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(54) Title: COMPOSITIONS AND METHODS FOR TARGETED CYTOKINE DELIVERY

(57) Abstract: The present disclosure encompasses compositions and methods for targeted cytokine delivery. The compositions disclosed herein comprise a cytokine linked to a ligand and may improve immunotherapy by limiting side effects associated with immunotherapy.

COMPOSITIONS AND METHODS FOR TARGETED CYTOKINE DELIVERY

GOVERNMENTAL RIGHTS

[0001] This invention was made with government support under R01 AI073552 and HHSN272200700058C awarded by the NIH/NIAID and R01 HL113931 awarded by the NIH/HLBI. The government has certain rights in the invention.

CROSS REFERENCE TO RELATED APPLICATIONS

[0002] This application claims the benefit of U.S. Provisional Application number 62/243,829, filed October 20, 2015 and U.S. Provisional Application number 62/091,898, filed December 15, 2014, each of the disclosures of which is hereby incorporated by reference in its entirety.

FIELD OF THE INVENTION

[0003] The present disclosure encompasses compositions and methods for targeted cytokine delivery. Through specific delivery of cytokines, the compositions disclosed herein may improve immunotherapy by limiting side effects associated with immunotherapy.

BACKGROUND OF THE INVENTION

[0004] Systemic administration of high dose interleukin 2 (IL2) is one of the most potent forms of immunotherapy and is currently approved by the FDA for treatment of several malignancies. Efficacy of this treatment depends on activating cytotoxic lymphocytes (CTLs) such as natural killer cells (NK) and $CD8^+$ T lymphocytes ($CD8^+$ CTLs). Clinical trials have demonstrated approximately 15% partial or complete tumor responses, with up to 5% of patients having a durable long-lasting response resembling a cure. Despite these encouraging results in a minority of patients, most do not achieve a benefit or stop IL2 therapy prematurely due to complications such as blood pressure changes and pulmonary or systemic capillary leak. It is thought that the direct action of IL2 on vascular endothelium contributes to the majority of these side effects. The efficacy of IL2 is also limited by preferential activation of $CD4^+Foxp3^+$ regulatory T cells (T_{regs}), which decrease

the tumor immune response. For these reasons treatment with high-dose IL2 has fallen out of favor clinically.

[0005] Side effects and deceased efficacy of IL2 therapy occur due to the high affinity trimeric αβγ IL2 receptor (IL2R), which is expressed by vascular endothelial cells and T_{regs} at baseline. Thus $CD4^{+}Foxp3^{+}$ T_{regs} and vascular endothelium are activated at much lower doses of IL2 than NK cells, which express the lower affinity βγ chains of the IL2R at rest. NK cells do express the high affinity α chain of IL2R after activation and depend on this trimeric receptor for peak cytolytic capacity. Mutant forms of IL2 with decreased affinity for IL2Rα have been described and offer a more favorable side effect profile. However, they also result in lower efficacy and decreased therapeutic potential due to decreased CTL activation. Therefore, there is a need in the art for a form of IL2 that could preferentially bind to and activate CTLs without activating T_{regs} and endothelial cells. Such an IL2 derivative might overcome such clinical barriers and result in more efficacious immunotherapy with fewer side effects.

SUMMARY OF THE INVENTION

[0006] In an aspect the disclosure provides, a composition comprising a cytokine linked to a ligand, wherein the ligand is not a corresponding binding partner to the cytokine.

[0007] In another aspect, the disclosure provides a method to deliver a cytokine to a target cell comprising contacting a target cell with a composition comprising a cytokine linked to a ligand. The ligand specifically binds to a receptor on the target cell and the ligand is not a corresponding binding partner to the cytokine.

[0008] In still another aspect, the disclosure provides a method to activate immune cells comprising contacting an immune cell with a composition comprising a proinflammatory cytokine linked to a ligand. The ligand specifically binds to a receptor on the immune cell thereby activating the cell and the ligand is not a corresponding binding partner to the cytokine.

[0009] In still yet another aspect, the disclosure provides a method to treat a tumor comprising identifying a subject with a tumor and administering to the subject a therapeutically effective amount of a composition comprising a proinflammatory

cytokine linked to a ligand. The ligand specifically binds to a receptor on a target cell and the ligand is not a corresponding binding partner to the cytokine.

[0010] In a different aspect, the disclosure provides a method to treat a viral infection comprising administering to the subject a therapeutically effective amount of a composition comprising a proinflammatory cytokine linked to a ligand. The ligand specifically binds to a receptor on a target cell and the ligand is not a corresponding binding partner to the cytokine.

[0011] In other aspects, the disclosure provides a chimeric peptide comprising a cytokine peptide and a ligand peptide. The cytokine peptide is not a binding partner of the ligand peptide.

[0012] In certain aspects, the disclosure provides a chimeric peptide comprising a cytokine peptide and a ligand peptide. The ligand peptide binds to an NKG2D receptor.

[0013] In another different aspect, the disclosure provides a nucleic acid molecule comprising a sequence encoding a chimeric peptide of the disclosure.

[0014] In yet another different aspect, the disclosure provides a pharmaceutical composition comprising a chimeric peptide of the disclosure.

[0015] In still yet another different aspect, the disclosure provides a method of treating a subject diagnosed with cancer comprising administering to the subject a pharmaceutical composition of the disclosure.

BRIEF DESCRIPTION OF THE FIGURES

[0016] The application file contains at least one drawing executed in color. Copies of this patent application publication with color drawing(s) will be provided by the Office upon request and payment of the necessary fee.

[0017] **FIG. 1A, FIG. 1B, FIG. 1C, FIG. 1D, FIG. 1E** and **FIG. 1F** depict a diagram, immunoblot and graphs showing the generation and *in vitro* evaluation of OMCP-mutIL-2. (**FIG. 1A**) Schematic structure of OMCP-mutIL-2. (**FIG. 1B**) Molecular weight of OMCP-mutIL-2 compared to mutIL-2 and wild-type IL-2. IL-2, mutIL-2, and OMCP-mutIL-2 were produced in mammalian cells and have higher molecular weights due to glycosylation. The lower migrating band for mutIL-2 corresponds to

unglycosylated protein, likely due to lysis of the producing cells. Based on differences in molecular weight all cytokines and construct were administered on a molar basis with 1 µl of 4.4 µM solution defined as 1000 IU equivalents (IUe) herein. This effectively allows for equimolar comparison between IL-2, mutIL-2 and OMCP-mutIL-2 despite different molecular weights. (**FIG. 1C, FIG. 1D**) *In vitro* activation of A/J lymphocyte subsets after 36 hours of culture in 100 IUe of cytokines or OMCP-mutIL-2 construct. (**FIG. 1E, FIG. 1F**) Proliferation of B6 lymphocyte subsets after 5-day culture in 1000 IUe/ml of cytokines or OMCP-mutIL-2 construct. Graphs representative of 3-6 replicates per condition. black=saline; blue=wtIL-2, red=OMCP-mutIL-2, green=mutIL-2.

[0018] **FIG. 2A, FIG. 2B, FIG. 2C, FIG. 2D, FIG. 2E, FIG. 2F, FIG. 2G, FIG. 2H, FIG. 2I, FIG. 2J, FIG. 2K, FIG. 2L, FIG. 2M, FIG. 2N** and **FIG. 2O** depict graphs and images showing *in vivo* dosing of IL-2 and IL-2 constructs. Animal mortality (**FIG. 2A**) and morbidity assessed by weight loss (**FIG. 2B**) accumulation of ascites and pleural fluid (representative syringe-**FIG. 2C**; average from all mice in the group-**FIG. 2D**) and (**FIG. 2E**) organ inflammation after administration of wtIL-2. Animal mortality (**FIG. 2F, FIG. 2H, FIG. 2J**) and morbidity as assessed by weight loss (**FIG. 2G, FIG. 2I, FIG. 2K**) after administration of high dose wtIL-2 (**FIG. 2F, FIG. 2G**), OMCP-mutIL-2 (**FIG. 2H, FIG. 2I**) and mutIL-2 (**FIG. 2J, FIG. 2K**) in anti-AsialoGM1 (solid line) or rabbit IgG-treated (dotted line) in A/J mice. Weight loss (**FIG. 2L**), ascites (representative syringe-**FIG. 2M**; average from all mice in the group-**FIG. 2N**) and organ inflammation (**FIG. 2O**) in mice treated with 200,000 IUe of either wt IL-2, OMCP-mutIL-2 or mutIL-2. All graphs represent 46 animals per treatment condition. ns $p>.05$; * $p<.05$; ** $p<.01$; *** $p<.001$; black=saline; blue=wtIL-2, red=OMCP-mutIL-2, green=mutIL-2.

[0019] **FIG. 3A, FIG. 3B, FIG. 3C, FIG. 3D, FIG. 3E, FIG. 3F, FIG. 3G, FIG. 3H, FIG. 3I and FIG. 3J** depict graphs and images showing immunologic changes associated with IL-2 and IL-2 construct administration *in vivo*. (**FIG. 3A, FIG. 3B**) Total splenocyte counts after a five-day course of 200,000 IUe of IL-2 (blue), mutIL-2 (green) and OMCP-mutIL-2 (red). (**FIG. 3C**) NK cell expansion and activation after IL-2, mutIL-2, OMCP-mutIL-2, high dose IL-2, high dose mutIL-2 and IL-2/anti-IL-2 complexes

measured by cell counts in the spleen (top) and KLRG1 upregulation (bottom). (**FIG. 3D**) $CD4^{+}Foxp3^{+}$ T_{reg} expansion and activation as measured by cell counts in the spleen (top) and ICOS upregulation (bottom) as well as (**FIG. 3E**) NK/T_{reg} ratio in the spleen. Expansion of splenocytes (**FIG. 3F, FIG. 3G**) and NK cells (**FIG. 3H**) in B6 mice treated with 750,000 IUe of cytokine or construct. T_{reg} expansion and activation (**FIG. 3I**) as well as $NK:T_{reg}$ ratio (**FIG. 3J**) in the spleen of B6 mice. All graphs represent an average cell count ± SEM from 5-10 mice per group. ns p>.05; * p<.05; ** p<.01; *** p<.001; black=saline; blue=wtIL-2, red=OMCP-mutIL-2, green=mutIL-2.

[0020] **FIG. 4A, FIG. 4B, FIG. 4C, FIG. 4D** and **FIG. 4E** depict graphs and images showing cytokine-mediated tumor immunotherapy. (**FIG. 4A**) *In vivo* cytotoxicity for YAC-1 lymphoma after intravenous injection. (**FIG. 4B, FIG. 4C**) LLC tumor growth after a five-day course of 750,000 IUe of cytokine treatment given as ten doses on days 5-10 post tumor injection. LLC tumor growth in mice depleted on NK cells (**FIG. 4D**) or mutant mice deficient in NKG2D (**FIG. 4E**). Data represents 5-6 mice per group. ns p>.05; * p<.05; ** p<.01; *** p<.001; black=saline; blue=wtIL-2, red=OMCP-mutIL-2, green=mutIL-2.

[0021] **FIG. 5A, FIG. 5B, FIG. 5C, FIG. 5D, FIG. 5E, FIG. 5F, FIG. 5G, FIG. 5H, FIG. 5I, FIG. 5J** and **FIG. 5K** depict graphs and a schematic showing IL-2 signaling in NK cells. (**FIG. 5A, FIG. 5B**) Serum levels after injection of $1x10^{6}$ IUe of fluorochrome-labeled cytokine or construct i.v. (**FIG. 5C**) Degranulation of NK cells in the presence of cytokines and pentameric OMCP-mediated crosslinking of NKG2D as measured by surface CD107a expression at 1000 IUe/ml. STAT5 phosphorylation in isolated NK cells from A/J (**FIG. 5D**) or B6 mice (**FIG. 5E**) by increasing doses of cytokine. Decay in STAT5 phosphorylation after a 15 minute stimulation by 1000 IUe/ml (**FIG. 5F**) or 100 IUe/ml (**FIG. 5G**) of IL-2 or OMCP-mutIL-2. (**FIG. 5H**) Proposed model of competition between NK cells and stromal cells for IL-2. (**FIG. 5I**) STAT5 phosphorylation of B6 NK cells in the presence of other splenocytes by wtIL-2 and OMCP-mutIL-2. (**FIG. 5J**) STAT5 phosphorylation of wild-type or $NKG2D^{-/-}$ NK cells by wtIL-2 and OMCP-mutIL-2 in the presence of competing splenocytes. (**FIG. 5K**) STAT5 phosphorylation, as measured by fold change over saline-treated controls, of wild-type NK cells in the

presence of competing splenocytes treated with saturating concentrations of rat anti-mouse CD25 (clone 3C7) or rat IgG isotype control.

[0022] **FIG. 6** depicts graphs showing B6 NK cells are preferentially activated by low dose OMCP-mutIL-2 but this selectivity disappears at the highest doses of cytokine or in the absence of NKG2D expression by NK cells. Left two graphs show B6 NK cells and right two graphs show BK NKG2D$^{-/-}$ NK cells.

[0023] **FIG. 7A, FIG. 7B** and **FIG. 7C** depict imaging showing that inspection of the viscera demonstrates limited food consumption after a 5-day course of 200,000 or 750,000 IUe of wtIL-2. **FIG. 7D** depicts a graph showing that unlike the A/J strain, B6 mice are able to tolerate higher doses of wtIL-2 with only moderate weight loss after 750,000 IUe. Higher doses of 1,500,000 IUe IL-2 resulted in increased weight loss. Doses above this regimen led to animal death.

[0024] **FIG. 8A** depicts a graph showing that A/J mice treated with IL-2/anti-IL-2 antibodies or high dose mutIL-2 lost significant weight during treatment. The majority of IL-2/anti-IL-2 treated mice could not survive the full 200,000 IUe dosing and were sacrificed four days after starting treatment thus receiving 160,000-180,000 IUe. **FIG. 8B** depicts a graph and flow cytometric plot showing NK expansion with ULBP3-mutIL-2 and lower doses of OMCP-mutIL-2 in A/J spleen (top). NK activation, as measured by surface KLRG1 expression on NK cells treated with 200,000 IUe of mutIL-2 (green) or ULBP3-mutIL-2 (purple) in A/J spleen (bottom). **FIG. 8C** and **FIG. 8D** depict graphs showing that unlike the case for NK cells, little expansion of CD8$^+$ or CD4$^+$ Foxp3$^-$ T cells was evident in either IL-2, OMCP-mut-IL-2, or mutIL-2 treated mice. **FIG. 8E** depicts a graph showing weight loss in B6 mice treated with high dose mutIL-2 or IL2/anti-IL-2 antibody complex. **FIG. 8F** and **FIG. 8G** depict graphs showing expansion of CD8$^+$ or CD4$^+$Foxp3$^-$ T cells in cytokine treated B6 mice. Graphs represent 5-10 mice per group.

[0025] **FIG. 9A** and **FIG. 9B** depict graphs showing *in vitro* lysis of A/J tumors, such as LM2 lung adenocarcinoma (**FIG. 9A**) or YAC-1 lymphoma (**FIG. 9B**) by bulk splenocytes after a five day course of 200,000 IUe of cytokine given over ten doses.

FIG. 9C shows *in vitro* lysis of LLC lung cancer by B6 splenocytes treated with 750,000 IUe of cytokines or constructs given over five days in ten doses.

[0026] **FIG. 10A** depicts flow cytometric plots showing that plate bound anti-NKG2D antibody (clone A10)-mediated augmentation of NK degranulation with cytokines added at 1000 IUe/ml. **FIG. 10B** depicts a flow cytometric plot showing CD69 levels on NK cells cultured at 100 IUe/ml of OMCP-mut-IL2 or mutIL-2 with pentameric OMCP.

[0027] **FIG. 11A, FIG. 11B** and **FIG. 11C** depict a schematic of the differential IL2 binding and activation *in vivo*. (**FIG. 11A**) Regular wild-type IL2 preferentially binds to cells such as $CD4^{+}Foxp3^{+}T_{regs}$ and vascular endothelium, both of which express the high affinity α chain along with the signaling β and γ chains of the IL2 receptor. (**FIG. 11B**) The R38A and F42K mutations in IL2 decrease affinity for the α chain of the IL2 receptor. (**FIG. 11C**) By linking R38A/F42K IL2 to the high affinity NKG2D ligand OMCP delivery and binding of this cytokine to NKG2D-expressing CTLs such as NK cells and activated $CD8^{+}$ T cells is increased. Width of arrows indicates proposed strength of IL2 binding and/or signaling.

[0028] **FIG. 12** depicts a schematic of the experimental design of immunotherapy experiments.

[0029] **FIG. 13** depicts a schematic of the experimental design of vaccination experiments.

[0030] **FIG. 14A** and **FIG. 14B** depict graphs showing lung cancer susceptible and resistant strains of mice. (**FIG. 14A**) AJ and 129 mouse strains are susceptible to lung cancer as evidenced by tumor burden whereas B6 and C3H mouse strains are resistant to lung cancer as evidenced by tumor burden. (**FIG. 14B**) Upon incubation with freshly isolated NK cells from the various mouse strains, B6 and C3H NK cells result in significantly more LM2 lung carcinoma cell lysis than AJ and 129 NK cells.

[0031] **FIG. 15** depicts a graph showing that in human men, a greater percentage of NK cells appear to produce TNFα in “resistant” patients versus “susceptible” patients.

[0032] **FIG 16** depicts a graph showing that ex vivo cytokine activation can reverse natural killer cell dysfunction. Mouse NK Cells that did not show significant lysis

of cancer cells (NK cells from 129 & AJ strains) were much more effective at lysis when treated with IL-2. NK cells from cancer-resistant strains also showed increase % of specific lysis.

[0033] **FIG. 17A, FIG. 17B, FIG. 17C, FIG. 17D, FIG. 17E** and **FIG. 17F** depict graphs showing binding of fluorescently labeled construct tested *in vitro* at 37 degrees in bulk splenocytes. The construct appears to only bind to NK cells (express NKG2D). Red line is OMCP-IL2 construct. (**FIG. 17A**) DX5+CD3- NK cell; (**FIG. 17B**) CD4+CD3+ T cells; (**FIG. 17C**) CD8+CD3+ T cells; (**FIG. 17D**) CD11C+CD11b- DCs; (**FIG. 17E**) CD11c-CD11b+ Macs; (**FIG. 17F**) CD19+CD3- B cells.

[0034] **FIG. 18** depicts a schematic dosing regimen for IL2 or IL2 constructs.

[0035] **FIG. 19** depicts a schematic dosing regimen for IL2 or IL2 constructs after irradiation.

[0036] **FIG. 20A, FIG. 20B** and **FIG. 20C** depict images and alignments of the OMCP structure. (**FIG. 20A**) Ribbon diagram of CPXV OMCP. Secondary structure elements are noted, S for beta strands and H for helix. The α1/α2 portions of the platform domain are indicated in cyan and magenta, respectively. (**FIG. 20B**) Ribbon diagram of the α1/α2 domain of MICA (PDB identifier 1HYR), with the α3 domain removed for clarity. Residues that contact NKG2D are colored yellow. (**FIG. 20C**) Structure alignment of OMCP with NKG2DLs. The mature sequences of $OMCP_{BR}$ (CPXV-BR-018; GenBank accession number NP_619807; PDB identifier 4FFE) and $OMCP_{MPX}$ (MPXV-ZAR_1979_005-198; N3R; GenBank accession number AAY97396) are aligned with the ectodomain sequences of MICA (1HYR), MICB (1JE6), ULBP3 (1KCG), and RAE-1β (1JFM). Known NKG2D contact residues for NKG2DLs are indicated in yellow. Asn residues likely to be glycosylated are noted by black boxes in panel C and as black side chains in panels A and B. OMCPbr=SEQ ID NO:13; OMCPmpx=SEQ ID NO:14; MICA=SEQ ID NO:15; MICB=SEQ ID NO:16; ULBP3=SEQ ID NO:17; and RAE-1B=SEQ ID NO:18

[0037] **FIG. 21** depicts a graph showing OMCP-targeted delivery of IL15. Higher levels of CD25 are evident when IL15 is delivered by OMCP vs naked cytokine alone in equimolar doses.

[0038] **FIG. 22** depicts a graph showing that the D132R mutation in OMCP significantly decreases its NKG2D binding. NK expansion and activation in the presence of mutIL2, OMCP-mutIL2, and D132ROMCP-mutIL2 was tested. The D132R mutation ameliorated the superiority of natural killer cell activation over cytokine alone.

