDl LEU H 96 12.554 24.028 2.122 1.00 12.84 B C
ATOM 4204 CD2 LEU H 96 13.281 25.453 0.197 1.00 13.38 B C
ATOM 4205 C LEU H 96 11.631 28.927 1.839 1.00 14.97 B C
ATOM 4206 O LEU H 96 10.836 28.843 0.903 1.00 15.21 B O
ATOM 4207 N MET H 97 11.500 29.832 2.808 1.00 16.74 B N
ATOM 4208 CA MET H 97 10.348 30.575 3.317 1.00 18.96 B C
ATOM 4209 CB MET H 97 10.619 31.1 13 4.726 1.00 19.12 B C
ATOM 4210 CG MET H 97 10.944 30.037 5.758 1.00 21.87 B C
ATOM 421 1 SD MET H 97 9.537 28.994 6.201 1.00 27.46 B S
ATOM 4212 CE MET H 97 8.667 28.891 4.638 1.00 24.25 B C
ATOM 4213 C MET H 97 9.912 31.705 2.386 1.00 20.09 B C
ATOM 4214 O MET H 97 8.725 32.019 2.294 1.00 20.58 B O
ATOM 4215 N GLN H 98 10.867 32.274 1.658 1.00 21.33 B N
ATOM 4216 CA GLN H 98 10.593 33.429 0.809 1.00 22.21 B C
ATOM 4217 CB GLN H 98 11.279 34.679 1.364 1.00 22.53 B C
ATOM 4218 CG GLN H 98 11.165 34.831 2.872 1.00 23.85 B C
ATOM 4219 CD GLN H 98 12.329 34.200 3.612 1.00 25.21 B C
ATOM 4220 OE1 GLN H 98 12.539 32.989 3.544 1.00 24.47 B O
ATOM 4221 NE2 GLN H 98 13.058 35.012 4.369 1.00 24.85 B N
ATOM 4222 C GLN H 98 11.035 33.183 -0.629 1.00 22.15 B C
ATOM 4223 O GLN H 98 11.448 32.080 -0.982 1.00 21.77 B O
ATOM 4224 N PHE H 137 5.312 39.031 -3.961 1.00 33.25 B N
ATOM 4225 CA PHE H 137 5.277 37.601 -4.244 1.00 36.79 B C
ATOM 4226 CB PHE H 137 3.903 37.193 -4.778 1.00 20.00 B C
ATOM 4227 CG PHE H 137 2.795 37.350 -3.779 1.00 20.00 B C
ATOM 4228 CDl PHE H 137 2.542 36.360 -2.843 1.00 20.00 B C
ATOM 4229 CE1 PHE H 137 1.524 36.503 -1.920 1.00 20.00 B C
ATOM 4230 CZ PHE H 137 0.751 37.645 -1.920 1.00 20.00 B C
ATOM 4231 CE2 PHE H 137 1.003 38.646 -2.836 1.00 20.00 B C
ATOM 4232 CD2 PHE H 137 2.015 38.493 -3.764 1.00 20.00 B C
ATOM 4233 C PHE H 137 6.359 37.207 -5.241 1.00 48.73 B C
ATOM 4234 O PHE H 137 6.595 36.022 -5.477 1.00 49.28 B O
ATOM 4235 N LEU H 138 6.975 38.204 -5.868 1.00 42.04 B N
ATOM 4236 CA LEU H 138 8.094 37.959 -6.768 1.00 44.26 B C
ATOM 4237 CB LEU H 138 8.582 39.268 -7.389 1.00 20.00 B C
ATOM 4238 CG LEU H 138 7.578 40.005 -8.278 1.00 20.00 B C
ATOM 4239 CDl LEU H 138 8.178 41.296 -8.816 1.00 20.00 B C
ATOM 4240 CD2 LEU H 138 7.101 39.1 12 -9.41 1 1.00 20.00 B C
ATOM 4241 C LEU H 138 9.234 37.274 -6.025 1.00 43.68 B C

ATOM 4242 O LEU H 138 10.107 36.658 -6.636 1.00 50.27 B O
ATOM 4243 N GLY H 139 9.188 37.343 -4.698 1.00 38.56 B N
ATOM 4244 CA GLY H 139 10.191 36.699 -3.860 1.00 47.99 B C
ATOM 4245 C GLY H 139 10.260 35.202 -4.081 1.00 44.53 B C
ATOM 4246 O GLY H 139 11.284 34.575 -3.815 1.00 32.21 B O
ATOM 4247 N PHE H 140 9.173 34.630 -4.590 1.00 46.33 B N
ATOM 4248 CA PHE H 140 9.070 33.183 -4.735 1.00 42.95 B C
ATOM 4249 CB PHE H 140 7.618 32.723 -4.576 1.00 20.00 B C
ATOM 4250 CG PHE H 140 7.058 32.941 -3.201 1.00 20.00 B C
ATOM 4251 CD1 PHE H 140 7.285 32.021 -2.190 1.00 20.00 B C
ATOM 4252 CE1 PHE H 140 6.763 32.217 -0.926 1.00 20.00 B C
ATOM 4253 CZ PHE H 140 5.992 33.332 -0.664 1.00 20.00 B C
ATOM 4254 CE2 PHE H 140 5.747 34.249 -1.667 1.00 20.00 B C
ATOM 4255 CD2 PHE H 140 6.271 34.047 -2.929 1.00 20.00 B C
ATOM 4256 C PHE H 140 9.632 32.695 -6.071 1.00 38.13 B C
ATOM 4257 O PHE H 140 9.693 31.490 -6.322 1.00 57.33 B O
ATOM 4258 N LEU H 141 10.017 33.631 -6.934 1.00 35.20 B N
ATOM 4259 CA LEU H 141 10.453 33.294 -8.288 1.00 27.01 B C
ATOM 4260 CB LEU H 141 11.557 32.235 -8.254 1.00 20.00 B C
ATOM 4261 CG LEU H 141 12.886 32.672 -7.636 1.00 20.00 B C
ATOM 4262 CD1 LEU H 141 13.836 31.493 -7.513 1.00 20.00 B C
ATOM 4263 CD2 LEU H 141 13.520 33.794 -8.445 1.00 20.00 B C
ATOM 4264 C LEU H 141 9.287 32.812 -9.144 1.00 35.79 B C
ATOM 4265 O LEU H 141 8.355 33.567 -9.417 1.00 46.92 B O
ATOM 4266 N LEU H 142 9.342 31.555 -9.570 1.00 38.67 B N
ATOM 4267 CA LEU H 142 8.195 30.927 -10.207 1.00 33.84 B C
ATOM 4268 CB LEU H 142 8.610 30.262 -11.517 1.00 20.00 B C
ATOM 4269 CG LEU H 142 9.069 31.205 -12.629 1.00 20.00 B C
ATOM 4270 CD1 LEU H 142 9.474 30.415 -13.865 1.00 20.00 B C
ATOM 4271 CD2 LEU H 142 7.974 32.209 -12.964 1.00 20.00 B C
ATOM 4272 C LEU H 142 7.541 29.910 -9.278 1.00 36.89 B C
ATOM 4273 O LEU H 142 8.215 29.038 -8.729 1.00 45.42 B O
ATOM 4274 N GLY H 143 6.268 30.132 -8.975 1.00 26.84 B N
ATOM 4275 CA GLY H 143 5.577 29.350 -7.958 1.00 27.41 B C
ATOM 4276 C GLY H 143 4.243 28.849 -8.463 1.00 29.08 B C
ATOM 4277 O GLY H 143 3.592 29.504 -9.277 1.00 40.24 B O
ATOM 4278 N VAL H 144 3.848 27.665 -8.010 1.00 30.17 B N
ATOM 4279 CA VAL H 144 2.550 27.121 -8.373 1.00 34.15 B C
ATOM 4280 CB VAL H 144 2.497 25.596 -8.195 1.00 20.00 B C
ATOM 4281 CGI VAL H 144 1.073 25.102, -8.370 1.00 20.00 B C
ATOM 4282 CG2 VAL H 144 3.426 24.913 -9.187 1.00 20.00 B C
ATOM 4283 C VAL H 144 1.449 27.759 -7.538 1.00 36.67 B C
ATOM 4284 O VAL H 144 1.723 28.490 -6.587 1.00 42.49 B O
ATOM 4285 N GLY H 145 0.204 27.526 -7.938 1.00 47.09 B N
ATOM 4286 CA GLY H 145 -0.946 27.979 -7.166 1.00 44.51 B C
ATOM 4287 C GLY H 145 -0.857 27.562 -5.712 1.00 44.94 B C
ATOM 4288 O GLY H 145 -1.097 28.365 -4.810 1.00 40.58 B O
ATOM 4289 N SER H 146 -0.529 26.297 -5.473 1.00 42.06 B N
ATOM 4290 CA SEPv H 146 -0.433 25.788 -4.109 1.00 47.39 B C
ATOM 4291 CB SEPv H 146 -0.198 24.275 -4.119 1.00 20.00 B C
ATOM 4292 OG SEPv H 146 1.004 23.951 -4.796 1.00 20.00 B O
ATOM 4293 C SEPv H 146 0.665 26.482 -3.307 1.00 51.48 B C
ATOM 4294 O SEPv H 146 0.481 26.809 -2.131 1.00 47.45 B O
ATOM 4295 N ALA H 147 1.807 26.710 -3.949 1.00 39.51 B N
ATOM 4296 CA ALA H 147 2.943 27.334 -3.282 1.00 43.38 B C
ATOM 4297 CB ALA H 147 4.162 27.326 -4.194 1.00 20.00 B C
ATOM 4298 C ALA H 147 2.633 28.754 -2.821 1.00 47.39 B C
ATOM 4299 O ALA H 147 2.997 29.147 -1.713 1.00 50.18 B O
ATOM 4300 N ILE H 148 1.952 29.520 -3.668 1.00 44.67 B N
ATOM 4301 CA ILE H 148 1.602 30.892 -3.323 1.00 43.56 B C

ATOM 4302 CB ILE H 148 0.921 31.615 -4.499 1.00 20.00 B C
ATOM 4303 CGI ILE H 148 1.854 31.657 -5.71 1 1.00 20.00 B C
ATOM 4304 CD1 ILE H 148 1.259 32.353 -6.916 1.00 20.00 B C
ATOM 4305 CG2 ILE H 148 0.504 33.020 -4.092 1.00 20.00 B C
ATOM 4306 C ILE H 148 0.672 30.913 -2.117 1.00 51.18 B C
ATOM 4307 O ILE H 148 0.830 31.730 -1.208 1.00 39.17 B O
ATOM 4308 N ALA H 149 -0.289 29.995 -2.109 1.00 42.17 B N
ATOM 4309 CA ALA H 149 -1.233 29.895 -1.007 1.00 36.76 B C
ATOM 4310 CB ALA H 149 -2.297 28.854 -1.312 1.00 20.00 B C
ATOM 4311 C ALA H 149 -0.490 29.541 0.272 1.00 45.19 B C
ATOM 4312 O ALA H 149 -0.771 30.090 1.340 1.00 47.83 B O
ATOM 4313 N SER H 150 0.471 28.630 0.157 1.00 43.64 B N
ATOM 4314 CA SER H 150 1.250 28.218 1.315 1.00 43.46 B C
ATOM 4315 CB SER H 150 2.211 27.088 0.943 1.00 20.00 B C
ATOM 4316 OG SER H 150 3.113 27.499 -0.069 1.00 20.00 B O
ATOM 4317 C SER H 150 2.024 29.408 1.865 1.00 44.80 B C
ATOM 4318 O SER H 150 2.095 29.610 3.077 1.00 41.55 B O
ATOM 4319 N GLY H 151 2.590 30.205 0.964 1.00 27.01 B N
ATOM 4320 CA GLY H 151 3.342 31.379 1.362 1.00 35.21 B C
ATOM 4321 C GLY H 151 2.454 32.375 2.078 1.00 42.40 B C
ATOM 4322 O GLY H 151 2.849 32.969 3.083 1.00 45.11 B O
ATOM 4323 N VAL H 152 1.241 32.551 1.563 1.00 40.20 B N
ATOM 4324 CA VAL H 152 0.293 33.471 2.174 1.00 46.73 B C
ATOM 4325 CB VAL H 152 -1.000 33.585 1.346 1.00 20.00 B C
ATOM 4326 CGI VAL H 152 -1.970 34.551 2.009 1.00 20.00 B C
ATOM 4327 CG2 VAL H 152 -0.682 34.029 -0.073 1.00 20.00 B C
ATOM 4328 C VAL H 152 -0.052 32.995 3.579 1.00 48.62 B C
ATOM 4329 O VAL H 152 -0.133 33.792 4.517 1.00 49.32 B O
ATOM 4330 N ALA H 153 -0.239 31.686 3.722 1.00 35.09 B N
ATOM 4331 CA ALA H 153 -0.567 31.112 5.018 1.00 42.37 B C
ATOM 4332 CB ALA H 153 -0.849 29.625 4.885 1.00 20.00 B C
ATOM 4333 C ALA H 153 0.578 31.353 5.992 1.00 37.79 B C
ATOM 4334 O ALA H 153 0.359 31.696 7.154 1.00 39.25 B O
ATOM 4335 N VAL H 154 1.802 31.189 5.502 1.00 38.88 B N
ATOM 4336 CA VAL H 154 2.982 31.394 6.328 1.00 35.53 B C
ATOM 4337 CB VAL H 154 4.274 31.042 5.568 1.00 20.00 B C
ATOM 4338 CGI VAL H 154 5.489 31.267 6.454 1.00 20.00 B C
ATOM 4339 CG2 VAL H 154 4.223 29.605 5.074 1.00 20.00 B C
ATOM 4340 C VAL H 154 3.053 32.842 6.791 1.00 41.00 B C
ATOM 4341 O VAL H 154 3.380 33.118 7.945 1.00 50.08 B O
ATOM 4342 N SER H 155 2.742 33.766 5.888 1.00 37.82 B N
ATOM 4343 CA SER H 155 2.753 35.181 6.232 1.00 44.68 B C
ATOM 4344 CB SER H 155 2.496 36.038 4.991 1.00 20.00 B C
ATOM 4345 OG SER H 155 1.238 35.736 4.414 1.00 20.00 B O
ATOM 4346 C SER H 155 1.706 35.477 7.300 1.00 41.82 B C
ATOM 4347 O SER H 155 1.960 36.224 8.245 1.00 49.37 B O
ATOM 4348 N LYS H 156 0.528 34.880 7.144 1.00 36.99 B N
ATOM 4349 CA LYS H 156 -0.559 35.059 8.102 1.00 35.11 B C
ATOM 4350 CB LYS H 156 -1.843 34.411 7.579 1.00 20.00 B C
ATOM 4351 CG LYS H 156 -2.334 34.983 6.259 1.00 20.00 B C
ATOM 4352 CD LYS H 156 -3.611 34.297 5.801 1.00 20.00 B C
ATOM 4353 CE LYS H 156 -4.102 34.869 4.481 1.00 20.00 B C
ATOM 4354 NZ LYS H 156 -5.353 34.206 4.020 1.00 20.00 B N
ATOM 4355 C LYS H 156 -0.210 34.493 9.476 1.00 35.98 B C
ATOM 4356 O LYS H 156 -0.535 35.081 10.507 1.00 42.31 B O
ATOM 4357 N VAL H 157 0.448 33.339 9.470 1.00 37.88 B N
ATOM 4358 CA VAL H 157 0.794 32.617 10.689 1.00 50.94 B C
ATOM 4359 CB VAL H 157 1.143 31.145 10.396 1.00 20.00 B C
ATOM 4360 CGI VAL H 157 1.572 30.439 11.672 1.00 20.00 B C
ATOM 4361 CG2 VAL H 157 -0.043 30.435 9.762 1.00 20.00 B C

```
ATOM   4362  C   VAL H 157      1.962  33.277  11.415  1.00 47.82      B    C
ATOM   4363  O   VAL H 157      2.296  32.905  12.541  1.00 56.87      B    o
ATOM   4364  N   LEU H 158      2.533  34.304  10.794  1.00 39.52      B    N
ATOM   4365  CA  LEU H 158      3.727  34.956  11.320  1.00 50.27      B    C
ATOM   4366  CB  LEU H 158      4.080  36.188  10.484  1.00 20.00      B    c
ATOM   4367  CG  LEU H 158      4.493  35.927   9.034  1.00 20.00      B    c
ATOM   4368  CD1 LEU H 158      4.688  37.237   8.287  1.00 20.00      B    c
ATOM   4369  CD2 LEU H 158      5.754  35.079   8.976  1.00 20.00      B    c
ATOM   4370  C   LEU H 158      3.589  35.334  12.794  1.00 54.47      B    c
ATOM   4371  O   LEU H 158      4.512  35.127  13.582  1.00 49.26      B    o
ATOM   4372  N   HIS H 159      2.448  35.754  13.309  1.00 59.45      B    N
ATOM   4373  CA  HIS H 159      2.473  36.028  14.762  1.00 49.1 1      B    c
ATOM   4374  CB  HIS H 159      1.136  36.614  15.221  1.00 20.00      B    c
ATOM   4375  CG  HIS H 159      0.780  37.903  14.548  1.00 20.00      B    c
ATOM   4376  ND1 HIS H 159      1.149  39. 132  15.051  1.00 20.00      B    N
ATOM   4377  CE1 HIS H 159      0.699  40.085  14.254  1.00 20.00      B    c
ATOM   4378  NE2 HIS H 159      0.052  39.519  13.252  1.00 20.00      B    N
ATOM   4379  CD2 HIS H 159      0.087  38.155  13.412  1.00 20.00      B    C
ATOM   4380  C   HIS H 159      2.830  34.775  15.616  1.00 44.09      B    C
ATOM   4381  O   HIS H 159      3.627  34.822  16.600  1.00 42.13      B    O
ATOM   4382  N   LEU H 160      2.261  33.646  15.207  1.00 37.55      B    N
ATOM   4383  CA  LEU H 160      2.402  32.391  15.934  1.00 43.52      B    C
ATOM   4384  CB  LEU H 160      1.521  31.310  15.302  1.00 20.00      B    C
ATOM   4385  CG  LEU H 160      0.018  31.596  15.268  1.00 20.00      B    c
ATOM   4386  CD1 LEU H 160     -0.734  30.443  14.620  1.00 20.00      B    c
ATOM   4387  CD2 LEU H 160     -0.509  31.865  16.668  1.00 20.00      B    c
ATOM   4388  C   LEU H 160      3.839  31.887  16.044  1.00 47.22      B    c
ATOM   4389  O   LEU H 160      4.233  31.383  17.091  1.00 43.25      B    o
ATOM   4390  N   GLU H 161      4.620  32.01 1  14.976  1.00 40.88      B    N
ATOM   4391  CA  GLU H 161      5.996  31.524  15.008  1.00 40.61      B    c
ATOM   4392  CB  GLU H 161      6.644  31.658  13.628  1.00 20.00      B    c
ATOM   4393  CG  GLU H 161      5.936  30.878  12.532  1.00 20.00      B    c
ATOM   4394  CD  GLU H 161      6.606  31.031  11.181  1.00 20.00      B    c
ATOM   4395  OE1 GLU H 161      6.1 13  30.437  10.200  1.00 20.00      B    o
ATOM   4396  OE2 GLU H 161      7.628  31.745  11.101  1.00 20.00      B    o
ATOM   4397  C   GLU H 161      6.833  32.259  16.054  1.00 39.76      B    c
ATOM   4398  O   GLU H 161      7.606  31.642  16.795  1.00 44.02      B    o
ATOM   4399  N   GLY H 162      6.679  33.566  16.21 1  1.00 34.18      B    N
ATOM   4400  CA  GLY H 162      7.497  34.204  17.230  1.00 35.01      B    c
ATOM   4401  C   GLY H 162      7.170  33.593  18.586  1.00 34.86      B    c
ATOM   4402  O   GLY H 162      8.065  33.226  19.372  1.00 47.81      B    o
ATOM   4403  N   GLU H 163      5.875  33.431  18.838  1.00 40.78      B    N
ATOM   4404  CA  GLU H 163      5.403  32.797  20.058  1.00 37.20      B    c
ATOM   4405  CB  GLU H 163      3.877  32.847  20.137  1.00 20.00      B    c
ATOM   4406  CG  GLU H 163      3.301  34.254  20.134  1.00 20.00      B    c
ATOM   4407  CD  GLU H 163      1.788  34.264  20.214  1.00 20.00      B    c
ATOM   4408  OE1 GLU H 163      1.199  35.365  20.219  1.00 20.00      B    o
ATOM   4409  OE2 GLU H 163      1.186  33.171  20.273  1.00 20.00      B    o
ATOM   4410  C   GLU H 163      5.884  31.355  20.065  1.00 46.12      B    c
ATOM   441 1  O   GLU H 163      6.295  30.824  21.098  1.00 58.66      B    o
ATOM   4412  N   VAL H 164      5.832  30.731  18.893  1.00 42.23      B    N
ATOM   4413  CA  VAL H 164      6.270  29.353  18.740  1.00 35.45      B    c
ATOM   4414  CB  VAL H 164      6.021  28.836  17.31 1  1.00 20.00      B    c
ATOM   4415  CGI VAL H 164      6.488  27.394  17.181  1.00 20.00      B    c
ATOM   4416  CG2 VAL H 164      4.549  28.962  16.951  1.00 20.00      B    c
ATOM   4417  C   VAL H 164      7.753  29.241  19.061  1.00 46.32      B    c
ATOM   4418  O   VAL H 164      8.180  28.290  19.709  1.00 45.08      B    o
ATOM   4419  N   ASN H 165      8.536  30.217  18.61 1  1.00 40.82      B    N
ATOM   4420  CA  ASN H 165      9.966  30.227  18.891  1.00 46.48      B    c
ATOM   4421  CB  ASN H 165     10.653  31.372  18. 145  1.00 20.00      B    c
```

ATOM 4422 CG ASN H 165 10.488 31.270 16.642 1.00 20.00 B C
ATOM 4423 OD1 ASN H 165 10.982 32.113 15.893 1.00 20.00 B O
ATOM 4424 ND2 ASN H 165 9.792 30.232 16.192 1.00 20.00 B N
ATOM 4425 C ASN H 165 10.227 30.342 20.389 1.00 50.90 B C
ATOM 4426 O ASN H 165 11.099 29.655 20.941 1.00 47.11 B O
ATOM 4427 N LYS H 166 9.453 31.198 21.052 1.00 48.36 B N
ATOM 4428 CA LYS H 166 9.605 31.351 22.495 1.00 38.71 B C
ATOM 4429 CB LYS H 166 8.692 32.461 23.019 1.00 20.00 B C
ATOM 4430 CG LYS H 166 8.968 33.828 22.414 1.00 20.00 B C
ATOM 4431 CD LYS H 166 8.030 34.881 22.980 1.00 20.00 B C
ATOM 4432 CE LYS H 166 8.306 36.249 22.376 1.00 20.00 B C
ATOM 4433 NZ LYS H 166 7.396 37.292 22.923 1.00 20.00 B N
ATOM 4434 C LYS H 166 9.284 30.029 23.192 1.00 45.07 B C
ATOM 4435 O LYS H 166 9.977 29.609 24.131 1.00 56.09 B O
ATOM 4436 N ILE H 167 8.238 29.366 22.709 1.00 42.02 B N
ATOM 4437 CA ILE H 167 7.817 28.091 23.272 1.00 43.86 B C
ATOM 4438 CB ILE H 167 6.527 27.577 22.607 1.00 20.00 B C
ATOM 4439 CGI ILE H 167 5.388 28.580 22.807 1.00 20.00 B C
ATOM 4440 CD1 ILE H 167 4.079 28.150 22.181 1.00 20.00 B C
ATOM 4441 CG2 ILE H 167 6.147 26.214 23.164 1.00 20.00 B C
ATOM 4442 C ILE H 167 8.916 27.053 23.099 1.00 49.02 B C
ATOM 4443 O ILE H 167 9.178 26.260 23.998 1.00 37.71 B O
ATOM 4444 N LYS H 168 9.557 27.068 21.935 1.00 33.87 B N
ATOM 4445 CA LYS H 168 10.644 26.146 21.640 1.00 35.11 B C
ATOM 4446 CB LYS H 168 11.103 26.304 20.189 1.00 20.00 B C
ATOM 4447 CG LYS H 168 10.014 26.040 19.162 1.00 20.00 B C
ATOM 4448 CD LYS H 168 10.535 26.220 17.746 1.00 20.00 B C
ATOM 4449 CE LYS H 168 9.445 25.959 16.719 1.00 20.00 B C
ATOM 4450 NZ LYS H 168 9.941 26.134 15.326 1.00 20.00 B N
ATOM 4451 C LYS H 168 11.813 26.380 22.588 1.00 39.27 B C
ATOM 4452 O LYS H 168 12.422 25.429 23.078 1.00 32.39 B O
ATOM 4453 N SER H 169 12.121 27.647 22.854 1.00 41.30 B N
ATOM 4454 CA SER H 169 13.203 27.963 23.783 1.00 43.23 B C
ATOM 4455 CB SER H 169 13.446 29.472 23.832 1.00 20.00 B C
ATOM 4456 OG SER H 169 12.284 30.162 24.259 1.00 20.00 B O
ATOM 4457 C SER H 169 12.865 27.436 25.178 1.00 41.44 B C
ATOM 4458 O SER H 169 13.723 26.871 25.883 1.00 44.82 B O
ATOM 4459 N ALA H 170 11.604 27.605 25.566 1.00 39.78 B N
ATOM 4460 CA ALA H 170 11.161 27.131 26.870 1.00 41.01 B C
ATOM 4461 CB ALA H 170 9.720 27.541 27.124 1.00 20.00 B C
ATOM 4462 C ALA H 170 11.308 25.615 26.948 1.00 46.04 B C
ATOM 4463 O ALA H 170 11.743 25.072 27.964 1.00 46.67 B O
ATOM 4464 N LEU H 171 10.955 24.940 25.859 1.00 34.26 B N
ATOM 4465 CA LEU H 171 11.050 23.489 25.782 1.00 37.69 B C
ATOM 4466 CB LEU H 171 10.458 22.982 24.466 1.00 20.00 B C
ATOM 4467 CG LEU H 171 8.984 23.305 24.216 1.00 20.00 B C
ATOM 4468 CD1 LEU H 171 8.529 22.743 22.878 1.00 20.00 B C
ATOM 4469 CD2 LEU H 171 8.118 22.773 25.348 1.00 20.00 B C
ATOM 4470 C LEU H 171 12.499 23.044 25.912 1.00 44.67 B C
ATOM 4471 O LEU H 171 12.797 22.054 26.579 1.00 34.27 B O
ATOM 4472 N LEU H 172 13.400 23.783 25.272 1.00 34.80 B N
ATOM 4473 CA LEU H 172 14.817 23.464 25.344 1.00 28.87 B C
ATOM 4474 CB LEU H 172 15.626 24.402 24.447 1.00 20.00 B C
ATOM 4475 CG LEU H 172 15.281 24.379 22.956 1.00 20.00 B C
ATOM 4476 CD1 LEU H 172 16.158 25.355 22.186 1.00 20.00 B C
ATOM 4477 CD2 LEU H 172 15.416 22.972 22.395 1.00 20.00 B C
ATOM 4478 C LEU H 172 15.291 23.577 26.786 1.00 29.90 B C
ATOM 4479 O LEU H 172 16.022 22.714 27.272 1.00 41.09 B O
ATOM 4480 N SER H 173 14.862 24.629 27.480 1.00 35.08 B N
ATOM 4481 CA SER H 173 15.184 24.754 28.902 1.00 35.53 B C

ATOM 4482 CB SER H 173 14.727 26.109 29.442 1.00 20.00 B C
ATOM 4483 OG SER H 173 13.328 26.272 29.294 1.00 20.00 B o
ATOM 4484 C SER H 173 14.506 23.618 29.673 1.00 35.07 B c
ATOM 4485 O SER H 173 15.056 23.037 30.609 1.00 51.28 B o
ATOM 4486 N THR H 174 13.286 23.341 29.234 1.00 46.35 B N
ATOM 4487 CA THR H 174 12.335 22.383 29.786 1.00 43.83 B c
ATOM 4488 CB THR H 174 10.885 22.764 29.429 1.00 20.00 B c
ATOM 4489 OG1 THR H 174 10.725 22.762 28.004 1.00 20.00 E; o
ATOM 4490 CG2 THR H 174 10.547 24.144 29.971 1.00 20.00 B, c
ATOM 4491 C THR H 174 12.616 20.979 29.263 1.00 52.54 B c
ATOM 4492 O THR H 174 12.523 20.726 28.063 1.00 64.10 B o
ATOM 4493 N ASN H 175 12.974 20.071 30. 165 1.00 55.57 B N
ATOM 4494 CA ASN H 175 13.072 18.660 29.817 1.00 40.58 B c
ATOM 4495 CB ASN H 175 13.942 17.915 30.831 1.00 20.00 B c
ATOM 4496 CG ASN H 175 15.405 18.303 30.740 1.00 20.00 B c
ATOM 4497 OD1 ASN H 175 15.868 18.788 29.708 1.00 20.00 E; o
ATOM 4498 ND2 ASN H 175 16.139 18.099 31.827 1.00 20.00 E; N
ATOM 4499 C ASN H 175 11.695 18.009 29.714 1.00 43.65 B c
ATOM 4500 O ASN H 175 10.972 17.912 30.705 1.00 53.1 1 B o
ATOM 4501 N LYS H 176 11.296 17.666 28.491 1.00 44.89 B N
ATOM 4502 CA LYS H 176 9.986 17.068 28.250 1.00 46.42 B C
ATOM 4503 CB LYS H 176 8.873 18.052 28.618 1.00 20.00 B c
ATOM 4504 CG LYS H 176 8.873 18.468 30.088 1.00 20.00 B c
ATOM 4505 CD LYS H 176 7.844 19.557 30.362 1.00 20.00 B c
ATOM 4506 CE LYS H 176 7.773 19.904 31.841 1.00 20.00 B c
ATOM 4507 NZ LYS H 176 6.701 20.899 32. 121 1.00 20.00 B N
ATOM 4508 C LYS H 176 9.829 16.596 26.806 1.00 45.00 B c
ATOM 4509 O LYS H 176 10.272 17.264 25.871 1.00 60.64 B o
ATOM 4510 N ALA H 177 9.245 15.415 26.634 1.00 46.01 B N
ATOM 451 1 CA ALA H 177 8.914 14.913 25.306 1.00 43.65 B c
ATOM 4512 CB ALA H 177 8.530 13.442 25.374 1.00 20.00 B c
ATOM 4513 C ALA H 177 7.789 15.731 24.686 1.00 41.42 B c
ATOM 4514 O ALA H 177 7.894 16.184 23.547 1.00 45.37 B o
ATOM 4515 N VAL H 178 6.736 15.960 25.463 1.00 35.70 B N
ATOM 4516 CA VAL H 178 5.642 16.820 25.037 1.00 43.93 B c
ATOM 4517 CB VAL H 178 4.383 15.999 24.710 1.00 20.00 B c
ATOM 4518 CGI VAL H 178 3.229 16.919 24.341 1.00 20.00 B c
ATOM 4519 CG2 VAL H 178 4.672 15.014 23.585 1.00 20.00 B c
ATOM 4520 C VAL H 178 5.313 17.836 26. 124 1.00 34.16 B c
ATOM 4521 O VAL H 178 5.395 17.527 27.31 1 1.00 44.45 B o
ATOM 4522 N VAL H 179 5.028 19.069 25.717 1.00 44.87 B N
ATOM 4523 CA VAL H 179 4.818 20.155 26.667 1.00 38.47 B c
ATOM 4524 CB VAL H 179 6.150 20.766 27.131 1.00 20.00 B c
ATOM 4525 CGI VAL H 179 5.908 21.808 28.221 1.00 20.00 B c
ATOM 4526 CG2 VAL H 179 7.097 19.678 27.609 1.00 20.00 B c
ATOM 4527 C VAL H 179 3.967 21.265 26.070 1.00 44.79 B c
ATOM 4528 O VAL H 179 4.226 21.727 24.959 1.00 51.88 B o
ATOM 4529 N SER H 180 3.025 21.765 26.862 1.00 45.23 B N
ATOM 4530 CA SER H 180 2.226 22.915 26.463 1.00 48.99 B c
ATOM 4531 CB SER H 180 0.976 23.033 27.340 1.00 20.00 B c
ATOM 4532 OG SER H 180 1.321 23.322 28.683 1.00 20.00 B o
ATOM 4533 C SER H 180 3.047 24.198 26.532 1.00 48.15 B c
ATOM 4534 O SER H 180 3.568 24.553 27.589 1.00 60.42 B o
ATOM 4535 N LEU H 181 3.261 24.821 25.378 1.00 42.42 B N
ATOM 4536 CA LEU H 181 3.872 26. 143 25.325 1.00 43.22 B c
ATOM 4537 CB LEU H 181 4.252 26.498 23.888 1.00 20.00 B c
ATOM 4538 CG LEU H 181 5.279 25.577 23.233 1.00 20.00 B c
ATOM 4539 CD1 LEU H 181 5.583 26.043 21.818 1.00 20.00 B c
ATOM 4540 CD2 LEU H 181 6.541 25.519 24.073 1.00 20.00 B c
ATOM 4541 C LEU H 181 2.929 27. 199 25.884 1.00 29.14 B c

ATOM 4542 O LEU H 181 1.891 27.494 25.291 1.00 43.42 B O
ATOM 4543 N SER H 182 3.271 27.735 27.051 1.00 41.83 B N
ATOM 4544 CA SER H 182 2.365 28.619 27.770 1.00 53.52 B C
ATOM 4545 CB SER H 182 2.034 28.053 29.152 1.00 20.00 B C
ATOM 4546 OG SER H 182 3.184 28.019 29.978 1.00 20.00 B o
ATOM 4547 C SER H 182 2.914 30.036 27.891 1.00 44.76 B c
ATOM 4548 O SER H 182 4.095 30.236 28.178 1.00 37.73 B o
ATOM 4549 N ASN H 183 2.072 31.008 27.556 1.00 47.84 B N
ATOM 4550 CA ASN H 183 2.258 32.384 27.996 1.00 59.45 B c
ATOM 4551 CB ASN H 183 2.304 33.316 26.782 1.00 20.00 B c
ATOM 4552 CG ASN H 183 3.512 33.066 25.897 1.00 20.00 B c
ATOM 4553 OD1 ASN H 183 4.574 32.671 26.379 1.00 20.00 B o
ATOM 4554 ND2 ASN H 183 3.384 33.386 24.615 1.00 20.00 B N
ATOM 4555 C ASN H 183 1.117 32.791 28.924 1.00 75.41 B c
ATOM 4556 O ASN H 183 -0.008 32.318 28.769 1.00102.31 B o
ATOM 4557 N GLY H 184 1.432 33.563 29.959 1.00 79.30 B N
ATOM 4558 CA GLY H 184 0.435 33.947 30.957 1.00 88.92 B c
ATOM 4559 C GLY H 184 -0.954 33.397 30.674 1.00101.85 B c
ATOM 4560 O GLY H 184 -1.760 34.037 29.999 1.00113.48 B o
ATOM 4561 N VAL H 185 -1.218 32.190 31.167 1.00 86.84 B N
ATOM 4562 CA VAL H 185 -2.573 31.636 31.236 1.00 81.80 B c
ATOM 4563 CB VAL H 185 -3.558 32.579 31.958 1.00 20.00 B c
ATOM 4564 CGI VAL H 185 -4.974 32.022 31.887 1.00 20.00 B c
ATOM 4565 CG2 VAL H 185 -3.135 32.783 33.405 1.00 20.00 B c
ATOM 4566 C VAL H 185 -3.164 31.228 29.887 1.00 81.69 B c
ATOM 4567 O VAL H 185 -4.347 30.900 29.801 1.00 99.84 B o
ATOM 4568 N SER H 186 -2.336 31.193 28.848 1.00 70.63 B N
ATOM 4569 CA SER H 186 -2.819 30.830 27.519 1.00 72.29 B c
ATOM 4570 CB SER H 186 -3.084 32.081 26.679 1.00 20.00 B c
ATOM 4571 OG SER H 186 -1.884 32.787 26.420 1.00 20.00 B o
ATOM 4572 C SER H 186 -1.865 29.891 26.789 1.00 62.99 B c
ATOM 4573 O SER H 186 -0.655 30.115 26.765 1.00 58.35 B o
ATOM 4574 N VAL H 187 -2.422 28.851 26.177 1.00 66.49 B N
ATOM 4575 CA VAL H 187 -1.627 27.877 25.438 1.00 57.36 B c
ATOM 4576 CB VAL H 187 -2.284 26.484 25.457 1.00 20.00 B c
ATOM 4577 CGI VAL H 187 -1.504 25.516 24.583 1.00 20.00 B c
ATOM 4578 CG2 VAL H 187 -2.383 25.963 26.883 1.00 20.00 B c
ATOM 4579 C VAL H 187 -1.432 28.317 23.991 1.00 53.67 B c
ATOM 4580 O VAL H 187 -2.401 28.531 23.262 1.00 50.10 B o
ATOM 4581 N LEU H 188 -0.176 28.476 23.588 1.00 43.20 B N
ATOM 4582 CA LEU H 188 0.143 28.854 22.217 1.00 41.76 B c
ATOM 4583 CB LEU H 188 1.487 29.581 22.160 1.00 20.00 B c
ATOM 4584 CG LEU H 188 1.549 30.938 22.862 1.00 20.00 B c
ATOM 4585 CD1 LEU H 188 2.957 31.507 22.799 1.00 20.00 B c
ATOM 4586 CD2 LEU H 188 0.548 31.907 22.250 1.00 20.00 B c
ATOM 4587 C LEU H 188 0.166 27.634 21.304 1.00 44.75 B c
ATOM 4588 O LEU H 188 -0.074 27.743 20.102 1.00 45.28 B o
ATOM 4589 N THR H 189 0.390 26.466 21.897 1.00 39.28 B N
ATOM 4590 CA THR H 189 0.552 25.235 21.133 1.00 36.51 B c
ATOM 4591 CB THR H 189 1.229 25.498 19.774 1.00 20.00 B c
ATOM 4592 OG1 THR H 189 2.554 26.001 19.986 1.00 20.00 B o
ATOM 4593 CG2 THR H 189 0.430 26.512 18.968 1.00 20.00 B c
ATOM 4594 C THR H 189 1.362 24.208 21.926 1.00 45.83 B c
ATOM 4595 O THR H 189 1.419 24.267 23.154 1.00 42.57 B o
ATOM 4596 N SER H 190 1.947 23.241 21.226 1.00 40.44 B N
ATOM 4597 CA SER H 190 2.691 22.171 21.881 1.00 41.82 B c
ATOM 4598 CB SER H 190 2.022 20.815 21.632 1.00 20.00 B c
ATOM 4599 OG SER H 190 2.225 20.376 20.300 1.00 20.00 B o
ATOM 4600 C SER H 190 4.152 22.141 21.437 1.00 33.81 B c
ATOM 4601 O SER H 190 4.473 22.505 20.306 1.00 49.61 B o

ATOM 4602 N LYS H 191 5.040 21.855 22.385 1.00 37.37 B N
ATOM 4603 CA LYS H 191 6.463 21.71 1 22.098 1.00 41.23 B C
ATOM 4604 CB LYS H 191 7.285 22.617 23.021 1.00 20.00 B C
ATOM 4605 CG LYS H 191 7.104 24.102 22.750 1.00 20.00 B C
ATOM 4606 CD LYS H 191 7.981 24.949 23.658 1.00 20.00 B C
ATOM 4607 CE LYS H 191 7.790 26.435 23.369 1.00 20.00 B C
ATOM 4608 NZ LYS H 191 8.364 27.306 24.434 1.00 20.00 B N
ATOM 4609 C LYS H 191 6.906 20.260 22.268 1.00 35.03 B C
ATOM 4610 O LYS H 191 6.828 19.710 23.365 1.00 40.06 B O
ATOM 461 1 N VAL H 192 7.443 19.670 21.205 1.00 33.70 B N
ATOM 4612 CA VAL H 192 7.787 18.250 2 1.221 1.00 27.61 B C
ATOM 4613 CB VAL H 192 6.974 17.456 20.182 1.00 20.00 B C
ATOM 4614 CGI VAL H 192 7.313 15.975 20.263 1.00 20.00 B C
ATOM 4615 CG2 VAL H 192 5.487 17.679 20.391 1.00 20.00 B C
ATOM 4616 C VAL H 192 9.277 18.01 1 20.985 1.00 31.74 B C
ATOM 4617 O VAL H 192 9.931 18.771 20.272 1.00 25.58 B O
ATOM 4618 N LEU H 193 9.792 16.921 21.550 1.00 28.88 B N
ATOM 4619 CA LEU H 193 11.190 16.530 21.360 1.00 34.36 B C
ATOM 4620 CB LEU H 193 12.061 17.069 22.505 1.00 20.00 B C
ATOM 4621 CG LEU H 193 12.332 18.577 22.614 1.00 20.00 B C
ATOM 4622 CD1 LEU H 193 12.987 18.914 23.949 1.00 20.00 B C
ATOM 4623 CD2 LEU H 193 13.194 19.076 21.459 1.00 20.00 B C
ATOM 4624 C LEU H 193 11.335 15.008 2 1.281 1.00 33.03 B C
ATOM 4625 O LEU H 193 11.373 14.331 22.310 1.00 44.93 B O
ATOM 4626 N ASP H 194 11.579 14.498 20.077 1.00 35.09 B N
ATOM 4627 CA ASP H 194 11.209 13.127 19.730 1.00 4 1.39 B C
ATOM 4628 CB ASP H 194 11.269 12.925 18.214 1.00 20.00 B C
ATOM 4629 CG ASP H 194 10. 132 13.626 17.485 1.00 20.00 B C
ATOM 4630 OD1 ASP H 194 9.081 13.873 18.1 15 1.00 20.00 B O
ATOM 4631 OD2 ASP H 194 10.305 13.969 16.296 1.00 20.00 B O
ATOM 4632 C ASP H 194 12.091 12.100 20.433 1.00 38.04 B C
ATOM 4633 O ASP H 194 11.796 10.904 20.429 1.00 48.03 B O
ATOM 4634 N LEU H 195 13. 174 12.576 21.039 1.00 43.64 B N
ATOM 4635 CA LEU H 195 14.206 11.690 21.555 1.00 35.97 B C
ATOM 4636 CB LEU H 195 15.532 11.935 20.832 1.00 20.00 B C
ATOM 4637 CG LEU H 195 15.563 11.586 19.340 1.00 20.00 B C
ATOM 4638 CD1 LEU H 195 16.947 11.852 18.750 1.00 20.00 B C
ATOM 4639 CD2 LEU H 195 15.1 18 10.144 19.081 1.00 20.00 B C
ATOM 4640 C LEU H 195 14.386 11.839 23.063 1.00 43.63 B C
ATOM 4641 O LEU H 195 15.068 11.036 23.699 1.00 34.71 B O
ATOM 4642 N ASN H 196 13.689 12.808 23.645 1.00 44.30 B N
ATOM 4643 CA ASN H 196 13.886 13.151 25.047 1.00 42.38 B C
ATOM 4644 CB ASN H 196 12.955 14.290 25.454 1.00 20.00 B C
ATOM 4645 CG ASN H 196 13.376 15.618 24.868 1.00 20.00 B C
ATOM 4646 OD1 ASN H 196 14.538 15.815 24.513 1.00 20.00 B O
ATOM 4647 ND2 ASN H 196 12.439 16.555 24.800 1.00 20.00 B N
ATOM 4648 C ASN H 196 13.721 11.972 26.000 1.00 43.66 B C
ATOM 4649 O ASN H 196 14.499 11.814 26.940 1.00 33.62 B O
ATOM 4650 N ASN H 197 12.649 11.208 25.817 1.00 34.31 B N
ATOM 4651 CA ASN H 197 12.370 10.074 26.691 1.00 38.83 B C
ATOM 4652 CB ASN H 197 11.043 9.417 26.318 1.00 20.00 B C
ATOM 4653 CG ASN H 197 9.848 10.251 26.729 1.00 20.00 B C
ATOM 4654 OD1 ASN H 197 9.957 11.129 27.585 1.00 20.00 B O
ATOM 4655 ND2 ASN H 197 8.722 10.042 26.059 1.00 20.00 B N
ATOM 4656 C ASN H 197 13.492 9.042 26.685 1.00 39.90 B C
ATOM 4657 O ASN H 197 14.026 8.687 27.735 1.00 39.04 B O
ATOM 4658 N TYR H 198 13.871 8.590 25.495 1.00 35.09 B N
ATOM 4659 CA TYPv H 198 14.992 7.672 25.355 1.00 41.03 B C
ATOM 4660 CB TYR H 198 15.246 7.355 23.882 1.00 20.00 B C
ATOM 4661 CG TYPv H 198 14.109 6.617 23.218 1.00 20.00 B C

ATOM 4662 CD1 TYR H 198 14.014 5.235 23.294 1.00 20.00 B C
ATOM 4663 CE1 TYR H 198 12.963 4.558 22.712 1.00 20.00 B C
ATOM 4664 CZ TYR H 198 11.999 5.265 22.024 1.00 20.00 B c
ATOM 4665 OH TYR H 198 10.967 4.598 21.403 1.00 20.00 B o
ATOM 4666 CE2 TYR H 198 12.073 6.638 21.934 1.00 20.00 B c
ATOM 4667 CD2 TYR H 198 13.120 7.305 22.533 1.00 20.00 B c
ATOM 4668 C TYR H 198 16.252 8.234 26.002 1.00 43.65 B c
ATOM 4669 O TYR H 198 16.940 7.533 26.744 1.00 52.37 B o
ATOM 4670 N ILE H 199 16.464 9.537 25.831 1.00 35.86 B N
ATOM 4671 CA ILE H 199 17.634 10.219 26.386 1.00 45.39 B c
ATOM 4672 CB ILE H 199 17.722 11.682 25.904 1.00 20.00 B c
ATOM 4673 CGI ILE H 199 18.102 11.741 24.425 1.00 20.00 B c
ATOM 4674 CD1 ILE H 199 18.674 13.078 24.004 1.00 20.00 B c
ATOM 4675 CG2 ILE H 199 18.730 12.457 26.735 1.00 20.00 B c
ATOM 4676 C ILE H 199 17.639 10.200 27.912 1.00 37.89 B c
ATOM 4677 O ILE H 199 18.667 9.941 28.538 1.00 45.28 B O
ATOM 4678 N ASP H 200 16.492 10.508 28.505 1.00 37.36 B N
ATOM 4679 CA ASP H 200 16.368 10.551 29.954 1.00 46.66 B c
ATOM 4680 CB ASP H 200 14.992 11.080 30.354 1.00 20.00 B c
ATOM 4681 CG ASP H 200 14.837 12.564 30.083 1.00 20.00 B c
ATOM 4682 OD1 ASP H 200 15.826 13.308 30.264 1.00 20.00 B o
ATOM 4683 OD2 ASP H 200 13.718 12.992 29.721 1.00 20.00 B o
ATOM 4684 C ASP H 200 16.600 9.181 30.581 1.00 51.05 B c
ATOM 4685 O ASP H 200 16.986 9.081 31.745 1.00 57.39 B o
ATOM 4686 N LYS H 201 16.346 8.129 29.810 1.00 57.68 B N
ATOM 4687 CA LYS H 201 16.517 6.766 30.299 1.00 44.02 B c
ATOM 4688 CB LYS H 201 15.747 5.778 29.423 1.00 20.00 B c
ATOM 4689 CG LYS H 201 14.242 5.854 29.602 1.00 20.00 B c
ATOM 4690 CD LYS H 201 13.531 4.795 28.781 1.00 20.00 B c
ATOM 4691 CE LYS H 201 12.030 5.042 28.737 1.00 20.00 B c
ATOM 4692 NZ LYS H 201 11.346 4.192 27.722 1.00 20.00 B N
ATOM 4693 C LYS H 201 17.985 6.366 30.373 1.00 43.56 B c
ATOM 4694 O LYS H 201 18.348 5.447 31.105 1.00 51.34 B o
ATOM 4695 N GLN H 202 18.832 7.074 29.633 1.00 46.06 B N
ATOM 4696 CA GLN H 202 20.216 6.648 29.445 1.00 44.95 B c
ATOM 4697 CB GLN H 202 20.507 6.398 27.963 1.00 20.00 B c
ATOM 4698 CG GLN H 202 19.685 5.270 27.351 1.00 20.00 B c
ATOM 4699 CD GLN H 202 19.894 5.134 25.853 1.00 20.00 B c
ATOM 4700 OE1 GLN H 202 20.323 6.075 25.184 1.00 20.00 B o
ATOM 4701 NE2 GLN H 202 19.513 3.984 25.309 1.00 20.00 B N
ATOM 4702 C GLN H 202 21.245 7.616 30.044 1.00 42.35 B c
ATOM 4703 O GLN H 202 22.376 7.224 30.335 1.00 47.00 B o
ATOM 4704 N LEU H 203 20.852 8.874 30.228 1.00 49.55 B N
ATOM 4705 CA LEU H 203 21.762 9.902 30.735 1.00 50.77 B c
ATOM 4706 CB LEU H 203 21.119 11.283 30.618 1.00 20.00 B c
ATOM 4707 CG LEU H 203 20.836 11.775 29.202 1.00 20.00 B c
ATOM 4708 CD1 LEU H 203 20.093 13.100 29.256 1.00 20.00 B c
ATOM 4709 CD2 LEU H 203 22.134 11.910 28.422 1.00 20.00 B c
ATOM 4710 C LEU H 203 22.148 9.656 32.190 1.00 52.51 B c
ATOM 4711 O LEU H 203 21.273 9.564 33.050 1.00 46.02 B o
ATOM 4712 N LEU H 204 23.439 9.786 32.490 1.00 51.45 B N
ATOM 4713 CA LEU H 204 23.928 9.661 33.865 1.00 58.44 B c
ATOM 4714 CB LEU H 204 25.423 9.333 33.885 1.00 20.00 B c
ATOM 4715 CG LEU H 204 25.848 7.919 33.484 1.00 20.00 B c
ATOM 4716 CD1 LEU H 204 27.346 7.764 33.658 1.00 20.00 B c
ATOM 4717 CD2 LEU H 204 25.112 6.874 34.306 1.00 20.00 B c
ATOM 4718 C LEU H 204 23.661 10.930 34.667 1.00 54.99 B c
ATOM 4719 O LEU H 204 23.740 12.035 34.131 1.00 55.13 B o
ATOM 4720 N PRO H 205 23.414 10.775 35.977 1.00 58.64 B N
ATOM 4721 CA PRO H 205 22.981 11.935 36.734 1.00 52.19 B c

ATOM 4722 CB PRO H 205 22.776 11.363 38.137 1.00 20.00 B C
ATOM 4723 CG PRO H 205 23.735 10.190 38.219 1.00 20.00 B C
ATOM 4724 CD PRO H 205 24.191 9.850 36.818 1.00 20.00 B c
ATOM 4725 C PRO H 205 24.112 12.948 36.754 1.00 54.30 B c
ATOM 4726 O PRO H 205 23.898 14.128 37.030 1.00 70.22 B o
ATOM 4727 N ILE H 206 25.316 12.460 36.481 1.00 62.70 B N
ATOM 4728 CA ILE H 206 26.487 13.308 36.354 1.00 68.19 B c
ATOM 4729 CB ILE H 206 27.225 13.445 37.696 1.00 20.00 B c
ATOM 4730 CGI ILE H 206 26.350 14.186 38.709 1.00 20.00 B c
ATOM 4731 CD1 ILE H 206 26.843 14.078 40.136 1.00 20.00 B c
ATOM 4732 CG2 ILE H 206 28.553 14.161 37.505 1.00 20.00 B c
ATOM 4733 C ILE H 206 27.439 12.723 35.321 1.00 62.35 B c
ATOM 4734 O ILE H 206 27.594 11.505 35.221 1.00 67.16 B o
ATOM 4735 N VAL H 207 28.023 13.596 34.510 1.00 52.22 B N
ATOM 4736 CA VAL H 207 28.952 13.168 33.480 1.00 51.31 B c
ATOM 4737 CB VAL H 207 28.568 13.742 32.111 1.00 20.00 B c
ATOM 4738 CGI VAL H 207 29.545 13.261 31.047 1.00 20.00 B C
ATOM 4739 CG2 VAL H 207 27.136 13.356 31.758 1.00 20.00 B C
ATOM 4740 C VAL H 207 30.378 13.582 33.821 1.00 62.09 B c
ATOM 4741 O VAL H 207 30.751 14.746 33.673 1.00 58.88 B o
ATOM 4742 N ASN H 208 31.140 12.641 34.367 1.00 71.72 B N
ATOM 4743 CA ASN H 208 32.533 12.886 34.707 1.00 70.92 B c
ATOM 4744 CB ASN H 208 32.855 12.307 36.086 1.00 20.00 B c
ATOM 4745 CG ASN H 208 32.187 13.074 37.209 1.00 20.00 B c
ATOM 4746 OD1 ASN H 208 31.862 14.252 37.065 1.00 20.00 B O
ATOM 4747 ND2 ASN H 208 31.993 12.411 38.344 1.00 20.00 B N
ATOM 4748 C ASN H 208 33.484 12.312 33.665 1.00 63.05 B c
ATOM 4749 O ASN H 208 33.051 11.778 32.645 1.00 61.34 B o
ATOM 4750 N LYS H 209 34.776 12.337 33.979 1.00 68.91 B N
ATOM 4751 CA LYS H 209 35.811 11.927 33.037 1.00 59.11 B c
ATOM 4752 CB LYS H 209 37.190 12.378 33.528 1.00 20.00 B c
ATOM 4753 CG LYS H 209 37.362 13.888 33.639 1.00 20.00 B c
ATOM 4754 CD LYS H 209 38.689 14.243 34.302 1.00 20.00 B c
ATOM 4755 CE LYS H 209 38.914 15.748 34.344 1.00 20.00 B c
ATOM 4756 NZ LYS H 209 40.286 16.091 34.815 1.00 20.00 B N
ATOM 4757 C LYS H 209 35.810 10.415 32.817 1.00 50.69 B c
ATOM 4758 O LYS H 209 36.500 9.910 31.932 1.00 51.01 B o
ATOM 4759 N GLN H 210 35.116 9.691 33.689 1.00 44.68 B N
ATOM 4760 CA GLN H 210 34.957 8.249 33.528 1.00 49.52 B c
ATOM 4761 CB GLN H 210 34.767 7.581 34.890 1.00 20.00 B c
ATOM 4762 CG GLN H 210 35.976 7.671 35.803 1.00 20.00 B c
ATOM 4763 CD GLN H 210 35.727 7.036 37.156 1.00 20.00 B c
ATOM 4764 OE1 GLN H 210 34.591 6.983 37.629 1.00 20.00 B o
ATOM 4765 NE2 GLN H 210 36.792 6.571 37.798 1.00 20.00 B N
ATOM 4766 C GLN H 210 33.765 7.937 32.632 1.00 62.08 B c
ATOM 4767 O GLN H 210 33.906 7.310 31.580 1.00 80.43 B o
ATOM 4768 N SER H 211 32.599 8.424 33.040 1.00 58.92 B N
ATOM 4769 CA SER H 211 31.384 8.297 32.251 1.00 47.88 B c
ATOM 4770 CB SER H 211 30.270 9.156 32.857 1.00 20.00 B c
ATOM 4771 OG SER H 211 30.733 10.462 33.169 1.00 20.00 B o
ATOM 4772 C SER H 211 31.609 8.665 30.783 1.00 57.32 B c
ATOM 4773 O SER H 211 31.138 7.967 29.884 1.00 50.74 B o
ATOM 4774 N CYS H 212 32.412 9.699 30.545 1.00 44.34 B N
ATOM 4775 CA CYS H 212 32.520 10.292 29.213 1.00 57.52 B c
ATOM 4776 CB CYS H 212 33.762 11.204 29.075 1.00 20.00 B c
ATOM 4777 SG CYS H 212 33.808 12.659 30.229 1.00 20.00 B s
ATOM 4778 C CYS H 212 32.395 9.264 28.073 1.00 60.91 B c
ATOM 4779 O CYS H 212 31.468 9.353 27.272 1.00 52.17 B o
ATOM 4780 N SER H 213 33.381 8.374 27.965 1.00 21.55 B N
ATOM 4781 CA SER H 213 33.462 7.484 26.814 1.00 21.67 B c

ATOM 4782 CB SER H 213 34.765 6.678 26.855 1.00 21.81 B C
ATOM 4783 OG SER H 213 35.892 7.530 26.960 1.00 23.00 B O
ATOM 4784 C SER H 213 32.284 6.537 26.686 1.00 21.45 B C
ATOM 4785 O SER H 213 31.711 6.410 25.603 1.00 21.98 B O
ATOM 4786 N ILE H 214 31.895 5.885 27.776 1.00 20.90 B N
ATOM 4787 CA ILE H 214 30.691 5.081 27.699 1.00 20.45 B C
ATOM 4788 CB ILE H 214 30.475 4.234 28.960 1.00 20.53 B C
ATOM 4789 CGI ILE H 214 31.411 3.025 28.946 1.00 20.46 B C
ATOM 4790 CD1 ILE H 214 31.049 1.951 29.952 1.00 21.75 B C
ATOM 4791 CG2 ILE H 214 29.021 3.787 29.052 1.00 20.34 B C
ATOM 4792 C ILE H 214 29.526 6.035 27.523 1.00 20.15 B C
ATOM 4793 O ILE H 214 28.694 5.870 26.631 1.00 19.91 B O
ATOM 4794 N SER H 215 29.528 7.080 28.346 1.00 19.84 B N
ATOM 4795 CA SER H 215 28.475 8.080 28.330 1.00 19.58 B C
ATOM 4796 CB SER H 215 28.663 9.070 29.478 1.00 19.76 B C
ATOM 4797 OG SER H 215 27.637 10.048 29.470 1.00 19.97 B O
ATOM 4798 C SER H 215 28.460 8.825 27.017 1.00 19.34 B C
ATOM 4799 O SER H 215 27.406 9.053 26.446 1.00 19.54 B O
ATOM 4800 N ASN H 216 29.638 9.187 26.527 1.00 18.80 B N
ATOM 4801 CA ASN H 216 29.724 9.885 25.258 1.00 18.36 B C
ATOM 4802 CB ASN H 216 31.156 10.336 24.972 1.00 18.41 B C
ATOM 4803 CG ASN H 216 31.647 11.377 25.959 1.00 19.55 B C
ATOM 4804 OD1 ASN H 216 31.028 12.428 26.133 1.00 20.52 B O
ATOM 4805 ND2 ASN H 216 32.779 11.100 26.597 1.00 20.43 B N
ATOM 4806 C ASN H 216 29.211 9.010 24.129 1.00 17.78 B C
ATOM 4807 O ASN H 216 28.481 9.479 23.255 1.00 17.91 B O
ATOM 4808 N ILE H 217 29.570 7.730 24.150 1.00 17.02 B N
ATOM 4809 CA ILE H 217 29.110 6.845 23.095 1.00 16.60 B C
ATOM 4810 CB ILE H 217 29.718 5.439 23.210 1.00 16.46 B C
ATOM 4811 CGI ILE H 217 31.093 5.403 22.540 1.00 16.26 B C
ATOM 4812 CD1 ILE H 217 31.610 4.001 22.276 1.00 16.44 B C
ATOM 4813 CG2 ILE H 217 28.791 4.408 22.591 1.00 16.70 B C
ATOM 4814 C ILE H 217 27.599 6.750 23.148 1.00 16.73 B C
ATOM 4815 O ILE H 217 26.923 6.809 22.116 1.00 16.80 B O
ATOM 4816 N GLU H 218 27.064 6.639 24.360 1.00 17.02 B N
ATOM 4817 CA GLU H 218 25.631 6.500 24.526 1.00 17.70 B C
ATOM 4818 CB GLU H 218 25.266 6.321 26.000 1.00 18.20 B C
ATOM 4819 CG GLU H 218 25.955 5.155 26.685 1.00 21.31 B C
ATOM 4820 CD GLU H 218 25.270 4.774 27.986 1.00 25.72 B C
ATOM 4821 OE1 GLU H 218 25.558 5.409 29.023 1.00 26.96 B O
ATOM 4822 OE2 GLU H 218 24.447 3.835 27.975 1.00 27.07 B O
ATOM 4823 C GLU H 218 24.951 7.742 23.995 1.00 17.29 B C
ATOM 4824 O GLU H 218 23.942 7.660 23.312 1.00 17.62 B O
ATOM 4825 N THR H 219 25.482 8.931 24.255 1.00 16.62 B N
ATOM 4826 CA THR H 219 24.786 10.141 23.789 1.00 15.95 B C
ATOM 4827 CB THR H 219 25.475 11.413 24.325 1.00 15.95 B C
ATOM 4828 OG1 THR H 219 25.394 11.438 25.756 1.00 15.63 B O
ATOM 4829 CG2 THR H 219 24.814 12.661 23.759 1.00 15.97 B C
ATOM 4830 C THR H 219 24.646 10.261 22.254 1.00 15.64 B C
ATOM 4831 O THR H 219 23.557 10.569 21.720 1.00 15.93 B O
ATOM 4832 N VAL H 220 25.737 9.974 21.550 1.00 14.98 B N
ATOM 4833 CA VAL H 220 25.773 10.074 20.093 1.00 14.51 B C
ATOM 4834 CB VAL H 220 27.177 9.738 19.559 1.00 14.29 B C
ATOM 4835 CGI VAL H 220 27.191 9.771 18.041 1.00 14.24 B C
ATOM 4836 CG2 VAL H 220 28.213 10.693 20.137 1.00 14.10 B C
ATOM 4837 C VAL H 220 24.779 9.088 19.498 1.00 14.64 B C
ATOM 4838 O VAL H 220 24.030 9.390 18.544 1.00 14.79 B O
ATOM 4839 N ILE H 221 24.762 7.904 20.097 1.00 14.43 B N
ATOM 4840 CA ILE H 221 23.860 6.856 19.674 1.00 14.36 B C
ATOM 4841 CB ILE H 221 24.067 5.569 20.487 1.00 14.03 B C

ATOM 4842 CGI ILE H 221 25.394 4.909 20.1 10 1.00 13.72 B C
ATOM 4843 CD1 ILE H 221 25.493 4.526 18.649 1.00 14.17 B C
ATOM 4844 CG2 ILE H 221 22.908 4.61 1 20.267 1.00 13.91 B c
ATOM 4845 C ILE H 221 22.443 7.351 19.869 1.00 14.82 B C
ATOM 4846 O ILE H 221 21.589 7.132 19.023 1.00 14.82 B O
ATOM 4847 N GLU H 222 22. 195 8.039 20.978 1.00 15.51 B N
ATOM 4848 CA GLU H 222 20.857 8.551 2 1.246 1.00 16.52 B c
ATOM 4849 CB GLU H 222 20.733 9.1 13 22.663 1.00 16.80 B c
ATOM 4850 CG GLU H 222 20.725 8.043 23.747 1.00 19.14 B c
ATOM 4851 CD GLU H 222 19.637 8.267 24.780 1.00 22.62 B c
ATOM 4852 OE1 GLU H 222 19.965 8.662 25.919 1.00 24.35 B o
ATOM 4853 OE2 GLU H 222 18.453 8.039 24.454 1.00 23.98 B o
ATOM 4854 C GLU H 222 20.400 9.566 20. 199 1.00 16.65 B c
ATOM 4855 O GLU H 222 19.255 9.541 19.792 1.00 16.95 B o
ATOM 4856 N PHE H 223 21.292 10.444 19.752 1.00 16.70 B N
ATOM 4857 CA PHE H 223 20.971 11.413 18.690 1.00 16.95 B c
ATOM 4858 CB PHE H 223 22.259 12.227 18.509 1.00 16.85 B c
ATOM 4859 CG PHE H 223 22. 154 13.406 17.593 1.00 17.23 B c
ATOM 4860 CD1 PHE H 223 21.522 14.570 17.995 1.00 17.98 B c
ATOM 4861 CE1 PHE H 223 21.467 15.667 17. 155 1.00 18.28 B c
ATOM 4862 CZ PHE H 223 22.071 15.616 15.914 1.00 18. 19 B c
ATOM 4863 CE2 PHE H 223 22.726 14.469 15.516 1.00 18.14 B c
ATOM 4864 CD2 PHE H 223 22.776 13.380 16.357 1.00 17.75 B c
ATOM 4865 C PHE H 223 20.601 10.675 17.371 1.00 17.28 B c
ATOM 4866 O PHE H 223 19.564 10.951 16.650 1.00 17.17 B o
ATOM 4867 N GLN H 224 21.422 9.671 17.091 1.00 17.62 B N
ATOM 4868 CA GLN H 224 21.209 8.880 15.894 1.00 18.16 B c
ATOM 4869 CB GLN H 224 22.390 7.930 15.652 1.00 18.51 B c
ATOM 4870 CG GLN H 224 23.751 8.594 15.888 1.00 20.06 B c
ATOM 4871 CD GLN H 224 24.867 8.009 15.039 1.00 22.03 B c
ATOM 4872 OE1 GLN H 224 24.920 6.800 14.806 1.00 22.15 B o
ATOM 4873 NE2 GLN H 224 25.783 8.864 14.595 1.00 22.1 1 B N
ATOM 4874 C GLN H 224 19.855 8.158 15.956 1.00 18.04 B c
ATOM 4875 O GLN H 224 19. 196 7.981 14.932 1.00 18.17 B o
ATOM 4876 N GLN H 225 19.488 7.701 17. 156 1.00 17.90 B N
ATOM 4877 CA GLN H 225 18.192 7.079 17.492 1.00 17.95 B c
ATOM 4878 CB GLN H 225 18.271 6.408 18.861 1.00 18. 13 B c
ATOM 4879 CG GLN H 225 19.251 5.257 18.893 1.00 19.04 B c
ATOM 4880 CD GLN H 225 18.854 4.196 19.891 1.00 21.22 B c
ATOM 4881 OE1 GLN H 225 17.834 4.321 20.569 1.00 22.55 B o
ATOM 4882 NE2 GLN H 225 19.651 3.142 19.985 1.00 22.48 B N
ATOM 4883 C GLN H 225 16.993 8.032 17.430 1.00 17.84 B c
ATOM 4884 O GLN H 225 15.872 7.657 17.090 1.00 17.71 B o
ATOM 4885 N LYS H 226 18.593 9.729 17.758 1.00 17.95 B N
ATOM 4886 CA LYS H 226 17.704 10.870 17.777 1.00 18.00 B c
ATOM 4887 CB LYS H 226 18.471 12.167 18.045 1.00 18.21 B c
ATOM 4888 CG LYS H 226 19.258 12.240 19.342 1.00 18.50 B c
ATOM 4889 CD LYS H 226 18.743 13.353 20.242 1.00 19.87 B c
ATOM 4890 CE LYS H 226 19.762 13.696 21.316 1.00 21.36 B c
ATOM 4891 NZ LYS H 226 19.374 14.909 22.085 1.00 2 1.83 B N
ATOM 4892 C LYS H 226 17.251 10.914 16.350 1.00 17.84 B c
ATOM 4893 O LYS H 226 16.195 11.458 16.046 1.00 17.94 B o
ATOM 4894 N ASN H 227 18.025 10.304 15.460 1.00 17.70 B N
ATOM 4895 CA ASN H 227 17.467 10.197 14.086 1.00 17.66 B c
ATOM 4896 CB ASN H 227 18.366 9.273 13.270 1.00 17.36 B c
ATOM 4897 CG ASN H 227 19.700 9.884 12.927 1.00 17.40 B c
ATOM 4898 OD1 ASN H 227 20.438 9.337 12.107 1.00 17.84 B o
ATOM 4899 ND2 ASN H 227 20.025 11.01 1 13.545 1.00 17.22 B, N
ATOM 4900 C ASN H 227 16.016 9.596 13.857 1.00 17.76 B c
ATOM 4901 O ASN H 227 15.214 10.239 13. 175 1.00 17.92 B o

ATOM 4902 N ASN H 228 15.655 8.431 14.418 1.00 17.78 B N
ATOM 4903 CA ASN H 228 14.290 7.922 14.435 1.00 17.59 B C
ATOM 4904 CB ASN H 228 14.003 7.185 15.743 1.00 17.89 B C
ATOM 4905 CG ASN H 228 14.845 5.934 15.903 1.00 18.43 B C
ATOM 4906 OD1 ASN H 228 15.432 5.698 16.959 1.00 18.74 B O
ATOM 4907 ND2 ASN H 228 14.908 5.124 14.852 1.00 18.61 B N
ATOM 4908 C ASN H 228 13.335 9.091 14.265 1.00 17.09 B C
ATOM 4909 O ASN H 228 12.380 9.032 13.490 1.00 17.17 B O
ATOM 4910 N ARG H 229 13.267 9.880 15.306 1.00 16.33 B N
ATOM 4911 CA ARG H 229 12.252 10.885 15.298 1.00 15.76 B C
ATOM 4912 CB ARG H 229 11.906 11.215 16.758 1.00 15.70 B C
ATOM 4913 CG ARG H 229 11.667 9.916 17.580 1.00 14.99 B C
ATOM 4914 CD ARG H 229 11.240 10.128 19.039 1.00 15.33 B C
ATOM 4915 NE ARG H 229 12.372 10.516 19.868 1.00 15.59 B N
ATOM 4916 CZ ARG H 229 13.209 9.663 20.448 1.00 15.85 B C
ATOM 4917 NH1 ARG H 229 13.045 8.350 20.313 1.00 16.20 B N
ATOM 4918 NH2 ARG H 229 14.216 10.134 21.168 1.00 16.63 B N
ATOM 4919 C ARG H 229 12.960 11.937 14.490 1.00 15.62 B C
ATOM 4920 O ARG H 229 12.436 12.586 13.561 1.00 15.73 B O
ATOM 4921 N LEU H 230 14.249 11.935 14.783 1.00 15.46 B N
ATOM 4922 CA LEU H 230 15.146 12.972 14.402 1.00 15.22 B C
ATOM 4923 CB LEU H 230 16.334 12.863 15.348 1.00 15.08 B C
ATOM 4924 CG LEU H 230 17.100 14.054 15.896 1.00 14.70 B C
ATOM 4925 CD1 LEU H 230 16.465 14.590 17.171 1.00 15.19 B C
ATOM 4926 CD2 LEU H 230 18.500 13.564 16.165 1.00 15.46 B C
ATOM 4927 C LEU H 230 15.658 12.853 12.989 1.00 15.31 B C
ATOM 4928 O LEU H 230 15.224 13.608 12.133 1.00 15.46 B O
ATOM 4929 N LEU H 231 16.533 11.890 12.727 1.00 15.48 B N
ATOM 4930 CA LEU H 231 17.158 11.825 11.423 1.00 15.75 B C
ATOM 4931 CB LEU H 231 18.215 10.722 11.423 1.00 15.90 B C
ATOM 4932 CG LEU H 231 19.366 10.875 12.416 1.00 16.63 B C
ATOM 4933 CD1 LEU H 231 20.443 9.836 12.133 1.00 18.45 B C
ATOM 4934 CD2 LEU H 231 19.953 12.276 12.366 1.00 16.67 B C
ATOM 4935 C LEU H 231 16.139 11.575 10.324 1.00 15.76 B C
ATOM 4936 O LEU H 231 16.121 12.269 9.309 1.00 15.84 B O
ATOM 4937 N GLU H 232 15.249 10.617 10.561 1.00 15.71 B N
ATOM 4938 CA GLU H 232 14.200 10.308 9.607 1.00 15.93 B C
ATOM 4939 CB GLU H 232 13.470 9.012 10.001 1.00 16.15 B C
ATOM 4940 CG GLU H 232 14.389 7.801 10.158 1.00 18.59 B C
ATOM 4941 CD GLU H 232 14.567 6.988 8.876 1.00 21.47 B C
ATOM 4942 OE1 GLU H 232 13.976 7.355 7.839 1.00 22.14 B O
ATOM 4943 OE2 GLU H 232 15.298 5.973 8.907 1.00 23.34 B O
ATOM 4944 C GLU H 232 13.241 11.482 9.456 1.00 15.45 B C
ATOM 4945 O GLU H 232 12.881 11.860 8.328 1.00 15.95 B O
ATOM 4946 N ILE H 233 12.855 12.113 10.564 1.00 14.54 B N
ATOM 4947 CA ILE H 233 11.941 13.221 10.375 1.00 13.69 B C
ATOM 4948 CB ILE H 233 11.444 13.775 11.699 1.00 13.63 B C
ATOM 4949 CGI ILE H 233 10.497 12.763 12.326 1.00 13.58 B C
ATOM 4950 CD1 ILE H 233 9.817 13.280 13.532 1.00 13.55 B C
ATOM 4951 CG2 ILE H 233 10.682 15.070 11.490 1.00 13.88 B C
ATOM 4952 C ILE H 233 12.605 14.309 9.526 1.00 13.28 B C
ATOM 4953 O ILE H 233 11.972 14.914 8.653 1.00 13.04 B O
ATOM 4954 N THR H 234 13.888 14.544 9.773 1.00 13.18 B N
ATOM 4955 CA THR H 234 14.620 15.575 9.063 1.00 13.39 B C
ATOM 4956 CB THR H 234 16.082 15.655 9.574 1.00 13.21 B C
ATOM 4957 OG1 THR H 234 16.099 15.927 10.978 1.00 13.15 B O
ATOM 4958 CG2 THR H 234 16.870 16.740 8.846 1.00 13.22 B C
ATOM 4959 C THR H 234 14.686 15.273 7.577 1.00 13.76 B C
ATOM 4960 O THR H 234 14.434 16.152 6.738 1.00 13.95 B O
ATOM 4961 N ARG H 235 14.994 14.024 7.240 1.00 14.26 B N

```
ATOM   4962  CA  ARG H 235      15.119  13.686   5.831  1.00 14.92      B    C
ATOM   4963  CB  ARG H 235      15.574  12.242   5.661  1.00 15.30      B    C
ATOM   4964  CG  ARG H 235      14.532  11.325   5.054  1.00 16.27      B    C
ATOM   4965  CD  ARG H 235      14.829   9.882   5.408  1.00 18.52      B    C
ATOM   4966  NE  ARG H 235      16.234   9.676   5.746  1.00 17.86      B    N
ATOM   4967  CZ  ARG H 235      17.190   9.425   4.858  1.00 16.91      B    C
ATOM   4968  NHl ARG H 235      16.898   9.354   3.566  1.00 16.59      B    N
ATOM   4969  NH2 ARG H 235      18.438   9.249   5.267  1.00 16.86      B    N
ATOM   4970  C   ARG H 235      13.766  13.887   5.176  1.00 15.05      B    C
ATOM   4971  O   ARG H 235      13.663  14.432   4.073  1.00 15.15      B    O
ATOM   4972  N   GLU H 236      12.727  13.474   5.894  1.00 15.18      B    N
ATOM   4973  CA  GLU H 236      11.375  13.527   5.376  1.00 15.24      B    C
ATOM   4974  CB  GLU H 236      10.415  12.920   6.403  1.00 15.69      B    C
ATOM   4975  CG  GLU H 236       9.176  12.265   5.822  1.00 18.22      B    C
ATOM   4976  CD  GLU H 236       8.355  11.543   6.875  1.00 21.59      B    C
ATOM   4977  OE1 GLU H 236       7.200  11.178   6.581  1.00 24.41      B    O
ATOM   4978  OE2 GLU H 236       8.857  11.345   8.000  1.00 21.59      B    O
ATOM   4979  C   GLU H 236      10.987  14.971   5.073  1.00 14.61      B    C
ATOM   4980  O   GLU H 236      10.396  15.253   4.031  1.00 14.82      B    O
ATOM   4981  N   PHE H 237      11.333  15.877   5.985  1.00 14.05      B    N
ATOM   4982  CA  PHE H 237      11.053  17.296   5.809  1.00 13.84      B    C
ATOM   4983  CB  PHE H 237      11.316  18.065   7.105  1.00 14.04      B    C
ATOM   4984  CG  PHE H 237      10.142  18.087   8.038  1.00 14.84      B    C
ATOM   4985  CD1 PHE H 237      10.224  17.516   9.297  1.00 15.30      B    C
ATOM   4986  CE1 PHE H 237       9.142  17.542  10.153  1.00 15.15      B    C
ATOM   4987  CZ  PHE H 237       7.961  18.135   9.755  1.00 15.19      B    C
ATOM   4988  CE2 PHE H 237       7.864  18.704   8.502  1.00 15.02      B    C
ATOM   4989  CD2 PHE H 237       8.949  18.677   7.651  1.00 15.03      B    C
ATOM   4990  C   PHE H 237      11.830  17.909   4.654  1.00 13.51      B    C
ATOM   4991  O   PHE H 237      11.293  18.687   3.866  1.00 13.43      B    O
ATOM   4992  N   SER H 238      13.100  17.534   4.554  1.00 13.11      B    N
ATOM   4993  CA  SER H 238      13.972  18.065   3.516  1.00 12.82      B    C
ATOM   4994  CB  SER H 238      15.404  17.546   3.691  1.00 12.86      B    C
ATOM   4995  OG  SER H 238      15.976  17.981   4.916  1.00 12.76      B    O
ATOM   4996  C   SER H 238      13.411  17.654   2.164  1.00 12.69      B    C
ATOM   4997  O   SER H 238      13.437  18.425   1.202  1.00 12.63      B    O
ATOM   4998  N   VAL H 239      12.910  16.426   2.107  1.00 12.59      B    N
ATOM   4999  CA  VAL H 239      12.361  15.865   0.883  1.00 12.80      B    C
ATOM   5000  CB  VAL H 239      12.065  14.358   1.041  1.00 12.71      B    C
ATOM   5001  CGI VAL H 239      11.359  13.819  -0.193  1.00 13.63      B    C
ATOM   5002  CG2 VAL H 239      13.349  13.588   1.316  1.00 13.57      B    C
ATOM   5003  C   VAL H 239      11.094  16.596   0.443  1.00 12.94      B    C
ATOM   5004  O   VAL H 239      10.722  16.546  -0.728  1.00 13.10      B    O
ATOM   5005  N   ASN H 240      10.430  17.274   1.372  1.00  4.15      B    N
ATOM   5006  CA  ASN H 240       9.074  17.741   1.109  1.00  4.33      B    C
ATOM   5007  CB  ASN H 240       8.110  17.268   2.199  1.00  4.59      B    C
ATOM   5008  CG  ASN H 240       7.810  15.784   2.106  1.00  5.36      B    C
ATOM   5009  OD1 ASN H 240       7.128  15.331   1.188  1.00  6.27      B    O
ATOM   5010  ND2 ASN H 240       8.343  15.016   3.047  1.00  7.15      B    N
ATOM   5011  C   ASN H 240       8.924  19.242   0.853  1.00  4.19      B    C
ATOM   5012  O   ASN H 240       7.843  19.707   0.490  1.00  4.19      B    O
ATOM   5013  N   ALA H 241      10.014  19.990   0.995  1.00  3.93      B    N
ATOM   5014  CA  ALA H 241       9.948  21.447   0.930  1.00  3.90      B    C
ATOM   5015  CB  ALA H 241       9.784  21.908  -0.511  1.00  3.86      B    C
ATOM   5016  C   ALA H 241       8.812  21.985   1.798  1.00  4.22      B    C
ATOM   5017  O   ALA H 241       7.932  22.697   1.314  1.00  4.47      B    O
ATOM   5018  N   GLY H 242       8.772  21.540   3.049  1.00  4.53      B    N
ATOM   5019  CA  GLY H 242       8.055  22.258   4.097  1.00  4.65      B    C
ATOM   5020  C   GLY H 242       6.563  21.980   4.122  1.00  4.67      B    C
ATOM   5021  O   GLY H 242       5.792  22.759   4.683  1.00  5.27      B    O
```

```
ATOM   5022  N   VAL H 243      6.159  20.841   3.570  1.00  4.37      B    N
ATOM   5023  CA  VAL H 243      4.755  20.449   3.577  1.00  4.32      B    C
ATOM   5024  CB  VAL H 243      3.961  21.182   2.477  1.00  3.99      B    C
ATOM   5025  CGI VAL H 243      2.519  21.398   2.915  1.00  4.22      B    c
ATOM   5026  CG2 VAL H 243      4.629  22.508   2.131  1.00  3.85      B    c
ATOM   5027  C   VAL H 243      4.595  18.943   3.393  1.00  4.61      B    c
ATOM   5028  O   VAL H 243      5.201  18.350   2.501  1.00  4.89      B    o
ATOM   5029  N   THR H 244      3.764  18.333   4.231  1.00  4.95      B    N
ATOM   5030  CA  THR H 244      3.600  16.886   4.220  1.00  5.71      B    c
ATOM   5031  CB  THR H 244      4.318  16.226   5.410  1.00  6.11      B    c
ATOM   5032  OG1 THR H 244      5.051  17.217   6.140  1.00  7.17      B    o
ATOM   5033  CG2 THR H 244      5.273  15.147   4.925  1.00  7.55      B    c
ATOM   5034  C   THR H 244      2.129  16.505   4.268  1.00  5.61      B    c
ATOM   5035  O   THR H 244      1.359  17.073   5.042  1.00  5.85      B    o
ATOM   5036  N   THR H 245      1.786  15.428   3.575  1.00  5.53      B    N
ATOM   5037  CA  THR H 245      0.617  14.647   3.939  1.00  5.81      B    c
ATOM   5038  CB  THR H 245     -0.404  14.592   2.788  1.00  6.13      B    c
ATOM   5039  OG1 THR H 245     -0.888  15.915   2.517  1.00  8.11      B    o
ATOM   5040  CG2 THR H 245     -1.577  13.695   3.154  1.00  6.63      B    c
ATOM   5041  C   THR H 245      1.032  13.245   4.370  1.00  5.73      B    c
ATOM   5042  O   THR H 245      2.189  12.861   4.202  1.00  5.86      B    o
ATOM   5043  N   PRO H 246      0.060  12.433   4.804  1.00  5.68      B    N
ATOM   5044  CA  PRO H 246      0.078  11.993   6.186  1.00  5.11      B    c
ATOM   5045  CB  PRO H 246      0.753  10.626   6.084  1.00  5.19      B    c
ATOM   5046  CG  PRO H 246      0.360  10.124   4.675  1.00  5.90      B    c
ATOM   5047  CD  PRO H 246     -0.256  11.297   3.926  1.00  6.36      B    c
ATOM   5048  C   PRO H 246      0.830  12.916   7.140  1.00  4.85      B    c
ATOM   5049  O   PRO H 246      1.927  13.379   6.825  1.00  5.25      B    o
ATOM   5050  N   VAL H 247      0.144  13.323   8.205  1.00  4.35      B    N
ATOM   5051  CA  VAL H 247      0.792  13.950   9.347  1.00  3.82      B    c
ATOM   5052  CB  VAL H 247     -0.198  14.817  10.157  1.00  3.52      B    c
ATOM   5053  CGI VAL H 247      0.558  15.754  11.087  1.00  3.62      B    c
ATOM   5054  CG2 VAL H 247     -1.091  15.615   9.217  1.00  3.60      B    c
ATOM   5055  C   VAL H 247      1.447  12.899  10.242  1.00  3.69      B    c
ATOM   5056  O   VAL H 247      0.761  12.124  10.913  1.00  3.36      B    o
ATOM   5057  N   SER H 248      2.748  12.721  10.040  1.00  3.72      B    N
ATOM   5058  CA  SER H 248      3.496  11.654  10.686  1.00  3.96      B    c
ATOM   5059  CB  SER H 248      4.995  11.840  10.451  1.00  4.07      B    c
ATOM   5060  OG  SER H 248      5.525  12.834  11.310  1.00  4.13      B    o
ATOM   5061  C   SER H 248      3.211  11.615  12.180  1.00  4.35      B    c
ATOM   5062  O   SER H 248      2.890  12.635  12.788  1.00  4.36      B    o
ATOM   5063  N   THR H 249      3.458  10.460  12.784  1.00  4.53      B    N
ATOM   5064  CA  THR H 249      3.489  10.350  14.231  1.00  4.61      B    c
ATOM   5065  CB  THR H 249      3.682   8.893  14.677  1.00  4.70      B    c
ATOM   5066  OG1 THR H 249      5.018   8.473  14.374  1.00  5.42      B    o
ATOM   5067  CG2 THR H 249      2.695   7.984  13.961  1.00  4.88      B    c
ATOM   5068  C   THR H 249      4.589  11.215  14.839  1.00  4.47      B    c
ATOM   5069  O   THR H 249      4.570  11.491  16.039  1.00  4.74      B    o
ATOM   5070  N   TYR H 250      5.518  11.684  14.009  1.00  4.32      B    N
ATOM   5071  CA  TYR H 250      6.544  12.619  14.475  1.00  4.42      B    c
ATOM   5072  CB  TYR H 250      7.811  12.531  13.625  1.00  4.91      B    c
ATOM   5073  CG  TYR H 250      8.409  11.148  13.525  1.00  6.81      B    c
ATOM   5074  CD1 TYR H 250      8.844  10.657  12.302  1.00  8.89      B    c
ATOM   5075  CE1 TYR H 250      9.480   9.437  12.205  1.00 10.73      B    c
ATOM   5076  CZ  TYR H 250      9.685   8.685  13.341  1.00 12.28      B    c
ATOM   5077  OH  TYR H 250     10.305   7.460  13.251  1.00 12.24      B    o
ATOM   5078  CE2 TYR H 250      9.284   9.161  14.571  1.00 12.15      B    c
ATOM   5079  CD2 TYR H 250      8.689  10.405  14.662  1.00  9.81      B    c
ATOM   5080  C   TYR H 250      6.053  14.064  14.516  1.00  4.21      B    c
ATOM   5081  O   TYR H 250      6.596  14.883  15.259  1.00  4.20      B    o
```

```
ATOM   5082  N   MET H 251      5.148  14.413  13.605  1.00  4.14      B    N
ATOM   5083  CA  MET H 251      4.517  15.732  13.632  1.00  4.15      B    C
ATOM   5084  CB  MET H 251      3.798  16.014  12.313  1.00  4.14      B    C
ATOM   5085  CG  MET H 251      4.720  16.097  11.115  1.00  4.51      B    c
ATOM   5086  SD  MET H 251      5.733  17.587  11.115  1.00  3.81      B    s
ATOM   5087  CE  MET H 251      5.601  18.077   9.395  1.00  4.55      B    c
ATOM   5088  C   MET H 251      3.519  15.806  14.775  1.00  4.13      B    c
ATOM   5089  O   MET H 251      3.510  16.759  15.555  1.00  4.24      B    o
ATOM   5090  N   LEU H 252      2.692  14.773  14.874  1.00  4.23      B    N
ATOM   5091  CA  LEU H 252      1.708  14.681  15.934  1.00  4.22      B    c
ATOM   5092  CB  LEU H 252      0.302  14.881  15.369  1.00  4.14      B    c
ATOM   5093  CG  LEU H 252     -0.295  16.282  15.515  1.00  4.05      B    c
ATOM   5094  CD1 LEU H 252     -1.813  16.216  15.561  1.00  5.22      B    c
ATOM   5095  CD2 LEU H 252      0.245  16.972  16.756  1.00  6.20      B    c
ATOM   5096  C   LEU H 252      1.818  13.314  16.589  1.00  4.62      B    c
ATOM   5097  O   LEU H 252      1.906  12.295  15.903  1.00  4.97      B    o
ATOM   5098  N   THR H 253      1.986  13.314  17.906  1.00  4.90      B    N
ATOM   5099  CA  THR H 253      1.718  12.126  18.704  1.00  5.57      B    c
ATOM   5100  CB  THR H 253      2.147  12.323  20.168  1.00  5.55      B    c
ATOM   5101  OG1 THR H 253      3.369  13.068  20.214  1.00  6.43      B    o
ATOM   5102  CG2 THR H 253      2.362  10.978  20.842  1.00  6.28      B    c
ATOM   5103  C   THR H 253      0.235  11.775  18.673  1.00  6.03      B    c
ATOM   5104  O   THR H 253     -0.621  12.663  18.679  1.00  6.68      B    o
ATOM   5105  N   ASN H 254     -0.066  10.483  18.746  1.00  6.39      B    N
ATOM   5106  CA  ASN H 254     -1.396  10.040  19.141  1.00  6.79      B    c
ATOM   5107  CB  ASN H 254     -1.375   8.564  19.534  1.00  6.85      B    c
ATOM   5108  CG  ASN H 254     -2.758   7.954  19.571  1.00  6.81      B    c
ATOM   5109  OD1 ASN H 254     -3.395   7.771  18.534  1.00  7.67      B    o
ATOM   5110  ND2 ASN H 254     -3.252   7.682  20.773  1.00  6.19      B    N
ATOM   5111  C   ASN H 254     -1.956  10.882  20.284  1.00  7.08      B    c
ATOM   5112  O   ASN H 254     -2.968  11.565  20.125  1.00  6.90      B    o
ATOM   5113  N   SER H 255     -1.282  10.843  21.430  1.00  7.21      B    N
ATOM   5114  CA  SER H 255     -1.689  11.633  22.588  1.00  7.37      B    c
ATOM   5115  CB  SER H 255     -0.561  11.714  23.619  1.00  8.09      B    c
ATOM   5116  OG  SER H 255      0.228  10.539  23.617  1.00 10.47      B    o
ATOM   5117  C   SER H 255     -2.102  13.036  22.163  1.00  6.82      B    c
ATOM   5118  O   SER H 255     -3.192  13.499  22.496  1.00  6.99      B    o
ATOM   5119  N   GLU H 256     -1.229  13.704  21.415  1.00  6.17      B    N
ATOM   5120  CA  GLU H 256     -1.485  15.072  20.981  1.00  6.13      B    c
ATOM   5121  CB  GLU H 256     -0.274  15.644  20.243  1.00  6.22      B    c
ATOM   5122  CG  GLU H 256      0.847  16.110  21.152  1.00  8.41      B    c
ATOM   5123  CD  GLU H 256      2.209  15.761  20.596  1.00 10.26      B    c
ATOM   5124  OE1 GLU H 256      2.292  15.472  19.384  1.00 11.90      B    o
ATOM   5125  OE2 GLU H 256      3.162  15.626  21.392  1.00  9.55      B    o
ATOM   5126  C   GLU H 256     -2.706  15.126  20.079  1.00  5.76      B    c
ATOM   5127  O   GLU H 256     -3.684  15.810  20.380  1.00  5.93      B    o
ATOM   5128  N   LEU H 257     -2.633  14.420  18.956  1.00  5.67      B    N
ATOM   5129  CA  LEU H 257     -3.729  14.411  18.002  1.00  5.37      B    c
ATOM   5130  CB  LEU H 257     -3.543  13.299  16.970  1.00  5.03      B    c
ATOM   5131  CG  LEU H 257     -4.781  13.003  16.121  1.00  3.65      B    c
ATOM   5132  CD1 LEU H 257     -5.114  14.184  15.222  1.00  2.00      B    c
ATOM   5133  CD2 LEU H 257     -4.592  11.737  15.305  1.00  2.14      B    c
ATOM   5134  C   LEU H 257     -5.050  14.223  18.732  1.00  5.64      B    c
ATOM   5135  O   LEU H 257     -6.020  14.934  18.475  1.00  5.81      B    o
ATOM   5136  N   LEU H 258     -5.061  13.300  19.687  1.00  5.75      B    N
ATOM   5137  CA  LEU H 258     -6.297  12.905  20.344  1.00  5.91      B    c
ATOM   5138  CB  LEU H 258     -6.063  11.693  21.242  1.00  6.10      B    c
ATOM   5139  CG  LEU H 258     -6.438  10.358  20.605  1.00  5.75      B    c
ATOM   5140  CD1 LEU H 258     -5.970   9.206  21.477  1.00  6.33      B    c
ATOM   5141  CD2 LEU H 258     -7.939  10.287  20.372  1.00  7.33      B    c
```

ATOM 5142 C LEU H 258 -6.908 14.049 21.142 1.00 6.03 B C
ATOM 5143 O LEU H 258 -8.113 14.290 21.071 1.00 5.73 B O
ATOM 5144 N SER H 259 -6.076 14.745 21.910 1.00 6.47 B N
ATOM 5145 CA SER H 259 -6.537 15.883 22.695 1.00 6.95 B C
ATOM 5146 CB SER H 259 -5.521 16.237 23.784 1.00 7.05 B C
ATOM 5147 OG SER H 259 -4.695 17.317 23.383 1.00 6.86 B O
ATOM 5148 C SER H 259 -6.782 17.086 21.795 1.00 6.74 B C
ATOM 5149 O SER H 259 -7.592 17.959 22.110 1.00 6.86 B O
ATOM 5150 N LEU H 260 -6.074 17.125 20.670 1.00 6.31 B N
ATOM 5151 CA LEU H 260 -6.295 18.149 19.657 1.00 6.09 B C
ATOM 5152 CB LEU H 260 -5.239 18.052 18.552 1.00 6.09 B C
ATOM 5153 CG LEU H 260 -4.235 19.203 18.446 1.00 6.24 B C
ATOM 5154 CD1 LEU H 260 -3.350 19.030 17.222 1.00 6.53 B C
ATOM 5155 CD2 LEU H 260 -4.944 20.549 18.407 1.00 5.98 B C
ATOM 5156 C LEU H 260 -7.692 18.026 19.056 1.00 6.25 B C
ATOM 5157 O LEU H 260 -8.428 19.010 18.963 1.00 6.37 B O
ATOM 5158 N ILE H 261 -8.024 16.825 18.596 1.00 6.63 B N
ATOM 5159 CA ILE H 261 -9.395 16.490 18.245 1.00 7.19 B C
ATOM 5160 CB ILE H 261 -9.568 14.975 18.078 1.00 7.09 B C
ATOM 5161 CGI ILE H 261 -9.037 14.528 16.715 1.00 7.46 B C
ATOM 5162 CD1 ILE H 261 -8.132 13.315 16.782 1.00 8.38 B C
ATOM 5163 CG2 ILE H 261 -11.024 14.579 18.262 1.00 6.61 B C
ATOM 5164 C ILE H 261 -10.352 16.980 19.322 1.00 8.01 B C
ATOM 5165 O ILE H 261 -11.255 17.770 19.051 1.00 8.26 B O
ATOM 5166 N ASN H 262 -10.081 16.586 20.560 1.00 9.05 B N
ATOM 5167 CA ASN H 262 -10.896 17.006 21.689 1.00 9.88 B C
ATOM 5168 CB ASN H 262 -10.175 16.714 23.001 1.00 9.99 B C
ATOM 5169 CG ASN H 262 -11.127 16.353 24.111 1.00 11.16 B C
ATOM 5170 OD1 ASN H 262 -12.345 16.408 23.936 1.00 12.70 B O
ATOM 5171 ND2 ASN H 262 -10.583 15.980 25.264 1.00 13.20 B N
ATOM 5172 C ASN H 262 -11.258 18.482 21.619 1.00 10.17 B C
ATOM 5173 O ASN H 262 -12.347 18.887 22.027 1.00 10.52 B O
ATOM 5174 N ASP H 263 -10.310 19.289 21.158 1.00 10.62 B N
ATOM 5175 CA ASP H 263 -10.437 20.734 21.247 1.00 11.02 B C
ATOM 5176 CB ASP H 263 -9.057 21.395 21.285 1.00 11.49 B C
ATOM 5177 CG ASP H 263 -9.138 22.905 21.401 1.00 12.80 B C
ATOM 5178 OD1 ASP H 263 -9.972 23.401 22.188 1.00 14.72 B O
ATOM 5179 OD2 ASP H 263 -8.354 23.596 20.717 1.00 13.88 B O
ATOM 5180 C ASP H 263 -11.261 21.293 20.091 1.00 10.92 B C
ATOM 5181 O ASP H 263 -11.686 22.446 20.130 1.00 10.96 B O
ATOM 5182 N MET H 264 -11.539 20.453 19.097 1.00 10.91 B N
ATOM 5183 CA MET H 264 -12.199 20.904 17.871 1.00 10.78 B C
ATOM 5184 CB MET H 264 -12.091 19.840 16.770 1.00 10.51 B C
ATOM 5185 CG MET H 264 -10.664 19.427 16.425 1.00 11.26 B C
ATOM 5186 SD MET H 264 -10.510 18.571 14.840 1.00 12.70 B S
ATOM 5187 CE MET H 264 -11.715 17.260 15.021 1.00 13.92 B C
ATOM 5188 C MET H 264 -13.666 21.240 18.119 1.00 10.85 B C
ATOM 5189 O MET H 264 -14.369 20.489 18.795 1.00 11.03 B O
ATOM 5190 N PRO H 265 -14.146 22.342 17.517 1.00 10.88 B N
ATOM 5191 CA PRO H 265 -15.522 22.802 17.700 1.00 11.09 B C
ATOM 5192 CB PRO H 265 -15.515 24.198 17.060 1.00 11.28 B C
ATOM 5193 CG PRO H 265 -14.322 24.216 16.167 1.00 11.24 B C
ATOM 5194 CD PRO H 265 -13.313 23.356 16.849 1.00 11.03 B C
ATOM 5195 C PRO H 265 -16.546 21.912 17.003 1.00 11.19 B C
ATOM 5196 O PRO H 265 -17.320 22.395 16.177 1.00 11.47 B O
ATOM 5197 N ILE H 266 -16.633 20.655 17.425 1.00 11.54 B N
ATOM 5198 CA ILE H 266 -17.540 19.710 16.786 1.00 12.15 B C
ATOM 5199 CB ILE H 266 -16.794 18.757 15.828 1.00 12.22 B C
ATOM 5200 CGI ILE H 266 -15.611 18.088 16.536 1.00 12.53 B C
ATOM 5201 CD1 ILE H 266 -15.044 16.895 15.789 1.00 12.40 B C