[0039] **FIG. 23** depicts various embodiments of the invention. 1. depicts OMCP helix 2 linked to cytokine. 2. depicts pegylation of the composition. 3. depicts a composition comprising engineered glycans. 4. depicts various linker lengths and compositions. 5. depicts an antibody linked to a cytokine. For example a Fab specific NKG2D antibody. 6. depicts a NKG2DL linked to a cytokine. For example, MIC or ULBP. 7 depicts an alternative OMCP linked to a cytokine. For example, $OMCP_{mpx}$ could represent a preferred variant of OMCP, and mutant OMCP could represent either a gain or loss of function for NKG2D binding. 8. depicts re-targeting of the OMCP in a composition. For example, a mutant OMCP may be directed to NKG2A, NKG2C, NKG2E, etc. 9. depicts other viral protein liked to a cytokine. For example, the other viral protein may also bind to receptors on immune cells. 10. depicts OMCP linked to mutant cytokines. It is understood that the OMCP sequence could be from various sources such as cowpox or monkeypox. Also, Fc-chimeras of OMCP and IL2, and variants thereof may be used.

[0040] **FIG. 24A** and **FIG. 24B** depict the structure of OMCP in complex with NKG2D. (**FIG. 24A**) OMCP bound to NKG2D. OMCP is colored magenta and the protomers of NKG2D are colored cyan ("A") and yellow ("B"). $NKG2D^A$ makes contacts primarily with the H2a helix and $NKG2D^B$ with H2b. Mutations introduced to facilitate alternate crystal packing are shown in red. The S193-S194 bond is shown as a ball on each NKG2D protomer. The asparagines of putative hNKG2D glycosylation sites are shown in orange. The asparagine of the confirmed N-glycan site of OMCP is shown green (data not shown) (**FIG. 24B**) View of the interface between OMCP-NKG2D. The α2 domain of OMCP is shown in the front with the α1 domain behind. OMCP and NKG2D are shown with cartoon representations for the main chain, with the side chains of contact residues shown as sticks. Hydrogen bonds and salt bridges are indicated with green dotted lines.

[0041] **FIG. 25A, FIG. 25B** and **FIG. 25C** depicts the interface of OMCP and NKG2D. (**FIG. 25A**) The local environment of the OMCP-NKG2D binding interface surrounding the D132R residue. The D132R mutation ablates OMCP-NKG2D binding. (**FIG. 25B**) A representative experiment for binding of WT and (D132R) OMCP to NKG2D by SPR. 100 nM of OMCP or (D132R) OMCP were injected at 50 µl/min over flowcells containing immobilized biotinylated murine NKG2D. (**FIG. 25C**) Ba/F3 cells transduced with NKG2D, FCRL5, or empty vector were stained with OMCP tetramers (solid line), D132R tetramers (dashed line), or WNV DIII tetramer control (gray histogram). Representative results from three independent experiments.

[0042] **FIG. 26A, FIG. 26B, FIG. 26C** and **FIG. 26D** depict the differences in the β5'-β5 loop (L2) of human and murine NKG2D. (**FIG. 26A, FIG. 26B**) Superimposition of mNKG2D (grey) (PDB ID: 1HQ8) with the structure of OMCP-hNKG2D (yellow and cyan). Core binding residues Y152 (Y168) and Y199 (Y215) are positionally conserved, while core binding residue M184 (I200) is not. (**FIG. 26C**) Surface representation of OMCP (magenta) interacting with the β5'-β5 loop. (**FIG. 26D**) Conservation of M184 and Q185. Only the NKG2D of mice, rats, guinea pigs, and flying foxes (not shown) differ. Conservation score is as computed by the ConSurf server. Human, organgutan, chimpanzee, gibbon, macaque-SEQ ID NO:19; Green monkey-SEQ ID NO:20; Marmoset-SEQ ID NO:21; Mouse-SEQ ID NO:22; Rat-SEQ ID NO:23; Guinea pig-SEQ ID NO:24; Ground squirrel-SEQ ID NO:25; Deer mouse-SEQ ID NO:26; Naked mole rat-SEQ ID NO:27; Prairie vole-SEQ ID NO:28; European shrew-SEQ ID NO:29; Star-nosed mole-SEQ ID NO:30; Chinese hamster-SEQ ID NO:31; Cat-SEQ ID NO:32.

[0043] **FIG. 27A, FIG. 27B, FIG 27C, FIG. 27D, FIG. 27E, FIG. 27F, FIG. 27G, FIG. 27H** and **FIG. 27I** depict a novel NKG2D binding adaptation. Surface representation of NKG2D and surface and cartoon representations of OMCP, MICA and ULBP3. Buried surface areas for $NKG2D^{A}$ and $NKG2D^{B}$ are indicated in cyan and yellow, respectively. Buried surface area by NKG2D is indicated for OMCP (magenta), MICA (green), and ULBP3 (orange). The core binding residues of NKG2D and NKG2D-binding elements of NKG2DLs are indicated. NKG2D (**FIG. 27A**) and OMCP (**FIG. 27B, FIG. 27C**) binding interactions. NKG2D (**FIG. 27D**) and MICA (**FIG. 27E, FIG. 27F**)

binding interactions. NKG2D (**FIG. 27G**) and ULBP3 (**FIG. 27H, FIG. 27I**) binding interactions. (**FIG. 27J**) Alignment by secondary structure of NKG2DLs (PDB ID: OMCP (4FFE), MICA (1HYR), MICB (1JE6), ULBP3 (1KCG) and RAE-1β (1JSK)). Contact residues are indicated for OMCP (magenta), MICA (green), ULBP3 (orange) and RAE-1β (bold and italics). Secondary structure elements are noted above the sequence (arrow for beta sheets, cylinders for alpha helices). Predicted glycan sites are highlighted in black. OMCPbr=SEQ ID NO:13; OMCPmpx=SEQ ID NO:14; MICA=SEQ ID NO:15; MICB=SEQ ID NO:16; ULBP3=SEQ ID NO:17; and RAE-1B=SEQ ID NO:18

[0044] **FIG. 28A, FIG. 28B, FIG. 28C, FIG. 28D** and **FIG. 28E** depict activation of NK cells by cell-associated OMCP. Model depicting NKG2D interaction with (**FIG. 28A**) host, (**FIG. 28B**) cancer-induced, (**FIG. 28C**) viral, or (**FIG. 28D**) chimeric ligands. Binding interactions that lead to NKG2D-mediated signaling are indicated by DAP10 tyrosine phosphorylation (red filled circles). (**FIG. 28E**) IL-2-activated splenocytes were used as cytotoxic effectors against stably transduced Ba/F3 cell lines. Splenocytes were activated with 200 U/ml of IL-2 for 24 hours. Labeled target cells were co-incubated with activated splenocytes for 4 hours at effector:target ratios of 10:1, 20:1, and 40:1. Killing was measured by incorporation of 7AAD by CFSE-labeled target cells using flow cytometry. Representative data from five independent experiments is shown

[0045] **FIG. 29A** and **FIG. 29B** depict the electron density supporting a *cis* peptide conformation. Stereo view of the β5-β6 loop of hNKG2D. Residues 193-Ala-Ser-Ser-Phe-Lys-197 (SEQ ID NO:33) is displayed for the OMCP-hNKG2D structure (yellow) and the structure of hNKG2D alone (grey). The 2Fo-Fc map for OMCP-hNKG2D is displayed at 2σ.

[0046] **FIG. 30A** and **FIG. 30B** depicts graphs showing survival curves of C57Bl/6J mice following infection with West Nile Virus (WNV). Mice were treated with OMCP-IL2, OMCP(D132R)-IL2, IL2, IL(38R/42A) or PBS after infection with WNV. Infection with OMCP-IL2 and IL2(38R/42A) resulted in survival beyond 21 days in 40% of mice compared to 0 mice following treatment with PBS or OMCP(D132R)-IL2.

[0047] **FIG. 31A, FIG. 31B, FIG. 31C** and **FIG. 31D** depicts flow cytometry data showing that OMCP-Mutant IL2 activates NK and CD8+ T cells. **FIG. 31A** shows that a

relatively higher proportion of NK cells was evident in the OMCP-mutant IL2 group. **FIG. 31B** shows that perforin levels were higher in OMCP-mutant IL2 treated NK cells (red) compared to saline (black), IL2 (blue) or mutant IL2 (green) treated ones. **FIG. 31C** shows that similar to NK cells, higher intracellular levels of perforin were evident in CD8+ T cells treated with OMCP-mutant IL2 compared to other conditions. **FIG. 31D** shows that when gating on CD4+Foxp3+CD45RA- T cells a relatively higher proportion of activated CD25+CD127- regulatory T cells was evident in IL2 treated peripheral blood lymphocyte cultures compared to other conditions.

[0048] **FIG. 32** depicts a schematic of the various IL18-OMCP constructs. Three versions were made, each having OMCP attached to either WT human IL-18, WT murine IL-18, or mutant human IL-18 (which inhibits its interaction with IL-18BP).

[0049] **FIG. 33** depicts a flow cytometry plot showing that IL18-OMCP activates NK cells. Peripheral blood lymphocytes were cultured for 48 hours in 4.4 μM of either wild-type IL18 (blue), OMCP-IL18 (red) or saline (black). Activation of CD56+CD3- Natural killer cells, as measured by surface CD69 expression, was superior by OMCP-IL18 compared to wild-type IL18.

DETAILED DESCRIPTION OF THE INVENTION

[0050] The compositions and methods described herein provide for delivery of cytokines to a defined cell via a ligand. The fusion of a cytokine to a ligand which specifically binds to a protein on the target cell creates an “address” for delivery of the cytokine. Specifically, using the invention disclosed herein, IL2 is directly targeted to lymphocytes, such as natural killer (NK) cells and CD8+ cytotoxic T lymphocytes (CTLs), via the orthopoxvirus major histocompatibility complex class I-like protein (OMCP) ligand. However other NKG2D ligands, including but not limited to ULBP1, ULBP2, ULBP3, H60, Rae-1α, Rae-1β, Rae-1δ, Rae-1γ, MICA, MICB, h-HLA-A, could also be used instead of OMCP. Specific delivery of IL2 to lymphocytes will enhance the efficacy of IL2, which could lead to reduced dosages and a significant decrease in associated toxicity. This methodology may be used for other cytokines, including, but not limited to, IL15, IL18 and interferons.

[0051] Specific aspects of the invention are described in detail below.

I. COMPOSITION

[0052] In an aspect, the invention encompasses a composition comprising a cytokine linked to a ligand. The composition may further comprise a linker to connect the cytokine to the ligand. The cytokine, ligand and linker are described in greater detail below. It should be understood that any of the cytokines described in detail below can be linked to any of the ligands described in detail below in the absence or presence of any of the linkers described below. In another aspect, the invention provides a nucleic acid molecule encoding a cytokine, a ligand, and optionally a linker.

(a) cytokine

[0053] As used herein, a "cytokine" is a small protein (~5-20 kDa) that is important in cell signaling. Cytokines are released by cells and affect the behavior of other cells and/or the cells that release the cytokine. Non-limiting examples of cytokines include chemokines, interferons, interleukins, lymphokines, tumor necrosis factor, monokines, and colony stimulating factors. Cytokines may be produced by a broad range of cells including, but not limited to, immune cells such as macrophages, B lymphocytes, T lymphocytes, mast cells and monocytes, endothelial cells, fibroblasts and stromal cells. A cytokine may be produced by more than one type of cell. Cytokines act through receptors and are especially important in the immune system, modulate the balance between humoral and cell-based immune responses, and regulate maturation, growth and responsiveness of cell populations. Cytokines are important in host responses to infection, immune responses, inflammation, trauma, sepsis, cancer and reproduction. A cytokine of the invention may be a naturally occurring cytokine or may be a mutated version of a naturally occurring cytokine. As used herein, "naturally occurring", which may also be referred to as wild-type, includes allelic variances. A mutated version or "mutant" of a naturally occurring cytokine refers to specific mutations that have been made to the naturally occurring sequence to alter the function, activity and/or specificity of the cytokine. In one embodiment, the mutations may enhance the function, activity and/or specificity of the cytokine. In another embodiment, the mutations may decrease the function, activity and/or specificity of the cytokine. The mutation may include deletions or additions of one or more amino acid residues of the cytokine.

[0054] Cytokines may be classified based on structure. For example, cytokines may be classified into four types: the four-α-helix bundle family, the IL1 family, the IL17 family and the cysteine-knot cytokines. Members of the four-α-helix bundle family have three-dimensional structures with four bundles of α-helices. This family is further divided into three sub-families: the IL2 subfamily, the interferon (IFN) subfamily and the IL10 subfamily. The IL2 subfamily is the largest and comprises several non-immunological cytokines including, but not limited to, erythropoietin (EPO) and thrombopoietin (TPO). In certain embodiments, a cytokine of the composition is a cytokine from the four-α-helix bundle family or a mutant thereof. A skilled artisan would be able to determine cytokines within the four-α-helix bundle family. In other embodiments, a cytokine of the composition is an IL2 subfamily cytokine or a mutant thereof. Non-limiting examples of members of the IL2 subfamily include IL2, IL4, IL7, IL9, IL15 and IL21. In a specific embodiment, a cytokine of the composition is IL2 or a mutant thereof. In certain embodiments, a cytokine of the composition is IL15 or a mutant thereof. The sequence information for the full length human IL15 amino acid sequence can be found using, for example, the GenBank accession number CAG46777.1, AAI00962.1 or AAI00963.1. The sequence information for the full length human IL15 mRNA sequence can be found using, for example, the GenBank accession number CR542007.1, KJ891469.1, NM_172175.2, NM_000585.4 or CR541980.1. A skilled artisan will appreciate that IL15 may be found in a variety of species and methods of identifying analogs or homologs of IL15 are known in the art as described in detail below.

[0055] In another embodiment, a cytokine of the invention is an IL1 family cytokine or a mutant thereof. The IL1 family is a group of 11 cytokines, which plays a central role in the regulation of immune and inflammatory responses. Generally, the IL1 family of cytokines are proinflammatory cytokines that regulate and initiate inflammatory responses. Non-limiting examples of IL1 family cytokines include IL1α, IL1β, IL1Ra, IL18, IL36Ra, IL36α, IL37, IL36β, IL36γ, IL38, and IL33. IL1 family members have a similar gene structure. A skilled artisan would be able to determine cytokines within the IL1 family. In certain embodiments, a cytokine of the composition is IL18 or a mutant thereof. The sequence information for the full length human IL18 amino acid sequence

can be found using, for example, the GenBank accession number CAG46771.1. The sequence information for the full length human IL18 mRNA sequence can be found using, for example, the GenBank accession number KR710147.1, CR542001.1, CR541973.1 or KJ897054.1. A skilled artisan will appreciate that IL18 may be found in a variety of species and methods of identifying analogs or homologs of IL18 are known in the art as described in detail below.

[0056] In other embodiments, a cytokine of the composition is an interferon subfamily cytokine or a mutant thereof. Interferons are named for their ability to "interfere" with viral replication by protecting cells from virus infection. IFNs also have other functions: they activate immune cells, such as natural killer cells and macrophages; they increase host defenses by up-regulating antigen presentation by virtue of increasing the expression of major histocompatibility complex (MHC) antigens. Based on the type of receptor through which they signal, human interferons have been classified into three major types: Type I IFN, Type II IFN, and Type III IFN. Type I IFNs bind to a specific cell surface receptor complex known as the IFN-α/β receptor (IFNAR) that consists of IFNAR1 and IFNAR2 chains. Non-limiting examples of type I interferons present in humans are IFN-α, IFN-β, IFN-ε, IFN-κ and IFN-ω. Thus, in certain embodiments, a cytokine of the composition is a Type 1 IFN cytokine or a mutant thereof, including, but not limited to wild-type and mutant forms of IFN-α, IFN-β, IFN-ε, IFN-κ and IFN-ω. Type II IFNs bind to IFNGR that consists of IFNGR1 and IFNGR2 chains. Non-limiting examples of type II interferons present in humans is IFN-γ. Thus, in certain embodiments, a cytokine of the composition is a Type II IFN cytokine or a mutant thereof, including, but not limited to wild-type and mutant forms of IFN-γ. Type III IFNs signal through a receptor complex consisting of IL10R2 (also called CRF2-4) and IFNLR1 (also called CRF2-12). Non-limiting examples of type III interferons include IFN-λ1, IFN-λ2 and IFN-λ3 (also called IL29, IL28A and IL28B respectively). Thus, in certain embodiments, a cytokine of the composition is a Type III IFN cytokine or a mutant thereof, including, but not limited to wild-type and mutant forms of IFN-λ1, IFN-λ2 and IFN-λ3.

[0057] In certain embodiments, a cytokine of the invention is an interleukin or mutant thereof. The majority of interleukins are synthesized by helper CD4 T lymphocytes, as well as through monocytes, macrophages, and endothelial cells. Interleukins may promote the development and differentiation of T and B lymphocytes and hematopoietic cells. Non-limiting examples of interleukins include IL1, IL2, IL3, IL4, IL5, IL6, IL7, IL8 (CXCL8), IL9, IL10, IL11, IL12, IL13, IL14, IL15, IL16, IL17, IL18, IL19, IL20, IL21, IL22, IL23, IL24, IL25, IL26, IL27, IL28, IL29, IL30, IL31, IL32, IL33, IL35, or IL36. Thus, in certain embodiments, a cytokine of the composition is an interleukin or a mutant thereof, including, but not limited to wild-type and mutant forms of IL1, IL2, IL3, IL4, IL5, IL6, IL7, IL8 (CXCL8), IL9, IL10, IL11, IL12, IL13, IL14, IL15, IL16, IL17, IL18, IL19, IL20, IL21, IL22, IL23, IL24, IL25, IL26, IL27, IL28, IL29, IL30, IL31, IL32, IL33, IL35, or IL36. In a specific embodiment, a cytokine of the composition is IL2 or a mutant thereof. IL2 is a lymphokine that induces the proliferation of responsive T cells. In addition, it acts on some B cells, via receptor-specific binding, as a growth factor and antibody production stimulant. The IL2 protein is secreted as a single glycosylated polypeptide, and cleavage of a signal sequence is required for its activity. The structure of IL2 comprises a bundle of 4 helices (termed A-D), flanked by 2 shorter helices and several poorly defined loops. Residues in helix A, and in the loop region between helices A and B, are important for receptor binding. Secondary structure analysis suggests similarity to IL4 and granulocyte-macrophage colony stimulating factor (GMCSF). In a specific embodiment, a cytokine of the composition is IL2 or a variant thereof. A variant may be a truncated or mutated IL2. The sequence information for the full length human IL2 amino acid sequence can be found using, for example, the GenBank accession number AAA59140.1 or AAH70338.1. The sequence information for the full length human IL2 mRNA sequence can be found using, for example, the GenBank accession number BC070338.1 or M22005.1.

[0058] A skilled artisan will appreciate that IL2 may be found in a variety of species. Non-limiting examples include mouse (AAI16874.1), pig (NP_999026.1), cattle (AAQ10670.1), rat (EDM01295.1), rabbit (AAC23838.1), goat (AAQ10671.1), sheep (ABK41601.1), chicken (AAV35056.1), hamster (ERE88380.1), and dog (AAA68969.1).

It is appreciated that the present invention is directed to analogs of IL2 in other organisms and is not limited to the human analog. Homologs can be found in other species by methods known in the art. For example, sequence similarity may be determined by conventional algorithms, which typically allow introduction of a small number of gaps in order to achieve the best fit. In particular, "percent identity" of two polypeptides or two nucleic acid sequences is determined using the algorithm of Karlin and Altschul (Proc. Natl. Acad. Sci. USA 87:2264-2268, 1993). Such an algorithm is incorporated into the BLASTN and BLASTX programs of Altschul et al. (J. Mol. Biol. 215:403-410, 1990). BLAST nucleotide searches may be performed with the BLASTN program to obtain nucleotide sequences homologous to a nucleic acid molecule of the invention. Equally, BLAST protein searches may be performed with the BLASTX program to obtain amino acid sequences that are homologous to a polypeptide of the invention. To obtain gapped alignments for comparison purposes, Gapped BLAST is utilized as described in Altschul et al. (Nucleic Acids Res. 25:3389-3402, 1997). When utilizing BLAST and Gapped BLAST programs, the default parameters of the respective programs (e.g., BLASTX and BLASTN) are employed. See www.ncbi.nlm.nih.gov for more details. Generally a homolog will have a least 80, 81, 82, 83, 84, 85, 86, 87, 88, or 89% homology. In another embodiment, the sequence may be at least 90, 91, 92, 93, 94, 95, 96, 97, 98, 99, or 100% homologous to IL2.

[0059] In a specific embodiment, a cytokine of the composition is a wildtype sequence of IL2 such as the sequence set forth in SEQ ID NO:5 (APTSSSTKKTQLQLEHLLLDLQMILNGINNYKNPKLTRMLTFKFYMPKKATELKHLQCL EEELKPLEEVLNLAQSKNFHLRPRDLISNINVIVLELKGSETTFMCEYADETATIVEFLNR WITFCQSIISTLT). In an alternative embodiment, a cytokine is a mutated version of IL2. In an embodiment, a mutation is a mutation that causes IL2 to preferentially bind the receptor IL2$\beta\gamma$. In another embodiment, a mutation is a mutation that alters the function of IL2 such that IL2 has a decreased affinity for the IL2 receptor alpha (IL2Rα). For example, a mutation may be one or more mutations selected from the group consisting of R38A, F42K and/or C125S relative to SEQ ID NO:5. The C125S mutation may be included to reduce protein aggregation. In a specific embodiment, a mutated version of

IL2 comprises at least one mutation selected from the group consisting of R38A, F42K and C125S relative to SEQ ID NO:5. In another specific embodiment, a mutated version of IL2 comprises the mutations R38A, F42K and C125S relative to SEQ ID NO:5. In a specific embodiment, a cytokine of the composition is a mutated sequence of IL2 such as the sequence set forth in SEQ ID NO:6 (APTSSSTKKTQLQLEHLLLDLQMILNGINNYKNPKLTAMLTKKFYMPKKATELKHLQCLEEELKPLEEVLNLAQSKNFHLRPRDLISNINVIVLELKGSETTFMCEYADETATIVEFLNRWITFSQSIISTLT).

[0060] In an alternative aspect, a toxin is substituted for a cytokine. The term "toxin" means the toxic material or product of plants, animals, microorganisms (including, but not limited to, bacteria, viruses, fungi, rickettsiae or protozoa), or infectious substances, or a recombinant or synthesized molecule, whatever their origin and method of production. A toxin may be a small molecule, peptide, or protein that is capable of causing disease on contact with or absorption by body tissues interacting with biological macromolecules such as enzymes or cellular receptors. A toxin may be a “biotoxin” which is used to explicitly identify the toxin as from biological origin. Biotoxins may be further classified into fungal biotoxins, or short mycotoxins, microbial biotoxins, plant biotoxins, short phytotoxins and animal biotoxins. Non-limiting examples of biotoxins include: cyanotoxins, produced by cyanobacteria, such as microcystins, nodularins, anatoxin-a, cylindrospermopsins, lyngbyatoxin-a, saxitoxin, lipopolysaccharides, aplysiatoxins, BMAA; dinotoxins, produced by dinoflagellates, such as saxitoxins and gonyautoxins; necrotoxins produced by, for example, the brown recluse or "fiddle back" spider, most rattlesnakes and vipers, the puff adder, *Streptococcus pyogenes*; neurotoxins, produced by, for example, the black widow spider, most scorpions, the box jellyfish, elapid snakes, the cone snail, the Blue-ringed octopus, venomous fish, frogs, palythoa coral, various different types of algae, cyanobacteria and dinoflagellates, such as botulinum toxin (e.g. Botox), tetanus toxin, tetrodotoxin, chlorotoxin, conotoxin, anatoxin-a, bungarotoxin, caramboxin, curare; myotoxins, found in, for example, snake and lizard venoms; and cytotoxins such as ricin, from castor beans, apitoxin, from honey bees, and T-2 mycotoxin, from certain

toxic mushrooms. In certain embodiments, a toxin is a cytotoxin. In an embodiment, a cytotoxin is selected from the group consisting of ricin, apitoxin, and T-2 mycotoxin. In a specific embodiment, a toxin is ricin.

[0061] In certain embodiments, a cytokine or toxin of the invention may be PEGylated for improved systemic half-life and reduced dosage frequency. In an embodiment, PEG may be added to a cytokine or toxin. As such, a composition of the invention may comprise a cytokine or toxin comprising PEG. In an embodiment, PEG may be selected from the group consisting of PEG-10K, PEG-20K and PEG-40K. Methods of conjugating PEG to a protein are standard in the art. For example, see Kolate et al, *Journal of Controlled Release* 2014; 192(28): 67-81, which is hereby incorporated by reference in its entirety. Still further, a cytokine or toxin of the invention may be modified to remove T cell epitopes. T cell epitopes can be the cause of an immunogenicity issue upon administration of a composition to a subject. Through their presentation to T cells, they activate the process of anti-drug antibody development. Preclinical screening for T cell epitopes may be performed *in silico*, followed by *in vitro* and *in vivo* validation. T cell epitope-mapping tools such as EpiMatrix can be highly accurate predictors of immune response. Deliberate removal of T cell epitopes may reduce immunogenicity. Other means of improving the safety and efficacy of a composition of the invention by reducing their immunogenicity include humanization and PEGylation.

(b) ligand

[0062] As used herein, a “ligand” is a protein that specifically binds to a receptor on a target cell and is not the corresponding binding partner to the cytokine linked to the ligand. A ligand may be from a eukaryote, a prokaryote or a virus. In certain embodiments, a ligand may be from a virus. The phrase "specifically binds" herein means ligands bind to the target protein with an affinity (K_d) in the range of at least 0.1 mM to 1 pM, or in the range of at least 0.1 pM to 200 nM, or in the range of at least 0.1 pM to 10 nM. A dissociation constant (K_d) measures the propensity of a larger object to separate (dissociate) reversibly into smaller components. The dissociation constant is the inverse of the association constant. The dissociation constant may be used to

describe the affinity between a ligand (L) and a target protein (P). As such, K_d = ([P] x [L]) / [C], wherein C is a ligand-target protein complex and wherein [P], [L] and [C] represent molar concentrations of the protein, ligand and complex, respectively. Methods of determining whether a ligand binds to a target protein are known in the art. For instance, see the Rossi and Taylor, *Nature Protocols* 2011; 6: 365-387.

[0063] A ligand may trigger a signal through its binding to a receptor on a target cell. A receptor is a protein molecule that may be embedded within the plasma membrane surface of a cell that receives chemical signals from outside the cell. When such chemical signals bind to a receptor, they cause some form of cellular/tissue response. In preferred embodiments, a target cell is an immune cell. Accordingly, a ligand of the composition binds to a receptor expressed on immune cells. Non-limiting example of immune cells include macrophages, B lymphocytes, T lymphocytes, mast cells, monocytes, dendritic cells, eosinophils, natural killer cells, basophils, neutrophils. Thus, in certain embodiments, immune cells include, but are not limited to, macrophages, B lymphocytes, T lymphocytes, mast cells, monocytes, dendritic cells, eosinophils, natural killer cells, basophils, neutrophils. In a specific embodiment, an immune cell is a natural killer cell or a T lymphocyte. Non-limiting examples of receptors expressed on immune cells include major histocompatibility complex (MHC; e.g. MHCI, MHCII, and MHCIII), toll-like receptors (TLRs; e.g. TLR1, TLR2, TLR3, TLR4, TLR5, TLR6, TLR7, TLR8, TLR9, TLR10, TLR11, TLR12, and TLR13), CD94/NKG2 family receptor, endothelin receptors, signaling lymphocytic activation molecule (SLAM) family of receptors. Thus, in certain embodiments, a receptor on a target cell includes, but is not limited to, major histocompatibility complex (MHC; e.g. MHCI, MHCII, and MHCIII), toll-like receptors (TLRs; e.g. TLR1, TLR2, TLR3, TLR4, TLR5, TLR6, TLR7, TLR8, TLR9, TLR10, TLR11, TLR12, and TLR13), CD94/NKG2 family receptor, endothelin receptors, signaling lymphocytic activation molecule (SLAM) family of receptors. In a specific embodiment, the receptor on a target cell is a CD94/NKG2 family receptor. In another specific embodiment, a ligand of the composition specifically binds to a receptor expressed on natural killer (NK) cells and CD8+ cytotoxic T lymphocytes (CTLs). In

preferred embodiments, a ligand of the composition does not specifically bind to a receptor on vascular endothelial cells or regulatory T cells (T_{regs}).

[0064] A receptor expressed on NK cells and CTLs may be a CD94/NKG2 family receptor or KLRG1. KLRG1 (Killer cell lectin-like receptor subfamily G member 1) is a protein that in humans is encoded by the KLRG1 gene. CD94/NKG2 family receptors are a family of C-type lectin receptors which are expressed predominantly on the surface of NK cells and a subset of CD8+ T-lymphocyte. These receptors stimulate or inhibit cytotoxic activity of NK cells, therefore they are divided into activating and inhibitory receptors according to their function. CD94/NKG2 recognize MHC class I-related glycoproteins. CD94/NKG2 family includes seven members: NKG2A, NKG2B, NKG2C, NKG2D, NKG2E, NKG2F and NKG2H. Thus, in certain embodiments, a ligand of the invention specifically binds to a receptor selected from the group consisting of NKG2A, NKG2B, NKG2C, NKG2D, NKG2E, NKG2F and NKG2H. NKG2 receptors are transmembrane proteins type II which dimerize with CD94 molecule. CD94 contains a short cytoplasmic domain and it is responsible for signal transduction. Therefore NKG2 receptors form disulfide bonded heterodimers. NKG2D represents an exception, it is a homodimer. NKG2A and NKG2B receptors transmit inhibitory signal. NKG2C, NKG2E and NKG2H are activating receptors. NKG2D is activating receptor as well but it couples with adaptor protein DAP10 which carries signaling motif YINM (SEQ ID NO:34). Src or Jak kinases phosphorylate DAP10, which can then associate with p85 subunit of PI(3)K or adaptor molecule Grb2. This signaling triggers actin reorganization (cell polarization) and degranulation. NKG2F receptor function has not been clarified yet.

[0065] In a specific embodiment, a ligand of the composition specifically binds to the NKG2D receptor. NKG2D is an activating receptor found on NK cells and CD8+ T cells (both αβ and γδ). The structure of NKG2D consists of two disulphide-linked type II transmembrane proteins with short intracellular domains incapable of transducing signals. The function of NKG2D on CD8+ T cells is to send co-stimulatory signals to activate them. In an embodiment, a ligand that binds to NKG2D may be an anti-NKG2D antibody. An “anti-NKG2D” includes all antibodies that specifically bind an epitope within NKG2D. The term “antibody’ includes the term “monoclonal antibody”. “Monoclonal

antibody" refers to an antibody that is derived from a single copy or clone, including e.g., any eukaryotic, prokaryotic, or phage clone. Monoclonal antibodies can be produced using e.g., hybridoma techniques well known in the art, as well as recombinant technologies, phage display technologies, synthetic technologies or combinations of such technologies and other technologies readily known in the art. Further by "antibody" is meant a functional monoclonal antibody, or an immunologically effective fragment thereof; such as an Fab, Fab', or F(ab')2 fragment thereof. As long as the protein retains the ability specifically to bind its intended target, it is included within the term "antibody." Also included within the definition "antibody" for example are single chain forms, generally designated Fv, regions, of antibodies with this specificity. These scFvs are comprised of the heavy and light chain variable regions connected by a linker. Methods of making and using scFvs are known in the art. Additionally, included within the definition "antibody" are single-domain antibodies, generally designated sdAb, which is an antibody fragment consisting of a single monomeric variable antibody domain. A sdAb antibody may be derived from camelids (V_HH fragments) or cartilaginous fishes (V_{NAR} fragments). As used herein "humanized antibody" includes an anti-NKG2D antibody that is composed partially or fully of amino acid sequence sequences derived from a human antibody germline by altering the sequence of an antibody having non-human complementarity determining regions ("CDR"). The simplest such alteration may consist simply of substituting the constant region of a human antibody for the murine constant region, thus resulting in a human/murine chimera which may have sufficiently low immunogenicity to be acceptable for pharmaceutical use. Preferably, however, the variable region of the antibody and even the CDR is also humanized by techniques that are by now well known in the art. The framework regions of the variable regions are substituted by the corresponding human framework regions leaving the non-human CDR substantially intact, or even replacing the CDR with sequences derived from a human genome. CDRs may also be randomly mutated such that binding activity and affinity for NKG2D is maintained or enhanced in the context of fully human germline framework regions or framework regions that are substantially human. In certain embodiments, an anti-NKG2D antibody is a Fab, Fab', or F(ab')2 fragment.

[0066] In another embodiment, ligands that bind to NKG2D share an MHC class I-related $\alpha1\alpha2$ superdomain that constitutes the common site for interaction with NKG2D. Non-limiting examples of ligands that bind to NKG2D include MHC class I-related glycoproteins such as MIC family proteins (i.e., MICA, MICB), UL16-binding family proteins (i.e., ULBP1, ULBP2, ULPB3, ULBP4, ULBP5, ULBP6), retinoid acid early induce gene 1 (Rae1)-like proteins (i.e., Rae1α, Rae1β, Rae1γ, Rae1δ, Rae1ε), members of the H60 protein family (i.e., H60a, H60b, H60c), h-HLA-A, as well as Mult1 in mice and orthopoxvirus major histocompatibility complex class I-like protein (OMCP). In certain embodiments, a ligand is a MHC class-I-related glycoprotein. In other embodiments, a ligand of the invention is selected from the group consisting of MICA, MICB, ULBP1, ULBP2, ULBP3, ULBP4, ULBP5, ULBP6, Rae1α, Rae1β, Rae1γ, Rae1δ, Rae1ε, H60a, H60b, H60c, h-HLA-A, Mult1 and OMCP. In an embodiment, a ligand is a UL16-binding family protein or a MIC family protein. In a specific embodiment, a ligand is selected from the group consisting of ULBP1, ULBP2, ULBP3, ULBP4, ULBP5, and ULBP6. In another specific embodiment, a ligand is ULBP3. In a specific embodiment, a ligand is orthopoxvirus major histocompatibility complex class I-like protein (OMCP) or a variant thereof. A variant may be a truncated or mutated OMCP that has about the same binding affinity of the full length OMCP. In an embodiment, a variant may be a truncated or mutated OMCP that has a slightly lower binding affinity relative to the binding affinity of the full length OMCP. In another embodiment, a variant is a truncated or mutated OMCP that has a slightly higher binding affinity relative to the binding affinity of the full length OMCP. Methods to determine binding affinity of a ligand to target protein are known in the art and described above. OMCP specifically binds to NKG2D with a binding affinity of about 0.1 to about 5 nM. For example, OMCP specially binds to human NKG2D with a binding affinity of about 0.2 nM and mouse NKG2D with a binding affinity of about 3 nM. In a preferred embodiment, OMCP or a variant thereof binds to human NKG2D with a binding affinity of about 1000 nM to about 0.1 nM. In certain embodiments, OMCP or a variant thereof binds to human NKG2D with a binding affinity of about 100 nM to about 0.1 nM, about 10 nM to about 0.1 nM, or about 1 nM to about 0.1 nM. In other embodiments, OMCP or a variant thereof binds to human NKG2D with

a binding affinity of about 1000 nM to about 1 nM, or about 1000 nM to about 10 nM, or about 1000 nM to about 100 nM. In still other embodiments, OMCP or a variant thereof binds to human NKG2D with a binding affinity of about 100 nM to about 1 nM, or about 100 nM to 10 nM. For example, OMCP or a variant thereof binds to human NKG2D with a binding affinity of about 1000 nM, about 500 nM, about 100 nM, about 50 nM, about 10 nM, about 9 nM, about 8 nM, about 7 nM, about 6 nM about 5 nM, about 4 nM, about 3 nM, about 2 nM, about 1 nM, about 0.9 nM, about 0.8 nM, about 0.7 nM, about 0.6 nM, about 0.5 nM, about 0.4 nM, about 0.3 nM, about 0.2 nM or about 0.1 nM. In another embodiment, a variant is a truncated or mutated OMCP that has binding affinity for one or more NKG2 family receptors other than NKG2D. For example, a variant is a truncated or mutated OMCP that has binding affinity for one or more NKG2 family receptors selected from the group consisting of NKG2A, NKG2B, NKG2C, NKG2E, NKG2F and NKG2H. Mutations to OMCP may be rationally selected via structure-based knowledge or mutations to OMCP may be identified via selection-based mutagenesis. In certain embodiments, mutations may be rationally selected to occur in the OMCP-NKG2D interface to either enhance or reduce binding affinity. Amino acids involved in binding at the OMCP-NKG2D interface are described in the Examples.

[0067] The structure of OMCP consists of an MHCI-like α1/α2 platform domain (**FIG. 20A**). The platform domain of OMCP has been trimmed to have only a six-stranded beta sheet with shorter flanking helices. The helix of the OMCP α1 domain (H1) is continuous, while the helix of the α2 domain is broken into two regions (H2a and H2b). The helices flank a six-stranded beta sheet and together form the characteristic platform that defines MHC proteins. Like other NKG2DLs (**FIG. 20B**), the alpha helices of OMCP are close together and thus have no groove for binding peptides or other ligands like antigen-presenting MHC platform domains. OMCP contains one disulfide bond between S5 and H2b, and this disulfide bond is conserved in most NKG2DLs (**FIG. 20C**). In certain embodiments, a ligand of the invention comprises one or more of the α helices of a MHC class I-related glycoprotein. In other embodiments, a ligand of the invention consists of one or more of the α helices of a MHC class I-related glycoprotein. More specifically, a ligand of the invention comprises the α1 domain (H1),

α2 domain (H2), H2a, H2b, or combinations thereof of a MHC class I-related glycoprotein. Or, a ligand of the invention consists of the α1 domain (H1), α2 domain (H2), H2a, H2b, or combinations thereof of a MHC class I-related glycoprotein. In a specific embodiment, a ligand of the invention comprises the α2 domain (H2) of a MHC class I-related glycoprotein. In another specific embodiment, a ligand of the invention consists of the α2 domain (H2) of a MHC class I-related glycoprotein. A skilled artisan would be able to determine the location of the α helices in other MHC class I-related glycoproteins, for example, using sequence alignment (see **FIG. 20C**, which is reproduced from Lazear et al. *J Virol* 2013; 87(2): 840-850, which is hereby incorporated by reference in its entirety). In an embodiment, a ligand of the invention comprises one or more of the α helices of OMCP. In another embodiment, a ligand of the invention comprises the α1 domain (H1), α2 domain (H2), H2a, H2b, or combinations thereof of OMCP. In still another embodiment, a ligand of the invention comprises the α2 domain (H2) of OMCP. In a specific embodiment, a ligand of the invention consists of one or more of the α helices of OMCP. In another specific embodiment, a ligand of the invention consists of the α1 domain (H1), α2 domain (H2), H2a, H2b, or combinations thereof of OMCP. In still another specific embodiment, a ligand of the invention consists of the α2 domain (H2) of OMCP.

[0068] The sequence information for the full length OMCP amino acid sequence can be found using, for example, the GenBank accession number 4FFE_Z, 4FFE_Y or 4FFE_X. A skilled artisan will appreciate that homologs of OMCP may be found in other species or viruses. For example, see Lefkowitz et al, *Nucleic Acids* Res 2005; 33: D311-316, which is herein incorporated by reference in its entirety, which describes eighteen OMCP variants between cowpox and monkeypox virus strains. In an embodiment, OMCP is from an orthopoxvirus. In a specific embodiment, OMCP is from a cowpox virus or a monkeypox virus. In another specific embodiment, OMCP is from the Brighton Red strain of cowpoxvirus. Homologs can be found in other species by methods known in the art. For example, sequence similarity may be determined by conventional algorithms, which typically allow introduction of a small number of gaps in order to achieve the best fit. In particular, "percent identity" of two polypeptides or two nucleic

acid sequences is determined using the algorithm of Karlin and Altschul (Proc. Natl. Acad. Sci. USA 87:2264-2268, 1993). Such an algorithm is incorporated into the BLASTN and BLASTX programs of Altschul et al. (J. Mol. Biol. 215:403-410, 1990). BLAST nucleotide searches may be performed with the BLASTN program to obtain nucleotide sequences homologous to a nucleic acid molecule of the invention. Equally, BLAST protein searches may be performed with the BLASTX program to obtain amino acid sequences that are homologous to a polypeptide of the invention. To obtain gapped alignments for comparison purposes, Gapped BLAST is utilized as described in Altschul et al. (Nucleic Acids Res. 25:3389-3402, 1997). When utilizing BLAST and Gapped BLAST programs, the default parameters of the respective programs (e.g., BLASTX and BLASTN) are employed. See www.ncbi.nlm.nih.gov for more details. Generally a homolog will have a least 80, 81, 82, 83, 84, 85, 86, 87, 88, or 89% homology. In another embodiment, the sequence may be at least 90, 91, 92, 93, 94, 95, 96, 97, 98, 99, or 100% homologous to OMCP.