ATOM 5202 CG2 ILE H 266 -16.337 19.507 14.588 1.00 12.74 B C
ATOM 5203 C ILE H 266 -18.353 18.902 17.793 1.00 12.29 B C
ATOM 5204 O ILE H 266 -18.068 18.913 18.991 1.00 12.36 B O
ATOM 5205 N THR H 267 -19.404 18.252 17.303 1.00 12.29 B N
ATOM 5206 CA THR H 267 -20.248 17.414 18.148 1.00 12.43 B C
ATOM 5207 CB THR H 267 -21.440 16.821 17.366 1.00 12.40 B C
ATOM 5208 OG1 THR H 267 -21.299 15.397 17.278 1.00 13.21 B O
ATOM 5209 CG2 THR H 267 -21.509 17.405 15.968 1.00 12.21 B C
ATOM 5210 C THR H 267 -19.432 16.276 18.740 1.00 12.37 B C
ATOM 5211 O THR H 267 -18.246 16.134 18.446 1.00 12.29 B O
ATOM 5212 N ASN H 268 -20.058 15.490 19.605 1.00 12.47 B N
ATOM 5213 CA ASN H 268 -19.325 14.501 20.377 1.00 12.57 B C
ATOM 5214 CB ASN H 268 -20.025 14.218 21.701 1.00 12.69 B C
ATOM 5215 CG ASN H 268 -19.461 15.041 22.832 1.00 13.65 B C
ATOM 5216 OD1 ASN H 268 -18.555 15.851 22.631 1.00 14.37 B O
ATOM 5217 ND2 ASN H 268 -20.005 14.856 24.028 1.00 15.74 B N
ATOM 5218 C ASN H 268 -19.084 13.207 19.621 1.00 12.43 B C
ATOM 5219 O ASN H 268 -18.038 12.576 19.776 1.00 12.51 B O
ATOM 5220 N ASP H 269 -20.107 12.747 18.912 1.00 12.34 B N
ATOM 5221 CA ASP H 269 -19.976 11.565 18.077 1.00 12.33 B C
ATOM 5222 CB ASP H 269 -21.316 11.222 17.431 1.00 12.89 B C
ATOM 5223 CG ASP H 269 -22.404 10.959 18.456 1.00 14.84 B C
ATOM 5224 OD1 ASP H 269 -22.145 10.209 19.422 1.00 16.90 B O
ATOM 5225 OD2 ASP H 269 -23.487 11.573 18.346 1.00 17.65 B O
ATOM 5226 C ASP H 269 -18.916 11.780 17.008 1.00 11.60 B C
ATOM 5227 O ASP H 269 -18.073 10.914 16.774 1.00 11.65 B O
ATOM 5228 N GLN H 270 -18.924 12.963 16.405 1.00 10.62 B N
ATOM 5229 CA GLN H 270 -17.836 13.371 15.530 1.00 10.01 B C
ATOM 5230 CB GLN H 270 -17.958 14.851 15.179 1.00 10.18 B C
ATOM 5231 CG GLN H 270 -17.709 15.154 13.718 1.00 11.49 B C
ATOM 5232 CD GLN H 270 -18.572 16.286 13.213 1.00 14.38 B C
ATOM 5233 OE1 GLN H 270 -18.076 17.238 12.613 1.00 16.38 B O
ATOM 5234 NE2 GLN H 270 -19.866 16.215 13.496 1.00 15.41 B N
ATOM 5235 C GLN H 270 -16.486 13.097 16.181 1.00 9.48 B C
ATOM 5236 O GLN H 270 -15.696 12.296 15.682 1.00 9.12 B O
ATOM 5237 N LYS H 271 -16.229 13.763 17.301 1.00 9.19 B N
ATOM 5238 CA LYS H 271 -15.004 13.541 18.056 1.00 8.89 B C
ATOM 5239 CB LYS H 271 -15.117 14.168 19.448 1.00 8.52 B C
ATOM 5240 CG LYS H 271 -15.410 15.663 19.445 1.00 9.14 B C
ATOM 5241 CD LYS H 271 -14.906 16.316 20.726 1.00 10.72 B C
ATOM 5242 CE LYS H 271 -15.469 17.718 20.900 1.00 10.79 B C
ATOM 5243 NZ LYS H 271 -14.711 18.506 21.916 1.00 9.77 B N
ATOM 5244 C LYS H 271 -14.699 12.049 18.175 1.00 8.83 B C
ATOM 5245 O LYS H 271 -13.660 11.577 17.713 1.00 9.05 B O
ATOM 5246 N LYS H 272 -15.653 11.301 18.719 1.00 8.65 B N
ATOM 5247 CA LYS H 272 -15.485 9.868 18.899 1.00 8.50 B C
ATOM 5248 CB LYS H 272 -16.766 9.240 19.443 1.00 9.14 B C
ATOM 5249 CG LYS H 272 -16.762 7.726 19.397 1.00 11.58 B C
ATOM 5250 CD LYS H 272 -18.170 7.167 19.394 1.00 15.78 B C
ATOM 5251 CE LYS H 272 -18.151 5.663 19.599 1.00 17.65 B C
ATOM 5252 NZ LYS H 272 -19.476 5.142 20.029 1.00 19.68 B N
ATOM 5253 C LYS H 272 -15.083 9.185 17.598 1.00 7.88 B C
ATOM 5254 O LYS H 272 -14.195 8.332 17.587 1.00 8.12 B O
ATOM 5255 N LEU H 273 -15.787 9.506 16.517 1.00 6.95 B N
ATOM 5256 CA LEU H 273 -15.456 8.939 15.216 1.00 5.70 B C
ATOM 5257 CB LEU H 273 -16.366 9.490 14.116 1.00 5.85 B C
ATOM 5258 CG LEU H 273 -15.894 9.204 12.683 1.00 4.65 B C
ATOM 5259 CD1 LEU H 273 -16.085 7.739 12.312 1.00 4.57 B C
ATOM 5260 CD2 LEU H 273 -16.569 10.123 11.669 1.00 3.69 B C
ATOM 5261 C LEU H 273 -14.005 9.227 14.877 1.00 5.14 B C

```
ATOM   5262  O   LEU H 273     -13.188   8.312  14.795  1.00  5.25      B    O
ATOM   5263  N   MET H 274     -13.668  10.509  14.775  1.00  4.52      B    N
ATOM   5264  CA  MET H 274     -12.307  10.910  14.447  1.00  4.59      B    C
ATOM   5265  CB  MET H 274     -12.147  12.429  14.567  1.00  4.35      B    C
ATOM   5266  CG  MET H 274     -12.862  13.219  13.479  1.00  4.50      B    C
ATOM   5267  SD  MET H 274     -12.547  14.992  13.574  1.00  5.51      B    S
ATOM   5268  CE  MET H 274     -10.875  15.078  12.935  1.00  5.26      B    C
ATOM   5269  C   MET H 274     -11.294  10.190  15.334  1.00  5.18      B    C
ATOM   5270  O   MET H 274     -10.272   9.703  14.851  1.00  5.61      B    O
ATOM   5271  N   SER H 275     -11.652  10.006  16.601  1.00  5.89      B    N
ATOM   5272  CA  SER H 275     -10.752   9.380  17.557  1.00  6.18      B    C
ATOM   5273  CB  SER H 275     -11.237   9.619  18.988  1.00  6.33      B    C
ATOM   5274  OG  SER H 275     -11.029  10.969  19.371  1.00  5.91      B    O
ATOM   5275  C   SER H 275     -10.583   7.886  17.288  1.00  6.58      B    C
ATOM   5276  O   SER H 275      -9.519   7.318  17.544  1.00  7.03      B    O
ATOM   5277  N   ASN H 276     -11.607   7.268  16.711  1.00  7.07      B    N
ATOM   5278  CA  ASN H 276     -11.525   5.857  16.369  1.00  7.86      B    C
ATOM   5279  CB  ASN H 276     -12.885   5.173  16.547  1.00  8.34      B    C
ATOM   5280  CG  ASN H 276     -13.108   4.676  17.969  1.00  9.77      B    C
ATOM   5281  OD1 ASN H 276     -12.161   4.307  18.666  1.00 11.84      B    O
ATOM   5282  ND2 ASN H 276     -14.351   4.748  18.433  1.00 11.15      B    N
ATOM   5283  C   ASN H 276     -10.959   5.605  14.971  1.00  7.71      B    C
ATOM   5284  O   ASN H 276     -10.950   4.468  14.498  1.00  7.84      B    O
ATOM   5285  N   ASN H 277     -10.386   6.643  14.363  1.00  7.77      B    N
ATOM   5286  CA  ASN H 277     -10.026   6.597  12.943  1.00  7.85      B    C
ATOM   5287  CB  ASN H 277     -11.209   7.021  12.073  1.00  7.58      B    C
ATOM   5288  CG  ASN H 277     -12.197   5.896  11.846  1.00  8.29      B    C
ATOM   5289  OD1 ASN H 277     -11.932   4.970  11.079  1.00  9.04      B    O
ATOM   5290  ND2 ASN H 277     -13.297   5.915  12.592  1.00  9.57      B    N
ATOM   5291  C   ASN H 277      -8.792   7.426  12.585  1.00  7.86      B    C
ATOM   5292  O   ASN H 277      -8.614   7.832  11.435  1.00  7.85      B    O
ATOM   5293  N   VAL H 278      -8.003   7.754  13.603  1.00  7.67      B    N
ATOM   5294  CA  VAL H 278      -6.682   8.354  13.425  1.00  7.77      B    C
ATOM   5295  CB  VAL H 278      -5.677   7.813  14.459  1.00  7.98      B    C
ATOM   5296  CGI VAL H 278      -5.763   8.615  15.749  1.00  7.21      B    C
ATOM   5297  CG2 VAL H 278      -5.932   6.336  14.725  1.00  8.99      B    C
ATOM   5298  C   VAL H 278      -6.095   8.223  12.019  1.00  7.76      B    C
ATOM   5299  O   VAL H 278      -5.641   9.211  11.444  1.00  7.84      B    O
ATOM   5300  N   GLN H 279      -5.935   6.989  11.553  1.00  7.47      B    N
ATOM   5301  CA  GLN H 279      -5.162   6.725  10.343  1.00  7.07      B    C
ATOM   5302  CB  GLN H 279      -5.291   5.256   9.938  1.00  7.62      B    C
ATOM   5303  CG  GLN H 279      -3.986   4.621   9.497  1.00 10.35      B    C
ATOM   5304  CD  GLN H 279      -4.194   3.335   8.725  1.00 13.70      B    C
ATOM   5305  OE1 GLN H 279      -5.319   2.986   8.367  1.00 15.06      B    O
ATOM   5306  NE2 GLN H 279      -3.105   2.622   8.460  1.00 13.97      B    N
ATOM   5307  C   GLN H 279      -5.610   7.621   9.192  1.00  6.02      B    C
ATOM   5308  O   GLN H 279      -4.795   8.297   8.563  1.00  5.45      B    O
ATOM   5309  N   ILE H 280      -6.881   7.492   8.829  1.00  5.25      B    N
ATOM   5310  CA  ILE H 280      -7.499   8.346   7.822  1.00  4.74      B    C
ATOM   5311  CB  ILE H 280      -9.022   8.133   7.775  1.00  4.58      B    C
ATOM   5312  CGI ILE H 280      -9.349   6.641   7.685  1.00  4.16      B    C
ATOM   5313  CD1 ILE H 280      -8.986   6.014   6.357  1.00  3.88      B    C
ATOM   5314  CG2 ILE H 280      -9.636   8.897   6.612  1.00  3.92      B    C
ATOM   5315  C   ILE H 280      -7.225   9.818   8.101  1.00  4.43      B    C
ATOM   5316  O   ILE H 280      -6.655  10.522   7.268  1.00  4.39      B    O
ATOM   5317  N   VAL H 281      -7.745  10.301   9.224  1.00  4.05      B    N
ATOM   5318  CA  VAL H 281      -7.502  11.671   9.651  1.00  3.58      B    C
ATOM   5319  CB  VAL H 281      -7.705  11.833  11.170  1.00  3.13      B    C
ATOM   5320  CGI VAL H 281      -7.901  13.299  11.526  1.00  2.34      B    C
ATOM   5321  CG2 VAL H 281      -8.890  11.002  11.638  1.00  2.21      B    C
```

ATOM 5322 C VAL H 281 -6.089 12.110 9.280 1.00 3.96 B C
ATOM 5323 O VAL H 281 -5.905 13.063 8.522 1.00 4.15 B O
ATOM 5324 N ARG H 282 -5.096 11.377 9.777 1.00 4.23 B N
ATOM 5325 CA ARG H 282 -3.697 11.649 9.454 1.00 4.45 B C
ATOM 5326 CB ARG H 282 -2.799 10.506 9.941 1.00 3.96 B C
ATOM 5327 CG ARG H 282 -2.843 10.255 11.440 1.00 2.99 B C
ATOM 5328 CD ARG H 282 -1.441 10.173 12.028 1.00 2.28 B C
ATOM 5329 NE ARG H 282 -1.470 9.891 13.460 1.00 2.00 B N
ATOM 5330 CZ ARG H 282 -0.687 10.483 14.358 1.00 2.44 B C
ATOM 5331 NH1 ARG H 282 0.219 11.371 13.970 1.00 2.04 B N
ATOM 5332 NH2 ARG H 282 -0.770 10.140 15.636 1.00 3.44 B N
ATOM 5333 C ARG H 282 -3.530 11.813 7.953 1.00 5.32 B C
ATOM 5334 O ARG H 282 -2.952 12.793 7.482 1.00 5.95 B O
ATOM 5335 N GLN H 283 -3.946 10.791 7.214 1.00 5.50 B N
ATOM 5336 CA GLN H 283 -3.837 10.802 5.766 1.00 5.80 B C
ATOM 5337 CB GLN H 283 -4.404 9.511 5.178 1.00 6.19 B C
ATOM 5338 CG GLN H 283 -3.531 8.297 5.431 1.00 9.68 B C
ATOM 5339 CD GLN H 283 -4.248 6.994 5.156 1.00 13.92 B C
ATOM 5340 OE1 GLN H 283 -5.408 6.984 4.745 1.00 16.20 B O
ATOM 5341 NE2 GLN H 283 -3.549 5.883 5.354 1.00 14.17 B N
ATOM 5342 C GLN H 283 -4.552 12.008 5.175 1.00 5.44 B C
ATOM 5343 O GLN H 283 -4.187 12.493 4.104 1.00 5.43 B O
ATOM 5344 N GLN H 284 -5.532 12.527 5.905 1.00 5.26 B N
ATOM 5345 CA GLN H 284 -6.361 13.609 5.396 1.00 5.18 B C
ATOM 5346 CB GLN H 284 -7.799 13.451 5.877 1.00 5.32 B C
ATOM 5347 CG GLN H 284 -8.666 12.649 4.933 1.00 6.85 B C
ATOM 5348 CD GLN H 284 -10.091 12.547 5.415 1.00 9.21 B C
ATOM 5349 OE1 GLN H 284 -10.340 12.297 6.595 1.00 9.74 B O
ATOM 5350 NE2 GLN H 284 -11.034 12.860 4.537 1.00 9.79 B N
ATOM 5351 C GLN H 284 -5.817 14.967 5.813 1.00 4.67 B C
ATOM 5352 O GLN H 284 -6.336 16.006 5.406 1.00 4.19 B O
ATOM 5353 N SER H 285 -4.758 14.950 6.614 1.00 4.51 B N
ATOM 5354 CA SER H 285 -4.240 16.170 7.212 1.00 4.39 B C
ATOM 5355 CB SER H 285 -4.020 15.979 8.713 1.00 4.13 B C
ATOM 5356 OG SER H 285 -5.177 15.446 9.334 1.00 4.40 B O
ATOM 5357 C SER H 285 -2.943 16.598 6.540 1.00 4.44 B C
ATOM 5358 O SER H 285 -2.286 15.804 5.866 1.00 4.82 B O
ATOM 5359 N TYR H 286 -2.600 17.870 6.704 1.00 4.53 B N
ATOM 5360 CA TYR H 286 -1.328 18.388 6.228 1.00 4.80 B C
ATOM 5361 CB TYR H 286 -1.560 19.527 5.236 1.00 4.88 B C
ATOM 5362 CG TYR H 286 -2.163 19.083 3.923 1.00 5.68 B C
ATOM 5363 CD1 TYR H 286 -3.448 18.558 3.868 1.00 7.34 B C
ATOM 5364 CE1 TYR H 286 -4.003 18.153 2.668 1.00 9.02 B C
ATOM 5365 CZ TYR H 286 -3.279 18.287 1.502 1.00 9.40 B C
ATOM 5366 OH TYR H 286 -3.829 17.892 0.304 1.00 10.44 B O
ATOM 5367 CE2 TYR H 286 -2.006 18.817 1.530 1.00 9.38 B C
ATOM 5368 CD2 TYR H 286 -1.458 19.214 2.735 1.00 7.39 B C
ATOM 5369 C TYR H 286 -0.501 18.884 7.404 1.00 4.76 B C
ATOM 5370 O TYR H 286 -1.036 19.160 8.478 1.00 5.25 B O
ATOM 5371 N SER H 287 0.803 19.011 7.194 1.00 4.52 B N
ATOM 5372 CA SER H 287 1.649 19.738 8.125 1.00 4.45 B C
ATOM 5373 CB SER H 287 2.518 18.768 8.927 1.00 4.57 B C
ATOM 5374 OG SER H 287 3.602 19.441 9.544 1.00 4.38 B O
ATOM 5375 C SER H 287 2.515 20.758 7.396 1.00 4.61 B C
ATOM 5376 O SER H 287 3.264 20.409 6.483 1.00 4.40 B O
ATOM 5377 N ILE H 288 2.294 22.033 7.710 1.00 5.11 B N
ATOM 5378 CA ILE H 288 3.067 23.130 7.131 1.00 5.81 B C
ATOM 5379 CB ILE H 288 2.176 24.349 6.825 1.00 5.52 B C
ATOM 5380 CGI ILE H 288 0.730 23.913 6.578 1.00 5.47 B C
ATOM 5381 CD1 ILE H 288 0.479 23.356 5.196 1.00 6.23 B C

ATOM 5382 CG2 ILE H 288 2.733 25.142 5.651 1.00 6.22 B C
ATOM 5383 C ILE H 288 4.170 23.581 8.080 1.00 6.71 B C
ATOM 5384 O ILE H 288 3.902 23.948 9.224 1.00 7.30 B O
ATOM 5385 N MET H 289 5.380 23.699 7.548 1.00 7.71 B N
ATOM 5386 CA MET H 289 6.487 24.307 8.274 1.00 8.57 B C
ATOM 5387 CB MET H 289 7.781 24.096 7.492 1.00 8.71 B C
ATOM 5388 CG MET H 289 9.038 24.181 8.326 1.00 9.70 B C
ATOM 5389 SD MET H 289 10.51 1 24.120 7.292 1.00 12.59 B S
ATOM 5390 CE MET H 289 10.168 25.446 6.138 1.00 12.41 B C
ATOM 5391 C MET H 289 6.245 25.801 8.468 1.00 9.12 B C
ATOM 5392 O MET H 289 5.976 26.513 7.501 1.00 9.31 B O
ATOM 5393 N SER H 290 6.457 26.293 9.688 1.00 9.80 B N
ATOM 5394 CA SER H 290 6.140 27.688 10.021 1.00 10.49 B C
ATOM 5395 CB SER H 290 5.283 27.777 11.287 1.00 10.64 B C
ATOM 5396 OG SER H 290 4.906 29.1 17 11.560 1.00 11.99 B O
ATOM 5397 C SER H 290 7.372 28.582 10.146 1.00 10.75 B C
ATOM 5398 O SER H 290 7.635 29.401 9.265 1.00 10.89 B O
ATOM 5399 N ILE H 291 8.095 28.469 11.258 1.00 11.04 B N
ATOM 5400 CA ILE H 291 9.405 29.1 12 11.361 1.00 11.41 B C
ATOM 5401 CB ILE H 291 9.335 30.523 11.981 1.00 11.80 B C
ATOM 5402 CG1 ILE H 291 8.071 30.680 12.828 1.00 11.81 B C
ATOM 5403 CD1 ILE H 291 8.273 30.362 14.291 1.00 11.76 B C
ATOM 5404 CG2 ILE H 291 9.390 31.586 10.891 1.00 12.39 B C
ATOM 5405 C ILE H 291 10.510 28.289 12.022 1.00 11.13 B C
ATOM 5406 O ILE H 291 10.337 27.742 13. 111 1.00 10.55 B O
ATOM 5407 N ILE H 292 11.678 28.302 11.388 1.00 11.36 B N
ATOM 5408 CA ILE H 292 12.827 27.544 11.855 1.00 11.82 B C
ATOM 5409 CB ILE H 292 13.483 26.752 10.710 1.00 11.86 B C
ATOM 5410 CGI ILE H 292 12.770 27.030 9.386 1.00 13.42 B C
ATOM 541 1 CD1 ILE H 292 11.373 27.593 9.542 1.00 15.86 B C
ATOM 5412 CG2 ILE H 292 13.500 25.262 11.022 1.00 10.85 B C
ATOM 5413 C ILE H 292 13.867 28.476 12.454 1.00 11.72 B C
ATOM 5414 O ILE H 292 14.414 29.343 11.771 1.00 11.28 B O
ATOM 5415 N LYS H 293 14.150 28.269 13.733 1.00 12.1 1 B N
ATOM 5416 CA LYS H 293 15.287 28.894 14.382 1.00 12.92 B C
ATOM 5417 CB LYS H 293 14.812 29.763 15.544 1.00 13.15 B C
ATOM 5418 CG LYS H 293 13.615 30.634 15.208 1.00 14. 17 B C
ATOM 5419 CD LYS H 293 13.793 32.037 15.758 1.00 15.37 B C
ATOM 5420 CE LYS H 293 12.940 33.041 15.001 1.00 16.68 B C
ATOM 5421 NZ LYS H 293 13. 111 34.421 15.532 1.00 18.18 B N
ATOM 5422 C LYS H 293 16.224 27.813 14.894 1.00 13.32 B C
ATOM 5423 O LYS H 293 15.800 26.689 15.167 1.00 13.17 B O
ATOM 5424 N GLU H 294 17.51 1 28.132 14.944 1.00 14.07 B N
ATOM 5425 CA GLU H 294 18.518 27.147 15.302 1.00 15.07 B C
ATOM 5426 CB GLU H 294 19.847 27.831 15.624 1.00 15.94 B C
ATOM 5427 CG GLU H 294 20.563 28.399 14.409 1.00 19.87 B C
ATOM 5428 CD GLU H 294 21.978 28.849 14.721 1.00 23.88 B C
ATOM 5429 OE1 GLU H 294 22.830 27.983 15.010 1.00 23.75 B O
ATOM 5430 OE2 GLU H 294 22.247 30.066 14.640 1.00 25.81 B O
ATOM 5431 C GLU H 294 18.056 26.299 16.482 1.00 14.40 B C
ATOM 5432 O GLU H 294 18.348 25.106 16.546 1.00 14.33 B O
ATOM 5433 N GLU H 295 17.279 26.904 17.378 1.00 13.97 B N
ATOM 5434 CA GLU H 295 16.914 26.255 18.635 1.00 13.84 B C
ATOM 5435 CB GLU H 295 17.570 26.953 19.830 1.00 14.67 B C
ATOM 5436 CG GLU H 295 18.047 28.366 19.550 1.00 17.56 B C
ATOM 5437 CD GLU H 295 16.928 29.281 19.096 1.00 21.41 B C
ATOM 5438 OE1 GLU H 295 16.816 29.524 17.876 1.00 22.35 B O
ATOM 5439 OE2 GLU H 295 16.190 29.795 19.962 1.00 23.20 B O
ATOM 5440 C GLU H 295 15.406 26.155 18.851 1.00 12.77 B C
ATOM 5441 O GLU H 295 14.956 25.743 19.919 1.00 12.58 B O

ATOM 5442 N VAL H 296 14.627 26.533 17.845 1.00 11.72 B N
ATOM 5443 CA VAL H 296 13.195 26.268 17.870 1.00 10.65 B C
ATOM 5444 CB VAL H 296 12.418 27.396 18.571 1.00 10.47 B C
ATOM 5445 CGI VAL H 296 10.974 26.983 18.804 1.00 9.77 B c
ATOM 5446 CG2 VAL H 296 13.090 27.760 19.884 1.00 11.31 B C
ATOM 5447 C VAL H 296 12.632 26.053 16.473 1.00 10.26 B c
ATOM 5448 O VAL H 296 12.887 26.838 15.561 1.00 10.09 B o
ATOM 5449 N LEU H 297 11.781 25.042 16.345 1.00 9.77 B N
ATOM 5450 CA LEU H 297 11.034 24.815 15.119 1.00 8.97 B c
ATOM 5451 CB LEU H 297 11.386 23.448 14.534 1.00 8.64 B c
ATOM 5452 CG LEU H 297 10.442 22.948 13.442 1.00 9.01 B c
ATOM 5453 CD1 LEU H 297 10.243 24.018 12.373 1.00 9.79 B c
ATOM 5454 CD2 LEU H 297 10.960 21.648 12.834 1.00 9.43 B c
ATOM 5455 C LEU H 297 9.535 24.885 15.388 1.00 8.34 B c
ATOM 5456 O LEU H 297 9.006 24.129 16.205 1.00 8.64 B o
ATOM 5457 N ALA H 298 8.848 25.771 14.675 1.00 7.21 B N
ATOM 5458 CA ALA H 298 7.396 25.872 14.777 1.00 6.33 B c
ATOM 5459 CB ALA H 298 6.987 27.268 15.238 1.00 6.68 B c
ATOM 5460 C ALA H 298 6.749 25.537 13.441 1.00 5.85 B c
ATOM 5461 O ALA H 298 7.310 25.823 12.384 1.00 5.96 B o
ATOM 5462 N TYR H 299 5.653 24.793 13.492 1.00 5.28 B N
ATOM 5463 CA TYR H 299 4.928 24.443 12.282 1.00 4.63 B c
ATOM 5464 CB TYR H 299 5.468 23.142 11.691 1.00 4.36 B c
ATOM 5465 CG TYR H 299 5.432 21.978 12.652 1.00 4.34 B c
ATOM 5466 CD1 TYR H 299 4.330 21.136 12.711 1.00 4.48 B c
ATOM 5467 CE1 TYR H 299 4.299 20.061 13.578 1.00 4.55 B c
ATOM 5468 CZ TYR H 299 5.373 19.826 14.410 1.00 3.72 B c
ATOM 5469 OH TYR H 299 5.343 18.762 15.282 1.00 2.38 B o
ATOM 5470 CE2 TYR H 299 6.475 20.651 14.374 1.00 4.13 B c
ATOM 5471 CD2 TYR H 299 6.494 21.727 13.509 1.00 4.38 B c
ATOM 5472 C TYR H 299 3.443 24.308 12.563 1.00 4.32 B c
ATOM 5473 O TYR H 299 3.034 24.068 13.699 1.00 4.67 B o
ATOM 5474 N VAL H 300 2.638 24.454 11.519 1.00 3.87 B N
ATOM 5475 CA VAL H 300 1.193 24.395 11.664 1.00 3.57 B c
ATOM 5476 CB VAL H 300 0.501 25.518 10.873 1.00 3.52 B c
ATOM 5477 CGI VAL H 300 -0.990 25.241 10.751 1.00 3.44 B c
ATOM 5478 CG2 VAL H 300 0.743 26.861 11.544 1.00 3.90 B c
ATOM 5479 C VAL H 300 0.654 23.049 11.203 1.00 3.53 B c
ATOM 5480 O VAL H 300 0.858 22.647 10.058 1.00 3.68 B o
ATOM 5481 N VAL H 301 -0.061 22.370 12.092 1.00 3.41 B N
ATOM 5482 CA VAL H 301 -0.857 21.216 11.704 1.00 3.36 B c
ATOM 5483 CB VAL H 301 -1.038 20.233 12.873 1.00 3.24 B c
ATOM 5484 CGI VAL H 301 -2.141 19.235 12.559 1.00 3.76 B c
ATOM 5485 CG2 VAL H 301 0.270 19.516 13.169 1.00 3.10 B c
ATOM 5486 C VAL H 301 -2.223 21.641 11.183 1.00 3.48 B c
ATOM 5487 O VAL H 301 -2.772 22.661 11.602 1.00 3.92 B o
ATOM 5488 N GLN H 302 -2.766 20.845 10.270 1.00 3.21 B N
ATOM 5489 CA GLN H 302 -3.989 21.201 9.569 1.00 3.01 B c
ATOM 5490 CB GLN H 302 -3.662 21.767 8.188 1.00 3.24 B c
ATOM 5491 CG GLN H 302 -4.875 21.992 7.307 1.00 5.21 B c
ATOM 5492 CD GLN H 302 -4.603 22.977 6.191 1.00 7.54 B c
ATOM 5493 OE1 GLN H 302 -3.715 23.822 6.297 1.00 7.28 B o
ATOM 5494 NE2 GLN H 302 -5.364 22.870 5.108 1.00 9.27 B N
ATOM 5495 C GLN H 302 -4.885 19.978 9.434 1.00 2.42 B c
ATOM 5496 O GLN H 302 -4.564 19.038 8.706 1.00 2.40 B o
ATOM 5497 N LEU H 303 -5.964 19.959 10.207 1.00 2.00 B N
ATOM 5498 CA LEU H 303 -6.802 18.775 10.329 1.00 2.00 B c
ATOM 5499 CB LEU H 303 -6.945 18.389 11.802 1.00 2.00 B c
ATOM 5500 CG LEU H 303 -5.634 18.464 12.590 1.00 2.00 B c
ATOM 5501 CD1 LEU H 303 -5.840 18.189 14.073 1.00 2.00 B c

```
ATOM   5502  CD2 LEU H 303     -4.598  17.517  11.999  1.00  2.00      B    C
ATOM   5503  C   LEU H 303     -8.172  19.024   9.704  1.00  2.00      B    C
ATOM   5504  O   LEU H 303     -8.499  20.159   9.359  1.00  2.45      B    O
ATOM   5505  N   PRO H 304     -8.955  17.949   9.506  1.00  2.00      B    N
ATOM   5506  CA  PRO H 304    -10.222  18.040   8.763  1.00  2.07      B    C
ATOM   5507  CB  PRO H 304    -10.407  16.623   8.206  1.00  2.00      B    C
ATOM   5508  CG  PRO H 304     -9.560  15.748   9.074  1.00  2.00      B    C
ATOM   5509  CD  PRO H 304     -8.390  16.589   9.469  1.00  2.06      B    C
ATOM   5510  C   PRO H 304    -11.449  18.462   9.590  1.00  2.11      B    C
ATOM   5511  O   PRO H 304    -11.353  18.606  10.812  1.00  2.13      B    O
ATOM   5512  N   ALA H 305    -12.622  18.425   8.953  1.00 30.00      B    N
ATOM   5513  CA  ALA H 305    -12.858  19.173   7.708  1.00 30.00      B    C
ATOM   5514  CB  ALA H 305    -11.532  19.487   7.023  1.00 30.00      B    C
ATOM   5515  C   ALA H 305    -13.809  18.445   6.733  1.00 30.00      B    C
ATOM   5516  O   ALA H 305    -13.601  17.265   6.429  1.00 30.00      B    O
ATOM   5517  N   TYR H 306    -14.925  19.101   6.370  1.00 13.49      B    N
ATOM   5518  CA  TYR H 306    -15.658  18.816   5.101  1.00 13.70      B    C
ATOM   5519  CB  TYR H 306    -16.947  18.016   5.303  1.00 13.93      B    C
ATOM   5520  CG  TYR H 306    -17.614  18.033   6.640  1.00 14.08      B    C
ATOM   5521  CD1 TYR H 306    -18.719  18.859   6.857  1.00 14.59      B    C
ATOM   5522  CE1 TYR H 306    -19.825  18.384   7.554  1.00 14.82      B    C
ATOM   5523  CZ  TYR H 306    -19.818  17.083   8.031  1.00 14.52      B    C
ATOM   5524  OH  TYR H 306    -20.780  16.679   8.925  1.00 13.02      B    O
ATOM   5525  CE2 TYR H 306    -18.727  16.282   7.818  1.00 15.22      B    C
ATOM   5526  CD2 TYR H 306    -17.583  16.855   7.363  1.00 14.61      B    C
ATOM   5527  C   TYR H 306    -16.111  19.916   4.144  1.00 13.68      B    C
ATOM   5528  O   TYR H 306    -15.500  20.982   4.051  1.00 13.95      B    O
ATOM   5529  N   GLY H 307    -17.412  19.756   3.831  1.00 13.54      B    N
ATOM   5530  CA  GLY H 307    -18.190  20.428   2.747  1.00 13.37      B    C
ATOM   5531  C   GLY H 307    -18.295  19.776   1.353  1.00 13.47      B    C
ATOM   5532  O   GLY H 307    -17.282  19.701   0.658  1.00 13.90      B    O
ATOM   5533  N   VAL H 308    -19.505  19.569   0.815  1.00 13.31      B    N
ATOM   5534  CA  VAL H 308    -19.608  19.371  -0.649  1.00 13.30      B    C
ATOM   5535  CB  VAL H 308    -18.352  18.643  -1.188  1.00 13.03      B    C
ATOM   5536  CGI VAL H 308    -17.948  19.190  -2.545  1.00 13.62      B    C
ATOM   5537  CG2 VAL H 308    -17.209  18.740  -0.205  1.00 12.86      B    C
ATOM   5538  C   VAL H 308    -20.720  18.501  -1.196  1.00 13.58      B    C
ATOM   5539  O   VAL H 308    -21.809  18.418  -0.627  1.00 13.71      B    o
ATOM   5540  N   ILE H 309    -20.173  17.489  -1.845  1.00  4.08      B    N
ATOM   5541  CA  ILE H 309    -19.600  16.440  -1.057  1.00  4.84      B    C
ATOM   5542  CB  ILE H 309    -19.530  16.902   0.426  1.00  4.89      B    c
ATOM   5543  CGI ILE H 309    -18.554  18.070   0.585  1.00  5.85      B    c
ATOM   5544  CD1 ILE H 309    -17.312  17.711   1.373  1.00  8.12      B    c
ATOM   5545  CG2 ILE H 309    -19.121  15.756   1.332  1.00  4.44      B    c
ATOM   5546  C   ILE H 309    -20.750  15.497  -1.251  1.00  5.23      B    c
ATOM   5547  O   ILE H 309    -21.670  15.818  -1.998  1.00  5.92      B    o
ATOM   5548  N   ASP H 310    -20.752  14.358  -0.584  1.00  5.33      B    N
ATOM   5549  CA  ASP H 310    -21.992  13.604  -0.482  1.00  5.83      B    c
ATOM   5550  CB  ASP H 310    -23.072  14.462   0.188  1.00  6.21      B    c
ATOM   5551  CG  ASP H 310    -22.698  14.894   1.595  1.00  7.19      B    c
ATOM   5552  OD1 ASP H 310    -22.903  16.084   1.920  1.00  7.74      B    o
ATOM   5553  OD2 ASP H 310    -22.425  14.005   2.428  1.00  7.58      B    o
ATOM   5554  C   ASP H 310    -22.524  13.115  -1.841  1.00  6.02      B    c
ATOM   5555  O   ASP H 310    -23.670  12.673  -1.927  1.00  6.05      B    o
ATOM   5556  N   THR H 311    -21.716  13.207  -2.897  1.00  6.24      B    N
ATOM   5557  CA  THR H 311    -22.015  12.488  -4.140  1.00  6.14      B    c
ATOM   5558  CB  THR H 311    -21.097  12.933  -5.305  1.00  5.69      B    c
ATOM   5559  OG1 THR H 311    -20.497  14.196  -4.994  1.00  5.34      B    O
ATOM   5560  CG2 THR H 311    -21.891  13.063  -6.599  1.00  7.10      B    C
ATOM   5561  C   THR H 311    -21.832  10.990  -3.911  1.00  6.78      B    C
```

```
ATOM   5562  O   THR H 311     -20.946  10.587  -3.160  1.00  7.33      B    O
ATOM   5563  N   PRO H 312     -22.611  10.155  -4.621  1.00  7.00      B    N
ATOM   5564  CA  PRO H 312     -22.351   8.718  -4.567  1.00  7.23      B    C
ATOM   5565  CB  PRO H 312     -23.560   8.115  -5.289  1.00  7.00      B    C
ATOM   5566  CG  PRO H 312     -24.053   9.200  -6.178  1.00  6.59      B    C
ATOM   5567  CD  PRO H 312     -23.800  10.475  -5.432  1.00  6.99      B    C
ATOM   5568  C   PRO H 312     -21.061   8.352  -5.298  1.00  7.69      B    C
ATOM   5569  O   PRO H 312     -20.796   8.881  -6.377  1.00  7.55      B    O
ATOM   5570  N   CYS H 313     -20.259   7.469  -4.712  1.00  8.10      B    N
ATOM   5571  CA  CYS H 313     -19.271   6.730  -5.491  1.00  8.54      B    C
ATOM   5572  CB  CYS H 313     -17.840   7.078  -5.071  1.00  8.77      B    C
ATOM   5573  SG  CYS H 313     -17.635   8.680  -4.269  1.00 10.74      B    S
ATOM   5574  C   CYS H 313     -19.470   5.222  -5.446  1.00  8.19      B    C
ATOM   5575  O   CYS H 313     -20.334   4.712  -4.734  1.00  8.07      B    O
ATOM   5576  N   TRP H 314     -18.571   4.517  -6.121  1.00  7.93      B    N
ATOM   5577  CA  TRP H 314     -18.564   3.067  -6.116  1.00  7.80      B    C
ATOM   5578  CB  TRP H 314     -19.648   2.528  -7.050  1.00  8.13      B    C
ATOM   5579  CG  TRP H 314     -19.582   3.091  -8.436  1.00  9.09      B    C
ATOM   5580  CD1 TRP H 314     -19.041   2.490  -9.536  1.00 10.26      B    C
ATOM   5581  NE1 TRP H 314     -19.247   3.268 -10.650  1.00 10.86      B    N
ATOM   5582  CE2 TRP H 314     -19.940   4.392 -10.285  1.00 10.68      B    C
ATOM   5583  CD2 TRP H 314     -20.172   4.313  -8.897  1.00 10.49      B    C
ATOM   5584  CE3 TRP H 314     -20.877   5.347  -8.271  1.00 11.67      B    C
ATOM   5585  CZ3 TRP H 314     -21.301   6.419  -9.037  1.00 12.98      B    C
ATOM   5586  CH2 TRP H 314     -21.048   6.472 -10.413  1.00 12.74      B    C
ATOM   5587  CZ2 TRP H 314     -20.369   5.472 -11.054  1.00 11.73      B    C
ATOM   5588  C   TRP H 314     -17.198   2.576  -6.563  1.00  7.34      B    C
ATOM   5589  O   TRP H 314     -16.485   3.272  -7.288  1.00  7.47      B    O
ATOM   5590  N   LYS H 315     -16.791   1.426  -6.041  1.00  6.75      B    N
ATOM   5591  CA  LYS H 315     -15.547   0.807  -6.462  1.00  6.37      B    C
ATOM   5592  CB  LYS H 315     -14.741   0.337  -5.252  1.00  6.38      B    C
ATOM   5593  CG  LYS H 315     -13.277   0.071  -5.554  1.00  6.55      B    C
ATOM   5594  CD  LYS H 315     -12.509  -0.282  -4.292  1.00  8.01      B    C
ATOM   5595  CE  LYS H 315     -11.014  -0.331  -4.556  1.00  8.78      B    C
ATOM   5596  NZ  LYS H 315     -10.337  -1.364  -3.726  1.00 10.21      B    N
ATOM   5597  C   LYS H 315     -15.825  -0.361  -7.392  1.00  6.32      B    C
ATOM   5598  O   LYS H 315     -16.746  -1.145  -7.164  1.00  6.21      B    O
ATOM   5599  N   LEU H 316     -15.089  -0.411  -8.495  1.00  6.58      B    N
ATOM   5600  CA  LEU H 316     -15.304  -1.435  -9.502  1.00  7.02      B    C
ATOM   5601  CB  LEU H 316     -15.491  -0.801 -10.880  1.00  6.64      B    C
ATOM   5602  CG  LEU H 316     -15.452  -1.767 -12.065  1.00  6.21      B    C
ATOM   5603  CD1 LEU H 316     -16.540  -2.822 -11.936  1.00  5.94      B    C
ATOM   5604  CD2 LEU H 316     -15.590  -1.011 -13.378  1.00  6.57      B    C
ATOM   5605  C   LEU H 316     -14.138  -2.409  -9.525  1.00  7.77      B    C
ATOM   5606  O   LEU H 316     -12.999  -2.024  -9.792  1.00  8.47      B    O
ATOM   5607  N   HIS H 317     -14.414  -3.656  -9.168  1.00  8.05      B    N
ATOM   5608  CA  HIS H 317     -13.460  -4.725  -9.388  1.00  8.21      B    C
ATOM   5609  CB  HIS H 317     -13.266  -5.547  -8.116  1.00  9.04      B    C
ATOM   5610  CG  HIS H 317     -13.449  -4.761  -6.856  1.00 11.41      B    C
ATOM   5611  ND1 HIS H 317     -12.392  -4.368  -6.063  1.00 13.62      B    N
ATOM   5612  CE1 HIS H 317     -12.854  -3.746  -4.993  1.00 14.91      B    C
ATOM   5613  NE2 HIS H 317     -14.172  -3.725  -5.060  1.00 14.25      B    N
ATOM   5614  CD2 HIS H 317     -14.570  -4.352  -6.216  1.00 12.67      B    C
ATOM   5615  C   HIS H 317     -13.904  -5.625 -10.528  1.00  7.39      B    C
ATOM   5616  O   HIS H 317     -15.085  -5.677 -10.870  1.00  7.23      B    O
ATOM   5617  N   THR H 318     -12.976  -6.451 -10.993  1.00  7.11      B    N
ATOM   5618  CA  THR H 318     -12.973  -6.913 -12.372  1.00  6.56      B    C
ATOM   5619  CB  THR H 318     -12.242  -5.919 -13.295  1.00  6.28      B    C
ATOM   5620  OG1 THR H 318     -13.197  -5.193 -14.078  1.00  6.33      B    O
ATOM   5621  CG2 THR H 318     -11.296  -6.662 -14.224  1.00  6.52      B    C
```

```
ATOM   5622  C   THR H 318     -12.254  -8.251 -12.438  1.00  6.58      B    C
ATOM   5623  O   THR H 318     -11.142  -8.393 -11.930  1.00  6.67      B    O
ATOM   5624  N   SER H 319     -12.919  -9.252 -13.001  1.00  6.81      B    N
ATOM   5625  CA  SER H 319     -12.328 -10.578 -13.115  1.00  7.31      B    C
ATOM   5626  CB  SER H 319     -12.902 -11.513 -12.047  1.00  7.14      B    C
ATOM   5627  OG  SER H 319     -12.244 -12.769 -12.052  1.00  6.84      B    O
ATOM   5628  C   SER H 319     -12.533 -11.169 -14.509  1.00  7.93      B    C
ATOM   5629  O   SER H 319     -13.583 -10.975 -15.124  1.00  8.65      B    O
ATOM   5630  N   PRO H 320     -11.534 -11.917 -15.002  1.00  8.08      B    N
ATOM   5631  CA  PRO H 320     -11.592 -12.459 -16.354  1.00  8.34      B    C
ATOM   5632  CB  PRO H 320     -10.339 -13.342 -16.442  1.00  7.99      B    C
ATOM   5633  CG  PRO H 320      -9.773 -13.404 -15.045  1.00  8.01      B    C
ATOM   5634  CD  PRO H 320     -10.230 -12.163 -14.367  1.00  8.10      B    C
ATOM   5635  C   PRO H 320     -12.848 -13.288 -16.610  1.00  9.03      B    C
ATOM   5636  O   PRO H 320     -13.372 -13.928 -15.697  1.00  8.74      B    O
ATOM   5637  N   LEU H 321     -13.224 -13.384 -17.881  1.00 10.31      B    N
ATOM   5638  CA  LEU H 321     -14.514 -13.933 -18.284  1.00 11.63      B    C
ATOM   5639  CB  LEU H 321     -15.543 -12.807 -18.448  1.00 11.31      B    C
ATOM   5640  CG  LEU H 321     -17.032 -13.163 -18.454  1.00 10.97      B    C
ATOM   5641  CD1 LEU H 321     -17.828 -12.071 -19.154  1.00 10.04      B    C
ATOM   5642  CD2 LEU H 321     -17.273 -14.514 -19.113  1.00 10.69      B    C
ATOM   5643  C   LEU H 321     -14.359 -14.687 -19.603  1.00 12.92      B    C
ATOM   5644  O   LEU H 321     -13.871 -14.135 -20.591  1.00 13.29      B    O
ATOM   5645  N   CYS H 322     -14.788 -15.947 -19.611  1.00 13.39      B    N
ATOM   5646  CA  CYS H 322     -14.579 -16.836 -20.751  1.00 14.16      B    C
ATOM   5647  CB  CYS H 322     -13.459 -17.833 -20.451  1.00 13.72      B    C
ATOM   5648  SG  CYS H 322     -11.996 -17.091 -19.704  1.00 13.42      B    S
ATOM   5649  C   CYS H 322     -15.859 -17.589 -21.115  1.00 15.46      B    C
ATOM   5650  O   CYS H 322     -16.561 -18.099 -20.241  1.00 15.94      B    O
ATOM   5651  N   THR H 323     -16.097 -17.735 -22.415  1.00 16.70      B    N
ATOM   5652  CA  THR H 323     -17.059 -18.703 -22.940  1.00 17.84      B    C
ATOM   5653  CB  THR H 323     -17.054 -18.690 -24.477  1.00 17.50      B    C
ATOM   5654  OG1 THR H 323     -15.767 -18.268 -24.947  1.00 15.70      B    O
ATOM   5655  CG2 THR H 323     -18.118 -17.740 -25.005  1.00 18.05      B    C
ATOM   5656  C   THR H 323     -16.755 -20.125 -22.469  1.00 19.54      B    C
ATOM   5657  O   THR H 323     -15.670 -20.389 -21.950  1.00 19.84      B    O
ATOM   5658  N   THR H 324     -17.625 -21.068 -22.825  1.00 21.17      B    N
ATOM   5659  CA  THR H 324     -17.251 -22.481 -22.774  1.00 22.89      B    C
ATOM   5660  CB  THR H 324     -17.589 -23.138 -21.426  1.00 22.69      B    C
ATOM   5661  OG1 THR H 324     -18.025 -22.141 -20.494  1.00 22.10      B    O
ATOM   5662  CG2 THR H 324     -16.365 -23.854 -20.871  1.00 22.03      B    C
ATOM   5663  C   THR H 324     -17.737 -23.375 -23.915  1.00 24.39      B    C
ATOM   5664  O   THR H 324     -17.251 -24.495 -24.070  1.00 24.53      B    O
ATOM   5665  N   ASN H 325     -18.633 -22.866 -24.755  1.00 25.72      B    N
ATOM   5666  CA  ASN H 325     -18.864 -23.475 -26.064  1.00 27.01      B    C
ATOM   5667  CB  ASN H 325     -19.924 -24.578 -25.977  1.00 27.37      B    C
ATOM   5668  CG  ASN H 325     -19.337 -25.925 -25.593  1.00 28.46      B    C
ATOM   5669  OD1 ASN H 325     -19.134 -26.792 -26.443  1.00 30.37      B    O
ATOM   5670  ND2 ASN H 325     -19.086 -26.114 -24.303  1.00 28.78      B    N
ATOM   5671  C   ASN H 325     -19.246 -22.460 -27.136  1.00 27.36      B    C
ATOM   5672  O   ASN H 325     -19.634 -21.334 -26.829  1.00 27.94      B    O
ATOM   5673  N   SER H 330     -15.365 -21.167 -24.863  1.00 35.76      B    N
ATOM   5674  CA  SER H 330     -14.200 -21.669 -25.580  1.00 35.01      B    C
ATOM   5675  CB  SER H 330     -14.630 -22.631 -26.690  1.00 35.47      B    C
ATOM   5676  OG  SER H 330     -15.521 -22.000 -27.595  1.00 33.31      B    O
ATOM   5677  C   SER H 330     -13.383 -20.522 -26.168  1.00 34.35      B    C
ATOM   5678  O   SER H 330     -13.938 -19.509 -26.593  1.00 34.33      B    O
ATOM   5679  N   ASN H 331     -12.062 -20.653 -26.123  1.00 32.48      B    N
ATOM   5680  CA  ASN H 331     -11.191 -19.933 -27.046  1.00 30.72      B    C
ATOM   5681  CB  ASN H 331     -11.577 -20.233 -28.504  1.00 31.31      B    C
```

ATOM 5682 CG ASN H 331 -11.276 -21.670 -28.918 1.00 32.11 B C
ATOM 5683 OD1 ASN H 331 -10.553 -22.391 -28.229 1.00 32.54 B O
ATOM 5684 ND2 ASN H 331 -11.753 -22.055 -30.097 1.00 31.30 B N
ATOM 5685 C ASN H 331 -11.120 -18.411 -26.826 1.00 28.71 B C
ATOM 5686 O ASN H 331 -10.495 -17.710 -27.621 1.00 29.07 B O
ATOM 5687 N ILE H 332 -11.797 -17.887 -25.802 1.00 25.44 B N
ATOM 5688 CA ILE H 332 -11.904 -16.424 -25.638 1.00 21.83 B C
ATOM 5689 CB ILE H 332 -12.919 -15.806 -26.624 1.00 21.42 B C
ATOM 5690 CGI ILE H 332 -12.916 -14.280 -26.511 1.00 19.89 B C
ATOM 5691 CD1 ILE H 332 -11.986 -13.596 -27.488 1.00 17.67 B C
ATOM 5692 CG2 ILE H 332 -14.314 -16.360 -26.374 1.00 20.61 B C
ATOM 5693 C ILE H 332 -12.204 -15.918 -24.217 1.00 20.37 B C
ATOM 5694 O ILE H 332 -13.219 -16.290 -23.624 1.00 19.95 B O
ATOM 5695 N CYS H 333 -11.425 -14.935 -23.761 1.00 18.27 B N
ATOM 5696 CA CYS H 333 -11.681 -14.282 -22.474 1.00 16.47 B C
ATOM 5697 CB CYS H 333 -10.802 -14.873 -21.371 1.00 16.14 B C
ATOM 5698 SG CYS H 333 -10.807 -16.672 -21.295 1.00 17.09 B S
ATOM 5699 C CYS H 333 -11.542 -12.763 -22.482 1.00 15.73 B C
ATOM 5700 O CYS H 333 -10.707 -12.206 -23.197 1.00 15.43 B O
ATOM 5701 N LEU H 334 -12.154 -12.155 -21.470 1.00 15.06 B N
ATOM 5702 CA LEU H 334 -12.256 -10.708 -21.353 1.00 13.79 B C
ATOM 5703 CB LEU H 334 -13.702 -10.264 -21.588 1.00 13.39 B C
ATOM 5704 CG LEU H 334 -14.262 -10.341 -23.008 1.00 13.93 B C
ATOM 5705 CD1 LEU H 334 -15.276 -9.230 -23.235 1.00 14.20 B C
ATOM 5706 CD2 LEU H 334 -13.143 -10.266 -24.035 1.00 14.52 B C
ATOM 5707 C LEU H 334 -11.868 -10.345 -19.930 1.00 13.22 B C
ATOM 5708 O LEU H 334 -12.324 -10.980 -18.980 1.00 13.31 B O
ATOM 5709 N THR H 335 -11.141 -9.246 -19.776 1.00 12.58 B N
ATOM 5710 CA THR H 335 -11.033 -8.596 -18.478 1.00 12.17 B C
ATOM 5711 CB THR H 335 -9.677 -8.904 -17.798 1.00 12.02 B C
ATOM 5712 OG1 THR H 335 -9.207 -10.191 -18.219 1.00 12.64 B O
ATOM 5713 CG2 THR H 335 -9.817 -8.893 -16.280 1.00 11.47 B C
ATOM 5714 C THR H 335 -11.203 -7.092 -18.639 1.00 11.97 B C
ATOM 5715 O THR H 335 -10.637 -6.493 -19.553 1.00 11.93 B O
ATOM 5716 N ARG H 336 -12.130 -6.526 -17.874 1.00 11.60 B N
ATOM 5717 CA ARG H 336 -12.411 -5.098 -17.949 1.00 12.15 B C
ATOM 5718 CB ARG H 336 -13.716 -4.767 -17.215 1.00 12.16 B C
ATOM 5719 CG ARG H 336 -14.525 -3.643 -17.849 1.00 12.67 B C
ATOM 5720 CD ARG H 336 -15.993 -4.018 -17.970 1.00 12.52 B C
ATOM 5721 NE ARG H 336 -16.736 -3.718 -16.750 1.00 12.35 B N
ATOM 5722 CZ ARG H 336 -17.058 -2.490 -16.355 1.00 12.54 B C
ATOM 5723 NH1 ARG H 336 -16.665 -1.439 -17.062 1.00 12.38 B N
ATOM 5724 NH2 ARG H 336 -17.761 -2.312 -15.246 1.00 12.48 B N
ATOM 5725 C ARG H 336 -11.252 -4.295 -17.361 1.00 12.71 B C
ATOM 5726 O ARG H 336 -10.891 -4.475 -16.198 1.00 12.62 B O
ATOM 5727 N THR H 337 -10.615 -3.475 -18.192 1.00 13.70 B N
ATOM 5728 CA THR H 337 -9.431 -2.733 -17.766 1.00 14.91 B C
ATOM 5729 CB THR H 337 -8.736 -2.032 -18.949 1.00 15.27 B C
ATOM 5730 OG1 THR H 337 -8.620 -2.946 -20.046 1.00 16.65 B O
ATOM 5731 CG2 THR H 337 -7.347 -1.560 -18.546 1.00 15.94 B C
ATOM 5732 C THR H 337 -9.759 -1.707 -16.681 1.00 15.16 B C
ATOM 5733 O THR H 337 -9.100 -1.659 -15.643 1.00 15.60 B O
ATOM 5734 N ASP H 338 -10.770 -0.880 -16.934 1.00 15.15 B N
ATOM 5735 CA ASP H 338 -10.988 0.325 -16.143 1.00 15.52 B C
ATOM 5736 CB ASP H 338 -11.999 1.250 -16.828 1.00 16.81 B C
ATOM 5737 CG ASP H 338 -13.028 0.489 -17.642 1.00 20.57 B C
ATOM 5738 OD1 ASP H 338 -13.670 1.103 -18.519 1.00 23.00 B O
ATOM 5739 OD2 ASP H 338 -13.224 -0.716 -17.378 1.00 22.92 B O
ATOM 5740 C ASP H 338 -11.453 -0.022 -14.733 1.00 14.21 B C
ATOM 5741 O ASP H 338 -12.651 -0.171 -14.482 1.00 14.00 B O

```
ATOM   5742  N   ARG H 339     -10.494  -0.189 -13.827  1.00 12.79      B    N
ATOM   5743  CA  ARG H 339     -10.792  -0.528 -12.440  1.00 11.71      B    C
ATOM   5744  CB  ARG H 339      -9.866  -1.630 -11.950  1.00 11.73      B    C
ATOM   5745  CG  ARG H 339      -9.941  -2.905 -12.727  1.00 12.49      B    C
ATOM   5746  CD  ARG H 339      -9.329  -3.991 -11.895  1.00 13.24      B    C
ATOM   5747  NE  ARG H 339      -8.677  -5.006 -12.705  1.00 12.04      B    N
ATOM   5748  CZ  ARG H 339      -8.332  -6.200 -12.239  1.00 11.74      B    C
ATOM   5749  NH1 ARG H 339      -8.540  -6.498 -10.964  1.00 13.43      B    N
ATOM   5750  NH2 ARG H 339      -7.784  -7.097 -13.045  1.00  9.80      B    N
ATOM   5751  C   ARG H 339     -10.626   0.666 -11.519  1.00 11.16      B    C
ATOM   5752  O   ARG H 339      -9.690   1.448 -11.681  1.00 11.37      B    O
ATOM   5753  N   GLY H 340     -11.290   0.573 -10.373  1.00 10.43      B    N
ATOM   5754  CA  GLY H 340     -11.038   1.481  -9.269  1.00  9.52      B    C
ATOM   5755  C   GLY H 340     -12.279   2.268  -8.916  1.00  8.80      B    C
ATOM   5756  O   GLY H 340     -13.397   1.759  -8.996  1.00  8.56      B    O
ATOM   5757  N   TRP H 341     -12.077   3.513  -8.506  1.00  8.25      B    N
ATOM   5758  CA  TRP H 341     -13.156   4.309  -7.953  1.00  7.98      B    C
ATOM   5759  CB  TRP H 341     -12.629   5.235  -6.865  1.00  7.79      B    C
ATOM   5760  CG  TRP H 341     -12.435   4.538  -5.579  1.00  7.67      B    C
ATOM   5761  CD1 TRP H 341     -11.275   3.990  -5.119  1.00  8.12      B    C
ATOM   5762  NE1 TRP H 341     -11.496   3.346  -3.928  1.00  8.60      B    N
ATOM   5763  CE2 TRP H 341     -12.834   3.401  -3.639  1.00  7.57      B    C
ATOM   5764  CD2 TRP H 341     -13.464   4.093  -4.691  1.00  7.52      B    C
ATOM   5765  CE3 TRP H 341     -14.848   4.291  -4.636  1.00  7.86      B    C
ATOM   5766  CZ3 TRP H 341     -15.545   3.797  -3.548  1.00  7.14      B    C
ATOM   5767  CH2 TRP H 341     -14.890   3.105  -2.522  1.00  6.39      B    C
ATOM   5768  CZ2 TRP H 341     -13.538   2.903  -2.546  1.00  7.30      B    C
ATOM   5769  C   TRP H 341     -13.835   5.117  -9.037  1.00  8.26      B    C
ATOM   5770  O   TRP H 341     -13.222   5.978  -9.666  1.00  8.35      B    O
ATOM   5771  N   TYR H 342     -15.113   4.840  -9.244  1.00  8.44      B    N
ATOM   5772  CA  TYR H 342     -16.000   5.809  -9.847  1.00  8.53      B    C
ATOM   5773  CB  TYR H 342     -16.948   5.116 -10.814  1.00  8.43      B    C
ATOM   5774  CG  TYR H 342     -16.214   4.338 -11.870  1.00  9.17      B    C
ATOM   5775  CD1 TYR H 342     -15.551   3.163 -11.540  1.00 10.32      B    C
ATOM   5776  CE1 TYR H 342     -14.766   2.503 -12.465  1.00 10.99      B    C
ATOM   5777  CZ  TYR H 342     -14.566   3.063 -13.709  1.00 11.00      B    C
ATOM   5778  OH  TYR H 342     -13.828   2.387 -14.653  1.00 12.82      B    O
ATOM   5779  CE2 TYR H 342     -15.115   4.288 -14.019  1.00 10.67      B    C
ATOM   5780  CD2 TYR H 342     -15.913   4.930 -13.091  1.00 10.41      B    C
ATOM   5781  C   TYR H 342     -16.781   6.535  -8.778  1.00  8.64      B    C
ATOM   5782  O   TYR H 342     -16.830   6.103  -7.628  1.00  8.40      B    O
ATOM   5783  N   CYS H 343     -17.373   7.657  -9.157  1.00  8.87      B    N
ATOM   5784  CA  CYS H 343     -17.812   8.625  -8.178  1.00  9.35      B    C
ATOM   5785  CB  CYS H 343     -16.702   8.901  -7.160  1.00  9.17      B    C
ATOM   5786  SG  CYS H 343     -17.204   9.963  -5.787  1.00 11.88      B    S
ATOM   5787  C   CYS H 343     -18.258   9.907  -8.863  1.00  9.42      B    C
ATOM   5788  O   CYS H 343     -17.552  10.444  -9.717  1.00  9.96      B    O
ATOM   5789  N   ASP H 344     -19.523  10.250  -8.643  1.00  9.36      B    N
ATOM   5790  CA  ASP H 344     -20.231  11.213  -9.477  1.00  9.24      B    C
ATOM   5791  CB  ASP H 344     -21.712  11.250  -9.097  1.00  9.34      B    C
ATOM   5792  CG  ASP H 344     -22.555  10.320  -9.943  1.00 10.72      B    C
ATOM   5793  OD1 ASP H 344     -22.582  10.500 -11.178  1.00 13.93      B    O
ATOM   5794  OD2 ASP H 344     -23.246   9.453  -9.367  1.00 11.87      B    O
ATOM   5795  C   ASP H 344     -19.632  12.607  -9.330  1.00  9.09      B    C
ATOM   5796  O   ASP H 344     -19.454  13.101  -8.216  1.00  9.39      B    O
ATOM   5797  N   ASN H 345     -19.416  13.274 -10.457  1.00  9.13      B    N
ATOM   5798  CA  ASN H 345     -19.165  14.709 -10.461  1.00  9.52      B    C
ATOM   5799  CB  ASN H 345     -17.833  15.011 -11.149  1.00  9.61      B    C
ATOM   5800  CG  ASN H 345     -17.166  16.258 -10.606  1.00  9.21      B    C
ATOM   5801  OD1 ASN H 345     -16.787  16.316  -9.437  1.00  6.21      B    O
```

```
ATOM   5802  ND2 ASN H 345     -17.023   17.268 -11.456  1.00 11.05      B    N
ATOM   5803  C   ASN H 345     -20.303   15.452 -11.152  1.00 10.06      B    C
ATOM   5804  O   ASN H 345     -21.347   14.867 -11.441  1.00 11.10      B    o
ATOM   5805  N   ALA H 346     -20.133   16.755 -11.352  1.00  9.74      B    N
ATOM   5806  CA  ALA H 346     -21.211   17.584 -11.877  1.00  9.58      B    C
ATOM   5807  CB  ALA H 346     -20.708   18.991 -12.164  1.00  9.60      B    c
ATOM   5808  C   ALA H 346     -21.825   16.968 -13.133  1.00  9.66      B    c
ATOM   5809  O   ALA H 346     -21.347   17.196 -14.244  1.00  9.39      B    o
ATOM   5810  N   GLY H 347     -22.883   16.182 -12.948  1.00 10.04      B    N
ATOM   5811  CA  GLY H 347     -23.684   15.689 -14.067  1.00 10.68      B    c
ATOM   5812  C   GLY H 347     -22.964   14.606 -14.846  1.00 10.90      B    c
ATOM   5813  O   GLY H 347     -23.490   14.064 -15.819  1.00 11.46      B    o
ATOM   5814  N   SER H 348     -21.714   14.370 -14.467  1.00 10.30      B    N
ATOM   5815  CA  SER H 348     -20.844   13.436 -15.165  1.00  9.94      B    c
ATOM   5816  CB  SER H 348     -19.833   14.200 -16.022  1.00  9.88      B    c
ATOM   5817  OG  SER H 348     -20.488   15.064 -16.934  1.00 10.09      B    o
ATOM   5818  C   SER H 348     -20.120   12.619 -14.104  1.00  9.60      B    c
ATOM   5819  O   SER H 348     -20.367   12.796 -12.912  1.00  9.59      B    o
ATOM   5820  N   VAL H 349     -19.286   11.677 -14.528  1.00  9.54      B    N
ATOM   5821  CA  VAL H 349     -18.647   10.766 -13.581  1.00  9.56      B    c
ATOM   5822  CB  VAL H 349     -19.075    9.305 -13.809  1.00  9.28      B    c
ATOM   5823  CGI VAL H 349     -18.659    8.442 -12.626  1.00  9.24      B    c
ATOM   5824  CG2 VAL H 349     -20.576    9.222 -14.033  1.00  9.94      B    c
ATOM   5825  C   VAL H 349     -17.126   10.861 -13.619  1.00  9.59      B    c
ATOM   5826  O   VAL H 349     -16.513   10.752 -14.681  1.00  9.69      B    o
ATOM   5827  N   SER H 350     -16.520   11.027 -12.449  1.00  9.93      B    N
ATOM   5828  CA  SER H 350     -15.073   11.104 -12.357  1.00 10.44      B    c
ATOM   5829  CB  SER H 350     -14.646   12.227 -11.408  1.00 10.04      B    c
ATOM   5830  OG  SER H 350     -14.584   13.468 -12.090  1.00  8.41      B    o
ATOM   5831  C   SER H 350     -14.459    9.773 -11.938  1.00 11.45      B    c
ATOM   5832  O   SER H 350     -15.000    9.062 -11.089  1.00 11.58      B    o
ATOM   5833  N   PHE H 351     -13.354    9.424 -12.587  1.00 12.28      B    N
ATOM   5834  CA  PHE H 351     -12.717    8.129 -12.403  1.00 13.04      B    c
ATOM   5835  CB  PHE H 351     -12.800    7.315 -13.697  1.00 12.87      B    c
ATOM   5836  CG  PHE H 351     -11.985    6.052 -13.677  1.00 13.52      B    c
ATOM   5837  CD1 PHE H 351     -12.081    5.165 -12.615  1.00 13.76      B    c
ATOM   5838  CE1 PHE H 351     -11.300    4.022 -12.574  1.00 14.10      B    c
ATOM   5839  CZ  PHE H 351     -10.453    3.726 -13.629  1.00 14.07      B    c
ATOM   5840  CE2 PHE H 351     -10.381    4.583 -14.715  1.00 14.14      B    c
ATOM   5841  CD2 PHE H 351     -11.134    5.744 -14.728  1.00 13.92      B    c
ATOM   5842  C   PHE H 351     -11.262    8.315 -11.993  1.00 13.84      B    c
ATOM   5843  O   PHE H 351     -10.528    9.090 -12.608  1.00 13.96      B    o
ATOM   5844  N   PHE H 352     -10.866    7.641 -10.919  1.00 14.72      B    N
ATOM   5845  CA  PHE H 352      -9.500    7.717 -10.418  1.00 15.98      B    c
ATOM   5846  CB  PHE H 352      -9.490    8.210  -8.966  1.00 15.75      B    c
ATOM   5847  CG  PHE H 352     -10.600    9.176  -8.638  1.00 15.51      B    c
ATOM   5848  CD1 PHE H 352     -11.835    8.713  -8.210  1.00 15.05      B    c
ATOM   5849  CE1 PHE H 352     -12.836    9.597  -7.837  1.00 14.05      B    c
ATOM   5850  CZ  PHE H 352     -12.592   10.955  -7.844  1.00 13.28      B    c
ATOM   5851  CE2 PHE H 352     -11.343   11.426  -8.201  1.00 13.71      B    c
ATOM   5852  CD2 PHE H 352     -10.347   10.536  -8.570  1.00 14.94      B    c
ATOM   5853  C   PHE H 352      -8.820    6.350 -10.511  1.00 17.56      B    c
ATOM   5854  O   PHE H 352      -9.259    5.390  -9.880  1.00 17.74      B    O
ATOM   5855  N   PRO H 353      -7.728    6.266 -11.288  1.00 19.05      B    N
ATOM   5856  CA  PRO H 353      -7.203    5.002 -11.802  1.00 20.40      B    c
ATOM   5857  CB  PRO H 353      -6.180    5.443 -12.859  1.00 20.26      B    c
ATOM   5858  CG  PRO H 353      -6.492    6.878 -13.145  1.00 19.71      B    c
ATOM   5859  CD  PRO H 353      -7.032    7.424 -11.869  1.00 18.97      B    c
ATOM   5860  C   PRO H 353      -6.522    4.135 -10.743  1.00 21.94      B    c
ATOM   5861  O   PRO H 353      -6.511    2.911 -10.873  1.00 22.29      B    o
```

ATOM 5862 N GLN H 354 -5.904 4.757 -9.742 1.00 23.38 B N
ATOM 5863 CA GLN H 354 -5.118 4.007 -8.760 1.00 24.64 B C
ATOM 5864 CB GLN H 354 -3.621 4.108 -9.064 1.00 24.93 B C
ATOM 5865 CG GLN H 354 -3.259 5.210 -10.038 1.00 26.00 B C
ATOM 5866 CD GLN H 354 -3.331 6.581 -9.407 1.00 25.92 B C
ATOM 5867 OE1 GLN H 354 -2.732 6.830 -8.360 1.00 25.67 B O
ATOM 5868 NE2 GLN H 354 -4.094 7.475 -10.025 1.00 24.27 B N
ATOM 5869 C GLN H 354 -5.393 4.393 -7.307 1.00 24.85 B C
ATOM 5870 O GLN H 354 -5.653 5.558 -7.007 1.00 24.51 B O
ATOM 5871 N ALA H 355 -5.162 3.446 -6.399 1.00 25.22 B N
ATOM 5872 CA ALA H 355 -5.563 3.599 -4.997 1.00 25.34 B C
ATOM 5873 CB ALA H 355 -5.112 2.400 -4.173 1.00 25.09 B C
ATOM 5874 C ALA H 355 -5.092 4.910 -4.354 1.00 24.92 B C
ATOM 5875 O ALA H 355 -5.901 5.647 -3.790 1.00 25.23 B O
ATOM 5876 N GLU H 356 -3.775 5.074 -4.242 1.00 23.93 B N
ATOM 5877 CA GLU H 356 -3.138 6.394 -4.141 1.00 22.77 B C
ATOM 5878 CB GLU H 356 -2.214 6.635 -5.339 1.00 23.22 B C
ATOM 5879 CG GLU H 356 -0.973 5.756 -5.344 1.00 26.33 B C
ATOM 5880 CD GLU H 356 -0.571 5.312 -3.948 1.00 30.93 B C
ATOM 5881 OE1 GLU H 356 -1.012 4.225 -3.516 1.00 31.97 B O
ATOM 5882 OE2 GLU H 356 0.074 6.111 -3.237 1.00 32.21 B O
ATOM 5883 C GLU H 356 -4.114 7.558 -3.990 1.00 21.31 B C
ATOM 5884 O GLU H 356 -4.098 8.270 -2.985 1.00 21.01 B O
ATOM 5885 N THR H 357 -4.868 7.819 -5.052 1.00 19.51 B N
ATOM 5886 CA THR H 357 -5.718 9.000 -5.138 1.00 17.55 B C
ATOM 5887 CB THR H 357 -6.391 9.086 -6.519 1.00 17.30 B C
ATOM 5888 OG1 THR H 357 -5.644 8.305 -7.462 1.00 17.32 B O
ATOM 5889 CG2 THR H 357 -6.472 10.531 -6.997 1.00 17.72 B C
ATOM 5890 C THR H 357 -6.801 9.006 -4.063 1.00 16.62 B C
ATOM 5891 O THR H 357 -7.346 10.058 -3.730 1.00 17.29 B O
ATOM 5892 N CYS H 358 -7.179 7.822 -3.594 1.00 14.88 B N
ATOM 5893 CA CYS H 358 -8.414 7.676 -2.833 1.00 13.15 B C
ATOM 5894 CB CYS H 358 -9.479 6.949 -3.655 1.00 13.04 B C
ATOM 5895 SG CYS H 358 -10.003 7.836 -5.144 1.00 14.02 B S
ATOM 5896 C CYS H 358 -8.202 6.982 -1.492 1.00 12.08 B C
ATOM 5897 O CYS H 358 -7.521 5.959 -1.408 1.00 12.15 B O
ATOM 5898 N LYS H 359 -8.741 7.585 -0.438 1.00 11.35 B N
ATOM 5899 CA LYS H 359 -8.861 6.922 0.853 1.00 11.01 B C
ATOM 5900 CB LYS H 359 -8.119 7.713 1.931 1.00 11.16 B C
ATOM 5901 CG LYS H 359 -7.413 8.953 1.414 1.00 13.28 B C
ATOM 5902 CD LYS H 359 -5.907 8.816 1.540 1.00 16.11 B C
ATOM 5903 CE LYS H 359 -5.199 10.088 1.104 1.00 17.91 B C
ATOM 5904 NZ LYS H 359 -3.719 9.952 1.184 1.00 20.99 B N
ATOM 5905 C LYS H 359 -10.325 6.777 1.242 1.00 10.46 B C
ATOM 5906 O LYS H 359 -11.191 7.462 0.697 1.00 10.70 B O
ATOM 5907 N VAL H 360 -10.579 5.977 2.270 1.00 9.99 B N
ATOM 5908 CA VAL H 360 -11.939 5.576 2.592 1.00 9.84 B C
ATOM 5909 CB VAL H 360 -12.406 4.401 1.712 1.00 9.42 B C
ATOM 5910 CGI VAL H 360 -11.411 3.253 1.784 1.00 10.07 B C
ATOM 5911 CG2 VAL H 360 -13.796 3.944 2.125 1.00 9.56 B C
ATOM 5912 C VAL H 360 -12.087 5.214 4.063 1.00 9.98 B C
ATOM 5913 O VAL H 360 -11.267 4.485 4.622 1.00 9.96 B O
ATOM 5914 N GLN H 361 -13.109 5.780 4.696 1.00 10.39 B N
ATOM 5915 CA GLN H 361 -13.322 5.606 6.125 1.00 11.53 B C
ATOM 5916 CB GLN H 361 -12.858 6.851 6.883 1.00 12.03 B C
ATOM 5917 CG GLN H 361 -13.051 6.769 8.385 1.00 16.44 B C
ATOM 5918 CD GLN H 361 -11.812 7.176 9.152 1.00 25.16 B C
ATOM 5919 OE1 GLN H 361 -11.763 8.257 9.738 1.00 29.01 B O
ATOM 5920 NE2 GLN H 361 -10.773 6.352 9.080 1.00 27.20 B N
ATOM 5921 C GLN H 361 -14.795 5.340 6.415 1.00 11.15 B C

```
ATOM   5922  O   GLN H 361     -15.620   6.253   6.355  1.00 11.80      B    O
ATOM   5923  N   SER H 362     -15.136   4.078   6.650  1.00 10.90      B    N
ATOM   5924  CA  SER H 362     -16.529   3.677   6.634  1.00 10.30      B    C
ATOM   5925  CB  SER H 362     -17.326   4.548   7.603  1.00 10.47      B    C
ATOM   5926  OG  SER H 362     -18.616   4.011   7.823  1.00 11.17      B    O
ATOM   5927  C   SER H 362     -17.074   3.846   5.224  1.00  9.58      B    C
ATOM   5928  O   SER H 362     -16.419   3.474   4.250  1.00  9.48      B    O
ATOM   5929  N   ASN H 363     -18.182   4.569   5.115  1.00  9.12      B    N
ATOM   5930  CA  ASN H 363     -18.810   4.826   3.826  1.00  8.73      B    C
ATOM   5931  CB  ASN H 363     -20.329   4.778   3.972  1.00  9.01      B    C
ATOM   5932  CG  ASN H 363     -20.850   5.801   4.965  1.00  9.29      B    C
ATOM   5933  OD1 ASN H 363     -20.079   6.555   5.561  1.00  9.82      B    O
ATOM   5934  ND2 ASN H 363     -22.162   5.818   5.163  1.00 10.08      B    N
ATOM   5935  C   ASN H 363     -18.382   6.185   3.277  1.00  8.12      B    C
ATOM   5936  O   ASN H 363     -18.996   6.720   2.352  1.00  8.10      B    O
ATOM   5937  N   ARG H 364     -17.346   6.749   3.890  1.00  7.20      B    N
ATOM   5938  CA  ARG H 364     -16.777   8.017   3.457  1.00  6.82      B    C
ATOM   5939  CB  ARG H 364     -16.307   8.821   4.671  1.00  6.91      B    C
ATOM   5940  CG  ARG H 364     -16.741  10.271   4.655  1.00  7.92      B    C
ATOM   5941  CD  ARG H 364     -18.197  10.397   4.249  1.00  8.20      B    C
ATOM   5942  NE  ARG H 364     -18.377  11.314   3.127  1.00  8.70      B    N
ATOM   5943  CZ  ARG H 364     -19.450  12.077   2.958  1.00  8.88      B    C
ATOM   5944  NHl ARG H 364     -20.420  12.062   3.862  1.00  8.57      B    N
ATOM   5945  NH2 ARG H 364     -19.546  12.867   1.897  1.00 10.59      B    N
ATOM   5946  C   ARG H 364     -15.603   7.775   2.519  1.00  6.58      B    C
ATOM   5947  O   ARG H 364     -14.680   7.030   2.847  1.00  6.65      B    O
ATOM   5948  N   VAL H 365     -15.619   8.448   1.375  1.00  6.64      B    N
ATOM   5949  CA  VAL H 365     -14.526   8.350   0.419  1.00  6.54      B    C
ATOM   5950  CB  VAL H 365     -15.000   7.763  -0.922  1.00  5.95      B    C
ATOM   5951  CGI VAL H 365     -13.934   7.950  -1.990  1.00  5.48      B    C
ATOM   5952  CG2 VAL H 365     -15.350   6.292  -0.762  1.00  6.22      B    C
ATOM   5953  C   VAL H 365     -13.914   9.719   0.166  1.00  7.35      B    C
ATOM   5954  O   VAL H 365     -14.617  10.729   0.128  1.00  8.33      B    O
ATOM   5955  N   PHE H 366     -12.611   9.733  -0.081  1.00  7.37      B    N
ATOM   5956  CA  PHE H 366     -11.904  10.969  -0.360  1.00  7.44      B    C
ATOM   5957  CB  PHE H 366     -11.137  11.431   0.874  1.00  7.30      B    C
ATOM   5958  CG  PHE H 366     -12.009  11.714   2.054  1.00  6.70      B    C
ATOM   5959  CD1 PHE H 366     -12.571  10.677   2.778  1.00  6.70      B    C
ATOM   5960  CE1 PHE H 366     -13.347  10.932   3.894  1.00  5.94      B    C
ATOM   5961  CZ  PHE H 366     -13.546  12.236   4.311  1.00  5.71      B    C
ATOM   5962  CE2 PHE H 366     -12.990  13.279   3.593  1.00  5.96      B    C
ATOM   5963  CD2 PHE H 366     -12.235  13.015   2.467  1.00  6.52      B    C
ATOM   5964  C   PHE H 366     -10.939  10.777  -1.511  1.00  7.45      B    C
ATOM   5965  O   PHE H 366      -9.931  10.082  -1.381  1.00  7.45      B    O
ATOM   5966  N   CYS H 367     -11.212  11.453  -2.618  1.00  8.00      B    N
ATOM   5967  CA  CYS H 367     -10.408  11.281  -3.809  1.00  8.90      B    C
ATOM   5968  CB  CYS H 367     -11.217  10.596  -4.909  1.00  9.46      B    C
ATOM   5969  SG  CYS H 367     -11.640   8.877  -4.545  1.00 10.79      B    S
ATOM   5970  C   CYS H 367      -9.870  12.612  -4.297  1.00  9.09      B    C
ATOM   5971  O   CYS H 367     -10.363  13.674  -3.919  1.00  9.24      B    O
ATOM   5972  N   ASP H 368      -8.892  12.540  -5.188  1.00  9.54      B    N
ATOM   5973  CA  ASP H 368      -8.190  13.724  -5.637  1.00 10.55      B    C
ATOM   5974  CB  ASP H 368      -6.693  13.584  -5.372  1.00 10.53      B    C
ATOM   5975  CG  ASP H 368      -5.983  14.917  -5.352  1.00 11.11      B    C
ATOM   5976  OD1 ASP H 368      -6.335  15.787  -6.177  1.00 11.42      B    O
ATOM   5977  OD2 ASP H 368      -5.158  15.138  -4.441  1.00 11.35      B    O
ATOM   5978  C   ASP H 368      -8.442  13.949  -7.118  1.00 11.45      B    C
ATOM   5979  O   ASP H 368      -8.036  13.143  -7.955  1.00 12.05      B    O
ATOM   5980  N   THR H 369      -9.222  14.980  -7.425  1.00 12.41      B    N
ATOM   5981  CA  THR H 369      -9.359  15.444  -8.796  1.00 13.00      B    C
```

```
ATOM   5982  CB  THR H 369      -9.723  16.934  -8.846  1.00 12.69      B    C
ATOM   5983  OG1 THR H 369     -10.937  17.158  -8.117  1.00 11.72      B    o
ATOM   5984  CG2 THR H 369      -9.896  17.390 -10.289  1.00 13.33      B    c
ATOM   5985  C   THR H 369      -8.052  15.254  -9.548  1.00 14.13      B    c
ATOM   5986  O   THR H 369      -7.986  14.504 -10.520  1.00 14.72      B    o
ATOM   5987  N   MET H 370      -6.996  15.868  -9.029  1.00 15.25      B    N
ATOM   5988  CA  MET H 370      -5.822  16.195  -9.825  1.00 16.60      B    c
ATOM   5989  CB  MET H 370      -4.542  15.983  -9.019  1.00 17.42      B    c
ATOM   5990  CG  MET H 370      -3.815  17.270  -8.673  1.00 20.31      B    c
ATOM   5991  SD  MET H 370      -3.256  18.144 -10.144  1.00 26.43      B    s
ATOM   5992  CE  MET H 370      -4.817  18.449 -10.970  1.00 24.07      B    c
ATOM   5993  C   MET H 370      -5.752  15.466 -11.165  1.00 16.54      B    c
ATOM   5994  O   MET H 370      -5.659  16.108 -12.209  1.00 16.74      B    o
ATOM   5995  N   ASN H 371      -5.730  14.137 -11.146  1.00 16.35      B    N
ATOM   5996  CA  ASN H 371      -5.564  13.390 -12.394  1.00 16.07      B    c
ATOM   5997  CB  ASN H 371      -4.271  12.573 -12.386  1.00 16.41      B    c
ATOM   5998  CG  ASN H 371      -3.047  13.428 -12.644  1.00 16.71      B    c
ATOM   5999  OD1 ASN H 371      -2.747  13.766 -13.790  1.00 15.75      B    O
ATOM   6000  ND2 ASN H 371      -2.401  13.874 -11.572  1.00 17.76      B    N
ATOM   6001  C   ASN H 371      -6.767  12.552 -12.827  1.00 15.55      B    C
ATOM   6002  O   ASN H 371      -6.757  11.959 -13.907  1.00 15.84      B    O
ATOM   6003  N   SER H 372      -7.879  12.750 -12.126  1.00 14.76      B    N
ATOM   6004  CA  SER H 372      -9.165  12.189 -12.526  1.00 13.91      B    C
ATOM   6005  CB  SER H 372     -10.309  12.932 -11.832  1.00 14.04      B    C
ATOM   6006  OG  SER H 372     -10.226  14.328 -12.061  1.00 15.09      B    O
ATOM   6007  C   SER H 372      -9.372  12.202 -14.037  1.00 13.07      B    C
ATOM   6008  O   SER H 372      -8.839  13.056 -14.743  1.00 13.02      B    O
ATOM   6009  N   LEU H 373     -10.112  11.213 -14.526  1.00 12.23      B    N
ATOM   6010  CA  LEU H 373     -10.687  11.256 -15.864  1.00 11.45      B    C
ATOM   6011  CB  LEU H 373     -10.417   9.939 -16.594  1.00 11.43      B    C
ATOM   6012  CG  LEU H 373      -9.204   9.880 -17.524  1.00 11.04      B    C
ATOM   6013  CD1 LEU H 373      -7.988  10.551 -16.888  1.00 11.76      B    C
ATOM   6014  CD2 LEU H 373      -8.894   8.435 -17.915  1.00 10.49      B    C
ATOM   6015  C   LEU H 373     -12.188  11.472 -15.762  1.00 11.17      B    C
ATOM   6016  O   LEU H 373     -12.847  10.886 -14.904  1.00 11.27      B    O
ATOM   6017  N   THR H 374     -12.733  12.289 -16.655  1.00 10.70      B    N
ATOM   6018  CA  THR H 374     -14.144  12.637 -16.586  1.00 10.23      B    C
ATOM   6019  CB  THR H 374     -14.367  14.151 -16.730  1.00 10.24      B    C
ATOM   6020  OG1 THR H 374     -13.177  14.850 -16.344  1.00 11.25      B    O
ATOM   6021  CG2 THR H 374     -15.521  14.604 -15.849  1.00 10.52      B    C
ATOM   6022  C   THR H 374     -14.953  11.896 -17.641  1.00  9.54      B    C
ATOM   6023  O   THR H 374     -14.580  11.855 -18.813  1.00  9.70      B    o
ATOM   6024  N   LEU H 375     -16.035  11.266 -17.198  1.00  8.83      B    N
ATOM   6025  CA  LEU H 375     -16.731  10.270 -18.000  1.00  7.83      B    C
ATOM   6026  CB  LEU H 375     -16.360   8.861 -17.540  1.00  7.38      B    c
ATOM   6027  CG  LEU H 375     -14.878   8.495 -17.551  1.00  5.06      B    c
ATOM   6028  CD1 LEU H 375     -14.710   7.045 -17.124  1.00  2.41      B    c
ATOM   6029  CD2 LEU H 375     -14.288   8.729 -18.934  1.00  4.31      B    c
ATOM   6030  C   LEU H 375     -18.236  10.456 -17.878  1.00  7.79      B    c
ATOM   6031  O   LEU H 375     -18.724  10.928 -16.850  1.00  7.92      B    o
ATOM   6032  N   PRO H 376     -18.982   9.954 -18.871  1.00  7.51      B    N
ATOM   6033  CA  PRO H 376     -20.439  10.009 -18.882  1.00  7.90      B    c
ATOM   6034  CB  PRO H 376     -20.780   9.837 -20.362  1.00  7.90      B    c
ATOM   6035  CG  PRO H 376     -19.657   9.033 -20.908  1.00  7.97      B    c
ATOM   6036  CD  PRO H 376     -18.435   9.468 -20.150  1.00  7.40      B    c
ATOM   6037  C   PRO H 376     -21.063   8.881 -18.064  1.00  8.35      B    c
ATOM   6038  O   PRO H 376     -20.569   7.753 -18.085  1.00  8.71      B    o
ATOM   6039  N   SER H 377     -22.190   9.172 -17.421  1.00  9.11      B    N
ATOM   6040  CA  SER H 377     -22.937   8.165 -16.673  1.00  9.91      B    c
ATOM   6041  CB  SER H 377     -24.272   8.737 -16.191  1.00 10.23      B    c
```

```
ATOM   6042  OG  SER H 377     -24.293   10.150 -16.304  1.00 10.90      B    O
ATOM   6043  C   SER H 377     -23.180   6.915 -17.513   1.00 10.14      B    C
ATOM   6044  O   SER H 377     -23.678   5.906 -17.013   1.00 10.08      B    O
ATOM   6045  N   GLU H 378     -22.875   7.010 -18.803   1.00 10.71      B    N
ATOM   6046  CA  GLU H 378     -23.057   5.893 -19.721   1.00 11.40      B    C
ATOM   6047  CB  GLU H 378     -22.970   6.377 -21. 170  1.00 11.65      B    C
ATOM   6048  CG  GLU H 378     -24.261   6.977 -21.706   1.00 13.46      B    c
ATOM   6049  CD  GLU H 378     -24.671   8.241 -20.972   1.00 16.20      B    c
ATOM   6050  OE1 GLU H 378     -23.922   8.681 -20.074   1.00 15.73      B    o
ATOM   6051  OE2 GLU H 378     -25.749   8.788 -21.285   1.00 18.38      B    o
ATOM   6052  C   GLU H 378     -22.019   4.805 -19.468   1.00 11.27      B    c
ATOM   6053  O   GLU H 378     -22.196   3.657 -19.877   1.00 11.28      B    o
ATOM   6054  N   VAL H 379     -20.943   5.170 -18.779   1.00 11.31      B    N
ATOM   6055  CA  VAL H 379     -19.977   4.192 -18.296   1.00 11.59      B    c
ATOM   6056  CB  VAL H 379     -18.973   4.824 -17.315   1.00 11.27      B    c
ATOM   6057  CGI VAL H 379     -18.343   3.752 -16.440   1.00 11.60      B    c
ATOM   6058  CG2 VAL H 379     -17.905   5.597 -18.073   1.00 11.54      B    c
ATOM   6059  C   VAL H 379     -20.675   3.023 -17.610   1.00 12. 16     B    c
ATOM   6060  O   VAL H 379     -20.260   1.872 -17.750   1.00 12.51      B    o
ATOM   6061  N   ASN H 380     -21.769   3.317 -16.915   1.00 12.98      B    N
ATOM   6062  CA  ASN H 380     -22.428   2.328 -16.068   1.00 14.00      B    c
ATOM   6063  CB  ASN H 380     -23.553   2.973 -15.258   1.00 14.59      B    c
ATOM   6064  CG  ASN H 380     -23.038   3.964 -14.234   1.00 17.09      B    c
ATOM   6065  OD1 ASN H 380     -22.893   3.637 -13.056   1.00 20.41      B    o
ATOM   6066  ND2 ASN H 380     -22.690   5.160 -14.693   1.00 18.86      B    N
ATOM   6067  C   ASN H 380     -22.954   1.1 15 -16.833   1.00 13.96      B    c
ATOM   6068  O   ASN H 380     -22.973   0.005 -16.302   1.00 14.38      B    o
ATOM   6069  N   LEU H 381     -23.459   1.343 -18.042   1.00 13.61      B    N
ATOM   6070  CA  LEU H 381     -24.024   0.261 -18.844   1.00 13.72      B    c
ATOM   6071  CB  LEU H 381     -24.514   0.792 -20.191   1.00 13.79      B    c
ATOM   6072  CG  LEU H 381     -25.004   2.240 -20.194   1.00 14.92      B    c
ATOM   6073  CD1 LEU H 381     -25.409   2.670 -21 .595  1.00 15.56      B    c
ATOM   6074  CD2 LEU H 381     -26.157   2.422 -19.218   1.00 15.78      B    c
ATOM   6075  C   LEU H 381     -22.982   -0.827 -19.060   1.00 13.62      B    c
ATOM   6076  O   LEU H 381     -23.314   -1.973 -19.365   1.00 13.57      B    o
ATOM   6077  N   CYS H 382     -21.729   -0.478 -18.796   1.00 13.47      B    N
ATOM   6078  CA  CYS H 382     -20.615   -1.367 -19.068   1.00 13.57      B    c
ATOM   6079  CB  CYS H 382     -19.321   -0.565 -19.165   1.00 13.62      B    c
ATOM   6080  SG  CYS H 382     -18.814   -0.217 -20.852   1.00 15.64      B    s
ATOM   6081  C   CYS H 382     -20.494   -2.432 -17.987   1.00 13.33      B    c
ATOM   6082  O   CYS H 382     -19.948   -3.510 -18.224   1.00 13.57      B    o
ATOM   6083  N   ASN H 383     -21.096   -2.163 -16.833   1.00 13.21      B    N
ATOM   6084  CA  ASN H 383     -21.267   -3.181 -15.803   1.00 13.22      B    c
ATOM   6085  CB  ASN H 383     -21.854   -2.568 -14.531   1.00 13.18      B    c
ATOM   6086  CG  ASN H 383     -21.059   -1.381 -14.034   1.00 13.42      B    c
ATOM   6087  OD1 ASN H 383     -19.830   -1.418 -13.985   1.00 13.68      B    o
ATOM   6088  ND2 ASN H 383     -21.761   -0.330 -13.626   1.00 14.32      B    N
ATOM   6089  C   ASN H 383     -22.159   -4.317 -16.277   1.00 13.28      B    c
ATOM   6090  O   ASN H 383     -22.096   -5.428 -15.751   1.00 13.50      B    o
ATOM   6091  N   VAL H 384     -23.092   -3.990 -17. 164  1.00 13.24      B    N
ATOM   6092  CA  VAL H 384     -24.065   -4.964 -17.630   1.00 13.29      B    c
ATOM   6093  CB  VAL H 384     -25.484   -4.367 -17.709   1.00 13.28      B    c
ATOM   6094  CGI VAL H 384     -26.371   -5.222 -18.601   1.00 13.73      B    c
ATOM   6095  CG2 VAL H 384     -26.083   -4.241 -16.315   1.00 12.76      B    c
ATOM   6096  C   VAL H 384     -23.677   -5.563 -18.977   1.00 13.57      B    c
ATOM   6097  O   VAL H 384     -23.940   -6.737 -19.233   1.00 13.31      B    o
ATOM   6098  N   ASP H 385     -23.060   -4.764 -19.843   1.00 14.07      B    N
ATOM   6099  CA  ASP H 385     -22.923   -5.172 -21.238   1.00 14.61      B    c
ATOM   6100  CB  ASP H 385     -23.915   -4.459 -22.154   1.00 14.71      B    c
ATOM   6101  CG  ASP H 385     -24.584   -5.410 -23. 130  1.00 16.69      B    c
```

```
ATOM   6102  OD1 ASP H 385     -24.093   -6.549 -23.281   1.00 18.63      B    O
ATOM   6103  OD2 ASP H 385     -25.614   -5.030 -23.724   1.00 19.10      B    O
ATOM   6104  C   ASP H 385     -21.525   -5.244 -21.851   1.00 14.63      B    C
ATOM   6105  O   ASP H 385     -21.203   -6.221 -22.526   1.00 14.34      B    O
ATOM   6106  N   ILE H 386     -20.722   -4.198 -21.691   1.00 14.54      B    N
ATOM   6107  CA  ILE H 386     -19.435   -4.146 -22.382   1.00 14.46      B    C
ATOM   6108  CB  ILE H 386     -18.772   -5.540 -22.417   1.00 13.83      B    C
ATOM   6109  CGI ILE H 386     -18.450   -6.032 -21.009   1.00 13.44      B    C
ATOM   6110  CD1 ILE H 386     -18.701   -7.516 -20.821   1.00 12.39      B    C
ATOM   6111  CG2 ILE H 386     -17.533   -5.525 -23.298   1.00 13.51      B    C
ATOM   6112  C   ILE H 386     -19.673   -3.755 -23.830   1.00 14.73      B    C
ATOM   6113  O   ILE H 386     -19.266   -2.682 -24.274   1.00 14.68      B    O
ATOM   6114  N   PHE H 387     -20.135   -4.733 -24.601   1.00 14.71      B    N
ATOM   6115  CA  PHE H 387     -20.696   -4.482 -25.915   1.00 14.78      B    C
ATOM   6116  CB  PHE H 387     -20.739   -5.766 -26.733   1.00 14.77      B    C
ATOM   6117  CG  PHE H 387     -19.482   -6.569 -26.647   1.00 14.75      B    C
ATOM   6118  CD1 PHE H 387     -19.407   -7.658 -25.797   1.00 15.03      B    C
ATOM   6119  CE1 PHE H 387     -18.229   -8.368 -25.662   1.00 14.62      B    C
ATOM   6120  CZ  PHE H 387     -17.093   -7.943 -26.318   1.00 14.55      B    C
ATOM   6121  CE2 PHE H 387     -17.136   -6.809 -27.103   1.00 14.68      B    C
ATOM   6122  CD2 PHE H 387     -18.316   -6.103 -27.227   1.00 14.61      B    C
ATOM   6123  C   PHE H 387     -22.080   -3.871 -25.821   1.00 14.91      B    C
ATOM   6124  O   PHE H 387     -22.992   -4.445 -25.228   1.00 14.86      B    O
ATOM   6125  N   ASN H 388     -22.144   -2.610 -26.216   1.00 15.11      B    N
ATOM   6126  CA  ASN H 388     -23.383   -1.869 -26.295   1.00 15.38      B    C
ATOM   6127  CB  ASN H 388     -23.968   -1.663 -24.897   1.00 14.86      B    C
ATOM   6128  CG  ASN H 388     -23.005   -0.958 -23.963   1.00 14.86      B    C
ATOM   6129  OD1 ASN H 388     -22.936    0.270 -23.935   1.00 12.80      B    O
ATOM   6130  ND2 ASN H 388     -22.213   -1.736 -23.234   1.00 15.97      B    N
ATOM   6131  C   ASN H 388     -23.023   -0.526 -26.906   1.00 16.11      B    C
ATOM   6132  O   ASN H 388     -21.965    0.024 -26.599   1.00 15.92      B    O
ATOM   6133  N   PRO H 389     -23.772   -0.117 -27.935   1.00 16.99      B    N
ATOM   6134  CA  PRO H 389     -23.716    1.289 -28.309   1.00 17.40      B    C
ATOM   6135  CB  PRO H 389     -24.965    1.468 -29.176   1.00 17.72      B    C
ATOM   6136  CG  PRO H 389     -25.904    0.425 -28.694   1.00 17.47      B    C
ATOM   6137  CD  PRO H 389     -25.041   -0.747 -28.339   1.00 17.05      B    C
ATOM   6138  C   PRO H 389     -23.810    2.170 -27.071   1.00 17.86      B    C
ATOM   6139  O   PRO H 389     -24.276    1.718 -26.025   1.00 18.45      B    O
ATOM   6140  N   LYS H 390     -23.335    3.406 -27.180   1.00 17.97      B    N
ATOM   6141  CA  LYS H 390     -23.325    4.318 -26.045   1.00 18.06      B    C
ATOM   6142  CB  LYS H 390     -24.373    3.904 -25.009   1.00 17.92      B    C
ATOM   6143  CG  LYS H 390     -25.807    4.197 -25.424   1.00 18.58      B    C
ATOM   6144  CD  LYS H 390     -26.259    5.564 -24.935   1.00 20.61      B    C
ATOM   6145  CE  LYS H 390     -27.775    5.656 -24.875   1.00 21.48      B    C
ATOM   6146  NZ  LYS H 390     -28.387    5.669 -26.232   1.00 23.16      B    N
ATOM   6147  C   LYS H 390     -21.946    4.403 -25.400   1.00 18.01      B    C
ATOM   6148  O   LYS H 390     -21.382    5.490 -25.279   1.00 18.43      B    O
ATOM   6149  N   TYR H 391     -21.391    3.261 -25.011   1.00 17.68      B    N
ATOM   6150  CA  TYR H 391     -20.012    3.232 -24.539   1.00 17.33      B    C
ATOM   6151  CB  TYR H 391     -19.948    3.140 -23.015   1.00 17.42      B    C
ATOM   6152  CG  TYR H 391     -18.847    3.986 -22.423   1.00 17.27      B    C
ATOM   6153  CD1 TYR H 391     -18.602    5.263 -22.911   1.00 17.29      B    C
ATOM   6154  CE1 TYR H 391     -17.553    6.021 -22.434   1.00 17.32      B    C
ATOM   6155  CZ  TYR H 391     -16.698    5.486 -21.496   1.00 16.51      B    C
ATOM   6156  OH  TYR H 391     -15.654    6.241 -21.015   1.00 16.65      B    O
ATOM   6157  CE2 TYR H 391     -16.878    4.195 -21.045   1.00 16.52      B    C
ATOM   6158  CD2 TYR H 391     -17.933    3.444 -21.530   1.00 17.24      B    C
ATOM   6159  C   TYR H 391     -19.179    2.130 -25.176   1.00 17.43      B    C
ATOM   6160  O   TYR H 391     -19.459    0.946 -24.993   1.00 17.70      B    O
ATOM   6161  N   ASP H 392     -18.075    2.522 -25.804   1.00 17.56      B    N
```

```
ATOM   6162  CA  ASP H 392     -16.973   1.599 -26.012  1.00 17.69      B    C
ATOM   6163  CB  ASP H 392     -16.119   2.003 -27.214  1.00 17.89      B    C
ATOM   6164  CG  ASP H 392     -16.587   3.290 -27.853  1.00 18.86      B    C
ATOM   6165  OD1 ASP H 392     -16.582   4.332 -27.165  1.00 20.34      B    O
ATOM   6166  OD2 ASP H 392     -16.931   3.269 -29.053  1.00 18.51      B    O
ATOM   6167  C   ASP H 392     -16.115   1.473 -24.767  1.00 17.11      B    C
ATOM   6168  O   ASP H 392     -15.801   2.460 -24.101  1.00 17.04      B    O
ATOM   6169  N   CYS H 393     -15.736   0.239 -24.468  1.00 16.33      B    N
ATOM   6170  CA  CYS H 393     -15.683  -0.240 -23.102  1.00 16.17      B    C
ATOM   6171  CB  CYS H 393     -16.818  -1.230 -22.851  1.00 16.11      B    C
ATOM   6172  SG  CYS H 393     -17.226  -1.449 -21.117  1.00 20.23      B    S
ATOM   6173  C   CYS H 393     -14.355  -0.941 -22.926  1.00 15.37      B    C
ATOM   6174  O   CYS H 393     -14.044  -1.876 -23.663  1.00 15.15      B    O
ATOM   6175  N   LYS H 394     -13.482  -0.332 -22.138  1.00 14.91      B    N
ATOM   6176  CA  LYS H 394     -12.100  -0.755 -22.107  1.00 14.50      B    C
ATOM   6177  CB  LYS H 394     -11.242   0.294 -21.405  1.00 14.60      B    C
ATOM   6178  CG  LYS H 394     -11.613   1.723 -21.788  1.00 16.44      B    C
ATOM   6179  CD  LYS H 394     -10.460   2.688 -21.576  1.00 20.45      B    C
ATOM   6180  CE  LYS H 394     -10.252   2.974 -20.099  1.00 23.05      B    C
ATOM   6181  NZ  LYS H 394      -9.330   1.988 -19.467  1.00 24.13      B    N
ATOM   6182  C   LYS H 394     -11.955  -2.130 -21.463  1.00 14.00      B    C
ATOM   6183  O   LYS H 394     -12.593  -2.434 -20.454  1.00 14.14      B    O
ATOM   6184  N   ILE H 395     -11.118  -2.957 -22.077  1.00 13.28      B    N
ATOM   6185  CA  ILE H 395     -11.238  -4.407 -22.026  1.00 12.89      B    C
ATOM   6186  CB  ILE H 395     -12.208  -4.925 -23.106  1.00 12.75      B    C
ATOM   6187  CGI ILE H 395     -13.660  -4.699 -22.690  1.00 13.58      B    C
ATOM   6188  CD1 ILE H 395     -14.633  -4.719 -23.849  1.00 15.33      B    C
ATOM   6189  CG2 ILE H 395     -11.947  -6.396 -23.399  1.00 12.16      B    C
ATOM   6190  C   ILE H 395      -9.860  -4.906 -22.407  1.00 13.15      B    C
ATOM   6191  O   ILE H 395      -9.242  -4.353 -23.312  1.00 13.45      B    O
ATOM   6192  N   MET H 396      -9.462  -6.054 -21.877  1.00 13.06      B    N
ATOM   6193  CA  MET H 396      -8.356  -6.773 -22.482  1.00 13.00      B    C
ATOM   6194  CB  MET H 396      -7.104  -6.717 -21.605  1.00 13.34      B    C
ATOM   6195  CG  MET H 396      -7.052  -7.752 -20.500  1.00 14.30      B    C
ATOM   6196  SD  MET H 396      -5.571  -7.581 -19.484  1.00 18.50      B    S
ATOM   6197  CE  MET H 396      -5.752  -5.895 -18.904  1.00 17.80      B    C
ATOM   6198  C   MET H 396      -8.702  -8.200 -22.867  1.00 12.96      B    C
ATOM   6199  O   MET H 396      -9.615  -8.808 -22.309  1.00 13.04      B    O
ATOM   6200  N   THR H 397      -7.935  -8.734 -23.808  1.00 12.78      B    N
ATOM   6201  CA  THR H 397      -8.350  -9.888 -24.585  1.00 12.51      B    C
ATOM   6202  CB  THR H 397      -8.389  -9.563 -26.087  1.00 12.39      B    C
ATOM   6203  OG1 THR H 397      -9.593  -8.851 -26.394  1.00 12.50      B    O
ATOM   6204  CG2 THR H 397      -8.335 -10.839 -26.912  1.00 12.55      B    C
ATOM   6205  C   THR H 397      -7.350 -11.005 -24.366  1.00 12.58      B    C
ATOM   6206  O   THR H 397      -6.143 -10.772 -24.327  1.00 12.88      B    O
ATOM   6207  N   SER H 398      -7.859 -12.210 -24.165  1.00 12.55      B    N
ATOM   6208  CA  SER H 398      -7.082 -13.401 -24.410  1.00 12.76      B    C
ATOM   6209  CB  SER H 398      -6.083 -13.627 -23.273  1.00 12.52      B    C
ATOM   6210  OG  SER H 398      -5.764 -15.001 -23.133  1.00 12.72      B    O
ATOM   6211  C   SER H 398      -8.070 -14.539 -24.456  1.00 12.99      B    C
ATOM   6212  O   SER H 398      -8.838 -14.672 -25.410  1.00 13.13      B    O
ATOM   6213  N   LYS H 399      -8.182 -15.232 -23.330  1.00 13.01      B    N
ATOM   6214  CA  LYS H 399      -7.890 -16.651 -23.342  1.00 13.29      B    C
ATOM   6215  CB  LYS H 399      -6.739 -17.020 -24.279  1.00 13.79      B    C
ATOM   6216  CG  LYS H 399      -6.786 -16.279 -25.618  1.00 14.34      B    C
ATOM   6217  CD  LYS H 399      -7.835 -16.868 -26.552  1.00 16.43      B    C
ATOM   6218  CE  LYS H 399      -7.864 -16.139 -27.889  1.00 17.37      B    C
ATOM   6219  NZ  LYS H 399      -8.770 -16.802 -28.867  1.00 16.62      B    N
ATOM   6220  C   LYS H 399      -8.128 -17.609 -22.171  1.00 13.09      B    C
ATOM   6221  O   LYS H 399      -9.087 -18.376 -22.216  1.00 12.87      B    O
```

ATOM 6222 N THR H 400 -7.140 -17.783 -21.300 1.00 13.04 B N
ATOM 6223 CA THR H 400 -7.133 -18.953 -20.420 1.00 13.38 B C
ATOM 6224 CB THR H 400 -5.703 -19.453 -20.133 1.00 13.74 B C
ATOM 6225 OG1 THR H 400 -4.773 -18.763 -20.977 1.00 14.38 B O
ATOM 6226 CG2 THR H 400 -5.601 -20.950 -20.394 1.00 14.32 B C
ATOM 6227 C THR H 400 -7.866 -18.687 -19.104 1.00 13.20 B C
ATOM 6228 O THR H 400 -7.913 -17.551 -18.630 1.00 13.12 B O
ATOM 6229 N ASP H 401 -8.478 -19.728 -18.545 1.00 12.97 B N
ATOM 6230 CA ASP H 401 -8.896 -19.715 -17.145 1.00 12.50 B C
ATOM 6231 CB ASP H 401 -9.622 -21.022 -16.798 1.00 12.73 B C
ATOM 6232 CG ASP H 401 -10.854 -21.261 -17.651 1.00 13.98 B C
ATOM 6233 OD1 ASP H 401 -10.870 -20.793 -18.808 1.00 16.55 B O
ATOM 6234 OD2 ASP H 401 -11.708 -22.076 -17.236 1.00 14.80 B O
ATOM 6235 C ASP H 401 -7.683 -19.567 -16.222 1.00 12.13 B C
ATOM 6236 O ASP H 401 -6.906 -20.508 -16.071 1.00 12.31 B O
ATOM 6237 N VAL H 402 -7.609 -18.459 -15.489 1.00 11.49 B N
ATOM 6238 CA VAL H 402 -7.400 -18.523 -14.044 1.00 10.74 B C
ATOM 6239 CB VAL H 402 -7.004 -17.151 -13.456 1.00 10.60 B C
ATOM 6240 CGI VAL H 402 -7.433 -17.045 -11.998 1.00 11.26 B C
ATOM 6241 CG2 VAL H 402 -5.504 -16.918 -13.602 1.00 10.99 B C
ATOM 6242 C VAL H 402 -8.707 -18.986 -13.423 1.00 10.24 B C
ATOM 6243 O VAL H 402 -9.515 -19.616 -14.104 1.00 10.30 B O
ATOM 6244 N SER H 403 -9.015 -18.516 -12.218 1.00 9.76 B N
ATOM 6245 CA SER H 403 -10.286 -18.897 -11.605 1.00 9.18 B C
ATOM 6246 CB SER H 403 -10.485 -20.406 -11.726 1.00 9.41 B C
ATOM 6247 OG SER H 403 -9.349 -21.015 -12.313 1.00 10.82 B O
ATOM 6248 C SER H 403 -10.528 -18.449 -10.162 1.00 8.51 B C
ATOM 6249 O SER H 403 -9.701 -18.699 -9.285 1.00 8.30 B O
ATOM 6250 N SER H 404 -11.773 -18.053 -9.888 1.00 8.35 B N
ATOM 6251 CA SER H 404 -12.352 -18.148 -8.541 1.00 8.18 B C
ATOM 6252 CB SER H 404 -11.585 -17.257 -7.564 1.00 8.18 B C
ATOM 6253 OG SER H 404 -12.250 -16.019 -7.382 1.00 8.83 B O
ATOM 6254 C SER H 404 -13.841 -17.789 -8.505 1.00 7.62 B C
ATOM 6255 O SER H 404 -14.505 -17.759 -9.541 1.00 7.57 B O
ATOM 6256 N SER H 405 -14.357 -17.506 -7.310 1.00 7.08 B N
ATOM 6257 CA SER H 405 -15.777 -17.210 -7.151 1.00 6.53 B C
ATOM 6258 CB SER H 405 -16.568 -18.475 -6.802 1.00 6.42 B C
ATOM 6259 OG SER H 405 -17.786 -18.156 -6.146 1.00 5.66 B O
ATOM 6260 C SER H 405 -16.070 -16.101 -6.144 1.00 6.28 B C
ATOM 6261 O SER H 405 -15.289 -15.847 -5.226 1.00 5.98 B O
ATOM 6262 N VAL H 406 -17.254 -15.514 -6.281 1.00 6.22 B N
ATOM 6263 CA VAL H 406 -17.629 -14.309 -5.557 1.00 6.50 B C
ATOM 6264 CB VAL H 406 -17.390 -13.053 -6.414 1.00 6.45 B C
ATOM 6265 CGI VAL H 406 -17.384 -11.811 -5.546 1.00 7.66 B C
ATOM 6266 CG2 VAL H 406 -16.090 -13.177 -7.191 1.00 7.38 B C
ATOM 6267 C VAL H 406 -19.115 -14.377 -5.237 1.00 6.24 B C
ATOM 6268 O VAL H 406 -19.946 -14.488 -6.138 1.00 6.14 B O
ATOM 6269 N ILE H 407 -19.450 -14.313 -3.955 1.00 6.32 B N
ATOM 6270 CA ILE H 407 -20.831 -14.478 -3.534 1.00 6.60 B C
ATOM 6271 CB ILE H 407 -20.925 -15.154 -2.163 1.00 6.27 B C
ATOM 6272 CGI ILE H 407 -20.643 -16.651 -2.296 1.00 6.19 B C
ATOM 6273 CD1 ILE H 407 -21.477 -17.514 -1.376 1.00 8.34 B C
ATOM 6274 CG2 ILE H 407 -22.294 -14.923 -1.550 1.00 6.42 B C
ATOM 6275 C ILE H 407 -21.570 -13.149 -3.497 1.00 7.20 B C
ATOM 6276 O ILE H 407 -21.094 -12.176 -2.913 1.00 7.42 B O
ATOM 6277 N THR H 408 -22.792 -13.155 -4.016 1.00 7.57 B N
ATOM 6278 CA THR H 408 -23.563 -11.933 -4.148 1.00 8.19 B C
ATOM 6279 CB THR H 408 -24.066 -11.739 -5.587 1.00 8.15 B C
ATOM 6280 OG1 THR H 408 -24.863 -12.866 -5.971 1.00 8.88 B O
ATOM 6281 CG2 THR H 408 -22.893 -11.606 -6.542 1.00 7.93 B C

```
ATOM   6282  C   THR H 408     -24.753 -11.933  -3.203  1.00  8.55      B    C
ATOM   6283  O   THR H 408     -24.998 -12.905  -2.488  1.00  9.07      B    O
ATOM   6284  N   SER H 409     -25.513 -10.844  -3.238  1.00  8.70      B    N
ATOM   6285  CA  SER H 409     -26.644 -10.667  -2.344  1.00  9.20      B    C
ATOM   6286  CB  SER H 409     -27.266  -9.284  -2.543  1.00  9.72      B    C
ATOM   6287  OG  SER H 409     -26.279  -8.269  -2.491  1.00 10.75      B    O
ATOM   6288  C   SER H 409     -27.686 -11.747  -2.596  1.00  9.01      B    C
ATOM   6289  O   SER H 409     -28.360 -12.203  -1.671  1.00  9.02      B    O
ATOM   6290  N   LEU H 410     -27.804 -12.160  -3.853  1.00  8.91      B    N
ATOM   6291  CA  LEU H 410     -28.962 -12.921  -4.302  1.00  9.29      B    C
ATOM   6292  CB  LEU H 410     -29.901 -12.033  -5.118  1.00  9.61      B    C
ATOM   6293  CG  LEU H 410     -31.317 -11.873  -4.558  1.00  9.70      B    C
ATOM   6294  CD1 LEU H 410     -31.289 -11.183  -3.203  1.00 11.11      B    C
ATOM   6295  CD2 LEU H 410     -32.204 -11.113  -5.532  1.00  9.16      B    C
ATOM   6296  C   LEU H 410     -28.533 -14.134  -5.119  1.00  9.12      B    C
ATOM   6297  O   LEU H 410     -29.364 -14.840  -5.690  1.00  9.08      B    O
ATOM   6298  N   GLY H 411     -27.228 -14.365  -5.173  1.00  9.03      B    N
ATOM   6299  CA  GLY H 411     -26.691 -15.606  -5.706  1.00  8.44      B    C
ATOM   6300  C   GLY H 411     -25.180 -15.615  -5.632  1.00  7.91      B    C
ATOM   6301  O   GLY H 411     -24.594 -15.123  -4.668  1.00  7.85      B    O
ATOM   6302  N   ALA H 412     -24.546 -16.095  -6.694  1.00  7.30      B    N
ATOM   6303  CA  ALA H 412     -23.095 -16.167  -6.738  1.00  6.92      B    C
ATOM   6304  CB  ALA H 412     -22.607 -17.439  -6.062  1.00  6.90      B    C
ATOM   6305  C   ALA H 412     -22.593 -16.098  -8.173  1.00  6.99      B    C
ATOM   6306  O   ALA H 412     -23.277 -16.525  -9.102  1.00  6.94      B    O
ATOM   6307  N   ILE H 413     -21.415 -15.510  -8.349  1.00  7.29      B    N
ATOM   6308  CA  ILE H 413     -20.705 -15.567  -9.622  1.00  7.49      B    C
ATOM   6309  CB  ILE H 413     -20.073 -14.207  -9.961  1.00  7.24      B    C
ATOM   6310  CGI ILE H 413     -21.142 -13.236 -10.466  1.00  7.18      B    C
ATOM   6311  CD1 ILE H 413     -20.589 -12.045 -11.233  1.00  7.70      B    C
ATOM   6312  CG2 ILE H 413     -18.958 -14.377 -10.983  1.00  7.70      B    C
ATOM   6313  C   ILE H 413     -19.596 -16.608  -9.554  1.00  7.94      B    C
ATOM   6314  O   ILE H 413     -18.965 -16.775  -8.512  1.00  8.39      B    O
ATOM   6315  N   VAL H 414     -19.276 -17.221 -10.687  1.00  8.22      B    N
ATOM   6316  CA  VAL H 414     -18.141 -18.134 -10.734  1.00  8.77      B    C
ATOM   6317  CB  VAL H 414     -18.558 -19.593 -10.482  1.00  8.57      B    C
ATOM   6318  CGI VAL H 414     -19.806 -19.936 -11.279  1.00  9.12      B;   C
ATOM   6319  CG2 VAL H 414     -17.416 -20.538 -10.825  1.00  8.90      B;   C
ATOM   6320  C   VAL H 414     -17.323 -18.031 -12.015  1.00  8.92      B    C
ATOM   6321  O   VAL H 414     -17.803 -18.347 -13.105  1.00  9.00      B    O
ATOM   6322  N   SER H 415     -16.058 -17.659 -11.853  1.00  8.97      B    N
ATOM   6323  CA  SER H 415     -15.120 -17.594 -12.962  1.00  9.02      B    C
ATOM   6324  CB  SER H 415     -14.260 -16.335 -12.855  1.00  8.98      B    C
ATOM   6325  OG  SER H 415     -15.043 -15.218 -12.473  1.00  9.54      B    O
ATOM   6326  C   SER H 415     -14.235 -18.832 -12.987  1.00  9.36      B    C
ATOM   6327  O   SER H 415     -13.326 -18.975 -12.170  1.00  9.61      B    O
ATOM   6328  N   CYS H 416     -14.602 -19.786 -13.834  1.00  9.57      B    N
ATOM   6329  CA  CYS H 416     -13.851 -21.023 -13.963  1.00  9.61      B    C
ATOM   6330  CB  CYS H 416     -14.801 -22.216 -14.038  1.00  9.62      B    C
ATOM   6331  SG  CYS H 416     -14.118 -23.727 -13.341  1.00 11.33      B    S
ATOM   6332  C   CYS H 416     -12.998 -20.973 -15.215  1.00  9.61      B    C
ATOM   6333  O   CYS H 416     -13.519 -20.829 -16.320  1.00  9.80      B    O
ATOM   6334  N   TYR H 417     -11.684 -20.941 -15.027  1.00  9.48      B    N
ATOM   6335  CA  TYR H 417     -10.772 -20.739 -16.142  1.00  9.28      B    C
ATOM   6336  CB  TYR H 417     -10.307 -19.281 -16.205  1.00  9.17      B    C
ATOM   6337  CG  TYR H 417     -11.358 -18.318 -16.714  1.00  8.71      B    C
ATOM   6338  CD1 TYR H 417     -11.483 -17.048 -16.167  1.00  8.54      B    C
ATOM   6339  CE1 TYR H 417     -12.425 -16.159 -16.635  1.00  9.56      B    C
ATOM   6340  CZ  TYR H 417     -13.230 -16.516 -17.693  1.00  9.83      B    C
ATOM   6341  OH  TYR H 417     -14.184 -15.638 -18.143  1.00 10.51      B;   O
```

ATOM 6342 CE2 TYR H 417 -13.122 -17.765 -18.263 1.00 9.36 B C
ATOM 6343 CD2 TYR H 417 -12.177 -18.651 -17.786 1.00 8.95 B C
ATOM 6344 C TYR H 417 -9.572 -21.677 -16.068 1.00 9.35 B c
ATOM 6345 O TYR H 417 -9.336 -22.318 -15.044 1.00 9.11 B o
ATOM 6346 N GLY H 418 -8.830 -21.762 -17.169 1.00 9.71 B N
ATOM 6347 CA GLY H 418 -7.678 -22.656 -17.263 1.00 9.95 B c
ATOM 6348 C GLY H 418 -8.045 -24.101 -16.993 1.00 10.09 B c
ATOM 6349 O GLY H 418 -9.082 -24.584 -17.450 1.00 10.17 B o
ATOM 6350 N LYS H 419 -7.251 -24.756 -16.154 1.00 10.17 B N
ATOM 6351 CA LYS H 419 -7.426 -26.177 -15.896 1.00 10.50 B c
ATOM 6352 CB LYS H 419 -6.086 -26.827 -15.545 1.00 11.09 B c
ATOM 6353 CG LYS H 419 -5.332 -27.389 -16.738 1.00 12.94 B c
ATOM 6354 CD LYS H 419 -4.265 -28.377 -16.297 1.00 15.52 B c
ATOM 6355 CE LYS H 419 -3.705 -29.152 -17.479 1.00 17.07 B c
ATOM 6356 NZ LYS H 419 -3.179 -28.247 -18.538 1.00 19.30 B N
ATOM 6357 C LYS H 419 -8.447 -26.465 -14.798 1.00 10.23 B c
ATOM 6358 O LYS H 419 -8.613 -27.616 -14.398 1.00 10.58 B o
ATOM 6359 N THR H 420 -9.070 -25.426 -14.250 1.00 10.10 B N
ATOM 6360 CA THR H 420 -9.805 -25.587 -12.997 1.00 9.74 B c
ATOM 6361 CB THR H 420 -9.938 -24.270 -12.223 1.00 9.28 B c
ATOM 6362 OG1 THR H 420 -9.022 -23.306 -12.754 1.00 9.21 B o
ATOM 6363 CG2 THR H 420 -9.633 -24.499 -10.752 1.00 9.03 B c
ATOM 6364 C THR H 420 -11.181 -26.223 -13.168 1.00 9.95 B c
ATOM 6365 O THR H 420 -11.779 -26.160 -14.242 1.00 10.35 B o
ATOM 6366 N LYS H 421 -11.652 -26.879 -12.111 1.00 10.07 B N
ATOM 6367 CA LYS H 421 -12.961 -27.527 -12.115 1.00 10.21 B c
ATOM 6368 CB LYS H 421 -12.835 -28.979 -11.649 1.00 10.30 B c
ATOM 6369 CG LYS H 421 -12.705 -29.989 -12.776 1.00 12.43 B c
ATOM 6370 CD LYS H 421 -12.482 -31.391 -12.234 1.00 15.12 B c
ATOM 6371 CE LYS H 421 -11.769 -32.267 -13.251 1.00 15.21 B c
ATOM 6372 NZ LYS H 421 -11.047 -33.396 -12.601 1.00 15.98 B N
ATOM 6373 C LYS H 421 -13.933 -26.782 -11.206 1.00 10.09 B c
ATOM 6374 O LYS H 421 -13.600 -26.456 -10.067 1.00 10.36 B o
ATOM 6375 N CYS H 422 -15.155 -26.574 -11.685 1.00 9.81 B N
ATOM 6376 CA CYS H 422 -16.153 -25.863 -10.898 1.00 9.56 B c
ATOM 6377 CB CYS H 422 -16.222 -24.392 -11.302 1.00 9.72 B c
ATOM 6378 SG CYS H 422 -14.611 -23.591 -11.379 1.00 11.42 B s
ATOM 6379 C CYS H 422 -17.535 -26.499 -10.939 1.00 9.18 B c
ATOM 6380 O CYS H 422 -17.952 -27.056 -11.954 1.00 9.27 B o
ATOM 6381 N THR H 423 -18.273 -26.311 -9.851 1.00 8.93 B N
ATOM 6382 CA THR H 423 -19.417 -27.147 -9.527 1.00 8.64 B c
ATOM 6383 CB THR H 423 -19.014 -28.315 -8.606 1.00 8.32 B c
ATOM 6384 OG1 THR H 423 -17.878 -28.993 -9.154 1.00 7.97 B o
ATOM 6385 CG2 THR H 423 -20.165 -29.297 -8.456 1.00 8.36 B c
ATOM 6386 C THR H 423 -20.441 -26.297 -8.791 1.00 8.86 B c
ATOM 6387 O THR H 423 -20.133 -25.694 -7.763 1.00 9.26 B o
ATOM 6388 N ALA H 424 -21.676 -26.306 -9.279 1.00 8.74 B N
ATOM 6389 CA ALA H 424 -22.803 -25.836 -8.487 1.00 8.79 B c
ATOM 6390 CB ALA H 424 -23.693 -24.926 -9.317 1.00 8.94 B c
ATOM 6391 C ALA H 424 -23.605 -27.008 -7.932 1.00 8.84 B c
ATOM 6392 O ALA H 424 -24.158 -27.807 -8.687 1.00 9.24 B o
ATOM 6393 N SER H 425 -23.649 -27.113 -6.608 1.00 8.81 B N
ATOM 6394 CA SER H 425 -24.412 -28.166 -5.950 1.00 8.85 B c
ATOM 6395 CB SER H 425 -23.530 -28.925 -4.957 1.00 8.94 B c
ATOM 6396 OG SER H 425 -22.166 -28.871 -5.341 1.00 7.69 B o
ATOM 6397 C SER H 425 -25.626 -27.584 -5.235 1.00 9.01 B c
ATOM 6398 O SER H 425 -25.593 -26.447 -4.763 1.00 8.63 B o
ATOM 6399 N ASN H 426 -26.716 -28.345 -5.208 1.00 9.54 B N
ATOM 6400 CA ASN H 426 -27.971 -27.851 -4.658 1.00 10.19 B c
ATOM 6401 CB ASN H 426 -29.166 -28.508 -5.356 1.00 9.77 B c

```
ATOM   6402  CG  ASN H 426     -29.499 -29.874  -4.787  1.00  9.43      B    C
ATOM   6403  OD1 ASN H 426     -28.998 -30.259  -3.730  1.00  9.01      B    o
ATOM   6404  ND2 ASN H 426     -30.349 -30.615  -5.488  1.00  9.01      B    N
ATOM   6405  C   ASN H 426     -28.074 -28.031  -3.146  1.00 11.16      B    C
ATOM   6406  O   ASN H 426     -27.072 -28.247  -2.463  1.00 11.06      B    o
ATOM   6407  N   LYS H 427     -29.285 -27.847  -2.628  1.00 12.38      B    N
ATOM   6408  CA  LYS H 427     -29.569 -27.993  -1.203  1.00 13.52      B    C
ATOM   6409  CB  LYS H 427     -31.082 -28.017  -0.968  1.00 14.00      B    c
ATOM   6410  CG  LYS H 427     -31.681 -26.675  -0.585  1.00 16.18      B    c
ATOM   6411  CD  LYS H 427     -33.105 -26.838  -0.078  1.00 18.24      B    c
ATOM   6412  CE  LYS H 427     -33.487 -25.714   0.870  1.00 19.72      B    c
ATOM   6413  NZ  LYS H 427     -32.873 -25.888   2.216  1.00 21.43      B    N
ATOM   6414  C   LYS H 427     -28.943 -29.256  -0.621  1.00 13.71      B    c
ATOM   6415  O   LYS H 427     -28.329 -29.220   0.446  1.00 13.63      B    o
ATOM   6416  N   ASN H 428     -29.233 -30.390  -1.252  1.00 14.28      B    N
ATOM   6417  CA  ASN H 428     -28.838 -31.694  -0.729  1.00 14.60      B    c
ATOM   6418  CB  ASN H 428     -29.715 -32.800  -1.324  1.00 14.57      B    c
ATOM   6419  CG  ASN H 428     -31.103 -32.312  -1.690  1.00 13.24      B    c
ATOM   6420  OD1 ASN H 428     -31.832 -31.790  -0.846  1.00  9.74      B    o
ATOM   6421  ND2 ASN H 428     -31.503 -32.546  -2.935  1.00 12.83      B    N
ATOM   6422  C   ASN H 428     -27.367 -32.009  -0.984  1.00 14.83      B    c
ATOM   6423  O   ASN H 428     -26.834 -32.982  -0.451  1.00 15.25      B    o
ATOM   6424  N   ARG H 429     -26.755 -31.260  -1.895  1.00 14.78      B    N
ATOM   6425  CA  ARG H 429     -25.364 -31.488  -2.275  1.00 14.74      B    c
ATOM   6426  CB  ARG H 429     -24.626 -32.268  -1.184  1.00 14.93      B    c
ATOM   6427  CG  ARG H 429     -24.252 -31.435   0.031  1.00 16.26      B    c
ATOM   6428  CD  ARG H 429     -22.869 -30.821  -0.119  1.00 19.79      B    c
ATOM   6429  NE  ARG H 429     -22.634 -29.760   0.857  1.00 22.68      B    N
ATOM   6430  CZ  ARG H 429     -22.532 -29.958   2.167  1.00 23.54      B    c
ATOM   6431  NHl ARG H 429     -22.640 -31.182   2.667  1.00 22.87      B    N
ATOM   6432  NH2 ARG H 429     -22.321 -28.932   2.980  1.00 23.53      B    N
ATOM   6433  C   ARG H 429     -25.252 -32.217  -3.611  1.00 14.35      B    C
ATOM   6434  O   ARG H 429     -24.175 -32.285  -4.203  1.00 14.62      B    o
ATOM   6435  N   GLY H 430     -26.373 -32.752  -4.085  1.00 13.67      B    N
ATOM   6436  CA  GLY H 430     -26.519 -33.087  -5.496  1.00 12.80      B    C
ATOM   6437  C   GLY H 430     -26.014 -31.977  -6.397  1.00 12.11      B    c
ATOM   6438  O   GLY H 430     -26.326 -30.805  -6.188  1.00 12.18      B    o
ATOM   6439  N   ILE H 431     -25.216 -32.346  -7.393  1.00 11.58      B    N
ATOM   6440  CA  ILE H 431     -24.551 -31.372  -8.251  1.00 10.76      B    c
ATOM   6441  CB  ILE H 431     -23.175 -31.896  -8.715  1.00 10.43      B    c
ATOM   6442  CGI ILE H 431     -22.220 -32.024  -7.527  1.00 10.95      B    c
ATOM   6443  CD1 ILE H 431     -21.220 -33.153  -7.665  1.00 12.08      B    c
ATOM   6444  CG2 ILE H 431     -22.592 -30.993  -9.791  1.00 10.07      B    c
ATOM   6445  C   ILE H 431     -25.406 -31.085  -9.484  1.00 10.68      B    C
ATOM   6446  O   ILE H 431     -25.703 -31.994 -10.258  1.00 10.40      B    o
ATOM   6447  N   ILE H 432     -25.852 -29.840  -9.636  1.00 10.90      B    N
ATOM   6448  CA  ILE H 432     -26.692 -29.481 -10.779  1.00 11.42      B    c
ATOM   6449  CB  ILE H 432     -27.709 -28.375 -10.448  1.00 11.63      B    c
ATOM   6450  CGI ILE H 432     -27.875 -28.224  -8.936  1.00 12.68      B    c
ATOM   6451  CD1 ILE H 432     -28.514 -26.915  -8.524  1.00 13.89      B    c
ATOM   6452  CG2 ILE H 432     -29.046 -28.664 -11.116  1.00 12.24      B    c
ATOM   6453  C   ILE H 432     -25.884 -29.045 -11.993  1.00 11.41      B    c
ATOM   6454  O   ILE H 432     -26.225 -29.395 -13.123  1.00 11.63      B    o
ATOM   6455  N   LYS H 433     -24.982 -28.093 -11.782  1.00 11.52      B    N
ATOM   6456  CA  LYS H 433     -24.226 -27.523 -12.888  1.00 11.96      B    c
ATOM   6457  CB  LYS H 433     -24.433 -26.010 -12.976  1.00 12.31      B    c
ATOM   6458  CG  LYS H 433     -23.850 -25.387 -14.237  1.00 14.42      B    c
ATOM   6459  CD  LYS H 433     -24.649 -24.175 -14.685  1.00 16.74      B    c
ATOM   6460  CE  LYS H 433     -24.112 -23.613 -15.993  1.00 17.08      B    c
ATOM   6461  NZ  LYS H 433     -24.993 -23.949 -17.146  1.00 17.30      B    N
```

```
ATOM   6462  C   LYS H 433     -22.743 -27.850 -12.793  1.00 11.65      B    C
ATOM   6463  O   LYS H 433     -22.248 -28.250 -11.740  1.00 11.48      B    O
ATOM   6464  N   THR H 434     -22.052 -27.731 -13.921  1.00 11.28      B    N
ATOM   6465  CA  THR H 434     -20.617 -27.970 -13.975  1.00 11.21      B    C
ATOM   6466  CB  THR H 434     -20.308 -29.467 -14.165  1.00 11.30      B    C
ATOM   6467  OG1 THR H 434     -18.945 -29.629 -14.574  1.00 11.83      B    O
ATOM   6468  CG2 THR H 434     -21.224 -30.071 -15.220  1.00 11.84      B    C
ATOM   6469  C   THR H 434     -20.009 -27.185 -15.131  1.00 10.94      B    C
ATOM   6470  O   THR H 434     -20.623 -27.060 -16.190  1.00 10.93      B    O
ATOM   6471  N   PHE H 435     -18.867 -26.549 -14.886  1.00 11.10      B    N
ATOM   6472  CA  PHE H 435     -18.610 -25.235 -15.464  1.00 11.96      B    C
ATOM   6473  CB  PHE H 435     -18.186 -24.223 -14.401  1.00 11.51      B    C
ATOM   6474  CG  PHE H 435     -19.344 -23.561 -13.710  1.00 11.19      B    C
ATOM   6475  CD1 PHE H 435     -19.580 -23.788 -12.365  1.00 10.86      B    C
ATOM   6476  CE1 PHE H 435     -20.692 -23.253 -11.741  1.00 10.24      B    C
ATOM   6477  CZ  PHE H 435     -21.613 -22.532 -12.474  1.00  9.89      B    C
ATOM   6478  CE2 PHE H 435     -21.420 -22.347 -13.828  1.00 10.78      B    C
ATOM   6479  CD2 PHE H 435     -20.304 -22.884 -14.445  1.00 11.14      B    C
ATOM   6480  C   PHE H 435     -17.694 -25.202 -16.684  1.00 13.00      B    C
ATOM   6481  O   PHE H 435     -16.525 -25.587 -16.618  1.00 13.03      B    O
ATOM   6482  N   SER H 436     -18.199 -24.569 -17.738  1.00 13.89      B    N
ATOM   6483  CA  SER H 436     -17.549 -24.549 -19.039  1.00 14.67      B    C
ATOM   6484  CB  SER H 436     -18.601 -24.438 -20.145  1.00 15.04      B    C
ATOM   6485  OG  SER H 436     -18.532 -25.539 -21.033  1.00 16.58      B    O
ATOM   6486  C   SER H 436     -16.586 -23.371 -19.134  1.00 14.75      B    C
ATOM   6487  O   SER H 436     -16.849 -22.398 -19.841  1.00 14.75      B    O
ATOM   6488  N   ASN H 437     -15.480 -23.451 -18.405  1.00 14.44      B    N
ATOM   6489  CA  ASN H 437     -14.306 -22.659 -18.736  1.00 14.35      B    C
ATOM   6490  CB  ASN H 437     -13.508 -23.354 -19.840  1.00 14.75      B    C
ATOM   6491  CG  ASN H 437     -12.101 -22.822 -19.966  1.00 15.51      B    C
ATOM   6492  OD1 ASN H 437     -11.290 -22.960 -19.049  1.00 16.85      B    O
ATOM   6493  ND2 ASN H 437     -11.757 -22.358 -21.162  1.00 16.10      B    N
ATOM   6494  C   ASN H 437     -14.692 -21.239 -19.161  1.00 13.69      B    C
ATOM   6495  O   ASN H 437     -14.402 -20.814 -20.280  1.00 13.40      B    O
ATOM   6496  N   GLY H 438     -15.374 -20.527 -18.267  1.00 13.39      B    N
ATOM   6497  CA  GLY H 438     -15.942 -19.216 -18.573  1.00 12.92      B    C
ATOM   6498  C   GLY H 438     -16.310 -18.455 -17.311  1.00 12.72      B    C
ATOM   6499  O   GLY H 438     -15.574 -18.495 -16.324  1.00 12.83      B    O
ATOM   6500  N   CYS H 439     -17.502 -17.863 -17.297  1.00 12.17      B    N
ATOM   6501  CA  CYS H 439     -17.969 -17.110 -16.134  1.00 11.52      B    C
ATOM   6502  CB  CYS H 439     -17.353 -15.712 -16.124  1.00 11.68      B    C
ATOM   6503  SG  CYS H 439     -18.500 -14.404 -16.619  1.00 12.89      B    S
ATOM   6504  C   CYS H 439     -19.492 -17.006 -16.079  1.00 10.95      B    C
ATOM   6505  O   CYS H 439     -20.102 -16.298 -16.880  1.00 10.77      B    O
ATOM   6506  N   ASP H 440     -20.089 -17.630 -15.066  1.00 10.41      B    N
ATOM   6507  CA  ASP H 440     -21.541 -17.762 -14.987  1.00 10.06      B    C
ATOM   6508  CB  ASP H 440     -21.953 -19.232 -15.091  1.00 10.85      B    C
ATOM   6509  CG  ASP H 440     -22.561 -19.576 -16.438  1.00 13.11      B    C
ATOM   6510  OD1 ASP H 440     -23.750 -19.260 -16.654  1.00 14.97      B    O
ATOM   6511  OD2 ASP H 440     -21.872 -20.227 -17.251  1.00 15.27      B    O
ATOM   6512  C   ASP H 440     -22.098 -17.161 -13.700  1.00  9.01      B    C
ATOM   6513  O   ASP H 440     -21.345 -16.790 -12.798  1.00  9.09      B    O
ATOM   6514  N   TYR H 441     -23.422 -17.184 -13.580  1.00  7.92      B    N
ATOM   6515  CA  TYR H 441     -24.117 -16.707 -12.387  1.00  7.24      B    C
ATOM   6516  CB  TYR H 441     -24.810 -15.371 -12.683  1.00  7.04      B    C
ATOM   6517  CG  TYR H 441     -25.669 -14.849 -11.556  1.00  6.77      B    C
ATOM   6518  CD1 TYR H 441     -25.145 -13.986 -10.605  1.00  7.41      B    C
ATOM   6519  CE1 TYR H 441     -25.927 -13.498  -9.579  1.00  6.79      B    C
ATOM   6520  CZ  TYR H 441     -27.270 -13.809  -9.539  1.00  6.49      B    C
ATOM   6521  OH  TYR H 441     -28.049 -13.340  -8.507  1.00  5.09      B    O
```

ATOM 6522 CE2 TYR H 441 -27.823 -14.634 -10.494 1.00 7.52 B C
ATOM 6523 CD2 TYR H 441 -27.029 -15.122 -11.512 1.00 7.12 B C
ATOM 6524 C TYR H 441 -25.153 -17.748 -11.974 1.00 6.89 B c
ATOM 6525 O TYR H 441 -25.720 -18.436 -12.823 1.00 7.12 B o
ATOM 6526 N VAL H 442 -25.353 -17.906 -10.670 1.00 6.73 B N
ATOM 6527 CA VAL H 442 -26.400 -18.784 -10.159 1.00 6.78 B c
ATOM 6528 CB VAL H 442 -25.808 -20.089 -9.596 1.00 6.51 B c
ATOM 6529 CGI VAL H 442 -25.394 -21.017 -10.729 1.00 7.38 B c
ATOM 6530 CG2 VAL H 442 -24.625 -19.786 -8.688 1.00 6.00 B c
ATOM 6531 C VAL H 442 -27.167 -18.062 -9.059 1.00 7.13 B c
ATOM 6532 O VAL H 442 -26.774 -16.973 -8.643 1.00 7.77 B o
ATOM 6533 N SER H 443 -28.229 -18.679 -8.552 1.00 7.12 B N
ATOM 6534 CA SER H 443 -29.017 -18.039 -7.504 1.00 7.64 B c
ATOM 6535 CB SER H 443 -30.184 -17.252 -8.104 1.00 7.83 B c
ATOM 6536 OG SER H 443 -31.411 -17.936 -7.922 1.00 7.99 B o
ATOM 6537 C SER H 443 -29.508 -18.989 -6.415 1.00 8.16 B c
ATOM 6538 O SER H 443 -29.421 -20.210 -6.552 1.00 8.69 B o
ATOM 6539 N ASN H 444 -29.959 -18.412 -5.306 1.00 8.73 B N
ATOM 6540 CA ASN H 444 -30.539 -19.184 -4.213 1.00 9.50 B c
ATOM 6541 CB ASN H 444 -30.766 -18.297 -2.984 1.00 9.65 B c
ATOM 6542 CG ASN H 444 -29.895 -17.053 -2.990 1.00 10.64 B c
ATOM 6543 OD1 ASN H 444 -28.780 -17.060 -3.516 1.00 12.28 B o
ATOM 6544 ND2 ASN H 444 -30.414 -15.966 -2.426 1.00 11.75 B N
ATOM 6545 C ASN H 444 -31.843 -19.863 -4.618 1.00 10.24 B c
ATOM 6546 O ASN H 444 -32.618 -19.317 -5.403 1.00 9.89 B o
ATOM 6547 N LYS H 445 -32.146 -20.975 -3.955 1.00 11.63 B N
ATOM 6548 CA LYS H 445 -32.826 -22.105 -4.588 1.00 13.07 B c
ATOM 6549 CB LYS H 445 -34.344 -21.990 -4.421 1.00 13.70 B c
ATOM 6550 CG LYS H 445 -35.131 -23.200 -4.915 1.00 15.80 B c
ATOM 6551 CD LYS H 445 -34.354 -24.501 -4.753 1.00 18.31 B c
ATOM 6552 CE LYS H 445 -33.508 -24.498 -3.490 1.00 19.03 B c
ATOM 6553 NZ LYS H 445 -34.316 -24.206 -2.274 1.00 20.02 B N
ATOM 6554 C LYS H 445 -32.459 -22.265 -6.060 1.00 12.96 B c
ATOM 6555 O LYS H 445 -32.290 -21.282 -6.780 1.00 13.24 B o
ATOM 6556 N GLY H 446 -32.350 -23.513 -6.504 1.00 13.08 B N
ATOM 6557 CA GLY H 446 -31.215 -23.936 -7.312 1.00 12.42 B c
ATOM 6558 C GLY H 446 -29.988 -24.163 -6.453 1.00 11.83 B c
ATOM 6559 O GLY H 446 -29.855 -25.209 -5.819 1.00 12.44 B o
ATOM 6560 N VAL H 447 -29.191 -23.114 -6.285 1.00 10.63 B N
ATOM 6561 CA VAL H 447 -27.809 -23.277 -5.857 1.00 10.01 B c
ATOM 6562 CB VAL H 447 -26.839 -22.442 -6.711 1.00 9.97 B c
ATOM 6563 CGI VAL H 447 -25.405 -22.896 -6.479 1.00 10.51 B c
ATOM 6564 CG2 VAL H 447 -27.204 -22.551 -8.183 1.00 10.50 B c
ATOM 6565 C VAL H 447 -27.603 -22.962 -4.380 1.00 9.53 B c
ATOM 6566 O VAL H 447 -28.099 -21.957 -3.868 1.00 9.61 B o
ATOM 6567 N ASP H 448 -26.719 -23.735 -3.760 1.00 9.16 B N
ATOM 6568 CA ASP H 448 -26.522 -23.714 -2.318 1.00 8.75 B c
ATOM 6569 CB ASP H 448 -27.139 -24.971 -1.698 1.00 9.22 B c
ATOM 6570 CG ASP H 448 -27.482 -24.795 -0.234 1.00 11.44 B c
ATOM 6571 OD1 ASP H 448 -26.877 -23.921 0.421 1.00 13.83 B o
ATOM 6572 OD2 ASP H 448 -28.319 -25.568 0.276 1.00 14.13 B o
ATOM 6573 C ASP H 448 -25.020 -23.714 -2.076 1.00 8.18 B c
ATOM 6574 O ASP H 448 -24.528 -23.151 -1.098 1.00 8.06 B o
ATOM 6575 N THR H 449 -24.298 -24.280 -3.036 1.00 7.63 B N
ATOM 6576 CA THR H 449 -22.858 -24.437 -2.940 1.00 6.80 B c
ATOM 6577 CB THR H 449 -22.485 -25.824 -2.386 1.00 6.89 B c
ATOM 6578 OG1 THR H 449 -22.377 -25.758 -0.959 1.00 6.16 B o
ATOM 6579 CG2 THR H 449 -21.163 -26.296 -2.970 1.00 7.55 B c
ATOM 6580 C THR H 449 -22.265 -24.297 -4.333 1.00 6.53 B c
ATOM 6581 O THR H 449 -22.828 -24.792 -5.309 1.00 6.59 B o

ATOM 6582 N VAL H 450 -21.145 -23.594 -4.428 1.00 6.07 B N
ATOM 6583 CA VAL H 450 -20.209 -23.829 -5.512 1.00 6.02 B C
ATOM 6584 CB VAL H 450 -20.064 -22.597 -6.420 1.00 5.61 B C
ATOM 6585 CGI VAL H 450 -21.429 -22.130 -6.904 1.00 5.32 B c
ATOM 6586 CG2 VAL H 450 -19.339 -21.481 -5.687 1.00 5.55 B c
ATOM 6587 C VAL H 450 -18.853 -24.210 -4.950 1.00 6.37 B c
ATOM 6588 O VAL H 450 -18.503 -23.827 -3.833 1.00 6.54 B o
ATOM 6589 N SER H 451 -18.176 -25.110 -5.649 1.00 6.41 B N
ATOM 6590 CA SER H 451 -16.786 -25.397 -5.362 1.00 6.70 B c
ATOM 6591 CB SER H 451 -16.602 -26.886 -5.069 1.00 7.13 B c
ATOM 6592 OG SER H 451 -17.729 -27.629 -5.498 1.00 9.26 B o
ATOM 6593 C SER H 451 -15.944 -24.990 -6.555 1.00 6.47 B c
ATOM 6594 O SER H 451 -16.363 -25.147 -7.701 1.00 6.54 B o
ATOM 6595 N VAL H 452 -14.861 -24.277 -6.276 1.00 6.56 B N
ATOM 6596 CA VAL H 452 -13.801 -24.112 -7.251 1.00 6.31 B c
ATOM 6597 CB VAL H 452 -13.469 -22.625 -7.471 1.00 5.74 B c
ATOM 6598 CGI VAL H 452 -12.757 -22.433 -8.801 1.00 5.06 B c
ATOM 6599 CG2 VAL H 452 -14.740 -21.787 -7.420 1.00 5.56 B c
ATOM 6600 C VAL H 452 -12.558 -24.861 -6.791 1.00 6.60 B c
ATOM 6601 O VAL H 452 -12.130 -24.726 -5.644 1.00 7.04 B o
ATOM 6602 N GLY H 453 -12.047 -25.732 -7.654 1.00 6.54 B N
ATOM 6603 CA GLY H 453 -11.013 -26.672 -7.250 1.00 6.43 B c
ATOM 6604 C GLY H 453 -11.329 -27.255 -5.889 1.00 6.09 B c
ATOM 6605 O GLY H 453 -12.396 -27.836 -5.690 1.00 5.90 B o
ATOM 6606 N ASN H 454 -10.479 -26.962 -4.913 1.00 6.02 B N
ATOM 6607 CA ASN H 454 -10.646 -27.533 -3.585 1.00 6.39 B c
ATOM 6608 CB ASN H 454 -9.330 -28.111 -3.073 1.00 6.81 B c
ATOM 6609 CG ASN H 454 -9.190 -29.585 -3.382 1.00 8.99 B c
ATOM 6610 OD1 ASN H 454 -9.587 -30.433 -2.584 1.00 11.67 B o
ATOM 6611 ND2 ASN H 454 -8.782 -29.893 -4.609 1.00 10.25 B N
ATOM 6612 C ASN H 454 -11.235 -26.563 -2.573 1.00 6.15 B c
ATOM 6613 O ASN H 454 -11.623 -26.963 -1.475 1.00 6.47 B o
ATOM 6614 N THR H 455 -11.406 -25.312 -2.985 1.00 5.40 B N
ATOM 6615 CA THR H 455 -12.129 -24.347 -2.172 1.00 4.53 B c
ATOM 6616 CB THR H 455 -11.775 -22.902 -2.551 1.00 4.70 B c
ATOM 6617 OG1 THR H 455 -10.351 -22.746 -2.567 1.00 5.28 B o
ATOM 6618 CG2 THR H 455 -12.374 -21.928 -1.542 1.00 5.57 B c
ATOM 6619 C THR H 455 -13.632 -24.543 -2.293 1.00 4.01 B c
ATOM 6620 O THR H 455 -14.139 -24.921 -3.349 1.00 3.78 B o
ATOM 6621 N LEU H 456 -14.338 -24.306 -1.194 1.00 3.87 B N
ATOM 6622 CA LEU H 456 -15.787 -24.419 -1.181 1.00 4.05 B c
ATOM 6623 CB LEU H 456 -16.232 -25.520 -0.219 1.00 3.95 B c
ATOM 6624 CG LEU H 456 -17.708 -25.915 -0.306 1.00 3.76 B c
ATOM 6625 CD1 LEU H 456 -18.042 -26.440 -1.694 1.00 5.35 B c
ATOM 6626 CD2 LEU H 456 -18.053 -26.944 0.758 1.00 4.10 B c
ATOM 6627 C LEU H 456 -16.439 -23.097 -0.802 1.00 4.47 B c
ATOM 6628 O LEU H 456 -16.186 -22.551 0.272 1.00 4.94 B o
ATOM 6629 N TYR H 457 -17.343 -22.634 -1.657 1.00 4.59 B N
ATOM 6630 CA TYR H 457 -18.102 -21.425 -1.386 1.00 4.60 B c
ATOM 6631 CB TYR H 457 -17.996 -20.463 -2.570 1.00 4.71 B c
ATOM 6632 CG TYR H 457 -16.594 -19.949 -2.820 1.00 5.62 B c
ATOM 6633 CD1 TYR H 457 -15.657 -20.727 -3.485 1.00 7.09 B c
ATOM 6634 CE1 TYR H 457 -14.388 -20.247 -3.748 1.00 8.22 B c
ATOM 6635 CZ TYR H 457 -14.029 -18.994 -3.305 1.00 8.06 B c
ATOM 6636 OH TYR H 457 -12.763 -18.520 -3.550 1.00 8.80 B o
ATOM 6637 CE2 TYR H 457 -14.933 -18.212 -2.622 1.00 7.18 B c
ATOM 6638 CD2 TYR H 457 -16.203 -18.694 -2.375 1.00 6.66 B c
ATOM 6639 C TYR H 457 -19.565 -21.758 -1.099 1.00 4.46 B c
ATOM 6640 O TYR H 457 -20.180 -22.551 -1.811 1.00 4.92 B o
ATOM 6641 N TYR H 458 -20.098 -21.196 -0.017 1.00 3.90 B N

```
ATOM   6642  CA  TYR H 458     -21.496 -21.408   0.366  1.00  3.26      B    C
ATOM   6643  CB  TYR H 458     -21.610 -21.544   1.885  1.00  3.16      B    C
ATOM   6644  CG  TYR H 458     -20.863 -22.722   2.457  1.00  3.29      B    c
ATOM   6645  CD1 TYR H 458     -19.547 -22.597   2.881  1.00  3.93      B    c
ATOM   6646  CE1 TYR H 458     -18.866 -23.672   3.419  1.00  4.90      B    c
ATOM   6647  CZ  TYR H 458     -19.501 -24.890   3.535  1.00  5.12      B    c
ATOM   6648  OH  TYR H 458     -18.826 -25.967   4.062  1.00  5.42      B    o
ATOM   6649  CE2 TYR H 458     -20.810 -25.036   3.128  1.00  4.72      B    c
ATOM   6650  CD2 TYR H 458     -21.483 -23.955   2.598  1.00  3.89      B    c
ATOM   6651  C   TYR H 458     -22.372 -20.242  -0.085  1.00  3.04      B    c
ATOM   6652  O   TYR H 458     -22.185 -19.119   0.378  1.00  3.37      B    0
ATOM   6653  N   VAL H 459     -23.453 -20.542  -0.800  1.00  2.71      B    N
ATOM   6654  CA  VAL H 459     -24.073 -19.546  -1.678  1.00  2.61      B    c
ATOM   6655  CB  VAL H 459     -24.381 -20.115  -3.067  1.00  2.22      B    c
ATOM   6656  CGI VAL H 459     -25.021 -19.042  -3.938  1.00  2.62      B    c
ATOM   6657  CG2 VAL H 459     -23.123 -20.656  -3.716  1.00  2.61      B    c
ATOM   6658  C   VAL H 459     -25.372 -18.924  -1.190  1.00  3.03      B    c
ATOM   6659  O   VAL H 459     -25.418 -18.348  -0.103  1.00  3.21      B    o
ATOM   6660  N   ASN H 460     -26.215 -18.648  -2.185  1.00106.93      B    N
ATOM   6661  CA  ASN H 460     -27.625 -18.431  -1.941  1.00 95.54      B    c
ATOM   6662  CB  ASN H 460     -27.810 -17.878  -0.542  1.00 20.00      B    c
ATOM   6663  CG  ASN H 460     -28.967 -18.507   0.162  1.00 20.00      B    c
ATOM   6664  ODl ASN H 460     -29.655 -19.349  -0.416  1.00 20.00      B    o
ATOM   6665  ND2 ASN H 460     -29.359 -17.912   1.280  1.00 20.00      B    N
ATOM   6666  C   ASN H 460     -28.426 -17.612  -2.969  1.00 99.41      B    c
ATOM   6667  O   ASN H 460     -29.222 -18.178  -3.718  1.00108.91      B    o
ATOM   6668  N   LYS H 461     -28.370 -16.283  -2.861  1.00 97.04      B    N
ATOM   6669  CA  LYS H 461     -29.458 -15.387  -3.306  1.00105.93      B    c
ATOM   6670  CB  LYS H 461     -29.011 -13.925  -3.219  1.00 20.00      B    c
ATOM   6671  CG  LYS H 461     -28.633 -13.460  -1.820  1.00 20.00      B    c
ATOM   6672  CD  LYS H 461     -27.794 -12.187  -1.865  1.00 20.00      B    c
ATOM   6673  CE  LYS H 461     -27.646 -11.565  -0.482  1.00 20.00      B    c
ATOM   6674  NZ  LYS H 461     -26.746 -10.375  -0.482  1.00 20.00      B    N
ATOM   6675  C   LYS H 461     -30.025 -15.676  -4.708  1.00102.28      B    c
ATOM   6676  O   LYS H 461     -29.779 -16.739  -5.276  1.00105.02      B    o
ATOM   6677  N   GLN H 462     -30.766 -14.715  -5.266  1.00 96.68      B    N
ATOM   6678  CA  GLN H 462     -31.286 -14.810  -6.641  1.00105.71      B    c
ATOM   6679  CB  GLN H 462     -32.787 -15.128  -6.624  1.00 20.00      B    c
ATOM   6680  CG  GLN H 462     -33.142 -16.522  -6.122  1.00 20.00      B    c
ATOM   6681  CD  GLN H 462     -34.637 -16.794  -6.159  1.00 20.00      B    c
ATOM   6682  OE1 GLN H 462     -35.450 -15.870  -6.115  1.00 20.00      B    o
ATOM   6683  NE2 GLN H 462     -35.006 -18.068  -6.230  1.00 20.00      B    N
ATOM   6684  C   GLN H 462     -31.052 -13.514  -7.429  1.00101.50      B    c
ATOM   6685  O   GLN H 462     -31.398 -12.430  -6.960  1.00105.94      B    o
ATOM   6686  N   GLU H 463     -30.565 -13.634  -8.663  1.00 98.92      B    N
ATOM   6687  CA  GLU H 463     -30.241 -12.453  -9.465  1.00108.59      B    c
ATOM   6688  CB  GLU H 463     -28.792 -12.505  -9.966  1.00 20.00      B    c
ATOM   6689  CG  GLU H 463     -27.767 -11.973  -8.957  1.00 20.00      B    c
ATOM   6690  CD  GLU H 463     -26.341 -11.973  -9.490  1.00 20.00      B    c
ATOM   6691  OE1 GLU H 463     -26.167 -11.917 -10.729  1.00 20.00      E;   o
ATOM   6692  OE2 GLU H 463     -25.399 -11.890  -8.672  1.00 20.00      B    o
ATOM   6693  C   GLU H 463     -31.208 -12.245 -10.629  1.001 16.39      B    c
ATOM   6694  O   GLU H 463     -31.442 -13.153 -11.426  1.001 18.70      B    o
ATOM   6695  N   GLY H 464     -31.759 -11.039 -10.722  1.00127.70      B    N
ATOM   6696  CA  GLY H 464     -32.671 -10.693 -11.806  1.00143.17      B    C
ATOM   6697  C   GLY H 464     -31.941 -10.347 -13.089  1.00149.77      B    C
ATOM   6698  O   GLY H 464     -30.719 -10.197 -13.098  1.00155.06      B    o
ATOM   6699  N   LYS H 465     -32.694 -10.223 -14.178  1.00153.73      B    N
ATOM   6700  CA  LYS H 465     -32.115  -9.929 -15.484  1.00153.69      B    C
ATOM   6701  CB  LYS H 465     -31.275  -8.651 -15.424  1.00 20.00      B    c
```

ATOM 6702 CG LYS H 465 -32.085 -7.385 -15.193 1.00 20.00 B C
ATOM 6703 CD LYS H 465 -31.186 -6.163 -15.106 1.00 20.00 B C
ATOM 6704 CE LYS H 465 -31.995 -4.898 -14.868 1.00 20.00 B C
ATOM 6705 NZ LYS H 465 -31.127 -3.692 -14.776 1.00 20.00 B N
ATOM 6706 C LYS H 465 -31.267 -11.091 -15.990 1.00155.37 B C
ATOM 6707 O LYS H 465 -31.276 -11.407 -17.180 1.00155.20 B O
ATOM 6708 N GLU H 472 -30.692 -9.899 -23.132 1.00145.47 B N
ATOM 6709 CA GLU H 472 -30.214 -9.535 -24.461 1.00151.12 B C
ATOM 6710 CB GLU H 472 -30.931 -8.281 -24.964 1.00 20.00 B C
ATOM 6711 CG GLU H 472 -32.419 -8.472 -25.209 1.00 20.00 B C
ATOM 6712 CD GLU H 472 -33.106 -7.192 -25.643 1.00 20.00 B C
ATOM 6713 OE1 GLU H 472 -32.477 -6.117 -25.554 1.00 20.00 B O
ATOM 6714 OE2 GLU H 472 -34.279 -7.260 -26.070 1.00 20.00 B O
ATOM 6715 C GLU H 472 -28.705 -9.310 -24.462 1.00153.35 B C
ATOM 6716 O GLU H 472 -28.208 -8.395 -23.805 1.00159.41 B O
ATOM 6717 N PRO H 473 -27.971 -10.164 -25.188 1.00150.51 B N
ATOM 6718 CA PRO H 473 -26.535 -10.028 -25.339 1.00141.97 B C
ATOM 6719 CB PRO H 473 -26.035 -11.435 -25.011 1.00 20.00 B C
ATOM 6720 CG PRO H 473 -27.175 -12.350 -25.428 1.00 20.00 B C
ATOM 6721 CD PRO H 473 -28.424 -11.506 -25.583 1.00 20.00 B C
ATOM 6722 C PRO H 473 -26.193 -9.688 -26.782 1.00135.14 B C
ATOM 6723 O PRO H 473 -26.968 -9.997 -27.687 1.00144.93 B O
ATOM 6724 N ILE H 474 -25.024 -9.096 -27.001 1.001 18.07 B N
ATOM 6725 CA ILE H 474 -24.617 -8.700 -28.344 1.00105.14 B C
ATOM 6726 CB ILE H 474 -25.549 -7.614 -28.919 1.00 20.00 B C
ATOM 6727 CGI ILE H 474 -26.957 -8.174 -29.133 1.00 20.00 B C
ATOM 6728 CD1 ILE H 474 -28.021 -7.109 -29.293 1.00 20.00 B C
ATOM 6729 CG2 ILE H 474 -24.988 -7.064 -30.222 1.00 20.00 B C
ATOM 6730 C ILE H 474 -23.184 -8.180 -28.352 1.00104.75 B C
ATOM 6731 O ILE H 474 -22.938 -7.013 -28.046 1.001 11.83 B O
ATOM 6732 N ILE H 475 -22.242 -9.045 -28.716 1.00 94.65 B N
ATOM 6733 CA ILE H 475 -20.826 -8.732 -28.565 1.00 79.88 B C
ATOM 6734 CB ILE H 475 -20.175 -9.577 -27.453 1.00 20.00 B C
ATOM 6735 CGI ILE H 475 -20.674 -9.120 -26.079 1.00 20.00 B C
ATOM 6736 CD1 ILE H 475 -20.434 -10.125 -24.972 1.00 20.00 B C
ATOM 6737 CG2 ILE H 475 -18.658 -9.507 -27.545 1.00 20.00 B C
ATOM 6738 C ILE H 475 -20.051 -8.909 -29.868 1.00 79.52 B C
ATOM 6739 O ILE H 475 -19.808 -10.032 -30.310 1.00 82.70 B O
ATOM 6740 N ASN H 476 -19.589 -7.793 -30.425 1.00 69.64 B N
ATOM 6741 CA ASN H 476 -18.756 -7.812 -31.623 1.00 68.88 B C
ATOM 6742 CB ASN H 476 -18.880 -6.487 -32.381 1.00 20.00 B C
ATOM 6743 CG ASN H 476 -20.247 -6.299 -33.011 1.00 20.00 B C
ATOM 6744 OD1 ASN H 476 -20.954 -7.268 -33.288 1.00 20.00 B O
ATOM 6745 ND2 ASN H 476 -20.618 -5.048 -33.257 1.00 20.00 B N
ATOM 6746 C ASN H 476 -17.290 -8.097 -31.306 1.00 67.13 B C
ATOM 6747 O ASN H 476 -16.718 -7.507 -30.389 1.00 73.10 B O
ATOM 6748 N PHE H 477 -16.677 -8.975 -32.096 1.00 64.95 B N
ATOM 6749 CA PHE H 477 -15.288 -9.380 -31.879 1.00 68.13 B C
ATOM 6750 CB PHE H 477 -14.918 -10.567 -32.776 1.00 20.00 B C
ATOM 6751 CG PHE H 477 -15.678 -11.822 -32.466 1.00 20.00 B C
ATOM 6752 CD1 PHE H 477 -15.266 -12.666 -31.448 1.00 20.00 B C
ATOM 6753 CE1 PHE H 477 -15.965 -13.820 -31.162 1.00 20.00 B C
ATOM 6754 CZ PHE H 477 -17.069 -14.158 -31.915 1.00 20.00 B C
ATOM 6755 CE2 PHE H 477 -17.473 -13.339 -32.949 1.00 20.00 B C
ATOM 6756 CD2 PHE H 477 -16.778 -12.181 -33.222 1.00 20.00 B C
ATOM 6757 C PHE H 477 -14.307 -8.232 -32.117 1.00 65.57 B C
ATOM 6758 O PHE H 477 -13.094 -8.412 -31.999 1.00 49.83 B O
ATOM 6759 N TYR H 478 -14.816 -7.113 -32.617 1.00 51.97 B N
ATOM 6760 CA TYR H 478 -13.996 -5.920 -32.779 1.00 52.01 B C
ATOM 6761 CB TYR H 478 -14.573 -5.017 -33.870 1.00 20.00 B C

ATOM 6762 CG TYR H 478 -14.579 -5.653 -35.247 1.00 20.00 B C
ATOM 6763 CD1 TYR H 478 -13.458 -5.593 -36.069 1.00 20.00 B C
ATOM 6764 CE1 TYR H 478 -13.453 -6.195 -37.316 1.00 20.00 B C
ATOM 6765 CZ TYR H 478 -14.585 -6.849 -37.766 1.00 20.00 B C
ATOM 6766 OH TYR H 478 -14.597 -7.434 -39.013 1.00 20.00 B O
ATOM 6767 CE2 TYR H 478 -15.689 -6.967 -36.948 1.00 20.00 B C
ATOM 6768 CD2 TYR H 478 -15.687 -6.360 -35.703 1.00 20.00 B C
ATOM 6769 C TYR H 478 -13.909 -5.178 -31.454 1.00 66.63 B C
ATOM 6770 O TYR H 478 -13.401 -4.059 -31.383 1.00 63.45 B O
ATOM 6771 N ASP H 479 -14.391 -5.828 -30.401 1.00 65.34 B N
ATOM 6772 CA ASP H 479 -14.256 -5.31 1 -29.049 1.00 65.32 B C
ATOM 6773 CB ASP H 479 -15.579 -5.450 -28.296 1.00 20.00 B C
ATOM 6774 CG ASP H 479 -16.664 -4.552 -28.856 1.00 20.00 B C
ATOM 6775 OD1 ASP H 479 -16.327 -3.593 -29.582 1.00 20.00 B O
ATOM 6776 OD2 ASP H 479 -17.854 -4.799 -28.568 1.00 20.00 B O
ATOM 6777 C ASP H 479 -13.144 -6.036 -28.300 1.00 64.83 B C
ATOM 6778 O ASP H 479 -12.738 -5.609 -27.220 1.00 60.42 B O
ATOM 6779 N PRO H 480 -12.610 -7.108 -28.903 1.00 47.60 B N
ATOM 6780 CA PRO H 480 -11.568 -7.902 -28.282 1.00 46.52 B C
ATOM 6781 CB PRO H 480 -11.905 -9.318 -28.742 1.00 20.00 B C
ATOM 6782 CG PRO H 480 -12.596 -9.131 -30.072 1.00 20.00 B C
ATOM 6783 CD PRO H 480 -13.021 -7.682 -30. 193 1.00 20.00 B C
ATOM 6784 C PRO H 480 -10.199 -7.497 -28.809 1.00 52.36 B C
ATOM 6785 O PRO H 480 -9.736 -8.035 -29.815 1.00 64.15 B O
ATOM 6786 N LEU H 481 -9.618 -6.472 -28.197 1.00 62.90 B N
ATOM 6787 CA LEU H 481 -8.285 -6.015 -28.562 1.00 54.24 B C
ATOM 6788 CB LEU H 481 -8.322 -4.544 -28.982 1.00 20.00 B C
ATOM 6789 CG LEU H 481 -9.202 -4.212 -30.186 1.00 20.00 B C
ATOM 6790 CD1 LEU H 481 -9.255 -2.706 -30.408 1.00 20.00 B C
ATOM 6791 CD2 LEU H 481 -8.698 -4.931 -31.425 1.00 20.00 B C
ATOM 6792 C LEU H 481 -7.315 -6.203 -27.402 1.00 59.81 B C
ATOM 6793 O LEU H 481 -7.682 -6.724 -26.348 1.00 64.98 B O
ATOM 6794 N VAL H 482 -6.058 -5.840 -27.628 1.00 59.66 B N
ATOM 6795 CA VAL H 482 -5.084 -5.781 -26.549 1.00 49.67 B C
ATOM 6796 CB VAL H 482 -3.786 -6.531 -26.91 1 1.00 20.00 B C
ATOM 6797 CGI VAL H 482 -2.81 1 -6.492 -25.742 1.00 20.00 B C
ATOM 6798 CG2 VAL H 482 -4.097 -7.973 -27.288 1.00 20.00 B C
ATOM 6799 C VAL H 482 -4.762 -4.337 -26. 191 1.00 53.03 B C
ATOM 6800 O VAL H 482 -4.706 -3.472 -27.064 1.00 46.27 B O
ATOM 6801 N PHE H 483 -4.641 -4.070 -24.894 1.00 61.61 B N
ATOM 6802 CA PHE H 483 -4.31 1 -2.732 -24.415 1.00 65.03 B C
ATOM 6803 CB PHE H 483 -5.338 -2.259 -23.391 1.00 20.00 B C
ATOM 6804 CG PHE H 483 -6.714 -2.064 -23.966 1.00 20.00 B C
ATOM 6805 CD1 PHE H 483 -7.021 -0.928 -24.695 1.00 20.00 B C
ATOM 6806 CE1 PHE H 483 -8.294 -0.739 -25.209 1.00 20.00 B C
ATOM 6807 CZ PHE H 483 -9.246 -1.731 -25.077 1.00 20.00 B C
ATOM 6808 CE2 PHE H 483 -8.937 -2.888 -24.397 1.00 20.00 B C
ATOM 6809 CD2 PHE H 483 -7.667 -3.065 -23.872 1.00 20.00 B C
ATOM 6810 C PHE H 483 -2.897 -2.662 -23.852 1.00 71.00 B C
ATOM 681 1 O PHE H 483 -2.704 -2.417 -22.659 1.00100.44 B O
ATOM 6812 N PRO H 484 -1.909 -2.972 -24.705 1.00 54.44 B N
ATOM 6813 CA PRO H 484 -0.512 -3.000 -24.329 1.00 47.46 B C
ATOM 6814 CB PRO H 484 -0.179 -4.492 -24.438 1.00 20.00 B C
ATOM 6815 CG PRO H 484 -1.142 -5.021 -25.513 1.00 20.00 B C
ATOM 6816 CD PRO H 484 -2.157 -3.926 -25.796 1.00 20.00 B C
ATOM 6817 C PRO H 484 0.323 -2.225 -25.346 1.00 41.56 B C
ATOM 6818 O PRO H 484 0.278 -2.527 -26.539 1.00 46.53 B O
ATOM 6819 N SER H 485 1.033 -1.202 -24.883 1.00 46.30 B N
ATOM 6820 CA SER H 485 1.824 -0.355 -25.768 1.00 49.30 B C
ATOM 6821 CB SER H 485 3.010 0.252 -25.015 1.00 20.00 B C

```
ATOM   6822  OG  SER H 485      3.864  -0.754 -24.502  1.00 20.00      B    O
ATOM   6823  C   SER H 485      2.307  -1.112 -27.003  1.00 41.24      B    C
ATOM   6824  O   SER H 485      1.964  -0.755 -28.131  1.00 46.93      B    O
ATOM   6825  N   ASP H 486      3.108  -2.150 -26.785  1.00 49.48      B    N
ATOM   6826  CA  ASP H 486      3.700  -2.909 -27.881  1.00 37.44      B    C
ATOM   6827  CB  ASP H 486      4.552  -4.054 -27.333  1.00 20.00      B    C
ATOM   6828  CG  ASP H 486      5.885  -3.576 -26.790  1.00 20.00      B    C
ATOM   6829  OD1 ASP H 486      6.284  -2.437 -27.115  1.00 20.00      B    O
ATOM   6830  OD2 ASP H 486      6.556  -4.355 -26.080  1.00 20.00      B    O
ATOM   6831  C   ASP H 486      2.628  -3.456 -28.818  1.00 45.66      B    C
ATOM   6832  O   ASP H 486      2.683  -3.252 -30.034  1.00 39.86      B    O
ATOM   6833  N   GLU H 487      1.627  -4.107 -28.238  1.00 49.20      B    N
ATOM   6834  CA  GLU H 487      0.525  -4.652 -29.013  1.00 45.70      B    C
ATOM   6835  CB  GLU H 487     -0.444  -5.410 -28.105  1.00 20.00      B    C
ATOM   6836  CG  GLU H 487      0.156  -6.664 -27.483  1.00 20.00      B    C
ATOM   6837  CD  GLU H 487     -0.814  -7.393 -26.576  1.00 20.00      B    C
ATOM   6838  OE1 GLU H 487     -1.852  -6.804 -26.214  1.00 20.00      B    O
ATOM   6839  OE2 GLU H 487     -0.514  -8.540 -26.183  1.00 20.00      B    O
ATOM   6840  C   GLU H 487     -0.203  -3.556 -29.783  1.00 41.48      B    C
ATOM   6841  O   GLU H 487     -0.411  -3.674 -30.989  1.00 48.92      B    o
ATOM   6842  N   PHE H 488     -0.486  -2.447 -29.110  1.00 42.16      B    N
ATOM   6843  CA  PHE H 488     -1.183  -1.339 -29.747  1.00 39.33      B    C
ATOM   6844  CB  PHE H 488     -1.438  -0.219 -28.745  1.00 20.00      B    c
ATOM   6845  CG  PHE H 488     -2.369  -0.602 -27.638  1.00 20.00      B    c
ATOM   6846  CD1 PHE H 488     -3.739  -0.595 -27.833  1.00 20.00      B    c
ATOM   6847  CE1 PHE H 488     -4.602  -0.873 -26.789  1.00 20.00      B    c
ATOM   6848  CZ  PHE H 488     -4.095  -1.193 -25.546  1.00 20.00      B    c
ATOM   6849  CE2 PHE H 488     -2.731  -1.192 -25.340  1.00 20.00      B    c
ATOM   6850  CD2 PHE H 488     -1.876  -0.912 -26.385  1.00 20.00      B    c
ATOM   6851  C   PHE H 488     -0.401  -0.804 -30.939  1.00 43.06      B    c
ATOM   6852  O   PHE H 488     -0.977  -0.505 -31.984  1.00 61.71      B    o
ATOM   6853  N   ASP H 489      0.915  -0.700 -30.782  1.00 41.95      B    N
ATOM   6854  CA  ASP H 489      1.766  -0.104 -31.808  1.00 42.75      B    c
ATOM   6855  CB  ASP H 489      3.172   0.134 -31.262  1.00 20.00      B    c
ATOM   6856  CG  ASP H 489      3.235   1.317 -30.327  1.00 20.00      B    c
ATOM   6857  OD1 ASP H 489      2.256   2.089 -30.288  1.00 20.00      B    o
ATOM   6858  OD2 ASP H 489      4.252   1.462 -29.617  1.00 20.00      B    o
ATOM   6859  C   ASP H 489      1.837  -0.980 -33.054  1.00 45.61      B    c
ATOM   6860  O   ASP H 489      2.110  -0.495 -34.154  1.00 54.39      B    o
ATOM   6861  N   ALA H 490      1.702  -2.287 -32.853  1.00 42.89      B    N
ATOM   6862  CA  ALA H 490      1.705  -3.238 -33.957  1.00 38.40      B    c
ATOM   6863  CB  ALA H 490      1.928  -4.653 -33.436  1.00 20.00      B    c
ATOM   6864  C   ALA H 490      0.413  -3.160 -34.770  1.00 39.67      B    c
ATOM   6865  O   ALA H 490      0.443  -3.194 -35.998  1.00 56.80      B    o
ATOM   6866  N   SER H 491     -0.717  -3.050 -34.080  1.00 40.38      B    N
ATOM   6867  CA  SER H 491     -2.003  -2.833 -34.737  1.00 41.77      B    c
ATOM   6868  CB  SER H 491     -3.155  -2.963 -33.731  1.00 20.00      B    c
ATOM   6869  OG  SER H 491     -3.173  -1.878 -32.817  1.00 20.00      B    o
ATOM   6870  C   SER H 491     -2.056  -1.474 -35.432  1.00 39.01      B    c
ATOM   6871  O   SER H 491     -2.701  -1.325 -36.472  1.00 36.91      B    o
ATOM   6872  N   ILE H 492     -1.440  -0.470 -34.812  1.00 38.11      B    N
ATOM   6873  CA  ILE H 492     -1.342   0.863 -35.402  1.00 41.21      B    c
ATOM   6874  CB  ILE H 492     -0.651   1.856 -34.446  1.00 20.00      B    c
ATOM   6875  CGI ILE H 492     -1.506   2.097 -33.203  1.00 20.00      B    c
ATOM   6876  CD1 ILE H 492     -0.883   3.081 -32.232  1.00 20.00      B    c
ATOM   6877  CG2 ILE H 492     -0.363   3.173 -35.150  1.00 20.00      B    c
ATOM   6878  C   ILE H 492     -0.561   0.826 -36.714  1.00 39.22      B    C
ATOM   6879  O   ILE H 492     -0.943   1.466 -37.696  1.00 47.54      B    O
ATOM   6880  N   SER H 493      0.535   0.073 -36.718  1.00 41.64      B    N
ATOM   6881  CA  SER H 493      1.307  -0.161 -37.933  1.00 35.15      B    C
```

ATOM 6882 CB SER H 493 2.587 -0.944 -37.618 1.00 20.00 B C
ATOM 6883 OG SER H 493 2.296 -2.250 -37.147 1.00 20.00 B o
ATOM 6884 C SER H 493 0.486 -0.880 -39.011 1.00 47.90 B c
ATOM 6885 O SER H 493 0.565 -0.538 -40.191 1.00 50.94 B o
ATOM 6886 N GLN H 494 -0.321 -1.855 -38.596 1.00 42.51 B N
ATOM 6887 CA GLN H 494 -1.175 -2.611 -39.517 1.00 41.96 B c
ATOM 6888 CB GLN H 494 -1.822 -3.801 -38.795 1.00 20.00 B c
ATOM 6889 CG GLN H 494 -0.843 -4.905 -38.423 1.00 20.00 B c
ATOM 6890 CD GLN H 494 -1.489 -6.019 -37.630 1.00 20.00 B c
ATOM 6891 OE1 GLN H 494 -2.536 -5.830 -37.011 1.00 20.00 B o
ATOM 6892 NE2 GLN H 494 -0.893 -7.205 -37.684 1.00 20.00 B N
ATOM 6893 C GLN H 494 -2.254 -1.721 -40.130 1.00 33.86 B c
ATOM 6894 O GLN H 494 -2.479 -1.743 -41.340 1.00 54.89 B o
ATOM 6895 N VAL H 495 -2.973 -1.005 -39.272 1.00 34.99 B N
ATOM 6896 CA VAL H 495 -3.955 -0.025 -39.718 1.00 38.42 B c
ATOM 6897 CB VAL H 495 -4.485 0.807 -38.536 1.00 20.00 B c
ATOM 6898 CGI VAL H 495 -5.501 1.828 -39.016 1.00 20.00 B c
ATOM 6899 CG2 VAL H 495 -5.088 -0.101 -37.479 1.00 20.00 B c
ATOM 6900 C VAL H 495 -3.344 0.912 -40.751 1.00 42.74 B c
ATOM 6901 O VAL H 495 -3.876 1.069 -41.850 1.00 44.00 B o
ATOM 6902 N ASN H 496 -2.171 1.447 -40.434 1.00 42.45 B N
ATOM 6903 CA ASN H 496 -1.500 2.382 -41.323 1.00 43.01 B c
ATOM 6904 CB ASN H 496 -0.202 2.880 -40.692 1.00 20.00 B c
ATOM 6905 CG ASN H 496 -0.446 3.770 -39.497 1.00 20.00 B c
ATOM 6906 OD1 ASN H 496 -1.517 4.360 -39.358 1.00 20.00 B o
ATOM 6907 ND2 ASN H 496 0.537 3.849 -38.608 1.00 20.00 B N
ATOM 6908 C ASN H 496 -1.227 1.780 -42.695 1.00 43.13 B c
ATOM 6909 O ASN H 496 -1.502 2.404 -43.720 1.00 54.76 B o
ATOM 6910 N GLU H 497 -0.737 0.544 -42.708 1.00 42.08 B N
ATOM 6911 CA GLU H 497 -0.453 -0.150 -43.957 1.00 43.13 B c
ATOM 6912 CB GLU H 497 0.151 -1.525 -43.678 1.00 20.00 B c
ATOM 6913 CG GLU H 497 1.651 -1.515 -43.476 1.00 20.00 B c
ATOM 6914 CD GLU H 497 2.193 -2.884 -43.108 1.00 20.00 B c
ATOM 6915 OE1 GLU H 497 1.402 -3.851 -43.058 1.00 20.00 B o
ATOM 6916 OE2 GLU H 497 3.419 -3.001 -42.899 1.00 20.00 B o
ATOM 6917 C GLU H 497 -1.724 -0.306 -44.781 1.00 49.77 B c
ATOM 6918 O GLU H 497 -1.680 -0.352 -46.011 1.00 42.88 B o
ATOM 6919 N LYS H 498 -2.846 -0.477 -44.088 1.00 41.82 B N
ATOM 6920 CA LYS H 498 -4.141 -0.621 -44.741 1.00 53.60 B c
ATOM 6921 CB LYS H 498 -5.174 -1.179 -43.761 1.00 20.00 B c
ATOM 6922 CG LYS H 498 -4.967 -2.641 -43.403 1.00 20.00 B c
ATOM 6923 CD LYS H 498 -6.078 -3.148 -42.491 1.00 20.00 B c
ATOM 6924 CE LYS H 498 -5.896 -4.624 -42.160 1.00 20.00 B c
ATOM 6925 NZ LYS H 498 -6.862 -5.090 -41.127 1.00 20.00 B N
ATOM 6926 C LYS H 498 -4.622 0.716 -45.298 1.00 55.29 B c
ATOM 6927 O LYS H 498 -5.273 0.766 -46.340 1.00 61.06 B o
ATOM 6928 N ILE H 499 -4.359 1.789 -44.558 1.00 52.22 B N
ATOM 6929 CA ILE H 499 -4.606 3.140 -45.052 1.00 48.26 B c
ATOM 6930 CB ILE H 499 -4.213 4.205 -44.012 1.00 20.00 B c
ATOM 6931 CGI ILE H 499 -5.137 4.139 -42.797 1.00 20.00 B c
ATOM 6932 CD1 ILE H 499 -4.719 5.058 -41.669 1.00 20.00 B c
ATOM 6933 CG2 ILE H 499 -4.246 5.594 -44.631 1.00 20.00 B c
ATOM 6934 C ILE H 499 -3.809 3.400 -46.323 1.00 49.07 B C
ATOM 6935 O ILE H 499 -4.273 4.090 -47.232 1.00 58.45 B O
ATOM 6936 N ASN H 500 -2.600 2.849 -46.371 1.00 51.02 B N
ATOM 6937 CA ASN H 500 -1.718 3.000 -47.524 1.00 52.06 B c
ATOM 6938 CB ASN H 500 -0.284 2.663 -47.120 1.00 20.00 B c
ATOM 6939 CG ASN H 500 0.707 2.898 -48.233 1.00 20.00 B c
ATOM 6940 OD1 ASN H 500 0.607 3.875 -48.973 1.00 20.00 B o
ATOM 6941 ND2 ASN H 500 1.740 2.071 -48.275 1.00 20.00 B N

ATOM 6942 C ASN H 500 -2.151 2.149 -48.719 1.00 48.31 B C
ATOM 6943 O ASN H 500 -1.841 2.469 -49.867 1.00 56.89 B o
ATOM 6944 N GLN H 501 -2.872 1.067 -48.438 1.00 55.87 B N
ATOM 6945 CA GLN H 501 -3.51 1 0.269 -49.480 1.00 53.55 B C
ATOM 6946 CB GLN H 501 -3.879 -1.1 16 -48.940 1.00 20.00 B c
ATOM 6947 CG GLN H 501 -2.685 -1.963 -48.513 1.00 20.00 B c
ATOM 6948 CD GLN H 501 -3.093 -3.333 -47.996 1.00 20.00 B c
ATOM 6949 OE1 GLN H 501 -4.169 -3.495 -47.420 1.00 20.00 B o
ATOM 6950 NE2 GLN H 501 -2.215 -4.317 -48. 162 1.00 20.00 B N
ATOM 6951 C GLN H 501 -4.755 0.964 -50.023 1.00 45.67 B c
ATOM 6952 O GLN H 501 -4.984 0.994 -51.232 1.00 58.31 B o
ATOM 6953 N SER H 502 -5.525 1.570 -49.124 1.00 43.44 B N
ATOM 6954 CA SER H 502 -6.702 2.345 -49.508 1.00 45.40 B c
ATOM 6955 CB SER H 502 -7.471 2.800 -48.264 1.00 20.00 B c
ATOM 6956 OG SER H 502 -6.684 3.664 -47.464 1.00 20.00 B o
ATOM 6957 C SER H 502 -6.319 3.555 -50.358 1.00 55.15 B c
ATOM 6958 O SER H 502 -7.049 3.943 -51 .270 1.00 52.57 B o
ATOM 6959 N LEU H 503 -5.160 4.135 -50.060 1.00 55.35 B N
ATOM 6960 CA LEU H 503 -4.662 5.286 -50.805 1.00 52.12 B c
ATOM 6961 CB LEU H 503 -3.529 5.973 -50.037 1.00 20.00 B c
ATOM 6962 CG LEU H 503 -3.896 6.598 -48.688 1.00 20.00 B c
ATOM 6963 CD1 LEU H 503 -2.646 7.032 -47.948 1.00 20.00 B c
ATOM 6964 CD2 LEU H 503 -4.847 7.769 -48.868 1.00 20.00 B c
ATOM 6965 C LEU H 503 -4.187 4.882 -52. 197 1.00 55.74 B c
ATOM 6966 O LEU H 503 -4.339 5.636 -53.159 1.00 57.75 B o
ATOM 6967 N ALA H 504 -3.608 3.691 -52.295 1.00 57.22 B N
ATOM 6968 CA ALA H 504 -3.204 3.150 -53.584 1.00 59.12 B c
ATOM 6969 CB ALA H 504 -2.319 1.930 -53.394 1.00 20.00 B c
ATOM 6970 C ALA H 504 -4.423 2.802 -54.427 1.00 58.10 B c
ATOM 6971 O ALA H 504 -4.488 3.145 -55.608 1.00 63.64 B o
ATOM 6972 N PHE H 505 -5.421 2.194 -53.793 1.00 58.17 B N
ATOM 6973 CA PHE H 505 -6.683 1.909 -54.464 1.00 56.56 B c
ATOM 6974 CB PHE H 505 -7.657 1.198 -53.517 1.00 20.00 B c
ATOM 6975 CG PHE H 505 -7.174 -0.142 -53.045 1.00 20.00 B c
ATOM 6976 CD1 PHE H 505 -7.297 -1.263 -53.851 1.00 20.00 B c
ATOM 6977 CE1 PHE H 505 -6.817 -2.490 -53.432 1.00 20.00 B c
ATOM 6978 CZ PHE H 505 -6.236 -2.610 -52.183 1.00 20.00 B c
ATOM 6979 CE2 PHE H 505 -6.106 -1.497 -51.373 1.00 20.00 B c
ATOM 6980 CD2 PHE H 505 -6.566 -0.272 -51 .809 1.00 20.00 B c
ATOM 6981 C PHE H 505 -7.307 3.189 -55.020 1.00 60.12 B c
ATOM 6982 O PHE H 505 -7.761 3.223 -56. 166 1.00 65.46 B o
ATOM 6983 N ILE H 506 -7.214 4.267 -54.247 1.00 56.10 B N
ATOM 6984 CA ILE H 506 -7.762 5.552 -54.667 1.00 57.32 B c
ATOM 6985 CB ILE H 506 -7.716 6.599 -53.536 1.00 20.00 B c
ATOM 6986 CGI ILE H 506 -8.610 6.163 -52.376 1.00 20.00 B c
ATOM 6987 CD1 ILE H 506 -8.728 7.191 -51 .274 1.00 20.00 B c
ATOM 6988 CG2 ILE H 506 -8.177 7.956 -54.049 1.00 20.00 B c
ATOM 6989 C ILE H 506 -7.013 6.084 -55.883 1.00 67.33 B C
ATOM 6990 O ILE H 506 -7.625 6.563 -56.839 1.00 76.99 B O
ATOM 6991 N ARG H 507 -5.694 5.913 -55.876 1.00 67.87 B N
ATOM 6992 CA ARG H 507 -4.858 6.338 -56.993 1.00 62. 11 B c
ATOM 6993 CB ARG H 507 -3.381 6.153 -56.657 1.00 20.00 B c
ATOM 6994 CG ARG H 507 -2.862 7.130 -55.630 1.00 20.00 B c
ATOM 6995 CD ARG H 507 -1.380 6.930 -55.386 1.00 20.00 B c
ATOM 6996 NE ARG H 507 -0.903 7.783 -54.303 1.00 20.00 B N
ATOM 6997 CZ ARG H 507 0.322 7.729 -53.792 1.00 20.00 B c
ATOM 6998 NH1 ARG H 507 1.215 6.883 -54.288 1.00 20.00 B N
ATOM 6999 NH2 ARG H 507 0.656 8.530 -52.791 1.00 20.00 B N
ATOM 7000 C ARG H 507 -5.191 5.565 -58.258 1.00 67.30 B C
ATOM 7001 O ARG H 507 -5.255 6.139 -59.344 1.00 67.02 B o

```
ATOM   7002  N   LYS H 508      -5.222   4.243 -58.139  1.00 66.83      B    N
ATOM   7003  CA  LYS H 508      -5.694   3.391 -59.220  1.00 68.12      B    C
ATOM   7004  CB  LYS H 508      -5.743   1.932 -58.763  1.00 20.00      B    C
ATOM   7005  CG  LYS H 508      -4.368   1.325 -58.543  1.00 20.00      B    c
ATOM   7006  CD  LYS H 508      -4.433  -0.159 -58.230  1.00 20.00      B    c
ATOM   7007  CE  LYS H 508      -3.037  -0.710 -57.973  1.00 20.00      B    c
ATOM   7008  NZ  LYS H 508      -3.053  -2.129 -57.525  1.00 20.00      B    N
ATOM   7009  C   LYS H 508      -7.065   3.839 -59.705  1.00 65.22      B    c
ATOM   7010  O   LYS H 508      -7.245   4.154 -60.881  1.00 72.34      B    o
ATOM   7011  N   SER H 509      -7.996   3.977 -58.767  1.00 64.87      B    N
ATOM   7012  CA  SER H 509      -9.366   4.349 -59.095  1.00 56.47      B    c
ATOM   7013  CB  SER H 509     -10.227   4.420 -57.832  1.00 20.00      B    c
ATOM   7014  OG  SER H 509      -9.862   5.523 -57.023  1.00 20.00      B    o
ATOM   7015  C   SER H 509      -9.418   5.673 -59.851  1.00 56.96      B    c
ATOM   7016  O   SER H 509     -10.124   5.796 -60.854  1.00 65.57      B    o
ATOM   7017  N   ASP H 510      -8.670   6.661 -59.368  1.00 64.34      B    N
ATOM   7018  CA  ASP H 510      -8.624   7.971 -60.009  1.00 64.83      B    c
ATOM   7019  CB  ASP H 510      -7.774   8.944 -59.192  1.00 20.00      B    c
ATOM   7020  CG  ASP H 510      -8.421   9.315 -57.872  1.00 20.00      B    c
ATOM   7021  OD1 ASP H 510      -9.589   8.927 -57.652  1.00 20.00      B    o
ATOM   7022  OD2 ASP H 510      -7.729   9.904 -57.015  1.00 20.00      B    o
ATOM   7023  C   ASP H 510      -8.087   7.873 -61.431  1.00 62.11      B    c
ATOM   7024  O   ASP H 510      -8.711   8.358 -62.373  1.00 67.61      B    o
ATOM   7025  N   GLU H 511      -6.939   7.222 -61.584  1.00 64.95      B    N
ATOM   7026  CA  GLU H 511      -6.330   7.042 -62.896  1.00 60.64      B    c
ATOM   7027  CB  GLU H 511      -5.117   6.109 -62.804  1.00 20.00      B    c
ATOM   7028  CG  GLU H 511      -3.959   6.673 -61.982  1.00 20.00      B    c
ATOM   7029  CD  GLU H 511      -2.858   5.655 -61.716  1.00 20.00      B    c
ATOM   7030  OE1 GLU H 511      -3.140   4.438 -61.756  1.00 20.00      B    o
ATOM   7031  OE2 GLU H 511      -1.749   6.076 -61.324  1.00 20.00      B    o
ATOM   7032  C   GLU H 511      -7.340   6.528 -63.928  1.00 59.91      B    c
ATOM   7033  O   GLU H 511      -7.417   7.043 -65.045  1.00 55.45      B    o
ATOM   7034  N   LEU H 512      -8.137   5.537 -63.533  1.00 44.35      B    N
ATOM   7035  CA  LEU H 512      -9.117   4.929 -64.432  1.00 49.60      B    c
ATOM   7036  CB  LEU H 512      -9.744   3.682 -63.796  1.00 20.00      B    c
ATOM   7037  CG  LEU H 512      -8.841   2.462 -63.572  1.00 20.00      B    c
ATOM   7038  CD1 LEU H 512      -9.594   1.368 -62.825  1.00 20.00      B    c
ATOM   7039  CD2 LEU H 512      -8.295   1.930 -64.892  1.00 20.00      B    c
ATOM   7040  C   LEU H 512     -10.208   5.920 -64.821  1.00 58.00      B    c
ATOM   7041  O   LEU H 512     -10.524   6.073 -66.000  1.00 55.11      B    o
ATOM   7042  N   LEU H 513     -10.814   6.552 -63.820  1.00 57.91      B    N
ATOM   7043  CA  LEU H 513     -11.866   7.536 -64.057  1.00 57.49      B    c
ATOM   7044  CB  LEU H 513     -12.390   8.097 -62.733  1.00 20.00      B    c
ATOM   7045  CG  LEU H 513     -13.077   7.088 -61.815  1.00 20.00      B    c
ATOM   7046  CD1 LEU H 513     -13.388   7.705 -60.461  1.00 20.00      B    c
ATOM   7047  CD2 LEU H 513     -14.336   6.556 -62.474  1.00 20.00      B    c
ATOM   7048  C   LEU H 513     -11.384   8.676 -64.949  1.00 58.78      B    c
ATOM   7049  O   LEU H 513     -12.154   9.220 -65.740  1.00 59.88      B    o
ATOM   7050  N   HIS H 514     -10.131   9.086 -64.764  1.00 60.07      B    N
ATOM   7051  CA  HIS H 514      -9.544  10.151 -65.578  1.00 62.82      B    c
ATOM   7052  CB  HIS H 514      -8.240  10.665 -64.951  1.00 20.00      B    c
ATOM   7053  CG  HIS H 514      -8.406  11.218 -63.567  1.00 20.00      B    c
ATOM   7054  ND1 HIS H 514      -9.083  12.390 -63.308  1.00 20.00      B    N
ATOM   7055  CE1 HIS H 514      -9.060  12.634 -62.010  1.00 20.00      B    c
ATOM   7056  NE2 HIS H 514      -8.393  11.660 -61.416  1.00 20.00      B    N
ATOM   7057  CD2 HIS H 514      -7.960  10.770 -62.368  1.00 20.00      B    C
ATOM   7058  C   HIS H 514      -9.305   9.679 -67.014  1.00 65.10      B    C
ATOM   7059  O   HIS H 514      -9.352  10.475 -67.953  1.00 66.73      B    o
ATOM   7060  N   ASN H 515      -9.179   8.365 -67.187  1.00 63.45      B    N
ATOM   7061  CA  ASN H 515      -9.028   7.768 -68.513  1.00 56.53      B    C
```

```
ATOM   7062  CB  ASN H 515      -8.367   6.392 -68.409  1.00 20.00      B    C
ATOM   7063  CG  ASN H 515      -6.901   6.476 -68.035  1.00 20.00      B    C
ATOM   7064  OD1 ASN H 515      -6.233   7.470 -68.319  1.00 20.00      B    o
ATOM   7065  ND2 ASN H 515      -6.375   5.399 -67.462  1.00 20.00      B    N
ATOM   7066  C   ASN H 515     -10.357   7.651 -69.254  1.00 60.06      B    C
ATOM   7067  O   ASN H 515     -10.414   7.816 -70.473  1.00 66.48      B    o
ATOM   7068  N   VAL H 516     -11.402   7.275 -68.522  1.00 54.29      B    N
ATOM   7069  CA  VAL H 516     -12.765   7.256 -69.056  1.00 52.70      B    C
ATOM   7070  CB  VAL H 516     -13.775   6.751 -68.001  1.00 20.00      B    c
ATOM   7071  CGI VAL H 516     -15.194   6.825 -68.541  1.00 20.00      B    c
ATOM   7072  CG2 VAL H 516     -13.431   5.333 -67.568  1.00 20.00      B    c
ATOM   7073  C   VAL H 516     -13.206   8.633 -69.557  1.00 60.10      B    c
ATOM   7074  O   VAL H 516     -13.761   8.759 -70.649  1.00 61.55      B    o
ATOM   7075  N   ASN H 517     -12.957   9.661 -68.752  1.00 69.10      B    N
ATOM   7076  CA  ASN H 517     -13.297  11.030 -69.125  1.00 67.75      B    c
ATOM   7077  CB  ASN H 517     -12.850  12.012 -68.038  1.00 20.00      B    c
ATOM   7078  CG  ASN H 517     -13.685  11.907 -66.774  1.00 20.00      B    c
ATOM   7079  OD1 ASN H 517     -14.835  11.471 -66.813  1.00 20.00      B,   o
ATOM   7080  ND2 ASN H 517     -13.126  12.355 -65.653  1.00 20.00      B,   N
ATOM   7081  C   ASN H 517     -12.686  11.424 -70.465  1.00 71.17      B    c
ATOM   7082  O   ASN H 517     -13.289  12.169 -71.238  1.00 66.42      B    o
ATOM   7083  N   ALA H 518     -11.489  10.912 -70.739  1.00 72.11      B    N
ATOM   7084  CA  ALA H 518     -10.794  11.202 -71.989  1.00 74.82      B    c
ATOM   7085  CB  ALA H 518      -9.318  10.855 -71.867  1.00 20.00      B    c
ATOM   7086  C   ALA H 518     -11.421  10.450 -73.155  1.00 70.11      B    c
ATOM   7087  O   ALA H 518     -11.593  11.001 -74.242  1.00 65.18      B    o
ATOM   7088  N   GLY H 519     -11.665   9.160 -72.952  1.00 56.07      B    N
ATOM   7089  CA  GLY H 519     -12.395   8.360 -73.926  1.00 53.01      B    c
ATOM   7090  C   GLY H 519     -13.763   8.941 -74.222  1.00 63.58      B    c
ATOM   7091  O   GLY H 519     -14.203   8.960 -75.371  1.00 69.35      B    o
ATOM   7092  N   LYS H 520     -14.422   9.444 -73.183  1.00 58.33      B    N
ATOM   7093  CA  LYS H 520     -15.716  10.101 -73.333  1.00 53.44      B    c
ATOM   7094  CB  LYS H 520     -16.241  10.557 -71.975  1.00 20.00      B    c
ATOM   7095  CG  LYS H 520     -16.441   9.429 -70.996  1.00 20.00      B    c
ATOM   7096  CD  LYS H 520     -16.739   9.961 -69.616  1.00 20.00      B    c
ATOM   7097  CE  LYS H 520     -17.296   8.868 -68.730  1.00 20.00      B    c
ATOM   7098  NZ  LYS H 520     -17.807   9.424 -67.452  1.00 20.00      B    N
ATOM   7099  C   LYS H 520     -15.623  11.296 -74.268  1.00 58.24      B    c
ATOM   7100  O   LYS H 520     -16.579  11.621 -74.972  1.00 48.60      B    o
ATOM   7101  N   SER H 521     -14.489  11.986 -74.219  1.00 67.19      B    N
ATOM   7102  CA  SER H 521     -14.232  13.101 -75.120  1.00 60.42      B    c
ATOM   7103  CB  SER H 521     -12.938  13.821 -74.727  1.00 20.00      B    c
ATOM   7104  OG  SER H 521     -11.894  12.898 -74.459  1.00 20.00      B    o
ATOM   7105  C   SER H 521     -14.167  12.636 -76.573  1.00 54.19      B    c
ATOM   7106  O   SER H 521     -14.886  13.151 -77.430  1.00 65.36      B    o
ATOM   7107  N   THR H 522     -13.362  11.609 -76.825  1.00 50.09      B    N
ATOM   7108  CA  THR H 522     -13.259  11.025 -78.158  1.00 57.59      B    c
ATOM   7109  CB  THR H 522     -12.299   9.817 -78.179  1.00 20.00      B    c
ATOM   7110  OG1 THR H 522     -12.774   8.810 -77.278  1.00 20.00      B    o
ATOM   7111  CG2 THR H 522     -10.894  10.235 -77.767  1.00 20.00      B    c
ATOM   7112  C   THR H 522     -14.625  10.565 -78.646  1.00 59.16      B    c
ATOM   7113  O   THR H 522     -15.044  10.893 -79.755  1.00 65.90      B    o
ATOM   7114  N   THR H 523     -15.338   9.849 -77.783  1.00 52.59      B    N
ATOM   7115  CA  THR H 523     -16.665   9.347 -78.112  1.00 42.19      B    c
ATOM   7116  CB  THR H 523     -17.298   8.599 -76.922  1.00 20.00      B    c
ATOM   7117  OG1 THR H 523     -17.543   9.516 -75.848  1.00 20.00      B    o
ATOM   7118  CG2 THR H 523     -16.373   7.492 -76.435  1.00 20.00      B    c
ATOM   7119  C   THR H 523     -17.596  10.466 -78.566  1.00 48.90      B    c
ATOM   7120  O   THR H 523     -18.331  10.314 -79.541  1.00 63.19      B    o
ATOM   7121  N   ASN H 524     -17.535  11.601 -77.881  1.00 52.51      B    N
```