[0069] A skilled artisan will appreciate that structural homologs of OMCP may be found in other species or viruses. A structural homolog may be a protein that is structurally related but the sequence is a distal homolog. For example, OMCP has low sequence identity for endogenous NKG2D ligands however it was discovered that OMCP would bind to NKG2D based on structural homology. Structural homologs can be found in other species by methods known in the art. For example, protein structure prediction may be determined by various databases, such as Phyre and Phyre2. Such databases generate reliable protein models that may be used to determine structural homologs. The main results table in Phyre2 provides confidence estimates, images and links to the three-dimensional predicted models and information derived from either Structural Classification of Proteins database (SCOP) or the Protein Data Bank (PDB) depending on the source of the detected template. For each match a link takes the user to a detailed view of the alignment between the user sequence and the sequence of known three-dimensional structure. See www.sbg.bio.ic.ac.uk/phyre2/ for more details. Generally, a structural homolog will have a least 50, 51, 52, 53, 54, 55, 56, 57, 58, or 59% confidence with OMCP. In an embodiment, a structural homolog will have a least

60, 61, 62, 63, 64, 65, 66, 67, 68, or 69% confidence with OMCP. In another embodiment, a structural homolog will have a least 70, 71, 72, 73, 74, 75, 76, 77, 78, or 79% confidence with OMCP. In still another embodiment, a structural homolog will have a least 80, 81, 82, 83, 64, 85, 86, 87, 88, or 89% confidence with OMCP. In still yet another embodiment, a structural homolog may have at least 90, 91, 92, 93, 94, 95, 96, 97, 98, 99, or 100% confidence with OMCP. The structural information for OMCP-human NKG2D may be found using the PDB ID: 4PDC.

[0070] In a specific embodiment, a ligand of the composition is a sequence of OMCP such as the sequence set forth in SEQ ID NO:7 (HKLAFNFNLEINGSDTHSTVDVYLDDSQIITFDGKDIRPTIPFMIGDEIFLPFYKNVFSEFFSLFRRVPTSTPYEDLTYFYECDYTDNKSTFDQFYLYNGEEYTVKTQEATNKNMWLTTSEFRLKKWFDGEDCIMHLRSLVRKMEDSKRNT). In an embodiment, a ligand of the composition is a sequence of OMCP comprising at least 80% identity to SEQ ID NO:7. For example, the ligand may have about 80%, about 81%, about 82%, about 83%, about 84%, about 85%, about 86%, about 87%, about 88%, about 89%, about 90%, about 91%, about 92%, about 93%, about 94%, about 95%, about 96%, about 97%, about 98%, about 99%, or about 100% identity to SEQ ID NO:7.

[0071] In another specific embodiment, a ligand of the composition is a sequence of OMCP such as the sequence set forth in SEQ ID NO:13 (GHKLAFNFNLEINGSDTHSTVDVYLDDSQIITFDGKDIRPTIPFMIGDEIFLPFYKNVFSEFFSLFRRVPTSTPYEDLTYFYECDYTDNKSTFDQFYLYNGEEYTVKTQEATNKNMWLTTSEFRLKKWFDGEDCIMHLRSLVRKMEDSKR). In an embodiment, a ligand of the composition is a sequence of OMCP comprising at least 80% identity to SEQ ID NO:13. For example, the ligand may have about 80%, about 81%, about 82%, about 83%, about 84%, about 85%, about 86%, about 87%, about 88%, about 89%, about 90%, about 91%, about 92%, about 93%, about 94%, about 95%, about 96%, about 97%, about 98%, about 99%, or about 100% identity to SEQ ID NO:13.

[0072] In still another specific embodiment, a ligand of the composition is a sequence of OMCP such as the sequence set forth in SEQ ID NO:14 (HKLVHYFNLKINGSDITNTADILLDNYPIMTFDGKDIYPSIAFMVGNKLFLDLYKNIFVEFFRLFRVSVSSQYEELEYYYSCDYTNNRPTIKQHYFYNGEEYTEIDRSKKATNKNSWLIT

SGFRLQKWFDSEDCIIYLRSLVRRMEDSNK). In an embodiment, a ligand of the composition is a sequence of OMCP comprising at least 80% identity to SEQ ID NO:14. For example, the ligand may have about 80%, about 81%, about 82%, about 83%, about 84%, about 85%, about 86%, about 87%, about 88%, about 89%, about 90%, about 91%, about 92%, about 93%, about 94%, about 95%, about 96%, about 97%, about 98%, about 99%, or about 100% identity to SEQ ID NO:14.

[0073] In an alternative aspect, a receptor expressed on immune cells may be PD1. PD1, also known as programmed cell death protein 1 and CD279 (cluster of differentiation 279), is a protein that in humans is encoded by the PDCD1 gene. PD1 is a cell surface receptor that belongs to the immunoglobulin superfamily and is expressed on T cells and pro-B cells. PD1 binds two ligands, PDL1 and PDL2. PD1, functioning as an immune checkpoint, plays an important role in down regulating the immune system by preventing the activation of T-cells. In certain embodiments, a ligand of the composition specifically binds to PD1. In an embodiment, a ligand that specifically binds to PD1 may be an anti-PD1 antibody. An "anti-PD1" includes all antibodies that specifically bind an epitope within PD1. The term "antibody" is described above. In another embodiment, a ligand that specifically binds to PD1 may be PDL1. PDL1 (programmed death-ligand 1also known as cluster of differentiation 274 (CD274) or B7 homolog 1 (B7-H1), is a protein that in humans is encoded by the CD274 gene. PDL1 binds to its receptor, PD1, found on activated T cells, B cells, and myeloid cells, to modulate activation or inhibition. The affinity between PDL1 and PD1, as defined by the dissociation constant K_d, is 770nM.

[0074] In another aspect, a ligand of the composition may be Glucocorticoid-induced TNFR-related (GITR) ligand (GITRL). GITR activation by GITRL influences the activity of effector and regulatory T cells, thus participating in the development of immune response against tumors and infectious agents, as well as in autoimmune and inflammatory diseases. GITR triggering stimulates T effector activity and inhibits Treg activity. GITR inhibition may ameliorate autoimmune/inflammatory diseases whereas GITR activation may treat viral, bacterial and parasitic infections, as well as boost

immune responses against tumors. GITRL is a type II transmembrane protein expressed at high levels on antigen presenting cells (APC) and endothelial cells.

[0075] In certain embodiments, a ligand of the invention is modified for improved systemic half-life and reduced dosage frequency. In an embodiment, N-glycans may be added to a ligand. While the biological function is typically determined by the protein component, carbohydrate can play a role in molecular stability, solubility, *in vivo* activity, serum half-life, and immunogenicity. The sialic acid component of carbohydrate in particular, can extend the serum half-life of protein therapeutics. Accordingly, new N-linked glycosylation consensus sequences may be introduced into desirable positions in the peptide backbone to generate proteins with increased sialic acid containing carbohydrate, thereby increasing *in vivo* activity due to a longer serum half-life. In another embodiment, PEG may be added to a ligand. Methods of conjugating PEG to a protein are standard in the art. For example, see Kolate et al, *Journal of Controlled Release* 2014; 192(28): 67-81, which is hereby incorporated by reference in its entirety. In an embodiment, a composition of the invention may comprise a ligand comprising PEG and/or one or more N-glycans. In an embodiment, PEG is selected from the group consisting of PEG-10K, PEG-20K and PEG-40K. Still further, a ligand of the invention may be modified to remove T cell epitopes. T cell epitopes can be the cause of an immunogenicity issue upon administration of a composition to a subject. Through their presentation to T cells, they activate the process of anti-drug antibody development. Preclinical screening for T cell epitopes may be performed *in silico*, followed by *in vitro* and *in vivo* validation. T cell epitope-mapping tools such as EpiMatrix can be highly accurate predictors of immune response. Deliberate removal of T cell epitopes may reduce immunogenicity. Other means of improving the safety and efficacy of a composition of the invention by reducing their immunogenicity include humanization and PEGylation.

(c) linker

[0076] In an aspect, a composition of the invention further comprises a linker. The linker may be used to connect the cytokine to the ligand. It is to be understood that linking the cytokine to the ligand will not adversely affect the function of the cytokine or

the ligand. Suitable linkers include amino acid chains and alkyl chains functionalized with reactive groups for coupling to both the cytokine and the ligand or combinations thereof.

[0077] In an embodiment, the linker may include amino acid side chains, referred to as a peptide linker. Amino acid residue linkers are usually at least one residue and can be 50 or more residues, but alone do not specifically bind to the target protein. In an embodiment, a linker may be about 1 to about 10 amino acids. In another embodiment, a linker may be about 10 to about 20 amino acids. In still another embodiment, a linker may be about 20 to about 30 amino acids. In still yet another embodiment, a linker may be about 30 to about 40 amino acids. In different embodiments, a linker may be about 40 to about 50 amino acids. In other embodiments, a linker may be more than 50 amino acids. For instance, a linker may be 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, 31, 32, 33, 34, 35, 36, 37, 38, 39, 40, 41, 42, 43, 44, 45, 46, 47, 48, 49 or 50 amino acids. In a specific embodiment, a linker is about 20 to about 30 amino acids. In another specific embodiment, a linker is about 26 amino acids.

[0078] Any amino acid residue may be used for the linker provided the linker does not specifically bind to the target protein. Typical amino acid residues used for linking are glycine, serine, alanine, leucine, tyrosine, cysteine, lysine, glutamic and aspartic acid, or the like. For example, a linker may be $(AAS)_n$, $(AAAL)_n$, $(G_nS)_n$ or $(G_2S)_n$, wherein A is alanine, S is serine, L is leucine, and G is glycine and wherein n is an integer from 1-20, or 1-10, or 3-10. Accordingly, n may be 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19 or 20. Thus, in certain embodiments, a linker includes, but is not limited to, $(AAS)_n$, $(AAAL)_n$, $(G_nS)_n$ or $(G_2S)_n$, wherein A is alanine, S is serine, L is leucine, and G is glycine and wherein n is an integer from 1-20, or 1-10, or 3-10. A linker may comprise one or more epitope tags. For instance, a linker may comprise 1, 2, 3, 4, 5, 6, 7 or 8 epitope tags. In a specific embodiment, a linker comprises 2 epitope tags. Non-limiting examples of epitope tags include FLAG tag (DYKDDDK epitope (SEQ ID NO:9)), HA tag (YPYDVPDYA epitope (SEQ ID NO:10)), His tag (6x-His or 8x-His), Myc tag (EQKLISEEDL epitope (SEQ ID NO:11)) and V5 tag (GKPIPNPLLGLDST

epitope (SEQ ID NO:12)). In an embodiment, a linker may comprise at least one tag selected from the group consisting of a FLAG tag and a His tag. In a specific embodiment, a linker comprises a FLAG tag and a His tag. In another specific embodiment, a linker comprises the sequence set forth in SEQ ID NO:8 (GSSGSSDYKDDDDKHHHHHHHHHGSSGSS).

[0079] In another embodiment, an alkyl chain linking group may be coupled to the cytokine by reacting the terminal amino group or the terminal carboxyl group with a functional group on the alkyl chain, such as a carboxyl group or an activated ester. Subsequently the ligand is attached to the alkyl chain to complete the formation of the complex by reacting a second functional group on the alkyl chain with an appropriate group on the ligand. The second functional group on the alkyl chain is selected from substituents that are reactive with a functional group on the ligand while not being reactive with the cytokine. For example, when the ligand incorporates a functional group, such as a carboxyl group or an activated ester, the second functional group of the alkyl chain linking group can be an amino group or vice versa. It will be appreciated that formation of the conjugate may require protection and deprotection of the functional groups present in order to avoid formation of undesired products. Protection and deprotection are accomplished using protecting groups, reagents, and protocols common in the art of organic synthesis. Particularly, protection and deprotection techniques employed in solid phase peptide synthesis may be used. It will be appreciated that linking groups may alternatively be coupled first to the ligand and then to the cytokine.

[0080] An alternative chemical linking group to an alkyl chain is polyethylene glycol (PEG), which is functionalized in the same manner as the alkyl chain described above. Such a linker may be referred to as a heterobifunctional PEG linker or a homobifunctional PEG linker. Non-limiting examples of heterobifunctional PEG linkers include: O-(2-Aminoethyl)-O′-[2-(biotinylamino)ethyl]octaethylene glycol; O-(2-Aminoethyl)-O′-(2-carboxyethyl)polyethylene glycol hydrochloride M_p 3000; O-(2-Aminoethyl)-O′-(2-carboxyethyl)polyethylene glycol 5,000 hydrochloride M_p 5,000; O-(2-Aminoethyl)polyethylene glycol 3,000 Mp 3,000; O-(2-Aminoethyl)-O′-(2-

(succinylamino)ethyl)polyethylene glycol hydrochloride M_p 10,000; O-(2-Azidoethyl)heptaethylene glycol; O-[2-(Biotinylamino)ethyl]-O′-(2-carboxyethyl)undecaethylene glycol; 21-[D(+)-Biotinylamino]-4,7,10,13,16,19-hexaoxaheneicosanoic acid; O-(2-Carboxyethyl)-O′-[2-(Fmoc-amino)-ethyl]heptacosaethylene glycol; O-(2-Carboxyethyl)-O′-(2-mercaptoethyl)heptaethylene glycol; O-(3-Carboxypropyl)-O′-[2-(3-mercaptopropionylamino)ethyl]-polyethylene glycol M_w 3000; O-(3-Carboxypropyl)-O′-[2-(3-mercaptopropionylamino)ethyl]-polyethylene glycol M_w 5000; O-[N-(3-Maleimidopropionyl)aminoethyl]-O′-[3-(N-succinimidyloxy)-3-oxopropyl]heptacosaethylene glycol; and O-[2-(3-Tritylthiopropionylamino)ethyl]polyethylene glycol M_p 3,000. Non-limiting examples of homobifunctional PEG linkers include: MAL-PEG-MAL (Bifunctional Maleimide PEG Maleimide); OPSS-PEG-OPSS (OPSS: orthopyridyl disulfide; PDP-PEG-PDP); HS-PEG-SH (Bifunctional Thiol PEG Thiol); SG-PEG-SG (Bifunctional PEG Succinimidyl Glutarate NHS ester); SS-PEG-SS (Bifunctional PEG Succinimidyl Succinate NHS ester); GAS-PEG-GAS (Bifunctional PEG Succinimidyl ester NHS-PEG-NHS); SAS-PEG-SAS (Bifunctional PEG Succinimidyl ester NHS-PEG-NHS); Amine-PEG-Amine (Bifunctional PEG Amine NH2-PEG-NH2); AC-PEG-AC (Bifunctional Acrylate PEG Acrylate); ACA-PEG-ACA (Bifunctional Polymerizable PEG Acrylate Acrylamide); Epoxide-PEG-Epoxide (Bifunctional PEG Epoxide or EP); NPC-PEG-NPC (Bifunctional NPC PEG, Nitrophenyl Carbonate); Aldehyde-PEG-Aldehyde (ALD-PEG-ALD, bifunctional PEG propionaldehyde); AA-PEG-AA (Acid-PEG-Acid, AA - acetic acid or carboxyl methyl); GA-PEG-GA (Acid - PEG - Acid, GA: Glutaric acid); SA-PEG-SA (Bifunctional PEG carboxylic acid - Succinic Acid); GAA-PEG-GAA (Bifunctional PEG carboxylic acid, Glutaramide Acid); SAA-PEG-SAA (Bifunctional PEG carboxylic acid, Succinamide Acid); Azide-PEG-Azide (Bifunctional PEG azide, N3-PEG-N3); Alkyne-PEG-Alkyne (Bifunctional alkyne or acetylene PEG); Biotin-PEG-Biotin (Bifunctional biotin PEG linker); Silane-PEG-Silane (Bifunctional silane PEG); Hydrazide-PEG-Hydrazide (Bifunctional PEG Hydrazide); Tosylate-PEG-Tosylate (Bifunctional PEG Tosyl); and Chloride-PEG-Chloride (Bifunctional PEG Halide).

[0081] In certain embodiments, a linker of the invention may be modified for improved systemic half-life and reduced dosage frequency. In an embodiment, N-glycans are added to a linker. While the biological function is typically determined by the protein component, carbohydrates can play a role in molecular stability, solubility, *in vivo* activity, serum half-life, and immunogenicity. The sialic acid component of carbohydrate in particular, can extend the serum half-life of protein therapeutics. Accordingly, new N-linked glycosylation consensus sequences may be introduced into desirable positions in the peptide backbone to generate proteins with increased sialic acid containing carbohydrate, thereby increasing *in vivo* activity due to a longer serum half-life. In another embodiment, PEG is added to a linker. Methods of conjugating PEG to a protein are standard in the art. For example, see Kolate et al, *Journal of Controlled Release* 2014; 192(28): 67-81, which is hereby incorporated by reference in its entirety. In an embodiment, a composition of the invention comprises a ligand comprising PEG and/or one or more N-glycans. In an embodiment, PEG is selected from the group consisting of PEG-10K, PEG-20K and PEG-40K.

[0082] Another aspect of the invention involves cross-linking the peptides of the invention to improve their pharmacokinetic, immunogenic, diagnostic, and/or therapeutic attributes. Cross-linking involves joining two molecules by a covalent bond through a chemical reaction at suitable site(s) (e.g., primary amines, sulfhydryls) on the cytokine and ligand of the invention. In an embodiment, the cytokine and ligand may be cross-linked together. The cross-linking agents may form a cleavable or non-cleavable linker between the cytokine and the ligand. Cross-linking agents that form non-cleavable linkers between the cytokine and the ligand may comprise a maleimido- or haloacetyl-based moiety. According to the present invention, such non-cleavable linkers are said to be derived from maleimido- or haloacetyl-based moiety. Cross-linking agents comprising a maleimido-based moiety include N-succinimidyl 4-(maleimidomethyl)cyclohexanecarboxylate (SMCC), N-succinimidyl-4-(N-maleimidomethyl)-cyclohexane-1-carboxy-(6-amidocaproate), which is a “long chain” analog of SMCC (LC-SMCC), κ-maleimidoundecanoic acid N-succinimidyl ester (KMUA), γ-maleimidobutyric acid N-succinimidyl ester (GMBS), ε-maleimidocaproic acid

N-hydroxysuccinimide ester (EMCS), m-maleimidobenzoyl-N-hydroxysuccinimide ester (MBS), N-(α-maleimidoacetoxy)-succinimide ester [AMAS], succinimidyl-6-(β-maleimidopropionamido)hexanoate (SMPH), N-succinimidyl 4-(p-maleimidophenyl)-butyrate (SMPB), and N-(p-maleimidophenyl)isocyanate (PMPI). These cross-linking agents form non-cleavable linkers derived from maleimido-based moieties. Cross-linking agents comprising a haloacetyl-based moiety include N-succinimidyl-4-(iodoacetyl)-aminobenzoate (SIAB), N-succinimidyl iodoacetate (SIA), N-succinimidyl bromoacetate (SBA) and N-succinimidyl 3-(bromoacetamido)propionate (SBAP). These cross-linking agents form non-cleavable linkers derived from haloacetyl-based moieties. Cross-linking agents that form non-cleavable linkers between the cytokine and the ligand may comprise N-succinimidyl 3-(2-pyridyldithio)propionate, 4-succinimidyl-oxycarbonyl-α-methyl-alpha-(2-pyridyldithio)-toluene (SMPT), N-succinimidyl-3-(2-pyridyldithio)-butyrate (SDPB), 2-iminothiolane, or acetylsuccinic anhydride.

(d) chimeric peptide

[0083] In another aspect, the invention encompasses a chimeric peptide comprising a cytokine peptide and a ligand peptide, wherein the cytokine peptide is not a binding partner of the ligand peptide. In still another aspect, the invention encompasses a chimeric peptide comprising a cytokine peptide and a ligand peptide, wherein the ligand peptide binds to an NKG2D receptor. It should be understood that "ligand peptide" is used interchangeably with "ligand" and "cytokine peptide" is used interchangeably with "cytokine" for purposes of descriptions herein of various cytokines and ligands that are suitable for use in the present compositions and methods.

[0084] In certain embodiments, the cytokine peptide is in the IL2 subfamily. More specifically, the cytokine peptide is selected from the group consisting of IL2, IL7, IL15 and IL21. In a specific embodiment, the cytokine peptide is IL15 or a mutant thereof. In another specific embodiment, the cytokine peptide is IL2 or a mutant thereof. In another embodiment, the cytokine peptide is mutant IL2 comprising at least one mutation selected from the group consisting of R38A, F42K and C125S. In a specific embodiment, the cytokine peptide comprises the amino acid sequence set forth in SEQ ID NO:5 or SEQ ID NO:6. In other embodiments, the cytokine peptide is in the IL1

family. More specifically, the cytokine peptide is selected from the group consisting of IL1α, IL1β, IL1Ra, IL18, IL36Ra, IL36α, IL37, IL36β, IL36γ, IL38, and IL33. In a specific embodiment, the cytokine peptide is IL18 or a mutant thereof.

[0085] In certain embodiments, the ligand peptide is a MHC class-I-related glycoprotein. In another embodiment, the ligand peptide is OMCP, a portion thereof, or a mutant thereof. In an embodiment, the ligand peptide binds to a receptor expressed on NK cells and CD8+ CTLs. In a specific embodiment, the ligand peptide binds to an NKG2D receptor. In certain embodiments, the ligand peptide comprises the amino acid sequence set forth in SEQ ID NO:7 or a portion thereof that is capable of binding to the NKG2D receptor.