ATOM 7122 CA ASN H 524 -18.341 12.752 -78.258 1.00 57.54 B C
ATOM 7123 CB ASN H 524 -18.235 13.853 -77.202 1.00 20.00 B C
ATOM 7124 CG ASN H 524 -19.015 13.528 -75.945 1.00 20.00 B C
ATOM 7125 OD1 ASN H 524 -19.910 12.682 -75.959 1.00 20.00 B O
ATOM 7126 ND2 ASN H 524 -18.683 14.203 -74.850 1.00 20.00 B N
ATOM 7127 C ASN H 524 -17.956 13.287 -79.633 1.00 54.12 B C
ATOM 7128 O ASN H 524 -18.812 13.463 -80.500 1.00 61.31 B O
ATOM 7129 N SER H 525 -16.656 13.422 -79.866 1.00 48.97 B N
ATOM 7130 CA SER H 525 -16.165 13.913 -81.145 1.00 64.81 B C
ATOM 7131 CB SER H 525 -14.636 13.940 -81.151 1.00 61.22 B C
ATOM 7132 OG SER H 525 -14.141 14.856 -80.191 1.00 85.90 B O
ATOM 7133 C SER H 525 -16.689 13.053 -82.292 1.00 69.67 B C
ATOM 7134 O SER H 525 -17.013 13.563 -83.367 1.00 72.60 B O
ATOM 7135 N LYS H 526 -16.849 11.760 -82.029 1.00 66.06 B N
ATOM 7136 CA LYS H 526 -17.335 10.831 -83.043 1.00 63.67 B C
ATOM 7137 CB LYS H 526 -17.003 9.383 -82.660 1.00 70.55 B C
ATOM 7138 CG LYS H 526 -15.562 8.963 -82.939 1.00 75.29 B C
ATOM 7139 CD LYS H 526 -15.205 7.681 -82.194 1.00 85.03 B C
ATOM 7140 CE LYS H 526 -13.700 7.525 -82.041 1.00 82.65 B C
ATOM 7141 NZ LYS H 526 -13.347 6.537 -80.984 1.00 73.89 B N
ATOM 7142 C LYS H 526 -18.838 10.987 -83.239 1.00 55.36 B C
ATOM 7143 O LYS H 526 -19.333 10.950 -84.365 1.00 70.69 B O
ATOM 7144 N ILE H 527 -19.560 11.149 -82.135 1.00 57.52 B N
ATOM 7145 CA ILE H 527 -20.995 11.389 -82.189 1.00 58.48 B C
ATOM 7146 CB ILE H 527 -21.569 11.642 -80.787 1.00 57.00 B C
ATOM 7147 CGI ILE H 527 -21.356 10.420 -79.891 1.00 49.07 B C
ATOM 7148 CD1 ILE H 527 -21.790 9.118 -80.517 1.00 46.18 B C
ATOM 7149 CG2 ILE H 527 -23.035 12.029 -80.872 1.00 52.63 B C
ATOM 7150 C ILE H 527 -21.317 12.586 -83.075 1.00 65.20 B C
ATOM 7151 O ILE H 527 -22.228 12.532 -83.900 1.00 66.48 B O
ATOM 7152 N TYR H 528 -20.590 13.681 -82.870 1.00 69.78 B N
ATOM 7153 CA TYR H 528 -20.780 14.884 -83.673 1.00 72.52 B C
ATOM 7154 CB TYR H 528 -19.738 15.948 -83.316 1.00 73.16 B C
ATOM 7155 CG TYR H 528 -19.707 16.343 -81.856 1.00 76.94 B C
ATOM 7156 CD1 TYR H 528 -18.615 17.018 -81.327 1.00 70.95 B C
ATOM 7157 CE1 TYR H 528 -18.584 17.406 -80.000 1.00 67.73 B C
ATOM 7158 CZ TYR H 528 -19.653 17.114 -79.180 1.00 71.89 B C
ATOM 7159 OH TYR H 528 -19.626 17.490 -77.856 1.00 75.44 B O
ATOM 7160 CE2 TYR H 528 -20.759 16.464 -79.687 1.00 77.03 B C
ATOM 7161 CD2 TYR H 528 -20.782 16.084 -81.018 1.00 77.84 B C
ATOM 7162 C TYR H 528 -20.678 14.551 -85.157 1.00 71.63 B C
ATOM 7163 O TYR H 528 -21.609 14.797 -85.925 1.00 84.20 B O
ATOM 7164 N HIS H 529 -19.526 14.025 -85.559 1.00 67.69 B N
ATOM 7165 CA HIS H 529 -19.265 13.733 -86.962 1.00 60.28 B C
ATOM 7166 CB HIS H 529 -17.883 13.102 -87.131 1.00 67.84 B C
ATOM 7167 CG HIS H 529 -16.752 14.042 -86.853 1.00 88.54 B C
ATOM 7168 ND1 HIS H 529 -15.514 13.914 -87.444 1.00 93.34 B N
ATOM 7169 CE1 HIS H 529 -14.718 14.874 -87.007 1.00 86.23 B C
ATOM 7170 NE2 HIS H 529 -15.394 15.614 -86.145 1.00 91.95 B N
ATOM 7171 CD2 HIS H 529 -16.667 15.110 -86.026 1.00 93.77 B C
ATOM 7172 C HIS H 529 -20.333 12.817 -87.546 1.00 63.30 B C
ATOM 7173 O HIS H 529 -20.803 13.034 -88.663 1.00 61.02 B O
ATOM 7174 N ILE H 530 -20.710 11.791 -86.791 1.00 59.79 B N
ATOM 7175 CA ILE H 530 -21.800 10.915 -87.201 1.00 45.70 B C
ATOM 7176 CB ILE H 530 -22.019 9.780 -86.190 1.00 40.57 B C
ATOM 7177 CGI ILE H 530 -20.879 8.765 -86.292 1.00 42.86 B C
ATOM 7178 CD1 ILE H 530 -20.826 7.775 -85.154 1.00 51.01 B C
ATOM 7179 CG2 ILE H 530 -23.360 9.108 -86.437 1.00 35.31 B C
ATOM 7180 C ILE H 530 -23.085 11.717 -87.331 1.00 57.52 B C
ATOM 7181 O ILE H 530 -23.779 11.645 -88.345 1.00 71.18 B O

ATOM 7182 N GLU H 531 -23.322 12.569 -86.341 1.00 67.55 B N
ATOM 7183 CA GLU H 531 -24.479 13.449 -86.325 1.00 69.79 B C
ATOM 7184 CB GLU H 531 -24.440 14.327 -85.074 1.00 84.02 B C
ATOM 7185 CG GLU H 531 -25.803 14.718 -84.541 1.00104.22 B C
ATOM 7186 CD GLU H 531 -25.706 15.531 -83.270 1.001 16.08 B C
ATOM 7187 OE1 GLU H 531 -25.017 15.079 -82.331 1.001 18.71 B O
ATOM 7188 OE2 GLU H 531 -26.222 16.669 -83.251 1.001 19.69 B O
ATOM 7189 C GLU H 531 -24.506 14.328 -87.569 1.00 64.87 B C
ATOM 7190 O GLU H 531 -25.517 14.404 -88.269 1.00 55.58 B O
ATOM 7191 N ASN H 532 -23.394 15.01 1 -87.821 1.00 65.70 B N
ATOM 7192 CA ASN H 532 -23.273 15.890 -88.979 1.00 64.16 B C
ATOM 7193 CB ASN H 532 -21.931 16.625 -88.953 1.00 60.58 B C
ATOM 7194 CG ASN H 532 -21.793 17.621 -90.085 1.00 67.75 B C
ATOM 7195 OD1 ASN H 532 -22.591 18.550 -90.206 1.00 53.59 B O
ATOM 7196 ND2 ASN H 532 -20.822 17.392 -90.961 1.00 61.81 B N
ATOM 7197 C ASN H 532 -23.418 15.1 19 -90.284 1.00 72.17 B C
ATOM 7198 O ASN H 532 -24.041 15.593 -91.233 1.00 85.75 B O
ATOM 7199 N GLU H 533 -22.870 13.909 -90.300 1.00 79.68 B N
ATOM 7200 CA GLU H 533 -22.922 13.044 -91 .468 1.00 7 1.96 B C
ATOM 7201 CB GLU H 533 -22.010 11.837 -91.264 1.00 67.87 B C
ATOM 7202 CG GLU H 533 -21.638 11.131 -92.547 1.00 81.94 B C
ATOM 7203 CD GLU H 533 -20.906 12.037 -93.515 1.00 92.79 B C
ATOM 7204 OE1 GLU H 533 -19.930 12.692 -93.094 1.00 95.90 B O
ATOM 7205 OE2 GLU H 533 -21.247 12.025 -94.716 1.00 93.14 B O
ATOM 7206 C GLU H 533 -24.342 12.570 -91.747 1.00 68.54 B C
ATOM 7207 O GLU H 533 -24.667 12.175 -92.866 1.00 79.29 B O
ATOM 7208 N ILE H 534 -25.137 12.470 -90.688 1.00 69.50 B N
ATOM 7209 CA ILE H 534 -26.529 12.076 -90.817 1.00 72.55 B C
ATOM 7210 CB ILE H 534 -27.056 11.467 -89.514 1.00 79.55 B C
ATOM 721 1 CGI ILE H 534 -26.263 10.209 -89. 164 1.00 80.41 B C
ATOM 7212 CD1 ILE H 534 -25.562 9.592 -90.348 1.00 89.38 B C
ATOM 7213 CG2 ILE H 534 -28.526 11.138 -89.645 1.00 78.63 B C
ATOM 7214 C ILE H 534 -27.389 13.273 -91.189 1.00 74.92 B C
ATOM 7215 O ILE H 534 -28.479 13. 120 -91.740 1.00 81.01 B O
ATOM 7216 N ALA H 535 -26.880 14.465 -90.903 1.00 79.52 B N
ATOM 7217 CA ALA H 535 -27.559 15.690 -91 .290 1.00 82.64 B C
ATOM 7218 CB ALA H 535 -27.016 16.867 -90.498 1.00 75.39 B C
ATOM 7219 C ALA H 535 -27.440 15.939 -92.795 1.00 81.39 B C
ATOM 7220 O ALA H 535 -28.408 16.341 -93.443 1.00 85.54 B O
ATOM 7221 N ARG H 536 -26.274 15.630 -93.358 1.00 78.41 B N
ATOM 7222 CA ARG H 536 -26.044 15.812 -94.791 1.00 83.27 B C
ATOM 7223 CB ARG H 536 -24.545 15.814 -95. 106 1.00 84.58 B C
ATOM 7224 CG ARG H 536 -23.776 16.993 -94.527 1.00103.24 B C
ATOM 7225 CD ARG H 536 -22.638 17.422 -95.449 1.001 14.72 B C
ATOM 7226 NE ARG H 536 -21.692 16.343 -95.722 1.001 17.80 B N
ATOM 7227 CZ ARG H 536 -20.692 16.430 -96.594 1.001 16.66 B C
ATOM 7228 NH1 ARG H 536 -20.522 17.538 -97.303 1.001 14.57 B N
ATOM 7229 NH2 ARG H 536 -19.885 15.396 -96.786 1.001 16.38 B N
ATOM 7230 C ARG H 536 -26.744 14.727 -95.606 1.00 82.20 B C
ATOM 7231 O ARG H 536 -27.369 15.01 1 -96.627 1.00 86.28 B O
ATOM 7232 N ILE H 537 -26.598 13.479 -95.172 1.00 77.08 B N
ATOM 7233 CA ILE H 537 -27.315 12.371 -95.782 1.00 66.79 B C
ATOM 7234 CB ILE H 537 -26.955 11.038 -95.1 13 1.00 64.76 B C
ATOM 7235 CGI ILE H 537 -25.523 10.627 -95.476 1.00 66.92 B C
ATOM 7236 CD1 ILE H 537 -24.906 9.625 -94.519 1.00 70.83 B C
ATOM 7237 CG2 ILE H 537 -27.960 9.964 -95.497 1.00 51.02 B C
ATOM 7238 C ILE H 537 -28.817 12.585 -95.674 1.00 74.94 B C
ATOM 7239 O ILE H 537 -29.587 12.070 -96.482 1.00 97.16 B O
ATOM 7240 N LYS H 538 -29.232 13.337 -94.661 1.00 75.09 B N
ATOM 7241 CA LYS H 538 -30.640 13.666 -94.485 1.00 90.28 B C

ATOM 7242 CB LYS H 538 -30.958 13.868 -93.003 1.00 93.73 B C
ATOM 7243 CG LYS H 538 -32.344 13.390 -92.575 1.00 96.60 B C
ATOM 7244 CD LYS H 538 -32.640 13.787 -91 .126 1.00 95.37 B C
ATOM 7245 CE LYS H 538 -34.127 13.714 -90.798 1.00100.63 B C
ATOM 7246 NZ LYS H 538 -34.398 14.067 -89.375 1.00 99.58 B N
ATOM 7247 C LYS H 538 -31 .022 14.91 1 -95.284 1.00102.20 B C
ATOM 7248 O LYS H 538 -32.166 15.360 -95.235 1.001 12. 11 B O
ATOM 7249 N LYS H 539 -30.069 15.444 -96.043 1.00105. 15 B N
ATOM 7250 CA LYS H 539 -30.317 16.603 -96.899 1.00105.65 B C
ATOM 7251 CB LYS H 539 -29.144 17.589 -96.823 1.001 10.12 B C
ATOM 7252 CG LYS H 539 -29.408 18.944 -97.481 1.001 13.31 B C
ATOM 7253 CD LYS H 539 -28.182 19.854 -97.435 1.001 14.26 B C
ATOM 7254 CE LYS H 539 -28.426 2 1.145 -98.205 1.001 18.39 B C
ATOM 7255 NZ LYS H 539 -27.168 21.897 -98.470 1.00121.77 B N
ATOM 7256 C LYS H 539 -30.572 16.187 -98.347 1.00108.88 B C
ATOM 7257 O LYS H 539 -30.886 17.021 -99. 195 1.001 10.77 B O
ATOM 7258 N LEU H 540 -30.515 14.884 -98.605 1.001 11.50 B N
ATOM 7259 CA LEU H 540 -30.796 14.356 -99.935 1.001 10.31 B C
ATOM 7260 CB LEU H 540 -29.690 13.389-100.368 1.00101.19 B C
ATOM 7261 CG LEU H 540 -28.270 13.889-100.078 1.00 94.26 B C
ATOM 7262 CD 1 LEU H 540 -27.249 12.769-100. 179 1.00 86.40 B C
ATOM 7263 CD2 LEU H 540 -27.896 15.059-100.984 1.00 84.54 B C
ATOM 7264 C LEU H 540 -32.157 13.675 -99.961 1.001 18.37 B C
ATOM 7265 O LEU H 540 -32.531 13.039-100.945 1.001 16.71 B O
ATOM 7266 N ILE H 541 -32.923 13.883 -98.896 1.00130.80 B N
ATOM 7267 CA ILE H 541 -34.267 13.339 -98.801 1.00140.48 B C
ATOM 7268 CB ILE H 541 -34.250 11.862 -98.372 1.00138.99 B C
ATOM 7269 CGI ILE H 541 -33.319 11.059 -99.282 1.00133.30 B C
ATOM 7270 CD 1 ILE H 541 -33.895 10.789-100.656 1.00136.26 B C
ATOM 7271 CG2 ILE H 541 -35.653 11.281 -98.432 1.00136.12 B C
ATOM 7272 C ILE H 541 -35.146 14. 139 -97.839 1.00144.97 B C
ATOM 7273 O ILE H 541 -36.372 14.063 -97.905 1.00145.83 B O
ATOM 7274 N GLY H 542 -34.523 14.940 -96.979 1.00148.77 B N
ATOM 7275 CA GLY H 542 -35.267 15.725 -95.991 1.00153.58 B C
ATOM 7276 C GLY H 542 -35.358 17.210 -96.308 1.00160.45 B C
ATOM 7277 O GLY H 542 -35.594 17.599 -97.454 1.00163.41 B O
ATOM 7278 N GLU H 543 -35.275 18.034 -95.267 1.00163.83 B N
ATOM 7279 CA GLU H 543 -35.152 19.480 -95.430 1.00165.52 B C
ATOM 7280 CB GLU H 543 -35.727 20.205 -94.21 1 1.00158.94 B C
ATOM 7285 C GLU H 543 -33.698 19.890 -95.644 1.00168.27 B C
ATOM 7286 O GLU H 543 -32.778 19.1 16 -95.373 1.00167.37 B O
ATOM 7287 N GLN I 26 21.181 -26.937 -9.836 1.00 23.62 C N
ATOM 7288 CA GLN I 26 21.159 -25.618 -10.530 1.00 23.82 C C
ATOM 7289 CB GLN I 26 21.607 -24.503 -9.580 1.00 23.94 C C
ATOM 7290 CG GLN I 26 20.888 -24.492 -8.237 1.00 28.83 C C
ATOM 7291 CD GLN I 26 21.323 -25.626 -7.329 1.00 36.36 C C
ATOM 7292 OE1 GLN I 26 20.813 -26.740 -7.428 1.00 39.09 C O
ATOM 7293 NE2 GLN I 26 22.207 -25.325 -6.384 1.00 37.86 C N
ATOM 7294 C GLN I 26 22.043 -25.641 - 11.774 1.00 23.09 C C
ATOM 7295 O GLN I 26 22.946 -26.471 - 11.888 1.00 24.21 C O
ATOM 7296 N ASN I 27 2 1.670 -24.835 -12.765 1.00 20.98 C N
ATOM 7297 CA ASN I 27 22.435 -24.709 -14.004 1.00 19.70 C C
ATOM 7298 CB ASN I 27 22.165 -25.904 -14.928 1.00 20.41 C C
ATOM 7299 CG ASN I 27 22.952 -25.833 -16.231 1.00 23.56 C C
ATOM 7300 OD1 ASN I 27 24.156 -25.579 -16. 199 1.00 24.42 C O
ATOM 7301 ND2 ASN I 27 22.227 -25.693 -17.339 1.00 27.70 C N
ATOM 7302 C ASN I 27 22.086 -23.414 -14.727 1.00 18.42 C C
ATOM 7303 O ASN I 27 2 1.539 -23.447 -15.830 1.00 18.47 C O
ATOM 7304 N ILE I 28 22.230 -22.288 -14.033 1.00 16.54 C N
ATOM 7305 CA ILE I 28 2 1.853 -21.004 -14.61 1 1.00 14.59 C C

ATOM 7306 CB ILE I 28 21.526 -19.932 -13.546 1.00 14.01 C C
ATOM 7307 CGI ILE I 28 22.461 -20.055 -12.343 1.00 15.60 C C
ATOM 7308 CD1 ILE I 28 23.710 -19.205 -12.454 1.00 16.26 C C
ATOM 7309 CG2 ILE I 28 20.065 -20.023 -13.122 1.00 12.57 C C
ATOM 7310 C ILE I 28 22.915 -20.484 -15.561 1.00 13.86 C C
ATOM 7311 O ILE I 28 24.111 -20.702 -15.363 1.00 13.70 C O
ATOM 7312 N THR I 29 22.442 -20.013 -16.703 1.00 13.23 C N
ATOM 7313 CA THR I 29 23.301 -19.589 -17.786 1.00 12.65 C C
ATOM 7314 CB THR I 29 23.241 -20.586 -18.948 1.00 12.69 C C
ATOM 7315 OG1 THR I 29 22.805 -21.861 -18.463 1.00 12.62 C O
ATOM 7316 CG2 THR I 29 24.603 -20.727 -19.608 1.00 12.92 C C
ATOM 7317 C THR I 29 22.740 -18.277 -18.281 1.00 12.47 C C
ATOM 7318 O THR I 29 21.531 -18.051 -18.220 1.00 12.53 C O
ATOM 7319 N GLU I 30 23.596 -17.467 -18.884 1.00 11.98 C N
ATOM 7320 CA GLU I 30 23.135 -16.364 -19.702 1.00 11.68 C C
ATOM 7321 CB GLU I 30 23.508 -15.035 -19.049 1.00 11.98 C C
ATOM 7322 CG GLU I 30 22.537 -13.901 -19.321 1.00 13.38 C C
ATOM 7323 CD GLU I 30 22.687 -12.767 -18.325 1.00 16.03 C C
ATOM 7324 OE1 GLU I 30 23.820 -12.269 -18.155 1.00 16.65 C O
ATOM 7325 OE2 GLU I 30 21.684 -12.412 -17.673 1.00 17.06 C O
ATOM 7326 C GLU I 30 23.814 -16.480 -21.047 1.00 11.39 C C
ATOM 7327 O GLU I 30 25.000 -16.799 -21.124 1.00 11.50 C O
ATOM 7328 N GLU I 31 23.036 -16.344 -22.111 1.00 11.11 C N
ATOM 7329 CA GLU I 31 23.626 -16.233 -23.427 1.00 11.06 C C
ATOM 7330 CB GLU I 31 23.376 -17.494 -24.251 1.00 11.48 C C
ATOM 7331 CG GLU I 31 22.395 -17.322 -25.391 1.00 13.90 C C
ATOM 7332 CD GLU I 31 22.329 -18.546 -26.280 1.00 17.27 C C
ATOM 7333 OE1 GLU I 31 22.658 -18.428 -27.478 1.00 17.55 C O
ATOM 7334 OE2 GLU I 31 21.999 -19.638 -25.769 1.00 18.73 C O
ATOM 7335 C GLU I 31 23.177 -14.989 -24.167 1.00 10.47 C C
ATOM 7336 O GLU I 31 22.010 -14.597 -24.118 1.00 10.12 C O
ATOM 7337 N PHE I 32 24.139 -14.352 -24.816 1.00 10.15 C N
ATOM 7338 CA PHE I 32 23.986 -12.994 -25.289 1.00 9.62 C C
ATOM 7339 CB PHE I 32 25.267 -12.204 -25.017 1.00 9.42 C C
ATOM 7340 CG PHE I 32 25.384 -10.939 -25.822 1.00 9.27 C C
ATOM 7341 CD1 PHE I 32 24.529 -9.871 -25.585 1.00 9.37 C C
ATOM 7342 CE1 PHE I 32 24.614 -8.713 -26.339 1.00 9.52 C C
ATOM 7343 CZ PHE I 32 25.594 -8.593 -27.306 1.00 9.82 C C
ATOM 7344 CE2 PHE I 32 26.458 -9.651 -27.548 1.00 10.13 C C
ATOM 7345 CD2 PHE I 32 26.372 -10.802 -26.786 1.00 10.06 C C
ATOM 7346 C PHE I 32 23.715 -13.038 -26.782 1.00 9.64 C C
ATOM 7347 O PHE I 32 24.336 -13.811 -27.512 1.00 9.84 C O
ATOM 7348 N TYR I 33 22.764 -12.229 -27.228 1.00 9.59 C N
ATOM 7349 CA TYR I 33 22.384 -12.221 -28.629 1.00 9.67 C C
ATOM 7350 CB TYR I 33 20.874 -12.414 -28.771 1.00 9.52 C C
ATOM 7351 CG TYR I 33 20.408 -13.802 -28.397 1.00 10.94 C C
ATOM 7352 CD1 TYR I 33 19.978 -14.084 -27.107 1.00 12.23 C C
ATOM 7353 CE1 TYR I 33 19.587 -15.359 -26.750 1.00 12.93 C C
ATOM 7354 CZ TYR I 33 19.675 -16.381 -27.670 1.00 13.47 C C
ATOM 7355 OH TYR I 33 19.297 -17.656 -27.315 1.00 14.54 C O
ATOM 7356 CE2 TYR I 33 20.151 -16.137 -28.941 1.00 13.56 C C
ATOM 7357 CD2 TYR I 33 20.538 -14.858 -29.288 1.00 12.96 C C
ATOM 7358 C TYR I 33 22.832 -10.933 -29.306 1.00 9.94 C C
ATOM 7359 O TYR I 33 22.138 -9.917 -29.257 1.00 10.16 C O
ATOM 7360 N GLN I 34 24.036 -10.964 -29.865 1.00 10.06 C N
ATOM 7361 CA GLN I 34 24.713 -9.751 -30.294 1.00 10.01 C C
ATOM 7362 CB GLN I 34 26.105 -10.085 -30.819 1.00 10.22 C C
ATOM 7363 CG GLN I 34 26.862 -8.884 -31.336 1.00 11.12 C C
ATOM 7364 CD GLN I 34 28.323 -9.187 -31.577 1.00 13.13 C C
ATOM 7365 OE1 GLN I 34 28.674 -9.887 -32.528 1.00 14.24 C O

```
ATOM   7366  NE2 GLN I  34      29.183  -8.693 -30.693  1.00 13.79      C    N
ATOM   7367  C   GLN I  34      23.914  -9.028 -31.370  1.00  9.94      C    C
ATOM   7368  O   GLN I  34      24.051  -7.818 -31.550  1.00 10.08      C    O
ATOM   7369  N   SER I  35      23.079  -9.781 -32.081  1.00  9.87      C    N
ATOM   7370  CA  SER I  35      22.336  -9.255 -33.225  1.00  9.91      C    C
ATOM   7371  CB  SER I  35      21.995 -10.382 -34.206  1.00 10.03      C    C
ATOM   7372  OG  SER I  35      21.241 -11.403 -33.574  1.00 10.81      C    O
ATOM   7373  C   SER I  35      21.059  -8.555 -32.775  1.00  9.56      C    C
ATOM   7374  O   SER I  35      20.248  -8.124 -33.595  1.00  9.59      C    O
ATOM   7375  N   THR I  36      20.823  -8.581 -31.472  1.00  9.21      C    N
ATOM   7376  CA  THR I  36      19.592  -8.066 -30.903  1.00  9.06      C    C
ATOM   7377  CB  THR I  36      18.648  -9.214 -30.517  1.00  9.49      C    C
ATOM   7378  OG1 THR I  36      18.292  -9.956 -31.691  1.00 10.82      C    O
ATOM   7379  CG2 THR I  36      17.392  -8.673 -29.860  1.00  9.45      C    C
ATOM   7380  C   THR I  36      19.966  -7.274 -29.661  1.00  8.77      C    C
ATOM   7381  O   THR I  36      19.112  -6.915 -28.848  1.00  8.60      C    O
ATOM   7382  N   CYS I  37      21.266  -7.035 -29.515  1.00  8.69      C    N
ATOM   7383  CA  CYS I  37      21.818  -6.428 -28.314  1.00  8.69      C    C
ATOM   7384  CB  CYS I  37      21.917  -4.911 -28.490  1.00  8.81      C    C
ATOM   7385  SG  CYS I  37      23.280  -4.138 -27.602  1.00 10.80      C    S
ATOM   7386  C   CYS I  37      20.954  -6.758 -27.107  1.00  8.27      C    C
ATOM   7387  O   CYS I  37      20.341  -5.872 -26.513  1.00  8.27      C    O
ATOM   7388  N   SER I  38      20.825  -8.045 -26.808  1.00  7.92      C    N
ATOM   7389  CA  SER I  38      19.990  -8.476 -25.699  1.00  7.51      C    C
ATOM   7390  CB  SER I  38      18.537  -8.626 -26.150  1.00  7.63      C    C
ATOM   7391  OG  SER I  38      18.429  -9.583 -27.190  1.00  8.54      C    O
ATOM   7392  C   SER I  38      20.496  -9.784 -25.110  1.00  7.02      C    C
ATOM   7393  O   SER I  38      21.196 -10.546 -25.776  1.00  6.83      C    O
ATOM   7394  N   ALA I  39      20.214  -9.995 -23.830  1.00  6.64      C    N
ATOM   7395  CA  ALA I  39      20.727 -11.159 -23.127  1.00  6.58      C    C
ATOM   7396  CB  ALA I  39      21.834 -10.761 -22.174  1.00  6.67      C    C
ATOM   7397  C   ALA I  39      19.615 -11.885 -22.388  1.00  6.93      C    C
ATOM   7398  O   ALA I  39      18.683 -11.263 -21.878  1.00  7.38      C    O
ATOM   7399  N   VAL I  40      19.675 -13.211 -22.415  1.00  6.87      C    N
ATOM   7400  CA  VAL I  40      18.707 -14.034 -21.706  1.00  6.55      C    C
ATOM   7401  CB  VAL I  40      17.905 -14.928 -22.668  1.00  6.22      C    C
ATOM   7402  CGI VAL I  40      17.196 -16.031 -21.899  1.00  6.52      C    C
ATOM   7403  CG2 VAL I  40      16.905 -14.098 -23.456  1.00  6.62      C    C
ATOM   7404  C   VAL I  40      19.394 -14.909 -20.670  1.00  6.73      C    C
ATOM   7405  O   VAL I  40      20.351 -15.620 -20.977  1.00  6.83      C    O
ATOM   7406  N   SER I  41      18.916 -14.822 -19.434  1.00  6.86      C    N
ATOM   7407  CA  SER I  41      19.298 -15.760 -18.388  1.00  6.75      C    C
ATOM   7408  CB  SER I  41      19.221 -15.082 -17.022  1.00  7.06      C    C
ATOM   7409  OG  SER I  41      18.745 -13.752 -17.148  1.00  7.50      C    O
ATOM   7410  C   SER I  41      18.399 -16.988 -18.409  1.00  6.56      C    C
ATOM   7411  O   SER I  41      17.174 -16.873 -18.403  1.00  6.08      C    O
ATOM   7412  N   LYS I  42      19.019 -18.163 -18.409  1.00  7.02      C    N
ATOM   7413  CA  LYS I  42      18.311 -19.409 -18.665  1.00  7.83      C    C
ATOM   7414  CB  LYS I  42      18.835 -20.066 -19.943  1.00  8.15      C    C
ATOM   7415  CG  LYS I  42      18.753 -19.192 -21.182  1.00  9.75      C    C
ATOM   7416  CD  LYS I  42      19.416 -19.872 -22.369  1.00 12.62      C    C
ATOM   7417  CE  LYS I  42      19.087 -19.162 -23.671  1.00 14.04      C    C
ATOM   7418  NZ  LYS I  42      19.298 -20.046 -24.851  1.00 14.96      C    N
ATOM   7419  C   LYS I  42      18.489 -20.367 -17.495  1.00  7.80      C    C
ATOM   7420  O   LYS I  42      19.512 -20.336 -16.810  1.00  8.15      C    O
ATOM   7421  N   GLY I  43      17.581 -21.330 -17.389  1.00  7.59      C    N
ATOM   7422  CA  GLY I  43      17.783 -22.472 -16.508  1.00  7.35      C    C
ATOM   7423  C   GLY I  43      17.031 -22.326 -15.202  1.00  7.10      C    C
ATOM   7424  O   GLY I  43      17.428 -22.883 -14.179  1.00  7.13      C    O
ATOM   7425  N   TYR I  44      15.907 -21.621 -15.253  1.00  7.01      C    N
```

ATOM 7426 CA TYR I 44 15.095 -21.391 -14.066 1.00 6.89 C c
ATOM 7427 CB TYR I 44 14.678 -19.924 -13.982 1.00 6.88 c c
ATOM 7428 CG TYR I 44 15.828 -18.979 -13.738 1.00 6.41 c c
ATOM 7429 CD1 TYR I 44 16.374 -18.238 -14.776 1.00 6.62 c c
ATOM 7430 CE1 TYR I 44 17.430 -17.376 -14.558 1.00 6.48 c c
ATOM 7431 CZ TYR I 44 17.946 -17.240 -13.287 1.00 6.88 c c
ATOM 7432 OH TYR I 44 18.989 -16.371 -13.062 1.00 7.50 c o
ATOM 7433 CE2 TYR I 44 17.438 -17.984 -12.245 1.00 6.68 c c
ATOM 7434 CD2 TYR I 44 16.388 -18.851 -12.475 1.00 5.91 c c
ATOM 7435 C TYR I 44 13.859 -22.275 -14.065 1.00 6.86 c c
ATOM 7436 O TYR I 44 13.320 -22.602 -15.122 1.00 7.14 c o
ATOM 7437 N LEU I 45 13.309 -22.498 -12.875 1.00 6.44 c N
ATOM 7438 CA LEU I 45 12.131 -23.342 -12.733 1.00 6.12 c c
ATOM 7439 CB LEU I 45 12.479 -24.650 -12.019 1.00 6.31 c c
ATOM 7440 CG LEU I 45 13.457 -25.536 -12.798 1.00 6.38 c c
ATOM 7441 CD1 LEU I 45 14.250 -26.452 -11.877 1.00 7.05 c c
ATOM 7442 CD2 LEU I 45 12.736 -26.332 -13.874 1.00 7.05 c c
ATOM 7443 C LEU I 45 10.924 -22.641 -12.096 1.00 5.84 C c
ATOM 7444 O LEU I 45 10.954 -22.268 -10.921 1.00 5.94 c o
ATOM 7445 N SER I 46 9.806 -22.689 -12.821 1.00 5.43 c N
ATOM 7446 CA SER I 46 8.639 -21.822 -12.611 1.00 5.26 c c
ATOM 7447 CB SER I 46 7.803 -21.796 -13.891 1.00 5.21 c c
ATOM 7448 OG SER I 46 7.441 -23.112 -14.280 1.00 4.95 c o
ATOM 7449 C SER I 46 7.793 -22.404 -11.485 1.00 5.51 c c
ATOM 7450 O SER I 46 8.086 -23.500 -11.013 1.00 6.03 c o
ATOM 7451 N ALA I 47 6.787 -21.679 -11.001 1.00 5.24 c N
ATOM 7452 CA ALA I 47 6.265 -22.042 -9.688 1.00 4.83 c c
ATOM 7453 CB ALA I 47 7.391 -22.094 -8.675 1.00 5.01 c c
ATOM 7454 C ALA I 47 5.061 -21.315 -9.106 1.00 4.35 c c
ATOM 7455 O ALA I 47 5.100 -20.099 -8.920 1.00 4.45 c o
ATOM 7456 N LEU I 48 4.246 -22.119 -8.428 1.00 3.67 c N
ATOM 7457 CA LEU I 48 3.120 -21.630 -7.645 1.00 3.15 c c
ATOM 7458 CB LEU I 48 1.802 -21.948 -8.359 1.00 2.78 c c
ATOM 7459 CG LEU I 48 1.785 -21.864 -9.889 1.00 2.18 c c
ATOM 7460 CD1 LEU I 48 0.350 -21.834 -10.383 1.00 2.00 c c
ATOM 7461 CD2 LEU I 48 2.544 -20.643 -10.386 1.00 3.94 c c
ATOM 7462 C LEU I 48 3.128 -22.240 -6.239 1.00 3.06 c c
ATOM 7463 O LEU I 48 3.433 -23.422 -6.065 1.00 3.27 c o
ATOM 7464 N ARG I 49 2.926 -21.394 -5.233 1.00 2.91 c N
ATOM 7465 CA ARG I 49 2.903 -21.846 -3.846 1.00 2.88 C c
ATOM 7466 CB ARG I 49 3.036 -20.658 -2.887 1.00 2.69 c c
ATOM 7467 CG ARG I 49 3.904 -20.942 -1.663 1.00 2.15 c c
ATOM 7468 CD ARG I 49 3.321 -20.322 -0.404 1.00 2.00 c c
ATOM 7469 NE ARG I 49 2.284 -21.163 0.190 1.00 5.18 c N
ATOM 7470 CZ ARG I 49 1.050 -20.748 0.463 1.00 7.68 c c
ATOM 7471 NH1 ARG I 49 0.699 -19.492, 0.217 1.00 8.32 c N
ATOM 7472 NH2 ARG I 49 0.181 -21.570 1.036 1.00 8.12 c N
ATOM 7473 C ARG I 49 1.625 -22.619 -3.544 1.00 3.09 c c
ATOM 7474 O ARG I 49 0.527 -22.170 -3.873 1.00 3.08 c o
ATOM 7475 N THR I 50 1.774 -23.803 -2.956 1.00 3.37 c N
ATOM 7476 CA THR I 50 0.625 -24.551 -2.456 1.00 3.55 c c
ATOM 7477 CB THR I 50 0.042 -25.503 -3.512 1.00 3.25 c c
ATOM 7478 OG1 THR I 50 1.091 -26.292 -4.086 1.00 2.66 c o
ATOM 7479 CG2 THR I 50 -0.670 -24.723 -4.605 1.00 3.46 c c
ATOM 7480 C THR I 50 0.919 -25.349 -1.195 1.00 4.07 c c
ATOM 7481 O THR I 50 0.137 -25.308 -0.247 1.00 4.35 c o
ATOM 7482 N GLY I 51 1.892 -26.248 -1.274 1.00 4.24 c N
ATOM 7483 CA GLY I 51 2.393 -26.864 -0.060 1.00 4.78 c c
ATOM 7484 C GLY I 51 2.414 -25.769 0.981 1.00 4.98 c c
ATOM 7485 O GLY I 51 3.082 -24.754 0.786 1.00 5.00 c o

```
ATOM   7486  N   TRP I  52      1.481 -25.829   1.923  1.00  5.34      C    N
ATOM   7487  CA  TRP I  52      1.440 -24.823   2.974  1.00  5.42      c    c
ATOM   7488  CB  TRP I  52      0.124 -24.048   2.951  1.00  5.75      c    c
ATOM   7489  CG  TRP I  52     -0.090 -23.284   1.696  1.00  6.38      c    c
ATOM   7490  CD1 TRP I  52     -1.020 -23.544   0.734  1.00  7.27      c    c
ATOM   7491  NE1 TRP I  52     -0.899 -22.647  -0.297  1.00  7.46      c    N
ATOM   7492  CE2 TRP I  52      0.129 -21.785  -0.018  1.00  7.15      c    c
ATOM   7493  CD2 TRP I  52      0.671 -22.164   1.228  1.00  7.02      c    c
ATOM   7494  CE3 TRP I  52      1.741 -21.428   1.752  1.00  6.83      c    c
ATOM   7495  CZ3 TRP I  52      2.221 -20.347   1.027  1.00  6.73      c    c
ATOM   7496  CH2 TRP I  52      1.664 -20.000  -0.214  1.00  7.13      c    c
ATOM   7497  CZ2 TRP I  52      0.621 -20.706  -0.751  1.00  6.82      c    c
ATOM   7498  C   TRP I  52      1.680 -25.408   4.354  1.00  5.34      c    c
ATOM   7499  O   TRP I  52      1.222 -26.507   4.667  1.00  5.47      c    o
ATOM   7500  N   TYR I  53      2.237 -24.581   5.227  1.00  5.29      c    N
ATOM   7501  CA  TYR I  53      2.492 -24.977   6.598  1.00  5.58      c    c
ATOM   7502  CB  TYR I  53      4.002 -25.087   6.829  1.00  5.51      c    c
ATOM   7503  CG  TYR I  53      4.401 -25.463   8.239  1.00  6.59      c    c
ATOM   7504  CD1 TYR I  53      4.613 -26.791   8.591  1.00  8.25      c    c
ATOM   7505  CE1 TYR I  53      5.010 -27.136   9.872  1.00  9.40      c    c
ATOM   7506  CZ  TYR I  53      5.280 -26.145  10.790  1.00  9.24      c    c
ATOM   7507  OH  TYR I  53      5.693 -26.480  12.058  1.00  9.61      c    o
ATOM   7508  CE2 TYR I  53      5.162 -24.818  10.437  1.00  8.78      c    c
ATOM   7509  CD2 TYR I  53      4.758 -24.485   9.157  1.00  7.93      c    c
ATOM   7510  C   TYR I  53      1.869 -23.950   7.539  1.00  5.74      c    c
ATOM   7511  O   TYR I  53      2.281 -22.790   7.558  1.00  6.19      c    o
ATOM   7512  N   THR I  54      0.756 -24.328   8.159  1.00  6.04      c    N
ATOM   7513  CA  THR I  54      0.075 -23.456   9.109  1.00  6.67      c    c
ATOM   7514  CB  THR I  54     -1.298 -24.028   9.513  1.00  6.97      c    c
ATOM   7515  OG1 THR I  54     -2.247 -23.782   8.467  1.00  7.51      c    o
ATOM   7516  CG2 THR I  54     -1.790 -23.384  10.800  1.00  7.98      c    c
ATOM   7517  C   THR I  54      0.928 -23.266  10.359  1.00  6.97      c    c
ATOM   7518  O   THR I  54      1.713 -24.141  10.723  1.00  7.32      c    o
ATOM   7519  N   SER I  55      0.775 -22.120  11.013  1.00  7.24      c    N
ATOM   7520  CA  SER I  55      1.085 -22.019  12.433  1.00  7.65      c    c
ATOM   7521  CB  SER I  55      2.589 -21.862  12.654  1.00  7.69      c    c
ATOM   7522  OG  SER I  55      2.868 -21.507  13.998  1.00  7.51      c    o
ATOM   7523  C   SER I  55      0.338 -20.878  13.104  1.00  8.03      c    c
ATOM   7524  O   SER I  55      0.238 -19.778  12.560  1.00  8.43      c    o
ATOM   7525  N   VAL I  56     -0.094 -21.121  14.335  1.00  8.14      c    N
ATOM   7526  CA  VAL I  56     -1.029 -20.234  15.006  1.00  8.41      c    c
ATOM   7527  CB  VAL I  56     -2.209 -21.014  15.598  1.00  8.72      c    c
ATOM   7528  CGI VAL I  56     -3.403 -20.094  15.787  1.00  9.29      c    c
ATOM   7529  CG2 VAL I  56     -2.569 -22.184  14.695  1.00  9.51      c    c
ATOM   7530  C   VAL I  56     -0.331 -19.478  16.123  1.00  8.19      c    c
ATOM   7531  O   VAL I  56      0.075 -20.066  17.122  1.00  8.54      c    o
ATOM   7532  N   ILE I  57     -0.187 -18.171  15.943  1.00  7.91      c    N
ATOM   7533  CA  ILE I  57      0.639 -17.368  16.832  1.00  7.64      c    c
ATOM   7534  CB  ILE I  57      1.675 -16.539  16.051  1.00  7.35      c    c
ATOM   7535  CGI ILE I  57      2.612 -17.461  15.262  1.00  7.25      c    c
ATOM   7536  CD1 ILE I  57      3.526 -16.730  14.294  1.00  8.42      c    c
ATOM   7537  CG2 ILE I  57      2.457 -15.632  16.993  1.00  7.52      c    c
ATOM   7538  C   ILE I  57     -0.222 -16.445  17.680  1.00  7.69      c    c
ATOM   7539  O   ILE I  57     -1.150 -15.810  17.178  1.00  7.79      C    O
ATOM   7540  N   THR I  58     -0.024 -16.523  18.989  1.00  7.85      C    N
ATOM   7541  CA  THR I  58     -0.929 -15.900  19.938  1.00  8.15      C    C
ATOM   7542  CB  THR I  58     -1.660 -16.954  20.777  1.00  8.14      C    C
ATOM   7543  OG1 THR I  58     -1.584 -18.225  20.120  1.00  8.62      C    O
ATOM   7544  CG2 THR I  58     -3.116 -16.566  20.957  1.00  7.94      C    C
ATOM   7545  C   THR I  58     -0.152 -14.983  20.869  1.00  8.20      C    C
```

ATOM 7546 O THR I 58 0.808 -15.408 21.510 1.00 8.18 C O
ATOM 7547 N ILE I 59 -0.539 -13.713 20.903 1.00 8.54 C N
ATOM 7548 CA ILE I 59 0.226 -12.694 21.616 1.00 9.23 C C
ATOM 7549 CB ILE I 59 0.863 -11.690 20.634 1.00 8.92 C C
ATOM 7550 CGI ILE I 59 1.868 -12.391 19.717 1.00 9.27 C C
ATOM 7551 CDHLE I 59 2.587 -11.453 18.770 1.00 10.89 C C
ATOM 7552 CG2 ILE I 59 1.516 -10.544 21.390 1.00 8.74 C C
ATOM 7553 C ILE I 59 -0.691 -11.920 22.553 1.00 10.02 C C
ATOM 7554 O ILE I 59 -1.692 -11.357 22.113 1.00 10.20 C O
ATOM 7555 N GLU I 60 -0.439 -12.007 23.853 1.00 10.95 C N
ATOM 7556 CA GLU I 60 -1.462 -11.602 24.808 1.00 12.13 C C
ATOM 7557 CB GLU I 60 -0.963 -11.829 26.248 1.00 12.44 C C
ATOM 7558 CG GLU I 60 -0.554 -13.288 26.547 1.00 15.04 C C
ATOM 7559 CD GLU I 60 -0.560 -13.630 28.036 1.00 19.34 C C
ATOM 7560 OE1 GLU I 60 0.413 -13.267 28.733 1.00 20.63 C O
ATOM 7561 OE2 GLU I 60 -1.469 -14.368 28.478 1.00 21.19 C O
ATOM 7562 C GLU I 60 -1.856 -10.131 24.547 1.00 12.46 C C
ATOM 7563 O GLU I 60 -0.984 -9.259 24.567 1.00 12.68 C O
ATOM 7564 N LEU I 61 -3.138 -9.818 24.298 1.00 12.80 C N
ATOM 7565 CA LEU I 61 -3.535 -8.473 24.718 1.00 12.71 C C
ATOM 7566 CB LEU I 61 -5.021 -8.120 24.699 1.00 12.55 C C
ATOM 7567 CG LEU I 61 -5.052 -6.753 25.421 1.00 12.39 C C
ATOM 7568 CD1 LEU I 61 -4.358 -5.650 24.625 1.00 13.14 C C
ATOM 7569 CD2 LEU I 61 -6.421 -6.318 25.899 1.00 12.50 C C
ATOM 7570 C LEU I 61 -3.097 -8.585 26.133 1.00 12.94 C C
ATOM 7571 O LEU I 61 -3.578 -9.474 26.843 1.00 12.78 C O
ATOM 7572 N SER I 62 -1.846 -8.190 26.260 1.00 13.61 C N
ATOM 7573 CA SER I 62 -1.183 -8.231 27.527 1.00 14.70 C C
ATOM 7574 CB SER I 62 0.326 -8.252 27.325 1.00 14.52 C C
ATOM 7575 OG SER I 62 0.724 -9.440 26.664 1.00 14.80 C O
ATOM 7576 C SER I 62 -1.605 -6.983 28.261 1.00 15.48 C C
ATOM 7577 O SER I 62 -1.206 -5.880 27.893 1.00 15.50 C O
ATOM 7578 N ASN I 63 -2.602 -7.135 29.121 1.00 16.61 C N
ATOM 7579 CA ASN I 63 -3.232 -5.978 29.716 1.00 17.77 C C
ATOM 7580 CB ASN I 63 -4.616 -6.314 30.263 1.00 17.73 C C
ATOM 7581 CG ASN I 63 -5.566 -5.142 30.175 1.00 18.52 C C
ATOM 7582 OD1 ASN I 63 -5.140 -3.987 30.185 1.00 18.29 C O
ATOM 7583 ND2 ASN I 63 -6.837 -5.433 29.933 1.00 19.40 C N
ATOM 7584 C ASN I 63 -2.369 -5.335 30.787 1.00 18.53 C C
ATOM 7585 O ASN I 63 -1.589 -6.007 31.463 1.00 18.82 C O
ATOM 7586 N ILE I 64 -2.403 -4.010 30.819 1.00 19.60 C N
ATOM 7587 CA ILE I 64 -1.812 -3.252 31.908 1.00 21.04 C C
ATOM 7588 CB ILE I 64 -1.433 -1.836 31.448 1.00 20.60 C C
ATOM 7589 CGI ILE I 64 -0.845 -1.878 30.038 1.00 20.13 C C
ATOM 7590 CDHLE I 64 -0.383 -0.534 29.522 1.00 20.19 C C
ATOM 7591 CG2 ILE I 64 -0.451 -1.211 32.416 1.00 20.74 C C
ATOM 7592 C ILE I 64 -2.778 -3.148 33.082 1.00 22.58 C C
ATOM 7593 O ILE I 64 -3.951 -2.832 32.900 1.00 23.07 C O
ATOM 7594 N LYS I 65 -2.259 -3.322 34.292 1.00 24.21 C N
ATOM 7595 CA LYS I 65 -2.904 -2.779 35.482 1.00 25.86 C C
ATOM 7596 CB LYS I 65 -2.929 -3.822 36.602 1.00 25.90 C C
ATOM 7597 CG LYS I 65 -2.083 -5.056 36.323 1.00 26.69 C C
ATOM 7598 CD LYS I 65 -0.616 -4.698 36.160 1.00 28.26 C C
ATOM 7599 CE LYS I 65 0.273 -5.606 36.992 1.00 28.67 C C
ATOM 7600 NZ LYS I 65 1.600 -4.983 37.247 1.00 28.95 C N
ATOM 7601 C LYS I 65 -2.215 -1.500 35.961 1.00 26.81 C C
ATOM 7602 O LYS I 65 -1.160 -1.557 36.591 1.00 26.72 C O
ATOM 7603 N GLU I 66 -2.903 -0.371 35.798 1.00 27.90 C N
ATOM 7604 CA GLU I 66 -2.291 0.962 35.878 1.00 28.82 C C
ATOM 7605 CB GLU I 66 -3.184 1.983 35.163 1.00 28.88 C C

```
ATOM   7606  CG  GLU I  66      -3.354   3.309  35.901  1.00 30.33      C    C
ATOM   7607  CD  GLU I  66      -4.570   4.084  35.431  1.00 33.17      C    C
ATOM   7608  OE1 GLU I  66      -4.590   5.323  35.595  1.00 35.05      C    O
ATOM   7609  OE2 GLU I  66      -5.488   3.457  34.860  1.00 33.14      C    O
ATOM   7610  C   GLU I  66      -2.102   1.393  37.333  1.00 29.12      C    C
ATOM   7611  O   GLU I  66      -3.002   1.204  38.148  1.00 29.28      C    O
ATOM   7612  N   ASN I  67      -0.975   2.029  37.653  1.00 29.32      C    N
ATOM   7613  CA  ASN I  67      -0.630   2.266  39.065  1.00 29.39      C    C
ATOM   7614  CB  ASN I  67       0.664   1.550  39.473  1.00 29.62      C    C
ATOM   7615  CG  ASN I  67       0.399   0.206  40.133  1.00 29.84      C    C
ATOM   7616  OD1 ASN I  67      -0.154   0.147  41.233  1.00 29.93      C    O
ATOM   7617  ND2 ASN I  67       0.655  -0.875  39.400  1.00 29.22      C    N
ATOM   7618  C   ASN I  67      -0.670   3.712  39.571  1.00 29.15      C    C
ATOM   7619  O   ASN I  67       0.352   4.281  39.962  1.00 29.06      C    O
ATOM   7620  N   LYS I  68      -1.872   4.284  39.584  1.00 28.87      C    N
ATOM   7621  CA  LYS I  68      -2.302   5.212  40.630  1.00 28.78      C    C
ATOM   7622  CB  LYS I  68      -3.436   4.596  41.454  1.00 28.89      C    C
ATOM   7623  CG  LYS I  68      -4.461   3.838  40.617  1.00 29.26      C    C
ATOM   7624  CD  LYS I  68      -5.357   2.964  41.483  1.00 29.68      C    C
ATOM   7625  CE  LYS I  68      -5.626   3.615  42.835  1.00 29.46      C    C
ATOM   7626  NZ  LYS I  68      -6.764   2.972  43.555  1.00 29.58      C    N
ATOM   7627  C   LYS I  68      -1.171   5.722  41.535  1.00 28.60      C    C
ATOM   7628  O   LYS I  68      -1.082   5.347  42.703  1.00 28.64      C    O
ATOM   7629  N   CYS I  69      -0.274   6.525  40.961  1.00 28.09      C    N
ATOM   7630  CA  CYS I  69       0.585   7.455  41.715  1.00 27.63      C    C
ATOM   7631  CB  CYS I  69       2.068   7.270  41.326  1.00 27.07      C    C
ATOM   7632  SG  CYS I  69       2.742   8.433  40.058  1.00 28.01      C    S
ATOM   7633  C   CYS I  69       0.143   8.893  41.433  1.00 27.69      C    C
ATOM   7634  O   CYS I  69      -0.588   9.134  40.473  1.00 27.41      C    O
ATOM   7635  N   ASN I  70       0.615   9.855  42.226  1.00 28.06      C    N
ATOM   7636  CA  ASN I  70       0.603  11.259  41.794  1.00 28.87      C    C
ATOM   7637  CB  ASN I  70      -0.364  12.119  42.626  1.00 30.52      C    C
ATOM   7638  CG  ASN I  70      -1.286  11.299  43.518  1.00 39.60      C    C
ATOM   7639  OD1 ASN I  70      -2.181  10.602  43.040  1.00 44.97      C    O
ATOM   7640  ND2 ASN I  70      -1.073  11.402  44.831  1.00 51.04      C    N
ATOM   7641  C   ASN I  70       1.978  11.934  41.727  1.00 26.97      C    C
ATOM   7642  O   ASN I  70       2.563  12.257  42.761  1.00 26.50      C    O
ATOM   7643  N   GLY I  71       2.371  12.349  40.523  1.00 25.46      C    N
ATOM   7644  CA  GLY I  71       3.643  13.052  40.316  1.00 23.67      C    C
ATOM   7645  C   GLY I  71       3.501  14.565  40.288  1.00 22.81      C    C
ATOM   7646  O   GLY I  71       2.415  15.094  40.516  1.00 22.79      C    O
ATOM   7647  N   THR I  72       4.585  15.268  39.975  1.00 21.93      C    N
ATOM   7648  CA  THR I  72       4.526  16.721  39.835  1.00 21.30      C    C
ATOM   7649  CB  THR I  72       5.923  17.363  39.940  1.00 21.12      C    C
ATOM   7650  OG1 THR I  72       6.624  17.194  38.702  1.00 19.87      C    O
ATOM   7651  CG2 THR I  72       6.725  16.723  41.063  1.00 20.76      C    C
ATOM   7652  C   THR I  72       3.864  17.132  38.518  1.00 21.50      C    C
ATOM   7653  O   THR I  72       4.384  16.852  37.438  1.00 21.85      C    O
ATOM   7654  N   ASP I  73       2.703  17.774  38.617  1.00 21.43      C    N
ATOM   7655  CA  ASP I  73       1.767  17.891  37.494  1.00 21.46      C    C
ATOM   7656  CB  ASP I  73       2.361  18.743  36.368  1.00 21.69      C    C
ATOM   7657  CG  ASP I  73       1.457  18.812  35.149  1.00 22.46      C    C
ATOM   7658  OD1 ASP I  73       0.542  17.969  35.035  1.00 23.01      C    O
ATOM   7659  OD2 ASP I  73       1.682  19.690  34.289  1.00 23.09      C    O
ATOM   7660  C   ASP I  73       1.323  16.536  36.950  1.00 20.96      C    C
ATOM   7661  O   ASP I  73       2.128  15.792  36.390  1.00 20.61      C    O
ATOM   7662  N   ALA I  74       0.019  16.285  36.989  1.00 20.42      C    N
ATOM   7663  CA  ALA I  74      -0.512  14.977  36.622  1.00 20.38      C    C
ATOM   7664  CB  ALA I  74      -1.027  14.248  37.855  1.00 20.11      C    C
ATOM   7665  C   ALA I  74      -1.602  15.058  35.556  1.00 20.45      C    C
```

ATOM 7666 O ALA I 74 -2.490 14.208 35.509 1.00 20.46 C o
ATOM 7667 N LYS I 75 -1.583 16.114 34.750 1.00 20.67 c N
ATOM 7668 CA LYS I 75 -2.473 16.188 33.596 1.00 20.99 c c
ATOM 7669 CB LYS I 75 -2.421 17.583 32.970 1.00 21.20 c c
ATOM 7670 CG LYS I 75 -2.967 18.684 33.865 1.00 22.02 c c
ATOM 7671 CD LYS I 75 -1.927 19.766 34.106 1.00 23.66 c c
ATOM 7672 CE LYS I 75 -1.971 20.263 35.542 1.00 24.93 c c
ATOM 7673 NZ LYS I 75 -0.622 20.658 36.036 1.00 25.55 c N
ATOM 7674 C LYS I 75 -2.025 15.144 32.587 1.00 20.92 c c
ATOM 7675 O LYS I 75 -2.801 14.680 31.751 1.00 20.92 c o
ATOM 7676 N VAL I 76 -0.731 14.853 32.634 1.00 20.63 c N
ATOM 7677 CA VAL I 76 -0.147 13.700 31.971 1.00 20.36 c c
ATOM 7678 CB VAL I 76 1.386 13.792 32.017 1.00 20.25 c c
ATOM 7679 CGI VAL I 76 2.009 12.475 31.612 1.00 20.82 c: c
ATOM 7680 CG2 VAL I 76 1.873 14.923 31.130 1.00 20.09 c: c
ATOM 7681 C VAL I 76 -0.586 12.393 32.629 1.00 20.29 c c
ATOM 7682 O VAL I 76 -0.452 12.225 33.840 1.00 20.21 c o
ATOM 7683 N LYS I 77 -1.106 11.471 31.826 1.00 20.17 c N
ATOM 7684 CA LYS I 77 -1.642 10.218 32.348 1.00 20.17 c c
ATOM 7685 CB LYS I 77 -3.103 10.393 32.760 1.00 20.62 c c
ATOM 7686 CG LYS I 77 -3.297 10.767 34.215 1.00 23.31 c c
ATOM 7687 CD LYS I 77 -4.508 11.664 34.388 1.00 26.74 c c
ATOM 7688 CE LYS I 77 -4.529 12.291 35.767 1.00 28.32 c c
ATOM 7689 NZ LYS I 77 -5.869 12.836 36.105 1.00 29.66 c N
ATOM 7690 C LYS I 77 -1.523 9.105 31.317 1.00 19.45 c c
ATOM 7691 O LYS I 77 -2.517 8.496 30.921 1.00 19.36 c o
ATOM 7692 N LEU I 78 -0.297 8.863 30.871 1.00 18.70 c N
ATOM 7693 CA LEU I 78 -0.064 8.098 29.659 1.00 17.98 c c
ATOM 7694 CB LEU I 78 1.419 7.775 29.528 1.00 17.72 c c
ATOM 7695 CG LEU I 78 2.275 9.033 29.591 1.00 17.51 c c
ATOM 7696 CD1 LEU I 78 3.746 8.676 29.494 1.00 17.41 c c
ATOM 7697 CD2 LEU I 78 1.859 9.984 28.480 1.00 17.62 c c
ATOM 7698 C LEU I 78 -0.882 6.820 29.656 1.00 17.77 c c
ATOM 7699 O LEU I 78 -1.665 6.576 28.739 1.00 17.89 c o
ATOM 7700 N ILE I 79 -0.749 6.036 30.717 1.00 17.29 C N
ATOM 7701 CA ILE I 79 -1.319 4.703 30.726 1.00 17.00 c c
ATOM 7702 CB ILE I 79 -0.968 3.948 32.005 1.00 16.96 c c
ATOM 7703 CGI ILE I 79 0.550 3.801 32.113 1.00 17.21 c c
ATOM 7704 CD1 ILE I 79 1.020 3.244 33.429 1.00 17.51 c c
ATOM 7705 CG2 ILE I 79 -1.643 2.587 32.005 1.00 17.30 c c
ATOM 7706 C ILE I 79 -2.828 4.750 30.547 1.00 16.83 c c
ATOM 7707 O ILE I 79 -3.365 4.160 29.609 1.00 17.02 c o
ATOM 7708 N LYS I 80 -3.616 5.565 31.220 1.00 16.55 c N
ATOM 7709 CA LYS I 80 -5.043 5.447 30.835 1.00 16.38 c c
ATOM 7710 CB LYS I 80 -5.918 6.332 31.725 1.00 16.73 c c
ATOM 7711 CG LYS I 80 -7.025 7.055 30.971 1.00 17.99 c c
ATOM 7712 CD LYS I 80 -8.237 7.295 31.854 1.00 20.71 c c
ATOM 7713 CE LYS I 80 -9.171 6.094 31.833 1.00 22.92 c c
ATOM 7714 NZ LYS I 80 -8.439 4.818 32.068 1.00 24.75 c N
ATOM 7715 C LYS I 80 -5.386 5.716 29.328 1.00 15.79 c c
ATOM 7716 O LYS I 80 -6.140 4.942 28.677 1.00 15.32 c o
ATOM 7717 N GLN I 81 -4.802 6.770 28.763 1.00 15.48 c N
ATOM 7718 CA GLN I 81 -5.092 7.178 27.383 1.00 15.33 c c
ATOM 7719 CB GLN I 81 -4.378 8.495 27.068 1.00 15.70 c c
ATOM 7720 CG GLN I 81 -4.522 9.557 28.146 1.00 17.88 c c
ATOM 7721 CD GLN I 81 -3.631 10.759 27.903 1.00 20.46 c c
ATOM 7722 OE1 GLN I 81 -3.065 10.916 26.822 1.00 21.59 c o
ATOM 7723 NE2 GLN I 81 -3.498 11.613 28.913 1.00 20.26 C N
ATOM 7724 C GLN I 81 -4.708 6.125 26.341 1.00 14.63 c c
ATOM 7725 O GLN I 81 -5.438 5.881 25.360 1.00 14.60 c o

```
ATOM   7726  N   GLU I  82      -3.556   5.500  26.560  1.00 13.81      C    N
ATOM   7727  CA  GLU I  82      -3.078   4.470  25.657  1.00 13.37      C    C
ATOM   7728  CB  GLU I  82      -1.705   3.958  26.094  1.00 13.20      C    C
ATOM   7729  CG  GLU I  82      -0.528   4.666  25.439  1.00 15.04      C    C
ATOM   7730  CD  GLU I  82      -0.472   4.436  23.942  1.00 17.51      C    C
ATOM   7731  OE1 GLU I  82       0.319   3.576  23.502  1.00 18.22      C    O
ATOM   7732  OE2 GLU I  82      -1.21 1   5.121  23.205  1.00 17.87      C    O
ATOM   7733  C   GLU I  82      -4.079   3.333  25.659  1.00 12.99      C    C
ATOM   7734  O   GLU I  82      -4.400   2.779  24.610  1.00 12.89      C    O
ATOM   7735  N   LEU I  83      -4.593   3.001  26.838  1.00 12.89      C    N
ATOM   7736  CA  LEU I  83      -5.558   1.919  26.944  1.00 13.08      C    C
ATOM   7737  CB  LEU I  83      -5.923   1.668  28.407  1.00 13.26      C    C
ATOM   7738  CG  LEU I  83      -4.774   1.250  29.325  1.00 14.18      C    C
ATOM   7739  CD1 LEU I  83      -5.293   0.948  30.721  1.00 15.1 1      C    C
ATOM   7740  CD2 LEU I  83      -4.036   0.051  28.748  1.00 14.79      C    C
ATOM   7741  C   LEU I  83      -6.808   2.252  26.144  1.00 13.18      C    C
ATOM   7742  O   LEU I  83      -7.310   1.410  25.386  1.00 13.05      C    O
ATOM   7743  N   ASP I  84      -7.286   3.490  26.251  1.00 13.56      C    N
ATOM   7744  CA  ASP I  84      -8.478   3.834  25.467  1.00 14.15      C    C
ATOM   7745  CB  ASP I  84      -8.946   5.258  25.781  1.00 14.80      C    C
ATOM   7746  CG  ASP I  84      -9.044   5.529  27.268  1.00 18.26      C    C
ATOM   7747  OD1 ASP I  84     -10.133   5.330  27.846  1.00 21.1 1      C    O
ATOM   7748  OD2 ASP I  84      -8.032   5.959  27.858  1.00 22.12      C    O
ATOM   7749  C   ASP I  84      -8.226   3.703  23.954  1.00 13.56      C    C
ATOM   7750  O   ASP I  84      -9.062   3.149  23.192  1.00 13.70      C    O
ATOM   7751  N   LYS I  85      -7.062   4.182  23.517  1.00 12.87      C    N
ATOM   7752  CA  LYS I  85      -6.752   4.121  22.089  1.00 12.31      C    C
ATOM   7753  CB  LYS I  85      -5.424   4.816  21.793  1.00 12.41      C    C
ATOM   7754  CG  LYS I  85      -5.1 18   4.954  20.308  1.00 12.26      C    C
ATOM   7755  CD  LYS I  85      -3.659   5.305  20.076  1.00 12.72      C    C
ATOM   7756  CE  LYS I  85      -2.751   4.171  20.519  1.00 14.40      C    C
ATOM   7757  NZ  LYS I  85      -1.316   4.445  20.230  1.00 16.45      C    N
ATOM   7758  C   LYS I  85      -6.691   2.671  21.621  1.00 11.85      C    C
ATOM   7759  O   LYS I  85      -7.187   2.312  20.537  1.00 11.66      C    O
ATOM   7760  N   TYR I  86      -6.085   1.836  22.457  1.00 11.32      C    N
ATOM   7761  CA  TYR I  86      -5.931   0.432  22.135  1.00 11.07      C    C
ATOM   7762  CB  TYR I  86      -5.1 15  -0.290  23.203  1.00 11.12      C    C
ATOM   7763  CG  TYR I  86      -5.391  -1.773  23.243  1.00 11.30      C    C
ATOM   7764  CDI TYR I  86      -4.884  -2.621  22.268  1.00 12.16      C    C
ATOM   7765  CE1 TYR I  86      -5.140  -3.977  22.297  1.00 12.39      C    C
ATOM   7766  CZ  TYR I  86      -5.916  -4.500  23.308  1.00 12.62      C    C
ATOM   7767  OH  TYR I  86      -6.174  -5.852  23.343  1.00 12.72      C    O
ATOM   7768  CE2 TYR I  86      -6.434  -3.680  24.286  1.00 11.38      C    C
ATOM   7769  CD2 TYR I  86      -6.173  -2.325  24.248  1.00 11.05      C    C
ATOM   7770  C   TYR I  86      -7.290  -0.219  22.008  1.00 10.75      C    C
ATOM   7771  O   TYR I  86      -7.517  -1.004  21.098  1.00 10.45      C    O
ATOM   7772  N   LYS I  87      -8.204   0.123  22.908  1.00 10.66      C    N
ATOM   7773  CA  LYS I  87      -9.533  -0.467  22.847  1.00 11.03      C    C
ATOM   7774  CB  LYS I  87     -10.389   0.010  24.021  1.00 11.36      C    C
ATOM   7775  CG  LYS I  87      -9.786  -0.270  25.384  1.00 12.79      C    C
ATOM   7776  CD  LYS I  87     -10.675   0.264  26.495  1.00 14.76      C    C
ATOM   7777  CE  LYS I  87     -10.068  -0.017  27.859  1.00 15.29      C    C
ATOM   7778  NZ  LYS I  87     -10.924   0.485  28.970  1.00 16.27      C    N
ATOM   7779  C   LYS I  87     -10.208  -0.098  21.530  1.00 10.83      C    C
ATOM   7780  O   LYS I  87     -10.800  -0.963  20.857  1.00 11.1 1      C    O
ATOM   7781  N   ASN I  88     -10.089   1.168  21.126  1.00 10.52      C    N
ATOM   7782  CA  ASN I  88     -10.721   1.545  19.858  1.00 10.21      C    C
ATOM   7783  CB  ASN I  88     -10.592   3.050  19.614  1.00 10.61      C    C
ATOM   7784  CG  ASN I  88     -11.178   3.480  18.281  1.00 11.81      C    C
ATOM   7785  OD1 ASN I  88     -12.1 14   2.864  17.772  1.00 12.97      C    O
```

ATOM 7786 ND2 ASN I 88 -10.625 4.543 17.709 1.00 13.82 C N
ATOM 7787 C ASN I 88 -10.128 0.767 18.674 1.00 9.42 C C
ATOM 7788 O ASN I 88 -10.858 0.237 17.796 1.00 8.94 C O
ATOM 7789 N ALA I 89 -8.802 0.652 18.677 1.00 8.77 C N
ATOM 7790 CA ALA I 89 -8.130 -0.041 17.586 1.00 8.21 C C
ATOM 7791 CB ALA I 89 -6.623 0.040 17.751 1.00 7.99 C C
ATOM 7792 C ALA I 89 -8.588 -1.493 17.543 1.00 7.78 C C
ATOM 7793 O ALA I 89 -8.826 -2.057 16.472 1.00 7.88 C O
ATOM 7794 N VAL I 90 -8.718 -2.086 18.724 1.00 7.01 C N
ATOM 7795 CA VAL I 90 -9.124 -3.474 18.849 1.00 6.26 C C
ATOM 7796 CB VAL I 90 -9.079 -3.943 20.313 1.00 5.91 C C
ATOM 7797 CGI VAL I 90 -9.557 -5.381 20.422 1.00 5.92 C C
ATOM 7798 CG2 VAL I 90 -7.671 -3.802 20.871 1.00 5.26 C C
ATOM 7799 C VAL I 90 -10.524 -3.689 18.299 1.00 6.25 C C
ATOM 7800 O VAL I 90 -10.765 -4.663 17.592 1.00 6.32 C O
ATOM 7801 N THR I 91 -11.445 -2.776 18.592 1.00 6.24 C N
ATOM 7802 CA THR I 91 -12.799 -2.932 18.065 1.00 6.68 C C
ATOM 7803 CB THR I 91 -13.734 -1.829 18.584 1.00 6.62 C C
ATOM 7804 OG1 THR I 91 -13.711 -1.819 20.017 1.00 7.19 C O
ATOM 7805 CG2 THR I 91 -15.157 -2.071 18.106 1.00 7.27 C C
ATOM 7806 C THR I 91 -12.768 -2.885 16.536 1.00 7.02 C C
ATOM 7807 O THR I 91 -13.430 -3.703 15.833 1.00 7.16 C O
ATOM 7808 N GLU I 92 -11.970 -1.955 16.011 1.00 7.31 C N
ATOM 7809 CA GLU I 92 -11.889 -1.863 14.558 1.00 7.81 C C
ATOM 7810 CB GLU I 92 -11.017 -0.680 14.131 1.00 8.23 C C
ATOM 7811 CG GLU I 92 -11.774 0.630 13.973 1.00 10.91 C C
ATOM 7812 CD GLU I 92 -12.907 0.529 12.969 1.00 14.95 C C
ATOM 7813 OE1 GLU I 92 -12.739 1.010 11.830 1.00 16.14 C O
ATOM 7814 OE2 GLU I 92 -13.968 -0.027 13.320 1.00 16.53 C O
ATOM 7815 C GLU I 92 -11.349 -3.164 13.959 1.00 7.47 C C
ATOM 7816 O GLU I 92 -11.911 -3.691 12.994 1.00 7.32 C O
ATOM 7817 N LEU I 93 -10.303 -3.716 14.568 1.00 7.30 C N
ATOM 7818 CA LEU I 93 -9.703 -4.950 14.062 1.00 7.47 C C
ATOM 7819 CB LEU I 93 -8.429 -5.299 14.830 1.00 7.15 C C
ATOM 7820 CG LEU I 93 -7.212 -4.438 14.490 1.00 7.20 C C
ATOM 7821 CD1 LEU I 93 -5.977 -4.957 15.204 1.00 7.93 C C
ATOM 7822 CD2 LEU I 93 -6.989 -4.392 12.984 1.00 6.91 C C
ATOM 7823 C LEU I 93 -10.705 -6.097 14.123 1.00 7.89 C C
ATOM 7824 O LEU I 93 -10.764 -6.947 13.235 1.00 7.94 C O
ATOM 7825 N GLN I 94 -11.486 -6.094 15.193 1.00 8.31 C N
ATOM 7826 CA GLN I 94 -12.514 -7.088 15.461 1.00 9.05 C C
ATOM 7827 CB GLN I 94 -13.131 -6.862 16.845 1.00 9.18 C C
ATOM 7828 CG GLN I 94 -12.158 -7.052 17.996 1.00 10.79 C C
ATOM 7829 CD GLN I 94 -12.831 -6.966 19.353 1.00 13.82 C C
ATOM 7830 OE1 GLN I 94 -14.042 -6.762 19.448 1.00 14.98 C O
ATOM 7831 NE2 GLN I 94 -12.047 -7.125 20.412 1.00 15.25 C N
ATOM 7832 C GLN I 94 -13.615 -7.127 14.405 1.00 9.25 C c
ATOM 7833 O GLN I 94 -14.122 -8.204 14.093 1.00 9.43 c o
ATOM 7834 N LEU I 95 -14.007 -5.977 13.858 1.00 9.55 c N
ATOM 7835 CA LEU I 95 -15.128 -6.009 12.888 1.00 10.17 c c
ATOM 7836 CB LEU I 95 -15.535 -4.582 12.510 1.00 9.79 c c
ATOM 7837 CG LEU I 95 -16.117 -3.716 13.628 1.00 8.86 c c
ATOM 7838 CD1 LEU I 95 -16.419 -2.315 13.117 1.00 8.31 c c
ATOM 7839 CD2 LEU I 95 -17.367 -4.359 14.211 1.00 7.62 c c
ATOM 7840 C LEU I 95 -14.958 -6.865 11.591 1.00 11.22 c c
ATOM 7841 O LEU I 95 -15.902 -7.505 11.125 1.00 11.55 c o
ATOM 7842 N LEU I 96 -13.751 -6.843 11.039 1.00 12.40 c N
ATOM 7843 CA LEU I 96 -13.313 -7.374 9.755 1.00 13.66 c c
ATOM 7844 CB LEU I 96 -11.796 -7.246 9.601 1.00 13.38 c c
ATOM 7845 CG LEU I 96 -11.288 -5.847 9.244 1.00 13.32 c c

ATOM 7846 CD1 LEU I 96 -9.901 -5.910 8.624 1.00 12.84 C C
ATOM 7847 CD2 LEU I 96 -12.256 -5.161 8.301 1.00 13.38 C C
ATOM 7848 C LEU I 96 -13.765 -8.817 9.534 1.00 14.97 C C
ATOM 7849 O LEU I 96 -13.908 -9.257 8.395 1.00 15.21 C O
ATOM 7850 N MET I 97 -14.125 -9.501 10.615 1.00 16.74 C N
ATOM 7851 CA MET I 97 -14.122 -10.962 10.625 1.00 18.96 C C
ATOM 7852 CB MET I 97 -13.987 -11.498 12.053 1.00 19.12 C C
ATOM 7853 CG MET I 97 -12.742 -11.021 12.784 1.00 21.87 C C
ATOM 7854 SD MET I 97 -11.220 -11.692 12.090 1.00 27.46 C S
ATOM 7855 CE MET I 97 -11.585 -11.630 10.338 1.00 24.25 C C
ATOM 7856 C MET I 97 -15.339 -11.576 9.929 1.00 20.09 C C
ATOM 7857 O MET I 97 -15.246 -12.655 9.343 1.00 20.58 C O
ATOM 7858 N GLN I 98 -16.462 -10.865 9.950 1.00 21.33 C N
ATOM 7859 CA GLN I 98 -17.706 -11.392 9.401 1.00 22.21 C C
ATOM 7860 CB GLN I 98 -18.708 -11.678 10.521 1.00 22.53 C C
ATOM 7861 CG GLN I 98 -18.099 -12.341 11.742 1.00 23.85 C C
ATOM 7862 CD GLN I 98 -17.673 -11.337 12.792 1.00 25.21 C C
ATOM 7863 OE1 GLN I 98 -16.838 -10.469 12.535 1.00 24.47 C O
ATOM 7864 NE2 GLN I 98 -18.199 -11.489 14.002 1.00 24.85 C N
ATOM 7865 C GLN I 98 -18.318 -10.439 8.378 1.00 22.15 C C
ATOM 7866 O GLN I 98 -17.765 -9.376 8.095 1.00 21.77 C O
ATOM 7867 N PHE I 137 -22.709 -16.921 4.271 1.00 33.25 C N
ATOM 7868 CA PHE I 137 -21.644 -16.142 3.651 1.00 36.79 C C
ATOM 7869 CB PHE I 137 -21.061 -16.892 2.453 1.00 20.00 C C
ATOM 7870 CG PHE I 137 -20.354 -18.166 2.825 1.00 20.00 C C
ATOM 7871 CD1 PHE I 137 -19.059 -18.134 3.318 1.00 20.00 C C
ATOM 7872 CE1 PHE I 137 -18.416 -19.301 3.700 1.00 20.00 C C
ATOM 7873 CZ PHE I 137 -19.092 -20.504 3.660 1.00 20.00 C C
ATOM 7874 CE2 PHE I 137 -20.414 -20.534 3.260 1.00 20.00 C C
ATOM 7875 CD2 PHE I 137 -21.046 -19.365 2.871 1.00 20.00 C C
ATOM 7876 C PHE 1 137 -22.138 -14.765 3.226 1.00 48.73 C C
ATOM 7877 O PHE I 137 -21.342 -13.888 2.890 1.00 49.28 C O
ATOM 7878 N LEU I 138 -23.454 -14.580 3.253 1.00 42.04 C N
ATOM 7879 CA LEU I 138 -24.055 -13.275 2.999 1.00 44.26 C C
ATOM 7880 CB LEU I 138 -25.581 -13.366 3.047 1.00 20.00 C C
ATOM 7881 CG LEU I 138 -26.248 -14.219 1.966 1.00 20.00 C C
ATOM 7882 CD1 LEU I 138 -27.748 -14.301 2.197 1.00 20.00 C C
ATOM 7883 CD2 LEU I 138 -25.944 -13.673 0.580 1.00 20.00 C C
ATOM 7884 C LEU 1 138 -23.565 -12.242 4.006 1.00 43.68 C C
ATOM 7885 O LEU I 138 -23.730 -11.038 3.804 1.00 50.27 C O
ATOM 7886 N GLY I 139 -22.983 -12.724 5.100 1.00 38.56 C N
ATOM 7887 CA GLY I 139 -22.415 -11.853 6.126 1.00 47.99 C C
ATOM 7888 C GLY I 139 -21.274 -10.985 5.625 1.00 44.53 C C
ATOM 7889 O GLY I 139 -20.971 -9.947 6.213 1.00 32.21 C O
ATOM 7890 N PHE I 140 -20.649 -11.402 4.528 1.00 46.33 C N
ATOM 7891 CA PHE I 140 -19.494 -10.693 3.986 1.00 42.95 C C
ATOM 7892 CB PHE I 140 -18.549 -11.668 3.281 1.00 20.00 C C
ATOM 7893 CG PHE I 140 -17.916 -12.677 4.202 1.00 20.00 C C
ATOM 7894 CD1 PHE I 140 -16.781 -12.356 4.929 1.00 20.00 C C
ATOM 7895 CE1 PHE I 140 -16.194 -13.284 5.769 1.00 20.00 C C
ATOM 7896 CZ PHE I 140 -16.731 -14.551 5.879 1.00 20.00 C C
ATOM 7897 CE2 PHE I 140 -17.854 -14.888 5.150 1.00 20.00 C C
ATOM 7898 CD2 PHE I 140 -18.434 -13.958 4.308 1.00 20.00 C C
ATOM 7899 C PHE 1 140 -19.898 -9.568 3.032 1.00 38.13 C C
ATOM 7900 O PHE I 140 -19.052 -8.795 2.581 1.00 57.33 C O
ATOM 7901 N LEU I 141 -21.191 -9.475 2.736 1.00 35.20 C N
ATOM 7902 CA LEU I 141 -21.690 -8.512 1.759 1.00 27.01 C C
ATOM 7903 CB LEU I 141 -21.184 -7.103 2.079 1.00 20.00 C C
ATOM 7904 CG LEU I 141 -21.717 -6.450 3.356 1.00 20.00 C C
ATOM 7905 CD1 LEU I 141 -20.991 -5.144 3.632 1.00 20.00 C C

ATOM 7906 CD2 LEU I 141 -23.216 -6.216 3.252 1.00 20.00 C C
ATOM 7907 C LEU 1 141 -21 .292 -8.918 0.341 1.00 35.79 C C
ATOM 7908 O LEU I 141 -21.674 -9.989 -0.130 1.00 46.92 C O
ATOM 7909 N LEU I 142 -20.469 -8.099 -0.306 1.00 38.67 C N
ATOM 7910 CA LEU I 142 -19.832 -8.492 -1.559 1.00 33.84 C C
ATOM 791 1 CB LEU I 142 -20.017 -7.408 -2.618 1.00 20.00 C C
ATOM 7912 CG LEU I 142 -21.465 -7.163 -3.040 1.00 20.00 C C
ATOM 7913 CD1 LEU I 142 -21.584 -5.883 -3.848 1.00 20.00 C C
ATOM 7914 CD2 LEU I 142 -21.999 -8.350 -3.827 1.00 20.00 C C
ATOM 7915 C LEU 1 142 -18.352 -8.799 -1.363 1.00 36.89 C C
ATOM 7916 O LEU I 142 -17.604 -7.979 -0.831 1.00 45.42 C O
ATOM 7917 N GLY I 143 -17.970 -10.034 -1.673 1.00 26.84 C N
ATOM 7918 CA GLY 1 143 -16.624 -10.516 -1.387 1.00 27.41 C C
ATOM 7919 C GLY I 143 -15.977 -11.154 -2.599 1.00 29.08 C C
ATOM 7920 O GLY I 143 -16.645 -11.813 -3.396 1.00 40.24 C O
ATOM 7921 N VAL I 144 -14.672 -10.957 -2.742 1.00 30.17 C N
ATOM 7922 CA VAL 1 144 -13.928 -11.605 -3.814 1.00 34.15 C C
ATOM 7923 CB VAL I 144 -12.559 -10.921 -4.058 1.00 20.00 C C
ATOM 7924 CGI VAL I 144 -11.826 -11.591 -5.212 1.00 20.00 C C
ATOM 7925 CG2 VAL I 144 -12.750 -9.434 -4.339 1.00 20.00 C C
ATOM 7926 C VAL I 144 -13.732 -13.091 -3.508 1.00 36.67 C C
ATOM 7927 O VAL I 144 -14.071 -13.558 -2.419 1.00 42.49 C O
ATOM 7928 N GLY I 145 -13.320 -13.847 -4.521 1.00 47.09 C N
ATOM 7929 CA GLY 1 145 -12.893 -15.227 -4.321 1.00 44.51 C C
ATOM 7930 C GLY I 145 -11.950 -15.377 -3. 141 1.00 44.94 C C
ATOM 7931 O GLY I 145 -12.181 -16. 196 -2.253 1.00 40.58 C O
ATOM 7932 N SER I 146 -10.905 -14.560 -3.085 1.00 42.06 C N
ATOM 7933 CA SER I 146 -9.931 -14.673 -2.000 1.00 47.39 C C
ATOM 7934 CB SER I 146 -8.758 -13.718 -2.236 1.00 20.00 C C
ATOM 7935 OG SER I 146 -9.200 -12.373 -2.297 1.00 20.00 C O
ATOM 7936 C SER 1 146 -10.535 -14.425 -0.613 1.00 51.48 C C
ATOM 7937 O SER I 146 -10.21 1 -15. 129 0.351 1.00 47.45 C O
ATOM 7938 N ALA I 147 -11.415 -13.434 -0.514 1.00 39.51 C N
ATOM 7939 CA ALA 1 147 -12.026 -13.082 0.766 1.00 43.38 C C
ATOM 7940 CB ALA I 147 -12.866 -11.821 0.621 1.00 20.00 C C
ATOM 7941 C ALA I 147 -12.865 -14.218 1.348 1.00 47.39 C C
ATOM 7942 O ALA I 147 -12.823 -14.476 2.554 1.00 50.18 C O
ATOM 7943 N ILE I 148 -13.624 -14.894 0.492 1.00 44.67 C N
ATOM 7944 CA ILE I 148 -14.453 -16.007 0.937 1.00 43.56 C C
ATOM 7945 CB ILE I 148 -15.322 -16.558 -0.208 1.00 20.00 C C
ATOM 7946 CGI ILE 1 148 -16.249 -15.466 -0.746 1.00 20.00 C C
ATOM 7947 CD1 ILE 1 148 -17.141 -15.925 -1.878 1.00 20.00 C C
ATOM 7948 CG2 ILE 1 148 -16.127 -17.759 0.265 1.00 20.00 C C
ATOM 7949 C ILE I 148 -13.575 -17.126 1.483 1.00 51.18 C C
ATOM 7950 O ILE I 148 -13.886 -17.736 2.510 1.00 39.17 C O
ATOM 7951 N ALA I 149 -12.468 -17.382 0.794 1.00 42.17 C N
ATOM 7952 CA ALA 1 149 -11.531 -18.412 1.217 1.00 36.76 C C
ATOM 7953 CB ALA I 149 -10.424 -18.578 0.189 1.00 20.00 C C
ATOM 7954 C ALA I 149 -10.949 -18.044 2.574 1.00 45.19 C C
ATOM 7955 O ALA I 149 -10.806 -18.897 3.451 1.00 47.83 C O
ATOM 7956 N SER I 150 -10.632 -16.765 2.748 1.00 43.64 C N
ATOM 7957 CA SER I 150 -10.084 -16.296 4.014 1.00 43.46 C C
ATOM 7958 CB SER I 150 -9.701 -14.818 3.919 1.00 20.00 C C
ATOM 7959 OG SER I 150 -10.828 -14.018 3.605 1.00 20.00 C O
ATOM 7960 C SER I 150 -11.093 -16.507 5.138 1.00 44.80 C C
ATOM 7961 O SER I 150 -10.733 -16.932 6.238 1.00 41.55 C O
ATOM 7962 N GLY I 151 -12.361 -16.222 4.854 1.00 27.01 C N
ATOM 7963 CA GLY 1 151 -13.413 -16.410 5.836 1.00 35.21 C C
ATOM 7964 C GLY I 151 -13.553 -17.871 6.219 1.00 42.40 C C
ATOM 7965 O GLY I 151 -13.742 -18.212 7.394 1.00 45.1 1 C O

```
ATOM   7966  N   VAL I 152     -13.454 -18.742   5.219  1.00 40.20      C    N
ATOM   7967  CA  VAL 1 152     -13.548 -20.175   5.458  1.00 46.73      C    c
ATOM   7968  CB  VAL I 152     -13.505 -20.973   4.144  1.00 20.00      c    c
ATOM   7969  CGI VAL I 152     -13.606 -22.464   4.426  1.00 20.00      c    c
ATOM   7970  CG2 VAL I 152     -14.621 -20.523   3.214  1.00 20.00      c    c
ATOM   7971  C   VAL I 152     -12.396 -20.615   6.351  1.00 48.62      c    c
ATOM   7972  O   VAL I 152     -12.579 -21.41 1   7.273  1.00 49.32      c    o
ATOM   7973  N   ALA I 153     -11.212 -20.074   6.083  1.00 35.09      c    N
ATOM   7974  CA  ALA 1 153     -10.030 -20.403   6.867  1.00 42.37      c    c
ATOM   7975  CB  ALA I 153      -8.798 -19.741   6.274  1.00 20.00      c    c
ATOM   7976  C   ALA I 153     -10.231 -19.965   8.310  1.00 37.79      c    c
ATOM   7977  O   ALA I 153      -9.860 -20.676   9.244  1.00 39.25      c    o
ATOM   7978  N   VAL I 154     -10.825 -18.789   8.486  1.00 38.88      c    N
ATOM   7979  CA  VAL 1 154     -11.100 -18.270   9.819  1.00 35.53      c    c
ATOM   7980  CB  VAL I 154     -11.680 -16.845   9.762  1.00 20.00      c    c
ATOM   7981  CGI VAL I 154     -11.955 -16.328  11.165  1.00 20.00      c    c
ATOM   7982  CG2 VAL I 154     -10.731 -15.916   9.021  1.00 20.00      c    c
ATOM   7983  C   VAL I 154     -12.071 -19.175  10.572  1.00 41.00      c    c
ATOM   7984  O   VAL I 154     -11.884 -19.441  11.759  1.00 50.08      c    o
ATOM   7985  N   SER I 155     -13.105 -19.652   9.882  1.00 37.82      c    N
ATOM   7986  CA  SER I 155     -14.071 -20.556  10.508  1.00 44.68      c    c
ATOM   7987  CB  SER I 155     -15.239 -20.834   9.561  1.00 20.00      c    c
ATOM   7988  OG  SER I 155     -14.790 -21.436   8.360  1.00 20.00      c    o
ATOM   7989  C   SER 1 155     -13.400 -21.867  10.917  1.00 41.82      c    c
ATOM   7990  O   SER I 155     -13.667 -22.425  11.982  1.00 49.37      c    o
ATOM   7991  N   LYS I 156     -12.525 -22.338  10.038  1.00 36.99      c    N
ATOM   7992  CA  LYS I 156     -11.772 -23.575  10.184  1.00 35.1 1      c    c
ATOM   7993  CB  LYS I 156     -11.122 -23.965   8.856  1.00 20.00      c    c
ATOM   7994  CG  LYS I 156     -12.1 16 -24.339   7.768  1.00 20.00      c    c
ATOM   7995  CD  LYS I 156     -11.408 -24.786   6.499  1.00 20.00      c    c
ATOM   7996  CE  LYS I 156     -12.400 -25.265   5.452  1.00 20.00      c    c
ATOM   7997  NZ  LYS I 156     -11.733 -25.581   4.158  1.00 20.00      c    N
ATOM   7998  C   LYS I 156     -10.715 -23.451  11.275  1.00 35.98      c    c
ATOM   7999  O   LYS 1 156     -10.361 -24.436  11.922  1.00 42.31      c    o
ATOM   8000  N   VAL I 157     -10.260 -22.224  11.514  1.00 37.88      c    N
ATOM   8001  CA  VAL 1 157      -9.225 -21.960  12.515  1.00 50.94      c    c
ATOM   8002  CB  VAL I 157      -8.267 -20.831  12.062  1.00 20.00      c    c
ATOM   8003  CGI VAL I 157      -7.261 -20.505  13.162  1.00 20.00      c    c
ATOM   8004  CG2 VAL I 157      -7.552 -21.219  10.771  1.00 20.00      c    c
ATOM   8005  C   VAL I 157      -9.832 -21.596  13.871  1.00 47.82      c    c
ATOM   8006  O   VAL I 157      -9.1 16 -21.443  14.863  1.00 56.87      c    o
ATOM   8007  N   LEU I 158     -11.156 -21 .533  13.947  1.00 39.52      c    N
ATOM   8008  CA  LEU I 158     -11.838 -20.969  15.1 12  1.00 50.27      c    c
ATOM   8009  CB  LEU I 158     -13.351 -20.935  14.869  1.00 20.00      c    c
ATOM   8010  CG  LEU I 158     -13.827 -20.109  13.673  1.00 20.00      c    c
ATOM   801 1 CD1 LEU I 158     -15.343 -20.163  13.552  1.00 20.00      c    c
ATOM   8012  CD2 LEU I 158     -13.346 -18.671  13.788  1.00 20.00      c    c
ATOM   8013  C   LEU 1 158     -11.550 -21.631  16.465  1.00 54.47      c    c
ATOM   8014  O   LEU I 158     -11.417 -20.934  17.477  1.00 49.26      c    o
ATOM   8015  N   HIS I 159     -11.447 -22.954  16.501  1.00 59.45      c    N
ATOM   8016  CA  HIS I 159     -11.205 -23.636  17.768  1.00 49.1 1      c    c
ATOM   8017  CB  HIS I 159     -11.225 -25.153  17.573  1.00 20.00      c    c
ATOM   8018  CG  HIS I 159     -12.522 -25.676  17.038  1.00 20.00      c    c
ATOM   8019  ND1 HIS I 159     -13.559 -26.070  17.855  1.00 20.00      c    N
ATOM   8020  CE1 HIS I 159     -14.570 -26.484  17.1 12  1.00 20.00      c    c
ATOM   8021  NE2 HIS 1 159     -14.225 -26.373  15.842  1.00 20.00      c    N
ATOM   8022  CD2 HIS I 159     -12.949 -25.871  15.768  1.00 20.00      c    c
ATOM   8023  C   HIS I 159      -9.874 -23.203  18.385  1.00 44.09      c    c
ATOM   8024  O   HIS I 159      -9.780 -22.977  19.596  1.00 42.13      c    o
ATOM   8025  N   LEU I 160      -8.851 -23.072  17.546  1.00 37.55      c    N
```

ATOM 8026 CA LEU I 160 -7.536 -22.649 18.01 1 1.00 43.52 C c
ATOM 8027 CB LEU I 160 -6.520 -22.704 16.869 1.00 20.00 C c
ATOM 8028 CG LEU I 160 -6.299 -24.073 16.224 1.00 20.00 c c
ATOM 8029 CD1 LEU I 160 -5.268 -23.982 15.109 1.00 20.00 c c
ATOM 8030 CD2 LEU I 160 -5.877 -25.097 17.266 1.00 20.00 c c
ATOM 8031 C LEU 1 160 -7.599 -21.240 18.591 1.00 47.22 c c
ATOM 8032 O LEU I 160 -6.984 -20.951 19.619 1.00 43.25 c o
ATOM 8033 N GLU I 161 -8.351 -20.368 17.927 1.00 40.88 c N
ATOM 8034 CA GLU I 161 -8.512 -18.996 18.388 1.00 40.61 c c
ATOM 8035 CB GLU I 161 -9.325 -18.182 17.381 1.00 20.00 c c
ATOM 8036 CG GLU I 161 -8.702 -18.104 15.997 1.00 20.00 c c
ATOM 8037 CD GLU I 161 -9.537 -17.292 15.027 1.00 20.00 c c
ATOM 8038 OE1 GLU I 161 -9.126 -17.158 13.855 1.00 20.00 c o
ATOM 8039 OE2 GLU I 161 -10.604 -16.788 15.436 1.00 20.00 c: o
ATOM 8040 C GLU I 161 -9.195 -18.983 19.749 1.00 39.76 c c
ATOM 8041 O GLU I 161 -8.816 -18.221 20.642 1.00 44.02 c o
ATOM 8042 N GLY I 162 -10.199 -19.840 19.906 1.00 34.18 c N
ATOM 8043 CA GLY I 162 -10.907 -19.934 21. 169 1.00 35.01 c c
ATOM 8044 C GLY I 162 -9.967 -20.387 22.269 1.00 34.86 c c
ATOM 8045 O GLY I 162 -9.997 -19.864 23.386 1.00 47.81 c o
ATOM 8046 N GLU I 163 -9.1 12 -21.352 21.945 1.00 40.78 c N
ATOM 8047 CA GLU 1 163 -8.143 -21.856 22.91 1 1.00 37.20 c c
ATOM 8048 CB GLU I 163 -7.365 -23.036 22.326 1.00 20.00 c c
ATOM 8049 CG GLU 1 163 -8.235 -24.218 21.931 1.00 20.00 c c
ATOM 8050 CD GLU 1 163 -7.430 -25.368 21.357 1.00 20.00 c c
ATOM 8051 OE1 GLU I 163 -8.037 -26.397 20.995 1.00 20.00 c o
ATOM 8052 OE2 GLU I 163 -6.191 -25.241 21.268 1.00 20.00 c o
ATOM 8053 C GLU I 163 -7.183 -20.745 23.324 1.00 46.12 c c
ATOM 8054 O GLU I 163 -6.837 -20.61 1 24.501 1.00 58.66 c o
ATOM 8055 N VAL I 164 -6.761 -19.944 22.350 1.00 42.23 c N
ATOM 8056 CA VAL I 164 -5.857 -18.834 22.620 1.00 35.45 c c
ATOM 8057 CB VAL I 164 -5.429 -18.124 21.323 1.00 20.00 c c
ATOM 8058 CGI VAL I 164 -4.487 -16.971 21.635 1.00 20.00 c c
ATOM 8059 CG2 VAL I 164 -4.775 -19.1 12 20.369 1.00 20.00 c c
ATOM 8060 C VAL I 164 -6.522 -17.823 23.548 1.00 46.32 c c
ATOM 8061 O VAL I 164 -5.892 -17.301 24.472 1.00 45.08 c o
ATOM 8062 N ASN I 165 -7.802 -17.558 23.304 1.00 40.82 c N
ATOM 8063 CA ASN I 165 -8.548 -16.631 24.144 1.00 46.48 c c
ATOM 8064 CB ASN I 165 -9.952 -16.403 23.581 1.00 20.00 c c
ATOM 8065 CG ASN I 165 -9.930 -15.822 22.181 1.00 20.00 c c
ATOM 8066 OD1 ASN I 165 -10.975 -15.504 21.612 1.00 20.00 c o
ATOM 8067 ND2 ASN I 165 -8.736 -15.681 21.617 1.00 20.00 c N
ATOM 8068 C ASN I 165 -8.631 -17.160 25.569 1.00 50.90 c c
ATOM 8069 O ASN I 165 -8.474 -16.412 26.536 1.00 47.1 1 c o
ATOM 8070 N LYS I 166 -8.857 -18.464 25.688 1.00 48.36 c N
ATOM 8071 CA LYS I 166 -8.945 -19.120 26.986 1.00 38.71 c c
ATOM 8072 CB LYS I 166 -9.329 -20.592 26.818 1.00 20.00 c c
ATOM 8073 CG LYS I 166 -10.649 -20.81 1 26.097 1.00 20.00 c c
ATOM 8074 CD LYS I 166 -10.952 -22.292 25.936 1.00 20.00 c c
ATOM 8075 CE LYS I 166 -12.264 -22.51 1 25.200 1.00 20.00 c c
ATOM 8076 NZ LYS I 166 -12.569 -23.958 25.028 1.00 20.00 c N
ATOM 8077 C LYS I 166 -7.623 -19.006 27.738 1.00 45.07 c c
ATOM 8078 O LYS 1 166 -7.600 -18.823 28.955 1.00 56.09 c o
ATOM 8079 N ILE I 167 -6.525 -19.121 26.999 1.00 42.02 C N
ATOM 8080 CA ILE I 167 -5.184 -19.080 27.576 1.00 43.86 c c
ATOM 8081 CB ILE I 167 -4.207 -19.975 26.789 1.00 20.00 c c
ATOM 8082 CGI ILE 1 167 -4.685 -21.429 26.804 1.00 20.00 c c
ATOM 8083 CD1 ILE 1 167 -3.778 -22.377 26.050 1.00 20.00 c c
ATOM 8084 CG2 ILE I 167 -2.803 -19.865 27.362 1.00 20.00 c c
ATOM 8085 C ILE I 167 -4.599 -17.669 27.665 1.00 49.02 c c

```
ATOM   8086  O   ILE I 167     -3.448 -17.497  28.066  1.00 37.71      C    O
ATOM   8087  N   LYS 1 168     -5.382 -16.664  27.282  1.00 33.87      C    N
ATOM   8088  CA  LYS I 168     -4.890 -15.285  27.251  1.00 35.1 1     C    C
ATOM   8089  CB  LYS I 168     -5.939 -14.363  26.622  1.00 20.00      C    C
ATOM   8090  CG  LYS I 168     -6.275 -14.698  25.178  1.00 20.00      C    C
ATOM   8091  CD  LYS I 168     -7.292 -13.723  24.607  1.00 20.00      C    C
ATOM   8092  CE  LYS I 168     -7.612 -14.046  23. 157  1.00 20.00     C    C
ATOM   8093  NZ  LYS I 168     -8.599 -13.092  22.580  1.00 20.00      C    N
ATOM   8094  C   LYS I 168     -4.431 -14.704  28.600  1.00 39.27      C    C
ATOM   8095  O   LYS 1 168     -3.414 -14.012  28.655  1.00 32.39      C    O
ATOM   8096  N   SER I 169     -5.164 -14.973  29.677  1.00 41.30      C    N
ATOM   8097  CA  SER I 169     -4.797 -14.446  30.987  1.00 43.23      C    C
ATOM   8098  CB  SER I 169     -5.756 -14.957  32.064  1.00 20.00      C    C
ATOM   8099  OG  SER I 169     -5.739 -16.371  32.127  1.00 20.00      C    O
ATOM   8100  C   SER 1 169     -3.359 -14.795  31.353  1.00 41.44      C    C
ATOM   8101  O   SER I 169     -2.580 -13.924  31.740  1.00 44.82      C    O
ATOM   8102  N   ALA I 170     -3.013 -16.072  31.235  1.00 39.78      C    N
ATOM   8103  CA  ALA 1 170     -1.644 -16.517  31.469  1.00 4 1.01     C    C
ATOM   8104  CB  ALA I 170     -1.541 -18.025  31.320  1.00 20.00      C    C
ATOM   8105  C   ALA I 170     -0.674 -15.820  30.523  1.00 46.04      C    C
ATOM   8106  O   ALA I 170      0.396 -15.373  30.935  1.00 46.67      C    O
ATOM   8107  N   LEU I 171     -1.061 -15.718  29.258  1.00 34.26      C    N
ATOM   8108  CA  LEU I 171     -0.245 -15.030  28.269  1.00 37.69      C    C
ATOM   8109  CB  LEU I 171     -0.942 -15.036  26.912  1.00 20.00      C    C
ATOM   8110  CG  LEU I 171     -1.226 -16.424  26.346  1.00 20.00      C    C
ATOM   8111  CD1 LEU I 171     -1.873 -16.31 1  24.972  1.00 20.00     C    C
ATOM   8112  CD2 LEU I 171      0.060 -17.242  26.293  1.00 20.00      C    C
ATOM   8113  C   LEU 1 171      0.053 -13.598  28.702  1.00 44.67      C    C
ATOM   8114  O   LEU I 171      1.173 -13. 109  28.538  1.00 34.27      C    O
ATOM   8115  N   LEU I 172     -0.935 -12.955  29.314  1.00 34.80      C    N
ATOM   8116  CA  LEU I 172     -0.817 -11.555  29.692  1.00 28.87      C    C
ATOM   8117  CB  LEU I 172     -2.199 -10.971  29.993  1.00 20.00      C    C
ATOM   8118  CG  LEU I 172     -3.198 -10.968  28.835  1.00 20.00      C    C
ATOM   8119  CD1 LEU I 172     -4.534 -10.393  29.283  1.00 20.00      C    C
ATOM   8120  CD2 LEU I 172     -2.643 -10.187  27.668  1.00 20.00      C    C
ATOM   8121  C   LEU 1 172      0.099 -11.400  30.901  1.00 29.90      C    C
ATOM   8122  O   LEU I 172      0.896 -10.462  30.972  1.00 4 1.09     C    O
ATOM   8123  N   SER I 173      0.016 -12.355  31.824  1.00 35.08      C    N
ATOM   8124  CA  SER I 173      0.740 -12.276  33.092  1.00 35.53      C    C
ATOM   8125  CB  SER I 173      0.1 10 -13.206  34. 132  1.00 20.00     C    C
ATOM   8126  OG  SER I 173      0.148 -14.555  33.701  1.00 20.00      C    O
ATOM   8127  C   SER 1 173      2.218 -12.610  32.919  1.00 35.07      C    C
ATOM   8128  O   SER I 173      3.042 -12.300  33.779  1.00 5 1.28     C    O
ATOM   8129  N   THR I 174      2.537 -13.275  31.817  1.00 46.35      C    N
ATOM   8130  CA  THR I 174      3.894 -13.733  31.561  1.00 43.83      C    C
ATOM   8131  CB  THR I 174      3.889 -14.970  30.641  1.00 20.00      C    C
ATOM   8132  OG1 THR I 174      3.327 -14.620  29.371  1.00 20.00     C    O
ATOM   8133  CG2 THR I 174      3.056 -16.081  31.260  1.00 20.00      C    C
ATOM   8134  C   THR I 174      4.722 -12.626  30.910  1.00 52.54      C    C
ATOM   8135  O   THR I 174      4.393 -12.154  29.821  1.00 64.10      C    O
ATOM   8136  N   ASN I 175      5.771 -12.188  31.599  1.00 55.57      C    N
ATOM   8137  CA  ASN I 175      6.735 -11.267  31.008  1.00 40.58      C    C
ATOM   8138  CB  ASN I 175      7.507 -10.521  32.099  1.00 20.00      C    C
ATOM   8139  CG  ASN I 175      6.646  -9.518  32.845  1.00 20.00      C    C
ATOM   8140  OD1 ASN I 175      5.640  -9.033  32.324  1.00 20.00      C    O
ATOM   8141  ND2 ASN I 175      7.043  -9.196  34.072  1.00 20.00      C    N
ATOM   8142  C   ASN I 175      7.708 -11.986  30.075  1.00 43.65      C    C
ATOM   8143  O   ASN I 175      8.525 -12.793  30.521  1.00 53.1 1     C    O
ATOM   8144  N   LYS 1 176      7.546 -11.768  28.773  1.00 44.89      C    N
ATOM   8145  CA  LYS I 176      8.402 -12.407  27.776  1.00 46.42      C    C
```

ATOM 8146 CB LYS I 176 8.150 -13.917 27.740 1.00 20.00 C C
ATOM 8147 CG LYS I 176 8.510 -14.625 29.034 1.00 20.00 C C
ATOM 8148 CD LYS I 176 8.270 -16.122 28.943 1.00 20.00 C C
ATOM 8149 CE LYS I 176 8.994 -16.863 30.063 1.00 20.00 C C
ATOM 8150 NZ LYS I 176 9.447 -18.223 29.648 1.00 20.00 C N
ATOM 8151 C LYS I 176 8.192 -11.798 26.392 1.00 45.00 C C
ATOM 8152 O LYS 1 176 7.084 -11.379 26.053 1.00 60.64 C O
ATOM 8153 N ALA I 177 9.280 -11.645 25.643 1.00 46.01 C N
ATOM 8154 CA ALA 1 177 9.189 -11.237 24.242 1.00 43.65 C C
ATOM 8155 CB ALA I 177 10.555 -10.847 23.706 1.00 20.00 C C
ATOM 8156 C ALA I 177 8.592 -12.349 23.395 1.00 41.42 C C
ATOM 8157 O ALA I 177 7.695 -12. 116 22.584 1.00 45.37 C O
ATOM 8158 N VAL I 178 9.140 -13.549 23.545 1.00 35.70 C N
ATOM 8159 CA VAL 1 178 8.580 -14.725 22.902 1.00 43.93 C C
ATOM 8160 CB VAL I 178 9.495 -15.243 21.780 1.00 20.00 C C
ATOM 8161 CGI VAL I 178 8.898 -16.490 21.143 1.00 20.00 C C
ATOM 8162 CG2 VAL I 178 9.714 -14.159 20.734 1.00 20.00 C C
ATOM 8163 C VAL I 178 8.363 -15.829 23.922 1.00 34.16 C C
ATOM 8164 O VAL I 178 9.1 15 -15.950 24.889 1.00 44.45 C O
ATOM 8165 N VAL I 179 7.271 -16.565 23.760 1.00 44.87 C N
ATOM 8166 CA VAL 1 179 6.916 -17.608 24.708 1.00 38.47 C C
ATOM 8167 CB VAL I 179 6.234 -17.027 25.960 1.00 20.00 C C
ATOM 8168 CGI VAL I 179 5.785 -18.147 26.887 1.00 20.00 C C
ATOM 8169 CG2 VAL I 179 7.174 -16.076 26.680 1.00 20.00 C C
ATOM 8170 C VAL I 179 6.003 -18.648 24.074 1.00 44.79 C C
ATOM 8171 O VAL I 179 5.097 -18.317 23.310 1.00 51.88 C O
ATOM 8172 N SER I 180 6.270 -19.91 1 24.378 1.00 45.23 C N
ATOM 8173 CA SER I 180 5.428 -21 .002 23.914 1.00 48.99 C C
ATOM 8174 CB SER I 180 6.171 -22.334 24.038 1.00 20.00 C C
ATOM 8175 OG SER I 180 6.627 -22.542 25.364 1.00 20.00 C O
ATOM 8176 C SER I 180 4.1 18 -21.053 24.698 1.00 48.15 C C
ATOM 8177 O SER I 180 4.1 16 -21.309 25.901 1.00 60.42 C O
ATOM 8178 N LEU I 181 3.009 -20.782 24.016 1.00 42.42 C N
ATOM 8179 CA LEU I 181 1.684 -20.959 24.605 1.00 43.22 c c
ATOM 8180 CB LEU I 181 0.610 -20.369 23.693 1.00 20.00 c c
ATOM 8181 CG LEU I 181 0.738 -18.866 23.467 1.00 20.00 c c
ATOM 8182 CD1 LEU I 181 -0.514 -18.314 22.808 1.00 20.00 c c
ATOM 8183 CD2 LEU I 181 1.008 -18.184 24.795 1.00 20.00 c c
ATOM 8184 C LEU 1 181 1.388 -22.428 24.863 1.00 29.14 c c
ATOM 8185 O LEU I 181 1.144 -23. 194 23.931 1.00 43.42 c o
ATOM 8186 N SER I 182 1.361 -22.807 26.136 1.00 4 1.83 c N
ATOM 8187 CA SER I 182 1.272 -24.214 26.503 1.00 53.52 c c
ATOM 8188 CB SER I 182 2.491 -24.642 27.324 1.00 20.00 c c
ATOM 8189 OG SER I 182 2.601 -23.890 28.521 1.00 20.00 c o
ATOM 8190 C SER I 182 -0.025 -24.557 27.236 1.00 44.76 c c
ATOM 8191 O SER I 182 -0.492 -23.802 28.090 1.00 37.73 c o
ATOM 8192 N ASN I 183 -0.652 -25.649 26.815 1.00 47.84 c N
ATOM 8193 CA ASN I 183 -1.684 -26.308 27.603 1.00 59.45 c c
ATOM 8194 CB ASN I 183 -3.002 -26.334 26.822 1.00 20.00 c c
ATOM 8195 CG ASN I 183 -3.598 -24.951 26.632 1.00 20.00 c c
ATOM 8196 OD1 ASN I 183 -3.426 -24.069 27.473 1.00 20.00 c o
ATOM 8197 ND2 ASN I 183 -4.381 -24.785 25.572 1.00 20.00 c N
ATOM 8198 C ASN I 183 -1.232 -27.732 27.905 1.00 75.41 c c
ATOM 8199 O ASN I 183 -0.535 -28.342 27.096 1.00102.31 c o
ATOM 8200 N GLY I 184 -1.489 -28.200 29. 121 1.00 79.30 c N
ATOM 8201 CA GLY I 184 -1.001 -29.510 29.549 1.00 88.92 c c
ATOM 8202 C GLY I 184 -0.204 -30.239 28.479 1.00101.85 c c
ATOM 8203 O GLY I 184 -0.764 -30.990 27.680 1.001 13.48 c o
ATOM 8204 N VAL I 185 1.103 -29.994 28.448 1.00 86.84 c N
ATOM 8205 CA VAL 1 185 2.047 -30.825 27.696 1.00 81.80 c c

ATOM 8206 CB VAL I 185 1.899 -32.323 28.027 1.00 20.00 C c
ATOM 8207 CGI VAL I 185 2.803 -33.155 27.126 1.00 20.00 c c
ATOM 8208 CG2 VAL I 185 2.219 -32.578 29.491 1.00 20.00 c c
ATOM 8209 C VAL I 185 1.997 -30.638 26.179 1.00 81.69 c c
ATOM 8210 O VAL I 185 2.634 -31.388 25.439 1.00 99.84 c o
ATOM 8211 N SER I 186 1.282 -29.618 25.718 1.00 70.63 c N
ATOM 8212 CA SER I 186 1.132 -29.398 24.284 1.00 72.29 c c
ATOM 8213 CB SER I 186 -0.201 -29.962 23.792 1.00 20.00 c c
ATOM 8214 OG SER I 186 -1.291 -29.357 24.467 1.00 20.00 c o
ATOM 8215 C SER I 186 1.247 -27.923 23.915 1.00 62.99 c c
ATOM 8216 O SER I 186 0.649 -27.064 24.565 1.00 58.35 c o
ATOM 8217 N VAL I 187 2.013 -27.638 22.865 1.00 66.49 c N
ATOM 8218 CA VAL I 187 2.203 -26.266 22.398 1.00 57.36 c c
ATOM 8219 CB VAL I 187 3.581 -26.078 21.735 1.00 20.00 c c
ATOM 8220 CGI VAL I 187 3.748 -24.643 21.256 1.00 20.00 c c
ATOM 8221 CG2 VAL I 187 4.691 -26.452 22.699 1.00 20.00 c c
ATOM 8222 C VAL I 187 1.116 -25.863 21.405 1.00 53.67 c c
ATOM 8223 O VAL I 187 0.949 -26.501 20.365 1.00 50.10 c o
ATOM 8224 N LEU I 188 0.381 -24.803 21.731 1.00 43.20 c N
ATOM 8225 CA LEU I 188 -0.676 -24.302 20.858 1.00 41.76 c c
ATOM 8226 CB LEU I 188 -1.749 -23.580 21.674 1.00 20.00 c c
ATOM 8227 CG LEU I 188 -2.557 -24.455 22.632 1.00 20.00 c c
ATOM 8228 CD1 LEU I 188 -3.533 -23.609 23.429 1.00 20.00 c c
ATOM 8229 CD2 LEU I 188 -3.287 -25.542 21.865 1.00 20.00 c c
ATOM 8230 C LEU I 188 -0.102 -23.361 19.813 1.00 44.75 c c
ATOM 8231 O LEU I 188 -0.674 -23.184 18.738 1.00 45.28 c o
ATOM 8232 N THR I 189 1.054 -22.786 20.124 1.00 39.28 c N
ATOM 8233 CA THR I 189 1.675 -21.805 19.250 1.00 36.51 c c
ATOM 8234 CB THR I 189 0.614 -20.957 18.526 1.00 20.00 c c
ATOM 8235 OG1 THR I 189 -0.113 -20.177 19.481 1.00 20.00 c o
ATOM 8236 CG2 THR I 189 -0.360 -21.858 17.785 1.00 20.00 c c
ATOM 8237 C THR I 189 2.615 -20.901 20.039 1.00 45.83 c c
ATOM 8238 O THR I 189 3.150 -21.304 21.072 1.00 42.57 c o
ATOM 8239 N SER I 190 2.853 -19.698 19.530 1.00 40.44 c N
ATOM 8240 CA SER I 190 3.792 -18.785 20.166 1.00 41.82 c c
ATOM 8241 CB SER I 190 5.022 -18.584 19.283 1.00 20.00 c c
ATOM 8242 OG SER I 190 4.664 -18.015 18.038 1.00 20.00 c o
ATOM 8243 C SER I 190 3.146 -17.444 20.491 1.00 33.81 c c
ATOM 8244 O SER I 190 2.391 -16.897 19.687 1.00 49.61 c o
ATOM 8245 N LYS I 191 3.454 -16.920 21.674 1.00 37.37 c N
ATOM 8246 CA LYS I 191 2.986 -15.598 22.086 1.00 41.23 c c
ATOM 8247 CB LYS I 191 2.358 -15.664 23.478 1.00 20.00 c c
ATOM 8248 CG LYS I 191 1.069 -16.459 23.525 1.00 20.00 c c
ATOM 8249 CD LYS I 191 0.505 -16.514 24.931 1.00 20.00 c c
ATOM 8250 CE LYS I 191 -0.626 -17.531 25.037 1.00 20.00 c c
ATOM 8251 NZ LYS I 191 -0.791 -18.032 26.435 1.00 20.00 c N
ATOM 8252 C LYS I 191 4.112 -14.568 22.069 1.00 35.03 c c
ATOM 8253 O LYS I 191 5.120 -14.728 22.757 1.00 40.06 c o
ATOM 8254 N VAL I 192 3.920 -13.495 21.308 1.00 33.70 c N
ATOM 8255 CA VAL I 192 4.967 -12.498 21.120 1.00 27.61 c c
ATOM 8256 CB VAL I 192 5.392 -12.392 19.646 1.00 20.00 c c
ATOM 8257 CGI VAL I 192 6.395 -11.267 19.465 1.00 20.00 c c
ATOM 8258 CG2 VAL I 192 5.972 -13.709 19.165 1.00 20.00 c c
ATOM 8259 C VAL I 192 4.550 -11.121 21.624 1.00 31.74 c c
ATOM 8260 O VAL I 192 3.376 -10.755 21.573 1.00 25.58 c o
ATOM 8261 N LEU I 193 5.526 -10.364 22.114 1.00 28.88 c N
ATOM 8262 CA LEU I 193 5.316 -8.973 22.488 1.00 34.36 c c
ATOM 8263 CB LEU I 193 5.118 -8.855 23.998 1.00 20.00 c c
ATOM 8264 CG LEU I 193 3.893 -9.566 24.567 1.00 20.00 c c
ATOM 8265 CD1 LEU I 193 3.915 -9.514 26.084 1.00 20.00 c c

ATOM 8266 CD2 LEU I 193 2.623 -8.947 24.019 1.00 20.00 C C
ATOM 8267 C LEU 1 193 6.507 -8.126 22.059 1.00 33.03 C C
ATOM 8268 O LEU I 193 7.592 -8.238 22.627 1.00 44.93 C O
ATOM 8269 N ASP 1 194 6.304 -7.294 21.042 1.00 35.09 C N
ATOM 8270 CA ASP I 194 7.409 -6.702 20.288 1.00 41.39 C C
ATOM 8271 CB ASP I 194 6.892 -6.027 19.014 1.00 20.00 C C
ATOM 8272 CG ASP I 194 6.375 -7.023 17.994 1.00 20.00 C C
ATOM 8273 OD1 ASP I 194 6.659 -8.229 18. 141 1.00 20.00 C O
ATOM 8274 OD2 ASP I 194 5.654 -6.606 17.064 1.00 20.00 C O
ATOM 8275 C ASP 1 194 8.255 -5.712 21.094 1.00 38.04 C C
ATOM 8276 O ASP 1 194 9.349 -5.339 20.670 1.00 48.03 C O
ATOM 8277 N LEU I 195 7.723 -5.232 22.215 1.00 43.64 C N
ATOM 8278 CA LEU I 195 8.360 -4.139 22.947 1.00 35.97 C C
ATOM 8279 CB LEU I 195 7.417 -2.935 23.045 1.00 20.00 C C
ATOM 8280 CG LEU I 195 7.024 -2.281 21.714 1.00 20.00 C C
ATOM 8281 CD1 LEU I 195 5.965 -1.195 21.915 1.00 20.00 C C
ATOM 8282 CD2 LEU I 195 8.249 -1.730 20.980 1.00 20.00 C C
ATOM 8283 C LEU 1 195 8.858 -4.546 24.335 1.00 43.63 C C
ATOM 8284 O LEU I 195 9.609 -3.81 1 24.972 1.00 34.71 C O
ATOM 8285 N ASN I 196 8.535 -5.769 24.742 1.00 44.30 C N
ATOM 8286 CA ASN I 196 8.824 -6.238 26.095 1.00 42.38 C C
ATOM 8287 CB ASN I 196 8.399 -7.701 26.254 1.00 20.00 C C
ATOM 8288 CG ASN I 196 6.892 -7.874 26.221 1.00 20.00 C C
ATOM 8289 OD1 ASN I 196 6.146 -6.952 26.545 1.00 20.00 C O
ATOM 8290 ND2 ASN I 196 6.438 -9.055 25.817 1.00 20.00 C N
ATOM 8291 C ASN I 196 10.282 -6.058 26.51 1 1.00 43.66 C C
ATOM 8292 O ASN I 196 10.568 -5.610 27.622 1.00 33.62 C O
ATOM 8293 N ASN I 197 11.199 -6.448 25.633 1.00 34.31 C N
ATOM 8294 CA ASN I 197 12.621 -6.414 25.950 1.00 38.83 C C
ATOM 8295 CB ASN I 197 13.437 -7.021 24.812 1.00 20.00 C C
ATOM 8296 CG ASN I 197 13.306 -8.527 24.747 1.00 20.00 C C
ATOM 8297 OD1 ASN I 197 13.064 -9.180 25.764 1.00 20.00 C O
ATOM 8298 ND2 ASN I 197 13.315 -9.069 23.533 1.00 20.00 C N
ATOM 8299 C ASN I 197 13.106 -5.005 26.239 1.00 39.90 C C
ATOM 8300 O ASN I 197 13.745 -4.752 27.261 1.00 39.04 C O
ATOM 8301 N TYR I 198 12.824 -4.095 25.314 1.00 35.09 C N
ATOM 8302 CA TYR I 198 13.109 -2.682 25.518 1.00 41.03 C C
ATOM 8303 CB TYR I 198 12.610 -1.859 24.332 1.00 20.00 C C
ATOM 8304 CG TYR I 198 13.298 -2.189 23.031 1.00 20.00 C C
ATOM 8305 CD 1 TYR I 198 14.497 -1.579 22.687 1.00 20.00 C C
ATOM 8306 CE1 TYR I 198 15.1 10 -1.847 21.488 1.00 20.00 C C
ATOM 8307 CZ TYR I 198 14.536 -2.752 20.620 1.00 20.00 C C
ATOM 8308 OH TYR 1 198 15.138 -3.016 19.41 1 1.00 20.00 C O
ATOM 8309 CE2 TYR I 198 13.349 -3.378 20.941 1.00 20.00 C C
ATOM 8310 CD2 TYR I 198 12.749 -3.109 22.148 1.00 20.00 C C
ATOM 831 1 C TYR I 198 12.490 -2.163 26.81 1 1.00 43.65 C C
ATOM 8312 O TYR I 198 13.128 -1.410 27.549 1.00 52.37 C O
ATOM 8313 N ILE I 199 11.279 -2.622 27. 115 1.00 35.86 C N
ATOM 8314 CA ILE I 199 10.573 -2.185 28.316 1.00 45.39 C C
ATOM 8315 CB ILE I 199 9.108 -2.624 28.306 1.00 20.00 C C
ATOM 8316 CGI ILE 1 199 8.330 -1.808 27.272 1.00 20.00 C C
ATOM 8317 CD1 ILE I 199 7.307 -2.607 26.505 1.00 20.00 C C
ATOM 8318 CG2 ILE I 199 8.502 -2.461 29.691 1.00 20.00 C C
ATOM 8319 C ILE I 199 11.232 -2.684 29.595 1.00 37.89 C C
ATOM 8320 O ILE I 199 11.344 -1.943 30.572 1.00 45.28 C O
ATOM 8321 N ASP 1200 11.628 -3.953 29.597 1.00 37.36 C N
ATOM 8322 CA ASP 1200 12.325 -4.543 30.737 1.00 46.66 C C
ATOM 8323 CB ASP 1200 12.549 -6.040 30.507 1.00 20.00 C C
ATOM 8324 CG ASP 1200 11.269 -6.841 30.616 1.00 20.00 C C
ATOM 8325 OD1 ASP I 200 10.283 -6.314 31. 172 1.00 20.00 C O

```
ATOM   8326  OD2 ASP I 200      11.248  -7.996  30.143  1.00 20.00      C    o
ATOM   8327  C   ASP I 200      13.655  -3.842  31.033  1.00 51.05      C    c
ATOM   8328  O   ASP I 200      14.077  -3.753  32.188  1.00 57.39      c    o
ATOM   8329  N   LYS I 201      14.284  -3.306  29.989  1.00 57.68      c    N
ATOM   8330  CA  LYS I 201      15.560  -2.605  30.126  1.00 44.02      c    c
ATOM   8331  CB  LYS I 201      16.228  -2.417  28.760  1.00 20.00      c    c
ATOM   8332  CG  LYS I 201      16.590  -3.716  28.055  1.00 20.00      c    c
ATOM   8333  CD  LYS I 201      17.363  -3.463  26.764  1.00 20.00      c    c
ATOM   8334  CE  LYS I 201      17.644  -4.764  26.018  1.00 20.00      c    c
ATOM   8335  NZ  LYS I 201      18.195  -4.531  24.654  1.00 20.00      c    N
ATOM   8336  C   LYS I 201      15.409  -1.254  30.827  1.00 43.56      c    c
ATOM   8337  O   LYS I 201      16.366  -0.743  31.407  1.00 51.34      c    o
ATOM   8338  N   GLN I 202      14.202  -0.694  30.795  1.00 46.06      c    N
ATOM   8339  CA  GLN I 202      13.987   0.689  31.223  1.00 44.95      c    c
ATOM   8340  CB  GLN I 202      13.366   1.518  30.101  1.00 20.00      c    c
ATOM   8341  CG  GLN I 202      14.344   1.932  29.024  1.00 20.00      c    c
ATOM   8342  CD  GLN I 202      13.660   2.551  27.823  1.00 20.00      c    c
ATOM   8343  OE1 GLN I 202      12.435   2.519  27.702  1.00 20.00      c    o
ATOM   8344  NE2 GLN I 202      14.452   3.135  26.932  1.00 20.00      c    N
ATOM   8345  C   GLN I 202      13.142   0.816  32.489  1.00 42.35      c    c
ATOM   8346  O   GLN I 202      13.166   1.853  33.151  1.00 47.00      c    o
ATOM   8347  N   LEU I 203      12.318  -0.189  32.766  1.00 49.55      c    N
ATOM   8348  CA  LEU I 203      11.397  -0.111  33.895  1.00 50.77      c    c
ATOM   8349  CB  LEU I 203      10.332  -1.205  33.796  1.00 20.00      c    c
ATOM   8350  CG  LEU I 203       9.392  -1.066  32.594  1.00 20.00      c    c
ATOM   8351  CD1 LEU I 203       8.616  -2.347  32.316  1.00 20.00      c    c
ATOM   8352  CD2 LEU I 203       8.447   0.111  32.787  1.00 20.00      c    c
ATOM   8353  C   LEU I 203      12.134  -0.184  35.231  1.00 52.51      c    c
ATOM   8354  O   LEU I 203      13.096  -0.937  35.379  1.00 46.02      c    o
ATOM   8355  N   LEU I 204      11.747   0.686  36.159  1.00 51.45      c    N
ATOM   8356  CA  LEU I 204      12.308   0.682  37.507  1.00 58.44      c    c
ATOM   8357  CB  LEU I 204      12.055   2.021  38.187  1.00 20.00      c    c
ATOM   8358  CG  LEU I 204      12.780   3.206  37.565  1.00 20.00      c    c
ATOM   8359  CD1 LEU I 204      12.380   4.480  38.291  1.00 20.00      c    c
ATOM   8360  CD2 LEU I 204      14.286   2.982  37.637  1.00 20.00      c    c
ATOM   8361  C   LEU I 204      11.700  -0.425  38.354  1.00 54.99      c    c
ATOM   8362  O   LEU I 204      10.489  -0.633  38.319  1.00 55.13      c    o
ATOM   8363  N   PRO I 205      12.498  -0.979  39.277  1.00 58.64      c    N
ATOM   8364  CA  PRO I 205      12.014  -2.145  39.995  1.00 52.19      c    c
ATOM   8365  CB  PRO I 205      13.198  -2.496  40.896  1.00 20.00      c    c
ATOM   8366  CG  PRO I 205      13.924  -1.175  41.116  1.00 20.00      c    c
ATOM   8367  CD  PRO I 205      13.404  -0.175  40.112  1.00 20.00      c    c
ATOM   8368  C   PRO I 205      10.799  -1.765  40.840  1.00 54.30      c    c
ATOM   8369  O   PRO I 205      10.014  -2.630  41.235  1.00 70.22      c    o
ATOM   8370  N   ILE I 206      10.656  -0.465  41.096  1.00 62.70      c    N
ATOM   8371  CA  ILE I 206       9.491   0.087  41.787  1.00 68.19      c    c
ATOM   8372  CB  ILE I 206       9.725   0.181  43.311  1.00 20.00      c    c
ATOM   8373  CGI ILE I 206       9.753  -1.214  43.941  1.00 20.00      c    c
ATOM   8374  CD1 ILE I 206      10.200  -1.220  45.389  1.00 20.00      c    c
ATOM   8375  CG2 ILE I 206       8.656   1.047  43.966  1.00 20.00      c    c
ATOM   8376  C   ILE I 206       9.175   1.484  41.253  1.00 62.35      c    c
ATOM   8377  O   ILE I 206      10.081   2.268  40.973  1.00 67.16      C    0
ATOM   8378  N   VAL I 207       7.894   1.749  41.015  1.00 52.22      c    N
ATOM   8379  CA  VAL I 207       7.461   3.050  40.521  1.00 51.31      c    c
ATOM   8380  CB  VAL I 207       6.469   2.918  39.345  1.00 20.00      c    c
ATOM   8381  CGI VAL I 207       5.891   4.279  38.984  1.00 20.00      c    c
ATOM   8382  CG2 VAL I 207       7.149   2.291  38.139  1.00 20.00      c    c
ATOM   8383  C   VAL I 207       6.800   3.846  41.634  1.00 62.09      c    c
ATOM   8384  O   VAL I 207       5.644   3.607  41.980  1.00 58.88      c    o
ATOM   8385  N   ASN I 208       7.557   4.759  42.229  1.00 71.72      c    N
```

ATOM 8386 CA ASN I 208 7.023 5.625 43.267 1.00 70.92 C c
ATOM 8387 CB ASN I 208 8.004 5.721 44.433 1.00 20.00 c c
ATOM 8388 CG ASN I 208 8.100 4.428 45.222 1.00 20.00 c c
ATOM 8389 OD1 ASN I 208 7.170 3.620 45.228 1.00 20.00 c o
ATOM 8390 ND2 ASN I 208 9.234 4.221 45.884 1.00 20.00 c N
ATOM 8391 C ASN I 208 6.699 7.015 42.735 1.00 63.05 c c
ATOM 8392 O ASN I 208 6.780 7.264 41.532 1.00 61.34 c o
ATOM 8393 N LYS I 209 6.391 7.933 43.645 1.00 68.91 c N
ATOM 8394 CA LYS I 209 5.953 9.273 43.274 1.00 59.11 c c
ATOM 8395 CB LYS I 209 5.349 9.992 44.482 1.00 20.00 c c
ATOM 8396 CG LYS I 209 4.044 9.391 44.979 1.00 20.00 c c
ATOM 8397 CD LYS I 209 3.507 10.158 46.179 1.00 20.00 c c
ATOM 8398 CE LYS I 209 2.159 9.612 46.629 1.00 20.00 c c
ATOM 8399 NZ LYS I 209 1.583 10.385 47.765 1.00 20.00 c N
ATOM 8400 C LYS I 209 7.100 10.100 42.702 1.00 50.69 c c
ATOM 8401 O LYS I 209 6.883 11.178 42.152 1.00 51.01 c o
ATOM 8402 N GLN I 210 8.326 9.638 42.920 1.00 44.68 c N
ATOM 8403 CA GLN I 210 9.495 10.293 42.349 1.00 49.52 c c
ATOM 8404 CB GLN I 210 10.724 10.052 43.223 1.00 20.00 c c
ATOM 8405 CG GLN I 210 10.667 10.739 44.573 1.00 20.00 c c
ATOM 8406 CD GLN I 210 11.865 10.409 45.435 1.00 20.00 c c
ATOM 8407 OE1 GLN I 210 12.517 9.385 45.239 1.00 20.00 c o
ATOM 8408 NE2 GLN I 210 12.173 11.286 46.383 1.00 20.00 C N
ATOM 8409 C GLN I 210 9.755 9.786 40.938 1.00 62.08 c c
ATOM 8410 O GLN I 210 9.786 10.560 39.983 1.00 80.43 c o
ATOM 8411 N SER I 211 9.902 8.472 40.813 1.00 58.92 c N
ATOM 8412 CA SER I 211 10.076 7.840 39.514 1.00 47.88 c c
ATOM 8413 CB SER I 211 9.987 6.319 39.647 1.00 20.00 c c
ATOM 8414 OG SER I 211 8.735 5.930 40.184 1.00 20.00 c o
ATOM 8415 C SER I 211 9.050 8.344 38.503 1.00 57.32 c c
ATOM 8416 O SER I 211 9.372 8.538 37.331 1.00 50.74 c o
ATOM 8417 N CYS I 212 7.845 8.647 38.979 1.00 44.34 c N
ATOM 8418 CA CYS I 212 6.690 8.758 38.095 1.00 57.52 c c
ATOM 8419 CB CYS I 212 5.453 9.307 38.834 1.00 20.00 c c
ATOM 8420 SG CYS I 212 4.771 8.198 40.141 1.00 20.00 c s
ATOM 8421 C CYS I 212 7.005 9.537 36.808 1.00 60.91 c c
ATOM 8422 O CYS I 212 6.991 8.952 35.727 1.00 52.17 c o
ATOM 8423 N SER I 213 7.305 10.827 36.916 1.00 21.55 c N
ATOM 8424 CA SER I 213 7.501 11.624 35.711 1.00 21.67 c c
ATOM 8425 CB SER I 213 7.747 13.090 36.075 1.00 21.81 c c
ATOM 8426 OG SER I 213 6.648 13.630 36.788 1.00 23.00 c o
ATOM 8427 C SER I 213 8.650 11.098 34.858 1.00 21.45 c c
ATOM 8428 O SER I 213 8.509 10.969 33.640 1.00 21.98 c o
ATOM 8429 N ILE I 214 9.775 10.772 35.484 1.00 20.90 c N
ATOM 8430 CA ILE I 214 10.875 10.168 34.746 1.00 20.45 c c
ATOM 8431 CB ILE I 214 12.127 10.002 35.624 1.00 20.53 c c
ATOM 8432 CGI ILE I 214 12.599 11.363 36.141 1.00 20.46 c c
ATOM 8433 CD1 ILE I 214 13.831 11.289 37.016 1.00 21.75 c c
ATOM 8434 CG2 ILE I 214 13.235 9.309 34.846 1.00 20.34 c c
ATOM 8435 C ILE I 214 10.423 8.802 34.247 1.00 20.15 c c
ATOM 8436 O ILE I 214 10.647 8.427 33.090 1.00 19.91 c o
ATOM 8437 N SER I 215 9.751 8.075 35.136 1.00 19.84 c N
ATOM 8438 CA SER I 215 9.240 6.749 34.827 1.00 19.58 c c
ATOM 8439 CB SER I 215 8.632 6.104 36.073 1.00 19.76 c c
ATOM 8440 OG SER I 215 8.132 4.810 35.785 1.00 19.97 c o
ATOM 8441 C SER I 215 8.201 6.841 33.724 1.00 19.34 c c
ATOM 8442 O SER I 215 8.172 6.013 32.818 1.00 19.54 c o
ATOM 8443 N ASN I 216 7.351 7.858 33.804 1.00 18.80 c N
ATOM 8444 CA ASN I 216 6.324 8.059 32.796 1.00 18.36 c c
ATOM 8445 CB ASN I 216 5.406 9.218 33.187 1.00 18.41 c c

ATOM 8446 CG ASN I 216 4.701 8.983 34.508 1.00 19.55 C c
ATOM 8447 OD1 ASN I 216 3.922 9.819 34.967 1.00 20.52 c o
ATOM 8448 ND2 ASN I 216 4.971 7.840 35.128 1.00 20.43 c N
ATOM 8449 C ASN I 216 6.958 8.324 31.440 1.00 17.78 c c
ATOM 8450 O ASN I 216 6.509 7.800 30.421 1.00 17.91 c o
ATOM 8451 N ILE I 217 8.016 9.130 31.433 1.00 17.02 C N
ATOM 8452 CA ILE I 217 8.714 9.439 30.194 1.00 16.60 c c
ATOM 8453 CB ILE I 217 9.833 10.472 30.417 1.00 16.46 c c
ATOM 8454 CGI ILE I 217 9.252 11.776 30.969 1.00 16.26 c c
ATOM 8455 CD1 ILE I 217 10.289 12.849 31.217 1.00 16.44 c c
ATOM 8456 CG2 ILE I 217 10.589 10.727 29.122 1.00 16.70 c c
ATOM 8457 C ILE I 217 9.314 8.168 29.609 1.00 16.73 c c
ATOM 8458 O ILE I 217 9.247 7.931 28.398 1.00 16.80 c o
ATOM 8459 N GLU I 218 9.885 7.339 30.478 1.00 17.02 c N
ATOM 8460 CA GLU I 218 10.485 6.090 30.031 1.00 17.70 c c
ATOM 8461 CB GLU I 218 11.172 5.376 31.197 1.00 18.20 c c
ATOM 8462 CG GLU I 218 12.289 6.178 31.844 1.00 21.31 c c
ATOM 8463 CD GLU I 218 12.951 5.437 32.989 1.00 25.72 c c
ATOM 8464 OE1 GLU I 218 13.884 5.998 33.602 1.00 26.96 c o
ATOM 8465 OE2 GLU I 218 12.538 4.294 33.277 1.00 27.07 c o
ATOM 8466 C GLU I 218 9.419 5.192 29.418 1.00 17.29 c c
ATOM 8467 O GLU I 218 9.642 4.555 28.387 1.00 17.62 c o
ATOM 8468 N THR I 219 8.253 5.156 30.055 1.00 16.62 c N
ATOM 8469 CA THR I 219 7.146 4.342 29.577 1.00 15.95 c c
ATOM 8470 CB THR I 219 5.952 4.387 30.547 1.00 15.95 c c
ATOM 8471 OG1 THR I 219 6.356 3.894 31.831 1.00 15.63 c o
ATOM 8472 CG2 THR I 219 4.806 3.536 30.021 1.00 15.97 c c
ATOM 8473 C THR I 219 6.696 4.825 28.207 1.00 15.64 c c
ATOM 8474 O THR I 219 6.414 4.022 27.321 1.00 15.93 c o
ATOM 8475 N VAL I 220 6.639 6.141 28.037 1.00 14.98 c N
ATOM 8476 CA VAL I 220 6.235 6.720 26.764 1.00 14.51 c c
ATOM 8477 CB VAL I 220 6.143 8.254 26.844 1.00 14.29 c c
ATOM 8478 CGI VAL I 220 5.716 8.830 25.502 1.00 14.24 c c
ATOM 8479 CG2 VAL I 220 5.176 8.671 27.942 1.00 14.10 c c
ATOM 8480 C VAL I 220 7.233 6.334 25.682 1.00 14.64 c c
ATOM 8481 O VAL I 220 6.850 5.992 24.560 1.00 14.79 c o
ATOM 8482 N ILE I 221 8.516 6.375 26.028 1.00 14.43 C N
ATOM 8483 CA ILE I 221 9.556 6.013 25.075 1.00 14.36 c c
ATOM 8484 CB ILE I 221 10.962 6.235 25.661 1.00 14.03 c c
ATOM 8485 CGI ILE I 221 11.156 7.704 26.041 1.00 13.72 c c
ATOM 8486 CD1 ILE I 221 11.011 8.660 24.877 1.00 14.17 c c
ATOM 8487 CG2 ILE I 221 12.027 5.791 24.671 1.00 13.91 c c
ATOM 8488 C ILE I 221 9.404 4.552 24.672 1.00 14.82 c c
ATOM 8489 O ILE I 221 9.531 4.204 23.496 1.00 14.82 c o
ATOM 8490 N GLU I 222 9.112 3.703 25.652 1.00 15.51 c N
ATOM 8491 CA GLU I 222 8.936 2.281 25.392 1.00 16.52 c c
ATOM 8492 CB GLU I 222 8.730 1.517 26.701 1.00 16.80 c c
ATOM 8493 CG GLU I 222 9.889 1.635 27.677 1.00 19.14 c c
ATOM 8494 CD GLU I 222 9.653 0.861 28.959 1.00 22.62 c c
ATOM 8495 OE1 GLU I 222 10.539 0.882 29.840 1.00 24.35 c o
ATOM 8496 OE2 GLU I 222 8.583 0.230 29.086 1.00 23.98 c o
ATOM 8497 C GLU I 222 7.750 2.064 24.464 1.00 16.65 c c
ATOM 8498 O GLU I 222 7.802 1.238 23.553 1.00 16.95 c o
ATOM 8499 N PHE I 223 6.681 2.817 24.701 1.00 16.70 c N
ATOM 8500 CA PHE I 223 5.482 2.717 23.885 1.00 16.95 c c
ATOM 8501 CB PHE I 223 4.370 3.600 24.453 1.00 16.85 c c
ATOM 8502 CG PHE I 223 3.058 3.460 23.736 1.00 17.23 c c
ATOM 8503 CD1 PHE I 223 2.127 2.519 24.145 1.00 17.98 c c
ATOM 8504 CE1 PHE I 223 0.919 2.387 23.488 1.00 18.28 c c
ATOM 8505 CZ PHE I 223 0.629 3.199 22.409 1.00 18.19 c c

ATOM 8506 CE2 PHE I 223 1.548 4.140 21.991 1.00 18.14 C C
ATOM 8507 CD2 PHE I 223 2.755 4.267 22.653 1.00 17.75 C C
ATOM 8508 C PHE 1223 5.790 3.119 22.450 1.00 17.28 C C
ATOM 8509 O PHE 1223 5.324 2.482 21.506 1.00 17.17 C O
ATOM 8510 N GLN 1224 6.581 4.175 22.287 1.00 17.62 C N
ATOM 8511 CA GLN 1224 6.954 4.619 20.952 1.00 18.16 C C
ATOM 8512 CB GLN 1224 7.759 5.918 21.021 1.00 18.51 C C
ATOM 8513 CG GLN 1224 7.015 7.075 21.669 1.00 20.06 C C
ATOM 8514 CD GLN 1224 7.842 8.344 21.718 1.00 22.03 C C
ATOM 8515 OE1 GLN 1224 7.387 9.376 22.214 1.00 22.15 C O
ATOM 8516 NE2 GLN I 224 9.064 8.275 21.203 1.00 22.11 C N
ATOM 8517 C GLN 1224 7.767 3.532 20.261 1.00 18.04 C C
ATOM 8518 O GLN 1224 7.561 3.238 19.083 1.00 18.17 C O
ATOM 8519 N GLN 1225 8.688 2.933 21.009 1.00 17.90 C N
ATOM 8520 CA GLN 1225 9.508 1.840 20.500 1.00 17.95 C C
ATOM 8521 CB GLN 1225 10.599 1.474 21.509 1.00 18.13 C C
ATOM 8522 CG GLN 1225 11.551 2.613 21.833 1.00 19.04 C C
ATOM 8523 CD GLN 1225 12.619 2.213 22.831 1.00 21.22 C C
ATOM 8524 OE1 GLN 1225 12.659 1.072 23.292 1.00 22.55 C O
ATOM 8525 NE2 GLN 1225 13.493 3.154 23.172 1.00 22.48 C N
ATOM 8526 C GLN 1225 8.664 0.611 20.172 1.00 17.84 C C
ATOM 8527 O GLN 1225 8.892 -0.068 19.171 1.00 17.71 C O
ATOM 8528 N LYS 1226 7.693 0.334 21.036 1.00 17.95 C N
ATOM 8529 CA LYS 1226 6.848 -0.831 20.912 1.00 18.00 C C
ATOM 8530 CB LYS 1226 6.821 -1.593 22.234 1.00 18.21 C C
ATOM 8531 CG LYS 1226 8.189 -1.697 22.905 1.00 18.50 C C
ATOM 8532 CD LYS 1226 8.132 -2.591 24.132 1.00 19.87 C C
ATOM 8533 CE LYS 1226 9.357 -2.411 25.004 1.00 21.36 C C
ATOM 8534 NZ LYS 1226 9.268 -3.230 26.248 1.00 21.83 C N
ATOM 8535 C LYS 1226 5.446 -0.408 20.499 1.00 17.84 C C
ATOM 8536 O LYS 1226 4.672 -1.220 19.998 1.00 17.94 C O
ATOM 8537 N ASN 1227 5.209 0.900 20.514 1.00 17.70 C N
ATOM 8538 CA ASN 1227 4.173 1.494 19.683 1.00 17.66 C C
ATOM 8539 CB ASN 1227 3.153 2.256 20.549 1.00 17.36 C C
ATOM 8540 CG ASN 1227 2.612 1.411 21.710 1.00 17.40 C C
ATOM 8541 OD1 ASN 1227 2.451 0.196 21.589 1.00 17.84 C O
ATOM 8542 ND2 ASN I 227 2.333 2.059 22.834 1.00 17.22 C N
ATOM 8543 C ASN 1227 4.713 2.343 18.506 1.00 17.76 C C
ATOM 8544 O ASN 1227 3.943 2.750 17.635 1.00 17.92 C O
ATOM 8545 N ASN 1228 6.045 2.460 18.398 1.00 17.78 C N
ATOM 8546 CA ASN 1228 6.734 2.532 17.084 1.00 17.59 C C
ATOM 8547 CB ASN 1228 8.170 3.085 17.155 1.00 17.89 C C
ATOM 8548 CG ASN 1228 8.870 3.082 15.779 1.00 18.43 C C
ATOM 8549 OD1 ASN 1228 9.451 2.077 15.366 1.00 18.74 C O
ATOM 8550 ND2 ASN I 228 8.682 4.157 15.022 1.00 18.61 C N
ATOM 8551 C ASN 1228 6.765 1.204 16.358 1.00 17.09 C C
ATOM 8552 O ASN 1228 6.004 0.992 15.417 1.00 17.17 C O
ATOM 8553 N ARG 1229 7.685 0.328 16.745 1.00 16.33 C N
ATOM 8554 CA ARG 1229 7.664 -1.016 16.195 1.00 15.76 C C
ATOM 8555 CB ARG 1229 8.624 -1.952 16.933 1.00 15.70 C C
ATOM 8556 CG ARG 1229 9.369 -2.904 16.000 1.00 14.99 C C
ATOM 8557 CD ARG 1229 9.887 -4.135 16.728 1.00 15.33 C C
ATOM 8558 NE ARG 1229 9.601 -5.376 16.008 1.00 15.59 C N
ATOM 8559 CZ ARG 1229 9.926 -6.587 16.451 1.00 15.85 C C
ATOM 8560 NH1 ARG 1229 10.559 -6.725 17.609 1.00 16.20 C N
ATOM 8561 NH2 ARG 1229 9.650 -7.660 15.722 1.00 16.63 C N
ATOM 8562 C ARG 1229 6.238 -1.559 16.223 1.00 15.62 C C
ATOM 8563 O ARG 1229 5.666 -1.860 15.175 1.00 15.73 C O
ATOM 8564 N LEU 1230 5.601 -1.468 17.387 1.00 15.46 C N
ATOM 8565 CA LEU 1230 4.191 -1.829 17.511 1.00 15.22 C C

ATOM 8566 CB LEU I 230 3.735 -1.792 18.974 1.00 15.08 C c
ATOM 8567 CG LEU I 230 2.252 -2.079 19.224 1.00 14.70 c c
ATOM 8568 CD1 LEU I 230 2.003 -3.572 19.359 1.00 15.19 c c
ATOM 8569 CD2 LEU I 230 1.743 -1.335 20.449 1.00 15.46 c c
ATOM 8570 C LEU I 230 3.302 -0.931 16.655 1.00 15.31 c c
ATOM 8571 O LEU I 230 2.417 -1.415 15.950 1.00 15.46 c o
ATOM 8572 N LEU I 231 3.519 0.377 16.745 1.00 15.48 c N
ATOM 8573 CA LEU I 231 2.678 1.338 16.038 1.00 15.75 c c
ATOM 8574 CB LEU I 231 3.187 2.763 16.257 1.00 15.90 c c
ATOM 8575 CG LEU I 231 2.906 3.379 17.628 1.00 16.63 c c
ATOM 8576 CD1 LEU I 231 3.382 4.819 17.676 1.00 18.45 c c
ATOM 8577 CD2 LEU I 231 1.425 3.292 17.961 1.00 16.67 c c
ATOM 8578 C LEU I 231 2.653 1.025 14.551 1.00 15.76 c c
ATOM 8579 O LEU I 231 1.606 1.092 13.908 1.00 15.84 c o
ATOM 8580 N GLU I 232 3.828 0.750 13.997 1.00 15.71 c N
ATOM 8581 CA GLU I 232 3.973 0.563 12.562 1.00 15.93 c c
ATOM 8582 CB GLU I 232 5.447 0.626 12.163 1.00 16.15 c c
ATOM 8583 CG GLU I 232 6.142 1.913 12.568 1.00 18.59 c c
ATOM 8584 CD GLU I 232 6.407 2.823 11.387 1.00 21.47 c c
ATOM 8585 OE1 GLU I 232 5.892 2.532 10.286 1.00 22.14 c o
ATOM 8586 OE2 GLU I 232 7.214 3.765 11.530 1.00 23.34 c o
ATOM 8587 C GLU I 232 3.377 -0.767 12.124 1.00 15.45 c c
ATOM 8588 O GLU I 232 2.921 -0.908 10.990 1.00 15.95 c o
ATOM 8589 N ILE I 233 3.432 -1.757 13.007 1.00 14.54 C N
ATOM 8590 CA ILE I 233 2.713 -3.000 12.776 1.00 13.69 c c
ATOM 8591 CB ILE I 233 2.998 -4.028 13.873 1.00 13.63 c c
ATOM 8592 CGI ILE I 233 4.500 -4.093 14.151 1.00 13.58 c c
ATOM 8593 CD1 ILE I 233 4.854 -4.786 15.444 1.00 13.55 c c
ATOM 8594 CG2 ILE I 233 2.458 -5.392 13.469 1.00 13.88 c c
ATOM 8595 C ILE I 233 1.219 -2.728 12.735 1.00 13.28 c c
ATOM 8596 O ILE I 233 0.528 -3.137 11.802 1.00 13.04 C O
ATOM 8597 N THR I 234 0.764 -1.898 13.667 1.00 13.18 c N
ATOM 8598 CA THR I 234 -0.651 -1.590 13.796 1.00 13.39 c c
ATOM 8599 CB THR I 234 -0.913 -0.636 14.974 1.00 13.21 c c
ATOM 8600 OG1 THR I 234 -0.476 -1.248 16.193 1.00 13.15 c: o
ATOM 8601 CG2 THR I 234 -2.395 -0.311 15.078 1.00 13.22 c c
ATOM 8602 C THR I 234 -1.208 -0.981 12.514 1.00 13.76 c c
ATOM 8603 O THR I 234 -2.230 -1.432 11.997 1.00 13.95 c o
ATOM 8604 N ARG I 235 -0.535 0.045 12.003 1.00 14.26 c N
ATOM 8605 CA ARG I 235 -0.945 0.670 10.752 1.00 14.92 c c
ATOM 8606 CB ARG I 235 -0.051 1.874 10.432 1.00 15.30 c c
ATOM 8607 CG ARG I 235 0.875 1.681 9.240 1.00 16.27 c c
ATOM 8608 CD ARG I 235 2.190 2.436 9.413 1.00 18.52 c c
ATOM 8609 NE ARG I 235 2.083 3.558 10.344 1.00 17.86 c N
ATOM 8610 CZ ARG I 235 1.516 4.724 10.051 1.00 16.91 c c
ATOM 8611 NH1 ARG I 235 0.855 4.874 8.912 1.00 16.59 c N
ATOM 8612 NH2 ARG I 235 1.511 5.703 10.946 1.00 16.86 c N
ATOM 8613 C ARG I 235 -0.904 -0.353 9.620 1.00 15.05 c c
ATOM 8614 O ARG I 235 -1.939 -0.693 9.045 1.00 15.15 c o
ATOM 8615 N GLU I 236 0.240 -1.020 9.504 1.00 15.18 c N
ATOM 8616 CA GLU I 236 0.451 -2.047 8.490 1.00 15.24 c c
ATOM 8617 CB GLU I 236 1.725 -2.835 8.801 1.00 15.69 c c
ATOM 8618 CG GLU I 236 2.432 -3.396 7.580 1.00 18.22 c c
ATOM 8619 CD GLU I 236 3.760 -4.040 7.926 1.00 21.59 c c
ATOM 8620 OE1 GLU I 236 4.381 -4.645 7.027 1.00 24.41 c o
ATOM 8621 OE2 GLU I 236 4.182 -3.944 9.097 1.00 21.59 c o
ATOM 8622 C GLU I 236 -0.735 -2.999 8.400 1.00 14.61 c c
ATOM 8623 O GLU I 236 -1.191 -3.334 7.307 1.00 14.82 c o
ATOM 8624 N PHE I 237 -1.184 -3.485 9.552 1.00 14.05 c N
ATOM 8625 CA PHE I 237 -2.318 -4.397 9.602 1.00 13.84 c c

ATOM 8626 CB PHE 1237 -2.466 -4.996 11.003 1.00 14.04 C C
ATOM 8627 CG PHE 1237 -1.643 -6.235 11.225 1.00 14.84 C C
ATOM 8628 CD1 PHE I 237 -0.734 -6.296 12.267 1.00 15.30 C C
ATOM 8629 CE1 PHE I 237 -0.006 -7.446 12.503 1.00 15.15 C C
ATOM 8630 CZ PHE 1237 -0.197 -8.557 11.708 1.00 15.19 C C
ATOM 8631 CE2 PHE I 237 -1.110 -8.514 10.673 1.00 15.02 C C
ATOM 8632 CD2 PHE I 237 -1.831 -7.360 10.439 1.00 15.03 C C
ATOM 8633 C PHE 1237 -3.607 -3.689 9.195 1.00 13.51 C C
ATOM 8634 O PHE 1237 -4.387 -4.213 8.399 1.00 13.43 C O
ATOM 8635 N SER I 238 -3.830 -2.503 9.754 1.00 13.11 C N
ATOM 8636 CA SER I 238 -5.032 -1.729 9.460 1.00 12.82 C C
ATOM 8637 CB SER I 238 -5.049 -0.438 10.279 1.00 12.86 C C
ATOM 8638 OG SER 1238 -5.205 -0.711 11.660 1.00 12.76 C O
ATOM 8639 C SER 1238 -5.104 -1.400 7.977 1.00 12.69 C C
ATOM 8640 O SER 1238 -6.187 -1.237 7.414 1.00 12.63 C O
ATOM 8641 N VAL 1239 -3.937 -1.313 7.349 1.00 12.59 C N
ATOM 8642 CA VAL 1239 -3.858 -1.042 5.923 1.00 12.80 C C
ATOM 8643 CB VAL 1239 -2.482 -0.473 5.524 1.00 12.71 C C
ATOM 8644 CGI VAL 1239 -2.390 -0.321 4.012 1.00 13.63 C C
ATOM 8645 CG2 VAL 1239 -2.239 0.859 6.214 1.00 13.57 C C
ATOM 8646 C VAL 1239 -4.144 -2.286 5.090 1.00 12.94 C C
ATOM 8647 O VAL 1239 -4.320 -2.190 3.877 1.00 13.10 C O
ATOM 8648 N ASN 1240 -4.139 -3.458 5.721 1.00 4.15 C N
ATOM 8649 CA ASN 1240 -4.166 -4.709 4.966 1.00 4.33 C C
ATOM 8650 CB ASN 1240 -2.941 -5.569 5.281 1.00 4.59 C C
ATOM 8651 CG ASN 1240 -1.674 -5.027 4.647 1.00 5.36 C C
ATOM 8652 OD1 ASN 1240 -1.524 -5.043 3.423 1.00 6.27 C O
ATOM 8653 ND2 ASN I 240 -0.816 -4.427 5.465 1.00 7.15 C N
ATOM 8654 C ASN 1240 -5.454 -5.529 5.074 1.00 4.19 C C
ATOM 8655 O ASN 1240 -5.634 -6.507 4.347 1.00 4.19 C O
ATOM 8656 N ALA 1241 -6.385 -5.073 5.904 1.00 3.93 C N
ATOM 8657 CA ALA 1241 -7.593 -5.840 6.186 1.00 3.90 C C
ATOM 8658 CB ALA 1241 -8.563 -5.749 5.020 1.00 3.86 C C
ATOM 8659 C ALA 1241 -7.253 -7.297 6.491 1.00 4.22 C C
ATOM 8660 O ALA 1241 -7.778 -8.212 5.856 1.00 4.47 C O
ATOM 8661 N GLY 1242 -6.289 -7.497 7.386 1.00 4.53 C N
ATOM 8662 CA GLY 1242 -6.124 -8.774 8.078 1.00 4.65 C C
ATOM 8663 C GLY 1242 -5.398 -9.848 7.282 1.00 4.67 C C
ATOM 8664 O GLY 1242 -5.496 -11.034 7.600 1.00 5.27 C O
ATOM 8665 N VAL 1243 -4.611 -9.433 6.292 1.00 4.37 C N
ATOM 8666 CA VAL 1243 -3.780 -10.366 5.531 1.00 4.32 C C
ATOM 8667 CB VAL 1243 -4.570 -11.042 4.389 1.00 3.99 C C
ATOM 8668 CGI VAL 1243 -3.987 -12.411 4.078 1.00 4.22 C C
ATOM 8669 CG2 VAL 1243 -6.042 -11.154 4.748 1.00 3.85 C C
ATOM 8670 C VAL 1243 -2.571 -9.658 4.932 1.00 4.61 C C
ATOM 8671 O VAL 1243 -2.704 -8.607 4.308 1.00 4.89 C O
ATOM 8672 N THR 1244 -1.402 -10.269 5.072 1.00 4.95 C N
ATOM 8673 CA THR 1244 -0.168 -9.654 4.604 1.00 5.71 C C
ATOM 8674 CB THR 1244 0.678 -9.128 5.775 1.00 6.11 C C
ATOM 8675 OG1 THR I 244 -0.078 -9.209 6.989 1.00 7.17 C O
ATOM 8676 CG2 THR 1244 1.091 -7.686 5.532 1.00 7.55 C C
ATOM 8677 C THR 1244 0.664 -10.649 3.813 1.00 5.61 C C
ATOM 8678 O THR 1244 0.811 -11.803 4.214 1.00 5.85 C O
ATOM 8679 N THR 1245 1.346 -10.150 2.791 1.00 5.53 C N
ATOM 8680 CA THR 1245 2.556 -10.791 2.308 1.00 5.81 C C
ATOM 8681 CB THR 1245 2.426 -11.170 0.818 1.00 6.13 C C
ATOM 8682 OG1 THR 1245 1.421 -12.181 0.668 1.00 8.11 C O
ATOM 8683 CG2 THR 1245 3.746 -11.696 0.281 1.00 6.63 C C
ATOM 8684 C THR 1245 3.748 -9.865 2.542 1.00 5.73 C C
ATOM 8685 O THR 1245 3.568 -8.705 2.916 1.00 5.86 C O

```
ATOM   8686  N   PRO I 246      4.963 -10.337   2.223  1.00  5.68      C    N
ATOM   8687  CA  PRO I 246      5.942 -10.579   3.269  1.00  5.1 1      c    c
ATOM   8688  CB  PRO I 246      6.802  -9.317   3.210  1.00  5.19      c    c
ATOM   8689  CG  PRO I 246      6.717  -8.878   1.734  1.00  5.90      c    c
ATOM   8690  CD  PRO I 246      5.613  -9.691   1.074  1.00  6.36      c    c
ATOM   8691  C   PRO I 246      5.360 -10.786   4.664  1.00  4.85      c    c
ATOM   8692  O   PRO I 246      4.465 -10.053   5.084  1.00  5.25      c    o
ATOM   8693  N   VAL I 247      5.795 -11.859   5.316  1.00  4.35      c    N
ATOM   8694  CA  VAL I 247      5.555 -12.048   6.739  1.00  3.82      c    c
ATOM   8695  CB  VAL I 247      5.603 -13.536   7.127  1.00  3.52      c    c
ATOM   8696  CGI VAL I 247      5.206 -13.717   8.584  1.00  3.62      c    c
ATOM   8697  CG2 VAL I 247      4.694 -14.347   6.218  1.00  3.60      c    c
ATOM   8698  C   VAL I 247      6.576 -11.271   7.558  1.00  3.69      c    c
ATOM   8699  O   VAL I 247      7.744 -11.653   7.641  1.00  3.36      c    o
ATOM   8700  N   SER I 248      6.172 -10.077   7.973  1.00  3.72      c    N
ATOM   8701  CA  SER I 248      7.077  -9.138   8.61 1  1.00  3.96      c    c
ATOM   8702  CB  SER I 248      6.291  -7.973   9.214  1.00  4.07      c    c
ATOM   8703  OG  SER I 248      5.661  -8.356  10.425  1.00  4.13      c    o
ATOM   8704  C   SER I 248      7.885  -9.830   9.695  1.00  4.35      c    c
ATOM   8705  O   SER I 248      7.453 -10.838  10.257  1.00  4.36      c    o
ATOM   8706  N   THR I 249      9.008  -9.223  10.057  1.00  4.53      c    N
ATOM   8707  CA  THR I 249      9.752  -9.638  11.235  1.00  4.61      c    c
ATOM   8708  CB  THR I 249     11.104  -8.916  11.329  1.00  4.70      c    c
ATOM   8709  OG1 THR I 249     10.889  -7.544  11.679  1.00  5.42      c:   o
ATOM   8710  CG2 THR I 249     11.833  -8.984   9.999  1.00  4.88      c    c
ATOM   871 1 C   THR I 249      8.955  -9.383  12.509  1.00  4.47      c    c
ATOM   8712  O   THR I 249      9.321  -9.861  13.584  1.00  4.74      c    o
ATOM   8713  N   TYR I 250      7.864  -8.633  12.388  1.00  4.32      c    N
ATOM   8714  CA  TYR I 250      6.956  -8.435  13.512  1.00  4.42      c    c
ATOM   8715  CB  TYR I 250      6.195  -7.1 13  13.381  1.00  4.91      c    c
ATOM   8716  CG  TYR I 250      7.072  -5.881  13.272  1.00  6.81      c    c
ATOM   8717  CD1 TYR I 250      6.791  -4.897  12.333  1.00  8.89      c    c
ATOM   8718  CE1 TYR I 250      7.556  -3.752  12.243  1.00 10.73      c    c
ATOM   8719  CZ  TYR I 250      8.587  -3.549  13.137  1.00 12.28      c    c
ATOM   8720  OH  TYR I 250      9.370  -2.421  13.032  1.00 12.24      c    o
ATOM   8721  CE2 TYR I 250      8.851  -4.483  14. 121  1.00 12.15      c    c
ATOM   8722  CD2 TYR I 250      8.067  -5.621  14.209  1.00  9.81      c    c
ATOM   8723  C   TYR I 250      5.973  -9.592  13.662  1.00  4.21      c    c
ATOM   8724  O   TYR I 250      5.525  -9.893  14.768  1.00  4.20      c    o
ATOM   8725  N   MET I 251      5.574 -10.183  12.541  1.00  4.14      c    N
ATOM   8726  CA  MET I 251      4.731 -11.372  12.574  1.00  4.15      c    c
ATOM   8727  CB  MET I 251      4.160 -11.662  11.187  1.00  4.14      c    c
ATOM   8728  CG  MET I 251      3.297 -10.547  10.630  1.00  4.51      c    c
ATOM   8729  SD  MET I 251      1.731 -10.386  11.505  1.00  3.81      c    s
ATOM   8730  CE  MET I 251      0.800  -9.412  10.327  1.00  4.55      c    c
ATOM   8731  C   MET I 251      5.540 -12.565  13.057  1.00  4.13      c    c
ATOM   8732  O   MET I 251      5.127 -13.289  13.964  1.00  4.24      c    o
ATOM   8733  N   LEU I 252      6.728 -12.718  12.487  1.00  4.23      c    N
ATOM   8734  CA  LEU I 252      7.586 -13.848  12.792  1.00  4.22      c    c
ATOM   8735  CB  LEU I 252      7.586 -14.839  11.631  1.00  4.14      c    c
ATOM   8736  CG  LEU I 252      6.703 -16.071  11.816  1.00  4.05      c    c
ATOM   8737  CD1 LEU I 252      7.171 -17.204  10.918  1.00  5.22      c    c
ATOM   8738  CD2 LEU I 252      6.692 -16.508  13.273  1.00  6.20      c    c
ATOM   8739  C   LEU I 252      8.998 -13.356  13.040  1.00  4.62      c    c
ATOM   8740  O   LEU I 252      9.599 -12.712  12. 182  1.00  4.97      c    o
ATOM   8741  N   THR I 253      9.531 -13.670  14.212  1.00  4.90      c    N
ATOM   8742  CA  THR I 253     10.942 -13.463  14.472  1.00  5.57      c    c
ATOM   8743  CB  THR I 253     11.265 -13.708  15.946  1.00  5.55      c    c
ATOM   8744  OG1 THR I 253     10.337 -12.987  16.765  1.00  6.43      C    O
ATOM   8745  CG2 THR I 253     12.673 -13.251  16.259  1.00  6.28      C    C
```

ATOM 8746 C THR I 253 11.753 -14.424 13.622 1.00 6.03 C c
ATOM 8747 O THR I 253 11.315 -15.541 13.349 1.00 6.68 c o
ATOM 8748 N ASN I 254 12.961 -14.015 13.255 1.00 6.39 c N
ATOM 8749 CA ASN I 254 13.951 -14.973 12.800 1.00 6.79 c c
ATOM 8750 CB ASN I 254 15.341 -14.348 12.762 1.00 6.85 c c
ATOM 8751 CG ASN I 254 16.324 -15.177 11.964 1.00 6.81 c c
ATOM 8752 OD1 ASN I 254 16.152 -15.366 10.760 1.00 7.67 c o
ATOM 8753 ND2 ASN I 254 17.271 -15.799 12.657 1.00 6.19 c N
ATOM 8754 C ASN I 254 13.964 -16.21 1 13.686 1.00 7.08 c c
ATOM 8755 O ASN I 254 13.654 -17.312 13.231 1.00 6.90 c o
ATOM 8756 N SER I 255 14.283 -16.017 14.962 1.00 7.21 c N
ATOM 8757 CA SER I 255 14.292 -17.1 12 15.929 1.00 7.37 c c
ATOM 8758 CB SER I 255 14.338 -16.568 17.360 1.00 8.09 c c
ATOM 8759 OG SER I 255 14.953 -15.293 17.407 1.00 10.47 c o
ATOM 8760 C SER I 255 13.078 -18.024 15.750 1.00 6.82 c c
ATOM 8761 O SER I 255 13.205 -19.249 15.768 1.00 6.99 c o
ATOM 8762 N GLU I 256 11.901 -17.422 15.61 1 1.00 6.17 c N
ATOM 8763 CA GLU I 256 10.658 -18.184 15.544 1.00 6.13 c c
ATOM 8764 CB GLU I 256 9.452 -17.266 15.742 1.00 6.22 c c
ATOM 8765 CG GLU I 256 9.210 -16.863 17.185 1.00 8.41 c c
ATOM 8766 CD GLU I 256 8.527 -15.516 17.299 1.00 10.26 c c
ATOM 8767 OE1 GLU I 256 8.232 -14.907 16.248 1.00 11.90 c o
ATOM 8768 OE2 GLU I 256 8.275 -15.070 18.437 1.00 9.55 c o
ATOM 8769 C GLU I 256 10.535 -18.895 14.209 1.00 5.76 c c
ATOM 8770 O GLU I 256 10.154 -20.064 14. 154 1.00 5.93 c o
ATOM 8771 N LEU I 257 10.669 -18. 124 13. 134 1.00 5.67 c N
ATOM 8772 CA LEU I 257 10.638 -18.679 11.787 1.00 5.37 c c
ATOM 8773 CB LEU I 257 11.010 -17.613 10.753 1.00 5.03 c c
ATOM 8774 CG LEU I 257 11.316 -18.130 9.344 1.00 3.65 c c
ATOM 8775 CD1 LEU I 257 10.067 -18.702 8.689 1.00 2.00 c c
ATOM 8776 CD2 LEU I 257 11.917 -17.030 8.485 1.00 2.14 c c
ATOM 8777 C LEU I 257 11.580 -19.871 11.670 1.00 5.64 c c
ATOM 8778 O LEU I 257 11.234 -20.895 11.079 1.00 5.81 c o
ATOM 8779 N LEU I 258 12.764 -19.741 12.259 1.00 5.75 c N
ATOM 8780 CA LEU I 258 13.808 -20.739 12.081 1.00 5.91 c c
ATOM 8781 CB LEU I 258 15. 156 -20.215 12.583 1.00 6.10 c c
ATOM 8782 CG LEU I 258 16.059 -19.626 11.495 1.00 5.75 c c
ATOM 8783 CD1 LEU I 258 17.208 -18.836 12.101 1.00 6.33 c c
ATOM 8784 CD2 LEU I 258 16.577 -20.724 10.577 1.00 7.33 c c
ATOM 8785 C LEU I 258 13.464 -22.074 12.736 1.00 6.03 c c
ATOM 8786 O LEU I 258 13.589 -23. 125 12. 109 1.00 5.73 c o
ATOM 8787 N SER I 259 12.980 -22.030 13.974 1.00 6.47 c N
ATOM 8788 CA SER I 259 12.538 -23.243 14.662 1.00 6.95 c c
ATOM 8789 CB SER I 259 12.400 -23.000 16.168 1.00 7.05 c c
ATOM 8790 OG SER I 259 11. 147 -23.460 16.650 1.00 6.86 c o
ATOM 8791 C SER I 259 11.220 -23.759 14.097 1.00 6.74 c c
ATOM 8792 O SER I 259 10.905 -24.943 14.213 1.00 6.86 c o
ATOM 8793 N LEU I 260 10.41 1 -22.844 13.576 1.00 6.31 c N
ATOM 8794 CA LEU I 260 9.188 -23.21 1 12.880 1.00 6.09 c c
ATOM 8795 CB LEU I 260 8.407 -21.957 12.484 1.00 6.09 c c
ATOM 8796 CG LEU I 260 7.140 -21.665 13.291 1.00 6.24 c c
ATOM 8797 CD1 LEU I 260 6.291 -20.595 12.61 1 1.00 6.53 c c
ATOM 8798 CD2 LEU I 260 6.337 -22.944 13.521 1.00 5.98 c c
ATOM 8799 C LEU I 260 9.497 -24.047 11.644 1.00 6.25 c c
ATOM 8800 O LEU I 260 8.809 -25.028 11.361 1.00 6.37 c o
ATOM 8801 N ILE I 261 10.452 -23.580 10.847 1.00 6.63 c N
ATOM 8802 CA ILE I 261 10.952 -24.360 9.723 1.00 7.19 c c
ATOM 8803 CB ILE I 261 12.165 -23.681 9.061 1.00 7.09 c c
ATOM 8804 CGI ILE I 261 11.703 -22.635 8.046 1.00 7.46 c c
ATOM 8805 CD1 ILE I 261 12.646 -21 .460 7.909 1.00 8.38 c c

```
ATOM   8806  CG2 ILE I 261      13.055 -24.718   8.391  1.00  6.61      C    c
ATOM   8807  C   ILE I 261      11.389 -25.723  10.228  1.00  8.01      c    c
ATOM   8808  O   ILE I 261      10.967 -26.758   9.713  1.00  8.26      c    o
ATOM   8809  N   ASN I 262      12.206 -25.708  11.273  1.00  9.05      c    N
ATOM   8810  CA  ASN I 262      12.640 -26.935  11.912  1.00  9.88      c    c
ATOM   881 1  CB  ASN I 262      13.220 -26.636  13.292  1.00  9.99      c    c
ATOM   8812  CG  ASN I 262      14.327 -27.590  13.672  1.00 11.16      c    c
ATOM   8813  OD1 ASN I 262      14.709 -28.457  12.886  1.00 12.70      C    O
ATOM   8814  ND2 ASN I 262      14.912 -27.379  14.844  1.00 13.20      C    N
ATOM   8815  C   ASN I 262      11.500 -27.939  12.023  1.00 10.17      c    c
ATOM   8816  O   ASN I 262      11.661 -29.108  11.675  1.00 10.52      c    o
ATOM   8817  N   ASP I 263      10.315 -27.444  12.368  1.00 10.62      c    N
ATOM   8818  CA  ASP I 263       9.203 -28.31 1  12.741  1.00 11.02      c    c
ATOM   8819  CB  ASP I 263       8.230 -27.584  13.675  1.00 11.49      c    c
ATOM   8820  CG  ASP I 263       7.026 -28.435  14.040  1.00 12.80      c    c
ATOM   8821  OD1 ASP I 263       7.219 -29.586  14.487  1.00 14.72      c    o
ATOM   8822  OD2 ASP I 263       5.886 -27.978  13.81 1  1.00 13.88      c    o
ATOM   8823  C   ASP I 263       8.460 -28.855  11.520  1.00 10.92      c    c
ATOM   8824  O   ASP I 263       7.619 -29.748  11.642  1.00 10.96      c    o
ATOM   8825  N   MET I 264       8.807 -28.346  10.341  1.00 10.91      c    N
ATOM   8826  CA  MET I 264       8.105 -28.707   9.1 10  1.00 10.78      c    c
ATOM   8827  CB  MET I 264       8.397 -27.687   8.007  1.00 10.51      c    c
ATOM   8828  CG  MET I 264       7.934 -26.276   8.329  1.00 11.26      c    c
ATOM   8829  SD  MET I 264       8.142 -25.144   6.942  1.00 12.70      c    s
ATOM   8830  CE  MET I 264       9.799 -25.565   6.41 1  1.00 13.92      c    c
ATOM   8831  C   MET I 264       8.466 -30. 116  8.631  1.00 10.85      c    c
ATOM   8832  O   MET I 264       9.644 -30.472   8.578  1.00 11.03      c    o
ATOM   8833  N   PRO I 265       7.451 -30.900   8.230  1.00 10.88      c    N
ATOM   8834  CA  PRO I 265       7.647 -32.293   7.841  1.00 11.09      c    c
ATOM   8835  CB  PRO I 265       6.215 -32.820   7.685  1.00 11.28      c    c
ATOM   8836  CG  PRO I 265       5.387 -31.612   7.438  1.00 11.24      c    c
ATOM   8837  CD  PRO I 265       6.025 -30.534   8.255  1.00 11.03      c    c
ATOM   8838  C   PRO I 265       8.400 -32.420   6.521  1.00 11.19      c    c
ATOM   8839  O   PRO I 265       7.889 -33.027   5.580  1.00 11.47      c    o
ATOM   8840  N   ILE I 266       9.642 -31.940   6.488  1.00 11.54      C    N
ATOM   8841  CA  ILE I 266      10.448 -31.980   5.266  1.00 12.15      c    c
ATOM   8842  CB  ILE I 266      10.586 -30.587   4.621  1.00 12.22      c    c
ATOM   8843  CGI ILE I 266      11.051 -29.559   5.654  1.00 12.53      c    c
ATOM   8844  CD1 ILE I 266      11.557 -28.269   5.047  1.00 12.40      c    c
ATOM   8845  CG2 ILE I 266       9.271 -30.157   3.984  1.00 12.74      c    c
ATOM   8846  C   ILE I 266      11.839 -32.574   5.485  1.00 12.29      c    c
ATOM   8847  O   ILE I 266      12.291 -32.724   6.619  1.00 12.36      C    0
ATOM   8848  N   THR I 267      12.498 -32.936   4.388  1.00 12.29      c    N
ATOM   8849  CA  THR I 267      13.868 -33.435   4.440  1.00 12.43      c    c
ATOM   8850  CB  THR I 267      14.386 -33.809   3.039  1.00 12.40      c    c
ATOM   8851  OG1 THR I 267      15.460 -32.934   2.674  1.00 13.21      c    o
ATOM   8852  CG2 THR I 267      13.274 -33.699   2.010  1.00 12.21      c    c
ATOM   8853  C   THR I 267      14.797 -32.391   5.046  1.00 12.37      c    c
ATOM   8854  O   THR I 267      14.403 -31 .244   5.251  1.00 12.29      c    o
ATOM   8855  N   ASN I 268      16.045 -32.779   5.282  1.00 12.47      c    N
ATOM   8856  CA  ASN I 268      16.965 -31.945   6.045  1.00 12.57      c    c
ATOM   8857  CB  ASN I 268      18.041 -32.800   6.715  1.00 12.69      c    c
ATOM   8858  CG  ASN I 268      17.682 -33.171   8.138  1.00 13.65      c    c
ATOM   8859  OD1 ASN I 268      16.61 1 -32.820   8.631  1.00 14.37      c    o
ATOM   8860  ND2 ASN I 268      18.569 -33.905   8.800  1.00 15.74      c    N
ATOM   8861  C   ASN I 268      17.608 -30.843   5.21 1  1.00 12.43      c    c
ATOM   8862  O   ASN I 268      17.775 -29.717   5.680  1.00 12.51      c    o
ATOM   8863  N   ASP I 269      18.038 -31.194   4.005  1.00 12.34      c    N
ATOM   8864  CA  ASP I 269      18.574 -30.21 1   3.072  1.00 12.33      c    c
ATOM   8865  CB  ASP I 269      19.015 -30.891   1.777  1.00 12.89      c    c
```

ATOM 8866 CG ASP I 269 20.071 -31.950 2.007 1.00 14.84 C c
ATOM 8867 ODl ASP I 269 21.002 -31.699 2.800 1.00 16.90 c o
ATOM 8868 OD2 ASP I 269 19.952 -33.047 1.422 1.00 17.65 c o
ATOM 8869 C ASP I 269 17.539 -29.138 2.769 1.00 11.60 c c
ATOM 8870 O ASP I 269 17.861 -27.952 2.696 1.00 11.65 c o
ATOM 8871 N GLN I 270 16.295 -29.564 2.585 1.00 10.62 c N
ATOM 8872 CA GLN I 270 15.182 -28.633 2.501 1.00 10.01 c c
ATOM 8873 CB GLN I 270 13.853 -29.384 2.525 1.00 10.18 c c
ATOM 8874 CG GLN I 270 12.845 -28.862 1.525 1.00 11.49 c c
ATOM 8875 CD GLN I 270 12.012 -29.968 0.918 1.00 14.38 c c
ATOM 8876 OE1 GLN I 270 10.789 -29.863 0.836 1.00 16.38 c: o
ATOM 8877 NE2 GLN I 270 12.665 -31.057 0.530 1.00 15.41 c: N
ATOM 8878 C GLN I 270 15.228 -27.620 3.636 1.00 9.48 c c
ATOM 8879 O GLN I 270 15.310 -26.415 3.400 1.00 9.12 c o
ATOM 8880 N LYS I 271 15.170 -28.112 4.868 1.00 9.19 c N
ATOM 8881 CA LYS I 271 15.211 -27.240 6.035 1.00 8.89 c c
ATOM 8882 CB LYS I 271 15.253 -28.064 7.322 1.00 8.52 c c
ATOM 8883 CG LYS I 271 13.948 -28.773 7.643 1.00 9.14 c c
ATOM 8884 CD LYS I 271 13.927 -29.280 9.076 1.00 10.72 c c
ATOM 8885 CE LYS 1271 13.274 -30.648 9.163 1.00 10.79 c c
ATOM 8886 NZ LYS 1271 12.712 -30.914 10.514 1.00 9.77 c N
ATOM 8887 C LYS I 271 16.405 -26.295 5.973 1.00 8.83 c c
ATOM 8888 O LYS I 271 16.257 -25.082 6.127 1.00 9.05 c o
ATOM 8889 N LYS I 272 17.583 -26.854 5.707 1.00 8.65 c N
ATOM 8890 CA LYS I 272 18.796 -26.058 5.548 1.00 8.50 c c
ATOM 8891 CB LYS I 272 19.977 -26.948 5.145 1.00 9.14 c c
ATOM 8892 CG LYS I 272 21.158 -26.189 4.547 1.00 11.58 c c
ATOM 8893 CD LYS I 272 22.213 -27.138 3.991 1.00 15.78 c c
ATOM 8894 CE LYS I 272 23.576 -26.464 3.891 1.00 17.65 c c
ATOM 8895 NZ LYS I 272 24.667 -27.446 3.641 1.00 19.68 c N
ATOM 8896 C LYS I 272 18.599 -24.956 4.514 1.00 7.88 c c
ATOM 8897 O LYS I 272 18.919 -23.794 4.761 1.00 8.12 c o
ATOM 8898 N LEU I 273 18.111 -25.336 3.338 1.00 6.95 c N
ATOM 8899 CA LEU I 273 17.867 -24.375 2.271 1.00 5.70 c c
ATOM 8900 CB LEU I 273 17.235 -25.063 1.060 1.00 5.85 c c
ATOM 8901 CG LEU I 273 16.754 -24.131 -0.054 1.00 4.65 c c
ATOM 8902 CD1 LEU I 273 17.928 -23.571 -0.841 1.00 4.57 c c
ATOM 8903 CD2 LEU I 273 15.777 -24.846 -0.972 1.00 3.69 c c
ATOM 8904 C LEU I 273 16.969 -23.244 2.755 1.00 5.14 c c
ATOM 8905 O LEU I 273 17.345 -22.074 2.702 1.00 5.25 c o
ATOM 8906 N MET I 274 15.776 -23.601 3.221 1.00 4.52 c N
ATOM 8907 CA MET I 274 14.828 -22.616 3.723 1.00 4.59 c c
ATOM 8908 CB MET I 274 13.599 -23.308 4.314 1.00 4.35 c c
ATOM 8909 CG MET I 274 12.709 -23.975 3.279 1.00 4.50 c c
ATOM 8910 SD MET I 274 11.194 -24.645 3.989 1.00 5.51 c s
ATOM 8911 CE MET I 274 10.326 -23.138 4.417 1.00 5.26 c c
ATOM 8912 C MET I 274 15.479 -21.720 4.768 1.00 5.18 c c
ATOM 8913 O MET I 274 15.279 -20.505 4.771 1.00 5.61 c o
ATOM 8914 N SER I 275 16.315 -22.319 5.610 1.00 5.89 c N
ATOM 8915 CA SER I 275 16.961 -21.588 6.688 1.00 6.18 c c
ATOM 8916 CB SER I 275 17.607 -22.555 7.682 1.00 6.33 c c
ATOM 8917 OG SER I 275 16.654 -23.470 8.193 1.00 5.91 c o
ATOM 8918 C SER I 275 17.996 -20.603 6.157 1.00 6.58 c c
ATOM 8919 O SER I 275 18.181 -19.526 6.721 1.00 7.03 c o
ATOM 8920 N ASN I 276 18.615 -20.940 5.030 1.00 7.07 c N
ATOM 8921 CA ASN I 276 19.593 -20.050 4.412 1.00 7.86 c c
ATOM 8922 CB ASN I 276 20.696 -20.854 3.711 1.00 8.34 c c
ATOM 8923 CG ASN I 276 21.868 -21.177 4.633 1.00 9.77 c c
ATOM 8924 ODl ASN I 276 22.167 -20.430 5.567 1.00 11.84 c o
ATOM 8925 ND2 ASN I 276 22.557 -22.278 4.349 1.00 11.15 C N

```
ATOM   8926  C   ASN I 276      18.976 -19.029   3.453  1.00  7.71      C    C
ATOM   8927  O   ASN I 276      19.695 -18.349   2.722  1.00  7.84      C    O
ATOM   8928  N   ASN 1277       17.655 -18.870   3.509  1.00  7.77      C    N
ATOM   8929  CA  ASN 1277        16.938 -18.098   2.491  1.00  7.85      C    C
ATOM   8930  CB  ASN 1277        16.575 -18.987   1.304  1.00  7.58      C    C
ATOM   8931  CG  ASN 1277        17.725 -19.157   0.335  1.00  8.29      C    C
ATOM   8932  OD1 ASN I 277       18.053 -18.240  -0.417  1.00  9.04      C    O
ATOM   8933  ND2 ASN I 277       18.427 -20.279   0.443  1.00  9.57      C    N
ATOM   8934  C   ASN 1277       15.697 -17.371   3.006  1.00  7.86      C    C
ATOM   8935  O   ASN 1277       14.826 -16.977   2.229  1.00  7.85      C    O
ATOM   8936  N   VAL 1278       15.593 -17.272   4.328  1.00  7.67      C    N
ATOM   8937  CA  VAL 1278        14.554 -16.489   4.998  1.00  7.77      C    C
ATOM   8938  CB  VAL 1278        15.120 -15.739   6.215  1.00  7.98      C    C
ATOM   8939  CGI VAL 1278        15.1 16 -16.638   7.440  1.00  7.21      C    C
ATOM   8940  CG2 VAL I 278       16.524 -15.234   5.918  1.00  8.99      C    C
ATOM   8941  C   VAL 1278       13.813 -15.497   4.105  1.00  7.76      C    C
ATOM   8942  O   VAL 1278       12.583 -15.441   4.123  1.00  7.84      C    O
ATOM   8943  N   GLN 1279       14.562 -14.581   3.501  1.00  7.47      C    N
ATOM   8944  CA  GLN 1279        13.966 -13.446   2.809  1.00  7.07      C    C
ATOM   8945  CB  GLN 1279        15.038 -12.668   2.045  1.00  7.62      C    C
ATOM   8946  CG  GLN 1279        14.870 - 11.159   2.1 16  1.00 10.35      C    C
ATOM   8947  CD  GLN 1279        15.712 -10.430   1.091  1.00 13.70      C    C
ATOM   8948  OE1 GLN 1279        16. 199 - 11.027   0.132  1.00 15.06      C    O
ATOM   8949  NE2 GLN 1279        15.865  -9.124   1.275  1.00 13.97      C    N
ATOM   8950  C   GLN 1279       12.868 -13.901   1.851  1.00  6.02      C    C
ATOM   8951  O   GLN 1279       11.734 -13.423   1.912  1.00  5.45      C    O
ATOM   8952  N   ILE 1280      13.249 -14.748   0.901  1.00  5.25      C    N
ATOM   8953  CA  ILE 1280       12.304 -15.343  -0.031  1.00  4.74      C    C
ATOM   8954  CB  ILE 1280       12.978 -16.451  -0.860  1.00  4.58      C    C
ATOM   8955  CGI ILE 1280        14.333 -15.973  -1.385  1.00  4.16      C    C
ATOM   8956  CD 1 ILE I 280       14.238 -15.065  -2.587  1.00  3.88      C    C
ATOM   8957  CG2 ILE 1280        12.065 -16.900  -1.996  1.00  3.92      C    C
ATOM   8958  C   ILE 1280      11.122 -15.946   0.716  1.00  4.43      C    C
ATOM   8959  O   ILE 1280       9.972 -15.547   0.516  1.00  4.39      C    O
ATOM   8960  N   VAL I 281       11.409 -16.970   1.513  1.00  4.05      C    N
ATOM   8961  CA  VAL 1281        10.390 -17.623   2.319  1.00  3.58      C    C
ATOM   8962  CB  VAL 1281        11.010 -18.335   3.534  1.00  3.13      C    C
ATOM   8963  CGI VAL 1281        10.006 -19.291   4.158  1.00  2.34      C    C
ATOM   8964  CG2 VAL 1281        12.277 -19.073   3.127  1.00  2.21      C    C
ATOM   8965  C   VAL 1281       9.373 -16.601   2.806  1.00  3.96      C    C
ATOM   8966  O   VAL 1281       8.186 -16.694   2.495  1.00  4.15      C    O
ATOM   8967  N   ARG 1282       9.857 -15.593   3.522  1.00  4.23      C    N
ATOM   8968  CA  ARG 1282        8.995 -14.530   4.016  1.00  4.45      C    C
ATOM   8969  CB  ARG 1282        9.829 -13.427   4.656  1.00  3.96      C    C
ATOM   8970  CG  ARG 1282        10.637 -13.896   5.841  1.00  2.99      C    C
ATOM   8971  CD  ARG 1282        10.550 -12.909   6.979  1.00  2.28      C    C
ATOM   8972  NE  ARG 1282        11.505 -13.236   8.029  1.00  2.00      C    N
ATOM   8973  CZ  ARG 1282        11.175 -13.463   9.297  1.00  2.44      C    C
ATOM   8974  NHl  ARG 1282       9.914 -13.339   9.690  1.00  2.04      C    N
ATOM   8975  NH2 ARG 1282       12.099 -13.847  10.167  1.00  3.44      C    N
ATOM   8976  C   ARG 1282       8.144 -13.952   2.898  1.00  5.32      C    C
ATOM   8977  O   ARG 1282       6.924 -13.854   3.022  1.00  5.95      C    O
ATOM   8978  N   GLN 1283       8.794 -13.551   1.812  1.00  5.50      C    N
ATOM   8979  CA  GLN 1283        8.083 -12.995   0.671  1.00  5.80      C    C
ATOM   8980  CB  GLN 1283        9.064 -12.580  -0.421  1.00  6.19      C    C
ATOM   8981  CG  GLN 1283        9.908 - 11.381  -0.047  1.00  9.68      C    C
ATOM   8982  CD  GLN 1283        11.088 - 11.192  -0.971  1.00 13.92      C    C
ATOM   8983  OE1 GLN I 283       11.266 - 11.939  -1.934  1.00 16.20      C    O
ATOM   8984  NE2 GLN I 283       11.885 -10.164  -0.706  1.00 14. 17      C    N
ATOM   8985  C   GLN 1283       7.071 -13.988   0.120  1.00  5.44      C    C
```

```
ATOM   8986  O   GLN I 283      6.069 -13.598  -0.479  1.00  5.43      C    o
ATOM   8987  N   GLN I 284      7.302 -15.269   0.387  1.00  5.26      c    N
ATOM   8988  CA  GLN I 284      6.465 -16.321  -0. 172  1.00  5.18      c    c
ATOM   8989  CB  GLN I 284      7.303 -17.549  -0.517  1.00  5.32      c    c
ATOM   8990  CG  GLN I 284      7.689 -17.619  -1.981  1.00  6.85      c    c
ATOM   8991  CD  GLN I 284      8.548 -18.821  -2.304  1.00  9.21      c    c
ATOM   8992  OE1 GLN I 284      9.398 -19.227  -1.51 1  1.00  9.74      c    o
ATOM   8993  NE2 GLN I 284      8.332 -19.400  -3.477  1.00  9.79      c    N
ATOM   8994  C   GLN I 284      5.345 -16.705   0.779  1.00  4.67      c    c
ATOM   8995  O   GLN I 284      4.485 -17.520   0.447  1.00  4.19      c    o
ATOM   8996  N   SER I 285      5.367 -16. 116   1.968  1.00  4.51      c    N
ATOM   8997  CA  SER I 285      4.457 -16.516   3.027  1.00  4.39      c    c
ATOM   8998  CB  SER I 285      5.218 -16.729   4.336  1.00  4.13      c    c
ATOM   8999  OG  SER I 285      6.328 -17.588   4.146  1.00  4.40      c    o
ATOM   9000  C   SER I 285      3.359 -15.481   3.220  1.00  4.44      c    c
ATOM   9001  O   SER I 285      3.483 -14.335   2.785  1.00  4.82      c    o
ATOM   9002  N   TYR I 286      2.268 -15.908   3.842  1.00  4.53      c    N
ATOM   9003  CA  TYR I 286      1.194 -15.002   4.213  1.00  4.80      c    c
ATOM   9004  CB  TYR I 286     -0.1 16 -15.441   3.559  1.00  4.88      c    c
ATOM   9005  CG  TYR I 286     -0.135 -15.272   2.059  1.00  5.68      c    c
ATOM   9006  CD1 TYR I 286      0.713 -16.013   1.245  1.00  7.34      c    c
ATOM   9007  CE1 TYR I 286      0.695 -15.864  -0.126  1.00  9.02      c    c
ATOM   9008  CZ  TYR I 286     -0.190 -14.979  -0.701  1.00  9.40      c    c
ATOM   9009  OH  TYR I 286     -0.206 -14.824  -2.066  1.00 10.44      c'   o
ATOM   9010  CE2 TYR I 286     -1.054 -14.244   0.083  1.00  9.38      c    c
ATOM   901 1 CD2 TYR I 286     -1.024 -14.395   1.453  1.00  7.39      c    c
ATOM   9012  C   TYR I 286      1.037 -14.978   5.726  1.00  4.76      C    c
ATOM   9013  O   TYR I 286      1.499 -15.883   6.421  1.00  5.25      c    o
ATOM   9014  N   SER I 287      0.403 -13.929   6.234  1.00  4.52      c    N
ATOM   9015  CA  SER I 287     -0.072 -13.924   7.609  1.00  4.45      c    c
ATOM   9016  CB  SER I 287      0.779 -12.989   8.470  1.00  4.57      c    c
ATOM   9017  OG  SER I 287      0.1 13 -12.662   9.678  1.00  4.38      c    o
ATOM   9018  C   SER I 287     -1.535 -13.516   7.675  1.00  4.61      c    c
ATOM   9019  O   SER I 287     -1.920 -12.460   7.172  1.00  4.40      c    o
ATOM   9020  N   ILE I 288     -2.364 -14.425   8.171  1.00  5.1 1      c    N
ATOM   9021  CA  ILE I 288     -3.788 -14. 171   8.302  1.00  5.81      c    c
ATOM   9022  CB  ILE I 288     -4.610 -15.393   7.863  1.00  5.52      c    c
ATOM   9023  CGI ILE I 288     -3.81 1 -16.253   6.878  1.00  5.47      c    c
ATOM   9024  CD1 ILE I 288     -3.975 -15.852   5.429  1.00  6.23      c    c
ATOM   9025  CG2 ILE I 288     -5.939 -14.957   7.271  1.00  6.22      c    c
ATOM   9026  C   ILE I 288     -4.123 -13.848   9.750  1.00  6.71      c    c
ATOM   9027  O   ILE I 288     -3.759 -14.593  10.660  1.00  7.30      c    o
ATOM   9028  N   MET I 289     -4.874 -12.771   9.952  1.00  7.71      c    N
ATOM   9029  CA  MET I 289     -5.451 -12.476  11.257  1.00  8.57      C    C
ATOM   9030  CB  MET I 289     -6.099 -1 1.090  11.246  1.00  8.71      C    C
ATOM   9031  CG  MET I 289     -6.131 -10.412  12.603  1.00  9.70      C    C
ATOM   9032  SD  MET I 289     -7.100  -8.895  12.581  1.00 12.59      C    S
ATOM   9033  CE  MET I 289     -8.569  -9.452  11.721  1.00 12.41      C    C
ATOM   9034  C   MET I 289     -6.477 -13.538  11.658  1.00  9.12      C    C
ATOM   9035  O   MET I 289     -7.322 -13.925  10.851  1.00  9.31      C    O
ATOM   9036  N   SER I 290     -6.406 -13.998  12.907  1.00  9.80      C    N
ATOM   9037  CA  SER I 290     -7.290 -15.062  13.388  1.00 10.49      C    C
ATOM   9038  CB  SER I 290     -6.494 -16.195  14.035  1.00 10.64      C    C
ATOM   9039  OG  SER I 290     -7.316 -17.328  14.257  1.00 11.99      C    O
ATOM   9040  C   SER 1290     -8.385 -14.573  14.335  1.00 10.75      C    C
ATOM   9041  O   SER 1290     -9.563 -14.595  13.980  1.00 10.89      C    O
ATOM   9042  N   ILE I 291     -8.018 -14.243  15.571  1.00 11.04      C    N
ATOM   9043  CA  ILE I 291     -8.955 -13.562  16.461  1.00 11.41      C    C
ATOM   9044  CB  ILE I 291     -9.796 -14.539  17.305  1.00 11.80      C    C
ATOM   9045  CGI ILE I 291     -9.096 -15.893  17.419  1.00 11.81      C    C
```