[0086] In other embodiments, a chimeric peptide further comprises a linker peptide. In certain embodiments, a linker peptide comprises the amino acid sequence selected from the group consisting of $(AAS)_n$, $(AAAL)_n$, $(G_nS)_n$ or $(G_2S)_n$, wherein A is alanine, S is serine, L is leucine, and G is glycine and wherein n is an integer from 1-20, or 1-10, or 3-10. In a different embodiment, a linker peptide comprises at least one tag selected from the group consisting of a FLAG tag and a His tag. In an embodiment, a linker peptide is about 20 to about 30 amino acids. In a specific embodiment, a linker peptide comprises the amino acid sequence set forth in SEQ ID NO:8.

[0087] The invention also encompasses a nucleic acid molecule encoding a chimeric peptide as described herein. Additionally, the invention encompasses a pharmaceutical composition comprising a chimeric peptide as described herein. Pharmaceutical compositions are described in more detail in **Section I(f)**.

(e) preferred embodiments

[0088] By way of non-limiting example, several preferred compositions of the invention are depicted in **FIG. 23**. 1. depicts a composition comprising α2 domain (H2) of OMCP linked to a cytokine. 2. depicts a composition comprising OMCP linked to a cytokine, wherein the composition is pegylated. 3. depicts a composition comprising OMCP linked to a cytokine, wherein the composition comprises N-glycan. 4. depicts a composition comprising, OMCP linked to a cytokine, wherein the linker comprises various sequences and various lengths. 5. depicts a composition comprising a Fab

specific antibody for NKG2D linked to a cytokine. 6. depicts a composition comprising various NKG2D ligands linked to a cytokine. 7. depicts a composition comprising a mutated version of OMCP linked to a cytokine, wherein the OMCP may be mutated to have improved binding affinity or weaker binding affinity. 8. depicts a composition comprising a mutated version of OMCP linked to a cytokine, wherein the OMCP may be mutated to have binding affinity for other NKG2 receptors. 9. depicts a composition comprising a viral protein liked to a cytokine. For example, OMCP binds to NKG2D. Additionally, CPXV203 binds to MHCI. 10. depicts a composition comprising OMCP linked to a mutated cytokine. It is understood that the OMCP sequence could be from various sources such as cowpox or monkeypox. Also, Fc-chimeras of OMCP and IL2, and variants thereof may be used.

[0089] In a preferred embodiment, the composition comprises IL2, IL15 or IL18 linked to OMCP. In another preferred embodiment, the composition comprises IL2, IL15 or IL18 linked to OMCP via a peptide linker. In still another preferred embodiment, the composition comprises IL2, IL15 or IL18 linked to OMCP via a peptide linker comprising about 20 to about 30 amino acids. In still yet another preferred embodiment, the composition comprises IL2, IL15 or IL18 linked to OMCP via a peptide linker comprising a FLAG tag and a His tag. In each of the foregoing embodiments, the IL2 may be a mutated version of IL2 comprising the mutations R38A and F42K.

[0090] In a different preferred embodiment, the composition comprises IL2 linked to OMCP. In another preferred embodiment, the composition comprises IL2 linked to OMCP via a peptide linker. In still another preferred embodiment, the composition comprises IL2 linked to OMCP via a peptide linker comprising about 20 to about 30 amino acids. In still yet another preferred embodiment, the composition comprises IL2 linked to OMCP via a peptide linker comprising a FLAG tag and a His tag. In each of the foregoing embodiments, the IL2 may be a mutated version of IL2 comprising the mutations R38A and F42K.

[0091] In an exemplary embodiment, the composition comprises the DNA sequence set forth in SEQ ID NO:1
(CACAAACTCGCATTCAACTTCAATCTAGAAATAAATGGCAGTGATACACATTCTAC

AGTAGATGTATATCTTGATGATTCTCAAATTATAACGTTTGATGGAAAAGATAT
CCGTCCAACCATCCCGTTCATGATAGGTGATGAAATTTTCTTACCGTTTTATAAAA
ATGTGTTTAGTGAGTTTTTCTCTCTGTTTAGAAGAGTTCCTACAAGTACTCCATATG
AAGACTTGACATATTTTTATGAATGCGACTATACAGACAATAAATCTACATTTGATCA
GTTTTATCTTTATAATGGCGAAGAATATACTGTCAAAACACAGGAGGCCACTAATAA
AAATATGTGGCTAACTACTTCCGAGTTTAGACTAAAAAAATGGTTCGATGGCGAAG
ATTGTATAATGCATCTTAGATCGTTAGTTAGAAAAATGGAGGACAGTAAACGAAACA
CTGGTGGTACCGGAAGTAGCGGTAGTAGTGATTACAAGGACGATGACGACAAGCA
CCACCATCATCATCATCACCACGGTAGCAGCGGCAGCAGTGCCCCCACCTCTAGC
AGCACAAAGAAGACCCAGCTGCAACTGGAACACCTCCTGCTGGACCTGCAGATGA
TCCTGAACGGCATCAACAACTACAAGAACCCCAAGCTGACCGCCATGCTGACCAA
AAAGTTTTACATGCCCAAGAAGGCCACCGAGCTTAAACACCTGCAATGCCTTGAGG
AGGAGCTGAAGCCCTGGAGGAGGTACTGAACCTGGCCCAGAGCAAGAACTTTCAT
CTGAGGCCCAGGGACCTGATTAGCAACATCAACGTGATCGTGTTGGAGTTGAAGG
GCAGCGAGACCACGTTCATGTGCGAGTACGCCGACGAGACGGCCACCATAGTGG
AGTTTCTTAACAGGTGGATCACCTTCTCACAGTCTATCATCAGCACCCTGACC).

[0092] In another exemplary embodiment, the composition comprises the amino acid sequence set forth in SEQ ID NO:2 (HKLAFNFNLEINGSDTHSTVDVYLDDSQIITFDGKDIRPTIPFMIGDEIFLPFYKNVFSEF FSLFRRVPTSTPYEDLTYFYECDYTDNKSTFDQFYLYNGEEYTVKTQEATNKNMWLTT SEFRLKKWFDGEDCIMHLRSLVRKMEDSKRNTGGTGSSGSSDYKDDDDKHHHHHHH HGSSGSSAPTSSSTKKTQLQLEHLLLDLQMILNGINNYKNPKLTAMLTKKFYMPKKATE LKHLQCLEEELKPLEEVLNLAQSKNFHLRPRDLISNINVIVLELKGSETTFMCEYADETA TIVEFLNRWITFSQSIISTLT).

(f) pharmaceutical compositions

[0093] The present disclosure also provides pharmaceutical compositions. The pharmaceutical composition comprises a composition of the invention which is detailed above, as an active ingredient and at least one pharmaceutically acceptable excipient.

[0094] The pharmaceutically acceptable excipient may be a diluent, a binder, a filler, a buffering agent, a pH modifying agent, a disintegrant, a dispersant, a

preservative, a lubricant, taste-masking agent, a flavoring agent, or a coloring agent. The amount and types of excipients utilized to form pharmaceutical compositions may be selected according to known principles of pharmaceutical science.

[0095] In one embodiment, the excipient may be a diluent. The diluent may be compressible (i.e., plastically deformable) or abrasively brittle. Non-limiting examples of suitable compressible diluents include microcrystalline cellulose (MCC), cellulose derivatives, cellulose powder, cellulose esters (i.e., acetate and butyrate mixed esters), ethyl cellulose, methyl cellulose, hydroxypropyl cellulose, hydroxypropyl methylcellulose, sodium carboxymethylcellulose, corn starch, phosphated corn starch, pregelatinized corn starch, rice starch, potato starch, tapioca starch, starch-lactose, starch-calcium carbonate, sodium starch glycolate, glucose, fructose, lactose, lactose monohydrate, sucrose, xylose, lactitol, mannitol, malitol, sorbitol, xylitol, maltodextrin, and trehalose. Non-limiting examples of suitable abrasively brittle diluents include dibasic calcium phosphate (anhydrous or dihydrate), calcium phosphate tribasic, calcium carbonate, and magnesium carbonate.

[0096] In another embodiment, the excipient may be a binder. Suitable binders include, but are not limited to, starches, pregelatinized starches, gelatin, polyvinylpyrrolidone, cellulose, methylcellulose, sodium carboxymethylcellulose, ethylcellulose, polyacrylamides, polyvinyloxoazolidone, polyvinylalcohols, C_{12}-C_{18} fatty acid alcohol, polyethylene glycol, polyols, saccharides, oligosaccharides, polypeptides, oligopeptides, and combinations thereof.

[0097] In another embodiment, the excipient may be a filler. Suitable fillers include, but are not limited to, carbohydrates, inorganic compounds, and polyvinylpyrrolidone. By way of non-limiting example, the filler may be calcium sulfate, both di- and tri-basic, starch, calcium carbonate, magnesium carbonate, microcrystalline cellulose, dibasic calcium phosphate, magnesium carbonate, magnesium oxide, calcium silicate, talc, modified starches, lactose, sucrose, mannitol, or sorbitol.

[0100] In still another embodiment, the excipient may be a buffering agent. Representative examples of suitable buffering agents include, but are not limited to,

phosphates, carbonates, citrates, tris buffers, and buffered saline salts (e.g., Tris buffered saline or phosphate buffered saline).

[0101] In various embodiments, the excipient may be a pH modifier. By way of non-limiting example, the pH modifying agent may be sodium carbonate, sodium bicarbonate, sodium citrate, citric acid, or phosphoric acid.

[0102] In a further embodiment, the excipient may be a disintegrant. The disintegrant may be non-effervescent or effervescent. Suitable examples of non-effervescent disintegrants include, but are not limited to, starches such as corn starch, potato starch, pregelatinized and modified starches thereof, sweeteners, clays, such as bentonite, micro-crystalline cellulose, alginates, sodium starch glycolate, gums such as agar, guar, locust bean, karaya, pecitin, and tragacanth. Non-limiting examples of suitable effervescent disintegrants include sodium bicarbonate in combination with citric acid and sodium bicarbonate in combination with tartaric acid.

[0103] In yet another embodiment, the excipient may be a dispersant or dispersing enhancing agent. Suitable dispersants may include, but are not limited to, starch, alginic acid, polyvinylpyrrolidones, guar gum, kaolin, bentonite, purified wood cellulose, sodium starch glycolate, isoamorphous silicate, and microcrystalline cellulose.

[0104] In another alternate embodiment, the excipient may be a preservative. Non-limiting examples of suitable preservatives include antioxidants, such as BHA, BHT, vitamin A, vitamin C, vitamin E, or retinyl palmitate, citric acid, sodium citrate; chelators such as EDTA or EGTA; and antimicrobials, such as parabens, chlorobutanol, or phenol.

[0105] In a further embodiment, the excipient may be a lubricant. Non-limiting examples of suitable lubricants include minerals such as talc or silica; and fats such as vegetable stearin, magnesium stearate or stearic acid.

[0106] In yet another embodiment, the excipient may be a taste-masking agent. Taste-masking materials include cellulose ethers; polyethylene glycols; polyvinyl alcohol; polyvinyl alcohol and polyethylene glycol copolymers; monoglycerides or triglycerides; acrylic polymers; mixtures of acrylic polymers with cellulose ethers; cellulose acetate phthalate; and combinations thereof.

[0107] In an alternate embodiment, the excipient may be a flavoring agent. Flavoring agents may be chosen from synthetic flavor oils and flavoring aromatics and/or natural oils, extracts from plants, leaves, flowers, fruits, and combinations thereof.

[0108] In still a further embodiment, the excipient may be a coloring agent. Suitable color additives include, but are not limited to, food, drug and cosmetic colors (FD&C), drug and cosmetic colors (D&C), or external drug and cosmetic colors (Ext. D&C).

[0109] The weight fraction of the excipient or combination of excipients in the composition may be about 99% or less, about 97% or less, about 95% or less, about 90% or less, about 85% or less, about 80% or less, about 75% or less, about 70% or less, about 65% or less, about 60% or less, about 55% or less, about 50% or less, about 45% or less, about 40% or less, about 35% or less, about 30% or less, about 25% or less, about 20% or less, about 15% or less, about 10% or less, about 5% or less, about 2%, or about 1% or less of the total weight of the composition.

[0110] The composition can be formulated into various dosage forms and administered by a number of different means that will deliver a therapeutically effective amount of the active ingredient. Such compositions can be administered orally, parenterally, or topically in dosage unit formulations containing conventional nontoxic pharmaceutically acceptable carriers, adjuvants, and vehicles as desired. Topical administration may also involve the use of transdermal administration such as transdermal patches or iontophoresis devices. The term parenteral as used herein includes subcutaneous, intravenous, intramuscular, or intrasternal injection, or infusion techniques. Formulation of drugs is discussed in, for example, Gennaro, A. R., Remington's Pharmaceutical Sciences, Mack Publishing Co., Easton, Pa. (18^{th} ed, 1995), and Liberman, H. A. and Lachman, L., Eds., Pharmaceutical Dosage Forms, Marcel Dekker Inc., New York, N.Y. (1980).

[0111] Solid dosage forms for oral administration include capsules, tablets, caplets, pills, powders, pellets, and granules. In such solid dosage forms, the active ingredient is ordinarily combined with one or more pharmaceutically acceptable

excipients, examples of which are detailed above. Oral preparations may also be administered as aqueous suspensions, elixirs, or syrups. For these, the active ingredient may be combined with various sweetening or flavoring agents, coloring agents, and, if so desired, emulsifying and/or suspending agents, as well as diluents such as water, ethanol, glycerin, and combinations thereof.

[0112] For parenteral administration (including subcutaneous, intradermal, intravenous, intramuscular, and intraperitoneal), the preparation may be an aqueous or an oil-based solution. Aqueous solutions may include a sterile diluent such as water, saline solution, a pharmaceutically acceptable polyol such as glycerol, propylene glycol, or other synthetic solvents; an antibacterial and/or antifungal agent such as benzyl alcohol, methyl paraben, chlorobutanol, phenol, thimerosal, and the like; an antioxidant such as ascorbic acid or sodium bisulfite; a chelating agent such as etheylenediaminetetraacetic acid; a buffer such as acetate, citrate, or phosphate; and/or an agent for the adjustment of tonicity such as sodium chloride, dextrose, or a polyalcohol such as mannitol or sorbitol. The pH of the aqueous solution may be adjusted with acids or bases such as hydrochloric acid or sodium hydroxide. Oil-based solutions or suspensions may further comprise sesame, peanut, olive oil, or mineral oil.

[0113] For topical (e.g., transdermal or transmucosal) administration, penetrants appropriate to the barrier to be permeated are generally included in the preparation. Transmucosal administration may be accomplished through the use of nasal sprays, aerosol sprays, tablets, or suppositories, and transdermal administration may be via ointments, salves, gels, patches, or creams as generally known in the art.

[0114] In certain embodiments, a composition comprising a compound of the invention is encapsulated in a suitable vehicle to either aid in the delivery of the compound to target cells, to increase the stability of the composition, or to minimize potential toxicity of the composition. As will be appreciated by a skilled artisan, a variety of vehicles are suitable for delivering a composition of the present invention. Non-limiting examples of suitable structured fluid delivery systems may include nanoparticles, liposomes, microemulsions, micelles, dendrimers and other phospholipid-

containing systems. Methods of incorporating compositions into delivery vehicles are known in the art.

[0115] In one alternative embodiment, a liposome delivery vehicle may be utilized. Liposomes, depending upon the embodiment, are suitable for delivery of the compound of the invention in view of their structural and chemical properties. Generally speaking, liposomes are spherical vesicles with a phospholipid bilayer membrane. The lipid bilayer of a liposome may fuse with other bilayers (e.g., the cell membrane), thus delivering the contents of the liposome to cells. In this manner, the compound of the invention may be selectively delivered to a cell by encapsulation in a liposome that fuses with the targeted cell's membrane.

[0116] Liposomes may be comprised of a variety of different types of phospholipids having varying hydrocarbon chain lengths. Phospholipids generally comprise two fatty acids linked through glycerol phosphate to one of a variety of polar groups. Suitable phospholipids include phosphatidic acid (PA), phosphatidylserine (PS), phosphatidylinositol (PI), phosphatidylglycerol (PG), diphosphatidylglycerol (DPG), phosphatidylcholine (PC), and phosphatidylethanolamine (PE). The fatty acid chains comprising the phospholipids may range from about 6 to about 26 carbon atoms in length, and the lipid chains may be saturated or unsaturated. Suitable fatty acid chains include (common name presented in parentheses) n-dodecanoate (laurate), n-tretradecanoate (myristate), n-hexadecanoate (palmitate), n-octadecanoate (stearate), n-eicosanoate (arachidate), n-docosanoate (behenate), n-tetracosanoate (lignocerate), cis-9-hexadecenoate (palmitoleate), cis-9-octadecanoate (oleate), cis,cis-9,12-octadecandienoate (linoleate), all cis-9, 12, 15-octadecatrienoate (linolenate), and all cis-5,8,11,14-eicosatetraenoate (arachidonate). The two fatty acid chains of a phospholipid may be identical or different. Acceptable phospholipids include dioleoyl PS, dioleoyl PC, distearoyl PS, distearoyl PC, dimyristoyl PS, dimyristoyl PC, dipalmitoyl PG, stearoyl, oleoyl PS, palmitoyl, linolenyl PS, and the like.

[0117] The phospholipids may come from any natural source, and, as such, may comprise a mixture of phospholipids. For example, egg yolk is rich in PC, PG, and PE, soy beans contains PC, PE, PI, and PA, and animal brain or spinal cord is enriched in

PS. Phospholipids may come from synthetic sources too. Mixtures of phospholipids having a varied ratio of individual phospholipids may be used. Mixtures of different phospholipids may result in liposome compositions having advantageous activity or stability of activity properties. The above mentioned phospholipids may be mixed, in optimal ratios with cationic lipids, such as N-(1-(2,3-dioleolyoxy)propyl)-N,N,N-trimethyl ammonium chloride, 1,1'-dioctadecyl-3,3,3',3'-tetramethylindocarbocyanine perchloarate, 3,3'-deheptyloxacarbocyanine iodide, 1,1'-dedodecyl-3,3,3',3'-tetramethylindocarbocyanine perchloarate, 1,1'-dioleyl-3,3,3',3'-tetramethylindo carbocyanine methanesulfonate, N-4-(delinoleylaminostyryl)-N-methylpyridinium iodide, or 1,1,-dilinoleyl-3,3,3',3'-tetramethylindocarbocyanine perchloarate.

[0118] Liposomes may optionally comprise sphingolipids, in which spingosine is the structural counterpart of glycerol and one of the one fatty acids of a phosphoglyceride, or cholesterol, a major component of animal cell membranes. Liposomes may optionally, contain pegylated lipids, which are lipids covalently linked to polymers of polyethylene glycol (PEG). PEGs may range in size from about 500 to about 10,000 daltons.

[0119] Liposomes may further comprise a suitable solvent. The solvent may be an organic solvent or an inorganic solvent. Suitable solvents include, but are not limited to, dimethylsulfoxide (DMSO), methylpyrrolidone, N-methylpyrrolidone, acetronitrile, alcohols, dimethylformamide, tetrahydrofuran, or combinations thereof.

[0120] Liposomes carrying the compound of the invention (i.e., having at least one methionine compound) may be prepared by any known method of preparing liposomes for drug delivery, such as, for example, detailed in U.S. Pat. Nos. 4,241,046, 4,394,448, 4,529,561, 4,755,388, 4,828,837, 4,925,661, 4,954,345, 4,957,735, 5,043,164, 5,064,655, 5,077,211 and 5,264,618, the disclosures of which are hereby incorporated by reference in their entirety. For example, liposomes may be prepared by sonicating lipids in an aqueous solution, solvent injection, lipid hydration, reverse evaporation, or freeze drying by repeated freezing and thawing. In a preferred embodiment the liposomes are formed by sonication. The liposomes may be multilamellar, which have many layers like an onion, or unilamellar. The liposomes may

be large or small. Continued high-shear sonication tends to form smaller unilamellar lipsomes.

[0121] As would be apparent to one of ordinary skill, all of the parameters that govern liposome formation may be varied. These parameters include, but are not limited to, temperature, pH, concentration of methionine compound, concentration and composition of lipid, concentration of multivalent cations, rate of mixing, presence of and concentration of solvent.