ATOM 9046 CD1 ILE I 291 -8.227 -16.028 18.647 1.00 11.76 C c
ATOM 9047 CG2 ILE I 291 -11.179 -14.707 16.700 1.00 12.39 c c
ATOM 9048 C ILE I 291 -8.349 -12.481 17.346 1.00 11.13 C c
ATOM 9049 O ILE I 291 -7.316 -12.681 17.986 1.00 10.55 c o
ATOM 9050 N ILE I 292 -9.034 -11.343 17.398 1.00 11.36 c N
ATOM 9051 CA ILE I 292 -8.605 -10.215 18.211 1.00 11.82 c c
ATOM 9052 CB ILE I 292 -8.651 -8.884 17.421 1.00 11.86 c c
ATOM 9053 CGI ILE I 292 -9.052 -9.127 15.963 1.00 13.42 c c
ATOM 9054 CD1 ILE I 292 -7.968 -9.771 15.126 1.00 15.86 c c
ATOM 9055 CG2 ILE I 292 -7.311 -8.160 17.508 1.00 10.85 c c
ATOM 9056 C ILE I 292 -9.486 -10.092 19.444 1.00 11.72 C c
ATOM 9057 O ILE I 292 -10.713 -10.029 19.346 1.00 11.28 c o
ATOM 9058 N LYS I 293 -8.857 -10.180 20.607 1.00 12.11 c N
ATOM 9059 CA LYS I 293 -9.479 -9.728 21.834 1.00 12.92 c c
ATOM 9060 CB LYS I 293 -9.599 -10.889 22.820 1.00 13.15 c c
ATOM 9061 CG LYS I 293 -10.034 -12.194 22.174 1.00 14.17 c c
ATOM 9062 CD LYS I 293 -10.958 -12.974 23.091 1.00 15.37 c c
ATOM 9063 CE LYS I 293 -11.869 -13.899 22.305 1.00 16.68 c c
ATOM 9064 NZ LYS I 293 -12.822 -14.614 23.197 1.00 18.18 c N
ATOM 9065 C LYS I 293 -8.670 -8.584 22.433 1.00 13.32 c c
ATOM 9066 O LYS I 293 -7.518 -8.366 22.055 1.00 13.17 c o
ATOM 9067 N GLU I 294 -9.337 -7.759 23.233 1.00 14.07 c N
ATOM 9068 CA GLU I 294 -8.714 -6.572 23.805 1.00 15.07 c c
ATOM 9069 CB GLU I 294 -9.608 -5.975 24.896 1.00 15.94 c c
ATOM 9070 CG GLU I 294 -10.872 -5.307 24.373 1.00 19.87 c c
ATOM 9071 CD GLU I 294 -11.569 -4.471 25.427 1.00 23.88 c c
ATOM 9072 OE1 GLU I 294 -10.994 -3.449 25.854 1.00 23.75 c: o
ATOM 9073 OE2 GLU I 294 -12.723 -4.799 25.777 1.00 25.81 c: o
ATOM 9074 C GLU I 294 -7.324 -6.878 24.362 1.00 14.40 c c
ATOM 9075 O GLU I 294 -6.433 -6.031 24.319 1.00 14.33 c o
ATOM 9076 N GLU I 295 -7.144 -8.092 24.879 1.00 13.97 c N
ATOM 9077 CA GLU I 295 -5.908 -8.452 25.568 1.00 13.84 c c
ATOM 9078 CB GLU I 295 -6.161 -8.721 27.055 1.00 14.67 c c
ATOM 9079 CG GLU I 295 -7.620 -8.914 27.427 1.00 17.56 c c
ATOM 9080 CD GLU I 295 -8.245 -10.112 26.743 1.00 21.41 c c
ATOM 9081 OE1 GLU I 295 -8.990 -9.909 25.761 1.00 22.35 c o
ATOM 9082 OE2 GLU I 295 -8.090 -11.241 27.257 1.00 23.20 c: o
ATOM 9083 C GLU I 295 -5.166 -9.630 24.933 1.00 12.77 c c
ATOM 9084 O GLU I 295 -4.166 -10.100 25.476 1.00 12.58 c o
ATOM 9085 N VAL I 296 -5.701 -10.162 23.838 1.00 11.72 c N
ATOM 9086 CA VAL I 296 -4.970 -11.150 23.051 1.00 10.65 c c
ATOM 9087 CB VAL I 296 -5.245 -12.589 23.517 1.00 10.47 c c
ATOM 9088 CGI VAL I 296 -4.277 -13.546 22.846 1.00 9.77 c c
ATOM 9089 CG2 VAL I 296 -5.118 -12.688 25.026 1.00 11.31 c c
ATOM 9090 C VAL I 296 -5.245 -11.039 21.562 1.00 10.26 c c
ATOM 9091 O VAL I 296 -6.395 -10.940 21.133 1.00 10.09 c o
ATOM 9092 N LEU I 297 -4.184 -11.178 20.777 1.00 9.77 c N
ATOM 9093 CA LEU I 297 -4.302 -11.269 19.332 1.00 8.97 c c
ATOM 9094 CB LEU I 297 -3.577 -10.097 18.672 1.00 8.64 c c
ATOM 9095 CG LEU I 297 -3.382 -10.209 17.160 1.00 9.01 c c
ATOM 9096 CD1 LEU I 297 -4.721 -10.384 16.459 1.00 9.79 c c
ATOM 9097 CD2 LEU I 297 -2.645 -8.994 16.620 1.00 9.43 c c
ATOM 9098 C LEU I 297 -3.725 -12.587 18.829 1.00 8.34 c c
ATOM 9099 O LEU I 297 -2.565 -12.908 19.089 1.00 8.64 c o
ATOM 9100 N ALA I 298 -4.545 -13.352 18.116 1.00 7.21 c N
ATOM 9101 CA ALA I 298 -4.095 -14.600 17.515 1.00 6.33 c c
ATOM 9102 CB ALA I 298 -4.908 -15.770 18.047 1.00 6.68 c c
ATOM 9103 C ALA I 298 -4.207 -14.524 16.002 1.00 5.85 c c
ATOM 9104 O ALA I 298 -5.179 -13.991 15.468 1.00 5.96 c o
ATOM 9105 N TYR I 299 -3.197 -15.040 15.314 1.00 5.28 c N

ATOM 9106 CA TYR I 299 -3.197 -15.042 13.861 1.00 4.63 C c
ATOM 9107 CB TYR I 299 -2.583 -13.749 13.324 1.00 4.36 c c
ATOM 9108 CG TYR I 299 -1.177 -13.490 13.812 1.00 4.34 c c
ATOM 9109 CD1 TYR I 299 -0.080 -13.970 13.110 1.00 4.48 c c
ATOM 9110 CE1 TYR I 299 1.207 -13.733 13.549 1.00 4.55 c c
ATOM 9111 CZ TYR I 299 1.409 -13.011 14.705 1.00 3.72 c c
ATOM 9112 OH TYR I 299 2.690 -12.775 15.149 1.00 2.38 c o
ATOM 9113 CE2 TYR I 299 0.336 -12.526 15.422 1.00 4.13 c c
ATOM 9114 CD2 TYR I 299 -0.947 -12.767 14.975 1.00 4.38 c c
ATOM 9115 C TYR I 299 -2.440 -16.243 13.322 1.00 4.32 c c
ATOM 9116 O TYR I 299 -1.602 -16.822 14.012 1.00 4.67 c o
ATOM 9117 N VAL I 300 -2.746 -16.622 12.087 1.00 3.87 c N
ATOM 9118 CA VAL I 300 -2.130 -17.792 11.486 1.00 3.57 c c
ATOM 9119 CB VAL I 300 -3.169 -18.702 10.805 1.00 3.52 c c
ATOM 9120 CGI VAL I 300 -2.475 -19.749 9.943 1.00 3.44 c c
ATOM 9121 CG2 VAL I 300 -4.053 -19.368 11.851 1.00 3.90 c c
ATOM 9122 C VAL I 300 -1.060 -17.392 10.482 1.00 3.53 c c
ATOM 9123 O VAL I 300 -1.299 -16.575 9.593 1.00 3.68 c o
ATOM 9124 N VAL I 301 0.148 -17.899 10.695 1.00 3.41 c N
ATOM 9125 CA VAL I 301 1.193 -17.816 9.689 1.00 3.36 c c
ATOM 9126 CB VAL I 301 2.593 -17.825 10.324 1.00 3.24 c c
ATOM 9127 CGI VAL I 301 3.655 -18.061 9.261 1.00 3.76 c c
ATOM 9128 CG2 VAL I 301 2.849 -16.519 11.059 1.00 3.10 c c
ATOM 9129 C VAL I 301 1.084 -18.962 8.695 1.00 3.48 c c
ATOM 9130 O VAL I 301 0.647 -20.061 9.037 1.00 3.92 c o
ATOM 9131 N GLN I 302 1.466 -18.684 7.456 1.00 3.21 c N
ATOM 9132 CA GLN I 302 1.274 -19.625 6.368 1.00 3.01 c c
ATOM 9133 CB GLN I 302 0.090 -19.202 5.504 1.00 3.24 c c
ATOM 9134 CG GLN I 302 -0.067 -20.021 4.239 1.00 5.21 c c
ATOM 9135 CD GLN I 302 -1.479 -19.984 3.701 1.00 7.54 c c
ATOM 9136 OE1 GLN I 302 -2.435 -19.784 4.449 1.00 7.28 c o
ATOM 9137 NE2 GLN I 302 -1.616 -20.143 2.390 1.00 9.27 c N
ATOM 9138 C GLN I 302 2.533 -19.693 5.523 1.00 2.42 c c
ATOM 9139 O GLN I 302 2.881 -18.736 4.832 1.00 2.40 c o
ATOM 9140 N LEU I 303 3.292 -20.765 5.707 1.00 2.00 c N
ATOM 9141 CA LEU I 303 4.607 -20.868 5.104 1.00 2.00 c c
ATOM 9142 CB LEU I 303 5.628 -21.358 6.130 1.00 2.00 c c
ATOM 9143 CG LEU I 303 5.663 -20.559 7.434 1.00 2.00 c c
ATOM 9144 CD1 LEU I 303 6.712 -21.118 8.382 1.00 2.00 c c
ATOM 9145 CD2 LEU I 303 5.918 -19.085 7.154 1.00 2.00 c c
ATOM 9146 C LEU I 303 4.564 -21.805 3.909 1.00 2.00 c c
ATOM 9147 O LEU I 303 3.658 -22.630 3.794 1.00 2.45 c o
ATOM 9148 N PRO I 304 5.499 -21.620 2.970 1.00 2.00 c N
ATOM 9149 CA PRO I 304 5.617 -22.519 1.840 1.00 2.07 c c
ATOM 9150 CB PRO I 304 6.326 -21.656 0.803 1.00 2.00 c c
ATOM 9151 CG PRO I 304 7.221 -20.775 1.620 1.00 2.00 c c
ATOM 9152 CD PRO I 304 6.564 -20.601 2.973 1.00 2.06 c c
ATOM 9153 C PRO I 304 6.492 -23.711 2.194 1.00 2.11 c c
ATOM 9154 O PRO I 304 7.544 -23.530 2.809 1.00 2.13 c o
ATOM 9155 N ALA I 305 5.903 -24.902 2.097 1.00 30.00 c N
ATOM 9156 CA ALA I 305 6.371 -25.959 1.180 1.00 30.00 c c
ATOM 9157 CB ALA I 305 5.841 -27.314 1.627 1.00 30.00 c c
ATOM 9158 C ALA I 305 6.011 -25.690 -0.310 1.00 30.00 c c
ATOM 9159 O ALA I 305 5.614 -24.571 -0.624 1.00 30.00 c o
ATOM 9160 N TYR I 306 5.840 -26.756 -1.125 1.00 13.49 c N
ATOM 9161 CA TYR I 306 6.433 -26.943 -2.522 1.00 13.70 c c
ATOM 9162 CB TYR I 306 7.412 -28.117 -2.435 1.00 13.93 c c
ATOM 9163 CG TYR I 306 8.486 -28.217 -3.491 1.00 14.08 c c
ATOM 9164 CD1 TYR I 306 8.717 -29.447 -4.102 1.00 14.59 c c
ATOM 9165 CE1 TYR I 306 9.982 -29.819 -4.531 1.00 14.82 c c

ATOM 9166 CZ TYR I 306 11.002 -28.893 -4.523 1.00 14.52 C c
ATOM 9167 OH TYR I 306 12.189 -29.164 -5.167 1.00 13.02 c o
ATOM 9168 CE2 TYR I 306 10.781 -27.632 -4.011 1.00 15.22 c c
ATOM 9169 CD2 TYR I 306 9.534 -27.303 -3.495 1.00 14.61 c c
ATOM 9170 C TYR I 306 5.391 -27.297 -3.661 1.00 13.68 c c
ATOM 9171 O TYR I 306 4.296 -27.738 -3.325 1.00 13.95 c o
ATOM 9172 N GLY I 307 5.786 -27.316 -4.962 1.00 13.54 c N
ATOM 9173 CA GLY I 307 5.057 -28.108 -6.046 1.00 13.37 c c
ATOM 9174 C GLY I 307 5.290 -27.995 -7.585 1.00 13.47 c c
ATOM 9175 O GLY I 307 5.871 -27.017 -8.054 1.00 13.90 c o
ATOM 9176 N VAL I 308 4.808 -28.976 -8.370 1.00 13.31 c N
ATOM 9177 CA VAL I 308 3.931 -28.717 -9.548 1.00 13.30 c c
ATOM 9178 CB VAL I 308 3.187 -27.383 -9.404 1.00 13.03 c c
ATOM 9179 CGI VAL I 308 1.935 -27.380 -10.261 1.00 13.62 c c
ATOM 9180 CG2 VAL I 308 2.849 -27.116 -7.951 1.00 12.86 c c
ATOM 9181 C VAL I 308 4.596 -28.668 -10.927 1.00 13.58 c c
ATOM 9182 O VAL I 308 5.407 -29.530 -11.271 1.00 13.71 c o
ATOM 9183 N ILE I 309 4.541 -27.470 -11.498 1.00 4.08 C N
ATOM 9184 CA ILE I 309 5.611 -26.532 -11.251 1.00 4.84 c c
ATOM 9185 CB ILE I 309 6.204 -26.810 -9.854 1.00 4.89 c c
ATOM 9186 CGI ILE I 309 5.086 -26.815 -8.801 1.00 5.85 c c
ATOM 9187 CD1 ILE I 309 4.233 -25.561 -8.803 1.00 8.12 c c
ATOM 9188 CG2 ILE I 309 7.308 -25.817 -9.517 1.00 4.44 c c
ATOM 9189 C ILE I 309 6.637 -26.814 -12.345 1.00 5.23 c c
ATOM 9190 O ILE I 309 6.299 -27.437 -13.352 1.00 5.92 c o
ATOM 9191 N ASP I 310 7.864 -26.330 -12.187 1.00 5.33 c N
ATOM 9192 CA ASP I 310 9.004 -26.924 -12.889 1.00 5.83 c c
ATOM 9193 CB ASP I 310 9.086 -28.423 -12.589 1.00 6.21 c c
ATOM 9194 CG ASP I 310 9.193 -28.716 -11.104 1.00 7.19 c c
ATOM 9195 OD1 ASP I 310 8.350 -29.478 -10.583 1.00 7.74 c o
ATOM 9196 OD2 ASP I 310 10.151 -28.228 -10.467 1.00 7.58 c o
ATOM 9197 C ASP I 310 8.997 -26.705 -14.408 1.00 6.02 c c
ATOM 9198 O ASP I 310 9.656 -27.438 -15.146 1.00 6.05 c o
ATOM 9199 N THR I 311 8.273 -25.687 -14.866 1.00 6.24 c N
ATOM 9200 CA THR I 311 8.429 -25.173 -16.229 1.00 6.14 c c
ATOM 9201 CB THR I 311 7.231 -24.299 -16.630 1.00 5.69 c c
ATOM 9202 OG1 THR I 311 6.093 -24.646 -15.830 1.00 5.34 c o
ATOM 9203 CG2 THR I 311 6.897 -24.500 -18.092 1.00 7.10 c c
ATOM 9204 C THR I 311 9.682 -24.313 -16.335 1.00 6.78 c c
ATOM 9205 O THR I 311 9.970 -23.530 -15.430 1.00 7.33 c o
ATOM 9206 N PRO I 312 10.330 -24.318 -17.509 1.00 7.00 c N
ATOM 9207 CA PRO I 312 11.470 -23.419 -17.668 1.00 7.23 c c
ATOM 9208 CB PRO I 312 12.060 -23.834 -19.020 1.00 7.00 c c
ATOM 9209 CG PRO I 312 10.936 -24.505 -19.747 1.00 6.59 c c
ATOM 9210 CD PRO I 312 10.098 -25.159 -18.697 1.00 6.99 c c
ATOM 9211 C PRO I 312 11.016 -21.962 -17.703 1.00 7.69 c c
ATOM 9212 O PRO I 312 9.943 -21.670 -18.228 1.00 7.55 c o
ATOM 9213 N CYS I 313 11.755 -21.077 -17.041 1.00 8.10 c N
ATOM 9214 CA CYS I 313 11.668 -19.654 -17.353 1.00 8.54 c c
ATOM 9215 CB CYS I 313 11.082 -18.852 -16.186 1.00 8.77 c c
ATOM 9216 SG CYS I 313 10.025 -19.785 -15.057 1.00 10.74 c s
ATOM 9217 C CYS I 313 13.000 -19.058 -17.780 1.00 8.19 c c
ATOM 9218 O CYS I 313 14.035 -19.725 -17.760 1.00 8.07 c o
ATOM 9219 N TRP I 314 12.964 -17.777 -18.126 1.00 7.93 c N
ATOM 9220 CA TRP I 314 14.162 -17.035 -18.473 1.00 7.80 c c
ATOM 9221 CB TRP I 314 14.563 -17.322 -19.919 1.00 8.13 c c
ATOM 9222 CG TRP I 314 13.457 -17.091 -20.902 1.00 9.09 c c
ATOM 9223 CD1 TRP I 314 13.295 -16.003 -21.710 1.00 10.26 c c
ATOM 9224 NE1 TRP I 314 12.219 -16.189 -22.546 1.00 10.86 c: N
ATOM 9225 CE2 TRP I 314 11.671 -17.421 -22.298 1.00 10.68 c c

```
ATOM   9226  CD2 TRP I 314      12.426 -18.020 -21.269  1.00 10.49      C    C
ATOM   9227  CE3 TRP I 314      12.083 -19.308 -20.842  1.00 11.67      C    C
ATOM   9228  CZ3 TRP I 314      11.009 -19.946 -21.447  1.00 12.98      C    C
ATOM   9229  CH2 TRP I 314      10.268 -19.318 -22.457  1.00 12.74      C    C
ATOM   9230  CZ2 TRP I 314      10.580 -18.059 -22.895  1.00 11.73      C    C
ATOM   9231  C   TRP I 314      13.899 -15.550 -18.298  1.00  7.34      C    C
ATOM   9232  O   TRP I 314      12.764 -15.091 -18.427  1.00  7.47      C    O
ATOM   9233  N   LYS I 315      14.936 -14.815 -17.920  1.00  6.75      C    N
ATOM   9234  CA  LYS I 315      14.833 -13.372 -17.823  1.00  6.37      C    C
ATOM   9235  CB  LYS I 315      15.493 -12.875 -16.541  1.00  6.38      C    C
ATOM   9236  CG  LYS I 315      14.992 -11.522 -16.065  1.00  6.55      C    C
ATOM   9237  CD  LYS I 315      15.692 -11.117 -14.778  1.00  8.01      C    C
ATOM   9238  CE  LYS I 315      15.198  -9.776 -14.269  1.00  8.78      C    C
ATOM   9239  NZ  LYS I 315      16.141  -9.189 -13.276  1.00 10.21      C    N
ATOM   9240  C   LYS I 315      15.468 -12.711 -19.036  1.00  6.32      C    C
ATOM   9241  O   LYS I 315      16.510 -13.153 -19.523  1.00  6.21      C    O
ATOM   9242  N   LEU I 316      14.766 -11.724 -19.584  1.00  6.58      C    N
ATOM   9243  CA  LEU I 316      15.231 -10.992 -20.758  1.00  7.02      C    C
ATOM   9244  CB  LEU I 316      14.122 -10.908 -21.809  1.00  6.64      C    C
ATOM   9245  CG  LEU I 316      14.308  -9.874 -22.922  1.00  6.21      C    C
ATOM   9246  CD1 LEU I 316      15.563 -10.150 -23.731  1.00  5.94      C    C
ATOM   9247  CD2 LEU I 316      13.082  -9.824 -23.819  1.00  6.57      C    C
ATOM   9248  C   LEU I 316      15.675  -9.588 -20.372  1.00  7.77      C    C
ATOM   9249  O   LEU I 316      14.865  -8.768 -19.941  1.00  8.47      C    O
ATOM   9250  N   HIS I 317      16.956  -9.302 -20.563  1.00  8.05      C    N
ATOM   9251  CA  HIS I 317      17.422  -7.929 -20.547  1.00  8.21      C    C
ATOM   9252  CB  HIS I 317      18.641  -7.786 -19.640  1.00  9.04      C    C
ATOM   9253  CG  HIS I 317      18.644  -8.734 -18.483  1.00 11.41      C    C
ATOM   9254  ND1 HIS I 317      18.314  -8.347 -17.202  1.00 13.62      C    N
ATOM   9255  CE1 HIS I 317      18.423  -9.383 -16.389  1.00 14.91      C    C
ATOM   9256  NE2 HIS I 317      18.811 -10.428 -17.097  1.00 14.25      C    N
ATOM   9257  CD2 HIS I 317      18.960 -10.048 -18.409  1.00 12.67      C    C
ATOM   9258  C   HIS I 317      17.760  -7.469 -21.950  1.00  7.39      C    C
ATOM   9259  O   HIS I 317      17.881  -8.278 -22.869  1.00  7.23      C    O
ATOM   9260  N   THR I 318      17.997  -6.172 -22.086  1.00  7.11      C    N
ATOM   9261  CA  THR I 318      17.745  -5.476 -23.333  1.00  6.56      C    C
ATOM   9262  CB  THR I 318      16.268  -5.093 -23.468  1.00  6.28      C    C
ATOM   9263  OG1 THR I 318      15.652  -5.909 -24.471  1.00  6.33      C    O
ATOM   9264  CG2 THR I 318      16.141  -3.634 -23.866  1.00  6.52      C    C
ATOM   9265  C   THR I 318      18.563  -4.201 -23.357  1.00  6.58      C    C
ATOM   9266  O   THR I 318      18.437  -3.356 -22.472  1.00  6.67      C    O
ATOM   9267  N   SER I 319      19.378  -4.044 -24.390  1.00  6.81      C    N
ATOM   9268  CA  SER I 319      20.173  -2.837 -24.533  1.00  7.31      C    C
ATOM   9269  CB  SER I 319      21.633  -3.105 -24.159  1.00  7.14      C    C
ATOM   9270  OG  SER I 319      22.309  -1.904 -23.825  1.00  6.84      C    O
ATOM   9271  C   SER I 319      20.069  -2.273 -25.945  1.00  7.93      C    C
ATOM   9272  O   SER I 319      19.736  -2.996 -26.887  1.00  8.65      C    O
ATOM   9273  N   PRO I 320      20.242  -0.952 -26.075  1.00  8.08      C    N
ATOM   9274  CA  PRO I 320      20.052  -0.299 -27.363  1.00  8.34      C    C
ATOM   9275  CB  PRO I 320      20.263   1.187 -27.047  1.00  7.99      C    C
ATOM   9276  CG  PRO I 320      20.887   1.228 -25.680  1.00  8.01      C    C
ATOM   9277  CD  PRO I 320      20.384   0.015 -24.977  1.00  8.10      C    C
ATOM   9278  C   PRO I 320      21.061  -0.770 -28.400  1.00  9.03      C    C
ATOM   9279  O   PRO I 320      22.135  -1.262 -28.053  1.00  8.74      C    O
ATOM   9280  N   LEU I 321      20.711  -0.594 -29.669  1.00 10.31      C    N
ATOM   9281  CA  LEU I 321      21.427  -1.228 -30.766  1.00 11.63      C    C
ATOM   9282  CB  LEU I 321      20.792  -2.576 -31.105  1.00 11.31      C    C
ATOM   9283  CG  LEU I 321      21.681  -3.600 -31.812  1.00 10.97      C    C
ATOM   9284  CD1 LEU I 321      20.835  -4.621 -32.549  1.00 10.04      C    C
ATOM   9285  CD2 LEU I 321      22.652  -2.914 -32.761  1.00 10.69      C    C
```

ATOM 9286 C LEU 1321 21.412 -0.317 -31.989 1.00 12.92 C C
ATOM 9287 O LEU 1321 20.351 0.114 -32.441 1.00 13.29 C O
ATOM 9288 N CYS 1322 22.601 0.013 -32.486 1.00 13.39 C N
ATOM 9289 CA CYS 1322 22.751 0.987 -33.563 1.00 14.16 C C
ATOM 9290 CB CYS 1322 23.359 2.288 -33.036 1.00 13.72 C C
ATOM 9291 SG CYS 1322 22.632 2.898 -31.504 1.00 13.42 C S
ATOM 9292 C CYS 1322 23.622 0.441 -34.690 1.00 15.46 C C
ATOM 9293 O CYS 1322 24.646 -0.196 -34.446 1.00 15.94 C O
ATOM 9294 N THR 1323 23.265 0.802 -35.919 1.00 16.70 C N
ATOM 9295 CA THR 1323 24.152 0.675 -37.075 1.00 17.84 C C
ATOM 9296 CB THR 1323 23.429 1.117 -38.359 1.00 17.50 C C
ATOM 9297 OG1 THR 1323 22.416 2.076 -38.031 1.00 15.70 C O
ATOM 9298 CG2 THR I 323 22.786 -0.076 -39.047 1.00 18.05 C C
ATOM 9299 C THR 1323 25.403 1.536 -36.918 1.00 19.54 C C
ATOM 9300 O THR 1323 25.408 2.477 -36.124 1.00 19.84 C O
ATOM 9301 N THR 1324 26.352 1.379 -37.840 1.00 21.17 C N
ATOM 9302 CA THR 1324 27.430 2.358 -37.967 1.00 22.89 C C
ATOM 9303 CB THR 1324 28.687 1.950 -37.188 1.00 22.69 C C
ATOM 9304 OG1 THR 1324 28.403 0.800 -36.381 1.00 22.10 C O
ATOM 9305 CG2 THR I 324 29.150 3.094 -36.300 1.00 22.03 C C
ATOM 9306 C THR 1324 27.815 2.806 -39.378 1.00 24.39 C C
ATOM 9307 O THR 1324 28.495 3.820 -39.537 1.00 24.53 C O
ATOM 9308 N ASN 1325 27.330 2.106 -40.398 1.00 25.72 C N
ATOM 9309 CA ASN 1325 27.321 2.661 -41.751 1.00 27.01 C C
ATOM 9310 CB ASN 1325 28.628 2.344 -42.484 1.00 27.37 C C
ATOM 9311 CG ASN 1325 29.720 3.360 -42.199 1.00 28.46 C C
ATOM 9312 OD1 ASN I 325 29.982 4.252 -43.007 1.00 30.37 C O
ATOM 9313 ND2 ASN I 325 30.364 3.229 -41.045 1.00 28.78 C N
ATOM 9314 C ASN 1325 26.125 2.199 -42.576 1.00 27.36 C C
ATOM 9315 O ASN 1325 25.455 1.228 -42.226 1.00 27.94 C O
ATOM 9316 N SER I 330 24.776 3.883 -38.461 1.00 35.76 C N
ATOM 9317 CA SER 1330 24.479 5.303 -38.606 1.00 35.01 C C
ATOM 9318 CB SER 1330 24.922 5.803 -39.983 1.00 35.47 C C
ATOM 9319 OG SER 1330 24.296 5.067 -41.019 1.00 33.31 C O
ATOM 9320 C SER 1330 22.992 5.574 -38.405 1.00 34.35 C C
ATOM 9321 O SER 1330 22.148 4.769 -38.798 1.00 34.33 C O
ATOM 9322 N ASN 1331 22.677 6.688 -37.752 1.00 32.48 C N
ATOM 9323 CA ASN 1331 21.365 7.314 -37.886 1.00 30.72 C C
ATOM 9324 CB ASN 1331 21.065 7.642 -39.357 1.00 31.31 C C
ATOM 9325 CG ASN I 331 21.961 8.740 -39.916 1.00 32.11 C C
ATOM 9326 OD1 ASN 1331 22.615 9.469 -39.170 1.00 32.54 C O
ATOM 9327 ND2 ASN I 331 21.941 8.901 -41.235 1.00 31.30 C N
ATOM 9328 C ASN 1331 20.188 6.532 -37.282 1.00 28.71 C C
ATOM 9329 O ASN 1331 19.038 6.940 -37.444 1.00 29.07 C O
ATOM 9330 N ILE 1332 20.450 5.399 -36.629 1.00 25.44 C N
ATOM 9331 CA ILE 1332 19.354 4.517 -36.200 1.00 21.83 C C
ATOM 9332 CB ILE 1332 18.777 3.711 -37.387 1.00 21.42 C C
ATOM 9333 CGI ILE 1332 17.534 2.929 -36.961 1.00 19.89 C C
ATOM 9334 CD1 ILE 1332 16.273 3.385 -37.652 1.00 17.67 C C
ATOM 9335 CG2 ILE 1332 19.828 2.777 -37.965 1.00 20.61 C C
ATOM 9336 C ILE 1332 19.679 3.570 -35.035 1.00 20.37 C C
ATOM 9337 O ILE 1332 20.593 2.751 -35.134 1.00 19.95 C O
ATOM 9338 N CYS 1333 18.816 3.561 -34.019 1.00 18.27 C N
ATOM 9339 CA CYS 1333 18.930 2.597 -32.921 1.00 16.47 C C
ATOM 9340 CB CYS 1333 19.646 3.216 -31.720 1.00 16.14 C C
ATOM 9341 SG CYS 1333 21.144 4.124 -32.136 1.00 17.09 C S
ATOM 9342 C CYS 1333 17.615 1.958 -32.475 1.00 15.73 C C
ATOM 9343 O CYS 1333 16.556 2.586 -32.511 1.00 15.43 C O
ATOM 9344 N LEU 1334 17.761 0.811 -31.819 1.00 15.06 C N
ATOM 9345 CA LEU I 334 16.643 -0.021 -31.394 1.00 13.79 C C

ATOM 9346 CB LEU I 334 16.607 -1.319 -32.203 1.00 13.39 C C
ATOM 9347 CG LEU I 334 16.482 -1.230 -33.725 1.00 13.93 C C
ATOM 9348 CD1 LEU I 334 15.861 -2.496 -34.287 1.00 14.20 C C
ATOM 9349 CD2 LEU I 334 15.686 -0.009 -34.151 1.00 14.52 C C
ATOM 9350 C LEU 1334 16.852 -0.366 -29.928 1.00 13.22 C C
ATOM 9351 O LEU 1334 17.968 -0.685 -29.520 1.00 13.31 C O
ATOM 9352 N THR 1335 15.768 -0.423 -29.167 1.00 12.58 C N
ATOM 9353 CA THR I 335 15.790 -1.126 -27.892 1.00 12.17 C C
ATOM 9354 CB THR 1335 15.955 -0.158 -26.706 1.00 12.02 C C
ATOM 9355 OG1 THR I 335 16.652 1.018 -27.139 1.00 12.64 C O
ATOM 9356 CG2 THR I 335 16.739 -0.825 -25.582 1.00 11.47 C C
ATOM 9357 C THR 1335 14.523 -1.942 -27.703 1.00 11.97 C C
ATOM 9358 O THR 1335 13.423 -1.471 -27.990 1.00 11.93 C O
ATOM 9359 N ARG I 336 14.700 -3.216 -27.379 1.00 11.60 C N
ATOM 9360 CA ARG I 336 13.573 -4.131 -27.260 1.00 12.15 C C
ATOM 9361 CB ARG I 336 14.066 -5.579 -27.235 1.00 12.16 C C
ATOM 9362 CG ARG I 336 13.124 -6.566 -27.906 1.00 12.67 C C
ATOM 9363 CD ARG I 336 13.876 -7.491 -28.846 1.00 12.52 C C
ATOM 9364 NE ARG I 336 14.414 -8.649 -28.144 1.00 12.35 C N
ATOM 9365 CZ ARG 1336 13.675 -9.665 -27.713 1.00 12.54 C C
ATOM 9366 NH1 ARG I 336 12.384 -9.718 -28.013 1.00 12.38 C N
ATOM 9367 NH2 ARG I 336 14.249 -10.681 -27.084 1.00 12.48 C N
ATOM 9368 C ARG 1336 12.761 -3.833 -26.004 1.00 12.71 C C
ATOM 9369 O ARG 1336 13.272 -3.932 -24.890 1.00 12.62 C O
ATOM 9370 N THR 1337 11.501 -3.457 -26.186 1.00 13.70 C N
ATOM 9371 CA THR 1337 10.696 -2.998 -25.065 1.00 14.91 C C
ATOM 9372 CB THR I 337 9.353 -2.405 -25.516 1.00 15.27 C C
ATOM 9373 OG1 THR I 337 9.571 -1.474 -26.584 1.00 16.65 C O
ATOM 9374 CG2 THR I 337 8.694 -1.678 -24.356 1.00 15.94 C C
ATOM 9375 C THR 1337 10.438 -4.115 -24.064 1.00 15.16 C C
ATOM 9376 O THR 1337 10.515 -3.902 -22.857 1.00 15.60 C O
ATOM 9377 N ASP 1338 10.036 -5.277 -24.566 1.00 15.15 C N
ATOM 9378 CA ASP I 338 9.394 -6.289 -23.732 1.00 15.52 C C
ATOM 9379 CB ASP I 338 8.653 -7.306 -24.602 1.00 16.81 C C
ATOM 9380 CG ASP I 338 9.242 -7.417 -26.000 1.00 20.57 C C
ATOM 9381 OD1 ASP I 338 8.554 -7.950 -26.895 1.00 23.00 C O
ATOM 9382 OD2 ASP I 338 10.395 -6.981 -26.200 1.00 22.92 C O
ATOM 9383 C ASP 1338 10.402 -7.004 -22.837 1.00 14.21 C C
ATOM 9384 O ASP 1338 10.930 -8.057 -23.196 1.00 14.00 C O
ATOM 9385 N ARG 1339 10.654 -6.432 -21.664 1.00 12.79 C N
ATOM 9386 CA ARG I 339 11.678 -6.949 -20.764 1.00 11.71 C C
ATOM 9387 CB ARG 1339 12.488 -5.810 -20.163 1.00 11.73 C C
ATOM 9388 CG ARG 1339 13.374 -5.080 -21.129 1.00 12.49 C C
ATOM 9389 CD ARG 1339 14.312 -4.211 -20.346 1.00 13.24 C C
ATOM 9390 NE ARG I 339 14.580 -2.944 -21.005 1.00 12.04 C N
ATOM 9391 CZ ARG 1339 15.717 -2.282 -20.858 1.00 11.74 C C
ATOM 9392 NH1 ARG I 339 16.664 -2.771 -20.072 1.00 13.43 C N
ATOM 9393 NH2 ARG I 339 15.904 -1.125 -21.475 1.00 9.80 C N
ATOM 9394 C ARG I 339 11.062 -7.727 -19.622 1.00 11.16 C C
ATOM 9395 O ARG 1339 10.029 -7.326 -19.087 1.00 11.37 C O
ATOM 9396 N GLY 1340 11.892 -8.572 -19.027 1.00 10.43 C N
ATOM 9397 CA GLY 1340 11.574 -9.178 -17.749 1.00 9.52 C C
ATOM 9398 C GLY 1340 11.463 -10.678 -17.876 1.00 8.80 C C
ATOM 9399 O GLY 1340 12.269 -11.313 -18.555 1.00 8.56 C O
ATOM 9400 N TRP I 341 10.532 -11.257 -17.129 1.00 8.25 C N
ATOM 9401 CA TRP I 341 10.462 -12.699 -17.005 1.00 7.98 C C
ATOM 9402 CB TRP I 341 10.018 -13.097 -15.605 1.00 7.79 C C
ATOM 9403 CG TRP I 341 11.120 -13.020 -14.622 1.00 7.67 C C
ATOM 9404 CD1 TRP I 341 11.382 -11.986 -13.775 1.00 8.12 C C
ATOM 9405 NE1 TRP I 341 12.511 -12.252 -13.042 1.00 8.60 C N

ATOM 9406 CE2 TRP I 341 13.037 -13.447 -13.459 1.00 7.57 C C
ATOM 9407 CD2 TRP I 341 12.217 -13.931 -14.495 1.00 7.52 C C
ATOM 9408 CE3 TRP I 341 12.541 -15.150 -15.098 1.00 7.86 C C
ATOM 9409 CZ3 TRP I 341 13.653 -15.837 -14.650 1.00 7.14 C C
ATOM 9410 CH2 TRP I 341 14.457 -15.323 -13.625 1.00 6.39 C C
ATOM 9411 CZ2 TRP I 341 14.164 -14.134 -13.017 1.00 7.30 C C
ATOM 9412 C TRP I 341 9.525 -13.288 -18.037 1.00 8.26 C C
ATOM 9413 O TRP I 341 8.322 -13.022 -18.031 1.00 8.35 C O
ATOM 9414 N TYR I 342 10.085 -14.100 -18.922 1.00 8.44 C N
ATOM 9415 CA TYR I 342 9.308 -15.102 -19.616 1.00 8.53 C C
ATOM 9416 CB TYR I 342 9.755 -15.202 -21.069 1.00 8.43 C C
ATOM 9417 CG TYR I 342 9.687 -13.885 -21.793 1.00 9.17 C C
ATOM 9418 CD1 TYR I 342 10.592 -12.874 -21.499 1.00 10.32 C C
ATOM 9419 CE1 TYR I 342 10.474 -11.625 -22.068 1.00 10.99 C C
ATOM 9420 CZ TYR I 342 9.395 -11.349 -22.873 1.00 11.00 C C
ATOM 9421 OH TYR I 342 9.267 -10.102 -23.435 1.00 12.82 C O
ATOM 9422 CE2 TYR I 342 8.433 -12.307 -23.105 1.00 10.67 C C
ATOM 9423 CD2 TYR I 342 8.569 -13.555 -22.542 1.00 10.41 C C
ATOM 9424 C TYR I 342 9.469 -16.437 -18.925 1.00 8.64 C C
ATOM 9425 O TYR I 342 10.376 -16.628 -18.115 1.00 8.40 C O
ATOM 9426 N CYS I 343 8.558 -17.351 -19.224 1.00 8.87 C N
ATOM 9427 CA CYS I 343 8.370 -18.516 -18.389 1.00 9.35 C C
ATOM 9428 CB CYS I 343 8.266 -18.116 -16.915 1.00 9.17 C C
ATOM 9429 SG CYS I 343 8.138 -19.512 -15.769 1.00 11.88 C S
ATOM 9430 C CYS I 343 7.151 -19.312 -18.831 1.00 9.42 C C
ATOM 9431 O CYS I 343 6.039 -18.788 -18.900 1.00 9.96 C O
ATOM 9432 N ASP I 344 7.408 -20.545 -19.254 1.00 9.36 C N
ATOM 9433 CA ASP I 344 6.483 -21.302 -20.083 1.00 9.24 C C
ATOM 9434 CB ASP I 344 7.122 -22.628 -20.500 1.00 9.34 C C
ATOM 9435 CG ASP I 344 7.796 -22.551 -21.856 1.00 10.72 C C
ATOM 9436 OD1 ASP I 344 7.123 -22.161 -22.833 1.00 13.93 C O
ATOM 9437 OD2 ASP I 344 9.003 -22.864 -21.942 1.00 11.87 C O
ATOM 9438 C ASP I 344 5.198 -21.576 -19.320 1.00 9.09 C C
ATOM 9439 O ASP I 344 5.233 -22.061 -18.192 1.00 9.39 C O
ATOM 9440 N ASN I 345 4.067 -21.385 -19.988 1.00 9.13 C N
ATOM 9441 CA ASN I 345 2.801 -21.924 -19.510 1.00 9.52 C C
ATOM 9442 CB ASN I 345 1.770 -20.804 -19.361 1.00 9.61 C C
ATOM 9443 CG ASN I 345 0.742 -21.101 -18.293 1.00 9.21 C C
ATOM 9444 OD1 ASN I 345 1.075 -21.251 -17.118 1.00 6.21 C O
ATOM 9445 ND2 ASN I 345 -0.511 -21.247 -18.706 1.00 11.05 C N
ATOM 9446 C ASN I 345 2.271 -23.022 -20.427 1.00 10.06 C C
ATOM 9447 O ASN I 345 3.005 -23.546 -21.267 1.00 11.10 C O
ATOM 9448 N ALA I 346 1.017 -23.411 -20.223 1.00 9.74 C N
ATOM 9449 CA ALA I 346 0.416 -24.492 -20.998 1.00 9.58 C C
ATOM 9450 CB ALA I 346 -1.062 -24.635 -20.650 1.00 9.60 C C
ATOM 9451 C ALA I 346 0.593 -24.278 -22.502 1.00 9.66 C C
ATOM 9452 O ALA I 346 -0.241 -23.639 -23.145 1.00 9.39 C O
ATOM 9453 N GLY I 347 1.655 -24.849 -23.065 1.00 10.04 C N
ATOM 9454 CA GLY I 347 1.836 -24.857 -24.513 1.00 10.68 C C
ATOM 9455 C GLY I 347 1.879 -23.454 -25.085 1.00 10.90 C C
ATOM 9456 O GLY I 347 1.661 -23.251 -26.280 1.00 11.46 C O
ATOM 9457 N SER I 348 2.016 -22.477 -24.193 1.00 10.30 C N
ATOM 9458 CA SER I 348 2.256 -21.088 -24.567 1.00 9.94 C C
ATOM 9459 CB SER I 348 0.933 -20.322 -24.613 1.00 9.88 C C
ATOM 9460 OG SER I 348 0.000 -20.969 -25.461 1.00 10.09 C O
ATOM 9461 C SER I 348 3.194 -20.462 -23.538 1.00 9.60 C C
ATOM 9462 O SER I 348 3.700 -21.157 -22.660 1.00 9.59 C O
ATOM 9463 N VAL I 349 3.494 -19.178 -23.689 1.00 9.54 C N
ATOM 9464 CA VAL I 349 4.452 -18.532 -22.800 1.00 9.56 C C
ATOM 9465 CB VAL I 349 5.700 -18.047 -23.558 1.00 9.28 C C

ATOM 9466 CGI VAL I 349 6.722 -17.476 -22.589 1.00 9.24 C c
ATOM 9467 CG2 VAL I 349 6.303 -19.183 -24.370 1.00 9.94 c c
ATOM 9468 C VAL I 349 3.832 -17.367 -22.041 1.00 9.59 c c
ATOM 9469 O VAL I 349 3.179 -16.506 -22.631 1.00 9.69 c o
ATOM 9470 N SER I 350 4.073 -17.326 -20.735 1.00 9.93 c N
ATOM 9471 CA SER I 350 3.559 -16.252 -19.896 1.00 10.44 c c
ATOM 9472 CB SER I 350 2.926 -16.815 -18.620 1.00 10.04 c c
ATOM 9473 OG SER I 350 1.578 -17.196 -18.841 1.00 8.41 c o
ATOM 9474 C SER I 350 4.629 -15.218 -19.557 1.00 11.45 c c
ATOM 9475 O SER I 350 5.746 -15.561 -19.168 1.00 11.58 c o
ATOM 9476 N PHE I 351 4.259 -13.948 -19.679 1.00 12.28 c N
ATOM 9477 CA PHE I 351 5.200 -12.847 -19.543 1.00 13.04 c c
ATOM 9478 CB PHE I 351 5.320 -12.089 -20.867 1.00 12.87 c c
ATOM 9479 CG PHE I 351 6.094 -10.809 -20.763 1.00 13.52 c c
ATOM 9480 CD1 PHE I 351 7.344 -10.788 -20.172 1.00 13.76 c c
ATOM 9481 CE1 PHE I 351 8.066 -9.613 -20.085 1.00 14.10 c c
ATOM 9482 CZ PHE I 351 7.541 -8.442 -20.588 1.00 14.07 c c
ATOM 9483 CE2 PHE I 351 6.305 -8.452 -21.197 1.00 14.14 c c
ATOM 9484 CD2 PHE I 351 5.580 -9.629 -21.270 1.00 13.92 c c
ATOM 9485 C PHE I 351 4.742 -11.899 -18.441 1.00 13.84 c c
ATOM 9486 O PHE I 351 3.579 -11.499 -18.394 1.00 13.96 c o
ATOM 9487 N PHE I 352 5.655 -11.574 -17.534 1.00 14.72 c N
ATOM 9488 CA PHE I 352 5.344 -10.699 -16.412 1.00 15.98 c c
ATOM 9489 CB PHE I 352 5.570 -11.435 -15.093 1.00 15.75 c c
ATOM 9490 CG PHE I 352 5.295 -12.909 -15.169 1.00 15.51 c c
ATOM 9491 CD1 PHE I 352 6.188 -13.762 -15.803 1.00 15.05 c c
ATOM 9492 CE1 PHE I 352 5.926 -15.116 -15.902 1.00 14.05 c c
ATOM 9493 CZ PHE I 352 4.745 -15.624 -15.402 1.00 13.28 c c
ATOM 9494 CE2 PHE I 352 3.833 -14.777 -14.796 1.00 13.71 c c
ATOM 9495 CD2 PHE I 352 4.099 -13.425 -14.704 1.00 14.94 c c
ATOM 9496 C PHE I 352 6.195 -9.438 -16.453 1.00 17.56 c c
ATOM 9497 O PHE I 352 7.419 -9.509 -16.360 1.00 17.74 c o
ATOM 9498 N PRO I 353 5.541 -8.271 -16.525 1.00 19.05 c N
ATOM 9499 CA PRO I 353 6.188 -7.074 -17.055 1.00 20.40 c c
ATOM 9500 CB PRO I 353 5.010 -6.146 -17.365 1.00 20.26 c c
ATOM 9501 CG PRO I 353 3.839 -7.052 -17.522 1.00 19.71 c c
ATOM 9502 CD PRO I 353 4.073 -8.155 -16.545 1.00 18.97 c c
ATOM 9503 C PRO I 353 7.136 -6.408 -16.058 1.00 21.94 c c
ATOM 9504 O PRO I 353 8.087 -5.745 -16.470 1.00 22.29 c o
ATOM 9505 N GLN I 354 6.858 -6.544 -14.763 1.00 23.38 c N
ATOM 9506 CA GLN I 354 7.646 -5.847 -13.743 1.00 24.64 c c
ATOM 9507 CB GLN I 354 6.943 -4.569 -13.274 1.00 24.93 c c
ATOM 9508 CG GLN I 354 5.458 -4.509 -13.587 1.00 26.00 c c
ATOM 9509 CD GLN I 354 4.646 -5.481 -12.756 1.00 25.92 c c
ATOM 9510 OE1 GLN I 354 4.710 -5.474 -11.527 1.00 25.67 c o
ATOM 9511 NE2 GLN I 354 3.870 -6.324 -13.427 1.00 24.27 c N
ATOM 9512 C GLN I 354 8.048 -6.707 -12.543 1.00 24.85 c c
ATOM 9513 O GLN I 354 7.280 -7.556 -12.088 1.00 24.51 c o
ATOM 9514 N ALA I 355 9.200 -6.384 -11.959 1.00 25.22 c N
ATOM 9515 CA ALA I 355 9.818 -7.215 -10.926 1.00 25.34 c c
ATOM 9516 CB ALA I 355 10.949 -6.458 -10.245 1.00 25.09 c c
ATOM 9517 C ALA I 355 8.809 -7.711 -9.892 1.00 24.92 c c
ATOM 9518 O ALA I 355 8.679 -8.915 -9.669 1.00 25.23 c o
ATOM 9519 N GLU I 356 8.278 -6.771 -9.115 1.00 23.93 c N
ATOM 9520 CA GLU I 356 7.089 -6.998 -8.295 1.00 22.77 c c
ATOM 9521 CB GLU I 356 5.993 -5.995 -8.658 1.00 23.22 c c
ATOM 9522 CG GLU I 356 6.412 -4.545 -8.500 1.00 26.33 c c
ATOM 9523 CD GLU I 356 7.250 -4.314 -7.258 1.00 30.93 c c
ATOM 9524 OE1 GLU I 356 8.490 -4.231 -7.380 1.00 31.97 c o
ATOM 9525 OE2 GLU I 356 6.668 -4.227 -6.156 1.00 32.21 c o

ATOM 9526 C GLU I 356 6.547 -8.419 -8.377 1.00 21.31 C c
ATOM 9527 O GLU I 356 6.338 -9.070 -7.354 1.00 21.01 c o
ATOM 9528 N THR I 357 6.137 -8.809 -9.577 1.00 19.51 c N
ATOM 9529 CA THR I 357 5.358 -10.023 -9.766 1.00 17.55 c c
ATOM 9530 CB THR I 357 4.829 -10.115 -11.207 1.00 17.30 c c
ATOM 9531 OG1 THR I 357 5.071 -8.873 -11.882 1.00 17.32 c o
ATOM 9532 CG2 THR I 357 3.335 -10.387 -11.203 1.00 17.72 c: c
ATOM 9533 C THR I 357 6.178 -11.268 -9.433 1.00 16.62 c c
ATOM 9534 O THR I 357 5.631 -12.286 -9.008 1.00 17.29 c o
ATOM 9535 N CYS I 358 7.498 -11.146 -9.526 1.00 14.88 c N
ATOM 9536 CA CYS I 358 8.365 -12.317 -9.566 1.00 13.15 c c
ATOM 9537 CB CYS I 358 8.955 -12.501 -10.961 1.00 13.04 c c
ATOM 9538 SG CYS I 358 7.735 -12.899 -12.228 1.00 14.02 c s
ATOM 9539 C CYS I 358 9.478 -12.255 -8.529 1.00 12.08 c c
ATOM 9540 O CYS I 358 10.186 -11.252 -8.417 1.00 12.15 c o
ATOM 9541 N LYS I 359 9.640 -13.345 -7.788 1.00 11.35 c N
ATOM 9542 CA LYS I 359 10.793 -13.519 -6.918 1.00 11.01 c c
ATOM 9543 CB LYS I 359 10.349 -13.675 -5.460 1.00 11.16 c c
ATOM 9544 CG LYS I 359 8.858 -13.470 -5.229 1.00 13.28 c c
ATOM 9545 CD LYS I 359 8.607 -12.427 -4.150 1.00 16.11 c c
ATOM 9546 CE LYS I 359 7.124 -12.287 -3.850 1.00 17.91 c c
ATOM 9547 NZ LYS I 359 6.818 -11.012 -3.145 1.00 20.99 c N
ATOM 9548 C LYS I 359 11.592 -14.739 -7.349 1.00 10.46 c c
ATOM 9549 O LYS I 359 11.091 -15.589 -8.085 1.00 10.70 c o
ATOM 9550 N VAL I 360 12.791 -14.880 -6.798 1.00 9.99 c N
ATOM 9551 CA VAL I 360 13.720 -15.885 -7.282 1.00 9.84 c c
ATOM 9552 CB VAL I 360 14.452 -15.412 -8.541 1.00 9.42 c c
ATOM 9553 CGI VAL I 360 15.135 -14.066 -8.288 1.00 10.07 c c
ATOM 9554 CG2 VAL I 360 15.454 -16.473 -8.996 1.00 9.56 c c
ATOM 9555 C VAL I 360 14.738 -16.297 -6.229 1.00 9.98 c c
ATOM 9556 O VAL I 360 15.380 -15.457 -5.598 1.00 9.96 c o
ATOM 9557 N GLN I 361 14.900 -17.604 -6.071 1.00 10.39 c N
ATOM 9558 CA GLN I 361 15.781 -18.150 -5.052 1.00 11.53 c c
ATOM 9559 CB GLN I 361 14.966 -18.692 -3.880 1.00 12.03 c c
ATOM 9560 CG GLN I 361 15.810 -19.254 -2.750 1.00 16.44 c c
ATOM 9561 CD GLN I 361 15.388 -18.722 -1.398 1.00 25.16 c c
ATOM 9562 OE1 GLN I 361 14.773 -19.434 -0.604 1.00 29.01 c: o
ATOM 9563 NE2 GLN I 361 15.686 -17.453 -1.141 1.00 27.20 c: N
ATOM 9564 C GLN I 361 16.613 -19.271 -5.641 1.00 11.15 c c
ATOM 9565 O GLN I 361 16.114 -20.375 -5.854 1.00 11.80 c o
ATOM 9566 N SER I 362 17.877 -18.986 -5.925 1.00 10.90 c N
ATOM 9567 CA SER I 362 18.671 -19.921 -6.695 1.00 10.30 c c
ATOM 9568 CB SER I 362 18.610 -21.302 -6.040 1.00 10.47 c c
ATOM 9569 OG SER I 362 19.659 -22.138 -6.491 1.00 11.17 c o
ATOM 9570 C SER I 362 18.088 -19.980 -8.103 1.00 9.58 c c
ATOM 9571 O SER I 362 17.759 -18.946 -8.683 1.00 9.48 c o
ATOM 9572 N ASN I 363 17.806 -21.188 -8.577 1.00 9.12 c N
ATOM 9573 CA ASN I 363 17.229 -21.365 -9.904 1.00 8.73 c c
ATOM 9574 CB ASN I 363 17.821 -22.602 -10.568 1.00 9.01 c c
ATOM 9575 CG ASN I 363 17.547 -23.864 -9.781 1.00 9.29 c c
ATOM 9576 OD1 ASN I 363 16.903 -23.826 -8.732 1.00 9.82 c o
ATOM 9577 ND2 ASN I 363 17.981 -25.000 -10.314 1.00 10.08 C N
ATOM 9578 C ASN I 363 15.716 -21.503 -9.827 1.00 8.12 c c
ATOM 9579 O ASN I 363 15.084 -22.042 -10.736 1.00 8.10 c o
ATOM 9580 N ARG I 364 15.168 -21.165 -8.665 1.00 7.20 c N
ATOM 9581 CA ARG I 364 13.731 -21.222 -8.445 1.00 6.82 c c
ATOM 9582 CB ARG I 364 13.427 -21.658 -7.012 1.00 6.91 c c
ATOM 9583 CG ARG I 364 12.287 -22.649 -6.908 1.00 7.92 c c
ATOM 9584 CD ARG I 364 12.520 -23.817 -7.843 1.00 8.20 c c
ATOM 9585 NE ARG I 364 11.374 -24.061 -8.711 1.00 8.70 c N

ATOM 9586 CZ ARG I 364 11.056 -25.255 -9.196 1.00 8.88 C C
ATOM 9587 NH1 ARG I 364 11.800 -26.309 -8.894 1.00 8.57 C N
ATOM 9588 NH2 ARG I 364 9.976 -25.403 -9.950 1.00 10.59 C N
ATOM 9589 C ARG I 364 13.110 -19.861 -8.694 1.00 6.58 C C
ATOM 9590 O ARG I 364 13.540 -18.861 -8.121 1.00 6.65 C O
ATOM 9591 N VAL I 365 12.031 -19.846 -9.466 1.00 6.64 C N
ATOM 9592 CA VAL I 365 11.325 -18.609 -9.756 1.00 6.54 C C
ATOM 9593 CB VAL I 365 11.399 -18.261 -11.254 1.00 5.95 C C
ATOM 9594 CGI VAL I 365 10.374 -17.196 -11.608 1.00 5.48 C C
ATOM 9595 CG2 VAL I 365 12.801 -17.804 -11.623 1.00 6.22 C C
ATOM 9596 C VAL 1365 9.866 -18.723 -9.335 1.00 7.35 C C
ATOM 9597 O VAL 1365 9.271 -19.799 -9.416 1.00 8.33 C O
ATOM 9598 N PHE I 366 9.309 -17.619 -8.843 1.00 7.37 C N
ATOM 9599 CA PHE I 366 7.919 -17.584 -8.401 1.00 7.44 C C
ATOM 9600 CB PHE I 366 7.840 -17.604 -6.875 1.00 7.30 C C
ATOM 9601 CG PHE I 366 8.426 -18.834 -6.255 1.00 6.70 C C
ATOM 9602 CD1 PHE I 366 9.799 -18.991 -6.163 1.00 6.70 C C
ATOM 9603 CE1 PHE I 366 10.345 -20.120 -5.588 1.00 5.94 C C
ATOM 9604 CZ PHE I 366 9.520 -21.083 -5.055 1.00 5.71 C C
ATOM 9605 CE2 PHE I 366 8.149 -20.934 -5.130 1.00 5.96 C C
ATOM 9606 CD2 PHE I 366 7.609 -19.805 -5.710 1.00 6.52 C C
ATOM 9607 C PHE 1366 7.236 -16.335 -8.919 1.00 7.45 C C
ATOM 9608 O PHE I 366 7.530 -15.225 -8.476 1.00 7.45 C O
ATOM 9609 N CYS I 367 6.282 -16.524 -9.819 1.00 8.00 C N
ATOM 9610 CA CYS I 367 5.626 -15.400 -10.450 1.00 8.90 C C
ATOM 9611 CB CYS I 367 5.985 -15.338 -11.934 1.00 9.46 C C
ATOM 9612 SG CYS I 367 7.712 -14.929 -12.259 1.00 10.79 C S
ATOM 9613 C CYS 1367 4.121 -15.484 -10.268 1.00 9.09 C C
ATOM 9614 O CYS I 367 3.591 -16.493 -9.799 1.00 9.24 C O
ATOM 9615 N ASP 1368 3.449 -14.382 -10.568 1.00 9.54 C N
ATOM 9616 CA ASP I 368 2.034 -14.255 -10.285 1.00 10.55 C C
ATOM 9617 CB ASP I 368 1.792 -13.067 -9.349 1.00 10.53 C C
ATOM 9618 CG ASP I 368 0.421 -13.102 -8.698 1.00 11.11 C C
ATOM 9619 OD1 ASP I 368 -0.574 -13.335 -9.415 1.00 11.42 C O
ATOM 9620 OD2 ASP I 368 0.323 -12.765 -7.499 1.00 11.35 C O
ATOM 9621 C ASP 1368 1.266 -14.073 -11.590 1.00 11.45 C C
ATOM 9622 O ASP 1368 1.418 -13.061 -12.274 1.00 12.05 C O
ATOM 9623 N THR 1369 0.563 -15.122 -12.003 1.00 12.41 C N
ATOM 9624 CA THR 1369 -0.399 -15.013 -13.089 1.00 13.00 C C
ATOM 9625 CB THR 1369 -1.513 -16.063 -12.953 1.00 12.69 C C
ATOM 9626 OG1 THR I 369 -0.935 -17.374 -12.929 1.00 11.72 C O
ATOM 9627 CG2 THR I 369 -2.488 -15.962 -14.115 1.00 13.33 C C
ATOM 9628 C THR 1369 -1.034 -13.632 -13.093 1.00 14.13 C C
ATOM 9629 O THR 1369 -0.895 -12.874 -14.051 1.00 14.72 C O
ATOM 9630 N MET 1370 -1.675 -13.289 -11.984 1.00 15.25 C N
ATOM 9631 CA MET 1370 -2.681 -12.240 -11.975 1.00 16.60 C C
ATOM 9632 CB MET 1370 -2.538 -11.361 -10.734 1.00 17.42 C C
ATOM 9633 CG MET I 370 -3.744 -11.411 -9.811 1.00 20.31 C C
ATOM 9634 SD MET 1370 -5.284 -10.974 -10.642 1.00 26.43 C S
ATOM 9635 CE MET I 370 -5.320 -12.185 -11.963 1.00 24.07 C C
ATOM 9636 C MET 1370 -2.700 -11.396 -13.249 1.00 16.54 C C
ATOM 9637 O MET 1370 -3.707 -11.367 -13.953 1.00 16.74 C O
ATOM 9638 N ASN I 371 -1.610 -10.691 -13.540 1.00 16.35 C N
ATOM 9639 CA ASN I 371 -1.614 -9.772 -14.680 1.00 16.07 C C
ATOM 9640 CB ASN I 371 -1.375 -8.326 -14.232 1.00 16.41 C C
ATOM 9641 CG ASN I 371 -2.619 -7.690 -13.634 1.00 16.71 C C
ATOM 9642 OD1 ASN I 371 -3.501 -7.228 -14.356 1.00 15.75 C O
ATOM 9643 ND2 ASN I 371 -2.722 -7.724 -12.310 1.00 17.76 C N
ATOM 9644 C ASN I 371 -0.698 -10.167 -15.842 1.00 15.55 C C
ATOM 9645 O ASN I 371 -0.650 -9.478 -16.862 1.00 15.84 C O

```
ATOM   9646  N   SER I 372     -0.166 -11.383 -15.771  1.00 14.76      C    N
ATOM   9647  CA  SER I 372      0.540 -11.990 -16.894  1.00 13.91      c    c
ATOM   9648  CB  SER I 372      0.561 -13.512 -16.746  1.00 14.04      c    c
ATOM   9649  OG  SER I 372     -0.696 -14.071 -17.084  1.00 15.09      c    o
ATOM   9650  C   SER I 372     -0.071 -11.614 -18.242  1.00 13.07      c    c
ATOM   9651  O   SER I 372     -1.291 -11.511 -18.373  1.00 13.02      c    o
ATOM   9652  N   LEU I 373      0.781 -11.525 -19.263  1.00 12.23      c    N
ATOM   9653  CA  LEU I 373      0.352 -11.621 -20.658  1.00 11.45      c    c
ATOM   9654  CB  LEU I 373      0.999 -10.504 -21.485  1.00 11.43      c    c
ATOM   9655  CG  LEU I 373      0.250  -9.176 -21.636  1.00 11.04      c    c
ATOM   9656  CD1 LEU I 373     -0.580  -8.867 -20.406  1.00 11.76      c    c
ATOM   9657  CD2 LEU I 373      1.213  -8.035 -21.928  1.00 10.49      c    c
ATOM   9658  C   LEU I 373      0.727 -12.982 -21.247  1.00 11.17      c    c
ATOM   9659  O   LEU I 373      1.819 -13.492 -21.000  1.00 11.27      c    o
ATOM   9660  N   THR I 374     -0.164 -13.546 -22.056  1.00 10.70      c    N
ATOM   9661  CA  THR I 374      0.062 -14.869 -22.633  1.00 10.23      c    c
ATOM   9662  CB  THR I 374     -1.187 -15.768 -22.531  1.00 10.24      c    c
ATOM   9663  OG1 THR I 374     -1.999 -15.346 -21.429  1.00 11.25      c    o
ATOM   9664  CG2 THR I 374     -0.785 -17.224 -22.338  1.00 10.52      c:   c
ATOM   9665  C   THR I 374      0.481 -14.772 -24.091  1.00  9.54      c    c
ATOM   9666  O   THR I 374     -0.164 -14.097 -24.893  1.00  9.70      c    o
ATOM   9667  N   LEU I 375      1.576 -15.444 -24.422  1.00  8.83      c    N
ATOM   9668  CA  LEU I 375      2.236 -15.253 -25.704  1.00  7.83      c    c
ATOM   9669  CB  LEU I 375      3.470 -14.361 -25.547  1.00  7.38      c    c
ATOM   9670  CG  LEU I 375      3.309 -13.047 -24.780  1.00  5.06      c    c
ATOM   9671  CD1 LEU I 375      4.669 -12.411 -24.533  1.00  2.41      c    c
ATOM   9672  CD2 LEU I 375      2.397 -12.098 -25.535  1.00  4.31      c    c
ATOM   9673  C   LEU I 375      2.644 -16.600 -26.283  1.00  7.79      c    c
ATOM   9674  O   LEU I 375      2.703 -17.598 -25.565  1.00  7.92      c    o
ATOM   9675  N   PRO I 376      2.914 -16.629 -27.595  1.00  7.51      c    N
ATOM   9676  CA  PRO I 376      3.325 -17.826 -28.323  1.00  7.90      c    c
ATOM   9677  CB  PRO I 376      2.852 -17.538 -29.748  1.00  7.90      c    c
ATOM   9678  CG  PRO I 376      2.913 -16.062 -29.858  1.00  7.97      c    c
ATOM   9679  CD  PRO I 376      2.537 -15.534 -28.505  1.00  7.40      c    c
ATOM   9680  C   PRO I 376      4.838 -18.023 -28.310  1.00  8.35      c    c
ATOM   9681  O   PRO I 376      5.589 -17.062 -28.484  1.00  8.71      c    o
ATOM   9682  N   SER I 377      5.263 -19.283 -28.263  1.00  9.11      c    N
ATOM   9683  CA  SER I 377      6.682 -19.622 -28.207  1.00  9.91      c    c
ATOM   9684  CB  SER I 377      6.880 -21.137 -28.330  1.00 10.23      c    c
ATOM   9685  OG  SER I 377      5.713 -21.842 -27.939  1.00 10.90      c    o
ATOM   9686  C   SER I 377      7.438 -18.911 -29.319  1.00 10.14      c    c
ATOM   9687  O   SER I 377      8.660 -19.024 -29.425  1.00 10.08      c    o
ATOM   9688  N   GLU I 378      6.683 -18.286 -30.215  1.00 10.71      c    N
ATOM   9689  CA  GLU I 378      7.256 -17.563 -31.339  1.00 11.40      c    c
ATOM   9690  CB  GLU I 378      6.177 -17.256 -32.379  1.00 11.65      c    c
ATOM   9691  CG  GLU I 378      5.858 -18.418 -33.312  1.00 13.46      c    c
ATOM   9692  CD  GLU I 378      5.249 -19.608 -32.588  1.00 16.20      c    c
ATOM   9693  OE1 GLU I 378      4.999 -19.505 -31.368  1.00 15.73      c    o
ATOM   9694  OE2 GLU I 378      4.989 -20.636 -33.250  1.00 18.38      c    o
ATOM   9695  C   GLU I 378      7.922 -16.274 -30.873  1.00 11.27      c    c
ATOM   9696  O   GLU I 378      8.776 -15.722 -31.567  1.00 11.28      c    o
ATOM   9697  N   VAL I 379      7.570 -15.827 -29.672  1.00 11.31      c    N
ATOM   9698  CA  VAL I 379      8.268 -14.708 -29.056  1.00 11.59      c    c
ATOM   9699  CB  VAL I 379      7.849 -14.504 -27.591  1.00 11.27      c    c
ATOM   9700  CGI VAL I 379      8.894 -13.674 -26.858  1.00 11.60      c:   c
ATOM   9701  CG2 VAL I 379      6.486 -13.833 -27.520  1.00 11.54      c:   c
ATOM   9702  C   VAL I 379      9.779 -14.907 -29.124  1.00 12.16      c    c
ATOM   9703  O   VAL I 379     10.533 -13.943 -29.255  1.00 12.51      c    o
ATOM   9704  N   ASN I 380     10.219 -16.158 -29.030  1.00 12.98      c    N
ATOM   9705  CA  ASN I 380     11.637 -16.453 -28.854  1.00 14.00      c    c
```

ATOM 9706 CB ASN I 380 11.854 -17.947 -28.579 1.00 14.59 C C
ATOM 9707 CG ASN 1 380 11.318 -18.381 -27.224 1.00 17.09 C C
ATOM 9708 OD1 ASN I 380 12.070 -18.488 -26.256 1.00 20.41 C O
ATOM 9709 ND2 ASN I 380 10.045 -18.763 -27.186 1.00 18.86 C N
ATOM 9710 C ASN 1 380 12.477 -16.006 -30.051 1.00 13.96 C C
ATOM 971 1 O ASN 1 380 13.619 -15.576 -29.890 1.00 14.38 C O
ATOM 9712 N LEU I 381 11.925 -16. 159 -31.252 1.00 13.61 C N
ATOM 9713 CA LEU I 381 12.638 -15.798 -32.475 1.00 13.72 C C
ATOM 9714 CB LEU I 381 11.742 -15.996 -33.698 1.00 13.79 C C
ATOM 9715 CG LEU I 381 10.720 -17.130 -33.607 1.00 14.92 C C
ATOM 9716 CD1 LEU I 381 9.817 -17.138 -34.830 1.00 15.56 C C
ATOM 9717 CD2 LEU I 381 11.421 -18.470 -33.446 1.00 15.78 C C
ATOM 9718 C LEU 1 381 13.093 -14.349 -32.401 1.00 13.62 C C
ATOM 9719 O LEU 1 381 14.017 -13.934 -33. 100 1.00 13.57 C O
ATOM 9720 N CYS 1 382 12.473 -13.607 -31.494 1.00 13.47 C N
ATOM 9721 CA CYS I 382 12.727 -12.187 -31.357 1.00 13.57 C C
ATOM 9722 CB CYS I 382 11.613 - 11.538 -30.545 1.00 13.62 C C
ATOM 9723 SG CYS I 382 10.346 -10.770 -31.551 1.00 15.64 C S
ATOM 9724 C CYS 1 382 14.073 - 11.928 -30.696 1.00 13.33 C C
ATOM 9725 O CYS 1 382 14.690 -10.887 -30.923 1.00 13.57 C O
ATOM 9726 N ASN 1 383 14.565 -12.914 -29.948 1.00 13.21 C N
ATOM 9727 CA ASN 1 383 15.925 -12.865 -29.415 1.00 13.22 C C
ATOM 9728 CB ASN 1 383 16.191 -14.054 -28.491 1.00 13. 18 C C
ATOM 9729 CG ASN 1 383 15.154 -14.186 -27.400 1.00 13.42 C C
ATOM 9730 OD1 ASN I 383 14.774 -13.202 -26.769 1.00 13.68 C O
ATOM 9731 ND2 ASN I 383 14.660 -15.402 -27.199 1.00 14.32 C N
ATOM 9732 C ASN 1 383 16.959 -12.845 -30.530 1.00 13.28 C C
ATOM 9733 O ASN 1 383 18.081 -12.374 -30.344 1.00 13.50 C O
ATOM 9734 N VAL I 384 16.605 -13.451 -31 .657 1.00 13.24 C N
ATOM 9735 CA VAL I 384 17.532 -13.584 -32.767 1.00 13.29 C C
ATOM 9736 CB VAL I 384 17.484 -14.992 -33.387 1.00 13.28 C C
ATOM 9737 CGI VAL I 384 18.046 -14.970 -34.800 1.00 13.73 C C
ATOM 9738 CG2 VAL I 384 18.251 -15.977 -32.518 1.00 12.76 C C
ATOM 9739 C VAL 1 384 17.292 -12.529 -33.842 1.00 13.57 C C
ATOM 9740 O VAL 1 384 18.239 -12.070 -34.480 1.00 13.31 C O
ATOM 9741 N ASP 1 385 16.038 -12.140 -34.049 1.00 14.07 C N
ATOM 9742 CA ASP I 385 15.71 1 - 11.380 -35.249 1.00 14.61 C C
ATOM 9743 CB ASP I 385 15.049 -12.246 -36.318 1.00 14.71 C C
ATOM 9744 CG ASP I 385 15.608 - 11.980 -37.701 1.00 16.69 C C
ATOM 9745 OD1 ASP I 385 16.308 -10.959 -37.872 1.00 18.63 C O
ATOM 9746 OD2 ASP I 385 15.367 -12.800 -38.612 1.00 19.10 C O
ATOM 9747 C ASP 1 385 15.014 -10.029 -35.092 1.00 14.63 C C
ATOM 9748 O ASP 1 385 15.412 -9.054 -35.728 1.00 14.34 C O
ATOM 9749 N ILE 1 386 13.937 -9.980 -34.314 1.00 14.54 C N
ATOM 9750 CA ILE I 386 13.154 -8.752 -34.212 1.00 14.46 C C
ATOM 9751 CB ILE I 386 14.074 -7.521 -34. 137 1.00 13.83 C C
ATOM 9752 CGI ILE I 386 14.932 -7.584 -32.875 1.00 13.44 C C
ATOM 9753 CD1 ILE I 386 16.315 -7.018 -33.048 1.00 12.39 C C
ATOM 9754 CG2 ILE I 386 13.253 -6.241 -34. 161 1.00 13.51 C C
ATOM 9755 C ILE 1 386 12.274 -8.602 -35.443 1.00 14.73 C C
ATOM 9756 O ILE 1 386 11.048 -8.692 -35.369 1.00 14.68 C O
ATOM 9757 N PHE 1 387 12.917 -8.301 -36.564 1.00 14.71 C N
ATOM 9758 CA PHE I 387 12.294 -8.428 -37.868 1.00 14.78 C C
ATOM 9759 CB PHE I 387 12.993 -7.528 -38.876 1.00 14.77 C C
ATOM 9760 CG PHE I 387 13.269 -6.154 -38.354 1.00 14.75 C C
ATOM 9761 CD1 PHE I 387 14.538 -5.818 -37.909 1.00 15.03 C C
ATOM 9762 CE1 PHE I 387 14.790 -4.572 -37.366 1.00 14.62 C C
ATOM 9763 CZ PHE I 387 13.743 -3.702 -37. 131 1.00 14.55 C C
ATOM 9764 CE2 PHE I 387 12.452 -4.074 -37.463 1.00 14.68 C C
ATOM 9765 CD2 PHE I 387 12.219 -5.303 -38.052 1.00 14.61 C C

```
ATOM   9766  C   PHE I 387      12.291   -9.864  -38.352   1.00 14.91      C    c
ATOM   9767  O   PHE I 387      13.339  -10.461  -38.604   1.00 14.86      c    o
ATOM   9768  N   ASN I 388      11.102  -10.448  -38.325   1.00 15.11      c    N
ATOM   9769  CA  ASN I 388      10.866  -11.776  -38.850   1.00 15.38      c    c
ATOM   9770  CB  ASN I 388      11.522  -12.817  -37.947   1.00 14.86      c    c
ATOM   9771  CG  ASN I 388      11.029  -12.733  -36.519   1.00 14.86      c    c
ATOM   9772  OD1 ASN I 388      10.004  -13.318  -36.170   1.00 12.80      c    o
ATOM   9773  ND2 ASN I 388      11.708  -11.934  -35.707   1.00 15.97      C    N
ATOM   9774  C   ASN I 388       9.363  -11.982  -38.843   1.00 16.11      c    c
ATOM   9775  O   ASN I 388       8.688  -11.570  -37.902   1.00 15.92      c    o
ATOM   9776  N   PRO I 389       8.817  -12.450  -39.969   1.00 16.99      c    N
ATOM   9777  CA  PRO I 389       7.464  -12.988  -39.920   1.00 17.40      c    c
ATOM   9778  CB  PRO I 389       7.376  -13.815  -41.204   1.00 17.72      c    c
ATOM   9779  CG  PRO I 389       8.776  -14.223  -41.477   1.00 17.47      c    c
ATOM   9780  CD  PRO I 389       9.618  -13.063  -41.043   1.00 17.05      c    c
ATOM   9781  C   PRO I 389       7.304  -13.894  -38.706   1.00 17.86      c    c
ATOM   9782  O   PRO I 389       8.297  -14.397  -38.181   1.00 18.45      c    o
ATOM   9783  N   LYS I 390       6.068  -14.106  -38.269   1.00 17.97      c    N
ATOM   9784  CA  LYS I 390       5.813  -14.937  -37.098   1.00 18.06      c    c
ATOM   9785  CB  LYS I 390       6.986  -15.889  -36.844   1.00 17.92      c    c
ATOM   9786  CG  LYS I 390       7.066  -17.065  -37.806   1.00 18.58      c    c
ATOM   9787  CD  LYS I 390       6.331  -18.283  -37.264   1.00 20.61      c    c
ATOM   9788  CE  LYS I 390       6.758  -19.556  -37.982   1.00 21.48      c    c
ATOM   9789  NZ  LYS I 390       6.197  -19.645  -39.360   1.00 23.16      c    N
ATOM   9790  C   LYS I 390       5.557  -14.087  -35.858   1.00 18.01      c    c
ATOM   9791  O   LYS I 390       4.552  -14.267  -35.171   1.00 18.43      c    o
ATOM   9792  N   TYR I 391       6.490  -13.192  -35.548   1.00 17.68      c    N
ATOM   9793  CA  TYR I 391       6.267  -12.216  -34.492   1.00 17.33      c    c
ATOM   9794  CB  TYR I 391       7.026  -12.599  -33.224   1.00 17.42      c    c
ATOM   9795  CG  TYR I 391       6.220  -12.376  -31.971   1.00 17.27      c    c
ATOM   9796  CD1 TYR I 391       4.863  -12.657  -31.951   1.00 17.29      c    c
ATOM   9797  CE1 TYR I 391       4.108  -12.437  -30.822   1.00 17.32      c    c
ATOM   9798  CZ  TYR I 391       4.678  -11.809  -29.739   1.00 16.51      c    c
ATOM   9799  OH  TYR I 391       3.934  -11.601  -28.602   1.00 16.65      c    o
ATOM   9800  CE2 TYR I 391       6.005  -11.441  -29.765   1.00 16.52      c    c
ATOM   9801  CD2 TYR I 391       6.756  -11.689  -30.893   1.00 17.24      c    c
ATOM   9802  C   TYR I 391       6.623  -10.796  -34.910   1.00 17.43      c    c
ATOM   9803  O   TYR I 391       7.786  -10.491  -35.175   1.00 17.70      c    o
ATOM   9804  N   ASP I 392       5.647   -9.899  -34.813   1.00 17.56      c    N
ATOM   9805  CA  ASP I 392       5.944   -8.487  -34.609   1.00 17.69      c    c
ATOM   9806  CB  ASP I 392       4.779   -7.590  -35.045   1.00 17.89      c    c
ATOM   9807  CG  ASP I 392       3.556   -8.380  -35.472   1.00 18.86      c    c
ATOM   9808  OD1 ASP I 392       2.911   -8.993  -34.596   1.00 20.34      c    o
ATOM   9809  OD2 ASP I 392       3.162   -8.272  -36.653   1.00 18.51      c    o
ATOM   9810  C   ASP I 392       6.342   -8.188  -33.169   1.00 17.11      C    c
ATOM   9811  O   ASP I 392       5.674   -8.609  -32.222   1.00 17.04      c    o
ATOM   9812  N   CYS I 393       7.356   -7.342  -33.026   1.00 16.33      c    N
ATOM   9813  CA  CYS I 393       8.347   -7.491  -31.975   1.00 16.17      c    c
ATOM   9814  CB  CYS I 393       9.656   -8.022  -32.554   1.00 16.11      c    c
ATOM   9815  SG  CYS I 393      10.738   -8.792  -31.342   1.00 20.23      c    s
ATOM   9816  C   CYS I 393       8.587   -6.139  -31.330   1.00 15.37      c    c
ATOM   9817  O   CYS I 393       9.066   -5.209  -31.980   1.00 15.15      c    o
ATOM   9818  N   LYS I 394       8.077   -5.982  -30.115   1.00 14.91      c    N
ATOM   9819  CA  LYS I 394       7.988   -4.668  -29.502   1.00 14.50      c    c
ATOM   9820  CB  LYS I 394       7.163   -4.724  -28.214   1.00 14.60      c    c
ATOM   9821  CG  LYS I 394       5.909   -5.591  -28.313   1.00 16.44      c    c
ATOM   9822  CD  LYS I 394       4.799   -5.101  -27.382   1.00 20.45      c    c
ATOM   9823  CE  LYS I 394       4.989   -5.604  -25.955   1.00 23.05      c    c
ATOM   9824  NZ  LYS I 394       5.685   -4.608  -25.094   1.00 24.13      c    N
ATOM   9825  C   LYS I 394       9.370   -4.087  -29.239   1.00 14.00      c    c
```

ATOM 9826 O LYS 1394 10.260 -4.760 -28.720 1.00 14.14 C O
ATOM 9827 N ILE I 395 9.497 -2.797 -29.507 1.00 13.28 C N
ATOM 9828 CA ILE I 395 10.750 -2.193 -29.919 1.00 12.89 C C
ATOM 9829 CB ILE I 395 10.960 -2.334 -31.435 1.00 12.75 C C
ATOM 9830 CGI ILE I 395 11.556 -3.695 -31.786 1.00 13.58 C C
ATOM 9831 CD1 ILE I 395 11.347 -4.084 -33.236 1.00 15.33 C C
ATOM 9832 CG2 ILE I 395 11.838 -1.216 -31.951 1.00 12.16 C C
ATOM 9833 C ILE 1395 10.534 -0.722 -29.648 1.00 13.15 C C
ATOM 9834 O ILE 1395 9.437 -0.210 -29.867 1.00 13.45 C O
ATOM 9835 N MET 1396 11.597 -0.002 -29.330 1.00 13.06 C N
ATOM 9836 CA MET 1396 11.526 1.433 -29.454 1.00 13.00 C C
ATOM 9837 CB MET 1396 11.421 2.114 -28.088 1.00 13.34 C C
ATOM 9838 CG MET I 396 12.738 2.594 -27.506 1.00 14.30 C C
ATOM 9839 SD MET 1396 12.483 3.421 -25.925 1.00 18.50 C S
ATOM 9840 CE MET 1396 11.067 2.515 -25.304 1.00 17.80 C C
ATOM 9841 C MET 1396 12.646 2.009 -30.288 1.00 12.96 C C
ATOM 9842 O MET 1396 13.704 1.405 -30.453 1.00 13.04 C O
ATOM 9843 N THR 1397 12.360 3.167 -30.862 1.00 12.78 C N
ATOM 9844 CA THR 1397 13.158 3.744 -31.917 1.00 12.51 C C
ATOM 9845 CB THR 1397 12.261 4.048 -33.134 1.00 12.39 C C
ATOM 9846 OG1 THR I 397 12.048 2.845 -33.883 1.00 12.50 C O
ATOM 9847 CG2 THR I 397 12.895 5.107 -34.026 1.00 12.55 C C
ATOM 9848 C THR 1397 13.633 5.062 -31.330 1.00 12.58 C C
ATOM 9849 O THR 1397 12.815 5.911 -31.001 1.00 12.88 C O
ATOM 9850 N SER I 398 14.919 5.217 -31.088 1.00 12.55 C N
ATOM 9851 CA SER I 398 15.538 6.442 -31.506 1.00 12.76 C C
ATOM 9852 CB SER I 398 16.509 6.920 -30.432 1.00 12.52 C C
ATOM 9853 OG SER I 398 17.486 7.787 -30.978 1.00 12.72 C O
ATOM 9854 C SER 1398 16.262 5.826 -32.632 1.00 12.99 C C
ATOM 9855 O SER 1398 16.219 6.314 -33.761 1.00 13.13 C O
ATOM 9856 N LYS 1399 16.463 4.540 -32.418 1.00 13.01 C N
ATOM 9857 CA LYS I 399 17.619 4.000 -32.989 1.00 13.29 C C
ATOM 9858 CB LYS I 399 17.475 4.221 -34.500 1.00 13.79 C C
ATOM 9859 CG LYS I 399 15.997 4.359 -34.942 1.00 14.34 C C
ATOM 9860 CD LYS I 399 15.854 4.556 -36.445 1.00 16.43 C C
ATOM 9861 CE LYS 1399 15.114 3.394 -37.093 1.00 17.37 C C
ATOM 9862 NZ LYS I 399 15.524 3.199 -38.511 1.00 16.62 C N
ATOM 9863 C LYS 1399 18.632 4.961 -32.349 1.00 13.09 C C
ATOM 9864 O LYS 1399 19.670 5.257 -32.934 1.00 12.87 C O
ATOM 9865 N THR 1400 18.236 5.572 -31.225 1.00 13.04 C N
ATOM 9866 CA THR 1400 19.072 6.571 -30.513 1.00 13.38 C C
ATOM 9867 CB THR 1400 18.218 7.723 -29.906 1.00 13.74 C C
ATOM 9868 OG1 THR 1400 16.861 7.632 -30.365 1.00 14.38 C O
ATOM 9869 CG2 THR 1400 18.798 9.072 -30.296 1.00 14.32 C C
ATOM 9870 C THR 1400 19.991 5.980 -29.408 1.00 13.20 C C
ATOM 9871 O THR 1400 19.748 4.866 -28.945 1.00 13.12 C O
ATOM 9872 N ASP 1401 20.881 6.801 -28.834 1.00 12.97 C N
ATOM 9873 CA ASP 1401 22.197 6.333 -28.331 1.00 12.50 C C
ATOM 9874 CB ASP 1401 23.307 7.270 -28.816 1.00 12.73 C C
ATOM 9875 CG ASP 1401 24.212 6.623 -29.841 1.00 13.98 C C
ATOM 9876 OD1 ASP 1401 23.677 6.029 -30.801 1.00 16.55 C O
ATOM 9877 OD2 ASP 1401 25.430 6.903 -29.814 1.00 14.80 C O
ATOM 9878 C ASP 1401 22.414 6.066 -26.816 1.00 12.13 C C
ATOM 9879 O ASP 1401 21.541 6.376 -26.002 1.00 12.31 C O
ATOM 9880 N VAL 1402 23.721 6.022 -26.502 1.00 11.49 C N
ATOM 9881 CA VAL 1402 24.382 5.380 -25.316 1.00 10.74 C C
ATOM 9882 CB VAL 1402 23.454 5.112 -24.128 1.00 10.60 C C
ATOM 9883 CGI VAL 1402 24.200 4.335 -23.060 1.00 11.26 C C
ATOM 9884 CG2 VAL 1402 22.942 6.425 -23.556 1.00 10.99 C C
ATOM 9885 C VAL 1402 25.452 4.251 -25.504 1.00 10.24 C C

ATOM 9886 O VAL I 402 25.773 3.895 -26.638 1.00 10.30 C o
ATOM 9887 N SER I 403 25.962 3.665 -24.400 1.00 9.76 c N
ATOM 9888 CA SER I 403 27.019 2.595 -24.456 1.00 9.18 c c
ATOM 9889 CB SER I 403 28.324 3.145 -25.036 1.00 9.41 c c
ATOM 9890 OG SER I 403 28.274 4.554 -25.165 1.00 10.82 c o
ATOM 9891 C SER I 403 27.325 1.652 -23.238 1.00 8.51 c c
ATOM 9892 O SER I 403 27.347 2.099 -22.088 1.00 8.30 c o
ATOM 9893 N SER I 404 27.642 0.376 -23.530 1.00 8.35 c N
ATOM 9894 CA SER I 404 28.574 -0.482 -22.733 1.00 8.18 c c
ATOM 9895 CB SER I 404 28.123 -0.585 -21.276 1.00 8.18 c c
ATOM 9896 OG SER I 404 27.698 -1.901 -20.968 1.00 8.83 c o
ATOM 9897 C SER I 404 28.789 -1.907 -23.310 1.00 7.62 c c
ATOM 9898 O SER I 404 28.422 -2.171 -24.455 1.00 7.57 c o
ATOM 9899 N SER I 405 29.368 -2.817 -22.514 1.00 7.08 c N
ATOM 9900 CA SER I 405 29.672 -4.192 -22.973 1.00 6.53 c c
ATOM 9901 CB SER I 405 31.139 -4.335 -23.400 1.00 6.42 c c
ATOM 9902 OG SER I 405 31.467 -5.695 -23.651 1.00 5.66 c o
ATOM 9903 C SER I 405 29.300 -5.333 -22.012 1.00 6.28 c c
ATOM 9904 O SER I 405 29.334 -5.169 -20.791 1.00 5.98 c o
ATOM 9905 N VAL I 406 29.215 -6.535 -22.576 1.00 6.22 c N
ATOM 9906 CA VAL I 406 28.714 -7.705 -21.866 1.00 6.50 c c
ATOM 9907 CB VAL I 406 27.208 -7.894 -22.099 1.00 6.45 c c
ATOM 9908 CG1 VAL I 406 26.661 -8.972 -21.181 1.00 7.66 C C
ATOM 9909 CG2 VAL I 406 26.470 -6.577 -21.903 1.00 7.38 C C
ATOM 9910 C VAL I 406 29.424 -8.942 -22.388 1.00 6.24 C C
ATOM 9911 O VAL I 406 29.397 -9.228 -23.584 1.00 6.14 C O
ATOM 9912 N ILE 1407 30.041 -9.689 -21.485 1.00 6.32 C N
ATOM 9913 CA ILE 1407 30.831 -10.838 -21.881 1.00 6.60 C C
ATOM 9914 CB ILE 1407 32.035 -11.021 -20.959 1.00 6.27 C C
ATOM 9915 CGI ILE 1407 33.112 -9.989 -21.295 1.00 6.19 C C
ATOM 9916 CD1 ILE 1407 33.720 -9.323 -20.073 1.00 8.34 C C
ATOM 9917 CG2 ILE I 407 32.567 -12.438 -21.053 1.00 6.42 C C
ATOM 9918 C ILE 1407 29.995 -12.110 -21.882 1.00 7.20 C C
ATOM 9919 O ILE 1407 29.246 -12.376 -20.944 1.00 7.42 C O
ATOM 9920 N THR 1408 30.163 -12.914 -22.925 1.00 7.57 C N
ATOM 9921 CA THR 1408 29.355 -14.113 -23.103 1.00 8.19 C C
ATOM 9922 CB THR 1408 28.681 -14.138 -24.483 1.00 8.15 C C
ATOM 9923 OG1 THR 1408 29.684 -14.218 -25.503 1.00 8.88 C O
ATOM 9924 CG2 THR 1408 27.853 -12.888 -24.693 1.00 7.93 C C
ATOM 9925 C THR 1408 30.192 -15.376 -22.966 1.00 8.55 C C
ATOM 9926 O THR 1408 31.419 -15.333 -23.065 1.00 9.07 C O
ATOM 9927 N SER I 409 29.503 -16.512 -22.970 1.00 8.70 C N
ATOM 9928 CA SER 1409 30.146 -17.813 -22.838 1.00 9.20 C C
ATOM 9929 CB SER 1409 29.126 -18.935 -23.044 1.00 9.72 C C
ATOM 9930 OG SER 1409 27.946 -18.700 -22.297 1.00 10.75 C O
ATOM 9931 C SER I 409 31.268 -17.958 -23.848 1.00 9.01 C C
ATOM 9932 O SER 1409 32.299 -18.571 -23.567 1.00 9.02 C O
ATOM 9933 N LEU 1410 31.027 -17.458 -25.053 1.00 8.91 C N
ATOM 9934 CA LEU 1410 31.814 -17.858 -26.204 1.00 9.29 C C
ATOM 9935 CB LEU 1410 31.024 -18.828 -27.081 1.00 9.61 C C
ATOM 9936 CG LEU 1410 31.702 -20.180 -27.323 1.00 9.70 C C
ATOM 9937 CD1 LEU 1410 31.975 -20.908 -26.014 1.00 11.11 C C
ATOM 9938 CD2 LEU 1410 30.895 -21.057 -28.274 1.00 9.16 C C
ATOM 9939 C LEU 1410 32.250 -16.644 -27.009 1.00 9.12 C C
ATOM 9940 O LEU 1410 32.844 -16.774 -28.077 1.00 9.08 C O
ATOM 9941 N GLY I 411 32.016 -15.462 -26.454 1.00 9.03 C N
ATOM 9942 CA GLY I 411 32.612 -14.247 -26.984 1.00 8.44 C C
ATOM 9943 C GLY I 411 32.234 -13.047 -26.146 1.00 7.91 C C
ATOM 9944 O GLY I 411 32.175 -13.131 -24.921 1.00 7.85 C O
ATOM 9945 N ALA I 412 31.868 -11.961 -26.816 1.00 7.30 C N

ATOM 9946 CA ALA 1412 31.416 -10.757 -26. 130 1.00 6.92 C c
ATOM 9947 CB ALA I 412 32.609 -9.925 -25.672 1.00 6.90 C c
ATOM 9948 C ALA I 412 30.502 -9.934 -27.029 1.00 6.99 c c
ATOM 9949 O ALA I 412 30.597 -10.004 -28.255 1.00 6.94 c o
ATOM 9950 N ILE I 413 29.567 -9.216 -26.418 1.00 7.29 C N
ATOM 9951 CA ILE I 413 28.808 -8.200 -27.136 1.00 7.49 c c
ATOM 9952 CB ILE I 413 27.296 -8.285 -26.846 1.00 7.24 c c
ATOM 9953 CGI ILE I 413 26.703 -9.550 -27.480 1.00 7.18 c c
ATOM 9954 CD1 ILE I 413 25.397 -9.315 -28.241 1.00 7.70 c c
ATOM 9955 CG2 ILE I 413 26.585 -7.051 -27.397 1.00 7.70 c c
ATOM 9956 C ILE I 413 29.304 -6.81 1 -26.776 1.00 7.94 c c
ATOM 9957 O ILE I 413 29.806 -6.591 -25.674 1.00 8.39 c o
ATOM 9958 N VAL I 414 29.155 -5.871 -27.703 1.00 8.22 c N
ATOM 9959 CA VAL I 414 29.498 -4.485 -27.420 1.00 8.77 c c
ATOM 9960 CB VAL I 414 30.965 -4.158 -27.782 1.00 8.57 c c
ATOM 9961 CGI VAL I 414 31.293 -4.627 -29. 197 1.00 9.12 c c
ATOM 9962 CG2 VAL I 414 31.245 -2.669 -27.607 1.00 8.90 c c
ATOM 9963 C VAL I 414 28.536 -3.470 -28.028 1.00 8.92 c c
ATOM 9964 O VAL I 414 28.246 -3.497 -29.227 1.00 9.00 c o
ATOM 9965 N SER I 415 27.947 -2.665 -27. 152 1.00 8.97 c N
ATOM 9966 CA SER I 415 27.023 -1.623 -27.552 1.00 9.02 c c
ATOM 9967 CB SER I 415 25.805 -1.623 -26.629 1.00 8.98 c c
ATOM 9968 OG SER I 415 25.203 -2.903 -26.581 1.00 9.54 c o
ATOM 9969 C SER I 415 27.727 -0.277 -27.480 1.00 9.36 c c
ATOM 9970 O SER I 415 27.996 0.230 -26.392 1.00 9.61 c o
ATOM 9971 N CYS I 416 28.219 0.177 -28.626 1.00 9.57 c N
ATOM 9972 CA CYS I 416 28.920 1.447 -28.701 1.00 9.61 c c
ATOM 9973 CB CYS I 416 30. 167 1.320 -29.572 1.00 9.62 c c
ATOM 9974 SG CYS 1416 31.508 2.403 -29.060 1.00 11.33 c s
ATOM 9975 C CYS I 416 28.01 1 2.519 -29.270 1.00 9.61 c c
ATOM 9976 O CYS I 416 27.619 2.458 -30.434 1.00 9.80 c o
ATOM 9977 N TYR I 417 27.662 3.493 -28.441 1.00 9.48 c N
ATOM 9978 CA TYR I 417 26.667 4.475 -28.829 1.00 9.28 c c
ATOM 9979 CB TYR I 417 25.305 4.1 17 -28.235 1.00 9.17 c c
ATOM 9980 CG TYR I 417 24.629 2.955 -28.924 1.00 8.71 c c
ATOM 9981 CD1 TYR I 417 23.902 2.024 -28.199 1.00 8.54 c c
ATOM 9982 CE1 TYR I 417 23.228 0.999 -28.830 1.00 9.56 c c
ATOM 9983 CZ TYR I 417 23.289 0.886 -30.201 1.00 9.83 c c
ATOM 9984 OH TYR I 417 22.658 -0.162 -30.829 1.00 10.51 c o
ATOM 9985 CE2 TYR I 417 24.025 1.783 -30.942 1.00 9.36 c c
ATOM 9986 CD2 TYR I 417 24.675 2.818 -30.305 1.00 8.95 c c
ATOM 9987 C TYR I 417 27.076 5.885 -28.422 1.00 9.35 c c
ATOM 9988 O TYR I 417 28.046 6.075 -27.687 1.00 9.11 c o
ATOM 9989 N GLY I 418 26.357 6.872 -28.946 1.00 9.71 c N
ATOM 9990 CA GLY I 418 26.662 8.270 -28.679 1.00 9.95 c c
ATOM 9991 C GLY I 418 28.094 8.602 -29.035 1.00 10.09 c c
ATOM 9992 O GLY I 418 28.623 8.1 12 -30.033 1.00 10.17 c o
ATOM 9993 N LYS I 419 28.768 9.307 -28. 136 1.00 10.17 c N
ATOM 9994 CA LYS 1419 30. 104 9.810 -28.415 1.00 10.50 c c
ATOM 9995 CB LYS I 419 30.381 11.077 -27.607 1.00 11.09 c c
ATOM 9996 CG LYS 1419 29.942 12.351 -28.300 1.00 12.94 c c
ATOM 9997 CD LYS 1419 30.697 13.553 -27.770 1.00 15.52 c c
ATOM 9998 CE LYS 1419 30.546 14.735 -28.708 1.00 17.07 c c
ATOM 9999 NZ LYS 1419 29.200 14.756 -29.349 1.00 19.30 c N
ATOM 10000 C LYS I 419 31.201 8.777 -28. 168 1.00 10.23 c c
ATOM 10001 O LYS 1419 32.380 9.063 -28.374 1.00 10.58 c o
ATOM 10002 N THR I 420 30.823 7.592 -27.697 1.00 10.10 c N
ATOM 10003 CA THR I 420 31.789 6.687 -27.076 1.00 9.74 c c
ATOM 10004 CB THR I 420 31.106 5.656 -26. 158 1.00 9.28 c c
ATOM 10005 OG1 THR I 420 29.766 6.076 -25.878 1.00 9.21 c: o

```
ATOM  10006  CG2 THR I 420      31.870   5.521 -24.851  1.00  9.03      C  c
ATOM  10007  C   THR I 420      32.671   5.966 -28.096  1.00  9.95      c  c
ATOM  10008  O   THR I 420      32.289   5.800 -29.254  1.00 10.35      c  o
ATOM  10009  N   LYS I 421      33.880   5.608 -27.674  1.00 10.07      c  N
ATOM  10010  CA  LYS I 421      34.808   4.863 -28.521  1.00 10.21      c  c
ATOM  10011  CB  LYS I 421      36.194   5.513 -28.495  1.00 10.30      c  c
ATOM  10012  CG  LYS I 421      36.445   6.496 -29.626  1.00 12.43      c  c
ATOM  10013  CD  LYS I 421      37.766   7.225 -29.441  1.00 15.12      c  c
ATOM  10014  CE  LYS I 421      37.752   8.578 -30.134  1.00 15.21      c  c
ATOM  10015  NZ  LYS I 421      38.779   9.500 -29.575  1.00 15.98      c  N
ATOM  10016  C   LYS I 421      34.908   3.412 -28.063  1.00 10.09      c  c
ATOM  10017  O   LYS I 421      34.979   3.137 -26.866  1.00 10.36      c  o
ATOM  10018  N   CYS I 422      34.937   2.486 -29.017  1.00  9.81      c  N
ATOM  10019  CA  CYS I 422      35.063   1.075 -28.681  1.00  9.56      c  c
ATOM  10020  CB  CYS I 422      33.696   0.396 -28.633  1.00  9.72      c  c
ATOM  10021  SG  CYS I 422      32.479   1.300 -27.664  1.00 11.42      c  s
ATOM  10022  C   CYS I 422      36.012   0.311 -29.590  1.00  9.18      c  c
ATOM  10023  O   CYS I 422      36.111   0.582 -30.787  1.00  9.27      c  o
ATOM  10024  N   THR I 423      36.636  -0.710 -29.016  1.00  8.93      c  N
ATOM  10025  CA  THR I 423      37.825  -1.322 -29.583  1.00  8.64      c  c
ATOM  10026  CB  THR I 423      39.104  -0.757 -28.940  1.00  8.32      c  c
ATOM  10027  OG1 THR I 423      39.059   0.675 -28.954  1.00  7.97      c  o
ATOM  10028  CG2 THR I 423      40.336  -1.230 -29.695  1.00  8.36      c  c
ATOM  10029  C   THR I 423      37.771  -2.810 -29.287  1.00  8.86      c  c
ATOM  10030  O   THR I 423      37.514  -3.214 -28.153  1.00  9.26      c  o
ATOM  10031  N   ALA I 424      37.993  -3.625 -30.310  1.00  8.74      c  N
ATOM  10032  CA  ALA I 424      38.356  -5.018 -30.097  1.00  8.79      c  c
ATOM  10033  CB  ALA I 424      37.512  -5.927 -30.977  1.00  8.94      c  c
ATOM  10034  C   ALA I 424      39.839  -5.233 -30.371  1.00  8.84      c  c
ATOM  10035  O   ALA I 424      40.316  -4.985 -31.477  1.00  9.24      c  o
ATOM  10036  N   SER I 425      40.570  -5.661 -29.347  1.00  8.81      c  N
ATOM  10037  CA  SER I 425      41.990  -5.958 -29.492  1.00  8.85      c  c
ATOM  10038  CB  SER I 425      42.803  -5.192 -28.446  1.00  8.94      c  c
ATOM  10039  OG  SER I 425      42.091  -4.060 -27.976  1.00  7.69      c  o
ATOM  10040  C   SER I 425      42.253  -7.456 -29.368  1.00  9.01      c  c
ATOM  10041  O   SER I 425      41.541  -8.163 -28.656  1.00  8.63      c  o
ATOM  10042  N   ASN I 426      43.246  -7.944 -30.102  1.00  9.54      c  N
ATOM  10043  CA  ASN I 426      43.519  -9.374 -30.153  1.00 10.19      c  c
ATOM  10044  CB  ASN I 426      44.105  -9.764 -31.511  1.00  9.77      c  c
ATOM  10045  CG  ASN I 426      45.597  -9.506 -31.599  1.00  9.43      c  c
ATOM  10046  OD1 ASN I 426      46.249  -9.211 -30.597  1.00  9.01      c  o
ATOM  10047  ND2 ASN I 426      46.146  -9.616 -32.803  1.00  9.01      c  N
ATOM  10048  C   ASN I 426      44.434  -9.853 -29.029  1.00 11.16      c  c
ATOM  10049  O   ASN I 426      44.674  -9.138 -28.056  1.00 11.06      c  o
ATOM  10050  N   LYS I 427      44.921 -11.083 -29.170  1.00 12.38      c  N
ATOM  10051  CA  LYS I 427      45.803 -11.703 -28.185  1.00 13.52      c  c
ATOM  10052  CB  LYS I 427      46.418 -12.978 -28.765  1.00 14.00      c  c
ATOM  10053  CG  LYS I 427      45.683 -14.255 -28.398  1.00 16.18      c  c
ATOM  10054  CD  LYS I 427      46.510 -15.478 -28.758  1.00 18.24      c  c
ATOM  10055  CE  LYS I 427      46.211 -16.641 -27.828  1.00 19.72      c  c
ATOM  10056  NZ  LYS I 427      46.794 -16.434 -26.474  1.00 21.43      c  N
ATOM  10057  C   LYS I 427      46.915 -10.758 -27.741  1.00 13.71      c  c
ATOM  10058  O   LYS I 427      47.180 -10.611 -26.547  1.00 13.63      c  o
ATOM  10059  N   ASN I 428      47.634 -10.210 -28.716  1.00 14.28      c  N
ATOM  10060  CA  ASN I 428      48.816  -9.400 -28.447  1.00 14.60      c  c
ATOM  10061  CB  ASN I 428      49.709  -9.331 -29.689  1.00 14.57      c  c
ATOM  10062  CG  ASN I 428      49.589 -10.565 -30.563  1.00 13.24      c:  c
ATOM  10063  OD1 ASN I 428      49.765 -11.690 -30.096  1.00  9.74      c  o
ATOM  10064  ND2 ASN I 428      49.319 -10.358 -31.847  1.00 12.83      C  N
ATOM  10065  C   ASN I 428      48.466  -7.989 -27.982  1.00 14.83      c  c
```

```
ATOM  10066  O   ASN 1428     49.330  -7.255 -27.499  1.00 15.25      C    O
ATOM  10067  N   ARG 1429     47.225  -7.580 -28.226  1.00 14.78      C    N
ATOM  10068  CA  ARG 1429     46.775  -6.234 -27.885  1.00 14.74      C    C
ATOM  10069  CB  ARG 1429     47.695  -5.603 -26.837  1.00 14.93      C    C
ATOM  10070  CG  ARG 1429     47.475  -6.121 -25.424  1.00 16.26      C    C
ATOM  10071  CD  ARG 1429     46.452  -5.279 -24.677  1.00 19.79      C    C
ATOM  10072  NE  ARG 1429     45.979  -5.940 -23.464  1.00 22.68      C    N
ATOM  10073  CZ  ARG 1429     46.735  -6.172 -22.396  1.00 23.54      C    C
ATOM  10074  NH1 ARG I 429     48.013  -5.817 -22.394  1.00 22.87      C    N
ATOM  10075  NH2 ARG I 429     46.219  -6.777 -21.335  1.00 23.53      C    N
ATOM  10076  C   ARG 1429     46.689  -5.339 -29.1 17  1.00 14.35      C    C
ATOM  10077  O   ARG 1429     46.093  -4.262 -29.073  1.00 14.62      C    O
ATOM  10078  N   GLY 1430     47.270  -5.798 -30.221  1.00 13.67      C    N
ATOM  10079  CA  GLY 1430     46.898  -5.304 -31.540  1.00 12.80      C    C
ATOM  10080  C   GLY 1430     45.397  -5.149 -31.683  1.00 12.1 1      C    C
ATOM  10081  O   GLY 1430     44.634  -6.038 -31 .306  1.00 12.18      C    O
ATOM  10082  N   ILE I 431     44.972  -4.001 -32.199  1.00 11.58      C    N
ATOM  10083  CA  ILE I 431     43.552  -3.678 -32.300  1.00 10.76      C    C
ATOM  10084  CB  ILE I 431     43.321  -2. 162 -32. 138  1.00 10.43      C    C
ATOM  10085  CGI ILE 1431     43.649  -1.718 -30.71 1  1.00 10.95      C    C
ATOM  10086  CD1 ILE 1431     44.264  -0.337 -30.628  1.00 12.08      C    C
ATOM  10087  CG2 ILE I 431     41.892  -1.796 -32.507  1.00 10.07      C    C
ATOM  10088  C   ILE I 431     43.01 1  -4.108 -33.660  1.00 10.68      C    C
ATOM  10089  O   ILE 1431     43.474  -3.623 -34.693  1.00 10.40      C    O
ATOM  10090  N   ILE 1432     42.063  -5.041 -33.669  1.00 10.90      C    N
ATOM  10091  CA  ILE I 432     41.497  -5.518 -34.931  1.00 11.42      C    C
ATOM  10092  CB  ILE 1432     41.106  -7.008 -34.884  1.00 11.63      C    C
ATOM  10093  CGI ILE 1432     41.784  -7.712 -33.709  1.00 12.68      C    C
ATOM  10094  CD1 ILE I 432     41.172  -9.055 -33.369  1.00 13.89      C    C
ATOM  10095  CG2 ILE 1432     41.453  -7.689 -36.201  1.00 12.24      C    C
ATOM  10096  C   ILE 1432     40.290  -4.703 -35.381  1.00 11.41      C    C
ATOM  10097  O   ILE 1432     40.172  -4.362 -36.558  1.00 11.63      C    O
ATOM  10098  N   LYS I 433     39.315  -4.555 -34.492  1.00 11.52      C    N
ATOM  10099  CA  LYS I 433     38.076  -3.878 -34.848  1.00 11.96      C    C
ATOM  10100  CB  LYS I 433     36.864  -4.767 -34.566  1.00 12.31      C    C
ATOM  10101  CG  LYS 1433     35.552  -4.201 -35.092  1.00 14.42      C    C
ATOM  10102  CD  LYS 1433     34.622  -5.301 -35.578  1.00 16.74      C    C
ATOM  10103  CE  LYS 1433     33.367  -4.723 -36.216  1.00 17.08      C    C
ATOM  10104  NZ  LYS 1433     33.135  -5.263 -37.585  1.00 17.30      C    N
ATOM  10105  C   LYS 1433     37.934  -2.543 -34.128  1.00 11.65      C    C
ATOM  10106  O   LYS 1433     38.620  -2.281 -33. 140  1.00 11.48      C    O
ATOM  10107  N   THR 1434     37.059  -1.691 -34.651  1.00 11.28      C    N
ATOM  10108  CA  THR 1434     36.764  -0.407 -34.027  1.00 11.21      C    C
ATOM  10109  CB  THR 1434     37.809   0.653 -34.414  1.00 11.30      C    C
ATOM  101 10  OG1 THR 1434     37.324   1.955 -34.062  1.00 11.83      C    O
ATOM  101 11  CG2 THR 1434     38.088   0.608 -35.910  1.00 11.84      C    C
ATOM  101 12  C   THR 1434     35.380   0.083 -34.446  1.00 10.94      C    C
ATOM  101 13  O   THR 1434     34.982  -0.085 -35.597  1.00 10.93      C    O
ATOM  101 14  N   PHE I 435     34.604   0.572 -33.484  1.00 11.10      C    N
ATOM  101 15  CA  PHE 1435     33.176   0.281 -33.466  1.00 11.96      C    C
ATOM  101 16  CB  PHE 1435     32.726  -0.248 -32. 106  1.00 11.51      C    C
ATOM  101 17  CG  PHE 1435     32.896  -1.732 -31 .957  1.00 11.19      C    C
ATOM  101 18  CD1 PHE I 435     33.805  -2.246 -31.047  1.00 10.86      C    C
ATOM  101 19  CE1 PHE I 435     34.022  -3.608 -30.957  1.00 10.24      C    C
ATOM  10120  CZ  PHE 1435     33.375  -4.467 -31.823  1.00  9.89      C    C
ATOM  10121  CE2 PHE I 435     32.512  -3.963 -32.774  1.00 10.78      C    C
ATOM  10122  CD2 PHE I 435     32.300  -2.599 -32.858  1.00 11.14      C    C
ATOM  10123  C   PHE 1435     32.255   1.381 -33.984  1.00 13.00      C    C
ATOM  10124  O   PHE 1435     32.168   2.466 -33.407  1.00 13.03      C    O
ATOM  10125  N   SER I 436     31.429   1.001 -34.954  1.00 13.89      C    N
```

ATOM 10126 CA SER I 436 30.556 1.929 -35.657 1.00 14.67 C c
ATOM 10127 CB SER I 436 30.282 1.417 -37.074 1.00 15.04 c c
ATOM 10128 OG SER I 436 30.877 2.256 -38.049 1.00 16.58 c o
ATOM 10129 C SER I 436 29.240 2.105 -34.903 1.00 14.75 c c
ATOM 10130 O SER I 436 28.192 1.626 -35.340 1.00 14.75 c o
ATOM 10131 N ASN I 437 29.302 2.785 -33.764 1.00 14.44 c N
ATOM 10132 CA ASN I 437 28. 124 3.433 -33.203 1.00 14.35 c c
ATOM 10133 CB ASN I 437 27.891 4.781 -33.881 1.00 14.75 c c
ATOM 10134 CG ASN I 437 26.889 5.641 -33.139 1.00 15.51 c c
ATOM 10135 OD1 ASN I 437 27.054 5.920 -31.951 1.00 16.85 c o
ATOM 10136 ND2 ASN I 437 25.878 6.120 -33.856 1.00 16.10 c N
ATOM 10137 C ASN I 437 26.885 2.558 -33.345 1.00 13.69 c c
ATOM 10138 O ASN I 437 25.912 2.941 -33.995 1.00 13.40 c o
ATOM 10139 N GLY I 438 26.957 1.358 -32.782 1.00 13.39 c N
ATOM 10140 CA GLY I 438 25.931 0.345 -32.986 1.00 12.92 c c
ATOM 10141 C GLY I 438 26.000 -0.743 -31.934 1.00 12.72 c c
ATOM 10142 O GLY I 438 26. 154 -0.459 -30.747 1.00 12.83 c o
ATOM 10143 N CYS I 439 25.949 -1.996 -32.375 1.00 12.17 c N
ATOM 10144 CA CYS I 439 26.014 -3.126 -31.456 1.00 11.52 c c
ATOM 10145 CB CYS I 439 24.672 -3.321 -30.750 1.00 11.68 c c
ATOM 10146 SG CYS 1439 24.046 -5.015 -30.795 1.00 12.89 c s
ATOM 10147 C CYS 1439 26.437 -4.41 1 -32. 159 1.00 10.95 c c
ATOM 10148 O CYS I 439 25.714 -4.935 -33.007 1.00 10.77 c o
ATOM 10149 N ASP I 440 27.617 -4.909 -31.802 1.00 10.41 c N
ATOM 10150 CA ASP 1440 28.240 -6.017 -32.518 1.00 10.06 c c
ATOM 10151 CB ASP I 440 29.514 -5.548 -33.224 1.00 10.85 c c
ATOM 10152 CG ASP 1440 29.336 -5.417 -34.724 1.00 13.1 1 c c
ATOM 10153 OD1 ASP I 440 29.376 -6.453 -35.422 1.00 14.97 c o
ATOM 10154 OD2 ASP I 440 29.192 -4.275 -35.209 1.00 15.27 c o
ATOM 10155 C ASP I 440 28.566 -7.175 -31.578 1.00 9.01 C c
ATOM 10156 O ASP I 440 28.479 -7.040 -30.358 1.00 9.09 c 0
ATOM 10157 N TYR I 441 29.027 -8.280 -32. 159 1.00 7.92 c N
ATOM 10158 CA TYR I 441 29.448 -9.461 -31.403 1.00 7.24 c c
ATOM 10159 CB TYR I 441 28.448 -10.605 -31.610 1.00 7.04 c c
ATOM 10160 CG TYR I 441 28.862 -11.916 -30.979 1.00 6.77 c c
ATOM 10161 CD1 TYR I 441 28.439 -12.256 -29.701 1.00 7.41 c c
ATOM 10162 CE1 TYR I 441 28.805 -13.460 -29. 122 1.00 6.79 c c
ATOM 10163 CZ TYR I 441 29.529 -14.381 -29.855 1.00 6.49 c c
ATOM 10164 OH TYR I 441 29.907 -15.573 -29.277 1.00 5.09 c o
ATOM 10165 CE2 TYR I 441 29.946 -14.076 -31. 134 1.00 7.52 c c
ATOM 10166 CD2 TYR I 441 29.600 -12.853 -31.694 1.00 7.12 c c
ATOM 10167 C TYR I 441 30.833 -9.902 -31.872 1.00 6.89 c c
ATOM 10168 O TYR I 441 31.150 -9.809 -33.058 1.00 7.12 c o
ATOM 10169 N VAL I 442 31.664 -10.363 -30.944 1.00 6.73 c N
ATOM 10170 CA VAL I 442 32.959 -10.941 -31.301 1.00 6.78 c c
ATOM 10171 CB VAL I 442 34. 133 -10.008 -30.925 1.00 6.51 c c
ATOM 10172 CGI VAL I 442 34.206 -8.830 -31 .879 1.00 7.38 c c
ATOM 10173 CG2 VAL I 442 34.007 -9.530 -29.488 1.00 6.00 c c
ATOM 10174 C VAL I 442 33.142 -12.285 -30.609 1.00 7.13 c c
ATOM 10175 O VAL I 442 32.307 -12.689 -29.800 1.00 7.77 c o
ATOM 10176 N SER I 443 34.241 -12.970 -30.908 1.00 7.12 c N
ATOM 10177 CA SER I 443 34.476 -14.283 -30.321 1.00 7.64 c c
ATOM 10178 CB SER I 443 33.940 -15.391 -31.233 1.00 7.83 c c
ATOM 10179 OG SER I 443 34.994 -16.091 -31.870 1.00 7.99 c o
ATOM 10180 C SER I 443 35.932 -14.541 -29.940 1.00 8.16 c c
ATOM 10181 O SER I 443 36.841 -13.847 -30.399 1.00 8.69 c o
ATOM 10182 N ASN I 444 36.135 -15.517 -29.058 1.00 8.73 c N
ATOM 10183 CA ASN I 444 37.473 -15.972 -28.692 1.00 9.50 c c
ATOM 10184 CB ASN I 444 37.408 -16.989 -27.546 1.00 9.65 c c
ATOM 10185 CG ASN I 444 36. 105 -16.916 -26.772 1.00 10.64 c c

```
ATOM  10186  OD1 ASN I 444      35.530 -15.839 -26.602  1.00 12.28      C    O
ATOM  10187  ND2 ASN 1444       35.617 -18.069 -26.325  1.00 11.75      C    N
ATOM  10188  C   ASN 1444       38.240 -16.558 -29.877  1.00 10.24      C    C
ATOM  10189  O   ASN 1444       37.657 -17.206 -30.748  1.00  9.89      C    O
ATOM  10190  N   LYS 1445       39.565 -16.467 -29.809  1.00 11.63      C    N
ATOM  10191  CA  LYS 1445       40.394 -16.179 -30.979  1.00 13.07      C    C
ATOM  10192  CB  LYS 1445       40.843 -17.470 -31.664  1.00 13.70      C    C
ATOM  10193  CG  LYS 1445       41.782 -17.255 -32.848  1.00 15.80      C    C
ATOM  10194  CD  LYS 1445       42.771 -16.1 14 -32.613  1.00 18.31      C    C
ATOM  10195  CE  LYS 1445       42.855 -15.717 -31.146  1.00 19.03      C    C
ATOM  10196  NZ  LYS 1445       43.703 -16.652 -30.355  1.00 20.02      C    N
ATOM  10197  C   LYS 1445       39.701 -15.268 -31 .980  1.00 12.96      C    C
ATOM  10198  O   LYS 1445       38.486 -15.336 -32.159  1.00 13.24      C    O
ATOM  10199  N   GLY 1446       40.491 -14.448 -32.664  1.00 13.08      C    N
ATOM  10200  CA  GLY 1446       40.131 -13.057 -32.889  1.00 12.42      C    C
ATOM  10201  C   GLY I 446      40.305 -12.233 -31.631  1.00 11.83      C    C
ATOM  10202  O   GLY 1446       41.402 - 11.756 -31 .342  1.00 12.44      C    O
ATOM  10203  N   VAL 1447       39.264 -12.192 -30.808  1.00 10.63      C    N
ATOM  10204  CA  VAL 1447       39.157 - 11.162 -29.785  1.00 10.01      C    C
ATOM  10205  CB  VAL 1447       37.758 -10.516 -29.764  1.00  9.97      C    C
ATOM  10206  CGI VAL 1447       37.778  -9.225 -28.957  1.00 10.51      C    C
ATOM  10207  CG2 VAL I 447       37.287 -10.244 -31. 180  1.00 10.50      C    C
ATOM  10208  C   VAL 1447       39.548 - 11.648 -28.390  1.00  9.53      C    C
ATOM  10209  O   VAL 1447       39. 184 -12.747 -27.967  1.00  9.61      C    O
ATOM  10210  N   ASP 1448       40.21 1 -10.766 -27.652  1.00  9.16      C    N
ATOM  1021 1  CA  ASP I 448       40.803 - 11.093 -26.362  1.00  8.75      C    C
ATOM  10212  CB  ASP 1448       42.325 - 11.159 -26.502  1.00  9.22      C    C
ATOM  10213  CG  ASP 1448       42.975 -12.024 -25.443  1.00 11.44      C    C
ATOM  10214  OD1 ASP I 448       42.372 -12.204 -24.365  1.00 13.83      C    O
ATOM  10215  OD2 ASP I 448       44.1 19 -12.472 -25.665  1.00 14.13      C    O
ATOM  10216  C   ASP 1448       40.427  -9.976 -25.398  1.00  8.18      C    C
ATOM  10217  O   ASP 1448       40.203 -10.209 -24.21 1  1.00  8.06      C    O
ATOM  10218  N   THR 1449       40.201  -8.794 -25.964  1.00  7.63      C    N
ATOM  10219  CA  THR 1449       39.894  -7.592 -25.197  1.00  6.80      C    C
ATOM  10220  CB  THR 1449       41.165  -6.750 -24.940  1.00  6.89      C    C
ATOM  10221  OG1 THR 1449       4 1.805  -7.196 -23.738  1.00  6.16      C    O
ATOM  10222  CG2 THR 1449       40.815  -5.275 -24.804  1.00  7.55      C    C
ATOM  10223  C   THR 1449       38.898  -6.751 -25.987  1.00  6.53      C    C
ATOM  10224  O   THR 1449       38.949  -6.708 -27.216  1.00  6.59      C    O
ATOM  10225  N   VAL 1450       37.947  -6.147 -25.288  1.00  6.07      C    N
ATOM  10226  CA  VAL 1450       37.318  -4.934 -25.781  1.00  6.02      C    C
ATOM  10227  CB  VAL 1450       35.839  -5.158 -26.121  1.00  5.61      C    C
ATOM  10228  CGI VAL I 450       35.697  -6.278 -27.136  1.00  5.32      C    C
ATOM  10229  CG2 VAL 1450       35.047  -5.460 -24.860  1.00  5.55      C    C
ATOM  10230  C   VAL 1450       37.427  -3.837 -24.743  1.00  6.37      C    C
ATOM  10231  O   VAL 1450       37.359  -4.097 -23.542  1.00  6.54      C    O
ATOM  10232  N   SER I 451       37.704  -2.626 -25.207  1.00  6.41      C    N
ATOM  10233  CA  SER 1451       37.571  - 1.451 -24.366  1.00  6.70      C    C
ATOM  10234  CB  SER 1451       38.845  -0.607 -24.422  1.00  7.13      C    C
ATOM  10235  OG  SER 1451       39.573  -0.864 -25.610  1.00  9.26      C    O
ATOM  10236  C   SER 1451       36.373  -0.626 -24.802  1.00  6.47      C    C
ATOM  10237  O   SER 1451       36.100  -0.493 -25.994  1.00  6.54      C    O
ATOM  10238  N   VAL 1452       35.577  -0.203 -23.830  1.00  6.56      C    N
ATOM  10239  CA  VAL 1452       34.627   0.872 -24.050  1.00  6.31      C    C
ATOM  10240  CB  VAL 1452       33.205   0.448 -23.647  1.00  5.74      C    C
ATOM  10241  CGI VAL 1452       32.189   1.471 -24. 130  1.00  5.06      C    C
ATOM  10242  CG2 VAL 1452       32.891  -0.929 -24.212  1.00  5.56      C    C
ATOM  10243  C   VAL 1452       35.056   2.087 -23.242  1.00  6.60      C    C
ATOM  10244  O   VAL 1452       35.499   1.950 -22. 102  1.00  7.04      C    O
ATOM  10245  N   GLY 1453       35. 141   3.234 -23.907  1.00  6.54      C    N
```

ATOM 10246 CA GLY I 453 35.790 4.395 -23.314 1.00 6.43 C c
ATOM 10247 C GLY I 453 37.010 3.964 -22.525 1.00 6.09 c c
ATOM 10248 O GLY I 453 37.910 3.328 -23.071 1.00 5.90 c o
ATOM 10249 N ASN I 454 36.985 4.188 -21.216 1.00 6.02 c N
ATOM 10250 CA ASN I 454 38.156 3.904 -20.396 1.00 6.39 c c
ATOM 10251 CB ASN I 454 38.491 5.088 -19.491 1.00 6.81 c c
ATOM 10252 CG ASN I 454 39.518 6.009 -20.108 1.00 8.99 c c
ATOM 10253 OD1 ASN I 454 40.718 5.817 -19.912 1.00 11.67 c o
ATOM 10254 ND2 ASN I 454 39.073 6.836 -21.048 1.00 10.25 c N
ATOM 10255 C ASN I 454 38.053 2.617 -19.588 1.00 6.15 c c
ATOM 10256 O ASN I 454 39.041 2.154 -19.016 1.00 6.47 c o
ATOM 10257 N THR I 455 36.888 1.983 -19.635 1.00 5.40 c N
ATOM 10258 CA THR I 455 36.730 0.659 -19.057 1.00 4.53 c c
ATOM 10259 CB THR I 455 35.251 0.352 -18.737 1.00 4.70 c c
ATOM 10260 OG1 THR I 455 34.662 1.471 -18.063 1.00 5.28 c o
ATOM 10261 CG2 THR I 455 35.141 -0.878 -17.845 1.00 5.57 c c
ATOM 10262 C THR I 455 37.296 -0.399 -19.999 1.00 4.01 c c
ATOM 10263 O THR I 455 37.333 -0.204 -21.216 1.00 3.78 c o
ATOM 10264 N LEU I 456 37.885 -1.438 -19.414 1.00 3.87 c N
ATOM 10265 CA LEU I 456 38.439 -2.542 -20.189 1.00 4.05 c c
ATOM 10266 CB LEU I 456 39.946 -2.660 -19.955 1.00 3.95 c c
ATOM 10267 CG LEU I 456 40.690 -3.636 -20.868 1.00 3.76 c c
ATOM 10268 CD1 LEU I 456 40.594 -3.192 -22.319 1.00 5.35 c c
ATOM 10269 CD2 LEU 1456 42.142 -3.770 -20.440 1.00 4.10 c c
ATOM 10270 C LEU 1456 37.755 -3.858 -19.845 1.00 4.47 c c
ATOM 10271 O LEU I 456 37.769 -4.293 -18.694 1.00 4.94 c o
ATOM 10272 N TYR I 457 37.248 -4.534 -20.869 1.00 4.59 c N
ATOM 10273 CA TYR I 457 36.626 -5.839 -20.695 1.00 4.60 c c
ATOM 10274 CB TYR I 457 35.248 -5.861 -21.363 1.00 4.71 c c
ATOM 10275 CG TYR I 457 34.244 -4.912 -20.739 1.00 5.62 c c
ATOM 10276 CD1 TYR I 457 34.230 -3.563 -21.074 1.00 7.09 c c
ATOM 10277 CE1 TYR I 457 33.316 -2.697 -20.510 1.00 8.22 c c
ATOM 10278 CZ TYR I 457 32.408 -3.173 -19.588 1.00 8.06 c c
ATOM 10279 OH TYR I 457 31.469 -2.318 -19.059 1.00 8.80 c o
ATOM 10280 CE2 TYR I 457 32.381 -4.513 -19.262 1.00 7.18 c c
ATOM 10281 CD2 TYR I 457 33.302 -5.371 -19.827 1.00 6.66 c c
ATOM 10282 C TYR I 457 37.513 -6.932 -21.285 1.00 4.46 c c
ATOM 10283 O TYR I 457 38.049 -6.780 -22.383 1.00 4.92 c o
ATOM 10284 N TYR I 458 37.706 -8.009 -20.529 1.00 3.90 c N
ATOM 10285 CA TYR I 458 38.520 -9.138 -20.980 1.00 3.26 c c
ATOM 10286 CB TYR I 458 39.407 -9.632 -19.832 1.00 3.16 c c
ATOM 10287 CG TYR I 458 40.399 -8.610 -19.320 1.00 3.29 c c
ATOM 10288 CD1 TYR I 458 40.076 -7.762 -18.269 1.00 3.93 c c
ATOM 10289 CE1 TYR I 458 40.993 -6.848 -17.782 1.00 4.90 c c
ATOM 10290 CZ TYR I 458 42.245 -6.766 -18.354 1.00 5.12 c c
ATOM 10291 OH TYR I 458 43.156 -5.850 -17.881 1.00 5.42 c o
ATOM 10292 CE2 TYR I 458 42.590 -7.599 -19.395 1.00 4.72 c c
ATOM 10293 CD2 TYR I 458 41.677 -8.528 -19.858 1.00 3.89 c c
ATOM 10294 C TYR I 458 37.638 -10.293 -21.464 1.00 3.04 c c
ATOM 10295 O TYR I 458 36.897 -10.869 -20.672 1.00 3.37 c o
ATOM 10296 N VAL I 459 37.857 -10.755 -22.696 1.00 2.71 c N
ATOM 10297 CA VAL I 459 36.818 -11.487 -23.441 1.00 2.61 c c
ATOM 10298 CB VAL I 459 36.856 -11.172 -24.940 1.00 2.22 c c
ATOM 10299 CGI VAL I 459 35.936 -12.119 -25.698 1.00 2.62 c c
ATOM 10300 CG2 VAL I 459 36.459 -9.728 -25.187 1.00 2.61 c c
ATOM 10301 C VAL I 459 36.847 -13.006 -23.279 1.00 3.03 c c
ATOM 10302 O VAL I 459 37.324 -13.520 -22.267 1.00 3.21 c o
ATOM 10303 N ASN I 460 36.301 -13.724 -24.263 1.00106.93 c N
ATOM 10304 CA ASN I 460 36.733 -15.100 -24.460 1.00 95.54 c c
ATOM 10305 CB ASN I 460 37.469 -15.533 -23.198 1.00 20.00 c c

ATOM 10306 CG ASN I 460 38.132 -16.862 -23.352 1.00 20.00 C c
ATOM 10307 OD1 ASN I 460 38.781 -17.118 -24.365 1.00 20.00 c o
ATOM 10308 ND2 ASN I 460 37.824 -17.783 -22.448 1.00 20.00 c N
ATOM 10309 C ASN I 460 35.684 -16.173 -24.797 1.00 99.41 c c
ATOM 10310 O ASN I 460 35.555 -17.141 -24.047 1.00108.91 c o
ATOM 10311 N LYS I 461 35.174 -16.182 -26.023 1.00 97.04 c N
ATOM 10312 CA LYS 1461 34.426 -17.350 -26.495 1.00105.93 c c
ATOM 10313 CB LYS 1461 33.128 -17.516 -25.700 1.00 20.00 c c
ATOM 10314 CG LYS 1461 33.324 -18.050 -24.284 1.00 20.00 c c
ATOM 10315 CD LYS 1461 32.012 -18.071 -23.510 1.00 20.00 c c
ATOM 10316 CE LYS I 461 32.154 -18.798 -22.179 1.00 20.00 c c
ATOM 10317 NZ LYS 1461 30.869 -19.408 -21.736 1.00 20.00 c N
ATOM 10318 C LYS I 461 34.141 -17.231 -27.987 1.00102.28 c c
ATOM 10319 O LYS 1461 34.601 -16.289 -28.627 1.00105.02 c o
ATOM 10320 N GLN I 462 33.377 -18.164 -28.545 1.00 96.68 c N
ATOM 10321 CA GLN I 462 32.944 -18.040 -29.939 1.00105.71 c c
ATOM 10322 CB GLN I 462 33.693 -19.032 -30.836 1.00 20.00 c c
ATOM 10323 CG GLN I 462 35.184 -18.748 -30.976 1.00 20.00 c c
ATOM 10324 CD GLN I 462 35.922 -19.829 -31.741 1.00 20.00 c c
ATOM 10325 OE1 GLN I 462 35.456 -20.965 -31.841 1.00 20.00 c o
ATOM 10326 NE2 GLN I 462 37.071 -19.475 -32.303 1.00 20.00 c N
ATOM 10327 C GLN I 462 31.440 -18.235 -30.082 1.00101.50 c c
ATOM 10328 O GLN I 462 30.881 -19.193 -29.553 1.00105.94 c o
ATOM 10329 N GLU I 463 30.787 -17.335 -30.809 1.00 98.92 c N
ATOM 10330 CA GLU I 463 29.339 -17.413 -30.975 1.00108.59 c c
ATOM 10331 CB GLU I 463 28.684 -16.055 -30.712 1.00 20.00 c c
ATOM 10332 CG GLU I 463 28.617 -15.668 -29.238 1.00 20.00 c c
ATOM 10333 CD GLU I 463 28.032 -14.283 -29.019 1.00 20.00 c c
ATOM 10334 OE1 GLU I 463 27.535 -13.682 -29.995 1.00 20.00 c o
ATOM 10335 OE2 GLU I 463 27.975 -13.842 -27.851 1.00 20.00 c o
ATOM 10336 C GLU I 463 28.950 -17.934 -32.353 1.001 16.39 c c
ATOM 10337 O GLU I 463 29.396 -17.411 -33.375 1.001 18.70 c o
ATOM 10338 N GLY I 464 28.103 -18.957 -32.372 1.00127.70 c N
ATOM 10339 CA GLY I 464 27.598 -19.512 -33.621 1.00143.17 c c
ATOM 10340 C GLY I 464 26.466 -18.687 -34.200 1.00149.77 c c
ATOM 10341 O GLY I 464 25.945 -17.784 -33.545 1.00155.06 c o
ATOM 10342 N LYS 1465 26.088 -18.997 -35.435 1.00153.73 c N
ATOM 10343 CA LYS I 465 25.034 -18.261 -36.124 1.00153.69 c c
ATOM 10344 CB LYS 1465 23.750 -18.259 -35.293 1.00 20.00 c c
ATOM 10345 CG LYS I 465 23.099 -19.626 -35.151 1.00 20.00 c c
ATOM 10346 CD LYS I 465 21.848 -19.555 -34.292 1.00 20.00 c c
ATOM 10347 CE LYS I 465 21.188 -20.919 -34.164 1.00 20.00 c c
ATOM 10348 NZ LYS 1465 19.972 -20.869 -33.307 1.00 20.00 c N
ATOM 10349 C LYS I 465 25.466 -16.831 -36.426 1.00155.37 c c
ATOM 10350 O LYS 1465 25.158 -16.292 -37.489 1.00155.20 c o
ATOM 10351 N GLU I 472 20.477 -14.304 -43.583 1.00145.47 c N
ATOM 10352 CA GLU I 472 19.435 -13.563 -44.284 1.00151.12 c c
ATOM 10353 CB GLU I 472 18.367 -14.521 -44.821 1.00 20.00 c c
ATOM 10354 CG GLU I 472 18.856 -15.453 -45.922 1.00 20.00 c c
ATOM 10355 CD GLU I 472 17.778 -16.409 -46.402 1.00 20.00 c c
ATOM 10356 OE1 GLU I 472 16.723 -16.504 -45.739 1.00 20.00 c o
ATOM 10357 OE2 GLU I 472 17.996 -17.083 -47.430 1.00 20.00 c o
ATOM 10358 C GLU I 472 18.796 -12.521 -43.369 1.00153.35 c c
ATOM 10359 O GLU I 472 18.205 -12.866 -42.345 1.00159.41 c o
ATOM 10360 N PRO I 473 18.943 -11.236 -43.722 1.00150.51 c N
ATOM 10361 CA PRO I 473 18.346 -10.158 -42.958 1.00141.97 c c
ATOM 10362 CB PRO I 473 19.542 -9.243 -42.691 1.00 20.00 c c
ATOM 10363 CG PRO I 473 20.496 -9.502 -43.863 1.00 20.00 c c
ATOM 10364 CD PRO I 473 20.007 -10.730 -44.602 1.00 20.00 c c
ATOM 10365 C PRO 1473 17.331 -9.429 -43.824 1.00135.14 c c

ATOM 10366 O PRO I 473 17.408 -9.503 -45.051 1.00144.93 c o
ATOM 10367 N ILE I 474 16.371 -8.757 -43. 197 1.001 18.07 c N
ATOM 10368 CA ILE I 474 15.320 -8.071 -43.939 1.00105.14 c c
ATOM 10369 CB ILE I 474 14.440 -9.067 -44.737 1.00 20.00 c c
ATOM 10370 CGI ILE 1474 15.255 -9.730 -45.856 1.00 20.00 c c
ATOM 10371 CD1 ILE 1474 14.525 -10.842 -46.588 1.00 20.00 c c
ATOM 10372 CG2 ILE 1474 13.224 -8.354 -45.317 1.00 20.00 c c
ATOM 10373 C ILE I 474 14.436 -7.226 -43.022 1.00104.75 c c
ATOM 10374 O ILE I 474 13.471 -7.725 -42.443 1.001 11.83 c o
ATOM 10375 N ILE I 475 14.746 -5.934 -42.932 1.00 94.65 c N
ATOM 10376 CA ILE 1475 14.105 -5.051 -41.957 1.00 79.88 c c
ATOM 10377 CB ILE I 475 15.105 -4.568 -40.885 1.00 20.00 c c
ATOM 10378 CGI ILE 1475 15.576 -5.737 -40.014 1.00 20.00 c c
ATOM 10379 CD1 ILE 1475 16.791 -5.417 -39. 163 1.00 20.00 c c
ATOM 10380 CG2 ILE 1475 14.493 -3.458 -40.043 1.00 20.00 c c
ATOM 10381 C ILE I 475 13.459 -3.835 -42.617 1.00 79.52 c c
ATOM 10382 O ILE I 475 14.150 -2.913 -43.054 1.00 82.70 c o
ATOM 10383 N ASN I 476 12.133 -3.791 -42.590 1.00 69.64 c N
ATOM 10384 CA ASN I 476 11.404 -2.621 -43.048 1.00 68.88 c c
ATOM 10385 CB ASN I 476 9.979 -3.002 -43.442 1.00 20.00 c c
ATOM 10386 CG ASN I 476 9.939 -3.881 -44.672 1.00 20.00 c c
ATOM 10387 OD1 ASN I 476 10.854 -3.856 -45.496 1.00 20.00 c o
ATOM 10388 ND2 ASN I 476 8.918 -4.722 -44.762 1.00 20.00 c N
ATOM 10389 C ASN I 476 11.401 -1.512 -42.004 1.00 67.13 c c
ATOM 10390 O ASN I 476 11.491 -1.781 -40.806 1.00 73.10 c o
ATOM 10391 N PHE I 477 11.492 -0.273 -42.474 1.00 64.95 c N
ATOM 10392 CA PHE I 477 11.535 0.883 -41.585 1.00 68.13 c c
ATOM 10393 CB PHE I 477 12.064 2.118 -42.327 1.00 20.00 c c
ATOM 10394 CG PHE I 477 13.494 1.995 -42.778 1.00 20.00 c c
ATOM 10395 CD1 PHE I 477 14.532 2.409 -41.955 1.00 20.00 c c
ATOM 10396 CE1 PHE I 477 15.842 2.359 -42.391 1.00 20.00 c c
ATOM 10397 CZ PHE 1477 16. 127 1.910 -43.665 1.00 20.00 c c
ATOM 10398 CE2 PHE I 477 15. 100 1.529 -44.506 1.00 20.00 c c
ATOM 10399 CD2 PHE I 477 13.791 1.596 -44.070 1.00 20.00 c c
ATOM 10400 C PHE 1477 10.167 1.186 -40.968 1.00 65.57 c c
ATOM 10401 O PHE 1477 10.033 2.109 -40. 165 1.00 49.83 c o
ATOM 10402 N TYR I 478 9.136 0.485 -41.432 1.00 51.97 c N
ATOM 10403 CA TYR I 478 7.81 1 0.580 -40.824 1.00 52.01 c c
ATOM 10404 CB TYR I 478 6.729 0.140 -41.815 1.00 20.00 c c
ATOM 10405 CG TYR I 478 6.638 1.012 -43.045 1.00 20.00 c c
ATOM 10406 CD1 TYR I 478 5.883 2.179 -43.040 1.00 20.00 c c
ATOM 10407 CE1 TYR I 478 5.824 2.997 -44. 155 1.00 20.00 c c
ATOM 10408 CZ TYR I 478 6.512 2.642 -45.300 1.00 20.00 c c
ATOM 10409 OH TYR I 478 6.454 3.447 -46.414 1.00 20.00 c o
ATOM 10410 CE2 TYR I 478 7.260 1.484 -45.333 1.00 20.00 c c
ATOM 1041 1 CD2 TYR I 478 7.319 0.677 -44.210 1.00 20.00 c c
ATOM 10412 C TYR I 478 7.745 -0.269 -39.556 1.00 66.63 c c
ATOM 10413 O TYR I 478 6.674 -0.470 -38.983 1.00 63.45 c o
ATOM 10414 N ASP I 479 8.898 -0.790 -39. 146 1.00 65.34 c N
ATOM 10415 CA ASP 1479 9.013 -1.509 -37.886 1.00 65.32 c c
ATOM 10416 CB ASP I 479 9.879 -2.758 -38.061 1.00 20.00 c c
ATOM 10417 CG ASP 1479 9.210 -3.815 -38.916 1.00 20.00 c c
ATOM 10418 OD1 ASP I 479 7.967 -3.791 -39.028 1.00 20.00 c o
ATOM 10419 OD2 ASP I 479 9.920 -4.701 -39.436 1.00 20.00 c o
ATOM 10420 C ASP I 479 9.590 -0.614 -36.796 1.00 64.83 c c
ATOM 10421 O ASP I 479 9.572 -0.976 -35.620 1.00 60.42 c o
ATOM 10422 N PRO I 480 10.076 0.579 -37. 181 1.00 47.60 c N
ATOM 10423 CA PRO I 480 10.722 1.488 -36.253 1.00 46.52 c c
ATOM 10424 CB PRO I 480 11.789 2.143 -37. 124 1.00 20.00 c c
ATOM 10425 CG PRO I 480 11.140 2.219 -38.487 1.00 20.00 c c

ATOM 10426 CD PRO I 480 10.043 1.155 -38.536 1.00 20.00 c c
ATOM 10427 C PRO 1480 9.736 2.550 -35.806 1.00 52.36 c c
ATOM 10428 O PRO I 480 9.629 3.601 -36.438 1.00 64.15 c o
ATOM 10429 N LEU I 481 8.945 2.229 -34.792 1.00 62.90 c N
ATOM 10430 CA LEU I 481 8.005 3.187 -34.233 1.00 54.24 c c
ATOM 10431 CB LEU I 481 6.576 2.656 -34.340 1.00 20.00 c c
ATOM 10432 CG LEU I 481 6.056 2.404 -35.756 1.00 20.00 c c
ATOM 10433 CD1 LEU I 481 4.735 1.662 -35.704 1.00 20.00 c c
ATOM 10434 CD2 LEU I 481 5.91 1 3.71 1 -36.524 1.00 20.00 c c
ATOM 10435 C LEU 1481 8.346 3.496 -32.783 1.00 59.81 c c
ATOM 10436 O LEU I 481 9.346 3.015 -32.250 1.00 64.98 c o
ATOM 10437 N VAL I 482 7.562 4.375 -32.176 1.00 59.66 c N
ATOM 10438 CA VAL I 482 7.706 4.645 -30.761 1.00 49.67 c c
ATOM 10439 CB VAL I 482 7.767 6.146 -30.484 1.00 20.00 c c
ATOM 10440 CGI VAL I 482 8.060 6.388 -29.015 1.00 20.00 c c
ATOM 10441 CG2 VAL I 482 8.826 6.795 -31.358 1.00 20.00 c c
ATOM 10442 C VAL I 482 6.550 4.037 -29.987 1.00 53.03 c c
ATOM 10443 O VAL I 482 5.423 3.998 -30.476 1.00 46.27 c o
ATOM 10444 N PHE I 483 6.864 3.441 -28.842 1.00 61.61 c N
ATOM 10445 CA PHE I 483 5.847 2.831 -27.994 1.00 65.03 c c
ATOM 10446 CB PHE I 483 6.218 1.380 -27.662 1.00 20.00 c c
ATOM 10447 CG PHE I 483 6.212 0.463 -28.857 1.00 20.00 c c
ATOM 10448 CD1 PHE I 483 5.036 -0.124 -29.292 1.00 20.00 c c
ATOM 10449 CE1 PHE I 483 5.028 -0.963 -30.390 1.00 20.00 c c
ATOM 10450 CZ PHE 1483 6.201 -1.222 -31.068 1.00 20.00 c c
ATOM 10451 CE2 PHE I 483 7.379 -0.653 -30.639 1.00 20.00 c c
ATOM 10452 CD2 PHE I 483 7.382 0.185 -29.540 1.00 20.00 c c
ATOM 10453 C PHE 1483 5.627 3.653 -26.723 1.00 7 1.00 c c
ATOM 10454 O PHE 1483 5.934 3.199 -25.620 1.00100.44 c o
ATOM 10455 N PRO I 484 5.255 4.928 -26.903 1.00 54.44 c N
ATOM 10456 CA PRO I 484 5.000 5.815 -25.781 1.00 47.46 c c
ATOM 10457 CB PRO I 484 6.136 6.828 -25.903 1.00 20.00 c c
ATOM 10458 CG PRO I 484 6.468 6.851 -27.406 1.00 20.00 c c
ATOM 10459 CD PRO I 484 5.760 5.686 -28.058 1.00 20.00 c c
ATOM 10460 C PRO 1484 3.661 6.533 -25.944 1.00 41.56 c c
ATOM 10461 O PRO I 484 3.430 7.190 -26.959 1.00 46.53 c o
ATOM 10462 N SER I 485 2.779 6.380 -24.964 1.00 46.30 c N
ATOM 10463 CA SER I 485 1.436 6.938 -25.048 1.00 49.30 c c
ATOM 10464 CB SER I 485 0.892 7.220 -23.649 1.00 20.00 c c
ATOM 10465 OG SER I 485 1.684 8.188 -22.983 1.00 20.00 c o
ATOM 10466 C SER I 485 1.380 8.204 -25.901 1.00 41.24 c c
ATOM 10467 O SER I 485 0.643 8.262 -26.883 1.00 46.93 c o
ATOM 10468 N ASP I 486 2.103 9.238 -25.482 1.00 49.48 c N
ATOM 10469 CA ASP 1486 2.085 10.518 -26.185 1.00 37.44 c c
ATOM 10470 CB ASP I 486 3.029 11.514 -25.51 1 1.00 20.00 c c
ATOM 10471 CG ASP 1486 2.509 11.993 -24.173 1.00 20.00 c c
ATOM 10472 OD1 ASP I 486 1.314 11.773 -23.887 1.00 20.00 c o
ATOM 10473 OD2 ASP I 486 3.299 12.566 -23.395 1.00 20.00 c o
ATOM 10474 C ASP I 486 2.456 10.359 -27.656 1.00 45.66 c c
ATOM 10475 O ASP I 486 1.752 10.848 -28.539 1.00 39.86 c o
ATOM 10476 N GLU I 487 3.559 9.665 -27.914 1.00 49.20 C N
ATOM 10477 CA GLU I 487 4.006 9.422 -29.280 1.00 45.70 c c
ATOM 10478 CB GLU I 487 5.346 8.684 -29.288 1.00 20.00 c c
ATOM 10479 CG GLU I 487 6.491 9.481 -28.685 1.00 20.00 c c
ATOM 10480 CD GLU I 487 7.766 8.669 -28.551 1.00 20.00 c c
ATOM 10481 OE1 GLU I 487 7.722 7.447 -28.804 1.00 20.00 c o
ATOM 10482 OE2 GLU I 487 8.794 9.238 -28.122 1.00 20.00 c o
ATOM 10483 C GLU I 487 2.966 8.648 -30.085 1.00 41.48 c c
ATOM 10484 O GLU I 487 2.656 9.01 1 -31 .219 1.00 48.92 c o
ATOM 10485 N PHE 1488 2.402 7.606 -29.483 1.00 42.16 C N

```
ATOM  10486  CA  PHE I 488      1.397   6.789 -30.155  1.00 39.33      C   c
ATOM  10487  CB  PHE I 488      0.968   5.623 -29.268  1.00 20.00      C   c
ATOM  10488  CG  PHE I 488      2.059   4.633 -29.005  1.00 20.00      c   c
ATOM  10489  CD1 PHE I 488      2.403   3.694 -29.958  1.00 20.00      c   c
ATOM  10490  CE1 PHE I 488      3.409   2.779 -29.715  1.00 20.00      c   c
ATOM  10491  CZ  PHE 1488      4.089   2.807 -28.517  1.00 20.00      c   c
ATOM  10492  CE2 PHE I 488      3.752   3.737 -27.560  1.00 20.00      c   c
ATOM  10493  CD2 PHE I 488      2.752   4.652 -27.810  1.00 20.00      c   c
ATOM  10494  C   PHE 1488      0.182   7.618 -30.540  1.00 43.06      c   c
ATOM  10495  O   PHE 1488     -0.328   7.508 -31.654  1.00 61.71      c   o
ATOM  10496  N   ASP I 489     -0.261   8.471 -29.624  1.00 41.95      c   N
ATOM  10497  CA  ASP 1489     -1.454   9.273 -29.851  1.00 42.75      c   c
ATOM  10498  CB  ASP I 489     -1.837  10.023 -28.581  1.00 20.00      c   c
ATOM  10499  CG  ASP 1489     -2.352   9.102 -27.504  1.00 20.00      c   c
ATOM  10500  OD1 ASP I 489     -2.808   7.989 -27.848  1.00 20.00      c   o
ATOM  10501  OD2 ASP I 489     -2.184   9.435 -26.313  1.00 20.00      c   o
ATOM  10502  C   ASP I 489     -1.255  10.256 -30.994  1.00 45.61      c   c
ATOM  10503  O   ASP I 489     -2.206  10.617 -31.689  1.00 54.39      c   o
ATOM  10504  N   ALA I 490     -0.020  10.714 -31.160  1.00 42.89      c   N
ATOM  10505  CA  ALA I 490      0.306  11.663 -32.215  1.00 38.40      c   c
ATOM  10506  CB  ALA I 490      1.684  12.262 -31.976  1.00 20.00      c   c
ATOM  10507  C   ALA I 490      0.240  10.994 -33.585  1.00 39.67      c   c
ATOM  10508  O   ALA I 490     -0.356  11.529 -34.521  1.00 56.80      c   o
ATOM  10509  N   SER I 491      0.803   9.793 -33.676  1.00 40.38      c   N
ATOM  10510  CA  SER I 491      0.721   8.992 -34.893  1.00 41.77      c   c
ATOM  10511  CB  SER I 491      1.611   7.752 -34.784  1.00 20.00      c   c
ATOM  10512  OG  SER I 491      1.132   6.864 -33.788  1.00 20.00      c   o
ATOM  10513  C   SER I 491     -0.717   8.580 -35.187  1.00 39.01      c   c
ATOM  10514  O   SER I 491     -1.142   8.563 -36.342  1.00 36.91      c   o
ATOM  10515  N   ILE I 492     -1.474   8.286 -34.135  1.00 38.11      C   N
ATOM  10516  CA  ILE I 492     -2.896   8.000 -34.280  1.00 41.21      c   c
ATOM  10517  CB  ILE I 492     -3.539   7.629 -32.938  1.00 20.00      c   c
ATOM  10518  CGI ILE 1492     -2.964   6.311 -32.424  1.00 20.00      c   c
ATOM  10519  CD1 ILE 1492     -3.501   5.906 -31.076  1.00 20.00      c   c
ATOM  10520  CG2 ILE 1492     -5.050   7.533 -33.080  1.00 20.00      c   c
ATOM  10521  C   ILE I 492     -3.646   9.182 -34.883  1.00 39.22      c   c
ATOM  10522  O   ILE I 492     -4.494   9.008 -35.758  1.00 47.54      c   o
ATOM  10523  N   SER I 493     -3.334  10.383 -34.408  1.00 41.64      c   N
ATOM  10524  CA  SER I 493     -3.929  11.598 -34.952  1.00 35.15      c   c
ATOM  10525  CB  SER I 493     -3.483  12.820 -34.146  1.00 20.00      c   c
ATOM  10526  OG  SER I 493     -2.100  13.070 -34.322  1.00 20.00      c   o
ATOM  10527  C   SER I 493     -3.547  11.773 -36.416  1.00 47.90      c   c
ATOM  10528  O   SER I 493     -4.380  12.128 -37.250  1.00 50.94      c   o
ATOM  10529  N   GLN I 494     -2.296  11.457 -36.727  1.00 42.51      c   N
ATOM  10530  CA  GLN I 494     -1.784  11.587 -38.081  1.00 41.96      c   c
ATOM  10531  CB  GLN I 494     -0.263  11.405 -38.085  1.00 20.00      c   c
ATOM  10532  CG  GLN I 494      0.495  12.482 -37.308  1.00 20.00      c   c
ATOM  10533  CD  GLN I 494      1.989  12.210 -37.223  1.00 20.00      c   c
ATOM  10534  OE1 GLN I 494      2.410  11.104 -36.881  1.00 20.00      c   o
ATOM  10535  NE2 GLN I 494      2.790  13.248 -37.433  1.00 20.00      c   N
ATOM  10536  C   GLN I 494     -2.449  10.583 -39.023  1.00 33.86      c   c
ATOM  10537  O   GLN I 494     -2.944  10.950 -40.090  1.00 54.89      c   o
ATOM  10538  N   VAL I 495     -2.511   9.328 -38.594  1.00 34.99      c   N
ATOM  10539  CA  VAL I 495     -3.226   8.300 -39.341  1.00 38.42      c   c
ATOM  10540  CB  VAL I 495     -3.245   6.968 -38.576  1.00 20.00      c   c
ATOM  10541  CGI VAL I 495     -4.032   5.922 -39.349  1.00 20.00      c   c
ATOM  10542  CG2 VAL I 495     -1.828   6.497 -38.309  1.00 20.00      c   c
ATOM  10543  C   VAL I 495     -4.661   8.731 -39.618  1.00 42.74      c   c
ATOM  10544  O   VAL I 495     -5.144   8.634 -40.747  1.00 44.00      c   o
ATOM  10545  N   ASN I 496     -5.314   9.268 -38.592  1.00 42.45      c   N
```

```
ATOM  10546  CA  ASN I 496      -6.705   9.685 -38.697  1.00 43.01      C    c
ATOM  10547  CB  ASN I 496      -7.232  10.134 -37.333  1.00 20.00      c    c
ATOM  10548  CG  ASN I 496      -7.416   8.977 -36.374  1.00 20.00      c    c
ATOM  10549  OD1 ASN I 496      -7.439   7.817 -36.784  1.00 20.00      c    o
ATOM  10550  ND2 ASN I 496      -7.495   9.283 -35.083  1.00 20.00      c    N
ATOM  10551  C   ASN I 496      -6.906  10.790 -39.727  1.00 43.13      c    c
ATOM  10552  O   ASN I 496      -7.893  10.793 -40.462  1.00 54.76      c    o
ATOM  10553  N   GLU I 497      -5.990  11.752 -39.744  1.00 42.08      c    N
ATOM  10554  CA  GLU I 497      -6.038  12.828 -40.726  1.00 43.13      c    c
ATOM  10555  CB  GLU I 497      -4.947  13.863 -40.443  1.00 20.00      c    c
ATOM  10556  CG  GLU I 497      -5.172  14.672 -39.175  1.00 20.00      c    c
ATOM  10557  CD  GLU I 497      -4.045  15.647 -38.896  1.00 20.00      c    c
ATOM  10558  OE1 GLU I 497      -3.007  15.574 -39.587  1.00 20.00      c    o
ATOM  10559  OE2 GLU I 497      -4.192  16.480 -37.977  1.00 20.00      c    o
ATOM  10560  C   GLU I 497      -5.884  12.275 -42.137  1.00 49.77      c    c
ATOM  10561  O   GLU I 497      -6.542  12.736 -43.071  1.00 42.88      c    o
ATOM  10562  N   LYS I 498      -5.051  11.249 -42.273  1.00 41.82      c    N
ATOM  10563  CA  LYS I 498      -4.855  10.579 -43.552  1.00 53.60      c    c
ATOM  10564  CB  LYS 1498      -3.676   9.609 -43.471  1.00 20.00      c    c
ATOM  10565  CG  LYS I 498      -2.336  10.274 -43.228  1.00 20.00      c    c
ATOM  10566  CD  LYS I 498      -1.193   9.356 -43.638  1.00 20.00      c    c
ATOM  10567  CE  LYS I 498       0.160   9.937 -43.247  1.00 20.00      c    c
ATOM  10568  NZ  LYS 1498       1.285   9.250 -43.942  1.00 20.00      c    N
ATOM  10569  C   LYS I 498      -6.109   9.830 -43.994  1.00 55.29      C    c
ATOM  10570  O   LYS 1498      -6.409   9.763 -45.186  1.00 61.06      c    o
ATOM  10571  N   ILE I 499      -6.766   9.165 -43.047  1.00 52.22      C    N
ATOM  10572  CA  ILE I 499      -8.038   8.500 -43.323  1.00 48.26      c    c
ATOM  10573  CB  ILE I 499      -8.586   7.785 -42.076  1.00 20.00      c    c
ATOM  10574  CGI ILE 1499      -7.657   6.642 -41.667  1.00 20.00      c    c
ATOM  10575  CD1 ILE 1499      -7.934   6.102 -40.286  1.00 20.00      c    c
ATOM  10576  CG2 ILE 1499      -9.994   7.267 -42.333  1.00 20.00      c    c
ATOM  10577  C   ILE I 499      -9.067   9.516 -43.798  1.00 49.07      c    c
ATOM  10578  O   ILE I 499      -9.858   9.244 -44.701  1.00 58.45      c    o
ATOM  10579  N   ASN I 500      -8.961  10.726 -43.265  1.00 51.02      c    N
ATOM  10580  CA  ASN I 500      -9.845  11.812 -43.644  1.00 52.06      c    c
ATOM  10581  CB  ASN I 500      -9.741  12.940 -42.625  1.00 20.00      c    c
ATOM  10582  CG  ASN I 500     -10.861  13.933 -42.753  1.00 20.00      c    c
ATOM  10583  OD1 ASN I 500     -11.927  13.622 -43.286  1.00 20.00      C    O
ATOM  10584  ND2 ASN I 500     -10.647  15.126 -42.232  1.00 20.00      C    N
ATOM  10585  C   ASN I 500      -9.552  12.345 -45.041  1.00 48.31      C    c
ATOM  10586  O   ASN I 500     -10.448  12.834 -45.729  1.00 56.89      c    o
ATOM  10587  N   GLN I 501      -8.283  12.300 -45.434  1.00 55.87      c    N
ATOM  10588  CA  GLN I 501      -7.900  12.610 -46.807  1.00 53.55      c    c
ATOM  10589  CB  GLN I 501      -6.384  12.797 -46.917  1.00 20.00      c    c
ATOM  10590  CG  GLN I 501      -5.851  13.987 -46.136  1.00 20.00      c    c
ATOM  10591  CD  GLN I 501      -4.338  14.093 -46.191  1.00 20.00      c    c
ATOM  10592  OE1 GLN I 501      -3.648  13.146 -46.576  1.00 20.00      c    o
ATOM  10593  NE2 GLN I 501      -3.814  15.247 -45.793  1.00 20.00      c    N
ATOM  10594  C   GLN I 501      -8.383  11.531 -47.777  1.00 45.67      c    c
ATOM  10595  O   GLN I 501      -8.980  11.837 -48.810  1.00 58.31      c    o
ATOM  10596  N   SER I 502      -8.234  10.273 -47.378  1.00 43.44      c    N
ATOM  10597  CA  SER I 502      -8.704   9.157 -48.189  1.00 45.40      c    c
ATOM  10598  CB  SER I 502      -8.367   7.830 -47.512  1.00 20.00      c    c
ATOM  10599  OG  SER I 502      -9.001   7.735 -46.250  1.00 20.00      c    o
ATOM  10600  C   SER I 502     -10.206   9.254 -48.413  1.00 55.15      c    c
ATOM  10601  O   SER I 502     -10.708   8.934 -49.490  1.00 52.57      c    o
ATOM  10602  N   LEU I 503     -10.920   9.673 -47.376  1.00 55.35      c    N
ATOM  10603  CA  LEU I 503     -12.366   9.798 -47.447  1.00 52.12      c    c
ATOM  10604  CB  LEU I 503     -12.950  10.025 -46.053  1.00 20.00      c    c
ATOM  10605  CG  LEU I 503     -12.783   8.856 -45.082  1.00 20.00      c    c
```

```
ATOM  10606  CD1 LEU 1503     -13.061   9.290 -43.653  1.00 20.00      C    C
ATOM  10607  CD2 LEU I 503     -13.685   7.704 -45.481  1.00 20.00      C    C
ATOM  10608  C   LEU 1503     -12.761  10.938 -48.371  1.00 55.74      C    C
ATOM  10609  O   LEU 1503     -13.782  10.869 -49.052  1.00 57.75      C    O
ATOM  10610  N   ALA 1504     -11.951  11.991 -48.382  1.00 57.22      C    N
ATOM  1061 1 CA  ALA 1504     -12.187  13.129 -49.261  1.00 59. 12     C    C
ATOM  10612  CB  ALA 1504     -11.333  14.315 -48.831  1.00 20.00      C    C
ATOM  10613  C   ALA 1504     -11.902  12.760 -50.713  1.00 58.10      C    C
ATOM  10614  O   ALA 1504     -12.656  13.1 19 -51 .618  1.00 63.64      C    O
ATOM  10615  N   PHE 1505     -10.813  12.029 -50.922  1.00 58.17      C    N
ATOM  10616  CA  PHE I 505     -10.485  11.505 -52.240  1.00 56.56      C    C
ATOM  10617  CB  PHE 1505      -9.180  10.698 -52. 186  1.00 20.00      C    C
ATOM  10618  CG  PHE 1505      -7.971  11.517 -51 .817  1.00 20.00      C    C
ATOM  10619  CD1 PHE I 505      -7.307  12.270 -52.773  1.00 20.00      C    C
ATOM  10620  CE1 PHE I 505      -6.230  13.063 -52.426  1.00 20.00      C    C
ATOM  10621  CZ  PHE 1505      -5.768  13.067 -51.125  1.00 20.00      C    C
ATOM  10622  CE2 PHE I 505      -6.376  12.270 -50.176  1.00 20.00      C    C
ATOM  10623  CD2 PHE I 505      -7.471  11.499 -50.524  1.00 20.00      C    C
ATOM  10624  C   PHE 1505     -11.625  10.637 -52.769  1.00 60.12      C    C
ATOM  10625  O   PHE 1505     -12.014  10.746 -53.934  1.00 65.46      C    O
ATOM  10626  N   ILE 1506     -12.214   9.844 -51.875  1.00 56.10      C    N
ATOM  10627  CA  ILE 1506     -13.355   8.991 -52.213  1.00 57.32      C    C
ATOM  10628  CB  ILE 1506     -13.782   8.109 -51.013  1.00 20.00      C    C
ATOM  10629  CGI ILE 1506     -12.657   7.149 -50.619  1.00 20.00      C    C
ATOM  10630  CD1 ILE 1506     -12.804   6.591 -49.222  1.00 20.00      C    C
ATOM  10631  CG2 ILE I 506     -15.064   7.345 -51.330  1.00 20.00      C    C
ATOM  10632  C   ILE 1506     -14.556   9.818 -52.669  1.00 67.33      C    C
ATOM  10633  O   ILE 1506     -15.217   9.485 -53.652  1.00 76.99      C    O
ATOM  10634  N   ARG 1507     -14.855  10.878 -51.925  1.00 67.87      C    N
ATOM  10635  CA  ARG I 507     -15.936  11.788 -52.287  1.00 62. 11     C    C
ATOM  10636  CB  ARG 1507     -16.087  12.898 -51.240  1.00 20.00      C    C
ATOM  10637  CG  ARG I 507     -16.795  12.450 -49.963  1.00 20.00      C    C
ATOM  10638  CD  ARG 1507     -16.736  13.504 -48.861  1.00 20.00      C    C
ATOM  10639  NE  ARG 1507     -17.140  12.957 -47.566  1.00 20.00      C    N
ATOM  10640  CZ  ARG 1507     -17.292  13.683 -46.463  1.00 20.00      C    C
ATOM  10641  NH1 ARG I 507     -17.083  14.992 -46.499  1.00 20.00      C    N
ATOM  10642  NH2 ARG I 507     -17.687  13.106 -45.335  1.00 20.00      C    N
ATOM  10643  C   ARG 1507     -15.685  12.391 -53.659  1.00 67.30      C    C
ATOM  10644  O   ARG 1507     -16.488  12.224 -54.574  1.00 67.02      C    O
ATOM  10645  N   LYS 1508     -14.518  13.001 -53.823  1.00 66.83      C    N
ATOM  10646  CA  LYS I 508     -14.125  13.546 -55. 112  1.00 68.12     C    C
ATOM  10647  CB  LYS 1508     -12.693  14.086 -55.052  1.00 20.00      C    C
ATOM  10648  CG  LYS I 508     -12.522  15.286 -54. 117  1.00 20.00      C    C
ATOM  10649  CD  LYS I 508     -11.072  15.750 -54.046  1.00 20.00      C    C
ATOM  10650  CE  LYS I 508     -10.912  16.933 -53.098  1.00 20.00      C    C
ATOM  10651  NZ  LYS 1508      -9.486  17.329 -52.912  1.00 20.00      C    N
ATOM  10652  C   LYS 1508     -14.275  12.499 -56.215  1.00 65.22      C    C
ATOM  10653  O   LYS 1508     -15.005  12.710 -57.183  1.00 72.34      C    O
ATOM  10654  N   SER I 509     -13.727  11.312 -55.973  1.00 64.87      C    N
ATOM  10655  CA  SER 1509     -13.783  10.230 -56.949  1.00 56.47      C    C
ATOM  10656  CB  SER 1509     -13.014   9.008 -56.445  1.00 20.00      C    C
ATOM  10657  OG  SER 1509     -13.561   8.528 -55.232  1.00 20.00      C    O
ATOM  10658  C   SER 1509     -15.220   9.847 -57.299  1.00 56.96      C    C
ATOM  10659  O   SER 1509     -15.537   9.599 -58.461  1.00 65.57      C    O
ATOM  10660  N   ASP 1510     -16.077   9.760 -56.285  1.00 64.34      C    N
ATOM  10661  CA  ASP 1510     -17.478   9.402 -56.500  1.00 64.83      C    C
ATOM  10662  CB  ASP 1510     -18.217   9.244 -55. 161  1.00 20.00      C    C
ATOM  10663  CG  ASP 1510     -17.827   7.975 -54.416  1.00 20.00      C    C
ATOM  10664  OD1 ASP I 510     -17.292   7.044 -55.050  1.00 20.00      C    O
ATOM  10665  OD2 ASP I 510     -18.083   7.900 -53. 197  1.00 20.00      C    O
```

```
ATOM  10666  C   ASP 1510     -18.173  10.458 -57.356  1.00 62.11     C  C
ATOM  10667  O   ASP 1510     -18.723  10.150 -58.412  1.00 67.61     C  O
ATOM  10668  N   GLU I511     -18.078  11.713 -56.928  1.00 64.95     C  N
ATOM  10669  CA  GLU I511     -18.673  12.822 -57.664  1.00 60.64     C  C
ATOM  10670  CB  GLU I511     -18.175  14.162 -57.117  1.00 20.00     C  C
ATOM  10671  CG  GLU I511     -18.700  14.509 -55.736  1.00 20.00     C  C
ATOM  10672  CD  GLU I511     -18.061  15.767 -55.172  1.00 20.00     C  C
ATOM  10673  OE1 GLU I511     -17.166  16.329 -55.841  1.00 20.00     C  O
ATOM  10674  OE2 GLU I511     -18.506  16.237 -54.102  1.00 20.00     C  O
ATOM  10675  C   GLU 1511     -18.377  12.729 -59.159  1.00 59.91     C  C
ATOM  10676  O   GLU 1511     -19.245  13.008 -59.983  1.00 55.45     C  O
ATOM  10677  N   LEU 1512     -17.122  12.450 -59.503  1.00 44.35     C  N
ATOM  10678  CA  LEU I512     -16.712  12.392 -60.904  1.00 49.60     C  C
ATOM  10679  CB  LEU 1512     -15.196  12.240 -61.021  1.00 20.00     C  C
ATOM  10680  CG  LEU I512     -14.353  13.460 -60.658  1.00 20.00     C  C
ATOM  10681  CD1 LEU 1512     -12.894  13.181 -60.963  1.00 20.00     C  C
ATOM  10682  CD2 LEU I512     -14.831  14.678 -61.424  1.00 20.00     C  C
ATOM  10683  C   LEU 1512     -17.396  11.239 -61.621  1.00 58.00     C  C
ATOM  10684  O   LEU I512     -17.946  11.411 -62.708  1.00 55.11     C  O
ATOM  10685  N   LEU 1513     -17.306  10.051 -61.036  1.00 57.91     C  N
ATOM  10686  CA  LEU 1513     -17.901   8.870 -61.636  1.00 57.49     C  C
ATOM  10687  CB  LEU 1513     -17.632   7.629 -60.774  1.00 20.00     C  C
ATOM  10688  CG  LEU 1513     -16.169   7.179 -60.678  1.00 20.00     C  C
ATOM  10689  CD1 LEU I513     -15.992   6.055 -59.670  1.00 20.00     C  C
ATOM  10690  CD2 LEU 1513     -15.637   6.768 -62.042  1.00 20.00     C  C
ATOM  10691  C   LEU 1513     -19.399   9.075 -61.852  1.00 58.78     C  C
ATOM  10692  O   LEU 1513     -19.913   8.812 -62.940  1.00 59.88     C  O
ATOM  10693  N   HIS 1514     -20.054   9.718 -60.888  1.00 60.07     C  N
ATOM  10694  CA  HIS 1514     -21.494   9.975 -60.982  1.00 62.82     C  C
ATOM  10695  CB  HIS 1514     -22.058  10.454 -59.635  1.00 20.00     C  C
ATOM  10696  CG  HIS 1514     -21.878   9.472 -58.517  1.00 20.00     C  C
ATOM  10697  ND1 HIS 1514     -22.551   8.269 -58.465  1.00 20.00     C  N
ATOM  10698  CE1 HIS I514     -22.192   7.612 -57.376  1.00 20.00     C  C
ATOM  10699  NE2 HIS 1514     -21.304   8.342 -56.723  1.00 20.00     C  N
ATOM  10700  CD2 HIS I514     -21.104   9.517 -57.407  1.00 20.00     C  C
ATOM  10701  C   HIS 1514     -21.799  10.989 -62.087  1.00 65.10     C  C
ATOM  10702  O   HIS 1514     -22.898  11.002 -62.647  1.00 66.73     C  O
ATOM  10703  N   ASN I515     -20.795  11.787 -62.441  1.00 63.45     C  N
ATOM  10704  CA  ASN I515     -20.932  12.782 -63.499  1.00 56.53     C  C
ATOM  10705  CB  ASN I515     -19.903  13.909 -63.317  1.00 20.00     C  C
ATOM  10706  CG  ASN I515     -20.243  14.838 -62.159  1.00 20.00     C  C
ATOM  10707  OD1 ASN I515     -21.400  14.948 -61.756  1.00 20.00     C  O
ATOM  10708  ND2 ASN I515     -19.238  15.544 -61.652  1.00 20.00     C  N
ATOM  10709  C   ASN 1515     -20.765  12.134 -64.868  1.00 60.06     C  C
ATOM  10710  O   ASN 1515     -21.518  12.422 -65.799  1.00 66.48     C  O
ATOM  10711  N   VAL I516     -19.829  11.197 -64.959  1.00 54.29     C  N
ATOM  10712  CA  VAL I516     -19.617  10.460 -66.195  1.00 52.70     C  C
ATOM  10713  CB  VAL I516     -18.407   9.523 -66.097  1.00 20.00     C  C
ATOM  10714  CGI VAL I516     -18.398   8.554 -67.267  1.00 20.00     C  C
ATOM  10715  CG2 VAL I516     -17.122  10.330 -66.063  1.00 20.00     C  C
ATOM  10716  C   VAL 1516     -20.850   9.645 -66.551  1.00 60.10     C  C
ATOM  10717  O   VAL 1516     -21.306   9.662 -67.693  1.00 61.55     C  O
ATOM  10718  N   ASN 1517     -21.432   8.998 -65.549  1.00 69.10     C  N
ATOM  10719  CA  ASN 1517     -22.648   8.224 -65.749  1.00 67.75     C  C
ATOM  10720  CB  ASN 1517     -23.135   7.652 -64.421  1.00 20.00     C  C
ATOM  10721  CG  ASN 1517     -22.254   6.530 -63.914  1.00 20.00     C  C
ATOM  10722  OD1 ASN I517     -21.467   5.954 -64.667  1.00 20.00     C  O
ATOM  10723  ND2 ASN I517     -22.368   6.226 -62.627  1.00 20.00     C  N
ATOM  10724  C   ASN 1517     -23.751   9.051 -66.394  1.00 71.17     C  C
ATOM  10725  O   ASN 1517     -24.535   8.544 -67.196  1.00 66.42     C  O
```

ATOM 10726 N ALA 1518 -23.811 10.326 -66.028 1.00 72.11 C N
ATOM 10727 CA ALA 1518 -24.811 11.232 -66.571 1.00 74.82 C C
ATOM 10728 CB ALA 1518 -24.936 12.464 -65.692 1.00 20.00 C C
ATOM 10729 C ALA 1518 -24.471 11.628 -68.004 1.00 70.11 C C
ATOM 10730 O ALA 1518 -25.328 11.590 -68.886 1.00 65.18 C O
ATOM 10731 N GLY I 519 -23.212 11.989 -68.230 1.00 56.07 C N
ATOM 10732 CA GLY I 519 -22.709 12.224 -69.577 1.00 53.01 C C
ATOM 10733 C GLY I 519 -22.906 11.026 -70.483 1.00 63.58 C C
ATOM 10734 O GLY I 519 -23.221 11.174 -71.663 1.00 69.35 C O
ATOM 10735 N LYS 1520 -22.776 9.833 -69.912 1.00 58.33 C N
ATOM 10736 CA LYS 1520 -22.996 8.592 -70.647 1.00 53.44 C C
ATOM 10737 CB LYS 1520 -22.655 7.389 -69.767 1.00 20.00 C C
ATOM 10738 CG LYS 1520 -21.194 7.319 -69.368 1.00 20.00 C C
ATOM 10739 CD LYS 1520 -20.915 6.097 -68.525 1.00 20.00 C C
ATOM 10740 CE LYS 1520 -19.428 5.920 -68.314 1.00 20.00 C C
ATOM 10741 NZ LYS 1520 -19.148 4.767 -67.417 1.00 20.00 C N
ATOM 10742 C LYS 1520 -24.437 8.485 -71.121 1.00 58.24 C C
ATOM 10743 O LYS 1520 -24.714 7.920 -72.179 1.00 48.60 C O
ATOM 10744 N SER I 521 -25.354 8.971 -70.293 1.00 67.19 C N
ATOM 10745 CA SER I 521 -26.772 8.995 -70.632 1.00 60.42 C C
ATOM 10746 CB SER I 521 -27.588 9.481 -69.436 1.00 20.00 C C
ATOM 10747 OG SER I 521 -27.281 10.830 -69.130 1.00 20.00 C O
ATOM 10748 C SER I 521 -27.047 9.892 -71.837 1.00 54.19 C C
ATOM 10749 O SER I 521 -27.767 9.506 -72.758 1.00 65.36 C O
ATOM 10750 N THR 1522 -26.556 11.124 -71.770 1.00 50.09 C N
ATOM 10751 CA THR 1522 -26.650 12.048 -72.892 1.00 57.59 C C
ATOM 10752 CB THR 1522 -25.950 13.377 -72.579 1.00 20.00 C C
ATOM 10753 OG1 THR I 522 -24.538 13.159 -72.466 1.00 20.00 C O
ATOM 10754 CG2 THR I 522 -26.478 13.957 -71.275 1.00 20.00 C C
ATOM 10755 C THR I 522 -26.040 11.450 -74.153 1.00 59.16 C C
ATOM 10756 O THR I 522 -26.682 11.416 -75.202 1.00 65.90 C O
ATOM 10757 N THR 1523 -24.840 10.891 -74.020 1.00 52.59 C N
ATOM 10758 CA THR 1523 -24.151 10.267 -75.148 1.00 42.19 C C
ATOM 10759 CB THR 1523 -22.805 9.649 -74.725 1.00 20.00 C C
ATOM 10760 OG1 THR I 523 -23.027 8.645 -73.726 1.00 20.00 C O
ATOM 10761 CG2 THR I 523 -21.876 10.722 -74.172 1.00 20.00 C C
ATOM 10762 C THR I 523 -25.002 9.194 -75.822 1.00 48.90 C c
ATOM 10763 O THR I 523 -24.991 9.059 -77.047 1.00 63.19 c o
ATOM 10764 N ASN I 524 -25.694 8.395 -75.018 1.00 52.51 c N
ATOM 10765 CA ASN I 524 -26.597 7.386 -75.553 1.00 57.54 c c
ATOM 10766 CB ASN I 524 -27.089 6.458 -74.444 1.00 20.00 c c
ATOM 10767 CG ASN I 524 -26.002 5.533 -73.941 1.00 20.00 c c
ATOM 10768 OD1 ASN I 524 -25.000 5.316 -74.620 1.00 20.00 c o
ATOM 10769 ND2 ASN I 524 -26.153 5.050 -72.714 1.00 20.00 c N
ATOM 10770 C ASN I 524 -27.776 7.996 -76.302 1.00 54.12 c c
ATOM 10771 O ASN I 524 -28.076 7.601 -77.428 1.00 61.31 c o
ATOM 10772 N SER I 525 -28.372 9.027 -75.714 1.00 48.97 c N
ATOM 10773 CA SER I 525 -29.483 9.734 -76.336 1.00 64.81 c c
ATOM 10774 CB SER I 525 -29.930 10.885 -75.441 1.00 61.22 c c
ATOM 10775 OG SER I 525 -29.691 10.571 -74.078 1.00 85.90 c o
ATOM 10776 C SER I 525 -29.114 10.265 -77.713 1.00 69.67 c c
ATOM 10777 O SER I 525 -29.974 10.417 -78.580 1.00 72.60 c o
ATOM 10778 N LYS I 526 -27.853 10.647 -77.872 1.00 66.06 c N
ATOM 10779 CA LYS I 526 -27.365 11.130 -79.154 1.00 63.67 c c
ATOM 10780 CB LYS I 526 -26.043 11.874 -78.980 1.00 70.55 c c
ATOM 10781 CG LYS I 526 -26.196 13.332 -78.608 1.00 75.29 c c
ATOM 10782 CD LYS I 526 -24.898 13.870 -78.032 1.00 85.03 c c
ATOM 10783 CE LYS I 526 -25.144 15.017 -77.067 1.00 82.65 c c
ATOM 10784 NZ LYS I 526 -24.040 15.141 -76.075 1.00 73.89 c N
ATOM 10785 C LYS I 526 -27.182 9.975 -80.124 1.00 55.36 c c

ATOM 10786 O LYS 1526 -27.591 10.050 -81.283 1.00 70.69 C O
ATOM 10787 N ILE 1527 -26.593 8.892 -79.634 1.00 57.52 C N
ATOM 10788 CA ILE 1527 -26.355 7.723 -80.461 1.00 58.48 C C
ATOM 10789 CB ILE 1527 -25.712 6.589 -79.650 1.00 57.00 C C
ATOM 10790 CGI ILE 1527 -24.414 7.071 -78.993 1.00 49.07 C C
ATOM 10791 CD1 ILE 1527 -23.516 7.882 -79.906 1.00 46.18 C C
ATOM 10792 CG2 ILE 1527 -25.469 5.370 -80.530 1.00 52.63 C C
ATOM 10793 C ILE 1527 -27.649 7.230 -81.097 1.00 65.20 C C
ATOM 10794 O ILE 1527 -27.705 7.000 -82.304 1.00 66.48 C O
ATOM 10795 N TYR 1528 -28.705 7.141 -80.293 1.00 69.78 C N
ATOM 10796 CA TYR 1528 -30.027 6.783 -80.798 1.00 72.52 C C
ATOM 10797 CB TYR 1528 -31.080 6.916 -79.695 1.00 73.16 C C
ATOM 10798 CG TYR 1528 -30.768 6.138 -78.433 1.00 76.94 C C
ATOM 10799 CD1 TYR I 528 -31.402 6.444 -77.233 1.00 70.95 C C
ATOM 10800 CE1 TYR I 528 -31.123 5.739 -76.074 1.00 67.73 C C
ATOM 10801 CZ TYR 1528 -30.200 4.712 -76.103 1.00 71.89 C C
ATOM 10802 OH TYR 1528 -29.927 4.009 -74.954 1.00 75.44 C O
ATOM 10803 CE2 TYR I 528 -29.534 4.407 -77.273 1.00 77.03 C C
ATOM 10804 CD2 TYR I 528 -29.818 5.120 -78.431 1.00 77.84 C C
ATOM 10805 C TYR 1528 -30.414 7.661 -81.985 1.00 71.63 C C
ATOM 10806 O TYR 1528 -30.720 7.162 -83.069 1.00 84.20 C O
ATOM 10807 N HIS 1529 -30.470 8.966 -81.748 1.00 67.69 C N
ATOM 10808 CA HIS 1529 -30.934 9.902 -82.759 1.00 60.28 C C
ATOM 10809 CB HIS 1529 -30.900 11.336 -82.218 1.00 67.84 C C
ATOM 10810 CG HIS I 529 -31.927 11.615 -81.162 1.00 88.54 C C
ATOM 10811 ND1 HIS 1529 -32.439 12.875 -80.934 1.00 93.34 C N
ATOM 10812 CE1 HIS I 529 -33.289 12.828 -79.924 1.00 86.23 C C
ATOM 10813 NE2 HIS 1529 -33.346 11.583 -79.486 1.00 91.95 C N
ATOM 10814 CD2 HIS I 529 -32.495 10.807 -80.235 1.00 93.77 C C
ATOM 10815 C HIS 1529 -30.094 9.785 -84.029 1.00 63.30 C C
ATOM 10816 O HIS 1529 -30.632 9.642 -85.127 1.00 61.02 C O
ATOM 10817 N ILE 1530 -28.775 9.752 -83.867 1.00 59.79 C N
ATOM 10818 CA ILE 1530 -27.886 9.457 -84.984 1.00 45.70 C C
ATOM 10819 CB ILE 1530 -26.413 9.365 -84.536 1.00 40.57 C C
ATOM 10820 CGI ILE I 530 -25.854 10.764 -84.270 1.00 42.86 C C
ATOM 10821 CD1 ILE 1530 -24.376 10.902 -84.570 1.00 51.01 C C
ATOM 10822 CG2 ILE I 530 -25.575 8.662 -85.596 1.00 35.31 C C
ATOM 10823 C ILE 1530 -28.301 8.153 -85.660 1.00 57.52 C C
ATOM 10824 O ILE 1530 -28.637 8.136 -86.845 1.00 71.18 C O
ATOM 10825 N GLU I 531 -28.485 7.122 -84.841 1.00 67.55 C N
ATOM 10826 CA GLU 1531 -28.876 5.801 -85.321 1.00 69.79 C C
ATOM 10827 CB GLU 1531 -29.114 4.869 -84.134 1.00 84.02 C C
ATOM 10828 CG GLU 1531 -28.794 3.415 -84.402 1.00104.22 C C
ATOM 10829 CD GLU 1531 -28.980 2.551 -83.170 1.001 16.08 C C
ATOM 10830 OE1 GLU I 531 -28.474 2.927 -82.091 1.001 18.71 C O
ATOM 10831 OE2 GLU I 531 -29.736 1.564 -83.255 1.001 19.69 C O
ATOM 10832 C GLU 1531 -30.145 5.890 -86.151 1.00 64.87 C C
ATOM 10833 O GLU 1531 -30.218 5.343 -87.250 1.00 55.58 C O
ATOM 10834 N ASN 1532 -31.177 6.489 -85.566 1.00 65.70 C N
ATOM 10835 CA ASN 1532 -32.459 6.657 -86.240 1.00 64.16 C C
ATOM 10836 CB ASN 1532 -33.475 7.303 -85.296 1.00 60.58 C C
ATOM 10837 CG ASN 1532 -34.859 7.396 -85.905 1.00 67.75 C C
ATOM 10838 OD1 ASN I 532 -35.480 6.381 -86.221 1.00 53.59 C O
ATOM 10839 ND2 ASN I 532 -35.352 8.618 -86.072 1.00 61.81 C N
ATOM 10840 C ASN 1532 -32.330 7.486 -87.517 1.00 72.17 C C
ATOM 10841 O ASN 1532 -32.999 7.220 -88.517 1.00 85.75 C O
ATOM 10842 N GLU 1533 -31.469 8.495 -87.470 1.00 79.68 C N
ATOM 10843 CA GLU 1533 -31.248 9.372 -88.611 1.00 71.96 C C
ATOM 10844 CB GLU I 533 -30.422 10.590 -88.186 1.00 67.87 C C
ATOM 10845 CG GLU I 533 -30.518 11.797 -89.125 1.00 81.94 C C

ATOM 10846 CD GLU I 533 -31.932 12.348 -89.256 1.00 92.79 C C
ATOM 10847 OE1 GLU I 533 -32.529 12.729 -88.227 1.00 95.90 C O
ATOM 10848 OE2 GLU I 533 -32.399 12.511 -90.403 1.00 93.14 C O
ATOM 10849 C GLU I 533 -30.546 8.622 -89.738 1.00 68.54 C C
ATOM 10850 O GLU I 533 -30.737 8.928 -90.914 1.00 79.29 C O
ATOM 10851 N ILE I 534 -29.742 7.631 -89.367 1.00 69.50 C N
ATOM 10852 CA ILE I 534 -29.047 6.796 -90.342 1.00 72.55 C C
ATOM 10853 CB ILE I 534 -27.786 6.137 -89.729 1.00 79.55 C C
ATOM 10854 CGI ILE I 534 -26.779 7.205 -89.298 1.00 80.41 C C
ATOM 10855 CD1 ILE I 534 -26.687 8.374 -90.254 1.00 89.38 C C
ATOM 10856 CG2 ILE I 534 -27.138 5.186 -90.724 1.00 78.63 C C
ATOM 10857 C ILE I 534 -29.972 5.707 -90.883 1.00 74.92 C C
ATOM 10858 O ILE I 534 -29.725 5.139 -91.948 1.00 81.01 C O
ATOM 10859 N ALA I 535 -31.028 5.411 -90.130 1.00 79.52 C N
ATOM 10860 CA ALA I 535 -32.056 4.474 -90.573 1.00 82.64 C C
ATOM 10861 CB ALA I 535 -32.890 4.001 -89.386 1.00 75.39 C C
ATOM 10862 C ALA I 535 -32.956 5.093 -91.645 1.00 81.39 C C
ATOM 10863 O ALA I 535 -33.323 4.435 -92.622 1.00 85.54 C O
ATOM 10864 N ARG I 536 -33.274 6.373 -91.474 1.00 78.41 C N
ATOM 10865 CA ARG I 536 -34.100 7.098 -92.435 1.00 83.27 C C
ATOM 10866 CB ARG I 536 -34.664 8.372 -91.804 1.00 84.58 C C
ATOM 10867 CG ARG I 536 -35.623 8.123 -90.651 1.00103.24 C C
ATOM 10868 CD ARG I 536 -36.750 9.145 -90.630 1.001 14.72 C C
ATOM 10869 NE ARG I 536 -36.250 10.513 -90.521 1.001 17.80 C N
ATOM 10870 CZ ARG I 536 -37.009 11.598 -90.638 1.001 16.66 C C
ATOM 10871 NH1 ARG I 536 -38.311 11.478 -90.863 1.001 14.57 C N
ATOM 10872 NH2 ARG I 536 -36.470 12.803 -90.520 1.001 16.38 C N
ATOM 10873 C ARG I 536 -33.323 7.440 -93.703 1.00 82.20 C C
ATOM 10874 O ARG I 536 -33.838 7.298 -94.812 1.00 86.28 C O
ATOM 10875 N ILE I 537 -32.114 7.964 -93.532 1.00 77.08 C N
ATOM 10876 CA ILE I 537 -31.219 8.194 -94.659 1.00 66.79 C C
ATOM 10877 CB ILE I 537 -29.908 8.850 -94.204 1.00 64.76 C C
ATOM 10878 CGI ILE I 537 -30.176 10.251 -93.649 1.00 66.92 C C
ATOM 10879 CD1 ILE I 537 -29.017 10.829 -92.869 1.00 70.83 C C
ATOM 10880 CG2 ILE I 537 -28.926 8.905 -95.354 1.00 51.02 C C
ATOM 10881 C ILE I 537 -30.900 6.892 -95.397 1.00 74.94 C C
ATOM 10882 O ILE I 537 -30.628 6.898 -96.599 1.00 97.16 C O
ATOM 10883 N LYS I 538 -30.959 5.777 -94.675 1.00 75.09 C N
ATOM 10884 CA LYS I 538 -30.769 4.462 -95.275 1.00 90.28 C C
ATOM 10885 CB LYS I 538 -30.228 3.472 -94.240 1.00 93.73 C C
ATOM 10886 CG LYS I 538 -29.538 2.255 -94.850 1.00 96.60 C C
ATOM 10887 CD LYS I 538 -29.040 1.288 -93.786 1.00 95.37 C C
ATOM 10888 CE LYS I 538 -28.132 0.235 -94.399 1.00100.63 C C
ATOM 10889 NZ LYS I 538 -27.652 -0.753 -93.397 1.00 99.58 C N
ATOM 10890 C LYS I 538 -32.062 3.927 -95.884 1.00102.20 C C
ATOM 10891 O LYS I 538 -32.083 2.839 -96.461 1.001 12.11 C O
ATOM 10892 N LYS I 539 -33.126 4.722 -95.795 1.00105.15 C N
ATOM 10893 CA LYS I 539 -34.422 4.355 -96.360 1.00105.65 C C
ATOM 10894 CB LYS I 539 -35.548 4.745 -95.398 1.001 10.12 C C
ATOM 10895 CG LYS I 539 -36.926 4.269 -95.823 1.001 13.31 C C
ATOM 10896 CD LYS I 539 -38.013 4.785 -94.889 1.001 14.26 C C
ATOM 10897 CE LYS I 539 -39.395 4.373 -95.378 1.001 18.39 C C
ATOM 10898 NZ LYS I 539 -40.449 4.593 -94.352 1.00121.77 C N
ATOM 10899 C LYS I 539 -34.646 5.008 -97.726 1.00108.88 C C
ATOM 10900 O LYS I 539 -35.717 4.876 -98.321 1.001 10.77 C O
ATOM 10901 N LEU I 540 -33.612 5.675 -98.232 1.001 11.50 C N
ATOM 10902 CA LEU I 540 -33.668 6.309 -99.544 1.001 10.31 C C
ATOM 10903 CB LEU I 540 -33.272 7.777 -99.435 1.00101.19 C C
ATOM 10904 CG LEU I 540 -34.219 8.611 -98.581 1.00 94.26 C C
ATOM 10905 CD1 LEU I 540 -34.093 10.066 -98.978 1.00 86.40 C C

ATOM 10906 CD2 LEU 1540 -35.646 8.133 -98.783 1.00 84.54 C C
ATOM 10907 C LEU 1540 -32.738 5.601-100.513 1.001 18.37 C C
ATOM 10908 O LEU 1540 -32.526 6.059-101.634 1.001 16.71 C O
ATOM 10909 N ILE I 541 -32.163 4.493-100.056 1.00130.80 C N
ATOM 10910 CA ILE I 541 -31 .273 3.686-100.882 1.00140.48 C C
ATOM 1091 1 CB ILE I 541 -29.821 4.210-100.840 1.00138.99 C C
ATOM 10912 CGI ILE 1541 -29.770 5.686-101.240 1.00133.30 C C
ATOM 10913 CD1 ILE 1541 -30.650 6.027-102.420 1.00136.26 C C
ATOM 10914 CG2 ILE I 541 -28.924 3.372-101.744 1.00136.12 C C
ATOM 10915 C ILE 1541 -31.289 2.233-100.426 1.00144.97 C C
ATOM 10916 O ILE 1541 -30.938 1.333-101. 188 1.00145.83 C O
ATOM 10917 N GLY 1542 -31 .724 2.004 -99.191 1.00148.77 C N
ATOM 10918 CA GLY 1542 -31.789 0.655 -98.645 1.00153.58 C C
ATOM 10919 C GLY 1542 -33.208 0.136 -98.534 1.00160.45 C C
ATOM 10920 O GLY 1542 -34.109 0.602 -99.233 1.00163.41 C O
ATOM 10921 N GLU 1543 -33.412 -0.799 -97.61 1 1.00163.83 C N
ATOM 10922 CA GLU I 543 -34.718 -1.409 -97.392 1.00165.52 C C
ATOM 10923 CB GLU I 543 -34.576 -2.673 -96.538 1.00158.94 C C
ATOM 10928 C GLU 1543 -35.680 -0.430 -96.729 1.00168.27 C C
ATOM 10929 O GLU 1543 -35.373 0.753 -96.584 1.00167.37 C O
ATOM 10930 CI NAG J1535 24.849 -25.592 34.903 1.00 72.96 C
ATOM 10931 C2 NAG J1535 24.818 -27.046 34.438 1.00 83.63 C
ATOM 10932 N2 NAG J1535 23.774 -27.757 35. 160 1.00 85.81 N
ATOM 10933 C7 NAG J1535 23.087 -28.774 34.642 1.00 87.77 C
ATOM 10934 0 7 NAG J1535 23.376 -29.307 33.573 1.00 89.34 O
ATOM 10935 C8 NAG J1535 21.991 -29.339 35.498 1.00 86.84 C
ATOM 10936 C3 NAG J1535 26.183 -27.682 34.695 1.00 85.86 C
ATOM 10937 0 3 NAG J1535 27.009 -27.488 33.569 1.00 84.14 O
ATOM 10938 C4 NAG J1535 26.823 -27.025 35.913 1.00 88.88 C
ATOM 10939 0 4 NAG J1535 27.730 -27.923 36.530 1.00 96.14 O
ATOM 10940 C5 NAG J1535 25.692 -26.643 36.863 1.00 85.57 C
ATOM 10941 C6 NAG J1535 26.185 -26.278 38.259 1.00 85.54 C
ATOM 10942 0 6 NAG J1535 27.307 -25.431 38. 159 1.00 85.75 O
ATOM 10943 0 5 NAG J1535 24.941 -25.575 36.317 1.00 79.39 O
ATOM 10944 CI NAG J1536 29.076 -27.393 36.512 1.00101 .26 C
ATOM 10945 C2 NAG J1536 29.807 -27.737 37.810 1.00103.37 C
ATOM 10946 N2 NAG J1536 30.222 -26.531 38.504 1.00104.36 N
ATOM 10947 C7 NAG J1536 30.339 -26.483 39.830 1.00104.07 C
ATOM 10948 0 7 NAG J1536 30.062 -27.429 40.566 1.00103.82 O
ATOM 10949 C8 NAG J1536 30.810 -25. 183 40.413 1.00103.07 C
ATOM 10950 C3 NAG J1536 31.013 -28.638 37.568 1.00104.12 C
ATOM 10951 0 3 NAG J1536 31.41 1 -29.224 38.788 1.00103.63 O
ATOM 10952 C4 NAG J1536 30.689 -29.737 36.565 1.00104.68 C
ATOM 10953 0 4 NAG J1536 31.865 -30.456 36.266 1.00105.46 O
ATOM 10954 C5 NAG J1536 30.104 -29. 166 35.277 1.00104.39 C
ATOM 10955 C6 NAG J1536 28.856 -29.920 34.835 1.00104.32 C
ATOM 10956 0 6 NAG J1536 28.929 -30.178 33.450 1.00104.22 O
ATOM 10957 0 5 NAG J1536 29.840 -27.780 35.384 1.00103.22 O
ATOM 10958 CI NAG J1545 -15.969 -4.075 -43.033 1.00 56.85 C
ATOM 10959 C2 NAG J1545 -16.105 -5.488 -42.448 1.00 66.44 C
ATOM 10960 N2 NAG J1545 -14.794 -6.1 11 -42.415 1.00 69.47 N
ATOM 10961 C7 NAG J1545 -13.913 -5.853 -41 .453 1.00 72.43 C
ATOM 10962 0 7 NAG J1545 -14.178 -5.152 -40.481 1.00 73.31 O
ATOM 10963 C8 NAG J1545 -12.558 -6.484 -41 .587 1.00 72.22 C
ATOM 10964 C3 NAG J1545 -17.084 -6.379 -43.216 1.00 68.81 C
ATOM 10965 0 3 NAG J1545 -17.443 -7.508 -42.449 1.00 68.22 O
ATOM 10966 C4 NAG J1545 -18.314 -5.557 -43.561 1.00 71. 19 C
ATOM 10967 0 4 NAG J1545 -19.356 -6.295 -44. 161 1.00 76.87 O
ATOM 10968 C5 NAG J1545 -17.827 -4.416 -44.429 1.00 67.79 C
ATOM 10969 C6 NAG J1545 -18.955 -3.707 -45.166 1.00 67.71 C