[0122] In another embodiment, a composition of the invention may be delivered to a cell as a microemulsion. Microemulsions are generally clear, thermodynamically stable solutions comprising an aqueous solution, a surfactant, and “oil." The "oil" in this case, is the supercritical fluid phase. The surfactant rests at the oil-water interface. Any of a variety of surfactants are suitable for use in microemulsion formulations including those described herein or otherwise known in the art. The aqueous microdomains suitable for use in the invention generally will have characteristic structural dimensions from about 5 nm to about 100 nm. Aggregates of this size are poor scatterers of visible light and hence, these solutions are optically clear. As will be appreciated by a skilled artisan, microemulsions can and will have a multitude of different microscopic structures including sphere, rod, or disc shaped aggregates. In one embodiment, the structure may be micelles, which are the simplest microemulsion structures that are generally spherical or cylindrical objects. Micelles are like drops of oil in water, and reverse micelles are like drops of water in oil. In an alternative embodiment, the microemulsion structure is the lamellae. It comprises consecutive layers of water and oil separated by layers of surfactant. The “oil” of microemulsions optimally comprises phospholipids. Any of the phospholipids detailed above for liposomes are suitable for embodiments directed to microemulsions. The composition of the invention may be encapsulated in a microemulsion by any method generally known in the art.

[0123] In yet another embodiment, a composition of the invention may be delivered in a dendritic macromolecule, or a dendrimer. Generally speaking, a dendrimer is a branched tree-like molecule, in which each branch is an interlinked chain of molecules that divides into two new branches (molecules) after a certain length. This

branching continues until the branches (molecules) become so densely packed that the canopy forms a globe. Generally, the properties of dendrimers are determined by the functional groups at their surface. For example, hydrophilic end groups, such as carboxyl groups, would typically make a water-soluble dendrimer. Alternatively, phospholipids may be incorporated in the surface of a dendrimer to facilitate absorption across the skin. Any of the phospholipids detailed for use in liposome embodiments are suitable for use in dendrimer embodiments. Any method generally known in the art may be utilized to make dendrimers and to encapsulate compositions of the invention therein. For example, dendrimers may be produced by an iterative sequence of reaction steps, in which each additional iteration leads to a higher order dendrimer. Consequently, they have a regular, highly branched 3D structure, with nearly uniform size and shape. Furthermore, the final size of a dendrimer is typically controlled by the number of iterative steps used during synthesis. A variety of dendrimer sizes are suitable for use in the invention. Generally, the size of dendrimers may range from about 1 nm to about 100 nm

II. METHODS

[0124] In an aspect, the invention encompasses a method to deliver a cytokine to a target cell. The method comprises contacting a target cell with a composition comprising a cytokine linked to a ligand, wherein the ligand specifically binds to a receptor on the target cell. Additionally, the method comprises contacting a target cell with a composition comprising a chimeric peptide as described in **Section I**. A target cell may be any cell comprising a target receptor for which the ligand specifically binds to. The ligand and specific binding are described in **Section I**. In certain embodiments, a target cell may be an immune cell. Non-limiting example of immune cells include macrophages, B lymphocytes, T lymphocytes, mast cells, monocytes, dendritic cells, eosinophils, natural killer cells, basophils, neutrophils. In certain embodiments, an immune cell is selected from the group consisting of a macrophage, B lymphocyte, T lymphocyte, mast cell, monocyte, dendritic cell, eosinophil, natural killer cell, basophil, and neutrophil. In a specific embodiment, a target cell is a natural killer (NK) cell and/or a CD8+ T cell. In other embodiments, a target cell is a NKG2D-expressing cell. Non-

limiting examples of NKG2D-expressing cell include natural killer (NK) cells and CD8+ T cells (both αβ and γδ).

[0125] In another aspect, the invention encompasses a method to activate immune cells. The method comprises contacting an immune cell with a composition comprising a cytokine linked to a ligand, wherein the ligand specifically binds to a receptor on the immune cell thereby activating the cell. Additionally, the method comprises contacting an immune cell with a composition comprising a chimeric peptide as described in **Section I**. Non-limiting example of immune cells include macrophages, B lymphocytes, T lymphocytes, mast cells, monocytes, dendritic cells, eosinophils, natural killer cells, basophils, neutrophils. In certain embodiments, an immune cell is selected from the group consisting of a macrophage, B lymphocyte, T lymphocyte, mast cell, monocyte, dendritic cell, eosinophil, natural killer cell, basophil, and neutrophil. In a specific embodiment, an immune cell is a natural killer (NK) cell and/or a CD8+ T cell. To facilitate activation of immune cells, a cytokine may be a proinflammatory cytokine. The term "proinflammatory cytokine" is a cytokine which promotes systemic inflammation. A skilled artisan would be able to determine those cytokines that are proinflammatory. In certain embodiments, a proinflammatory cytokine is IL1α, IL1β, IL2, IL3, IL6, IL7, IL9, IL12, IL15, IL17, IL18, IL21, IFNα, IFNγ, TNFα, MIF, G-CSF, GM-CSF or mutants thereof. In an embodiment, a proinflammatory cytokine is an IL1 family cytokine. In certain embodiments, an IL1 family cytokine is selected from the group consisting of IL1α, IL1β, IL1Ra, IL18, IL36Ra, IL36α, IL37, IL36β, IL36γ, IL38, IL33 and mutants thereof. In a specific embodiment, a proinflammatory cytokine is selected from the group consisting of IL2, IL7, IL15, IL18, IL21 and mutants thereof. In another specific embodiment, a proinflammatory cytokine is selected from the group consisting of IL2, IL15, IL18, and mutants thereof. In an exemplary embodiment, a proinflammatory cytokine is IL2 or a mutant thereof. Activation of the immune cells may result in lysis of tumor cells. Accordingly, activation of immune cells may be measured by determining the amount of tumor cell lysis. In an embodiment, activation of the immune cells may result in about 10% to about 100% lysis of tumor cells. In another embodiment, activation of the immune cells may result in about 20% to about 80% lysis of tumor

cells. In still another embodiment, activation of the immune cells may result in greater than 40% lysis of tumor cells. For example, activation of the immune cells may result in greater than 40%, greater than 45%, greater than 50%, greater than 55%, greater than 60%, greater than 65%, greater than 70%, greater than 75%, greater than 80%, greater than 85%, greater than 90%, greater than 95%, or greater than 99% lysis of tumor cells. The lysis of tumor cells may be measured using any standard assay (e.g., caspase assays, TUNEL and DNA fragmentation assays, cell permeability assays, and Annexin V assays).

[0126] In still another aspect, the invention encompasses a method to treat a tumor. The method comprises identifying a subject with a tumor and administering to the subject a composition comprising a cytokine linked to a ligand, wherein the ligand specifically binds to a receptor on a target cell. Additionally, the method comprises administering to the subject a composition comprising a chimeric peptide as described in **Section I**. Specifically, the inventors have shown that delivering a cytokine to a target cell activates the cells bound by the composition, wherein the activated cells specifically lyse tumor cells thereby reducing the amount of cancer cells. In a specific embodiment, a cytokine is a proinflammatory cytokine as described in the preceding paragraph. Accordingly, a composition of the present invention, may be used in treating, stabilizing and preventing cancer and associated diseases in a subject. By “treating, stabilizing, or preventing cancer” is meant causing a reduction in the size of a tumor or in the number of cancer cells, slowing or preventing an increase in the size of a tumor or cancer cell proliferation, increasing the disease-free survival time between the disappearance of a tumor or other cancer and its reappearance, preventing an initial or subsequent occurrence of a tumor or other cancer, or reducing an adverse symptom associated with a tumor or other cancer. The inventors have shown that a composition of the invention activates natural killer (NK) cells bound by the composition, wherein the activated NK cells specifically lyse tumor cells thereby reducing the amount of tumor cells. For example, as cancerous cells are "stressed", NKG2D ligands become upregulated, rendering the cell susceptible to NK cell-mediated lysis. In a desired embodiment, the percent of tumor or cancerous cells surviving the treatment is at least 20, 30, 40, 50, 60,

70, 80, 90 or 100% lower than the initial number of tumor or cancerous cells, as measured using any standard assay (e.g., caspase assays, TUNEL and DNA fragmentation assays, cell permeability assays, and Annexin V assays). Desirably, the decrease in the number of tumor or cancerous cells induced by administration of a composition of the invention is at least 2, 5, 10, 15, 20, 25, 30, 35, 40, 45 or 50-fold greater than the decrease in the number of non-tumor or non-cancerous cells. Desirably, the methods of the present invention result in a decrease of 20, 30, 40, 50, 60, 50, 80, 90 or 100% in the size of a tumor or in the number of cancerous cells, as determined using standard methods. Desirably, at least 20, 30, 40, 50, 60, 70, 80, 90, or 95% of the treated subjects have a complete remission in which all evidence of the tumor or cancer disappears. Desirably, the tumor or cancer does not reappear or reappears after at least 1, 2, 3, 4, 5, 10, 15, or 20 years.

[0127] In another aspect, the invention encompasses a method to suppress immune cells. The method comprises contacting an immune cell with a composition comprising a cytokine linked to a ligand, wherein the ligand specifically binds to a receptor on the immune cell thereby suppressing the cell. Additionally, the method comprises contacting an immune cells with a composition comprising a chimeric peptide as described in **Section I**. Non-limiting example of immune cells include macrophages, B lymphocytes, T lymphocytes, mast cells, monocytes, dendritic cells, eosinophils, natural killer cells, basophils, neutrophils. In certain embodiments, an immune cell is selected from the group consisting of a macrophage, B lymphocyte, T lymphocyte, mast cell, monocyte, dendritic cell, eosinophil, natural killer cell, basophil, and neutrophil. In a specific embodiment, an immune cell is a natural killer (NK) cell and/or a CD8+ T cell. To facilitate suppression of immune cells, a cytokine may be an anti-inflammatory cytokine. The term “anti-inflammatory cytokine” is a cytokine that counteracts various aspects of inflammation, for example cell activation or the production of proinflammatory cytokines, and thus contributes to the control of the magnitude of the inflammatory response. A skilled artisan would be able to determine those cytokines that are anti-inflammatory. In certain embodiments, an anti-inflammatory cytokine is IL4, IL5, IL10, IL11, IL13, IL16, IL35, IFNα, TGFβ, G-CSF or a mutant thereof. In a specific

embodiment, an anti-inflammatory cytokine is IL10 or a mutant thereof. In another embodiment, the invention encompasses a method to kill immune cells. The method comprises contacting an immune cell with a composition comprising a toxin linked to a ligand, wherein the ligand specifically binds to a receptor on the immune cell thereby killing the cell. Suppression or killing of the immune cells may result in treatment, stabilization and prevention of autoimmune diseases caused by overactive immune cells. NKG2D-expressing cells and/or aberrant expression of host NKG2DLs have been implicated in diabetes, celiac disease and rheumatoid arthritis. For example, NK cells can recognize pancreatic beta cells and destroy them. The destruction of pancreatic beta cells may lead to type 1 diabetes. By way of another example, overactive immune cells are involved in transplant/graft rejection. Accordingly, a composition of the present invention, may be used in treating, stabilizing and preventing an automimmune disease in a subject. In a specific embodiment, the autoimmune disease is type 1 diabetes. In another specific embodiment, the autoimmune disease is transplant or graft rejection. In still another specific embodiment, the autoimmune disease is rheumatoid arthritis.

[0128] In still yet another aspect, the invention encompasses a method to treat an infection comprising administering a composition comprising a cytokine linked to a ligand. For example, a composition comprising a cytokine linked to a ligand may specifically bind an immune cell that is then activated to target and lyse the infected host cell. Additionally, the method comprises administering to the subject a composition comprising a chimeric peptide as described in **Section I**. The term "infection" as used herein includes the presence of pathogens in or on a subject, which, if its growth were inhibited, would result in a benefit to the subject. As such, the term "infection" in addition to referring to the presence of pathogens also refers to normal flora which are not desirable. The term “pathogen” as used herein refers to an infectious agent that can produce disease. Non-limiting examples of an infectious agent include virus, bacterium, prion, fungus, viroid, or parasite that cause disease in a subject. In a specific embodiment, an infection is caused by pathogens such as bacteria or viruses. In certain embodiments, the infection is an intracellular infection. In an embodiment, the infection is a viral infection. In another embodiment, the viral infection is caused by a flavivirus.

Flavivirus is a genus of viruses in the family Flaviviridae. Non-limiting examples of flaviviruses include Gadget's Gully virus, Kadam virus, Kyasanur Forrest disease virus, Langat virus, Omsk hemorrhagic fever virus, Tick-borne encephalitis virus, Louping ill virus, Aroa virus, Dengue viruses 1-4, Kedougou virus, Cacipacore virus, Koutango virus, Murray Valley encephalitis virus, St. Louis encephalitis virus, Usutu virus, West Nile virus, Yaounde virus, Kokobera virus group, Kokobera virus, Bagaza virus, Ilheus virus, Israel turkey meningoencephalomyelitis virus, Ntaya virus, Tembusu virus, Zika virus, Banzi virus, Bouboui virus, Edge Hill virus, Jugra virus, Saboya virus, Sepik virus, Uganda S virus, Wesselsbron virus, Yellow fever virus, Entebbe bat virus, Yokose virus, Apoi virus, Cowbone Ridge virus, Jutiapa virus, Modoc virus, Sal Vieja virus, San Perlita virus, Bukalasa bat virus, Carey Island virus, Dakar bat virus, Montana myotis leukoencephalitis virus, Phnom Penh bat virus, Rio Bravo virus, hepatitis C virus, e.g., hepatitis C virus genotypes 1-6, and GB virus A and B. In a certain embodiment, the flavivirus may be selected from the group consisting of West Nile virus, dengue virus, Japanese encephalitis virus, and yellow fever virus. In a specific embodiment, the viral infection is caused by West Nile virus. In certain embodiments, a pathogen, more specifically a virus, can induce the expression of proteins for which NKG2D binds. Accordingly, a composition comprising a cytokine linked to a ligand may specifically bind a NK cell that is then activated to target and lyse the infected host cell expressing NKG2D. In another embodiment, a composition comprising a cytokine linked to a ligand may activate cytotoxic T lymphocytes that recognize infected cells via other mechanisms for targeted killing.

[0129] In a different aspect, the invention encompasses a method to alleviate immunosuppression related to radiation exposure or lympotoxic substances comprising administering a composition comprising a cytokine linked to a ligand. Additionally, the method comprises administering a composition comprising a chimeric peptide as described in **Section I**. Additionally, a composition of the invention may be used to raise CD4 counts in HIV positive subjects. For example, a composition of the invention may be used to activate immune cells which can help restore the immune system of the subject.

[0130] In an alternative aspect, the invention encompasses a method of use as an adjuvant in a vaccine composition. For example, a composition of the invention may be used to expand CD8+ memory cells.

(a) administration

[0131] In certain aspects, a pharmacologically effective amount of a composition of the invention may be administered to a subject. Administration is performed using standard effective techniques, including peripherally (i.e. not by administration into the central nervous system) or locally to the central nervous system. Peripheral administration includes but is not limited to intravenous, intraperitoneal, subcutaneous, pulmonary, transdermal, intramuscular, intranasal, buccal, sublingual, or suppository administration. Local administration, including directly into the central nervous system (CNS) includes but is not limited to via a lumbar, intraventricular or intraparenchymal catheter or using a surgically implanted controlled release formulation. Pheresis may be used to deliver a composition of the invention. In certain embodiments, a composition of the invention may be administered via an infusion (continuous or bolus).

[0132] Pharmaceutical compositions for effective administration are deliberately designed to be appropriate for the selected mode of administration, and pharmaceutically acceptable excipients such as compatible dispersing agents, buffers, surfactants, preservatives, solubilizing agents, isotonicity agents, stabilizing agents and the like are used as appropriate. Remington's Pharmaceutical Sciences, Mack Publishing Co., Easton Pa., 16Ed ISBN: 0-912734-04-3, latest edition, incorporated herein by reference in its entirety, provides a compendium of formulation techniques as are generally known to practitioners.

[0133] Effective peripheral systemic delivery by intravenous or intraperitoneal or subcutaneous injection is a preferred method of administration to a living patient. Suitable vehicles for such injections are straightforward. In addition, however, administration may also be effected through the mucosal membranes by means of nasal aerosols or suppositories. Suitable formulations for such modes of administration are well known and typically include surfactants that facilitate cross-membrane transfer. Such surfactants are often derived from steroids or are cationic lipids, such as N-[1-(2,3-

dioleoyl)propyl]-N,N,N-trimethyl ammonium chloride (DOTMA) or various compounds such as cholesterol hemisuccinate, phosphatidyl glycerols and the like.

[0134] For therapeutic applications, a therapeutically effective amount of a composition of the invention is administered to a subject. A "therapeutically effective amount" is an amount of the therapeutic composition sufficient to produce a measurable response (e.g., an immunostimulatory, an anti-angiogenic response, a cytotoxic response, tumor regression, immunoinhibitory, immunosuppression, infection reduction). Actual dosage levels of active ingredients in a therapeutic composition of the invention can be varied so as to administer an amount of the active compound(s) that is effective to achieve the desired therapeutic response for a particular subject. The selected dosage level will depend upon a variety of factors including the activity of the therapeutic composition, formulation, the route of administration, combination with other drugs or treatments, tumor size and longevity, the autoimmune disease, infection, and the physical condition and prior medical history of the subject being treated. In some embodiments, a minimal dose is administered, and dose is escalated in the absence of dose-limiting toxicity. Determination and adjustment of a therapeutically effective dose, as well as evaluation of when and how to make such adjustments, are known to those of ordinary skill in the art of medicine. In an aspect, a typical dose contains from about 10 IU/kg to about 1,000,000 IU/kg of a cytokine described herein. In an embodiment, a typical dose contains from about 10 IU/kg to about 100 IU/kg. In another embodiment, a typical dose contains about 100 IU/kg to about 1,000 IU/kg. In still another embodiment, a typical dose contains about 1,000 IU/kg to about 10,000 IU/kg. In yet still another embodiment, a typical dose contains about 10,000 IU/kg to about 100,000 IU/kg. In a different embodiment, a typical dose contains about 100,000 IU/kg to about 1,000,000 IU/kg. In certain embodiments, a typical dose contains about 500,000 IU/kg to about 1,000,000 IU/kg. In other embodiments, a typical dose contains about 100,000 IU/kg to about 500,000 IU/kg. Alternatively, a typical dose contains about 50,000 IU/kg to about 100,000 IU/kg. In another embodiment, a typical dose contains about 10,000 IU/kg to about 50,000 IU/kg. In still another embodiment, a typical dose contains about 5,000 IU/kg to about 10,000 IU/kg. In a specific embodiment, a typical dose contains about

5,000 IU/kg to about 200,000 IU/kg. In another specific embodiment, a typical dose contains about 5,000 IU/kg to about 500,000 IU/kg. In still another specific embodiment, a typical dose contains about 50,000 IU/kg to about 500,000 IU/kg. In still yet another specific embodiment, a typical dose contains about 250,000 IU/kg to about 750,000 IU/kg.

[0135] The frequency of dosing may be once, twice, three times or more daily or once, twice, three times or more per week or per month, as needed as to effectively treat the symptoms or disease. In certain embodiments, the frequency of dosing may be once, twice or three times daily. For example, a dose may be administered every 24 hours, every 12 hours, or every 8 hours. In a specific embodiment, the frequency of dosing may be twice daily.

[0136] Duration of treatment could range from a single dose administered on a one-time basis to a life-long course of therapeutic treatments. The duration of treatment can and will vary depending on the subject and the cancer or autoimmune disease or infection to be treated. For example, the duration of treatment may be for 1 day, 2 days, 3 days, 4 days, 5 days, 6 days, or 7 days. Or, the duration of treatment may be for 1 week, 2 weeks, 3 weeks, 4 weeks, 5 weeks or 6 weeks. Alternatively, the duration of treatment may be for 1 month, 2 months, 3 months, 4 months, 5 months, 6 months, 7 months, 8 months, 9 months, 10 months, 11 months, or 12 months. In still another embodiment, the duration of treatment may be for 1 year, 2 years, 3 years, 4 years, 5 years, or greater than 5 years. It is also contemplated that administration may be frequent for a period of time and then administration may be spaced out for a period of time. For example, duration of treatment may be 5 days, then no treatment for 9 days, then treatment for 5 days.

[0137] The timing of administration of the treatment relative to the disease itself and duration of treatment will be determined by the circumstances surrounding the case. Treatment could begin immediately, such as at the time of diagnosis, or treatment could begin following surgery. Treatment could begin in a hospital or clinic itself, or at a later time after discharge from the hospital or after being seen in an outpatient clinic.

[0138] Although the foregoing methods appear the most convenient and most appropriate and effective for administration of a composition of the invention, by suitable adaptation, other effective techniques for administration, such as intraventricular administration, transdermal administration and oral administration may be employed provided proper formulation is utilized herein.

[0139] In addition, it may be desirable to employ controlled release formulations using biodegradable films and matrices, or osmotic mini-pumps, or delivery systems based on dextran beads, alginate, or collagen.