ATOM 10970 0 6 NAG J1545 -19.545 -2.754 -44.31 1 1.00 67.33 O
ATOM 10971 0 5 NAG J1545 -17.181 -3.544 -43.536 1.00 62.66 O
ATOM 10972 CI NAG J1546 -20.251 -6.690 -43.101 1.00 83. 18 C
ATOM 10973 C2 NAG J1546 -21 .616 -5.983 -43.168 1.00 85.51 C
ATOM 10974 N2 NAG J1546 -21.766 -5.147 -41.990 1.00 84.12 N
ATOM 10975 C7 NAG J1546 -21 .679 -3.817 -41 .993 1.00 82.64 C
ATOM 10976 0 7 NAG J1546 -21.413 -3.148 -42.990 1.00 81.92 O
ATOM 10977 C8 NAG J1546 -21 .866 -3.149 -40.663 1.00 80.96 C
ATOM 10978 C3 NAG J1546 -22.846 -6.884 -43.261 1.00 87.47 C
ATOM 10979 0 3 NAG J1546 -23.679 -6.482 -44.325 1.00 87.96 O
ATOM 10980 C4 NAG J1546 -22.495 -8.356 -43.377 1.00 87.61 C
ATOM 10981 0 4 NAG J1546 -23.635 -9.125 -43.071 1.00 86.77 O
ATOM 10982 C5 NAG J1546 -21 .399 -8.665 -42.371 1.00 87. 12 C
ATOM 10983 C6 NAG J1546 -21 .176 -10.167 -42.218 1.00 87.02 C
ATOM 10984 0 6 NAG J1546 -20.698 -10.439 -40.920 1.00 86.44 O
ATOM 10985 0 5 NAG J1546 -20.21 1 -8.081 -42.842 1.00 85.80 O
ATOM 10986 CI NAG J1525 19.621 34.609 -15.280 1.00 72.96 C
ATOM 10987 C2 NAG J1525 20.014 34.434 -16.749 1.00 83.63 C
ATOM 10988 N2 NAG J1525 21.459 34.306 -16.817 1.00 85.81 N
ATOM 10989 C7 NAG J1525 22.104 33.549 -17.705 1.00 87.77 C
ATOM 10990 0 7 NAG J1525 21.559 33.036 -18.682 1.00 89.34 O
ATOM 10991 C8 NAG J1525 23.597 33.493 -17.560 1.00 86.84 C
ATOM 10992 C3 NAG J1525 19.546 35.624 -17.590 1.00 85.86 C
ATOM 10993 0 3 NAG J1525 18.248 35.381 -18.082 1.00 84.14 O
ATOM 10994 C4 NAG J1525 19.548 36.890 -16.742 1.00 88.88 C
ATOM 10995 0 4 NAG J1525 19.800 38.032 -17.545 1.00 96.14 O
ATOM 10996 C5 NAG J1525 20.649 36.717 -15.706 1.00 85.57 C
ATOM 10997 C6 NAG J1525 20.983 38.020 -14.991 1.00 85.54 C
ATOM 10998 0 6 NAG J1525 19.792 38.678 -14.623 1.00 85.75 O
ATOM 10999 0 5 NAG J1525 20.253 35.757 -14.753 1.00 79.39 O
ATOM 11000 CI NAG J1526 18.686 38.953 -17.492 1.00101 .26 C
ATOM 11001 C2 NAG J1526 19.171 40.401 -17.403 1.00103.37 C
ATOM 11002 N2 NAG J1526 18.643 41.051 -16.216 1.00104.36 N
ATOM 11003 C7 NAG J1526 19.298 42.039 -15.609 1.00104.07 C
ATOM 11004 0 7 NAG J1526 20.406 42.432 -15.972 1.00103.82 O
ATOM 11005 C8 NAG J1526 18.641 42.635 -14.399 1.00103.07 C
ATOM 11006 C3 NAG J1526 18.781 41.209 -18.636 1.00104.12 C
ATOM 11007 0 3 NAG J1526 19.553 42.388 -18.684 1.00103.63 O
ATOM 11008 C4 NAG J1526 19.007 40.409 -19.91 1 1.00104.68 C
ATOM 11009 0 4 NAG J1526 18.509 41.133 -21.014 1.00105.46 O
ATOM 11010 C5 NAG J1526 18.320 39.050 -19.846 1.00104.39 C
ATOM 1101 1 C6 NAG J1526 19.260 37.926 -20.265 1.00104.32 C
ATOM 11012 0 6 NAG J1526 18.612 37.103 -21.209 1.00104.22 O
ATOM 11013 0 5 NAG J1526 17.776 38.800 -18.564 1.00103.22 O
ATOM 11014 CI NAG K1535 41.248 18.154 31.115 1.00 72.96 C
ATOM 11015 C2 NAG K1535 41.855 19.316 30.338 1.00 83.63 C
ATOM 11016 N2 NAG K1535 43.088 18.851 29.728 1.00 85.81 N
ATOM 11017 C7 NAG K1535 43.469 19.184 28.498 1.00 87.77 C
ATOM 11018 0 7 NAG K1535 42.908 20.051 27.830 1.00 89.34 O
ATOM 11019 C8 NAG K1535 44.735 18.550 28.004 1.00 86.84 C
ATOM 11020 C3 NAG K1535 42.1 18 20.499 31.270 1.00 85.86 C
ATOM 11021 0 3 NAG K1535 40.974 21.322 31.315 1.00 84.14 O
ATOM 11022 C4 NAG K1535 42.448 20.012 32.677 1.00 88.88 C
ATOM 11023 0 4 NAG K1535 43.310 20.930 33.331 1.00 96.14 O
ATOM 11024 C5 NAG K1535 43.123 18.655 32.535 1.00 85.57 C
ATOM 11025 C6 NAG K1535 43.778 18.188 33.832 1.00 85.54 C
ATOM 11026 0 6 NAG K1535 43.027 18.627 34.942 1.00 85.75 O
ATOM 11027 0 5 NAG K1535 42. 190 17.694 32.074 1.00 79.39 O
ATOM 11028 CI NAG K1536 42.680 21.487 34.509 1.00101.26 C
ATOM 11029 C2 NAG K1536 43.698 21.677 35.636 1.00103.37 C

```
ATOM  11030  N2  NAG K1536      43.310  20.938  36.825  1.00104.36           N
ATOM  11031  C7  NAG K1536      44.214  20.505  37.702  1.00104.07           C
ATOM  11032  07  NAG K1536      45.425  20.656  37.545  1.00103.82           O
ATOM  11033  C8  NAG K1536      43.689  19.781  38.906  1.00103.07           C
ATOM  11034  C3  NAG K1536      43.900  23.146  35.994  1.00104.12           C
ATOM  11035  03  NAG K1536      45.102  23.286  36.719  1.00103.63           O
ATOM  11036  C4  NAG K1536      43.966  24.019  34.748  1.00104.68           C
ATOM  11037  04  NAG K1536      43.988  25.378  35.126  1.00105.46           O
ATOM  11038  C5  NAG K1536      42.782  23.769  33.821  1.00104.39           C
ATOM  11039  C6  NAG K1536      43.229  23.554  32.380  1.00104.32           C
ATOM  11040  06  NAG K1536      42.483  24.396  31.530  1.00104.22           O
ATOM  11041  05  NAG K1536      41.980  22.692  34.267  1.00103.22           O
ATOM  11042  CI  NAG K1545       2.615   1.983 -49.407  1.00 56.85           C
ATOM  11043  C2  NAG K1545       2.918   2.869 -50.621  1.00 66.44           c
ATOM  11044  N2  NAG K1545       1.785   3.731 -50.894  1.00 69.47           N
ATOM  11045  C7  NAG K1545       1.517   4.812 -50.168  1.00 72.43           C
ATOM  11046  07  NAG K1545       2.154   5.121 -49.163  1.00 73.31           o
ATOM  11047  C8  NAG K1545       0.302   5.589 -50.579  1.00 72.22           c
ATOM  11048  C3  NAG K1545       3.247   2.088 -51.890  1.00 68.81           c
ATOM  11049  03  NAG K1545       3.890   2.929 -52.817  1.00 68.22           o
ATOM  11050  C4  NAG K1545       4.146   0.927 -51.513  1.00 71.19           c
ATOM  11051  04  NAG K1545       4.688   0.219 -52.606  1.00 76.87           o
ATOM  11052  C5  NAG K1545       3.310   0.066 -50.596  1.00 67.79           c
ATOM  11053  C6  NAG K1545       3.861  -1.348 -50.446  1.00 67.71           c
ATOM  11054  06  NAG K1545       4.940  -1.351 -49.538  1.00 67.33           o
ATOM  11055  05  NAG K1545       3.330   0.760 -49.372  1.00 62.66           o
ATOM  11056  CI  NAG K1546       5.996   0.777 -52.858  1.00 83.18           c
ATOM  11057  C2  NAG K1546       7.149  -0.188 -52.527  1.00 85.51           c
ATOM  11058  N2  NAG K1546       7.911   0.336 -51.403  1.00 84.12           N
ATOM  11059  C7  NAG K1546       8.044  -0.298 -50.234  1.00 82.64           c
ATOM  11060  07  NAG K1546       7.581  -1.414 -50.007  1.00 81.92           o
ATOM  11061  C8  NAG K1546       8.880   0.392 -49.197  1.00 80.96           c
ATOM  11062  C3  NAG K1546       8.093  -0.539 -53.684  1.00 87.47           c
ATOM  11063  03  NAG K1546       8.280  -1.934 -53.775  1.00 87.96           o
ATOM  11064  C4  NAG K1546       7.594   0.007 -55.013  1.00 87.61           c
ATOM  11065  04  NAG K1546       8.586  -0.124 -56.008  1.00 86.77           o
ATOM  11066  C5  NAG K1546       7.269   1.469 -54.777  1.00 87.12           c
ATOM  11067  C6  NAG K1546       7.145   2.266 -56.074  1.00 87.02           c
ATOM  11068  06  NAG K1546       7.707   3.548 -55.896  1.00 86.44           o
ATOM  11069  05  NAG K1546       6.050   1.508 -54.073  1.00 85.80           o
ATOM  11070  CI  NAG K1525     -29..090   1.326   0.431  1.00 56.85           c
ATOM  11071  C2  NAG K1525     -30..509   1.450   1.026  1.00 66.44           c
ATOM  11072  N2  NAG K1525     -30.921   0.195   1.623  1.00 69.47           N
ATOM  11073  C7  NAG K1525     -30..381  -0.257   2.752  1.00 72.43           c
ATOM  11074  07  NAG K1525     -29.481   0.332   3.347  1.00 73.31           o
ATOM  11075  C8  NAG K1525     -30..965  -1.518   3.317  1.00 72.22           c
ATOM  11076  C3  NAG K1525     -31.621   1.959   0.102  1.00 68.81           c
ATOM  11077  03  NAG K1525     -32.692   2.482   0.855  1.00 68.22           o
ATOM  11078  C4  NAG K1525     -31.056   3.022  -0.817  1.00 71.19           c
ATOM  11079  04  NAG K1525     -32.040   3.689  -1.591  1.00 76.87           o
ATOM  11080  C5  NAG K1525     -30..031   2.269  -1.642  1.00 67.79           c
ATOM  11081  C6  NAG K1525     -29..635   3.028  -2.906  1.00 67.71           c
ATOM  11082  06  NAG K1525     -28.857   4.152  -2.561  1.00 67.33           o
ATOM  11083  05  NAG K1525     -28.906   2.013  -0.814  1.00 62.66           o
ATOM  11084  CI  NAG K1526     -32..430   4.903  -0.902  1.00 83.18           c
ATOM  11085  C2  NAG K1526     -31.984   6.181  -1.635  1.00 85.51           c
ATOM  11086  N2  NAG K1526     -30.942   6.832  -0.859  1.00 84.12           N
ATOM  11087  C7  NAG K1526     -29..678   6.943  -1.267  1.00 82.64           c
ATOM  11088  07  NAG K1526     -29.276   6.528  -2.353  1.00 81.92           o
ATOM  11089  C8  NAG K1526     -28..739   7.632  -0.321  1.00 80.96           c
```

```
ATOM  11090  C3  NAG K1526     -33.070   7.210  -1.965  1.00 87.47      C
ATOM  11091  03  NAG K1526     -32.990   7.586  -3.320  1.00 87.96      O
ATOM  11092  C4  NAG K1526     -34.468   6.712  -1.644  1.00 87.61      C
ATOM  11093  04  NAG K1526     -35.385   7.783  -1.653  1.00 86.77      O
ATOM  11094  C5  NAG K1526     -34.395   6.107  -0.257  1.00 87.12      C
ATOM  11095  C6  NAG K1526     -35.779   5.918   0.354  1.00 87.02      C
ATOM  11096  06  NAG K1526     -35.724   6.194   1.736  1.00 86.44      O
ATOM  11097  05  NAG K1526     -33.754   4.862  -0.395  1.00 85.80      O
ATOM  11098  CI  NAG L1535      -2.070  11.341  45.870  1.00 72.96      C
ATOM  11099  C2  NAG L1535      -3.565  11.622  45.740  1.00 83.63      C
ATOM  11100  N2  NAG L1535      -3.793  13.060  45.821  1.00 85.81      N
ATOM  11101  C7  NAG L1535      -4.706  13.721  45.104  1.00 87.77      C
ATOM  11102  07  NAG L1535      -5.570  13.168  44.424  1.00 89.34      O
ATOM  11103  C8  NAG L1535      -4.727  15.213  45.270  1.00 86.84      C
ATOM  11104  C3  NAG L1535      -4.303  10.883  46.855  1.00 85.86      C
ATOM  11105  03  NAG L1535      -4.575   9.563  46.441  1.00 84.14      O
ATOM  11106  C4  NAG L1535      -3.441  10.862  48.115  1.00 88.88      C
ATOM  11107  04  NAG L1535      -4.260  10.849  49.273  1.00 96.14      O
ATOM  11108  C5  NAG L1535      -2.549  12.100  48.077  1.00 85.57      C
ATOM  11109  C6  NAG L1535      -1.872  12.404  49.410  1.00 85.54      C
ATOM  11110  06  NAG L1535      -1.282  11.235  49.931  1.00 85.75      O
ATOM  11111  05  NAG L1535      -1.585  11.956  47.052  1.00 79.39      O
ATOM  11112  CI  NAG L1536      -4.061   9.626  50.020  1.00101.26      C
ATOM  11113  C2  NAG L1536      -4.102   9.893  51.524  1.00103.37      C
ATOM  11114  N2  NAG L1536      -2.863   9.461  52.140  1.00104.36      N
ATOM  11115  C7  NAG L1536      -2.405  10.023  53.252  1.00104.07      C
ATOM  11116  07  NAG L1536      -2.958  10.972  53.807  1.00103.82      O
ATOM  11117  C8  NAG L1536      -1.111  9.476  53.773  1.00103.07      C
ATOM  11118  C3  NAG L1536      -5.265   9.179  52.199  1.00104.12      C
ATOM  11119  03  NAG L1536      -5.486   9.747  53.470  1.00103.63      O
ATOM  11120  C4  NAG L1536      -6.532   9.306  51.370  1.00104.68      C
ATOM  11121  04  NAG L1536      -7.534   8.514  51.963  1.00105.46      O
ATOM  11122  C5  NAG L1536      -6.309   8.841  49.937  1.00104.39      C
ATOM  11123  C6  NAG L1536      -6.864   9.838  48.932  1.00104.32      C
ATOM  11124  06  NAG L1536      -7.576   9.132  47.943  1.00104.22      O
ATOM  11125  05  NAG L1536      -4.947   8.581  49.669  1.00103.22      O
ATOM  11126  CI  NAG L1545     -11.652  16.132 -42.376  1.00 56.85      C
ATOM  11127  C2  NAG L1545     -11.811  17.208 -43.449  1.00 66.44      C
ATOM  11128  N2  NAG L1545     -10.485  17.531 -43.934  1.00 69.47      N
ATOM  11129  C7  NAG L1545      -9.803  16.702 -44.718  1.00 72.43      C
ATOM  11130  07  NAG L1545     -10.291  15.689 -45.219  1.00 73.31      O
ATOM  11131  C8  NAG L1545      -8.341  16.997 -44.865  1.00 72.22      C
ATOM  11132  C3  NAG L1545     -12.475  18.463 -42.898  1.00 68.81      C
ATOM  11133  03  NAG L1545     -12.890  19.301 -43.953  1.00 68.22      O
ATOM  11134  C4  NAG L1545     -13.667  18.017 -42.071  1.00 71.19      C
ATOM  11135  04  NAG L1545     -14.509  19.077 -41.672  1.00 76.87      O
ATOM  11136  C5  NAG L1545     -13.113  17.218 -40.907  1.00 67.79      C
ATOM  11137  C6  NAG L1545     -14.125  17.020 -39.786  1.00 67.71      C
ATOM  11138  06  NAG L1545     -15.086  16.069 -40.180  1.00 67.33      O
ATOM  11139  05  NAG L1545     -12.727  15.986 -41.467  1.00 62.66      O
ATOM  11140  CI  NAG L1546     -15.574  19.184 -42.644  1.00 83.18      C
ATOM  11141  C2  NAG L1546     -16.945  18.806 -42.055  1.00 85.51      C
ATOM  11142  N2  NAG L1546     -17.436  17.613 -42.723  1.00 84.12      N
ATOM  11143  C7  NAG L1546     -17.522  16.433 -42.114  1.00 82.64      C
ATOM  11144  07  NAG L1546     -17.214  16.256 -40.937  1.00 81.92      O
ATOM  11145  C8  NAG L1546     -18.068  15.302 -42.933  1.00 80.96      C
ATOM  11146  C3  NAG L1546     -18.033  19.883 -42.093  1.00 87.47      C
ATOM  11147  03  NAG L1546     -18.679  19.995 -40.846  1.00 87.96      O
ATOM  11148  C4  NAG L1546     -17.484  21.228 -42.533  1.00 87.61      C
ATOM  11149  04  NAG L1546     -18.538  22.132 -42.784  1.00 86.77      O
```

ATOM 11150 C5 NAG L1546 -16.723 20..935 -43..810 1.00 87.12 C
ATOM 11151 C6 NAG L1546 -16.525 22. 183 -44..663 1.00 87.02 C
ATOM 11152 0 6 NAG L1546 -17.041 21..939 -45..954 1.00 86.44 O
ATOM 11153 0 5 NAG L1546 -15.492 20..356 -43..444 1.00 85.80 O
ATOM 11154 CI NAG L1525 21.793 -26..723 -18..244 1.00 56.85 C
ATOM 11155 C2 NAG LI525 22.365 -27..060 -19..634 1.00 66.44 C
ATOM 11156 N2 NAG LI525 22.402 -25..862 -20..460 1.00 69.47 N
ATOM 11157 C7 NAG LI525 23.351 -24..934 -20..342 1.00 72.43 C
ATOM 11158 0 7 NAG LI525 24.279 -25..026 -19..540 1.00 73.31 O
ATOM 11159 C8 NAG L1525 23.280 -23..766 -21..282 1.00 72.22 C
ATOM 11160 C3 NAG L1525 21.624 -28. 181 -20..369 1.00 68.81 C
ATOM 11161 0 3 NAG L1525 22.407 -28..687 -21..427 1.00 68.22 O
ATOM 11162 C4 NAG LI525 21.308 -29..275 -19..364 1.00 71.19 C
ATOM 11163 0 4 NAG LI525 20.761 -30..454 -19..918 1.00 76.87 O
ATOM 11164 C5 NAG LI525 20.389 -28..631 -18..348 1.00 67.79 C
ATOM 11165 C6 NAG L1525 19.627 -29..660 -17..520 1.00 67.71 C
ATOM 11166 0 6 NAG L1525 20.442 -30..144 -16..478 1.00 67.33 O
ATOM 11167 0 5 NAG LI525 21.225 -27..824 -17..551 1.00 62.66 O
ATOM 11168 CI NAG L1526 21.846 -31..384 -20. 124 1.00 83.18 C
ATOM 11169 C2 NAG L1526 21.792 -32..604 -19. 182 1.00 85.51 C
ATOM 11170 N2 NAG L1526 22.928 -32..540 -18..274 1.00 84.12 N
ATOM 11171 C7 NAG L1526 22.851 -32..639 -16..945 1.00 82.64 C
ATOM 11172 0 7 NAG L1526 21.797 -32..785 -16..328 1.00 81.92 O
ATOM 11173 C8 NAG L1526 24.156 -32..563 -16..207 1.00 80.96 C
ATOM 11174 C3 NAG L1526 21.773 -33..981 -19..854 1.00 87.47 C
ATOM 11175 0 3 NAG L1526 20.751 -34..790 -19..316 1.00 87.96 O
ATOM 11176 C4 NAG L1526 21.648 -33..901 -21..365 1.00 87.61 C
ATOM 11177 0 4 NAG L1526 21.965 -35..150 -21..938 1.00 86.77 O
ATOM 11178 C5 NAG L1526 22.647 -32..860 -21..827 1.00 87.12 C
ATOM 11179 C6 NAG L1526 22.903 -32..944 -23..327 1.00 87.02 C
ATOM 11180 0 6 NAG L1526 24.294 -32..969 -23..563 1.00 86.44 O
ATOM 11181 0 5 NAG L1526 22.108 -31..604 -21..499 1.00 85.80 O
END

CLAIMS

What is claimed is:

1. A pre-fusion respiratory syncytial virus (RSV) F polypeptide comprising at least two introduced cysteine residues, wherein said cysteines are in close proximity to one another and form a disulfide bond that stabilizes the pre-fusion RSV F polypeptide.

2. The pre-fusion RSV F polypeptide of claim 1, wherein said cysteine mutations are not more than about 10 Å away from each other.

3. The pre-fusion RSV F polypeptide of claim 1 or 2, wherein the HRB region and the DI and/or DII region contain an introduced cysteine residue, and a disulfide bond is formed between the introduced cysteine residue in the HRB region and the introduced cysteine residue in the DI or DII region.

4. The pre-fusion RSV F polypeptide of claim 1 or 2, wherein the HRA region and the Dili region contain an introduced cysteine residue, and a disulfide bond is formed between the introduced cysteine residues in the HRA region and the Dili region.

5. The pre-fusion RSV F polypeptide of claim 1 or 2, wherein the HRA region contains at least two introduced cysteine residues, and a disulfide bond is formed between the introduced cysteine residues in the HRA region.

6. A pre-fusion respiratory syncytial virus (RSV) F polypeptide comprising a post-fusion modification selected from the group consisting of deletion of the HRA helix, deletion of the HRB helix, introduction of point mutations, addition of glycosylation sites and combinations thereof, wherein said post-fusion modification destabilizes the post-fusion conformation.

7. The pre-fusion RSV F polypeptide of claim 6, wherein said destabilizing post-fusion modification is deletion of the HRB helix.

8. The pre-fusion RSV F polypeptide of claim 7, further comprising deletion of the fusion peptide.

9. The pre-fusion RSV F polypeptide of claim 6, wherein said destabilizing post-fusion modification is addition of a glycosylation site.

10. The pre-fusion RSV F polypeptide of claim 9, wherein said glycosylation site is on a residue selected from the group consisting of position 173, position 175 and position 184.

11. A pre-fusion respiratory syncytial virus (RSV) F polypeptide comprising three RSV F monomers, wherein at least two of the monomers contain an introduced cysteine residue, said introduced cysteine residues are in close proximity to one another and form a disulfide bond that stabilizes the pre-fusion RSV F polypeptide.

12. The pre-fusion RSV F polypeptide of any one of claims 1-11, wherein the pre-fusion RSV F polypeptide is a soluble ectodomain of RSV F or a trimer of soluble ectodomain of RSV F.

13. A chimeric pre-fusion F protein comprising a stabilized F protein from a virus other than RSV that contains one or more neutralizing epitope of RSV F.

14. The chimeric pre-fusion F protein of claim 13, wherein said stabilized F protein is from a parainfluenza virus F polypeptide or a metapneumovirus virus F polypeptide.

15. The chimeric pre-fusion F protein of claim 13, wherein said stabilized F protein is a PIV5 pre-fusion F polypeptide or a NDV pre-fusion F polypeptide.

16. The chimeric pre-fusion F protein of any one of claims 13-15, wherein the stabilized F protein is the soluble ectodomain.

17. The chimeric pre-fusion F protein of any one of claims 13-16, wherein said neutralizing epitopes of RSV F are from the HRA region of RSV F.

18. The chimeric pre-fusion F protein of any one of claims 13-16, wherein the neutralizing epitopes are selcted from the group consisting of the epitopes that are recognized by motavizumab, palivizumab, mAb 11, mAb 151, mAb 1129, mAb 1153, mAb 1200, mAb 1214, mAb 1237, mAb 47F, mAb 7C2, mAb B4, Fab 19, mAb AK13A2, mAb 7.936, mAb 9.936, mAb 19, mAb 20, mAb 101F and combinations thereof.

19. The pre-fusion RSV F polypeptide or chimeric pre-fusion F protein of any one of claims 1-18, further comprising a heterologous oligomerization domain, an epitope, or a signal peptide.

20. The pre-fusion RSV F polypeptide or chimeric pre-fusion F protein of claim 19, wherein said heterologous oligomerization domain is a trimerization domain.

21. The pre-fusion RSV F polypeptide or chimeric pre-fusion F protein of claim 20 wherein the trimerization domain is from influenza hemagglutinin, SARS spike, HIV gp41, NadA, modified GCN4, GCN4 or ATCase.

22. An immunogenic composition comprising the pre-fusion RSV F polypeptide or chimeric pre-fusion F protein of any one of claim 1-21.

23. The immunogenic composition of claim 22, wherein said composition further comprises an adjuvant.

24. The immunogenic composition of claim 23, wherein the adjuvant is selected from the group consisting of: an aluminum salt, a squalene-in-water emulsion, a benzonaphthyridine compound, a phospholipid compound, a small molecule immunopotentiator and combinations of any of the foregoing.

25. An isolated nucleic acid encoding the pre-fusion RSV F polypeptide or chimeric pre-fusion F protein of any one of claims 1 - 21.

26. The isolated nucleic acid of claim 25, which is a self-replicating RNA molecule.

27. An immunogenic composition comprising the self-replicating RNA molecule of claim 26.

28. The immunogenic composition of claim 26, further comprising an RNA delivery system.

29. A method of inducing an immune response in a subject to RSV F comprising administering an immunogenic composition of any one of claims 22-24 to the subject.

29. A method of inducing an immune response in a subject to RSV F comprising administering an immunogenic composition of claim 27 or 28 to the subject.

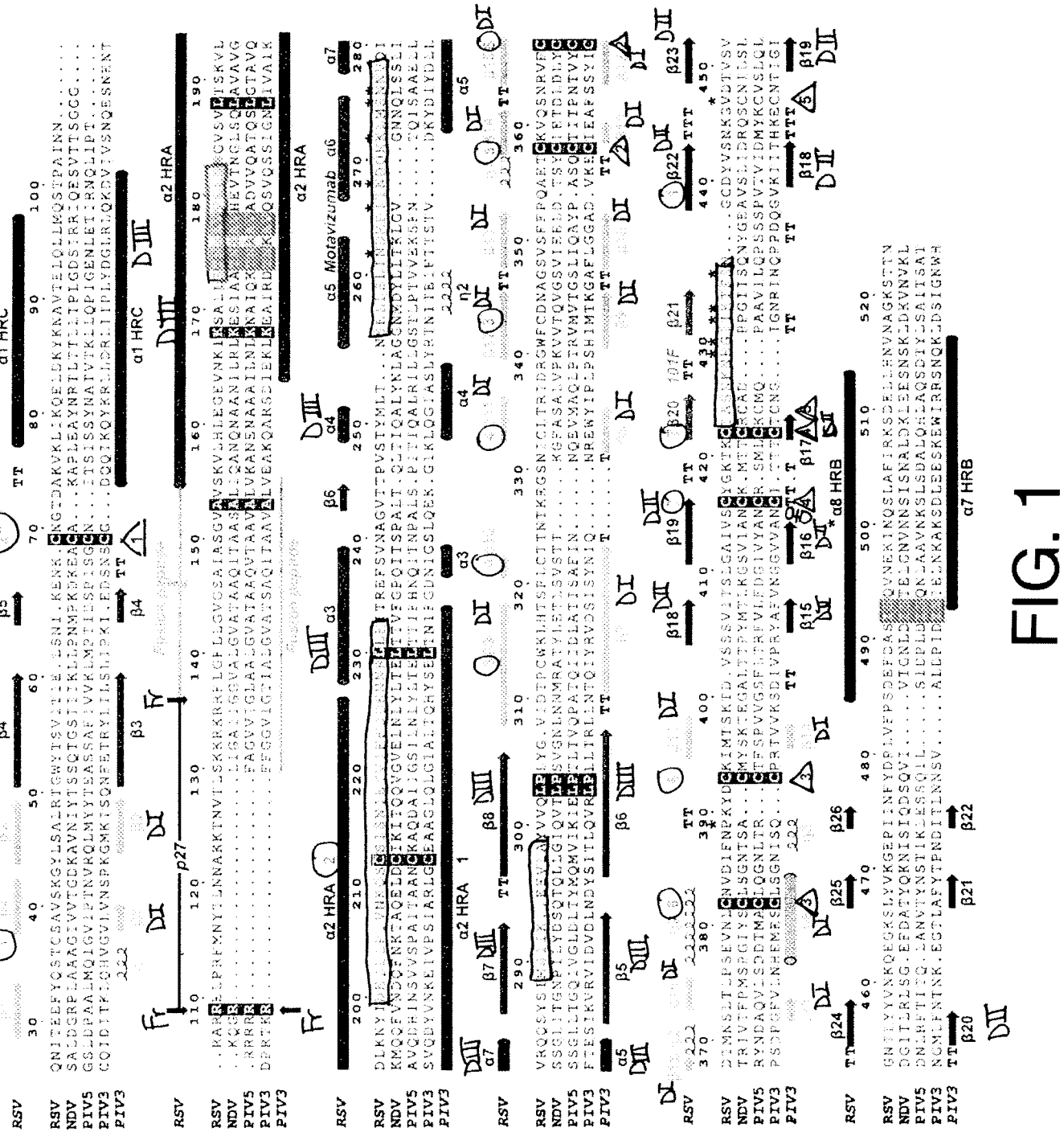

FIG. 1

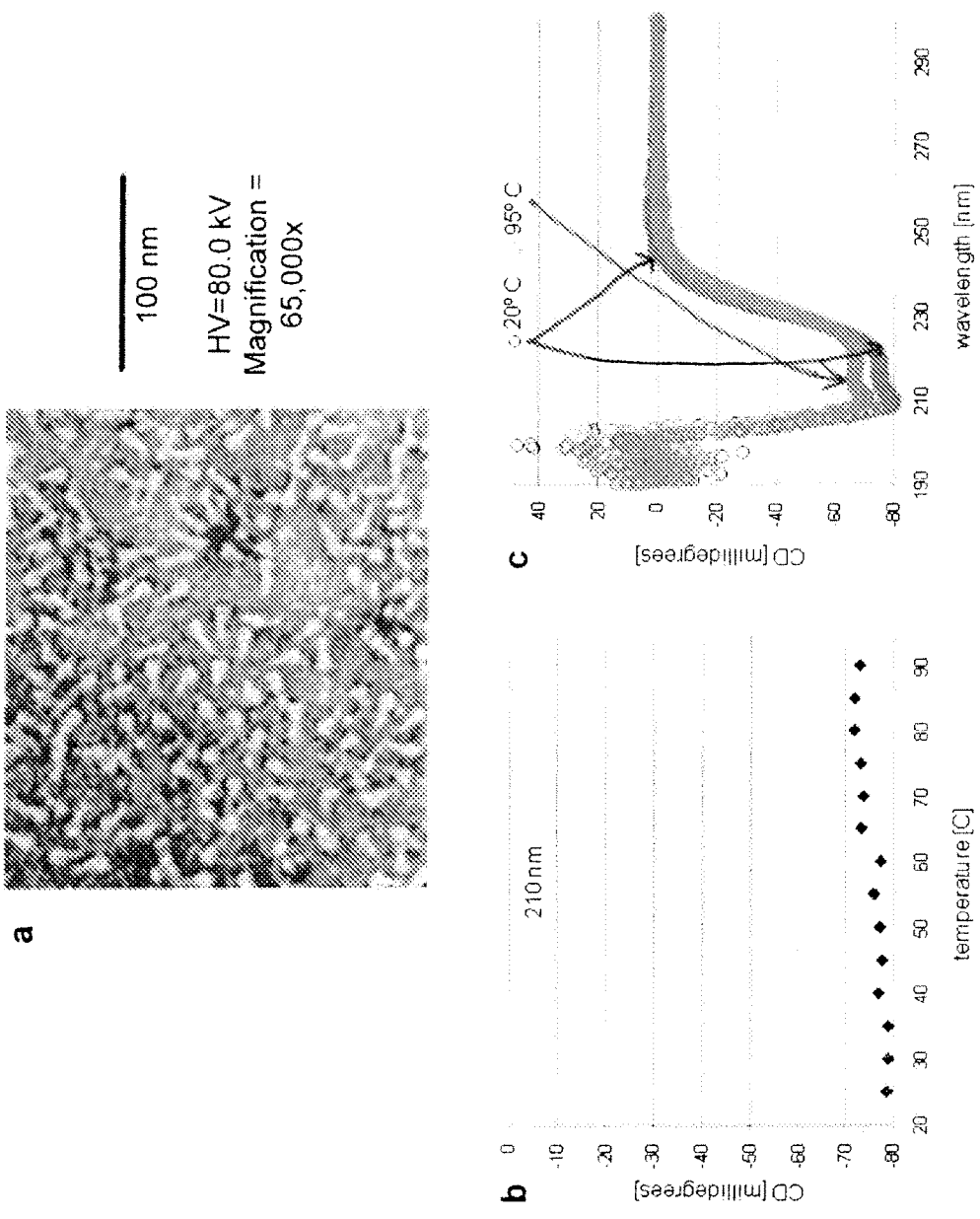
a
100 nm
HV=80.0 kV
Magnification = 65,000x
b
210 nm
CD [millidegrees]
temperature [C]
c
20° C
95° C
CD [millidegrees]
wavelength [nm]

FIG. 2

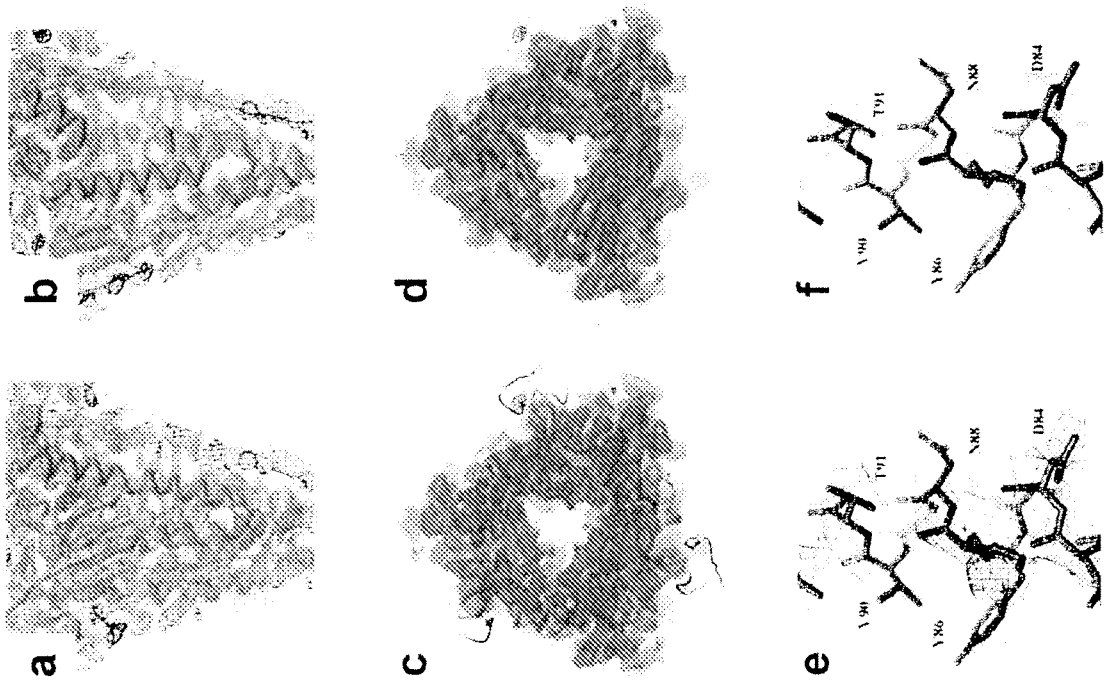

FIG. 3

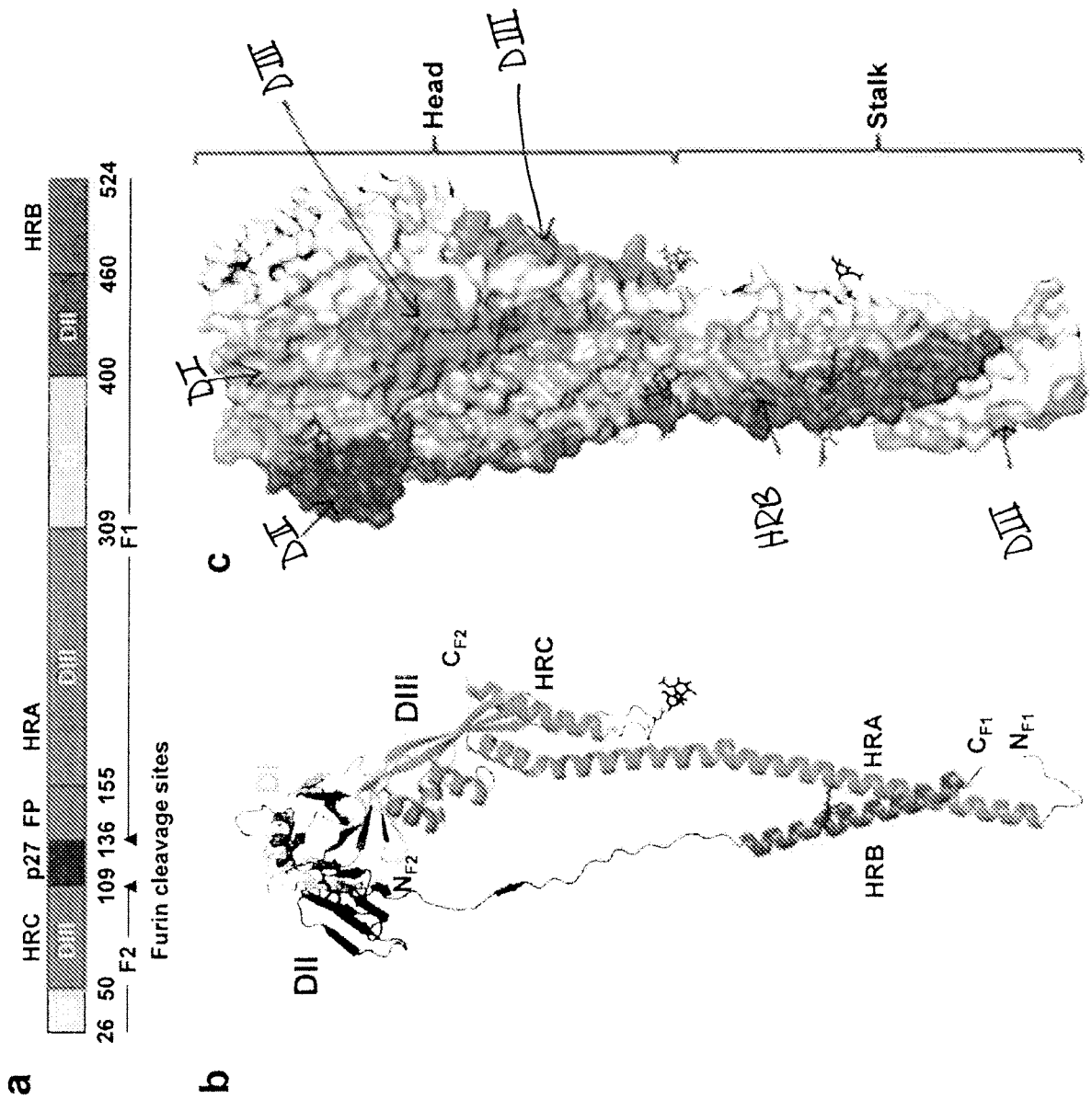
a
HRC
p27
FP
HRA
HRB
DIII
DII
DI
26
50
109
136
155
309
400
460
524
F2
F1
Furin cleavage sites
b
DII
DIII
C_{F2}
N_{F2}
HRC
HRA
HRB
C_{F1}
N_{F1}
c
DI
DII
DIII
Head
Stalk
HRB
DIII

FIG. 4

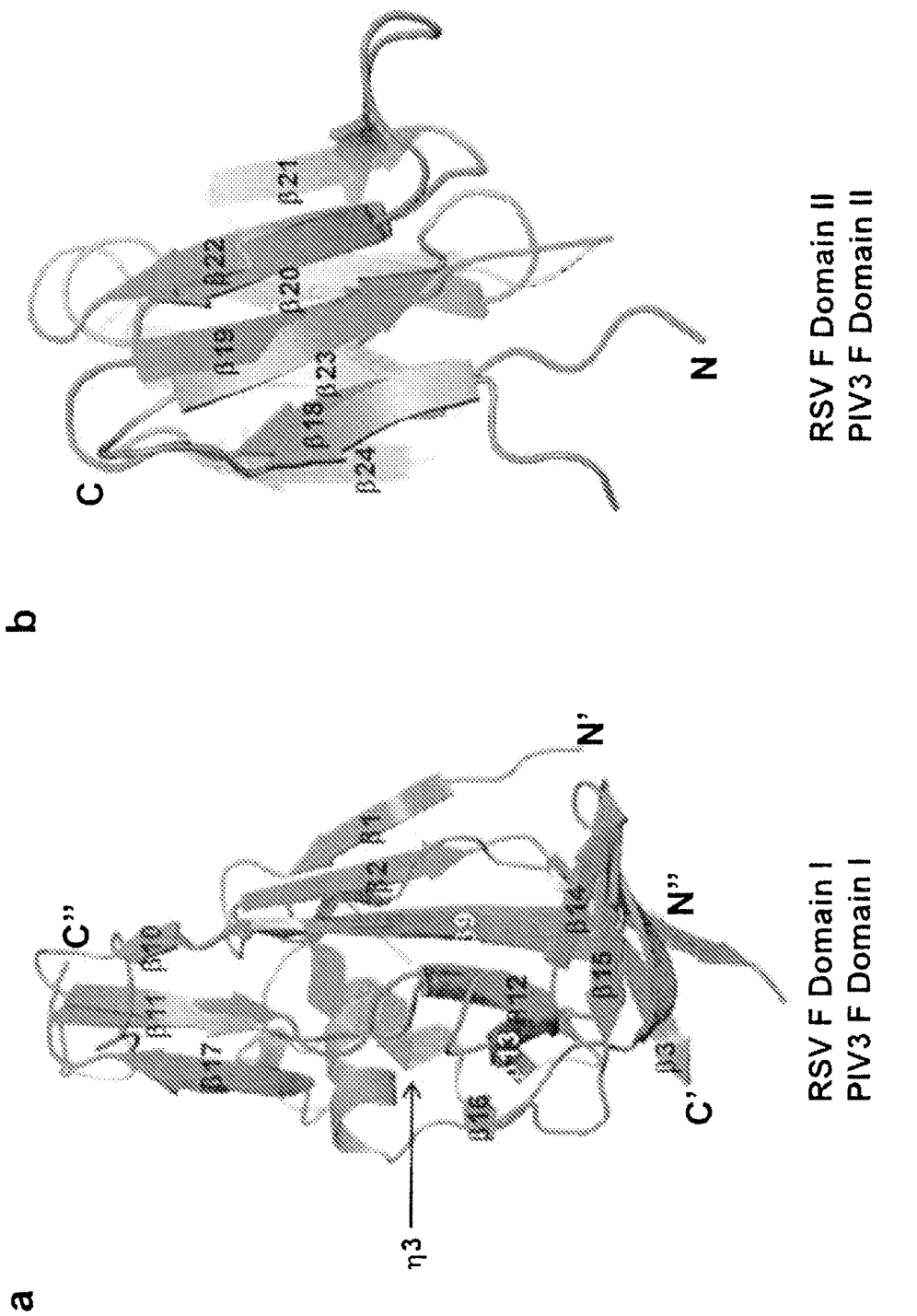
a
b
C
N
C''
N'
N''
C'
β21
β22
β20
β18
β23
β24
β17
β11
β10
β12
β13
β16
β15
η3
RSV F Domain II
PIV3 F Domain II
RSV F Domain I
PIV3 F Domain I

FIG. 5

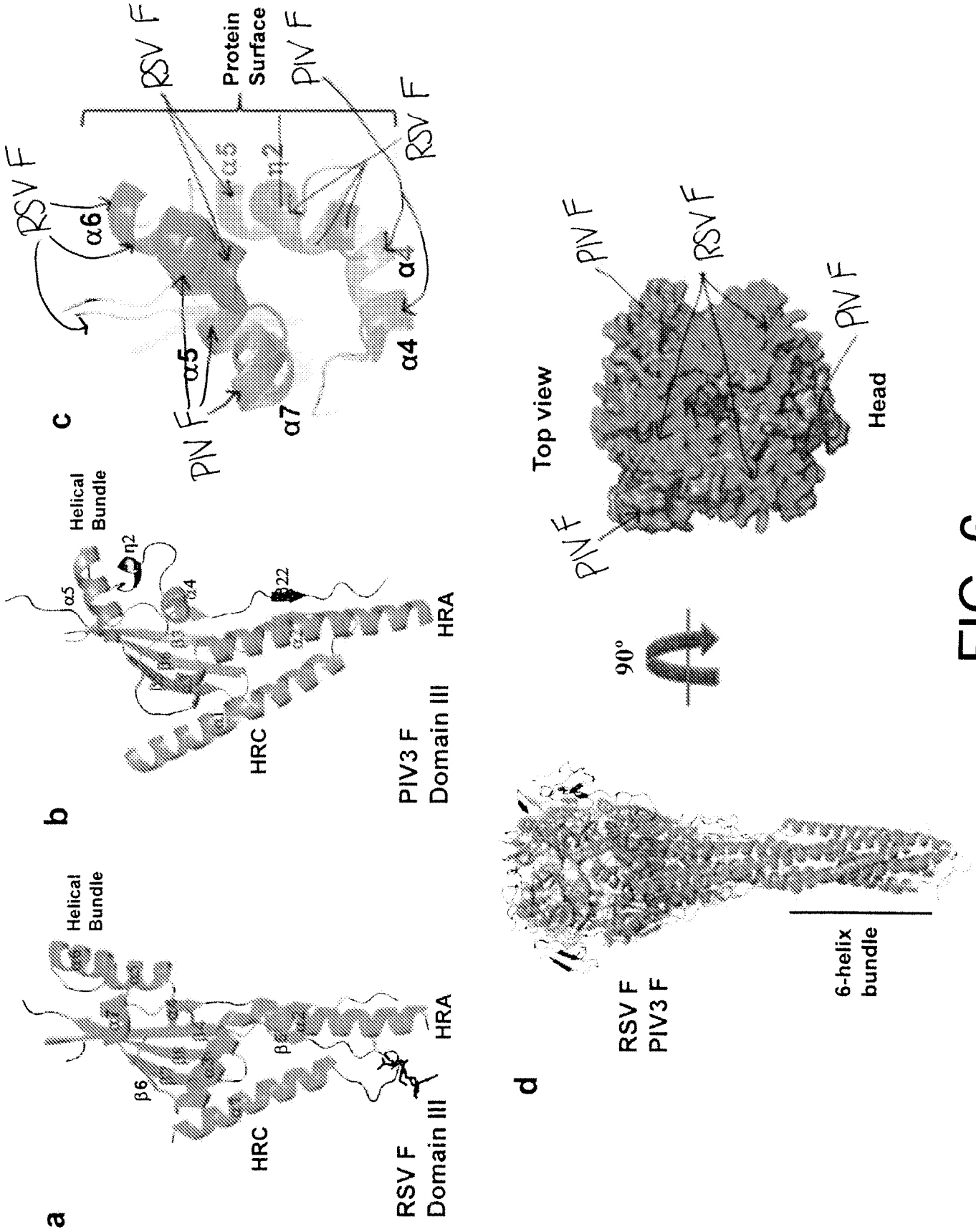
a
Helical Bundle
β6
HRC
RSV F
Domain III
HRA
b
Helical Bundle
α5
η2
α4
β22
HRC
PIV3 F
Domain III
HRA
c
RSV F
α6
α3
η2
Protein Surface
PIV F
RSV F
PIV F
α5
α7
α4
RSV F
d
Top view
PIV F
RSV F
PIV F
90°
RSV F
PIV3 F
Head
6-helix bundle

FIG. 6

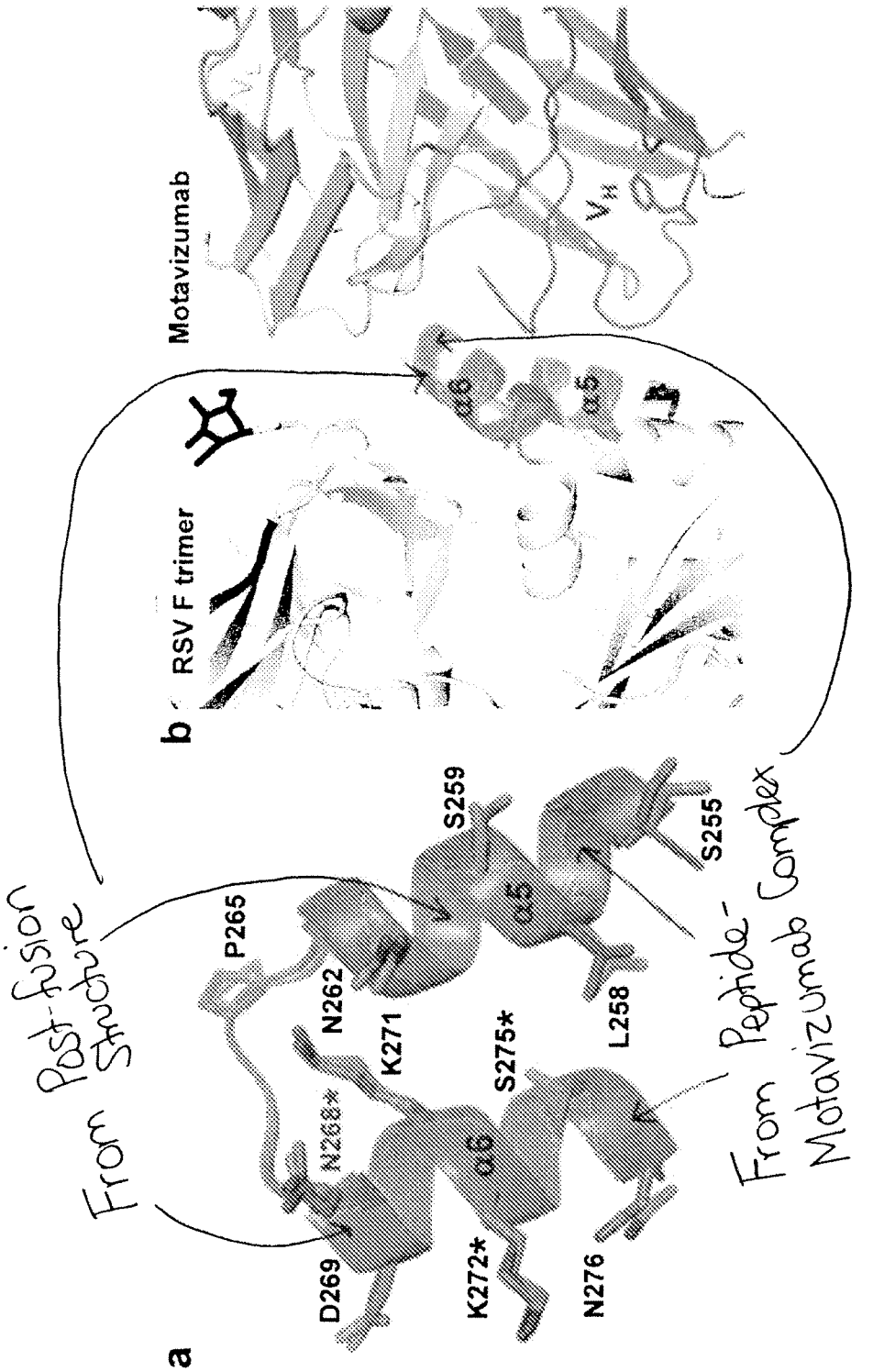
a
b
RSV F trimer
Motavizumab
V_H
V_L
α6
α5
From Post-fusion Structure
From Peptide-Motavizumab Complex
D269
K272*
N276
N268*
N262
P265
K271
S275*
L258
S259
S255

FIG. 7

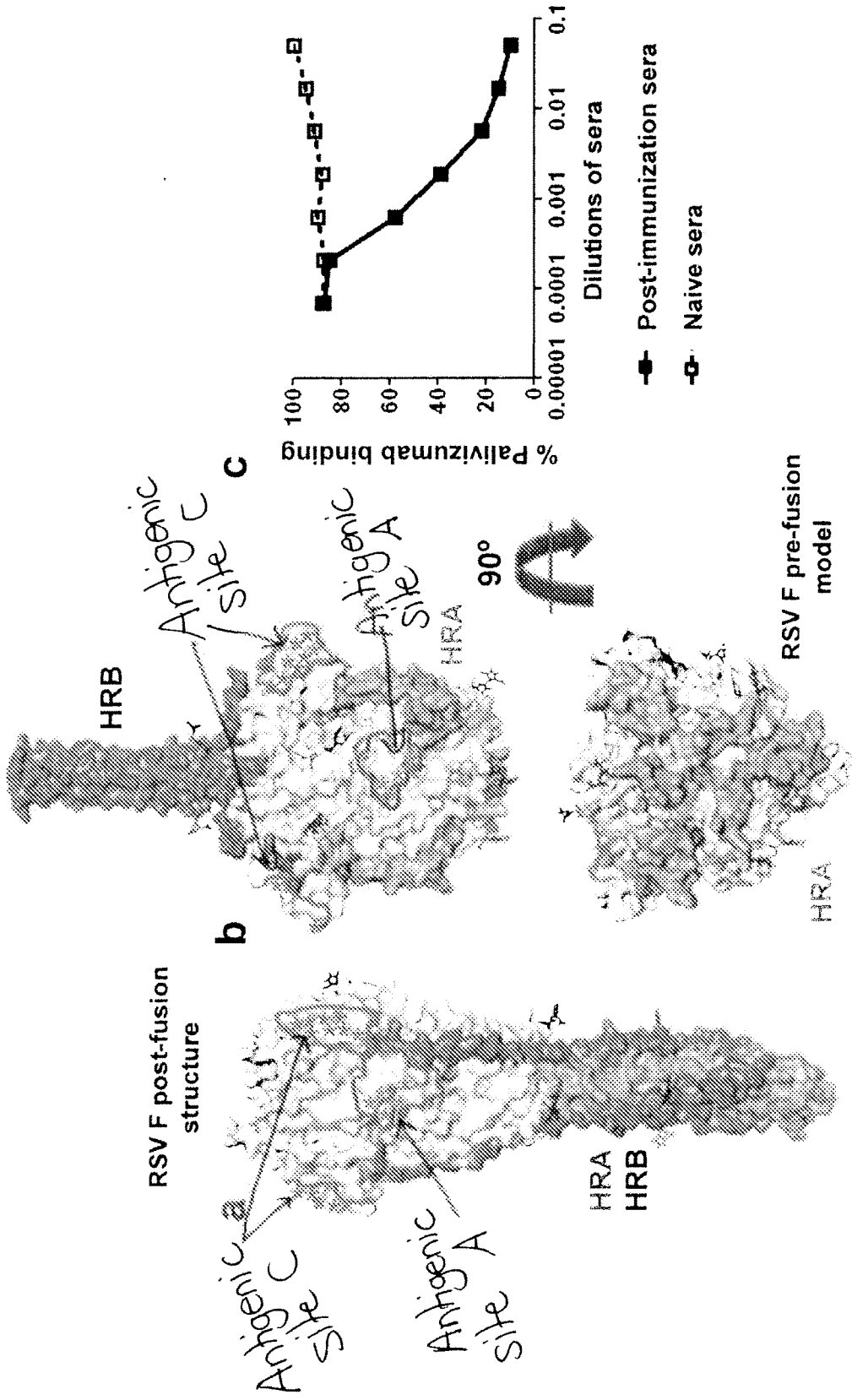
RSV F post-fusion structure
Antigenic site C
Antigenic site A
HRA
HRB
b
HRB
Antigenic site C
Antigenic site A
HRA
90°
RSV F pre-fusion model
HRA
c
% Palivizumab binding
100
80
60
40
20
0
0.00001
0.0001
0.001
0.01
0.1
Dilutions of sera
Post-immunization sera
Naive sera

FIG. 8

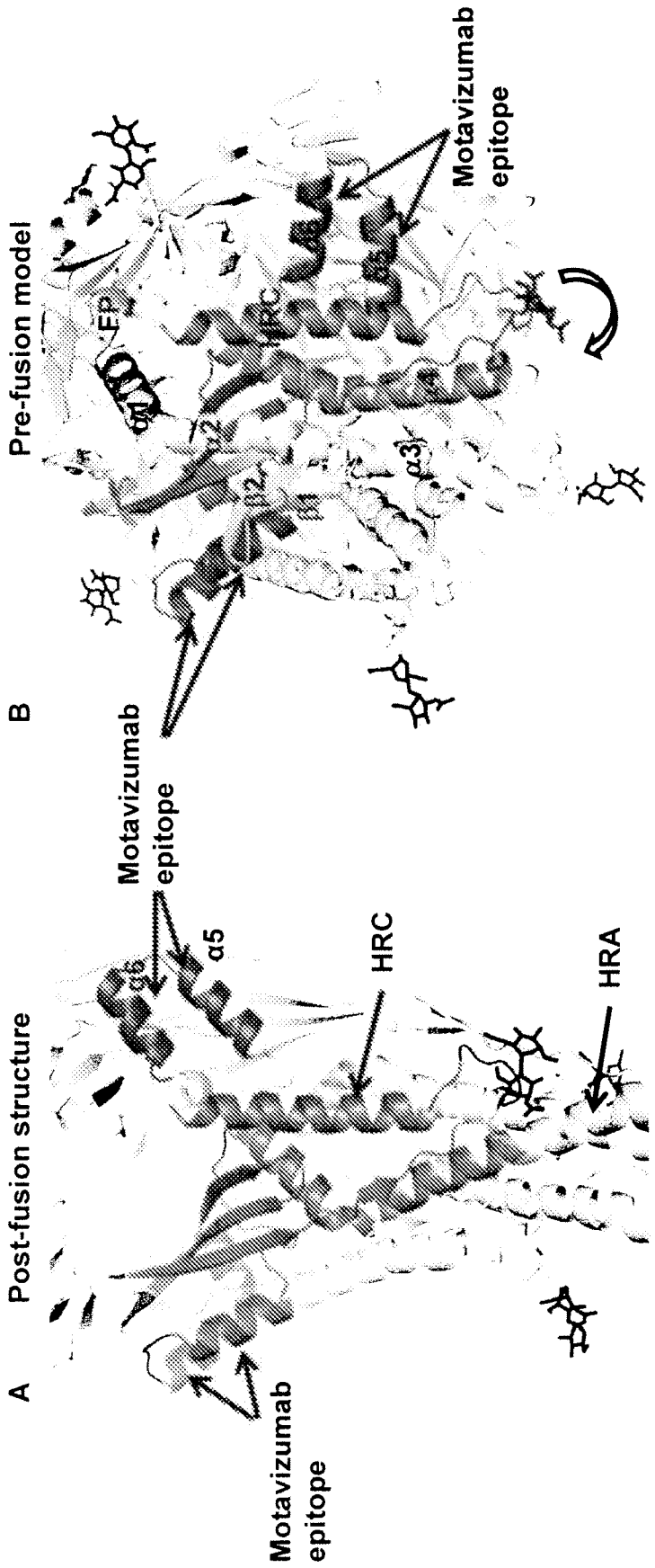
A
Post-fusion structure
Motavizumab epitope
α6
α5
HRC
HRA
Motavizumab epitope
B
Pre-fusion model
Motavizumab epitope
FP
HRC
α4
α3
β2
β1
β2

Figure 9

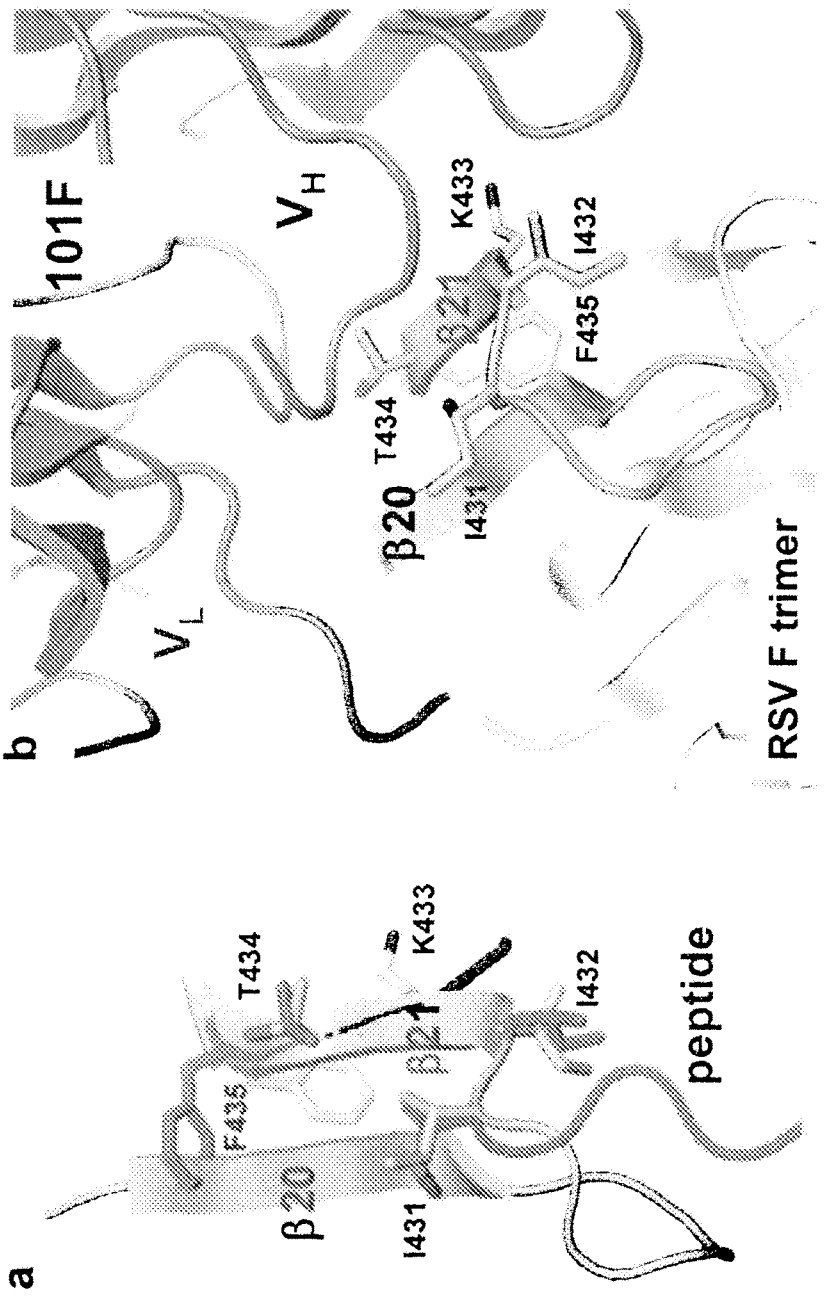
a
T434
K433
F435
β21
I432
β20
I431
peptide
b
101F
V_H
V_L
K433
I432
F435
β21
T434
β20
I431
RSV F trimer

FIG. 10

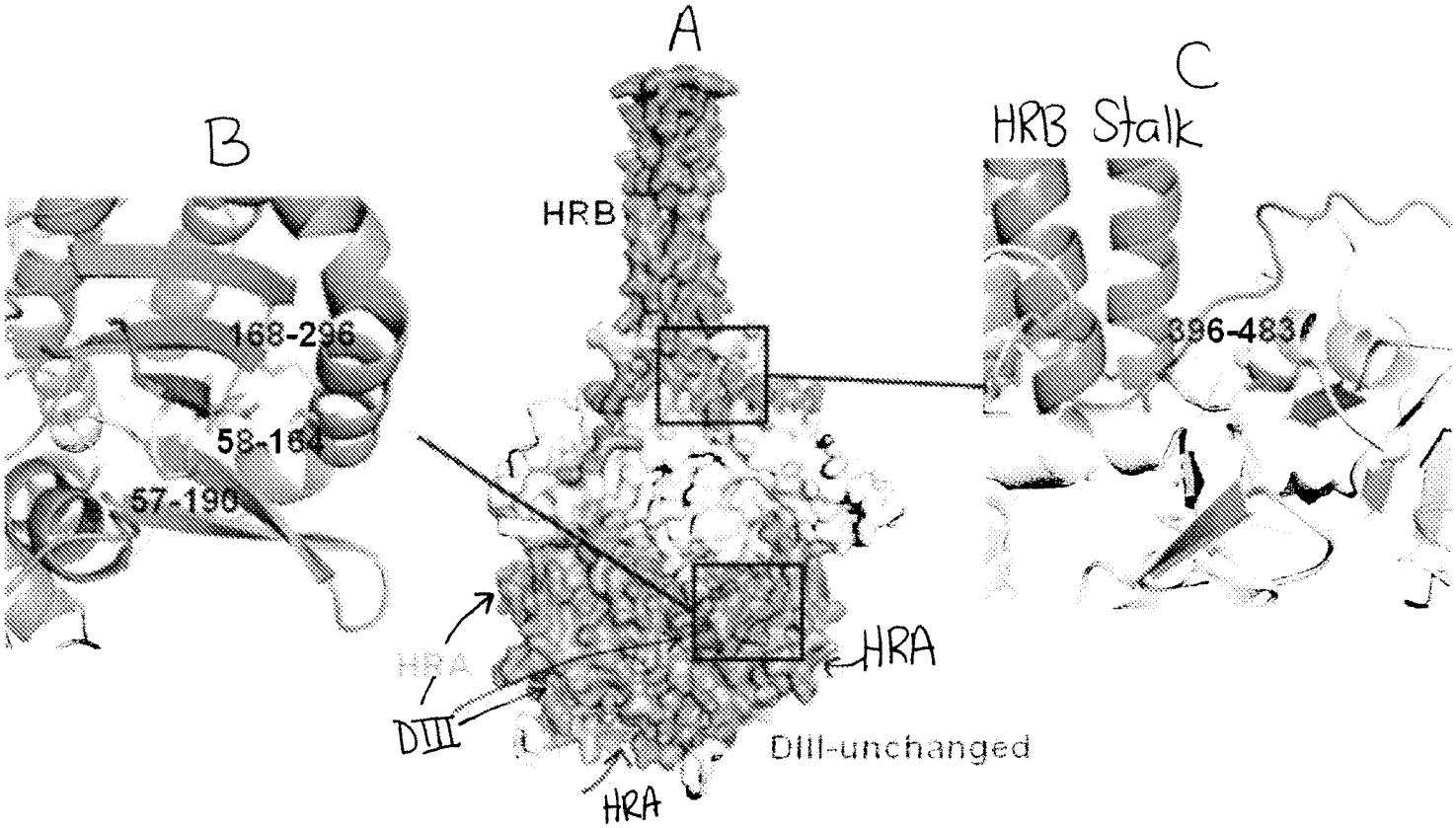
A
B
C
HRB
HRB Stalk
168-296
58-164
57-190
396-483
HRA
DIII
HRA
DIII-unchanged
HRA
165-296 and 56-164 proposed to account for potential model bias

FIG. 11

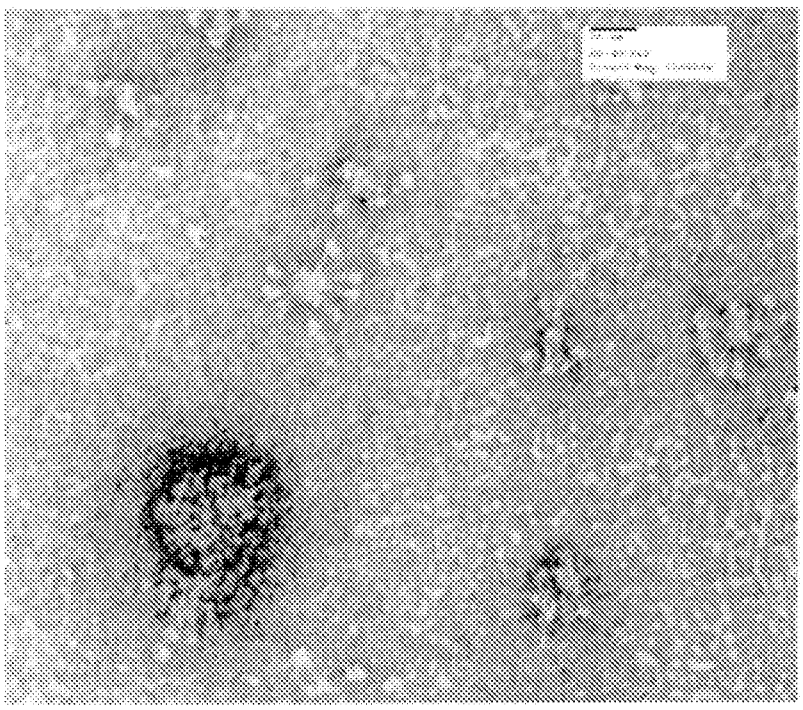

FIG. 12

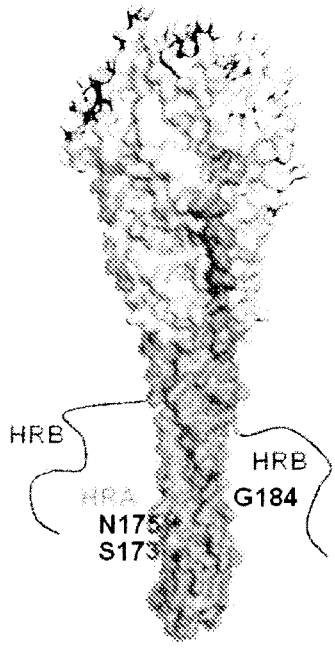

FIG. 13

R049 RSV-F fus del R429S I432T K433T S436F trunc
R050 RSV-F HRA Disulfide2 I57C S190C trunc
R051 RSV-F HRA Disulfide3 T58C V164C trunc
R052 RSV-F HRA Disulfide5 K168C V296C trunc
R053 RSV-F fus del N262Y N268I K272M R429S I432T K433T S436F trunc
R054 RSV-F HRA Disulfide1 V56C V164C trunc
R055 RSV-F HRA Disulfide4 N165C V296C trunc
R056 RSV-F HRB Disulfide M396C F483C trunc

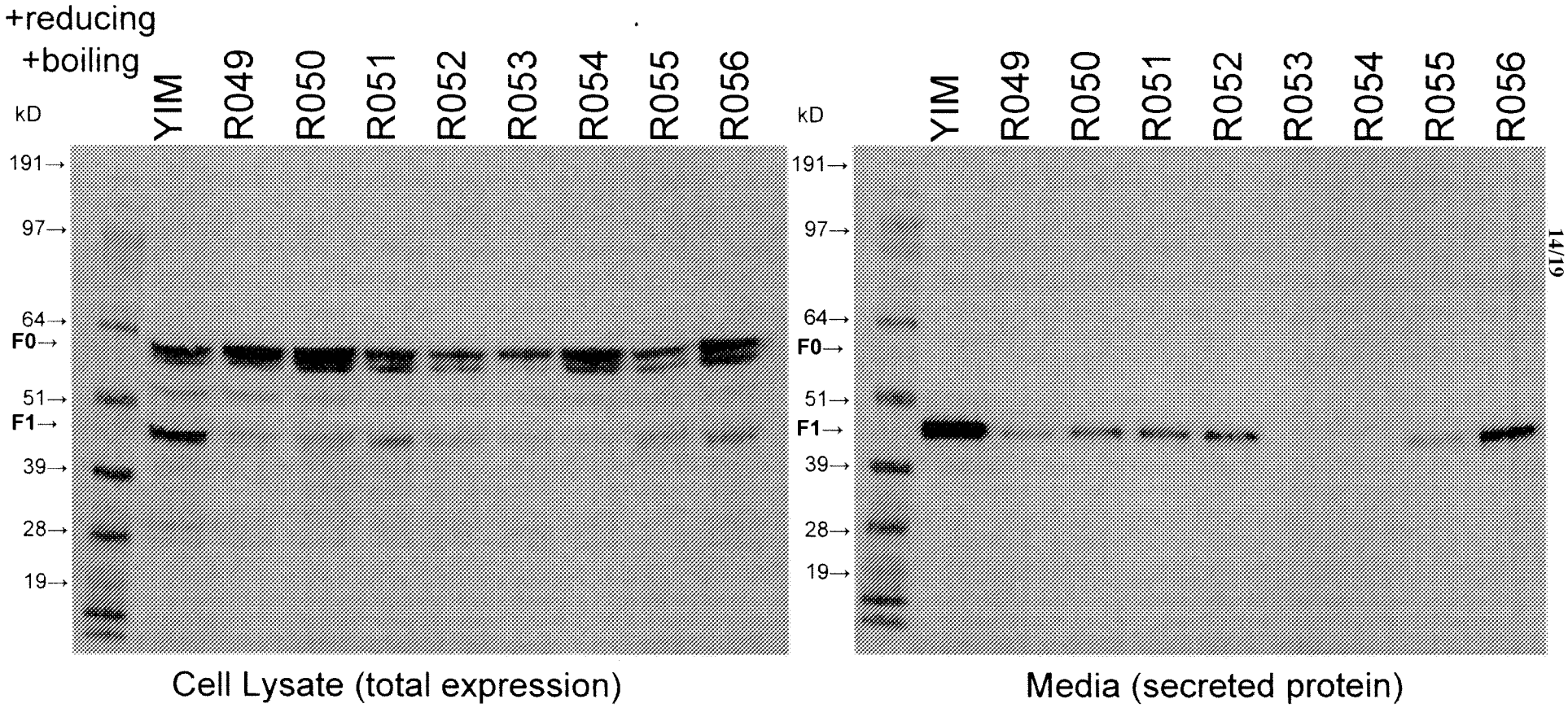

FIG. 14

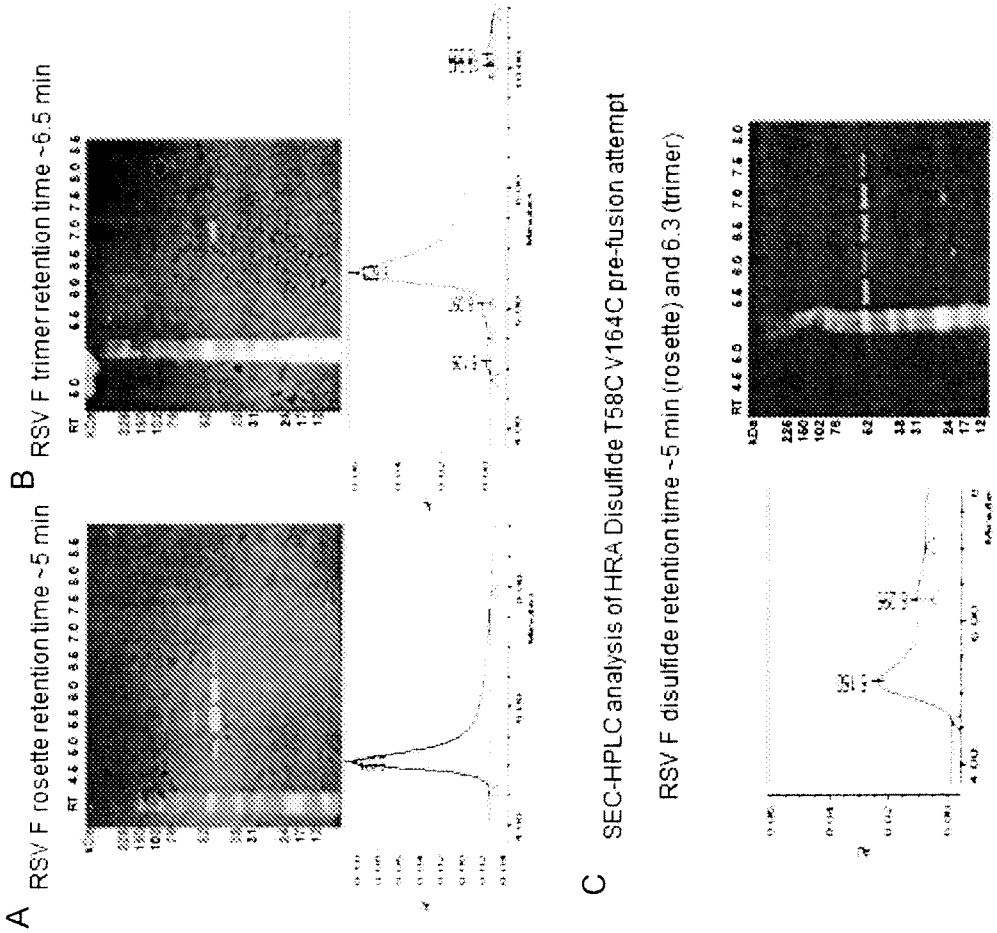
A
RSV F rosette retention time ~5 min
B
RSV F trimer retention time ~6.5 min
C
SEC-HPLC analysis of HRA Disulfide T58C V164C pre-fusion attempt
RSV F disulfide retention time ~5 min (rosette) and 6.3 (trimer)

FIG. 15

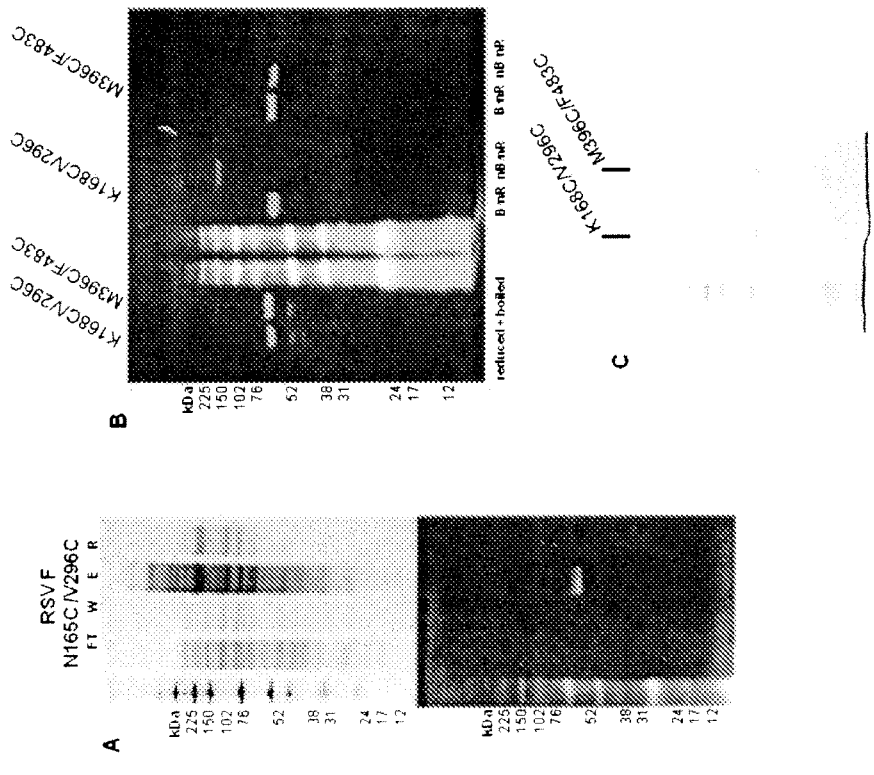
A
RSVF
N165C/N296C
FT W E R
kDa
225
150
102
76
52
38
31
24
17
12
B
K168C/N296C
M396C/F483C
K168C/N296C
M396C/F483C
reduced + boiled
B nR nB nP
B nR nB nP
C
K168C/N296C
M396C/F483C

FIG. 16

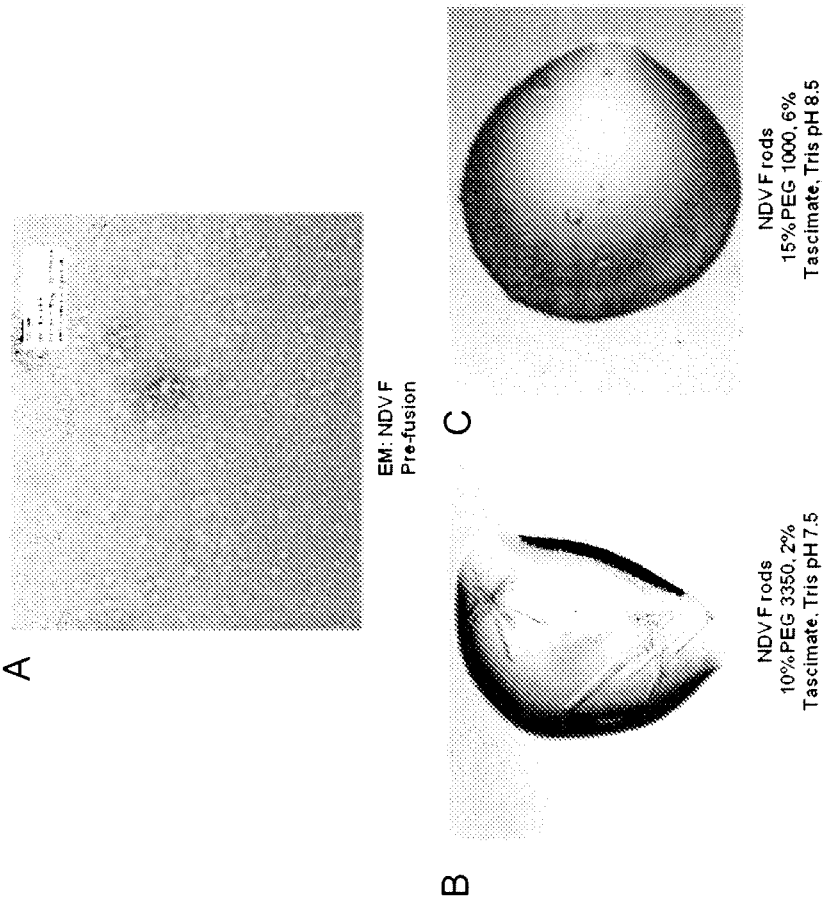
A
EM: NDV F
Pre-fusion
B
NDV F rods
10% PEG 3350, 2%
Tascimate, Tris pH 7.5
C
NDV F rods
15% PEG 1000, 6%
Tascimate, Tris pH 8.5

FIG. 17

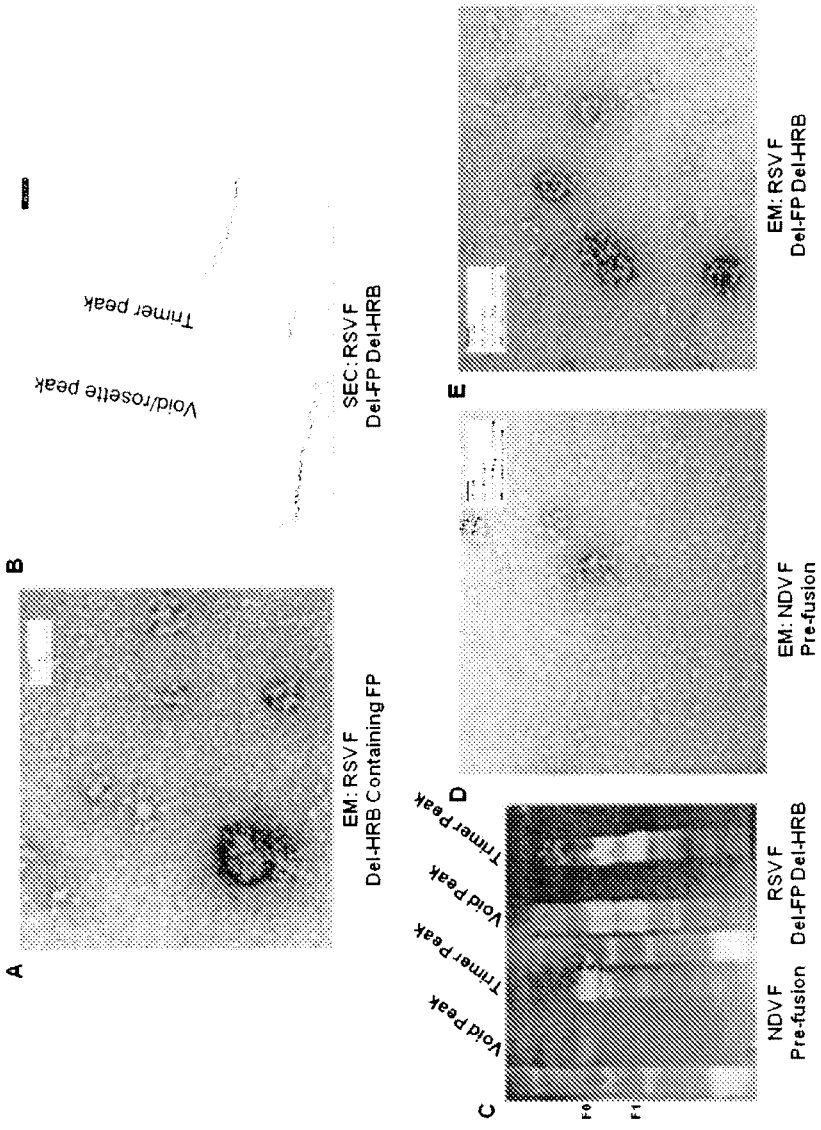
A
EM: RSV F
Del-HRB Containing FP
B
SEC: RSV F
Del-FP Del-HRB
Void/rosette peak
Trimer peak
C
NDV F
Pre-fusion
RSV F
Del-FP Del-HRB
Void peak
Trimer peak
Void peak
Trimer peak
D
EM: NDV F
Pre-fusion
E
EM: RSV F
Del-FP Del-HRB

FIG. 18

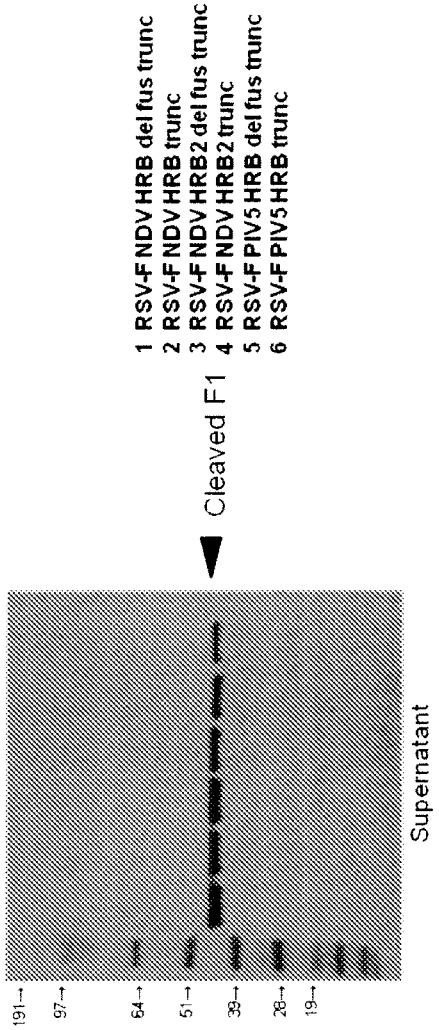
1 RSV-F NDV HRB del fus trunc
2 RSV-F NDV HRB trunc
3 RSV-F NDV HRB2 del fus trunc
4 RSV-F NDV HRB2 trunc
5 RSV-F PIV5 HRB del fus trunc
6 RSV-F PIV5 HRB trunc
Cleaved F1
1 2 3 4 5 6
Supernatant
191→
97→
64→
51→
39→
28→
19→

FIG. 19

INTERNATIONAL SEARCH REPORT

International application No
PCT/US2012/037773

A. CLASSIFICATION OF SUBJECT MATTER
INV. C07K14/135
ADD.

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)
C07K

Documentation searched other than minimum documentation to the extent that such documents are included in the fields searched

Electronic data base consulted during the international search (name of data base and, where practicable, search terms used)
EPO-Internal , BIOSIS, CHEM ABS Data, Sequence Search , EMBASE, WPI Data

C. DOCUMENTS CONSIDERED TO BE RELEVANT

Category*	Citation of document, with indication, where appropriate, of the relevant passages	Relevant to claim No.
X	WO 2011/008974 A2 (NOVARTIS AG [CH] ; SWANSON KURT [US] ; DORMITZER PHILIPP R [US]) 20 January 2011 (2011-01-20)	1-5 , 11 , 12 , 19-29
Y	the whole document	1-5 , 11 , 12 , 19-29

Y	WO 2010/149745 A1 (GLAXOSMITHKLINE BIOLOG SA [BE] ; ID BIOMEDICAL CORP QUEBEC [CA] ; BAUDOU) 29 December 2010 (2010-12-29) the whole document	1-5 , 11 , 12 , 19-29

Y	WO 2009/079796 A1 (ID BIOMEDICAL CORP QUEBEC [CA] ; GLAXOSMITHKLINE BIOLOG SA [BE] ; BAUDOU) 2 July 2009 (2009-07-02) the whole document	1-5 , 11 , 12 , 19-29

	-/-- ·	

[X] Further documents are listed in the continuation of Box C.

[X] See patent family annex.

* 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" documentwhich may throw doubts on priority claim(s) orwhich 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
30 October 2012	06/11/2012

Name and mailing address of the ISA/	Authorized officer
European Patent Office, P.B. 5818 Patentlaan 2 NL - 2280 HV Rijswijk Tel. (+31-70) 340-2040, Fax: (+31-70) 340-3016	Pilat, Daniel

4

Form PCT/ISA/210 (second sheet) (April 2005)

C(Continuation). DOCUMENTS CONSIDERED TO BE RELEVANT

Category*	Citation of document, with indication, where appropriate, of the relevant passages	Relevant to claim No.
X Y	WO 2010/149743 A2 (ID BIOMEDICAL CORP QUEBEC [CA]; GLAXOSMITHKLINE BI0L0G SA [BE]; BLAIS) 29 December 2010 (2010-12-29) the whole document	6,9, 10, 12, 19-25, 29 1-5, 11, 12, 19-29
Y	J. K. LEE ET AL: "Reversible Inhibition of the Fusion Activity of Measles Virus F Protein by an Engineered Intersubunit Disulfide Bridge", JOURNAL OF VIROLOGY, vol. 81, no. 16, 15 August 2007 (2007-08-15), pages 8821-8826, XP55032543, ISSN: 0022-538X, D0I: 10.1128/JVI.00754-07 abstract page 8821, column 1, last paragraph	1-5, 11, 12, 19-29
A	DAY NICOLE D ET AL: "Contribution of cysteine residues in the extracellular domain of the F protein of human respiratory syncytial virus to its function", VIROLOGY JOURNAL, BI0MED CENTRAL, LONDON, GB, vol. 3, no. 1, 24 May 2006 (2006-05-24), page 34, XP021019338, ISSN: 1743-422X, D0I: 10.1186/1743-422X-3-34 abstract	1-5, 11, 12, 19-29
A	YIN HSIEN-SHENG ET AL: "Structure of the parainfluenza virus 5 F protein in its metastable, prefusion conformation", NATURE: INTERNATIONAL WEEKLY JOURNAL OF SCIENCE, NATURE PUBLISHING GROUP, UNITED KINGDOM, vol. 439, no. 7072, 5 January 2006 (2006-01-05), pages 38-44, XP002600415, ISSN: 0028-0836, D0I: 10.1038/NATURE04322 cited in the application the whole document	1-5, 11, 12, 19-29
X, P	K. A. SWANS0N ET AL: "Structural basis for immunization with postfusion respiratory syncytial virus fusion F glycoprotein (RSV F) to elicit high neutralizing antibody titers", PROCEEDINGS OF THE NATIONAL ACADEMY OF SCIENCES, vol. 108, no. 23, 17 May 2011 (2011-05-17), pages 9619-9624, XP55032519, ISSN: 0027-8424, D0I: 10.1073/pnas.1106536108 the whole document	1-5, 11, 12, 19-29

4

INTERNATIONAL SEARCH REPORT

International application No.
PCT/US2012/037773

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.:
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:

see additional sheet

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 an 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.:

1-5, 9-11 (completely); 6, 12, 19-29 (partially)

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.

FURTHER INFORMATION CONTINUED FROM PCT/ISA/ 210

This International Searching Authority found multiple (groups of) inventions in this international application, as follows:

1. claims: 1-5, 11 (completely) ; 12, 19-29 (partially)

   a pre-fusion respiratory syncytial virus (RSV) F polypeptide comprising at least two introduced cysteine residues, wherein said cysteines are in close proximity to one another and form a disulfide bond that stabilizes the pre-fusion RSV F polypeptide and embodiments thereof.

   ---

2. claims: 6, 12, 19-29 (all partially)

   a pre-fusion respiratory syncytial virus (RSV) F polypeptide comprising a post-fusion modification consisting of a deletion of the HRA helix, wherein said post-fusion modification destabilizes the post-fusion conformation and embodiments thereof.

   ---

3. claims: 7, 8(completely) ; 6, 12, 19-29 (partially)

   a pre-fusion respiratory syncytial virus (RSV) F polypeptide comprising a post-fusion modification consisting of deletion of the HRB helix, wherein said post-fusion modification destabilizes the post-fusion conformation and embodiments thereof.

   ---

4. claims: 6, 12, 19-29 (all partially)

   a pre-fusion respiratory syncytial virus (RSV) F polypeptide comprising a post-fusion modification consisting of introduction of point mutations, wherein said post-fusion modification destabilizes the post-fusion conformation, and embodiments thereof.

   ---

5. claims: 9, lO(completely) ; 6, 12, 19-29 (partially)

   a pre-fusion respiratory syncytial virus (RSV) F polypeptide comprising a post-fusion modification consisting of addition of glycosylation sites, wherein said post-fusion modification destabilizes the post-fusion conformation and embodiments thereof.

   ---

6. claims: 13-18(completely) ; 19-29 (partially)

   a chimeric pre-fusion F protein comprising a stabilized F protein from a virus other than RSV that contains one or more neutralizing epitope of RSV F and embodiments thereof.

INTERNATIONAL SEARCH REPORT

Information on patent family members

International application No
PCT/US2012/037773

Patent document cited in search report	Publication date	Patent family member(s)	Publication date
WO 2011008974 A2	20-01-2011	AR 077757 Al	21-09-2011
		CA 2768186 Al	20-01-2011
		CN 102639147 A	15-08-2012
		CO 6491045 A2	31-07-2012
		EP 2453918 A2	23-05-2012
		SG 178026 Al	29-03-2012
		TW 201116294 A	16-05-2011
		US 2011305727 Al	15-12-2011
		US 2012164176 Al	28-06-2012
		WO 2011008974 A2	20-01-2011
WO 2010149745 Al	29-12-2010	AU 2010264688 Al	19-01-2012
		CA 2766211 Al	29-12-2010
		CN 102481359 A	30-05-2012
		CO 6480978 A2	16-07-2012
		CR 20120025 A	28-05-2012
		EA 201270063 Al	30-07-2012
		EP 2445526 Al	02-05-2012
		MA 33449 Bl	03-07-2012
		SG 176829 Al	30-01-2012
		US 2012093847 Al	19-04-2012
		WO 2010149745 Al	29-12-2010
WO 2009079796 Al	02-07-2009	AU 2008340949 Al	02-07-2009
		CA 2710600 Al	02-07-2009
		CN 101952321 A	19-01-2011
		EA 201070794 Al	28-02-2011
		EP 2222710 Al	01-09-2010
		JP 2011507533 A	10-03-2011
		KR 20100109933 A	11-10-2010
		US 2010291147 Al	18-11-2010
		WO 2009079796 Al	02-07-2009
WO 2010149743 A2	29-12-2010	AU 2010264686 Al	19-01-2012
		CA 2766205 Al	29-12-2010
		CN 102548578 A	04-07-2012
		EP 2445527 A2	02-05-2012
		KR 20120093811 A	23-08-2012
		SG 176807 Al	30-01-2012
		US 2012135028 Al	31-05-2012
		WO 2010149743 A2	29-12-2010