(b) tumor

[0140] A composition of the invention may be used to treat or recognize a tumor derived from a neoplasm or a cancer. The neoplasm may be malignant or benign, the cancer may be primary or metastatic; the neoplasm or cancer may be early stage or late stage. Non-limiting examples of neoplasms or cancers that may be treated include acute lymphoblastic leukemia, acute myeloid leukemia, adrenocortical carcinoma, AIDS-related cancers, AIDS-related lymphoma, anal cancer, appendix cancer, astrocytomas (childhood cerebellar or cerebral), basal cell carcinoma, bile duct cancer, bladder cancer, bone cancer, brainstem glioma, brain tumors (cerebellar astrocytoma, cerebral astrocytoma/malignant glioma, ependymoma, medulloblastoma, supratentorial primitive neuroectodermal tumors, visual pathway and hypothalamic gliomas), breast cancer, bronchial adenomas/carcinoids, Burkitt lymphoma, carcinoid tumors (childhood, gastrointestinal), carcinoma of unknown primary, central nervous system lymphoma (primary), cerebellar astrocytoma, cerebral astrocytoma/malignant glioma, cervical cancer, childhood cancers, chronic lymphocytic leukemia, chronic myelogenous leukemia, chronic myeloproliferative disorders, colon cancer, cutaneous T-cell lymphoma, desmoplastic small round cell tumor, endometrial cancer, ependymoma, esophageal cancer, Ewing's sarcoma in the Ewing family of tumors, extracranial germ cell tumor (childhood), extragonadal germ cell tumor, extrahepatic bile duct cancer, eye cancers (intraocular melanoma, retinoblastoma), gallbladder cancer, gastric (stomach) cancer, gastrointestinal carcinoid tumor, gastrointestinal stromal tumor, germ cell tumors (childhood extracranial, extragonadal, ovarian), gestational trophoblastic tumor,

gliomas (adult, childhood brain stem, childhood cerebral astrocytoma, childhood visual pathway and hypothalamic), gastric carcinoid, hairy cell leukemia, head and neck cancer, hepatocellular (liver) cancer, Hodgkin lymphoma, hypopharyngeal cancer, hypothalamic and visual pathway glioma (childhood), intraocular melanoma, islet cell carcinoma, Kaposi sarcoma, kidney cancer (renal cell cancer), laryngeal cancer, leukemias (acute lymphoblastic, acute myeloid, chronic lymphocytic, chronic myelogenous, hairy cell), lip and oral cavity cancer, liver cancer (primary), lung cancers (non-small cell, small cell), lymphomas (AIDS-related, Burkitt, cutaneous T-cell, Hodgkin, non-Hodgkin, primary central nervous system), macroglobulinemia (Waldenström), malignant fibrous histiocytoma of bone/osteosarcoma, medulloblastoma (childhood), melanoma, intraocular melanoma, Merkel cell carcinoma, mesotheliomas (adult malignant, childhood), metastatic squamous neck cancer with occult primary, mouth cancer, multiple endocrine neoplasia syndrome (childhood), multiple myeloma/plasma cell neoplasm, mycosis fungoides, myelodysplastic syndromes, myelodysplastic/myeloproliferative diseases, myelogenous leukemia (chronic), myeloid leukemias (adult acute, childhood acute), multiple myeloma, myeloproliferative disorders (chronic), nasal cavity and paranasal sinus cancer, nasopharyngeal carcinoma, neuroblastoma, non-Hodgkin lymphoma, non-small cell lung cancer, oral cancer, oropharyngeal cancer, osteosarcoma/malignant fibrous histiocytoma of bone, ovarian cancer, ovarian epithelial cancer (surface epithelial-stromal tumor), ovarian germ cell tumor, ovarian low malignant potential tumor, pancreatic cancer, pancreatic cancer (islet cell), paranasal sinus and nasal cavity cancer, parathyroid cancer, penile cancer, pharyngeal cancer, pheochromocytoma, pineal astrocytoma, pineal germinoma, pineoblastoma and supratentorial primitive neuroectodermal tumors (childhood), pituitary adenoma, plasma cell neoplasia, pleuropulmonary blastoma, primary central nervous system lymphoma, prostate cancer, rectal cancer, renal cell carcinoma (kidney cancer), renal pelvis and ureter transitional cell cancer, retinoblastoma, rhabdomyosarcoma (childhood), salivary gland cancer, sarcoma (Ewing family of tumors, Kaposi, soft tissue, uterine), Sézary syndrome, skin cancers (nonmelanoma, melanoma), skin carcinoma (Merkel cell), small cell lung cancer, small intestine cancer,

soft tissue sarcoma, squamous cell carcinoma, squamous neck cancer with occult primary (metastatic), stomach cancer, supratentorial primitive neuroectodermal tumor (childhood), T-Cell lymphoma (cutaneous), testicular cancer, throat cancer, thymoma (childhood), thymoma and thymic carcinoma, thyroid cancer, thyroid cancer (childhood), transitional cell cancer of the renal pelvis and ureter, trophoblastic tumor (gestational), unknown primary site (adult, childhood), ureter and renal pelvis transitional cell cancer, urethral cancer, uterine cancer (endometrial), uterine sarcoma, vaginal cancer, visual pathway and hypothalamic glioma (childhood), vulvar cancer, Waldenström macroglobulinemia, and Wilms tumor (childhood). In certain embodiments, the neoplasm or cancer may be selected from the group consisting of melanoma, renal cell carcinoma, lung cancer and blood cancer. As used herein, a "blood cancer" is a cancer that affects the blood, bone marrow and lymphatic system. There are three main groups of blood cancer: leukemia, lymphoma and myeloma. The four broad classification of leukemia are: acute lymphocytic leukemia (ALL), acute myelogenous leukemia (AML), chronic lymphocytic leukemia (CLL) and chronic myelogenous leukemia (CML). Lymphomas are divided into two categories: Hodgkin lymphoma and non-Hodgkin lymphoma. Most non-Hodgkin lymphomas are B-cell lymphomas, and either grow quickly (high-grade) or slowly (low-grade). There are 14 types of B-cell non-Hodgkin lymphomas. The rest are T-cell lymphomas, named after a different cancerous white blood cell, or lymphocyte. Because myeloma frequently occurs at many sites in the bone marrow, it is often referred to as multiple myeloma.

(c) subject

[0141] A suitable subject includes a human, a livestock animal, a companion animal, a lab animal, or a zoological animal. In one embodiment, the subject may be a rodent, e.g. a mouse, a rat, a guinea pig, etc. In another embodiment, the subject may be a livestock animal. Non-limiting examples of suitable livestock animals may include pigs, cows, horses, goats, sheep, llamas and alpacas. In yet another embodiment, the subject may be a companion animal. Non-limiting examples of companion animals may include pets such as dogs, cats, rabbits, and birds. In yet another embodiment, the subject may be a zoological animal. As used herein, a "zoological animal" refers to an

animal that may be found in a zoo. Such animals may include non-human primates, large cats, wolves, and bears. In a specific embodiment, the animal is a laboratory animal. Non-limiting examples of a laboratory animal may include rodents, canines, felines, and non-human primates. In certain embodiments, the animal is a rodent. Non-limiting examples of rodents may include mice, rats, guinea pigs, etc. In preferred embodiments, the subject is a human.

Table A. Sequences

SEQ ID NO	Name	Sequence	Source
1	R38A, F42K, C125S IL2-OMCP construct	CACAAACTCGCATTCAACTTCAATCTAGAAATAAATG GCAGTGATACACATTCTACAGTAGATGTATATCTTG ATGATTCTCAAATTATAACGTTTGATGGAAAAGAT ATCCGTCCAACCATCCCGTTCATGATAGGTGATGAA ATTTTCTTACCGTTTTATAAAAATGTGTTTAGTGAGTT TTTCTCTCTGTTTAGAAGAGTTCCTACAAGTACTCCAT ATGAAGACTTGACATATTTTTATGAATGCGACTATACA GACAATAAATCTACATTTGATCAGTTTTATCTTTATAA TGGCGAAGAATATACTGTCAAAACACAGGAGGCCAC TAATAAAAATATGTGGCTAACTACTTCCGAGTTTAGA CTAAAAAAATGGTTCGATGGCGAAGATTGTATAATGC ATCTTAGATCGTTAGTTAGAAAAATGGAGGACAGTAA ACGAAACACTGGTGGTACCGGAAGTAGCGGTAGTAG TGATTACAAGGACGATGACGACAAGCACCACCATCA TCATCATCACCACGGTAGCAGCGGCAGCAGTGCCCC CACCTCTAGCAGCACAAAGAAGACCCAGCTGCAACT GGAACACCTCCTGCTGGACCTGCAGATGATCCTGAA CGGCATCAACAACTACAAGAACCCCAAGCTGACCGC CATGCTGACCAAAAAGTTTTACATGCCCAAGAAGGC CACCGAGCTTAAACACCTGCAATGCCTTGAGGAGGA GCTGAAGCCCTGGAGGAGGTACTGAACCTGGCCCA GAGCAAGAACTTTCATCTGAGGCCCAGGGACCTGAT TAGCAACATCAACGTGATCGTGTTGGAGTTGAAGGG CAGCGAGACCACGTTCATGTGCGAGTACGCCGACGA GACGGCCACCATAGTGGAGTTTCTTAACAGGTGGAT CACCTTCTCACAGTCTATCATCAGCACCCTGACC	Synthesized
2	R38A, F42K, C125S IL2-OMCP construct	HKLAFNFNLEINGSDTHSTVDVYLDDSQIITFDGKDIRPT IPFMIGDEIFLPFYKNVFSEFFSLFRRVPTSTPYEDLTYF YECDYTDNKSTFDQFYLYNGEEYTVKTQEATNKNMWL TTSEFRLKKWFDGEDCIMHLRSLVRKMEDSKRNTGGT GSSGSSDYKDDDDKHHHHHHHHGSSGSSAPTSSSTK KTQLQLEHLLLDLQMILNGINNYKNPKLTAMLTKKFYMP KKATELKHLQCLEEELKPLEEVLNLAQSKNFHLRPRDLI SNINVIVLELKGSETTFMCEYADETATIVEFLNRWITFSQ SIISTLT	Synthesized
3	Melanoma tumor	SVYDFFVWL	Homo sapiens

	associate antigen tyrosinase-related protein 2 peptide		
4	Highly immunogenic peptide	SIINFEKL	Homo sapiens
5	WT IL2 (C125S)	APTSSSTKKTQLQLEHLLLDLQMILNGINNYKNPKLTRM LTFKFYMPKKATELKHLQCLEEELKPLEEVLNLAQSKNF HLRPRDLISNINVIVLELKGSETTFMCEYADETATIVEFL NRWITFCQSIISTLT	Homo sapiens
6	R38A, F42K, C125S IL2	APTSSSTKKTQLQLEHLLLDLQMILNGINNYKNPKLTAM LTKKFYMPKKATELKHLQCLEEELKPLEEVLNLAQSKNF HLRPRDLISNINVIVLELKGSETTFMCEYADETATIVEFL NRWITFSQSIISTLT	Synthesized
7	OMCP	HKLAFNFNLEINGSDTHSTVDVYLDDSQIITFDGKDIRPT IPFMIGDEIFLPFYKNVFSEFFSLFRRVPTSTPYEDLTYF YECDYTDNKSTFDQFYLYNGEEYTVKTQEATNKNMWL TTSEFRLKKWFDGEDCIMHLRSLVRKMEDSKRNT	Synthesized
8	Linker	GSSGSSDYKDDDDKHHHHHHHHGSSGSS	Synthesized
9	FLAG tag	DYKDDDK	Synthesized
10	HA tag	YPYDVPDYA	Synthesized
11	Myc tag	EQKLISEEDL	Synthesized
12	V5 tag	GKPIPNPLLGLDST	Synthesized
13	OMCPbr	GHKLAFNFNLEINGSDTHSTVDVYLDDSQIITFDGKDIRP TIPFMIGDEIFLPFYKNVFSEFFSLFRRVPTSTPYEDLTY FYECDYTDNKSTFDQFYLYNGEEYTVKTQEATNKNMW LTTSEFRLKKWFDGEDCIMHLRSLVRKMEDSKR	Cowpox virus
14	OMCPmpx	HKLVHYFNLKINGSDITNTADILLDNYPIMTFDGKDIYPSI AFMVGNKLFLDLYKNIFVEFFRLFRVSVSSQYEELEYYY SCDYTNNRPTIKQHYFYNGEEYTEIDRSKKATNKNSWLI TSGFRLQKWFDSEDCIIYLRSLVRRMEDSNK	Monkeypox virus
15	MICA	MEPHSLRYNLTVLSWDGSVQSGFLTEVHLDGQPFLRC RDRQKCRAKPQGQWAEDVLGNKTWDRETRDLTGNG KDLRMTLAHIKDQKEGLHSLQEIRVCEIHEDNSTRSSQH FYYDGELFLSQNLETKEWTMPQSSRAQTLAMNVRNFL KEDAMKTKTHYHAMHADCLQELRRYLKSGVVLR	Homo sapiens
16	MICB	MEPHSLRYNLMVLSQDGSVQSGFLAEGHLDGQPFLRY DRQKRRAKPQGQWAEDVLGAETWDTETEDLTENGQD LRRTLTHIKDQKGGLHSLQEIRVCEIHEDSSTRGSRHFY YNGELFLSQNLETQESTVPQSSRAQTLAMNVTNFWKE DAMKTKTHYRAMQADCLQKLQRYLKSGVAIR	Homo sapiens
17	ULBP3	DAHSLWYNFTIIHLPRHGQQWCEVQSQVDQKNFLSYD CGSDKVLSMGHLEEQLYATDAWGKQLEMLREVGQRL RLELADTELEDFTPSGPLTLQVRMSCECEADGYIRGSW QFSFDGRKFLLFDSNNRKWTVVHAGARRMKEKWEKD SGLTTFFKMVSMRDCKSWLRDFLMHRKKRLE	Homo sapiens

18	RAE-1B	DAHSLRCNLTIKDPTPADPLWYEAKCFVGEILILHLSNIN KTMTSGDPGETANATEVKKCLTQPLKNLCQKLRNKVS NTKVDTHKTNGYPHLQVTMIYPQSQGRTPSATWEFNIS DSYFFTFYTENMSWRSANDESGVIMNKWKDDGEFVK QLKFLIHECSQKMDEFLKQSKEK	Homo sapiens
19	NKG2D portion	LTIIEMQKGDCALYAS	Homo sapiens
20	NKG2D portion	LTIIEMQKGECALYAS	Green monkey
21	NKG2D portion	LTIIEMQKGDCAVYAS	Marmoset
22	NKG2D portion	LTLVEIPKGSCAVYGS	Mouse
23	NKG2D portion	LTLVKTPSGTCAVYGS	Rat
24	NKG2D portion	LTLMDTQNGKCALYGS	Guinea pig
25	NKG2D portion	LTLVEMQNGTCIVYGS	Ground squirrel
26	NKG2D portion	LTVVEMQSGSCAVYGS	Deer mouse
27	NKG2D portion	LSMVEMQNGTCAVYAS	Naked mole rat
28	NKG2D portion	LTLVEMQRGSCAVYGS	Prairie vole
29	NKG2D portion	VSIVEMQGGNCAVYGS	European shrew
30	NKG2D portion	VTVYEMQNGSCAVYGS	Star-nosed mole
31	NKG2D portion	LTLVEMQNGSCAVYGS	Chinese hamster
32	NKG2D portion	LTMVDMQNGTCAVYGS	Cat
33	OMCP portion	ASSFK	Cowpox virus
34	DAP10 signaling motif	YINM	Synthesized

EXAMPLES

[0142] The following examples are included to demonstrate preferred embodiments of the invention. It should be appreciated by those of skill in the art that the techniques disclosed in the examples that follow represent techniques discovered by the inventors to function well in the practice of the invention, and thus can be considered to constitute preferred modes for its practice. However, those of skill in the

art should, in light of the present disclosure, appreciate that many changes can be made in the specific embodiments which are disclosed and still obtain a like or similar result without departing from the spirit and scope of the invention.

Introduction to Examples 1-6.

[0143] The IL-2Rα chain serves to capture IL-2 at the cell surface to facilitate subsequent binding to the signaling part of the receptor, namely the IL-2Rβγ chains. Resting cytotoxic lymphocytes, such as natural killer (NK) and $CD8^+$ T cells, do not express appreciable IL-2Rα at the cell surface and are thus not activated by low levels of IL-2[1]. IL-2Rα is expressed on this population after initial activation, however, and is required for maximum cytotoxic lymphocyte expansion[2]. High dose IL-2 can induce the activation of all cytotoxic lymphocytes and is approved for treatment of several malignancies with an approximately 15% partial or complete tumor response[3-5]. Most patients do not benefit from such therapy due to activation of regulatory T cell (T_{regs}) and complications such as severe blood pressure alteration, generalized capillary leak, and end organ failure due to activation of vascular endothelium[6,3,7]. Both vascular endothelium and T_{regs} express IL-2Rα and are thus preferentially activated by IL-2 over cytotoxic lymphocytes[8]. Lowering the IL-2 dose can ameliorate side effects but also decreases efficacy. Mutant forms of IL-2, such as those with substitutions of alanine for arginine at the 38 position (R38A) and/or lysine for phenylalanine at the 42 position (F42K), decrease the affinity of IL-2 for IL-2Rα and thus eliminate many side effects[9]. Such IL-2α mutants may also decrease the efficacy of immunotherapy[2]. A form of IL-2 that could preferentially activate cytotoxic lymphocytes in the absence of IL-2Rα reactivity would be highly advantageous for clinical applications.

[0144] NKG2D recognizes MHC class-I-related stress ligands expressed by malignant or virally-transformed cells[10]. Of all the activating immunoreceptors NKG2D has the highest specificity for cytotoxic lymphocytes as it is constitutively expressed on both murine and human NK cells as well as activated $CD8^+$ T cells[11]. Consequentially it has been argued that tumors and virally infected cells utilize shed NKG2D ligands as a mechanism of immune evasion[12,13]. Orthopox major histocompatibility complex class I-like protein, or OMCP, is an NKG2D ligand decoy shed by monkeypox and cowpox

virus infected cells. It is not expressed by small pox or vaccinia virus and thus not recognized by those immunized with small pox vaccine. As OMCP binds to both human and murine NKG2D with the highest affinity of any known ligand we thought it might function as an ideal targeting vector to optimally deliver IL-2 to cytotoxic lymphocytes[14,15]. Here we describe the construction and function of a fusion protein designed to deliver an IL-2Rα mutant to NKG2D-expressing lymphocytes[15]. We demonstrate that this construct overcomes decreased efficacy associated with mutations in the IL-2Rα binding region while retaining a favorable safety profile. Systemic administration of this fusion protein improves immunotherapy against both solid and liquid tumors. Targeted delivery of IL-2 can thus be safely used to maximally activate NKG2D-expressing lymphocytes, such as NK cells, to optimize immunotherapy without systemic side effects.

Example 1. NKG2D-targeted delivery of an IL-2 mutant preferentially activates cytotoxic lymphocytes *in vitro*.

[0145] To overcome the preferential activation of IL-2Rα-expressing cells, we designed an IL-2 fusion protein that would target cytotoxic lymphocytes directly via the NKG2D receptor. This fusion protein combines the high affinity NKG2D ligand OMCP with an IL-2 mutated to reduce IL-2Rα reactivity. Our construct, termed OMCP-mutIL-2, consists of the 152 residue OMCP protein fused to the N-terminus of the 133 amino acid R38A/F42K mutant form of human IL-2 (mutIL-2) via a flexible 30 residue linker (**FIG. 1A-B**). The construct was first assessed for its *in vitro* binding ability. Binding of fluorescently labeled construct was tested *in vitro* at 37°C in bulk splenocytes. **FIG. 17** shows that the construct appears to only bind to NK cells which express NKG2D. The construct does not show binding to CD4+CD3+ T cells, CD8+CD3+ T cells, CD11C+CD11b- DCs, CD11c-CD11b+ Macs or CD19+CD3- B cells.

[0146] We have previously demonstrated strain-specific differences in murine NK cell cytotoxicity and lung cancer immunosurveillance[16] (and **Example 7**). Therefore, we set out to examine the efficacy of OMCP-mut-IL2 in activation of NK cells from two different strains of mice, namely A/J and B6 with poor and robust NK function, respectively. Compared to wild-type IL-2 (wtIL-2) or mutIL-2, OMCP-mutIL-2 strongly

upregulated CD69 on NK cells of both strains after 36-hour co-culture with 100 IUe/ml of cytokine (**FIG. 1C**, left; **FIG. 6**, left two graphs)[16,17]. At high concentrations a similar increase in CD69 expression was observed with OMCP-mut-IL-2, wtIL-2 or mutIL-2 (**FIG. 6**). Activation of $CD4^+Foxp3^+ T_{regs,,}$ as measured by upregulation of ICOS, was evident with wtIL-2 only, but not with mutIL-2 nor OMCP-mutIL-2 (**FIG. 1C-D**). $CD8^+$ and $CD4^+Foxp3^-$ effector T cells, on the other hand, demonstrated no upregulation of CD69 after 36 hours, even at highest doses of cytokines (**FIG. 1C-D** and data not shown). Longer exposure over a period of five days led to proliferation of both NK and $CD8^+$ T cells exposed to wtIL-2 and OMCP-mutIL-2 (**FIG. 1E-F**). Importantly, OMCP-mutIL-2 activated $CD8^+$ T cells and NK cells equivalently to mutIL-2 in $NKG2D^{-/-}$ splenocytes, indicating that the increased activation was due to the effect of OMCP targeting upon NKG2D-bearing cells (**FIG. 1F**; **FIG. 6,** right two graphs). Only incubation with wtIL-2 led to $CD4^+Foxp3^+ T_{regs}$ and $CD4^+Foxp3^-$ effector cell proliferation (**FIG. 1E-F**). Thus exposure to OMCP-mutIL-2 results in preferential NK activation that is superior or equivalent to wtIL-2 in a dose-dependent manner. $CD8^+$ T cells can also be activated but require prolonged exposure to higher doses of OMCP-mutIL-2.

Example 2. Low-dose cytokine therapy offers a favorable safety profile.

[0147] Dose-dependent toxicity can limit cytokine administration *in vivo*. To model human immunotherapy protocols we next treated A/J mice with wtIL-2 given as ten doses over a five day cycle[18]. While A/J mice tolerated 750,000 IUe of wtIL-2, significant mortality was evident at higher doses (**FIG. 2A-B**). Even after a 750,000 IUe dose mice demonstrated extreme distress, weight loss, decreased food consumption, ascites and hepatic inflammation (**FIG. 2A-E**; **FIG. 7A-C**). These side-effects mirror the capillary leak and distress associated with high dose IL-2 therapy in humans[7]. Treatment with anti-Asialo-GM1 ameliorated mortality, but not weight loss, induced by high dose wtIL-2 (1,500,000 IUe) in A/J mice, confirming that side effects of such therapy can occur independent of NK cells (**FIG. 2F-K**). Unlike the case for wtIL-2 no animal death was evident after 1,500,000 IUe of OMCP-mutIL-2 or mutIL-2 in the presence or absence of NK cells. Animal weight loss after 1,500,000 IUe of OMCP-mutIL-2 occurred only in NK-sufficient mice suggesting that toxicity of our construct was solely due to

immunoactivation (**FIG. 2F-K**). A regimen of 200,000 IUe was well tolerated in A/J mice with minimal weight loss, distress, or organ inflammation for all cytokines (**FIG. 2L-O**). Capillary leak, however, was still evident by accumulation of pleural effusion and ascites after wtIL-2, but not OMCP-mutIL-2 or mutIL-2, at this dose. B6 mice were able to tolerate higher doses of wtIL-2 but still suffered significant morbidity over 750,000 IUe (**FIG. 7D**).

Example 3. OMCP-mutIL-2 preferentially expands and activates NK cells *in vivo* compared to wtIL-2 or mutIL-2.

[0148] To evaluate immunologic changes associated with cytokine treatment, A/J mice received 200,000 IUe of cytokine or construct given as ten equal doses over five days. Splenic lymphocytes were evaluated flow cytometrically on day six. Both wtIL-2 and OMCP-mutIL-2 increased lymphocyte content and splenic size over saline-treated controls (**FIG. 3A-B**). OMCP-mutIL-2 led to a substantial expansion and activation of NK cells measured by cellularity and surface KLRG1 levels (**FIG. 3C**). In OMCP-mutIL-2 treated mice NK cells comprised close to half of all splenic lymphocytes, paralleling or even surpassing the total lymphocyte counts of saline or mutIL-2-treated mice (**FIG. 3A vs. FIG. 3C**). NK expansion by 200,000 IUe of OMCP-mutIL-2 was superior to near toxic doses of wtIL-2 (750,000IU), high dose mutIL-2 (3,500,000 IUe), or wtIL-2 complexed to anti-IL-2 antibody (clone MAB602)[19] (**FIG. 3C**). In fact, the majority of mice could not tolerate the full 200,000 IUe of wtIL-2/anti-IL-2 antibody and injections had to be terminated at 160,000 or 180,000 IUe with requisite animal sacrifice due to animal distress and rapid weight loss (**FIG. 8A**). WtIL-2 led to a significant expansion of $CD4^+Foxp3^+T_{regs}$, specifically the $ICOS^+$ subset[6] in A/J mice even when complexed to anti-IL-2 antibodies (**FIG. 3D**). Importantly the NK/T_{reg} ratio, which has been described as a predictive factor for success of immunotherapy[20], was dramatically increased in OMCP-mutIL-2 treated mice compared to all other treatment conditions (**FIG. 3E**). Superior expansion of NK cells by OMCP-mutIL-2 was even possible at doses 2-fold lower than wtIL-2 (**FIG. 8B**). However, targeting NKG2D with a ~500-fold lower affinity NKG2D ligand, ULBP3, ameliorated efficacy of the fusion construct for expansion but still offered superior NK activation compared to mutIL-2 alone (**FIG. 8B**). No statistically

significant increase in $CD4^+Foxp3^-$ or $CD8^+$ T lymphocytes was evident after wtIL-2 or OMCP-mutIL-2 treatment, although a trend for $CD8^+$ T cell expansion was evident (**FIG. 8C-D**). Such data is consistent with the prevalence of naïve T lymphocytes, expressing low levels of IL-2 receptors and NKG2D in specific pathogen-free mice.

[0149] Unlike the A/J strain little immunoactivation of lymphocytes was evident in B6 mice treated with 200,000 IUe of wtIL-2 (data not shown). At higher doses of 750,000 IUe OMCP-mutIL-2 expanded NK cells more robustly than wtIL-2 in this strain (**FIG. 3F-H**). IL-2/anti-IL-2 antibody complexes prevented T_{reg} expansion but, similar to the A/J strain, such treatment had toxicity and the majority of B6 mice could not tolerate the full 750,000 IUe dose (**FIG. 3I**). OMCP-mutIL-2, however, was well tolerated at this dose and led to a high NK/T_{reg} ratio (**FIG. 3J**). No expansion of NK cells was evident in OMCP-mutIL-2 treated B6 $NKG2D^{-/-}$ mutants, confirming the requirement for NKG2D in the function of our construct (data not shown). No statistically significant expansion of B6 $CD8^+$ or $CD4^+Foxp3^-$ T cells was evident in any treatment group although a trend for $CD8^+$ T cell expansion was evident after wtIL-2 administration (**FIG. 8F-G**). Identical data was obtained for lung resident lymphocytes in both the A/J and B6 strains (data not shown).

Example 4. OMCP-mutIL-2 preferentially expands and activates NK cells in human peripheral blood lymphocytes compared to wtIL-2 or mutIL-2.

[0150] To demonstrate the effectiveness of OMCP-mutIL-2 in human lymphocytes, human peripheral blood lymphocytes were co-cultured for 36 hours in 100IUe of either wild-type IL2, R38A/F42K mutant form of IL-2 or OMCP-mutant IL-2.

[0151] NK cells: The cells were flow cytometrically analyzed and relative prevalence of CD56+CD3- NK cells compared between conditions. A relatively higher proportion of NK cells was evident in the OMCP-mutant IL-2 group (**FIG. 31A**). Perforin levels were higher in OMCP-mutant IL-2 treated NK cells (red) compared to saline (black), IL-2 (blue) or mutant IL-2 (green) treated ones (**FIG. 31B**).

[0152] CD8+ T cells: Similar to NK cells, higher intracellular levels of perforin were evident in CD8+ T cells treated with OMCP-mutant IL-2 compared to other conditions (**FIG. 31C**).

[0153] Tregs: When gating on CD4+Foxp3+CD45RA- T cells a relatively higher proportion of activated CD25+CD127- regulatory T cells was evident in IL-2 treated peripheral blood lymphocyte cultures compared to other conditions (**FIG. 31D**). Taken together this data suggests that OMCP-mutIL-2 preferentially expands and activates NK cells and CD8+ cells in human peripheral blood lymphocytes compared to wtIL-2 or mutIL-2. Importantly, OMCP-mutIL-2 does not activated regulatory T cells significantly relative to IL2.

Example 5. Treatment with OMCP-mutIL-2 offers superior immunologic control of malignancies *in vivo*.

[0154] Unlike T lymphocytes, which require prior antigen encounter for optimal antigen-specific tumor cytotoxicity, NK cells can mediate natural cytotoxicity without prior sensitization. NK cells also form the primary barrier for expansion of select malignancies, such as lymphoma and lung cancer[16,17,21,22]. Treatment of A/J mice with OMCP-mutIL-2, compared to wtIL-2 or mutIL-2, led to enhanced *in vivo* clearance and *in vitro* lysis of YAC-1 cells by bulk splenocytes (**FIG. 4A**, **FIG. 9A-B**). Decreased growth of the highly aggressive Lewis Lung Carcinoma (LLC) cell line was evident in B6 mice after 750,000 IUe of OMCP-mutIL-2 compared to wtIL-2 or mutIL-2. Increased cytotoxicity was evident in OMCP-mutIL-2 treated splenocytes for the LLC cell line as well (**FIG. 4B-C**; **FIG. 9A-C**). Enhanced immunotherapy was lost in NKG2D$^{-/-}$ mice or following NK depletion (**FIG. 4D-E**). In the absence of host NKG2D mutIL-2 actually increased the rate of LLC growth. Thus OMCP-mediated targeting of mutIL-2 offers a safer and more efficacious form of immunotherapy for both solid and liquid tumors in various strains of mice.

Example 6. Impact of NKG2D targeting on IL-2 signaling.

[0155] Antibody-IL-2 conjugates, or IL-2/anti-IL-2 antibody complexes demonstrate improved biologic activity over purified cytokine by extending the duration of serum half-life[23,24]. To investigate whether linking IL-2 to OMCP increased serum half-life, we injected 500,000 IUe of fluorescently-labeled wtIL-2, mutIL-2 or OMCP-mutIL-2 into A/J and B6 mice and monitored serum clearance by serial blood draws.

While OMCP-mutIL-2 had a slightly higher serum concentration at early time points, all constructs were undetectable in the blood one hour post-injection (**FIG. 5A-B**). This is significantly shorter than the described 11-14 hour serum half-life of antibody-IL-2 conjugates[23]. Interestingly, despite the injection of identical amount of cytokine, lower cytokine levels were detected in B6 mice compared to A/J mice at all time points. Such data points to strain-specific differences in clearance of IL-2 and may explain why B6 mice are able to both tolerate and require higher doses of cytokine for NK expansion. Nevertheless, based on this data it is unlikely that prolonged circulation of construct was responsible for the increased activity of OMCP-mutIL-2 over wtIL-2.

[0156] We next considered the possibility that the superiority of OMCP-mutIL-2 was the result of signaling through NKG2D as antibody-mediated crosslinking of this receptor can activate NK cells (**FIG. 10A**)[25]. While the addition of purified OMCP to mutIL-2 did not augment NK activation or expansion *in vitro* or *in vivo* (data not shown) we would not expect a monomeric ligand to crosslink NKG2D. We thus directly compared NK cell activation in the presence of 1000 IUe of OMCP-mutIL-2, mutIL-2 and mutIL-2 combined with equimolar concentration of pentamerized OMCP. No increase in NK activation, as measured by CD69 upregulation or degranulation, was evident in the presence of pentamerized OMCP (**FIG. 5C, FIG. 10B**). This suggests that NKG2D crosslinking is not responsible for augmented NK cell activation by OMCP-mutIL-2 at physiologic concentrations.

[0157] To evaluate IL-2 signaling we next quantitated STAT5 phosphorylation after a 15 minute cytokine stimulation of freshly isolated NK cells *in vitro*. Lower levels of STAT5 phosphorylation were evident in A/J compared to B6 NK cells at all concentrations tested (**FIG. 5D-E**) suggesting that lymphocyte dysfunction of A/J mice may at least partially be the result of inefficient IL-2 signal transduction. Surprisingly, for both B6 and A/J NK cells wtIL-2 and OMCP-mutIL-2 demonstrated an identical dose-dependent pattern of STAT5 phosphorylation (**FIG. 5D-E**). In the absence of NKG2D reactivity OMCP-mutIL-2 failed to increase STAT5 phosphorylation over mutIL-2 alone. Taken together these data suggested that IL-2α reactivity is important for peak IL-2 signaling in resting NK cells, and that NKG2D-binding may effectively substitute for IL-

2Rα-binding in IL-2-mediated signal transduction. Such data, however, failed to explain the superior NK activation by OMCP-mutIL-2 *in vivo* or in bulk splenocyte cultures (**FIG. 1C-D, FIG. 3**).

[0158] IL-2 signaling results in the internalization of IL-2/IL-2R, with subsequent degradation of IL-2 and IL-2Rβγ. The binding of OMCP-mutIL-2 to both the IL-2 receptor and NKG2D could thus lead to altered internalization and enhanced NK cell activation by prolonging IL-2 signaling. To test this we stimulated freshly isolated NK cells for 15 minutes, replaced the culture media with cytokine free media, and monitored STAT5 phosphorylation for four hours. Identical decay of phospho-STAT5 was evident for both wtIL-2 and OMCP-mutIL-2 (**FIG. 5F-G**). Thus altering duration of IL-2 signaling is not responsible for superior NK activation by OMCP-mutIL-2.

[0159] We next considered the possibility that superior NK activation by OMCP-mutIL-2 may be the result of altered cytokine interaction with competing stromal cells (**FIG. 5H**). Indeed, in the presence of other splenocytes OMCP-mutIL-2 demonstrated a dose-dependent enhancement in NK STAT5 phosphorylation over wtIL-2 (**FIG. 5I**). We next explored the interplay between IL-2Rα expression by stromal cells and NKG2D expression by NK cells on IL-2 signal transduction. To accomplish this we isolated splenic NK cells from either wild-type or NKG2D$^{-/-}$ B6 mice and combined them with wild-type splenocytes depleted of NK cells. Cultures were recombined in a 1:20 NK:splenocyte ratio, resembling the proportion normally present in resting wild-type B6 mice. For some cultures NK cell depleted splenocytes were treated with saturating concentrations of IL-2Rα-blocking antibody (clone 3C7) prior to recombining with wild-type NK cells. The cultures were then stimulated with 1000 IUe of either wtIL-2 or OMCP-mutIL-2 for 15 minutes. STAT5 phosphorylation was identical in NKG2D$^{-/-}$ or wild type NK cells in the presence of wtIL-2 (**FIG. 5J,** left two columns). Wild-type NK cells cultured with OMCP-mutIL-2 demonstrated superior STAT5 phosphorylation to cultures with wtIL-2. Little STAT5 phosphorylation was evident in NKG2D$^{-/-}$ NK cells cultured with OMCP-mutIL-2 (**FIG. 5J,** right two columns). In the presence of IL-2Rα-blockade of competing splenocyte stromal cells, NK cell STAT5 phosphorylation by wtIL-2 increased to levels comparable to OMCP-mutIL-2 (**FIG. 5K**). Taken together these data

demonstrate that IL-2-Rα expression by "competing" stromal cells limits NK cell activation by wtIL-2 and this competition can be eliminated by the NKG2D-targeted, IL-2Rα-binding impaired OMCP-mutIL-2 construct.

Discussion for Examples 1-6.

[0160] While IL-2 therapy initially showed great promise, it has been limited by activation of T_{regs} and toxic side effects associated with activation of vascular endothelium. Several strategies have been proposed to preferentially activate cytotoxic lymphocytes. One strategy has been to create mutants with increased affinity for IL-2Rβ to remove the preference for IL-2Rα[26,27]. Importantly, these IL-2 mutants retain wild type binding for IL-2Rα, and would therefore still be recognized by T_{reg} cells and vascular endothelium. Our results also suggest that competition with IL2-Rα^{+}-expressing cells limits bioavailability of wtIL-2 to cytotoxic lymphocytes.

[0161] Another promising therapy involves anti-IL2 antibodies that sterically inhibit wtIL-2 binding to IL-2Rα[1,28,29]. Such treatment can extend serum half-life[24] due to the Fc region of the antibody and potentially due to reduced competition for wtIL-2 from IL-2Rα-expressing cells. Antibody-IL-2 fusion proteins have also been designed to target IL-2 to specific tumor antigens[30,31]. While offering the potential for personalized therapy such antibody-mediated delivery of IL-2 to the tumor depends on the expression of a known tumor associated antigen, a situation that often does not exist. This approach could potentially be further limited by tumor-mediated alteration of the targeted antigen.

[0162] Finally, IL-2 mutants with reduced affinity for IL-2Rα have been tested extensively. Compared to wtIL-2 these mutants can be administered in supratherapeutic doses without IL-2Rα-mediated capillary leak or systemic toxicity[32]. While these mutants have excellent safety profiles, they activate cytotoxic lymphocytes poorly (**FIG. 5C-E**)[33]. Our approach combines several of the concepts above to target a safe form of IL-2 directly to cytotoxic lymphocytes, instead of tumors. This is accomplished by replacing the normal targeting of IL-2 to IL-2Rα with NKG2D. The combination of an IL-2Rα-deficient IL-2 fused to a high affinity NKG2D-ligand improves upon previous strategies by specifically expanding NK cells without any apparent

activation of T_{regs} or capillary leak. These findings offer the promise of a potentially safe and highly efficacious form of IL-2.

[0163] One limitation in translating results from inbred lab animals to humans is the natural diversity in cytokine reactivity and environmentally dependent threshold for lymphocyte activation. Previous studies have demonstrated a correlation between *ex vivo* killing of tumor cells and enhanced long-term cancer immunity[34]. Therefore, any potential therapy needs to account for a population that has differential levels of cytotoxic lymphocyte activity. We have thus attempted to model this natural variation by using two strains of mice known to be highly resistant (B6) or susceptible (A/J) to carcinogenesis. For example, NK cells from B6 mice, are activated by wtIL-2 and extreme doses of mutIL-2. In contrast, IL-2/anti-IL-2 antibody complexes resulted in expansion of NK cells in A/J but not in B6 mice. Such variations highlight the limitations of translating results derived from a single strain of mice to immunologically diverse humans. Importantly, the OMCP-mutIL-2 construct was able to expand NK cells in both strains of mice, indicating that this therapy could be efficacious in populations with diverse NK function and cytokine reactivity.

[0164] Since OMCP has been described as an evolutionary antagonist of NKG2D[35] blockade of this immunoreceptor at the time of tumor therapy may be construed as counterproductive. Nevertheless, natural cytotoxicity and tumor clearance was augmented in OMCP-mutIL-2-treated mice even in the presence of established tumors. This suggests minimal or transient NKG2D receptor occupancy and preservation of function. Alternatively recent reports have demonstrated that shed NKG2D ligands may actually promote tumor immunity through reversal of NK desensitization imposed by chronic agonistic engagement[36]. While we did not detect NK activation or expansion by monomeric or even pentameric OMCP, it is possible that within the tumor bed such competitive antagonism plays a paradoxical role in NK activation. In addition, IL-2 may upregulate receptors necessary for NK migration and tumor infiltration. It is thus possible that anti-tumor immunity mediated by OMCP-mutIL-2 may depend on NK cells located outside the tumor bed and not subject to local tumor-

specific tolerance or anergy. Furthermore, OMCP maybe the ideal "targeting vector" due to its high affinity and long half-life of binding to human NKG2D.

[0165] While NK cells from two separate strains of mice were activated by OMCP-mutIL-2 we did not detect global expansion of activation of $CD8^+$ T cells by our construct. This is most likely due to the fact that NKG2D is expressed only on select subsets of $CD8^+$ T cells, namely memory or activated cytotoxic lymphocytes. Based on the paucity of this cell population in mice raised in specific pathogen-free environment, OMCP-mutIL-2-mediated activation was limited in our system to NK cells. To this end we focused on immunotherapy for lung cancer and lymphoma, whose growth is regulated primarily by NK cells[16,17,22,37]. Nevertheless OMCP-mutIL-2 was able to expand $CD8^+$ T cells when administered in high concentrations *in vitro* (**FIG. 1E-F**). Thus, it may be possible that NKG2D-targeted delivery of immunostimulatory cytokines may lead to the expansion and/or activation of antigen-specific $CD8^+$ memory cells for long-term tumor immunity under normal immunologic conditions.

Methods for Examples 1-6.

[0166] *Cytokine and Construct Generation:* The sequences encoding human IL-2 (1-133; C125S) and mutant IL2 (1-133; R38A, F42K, C125S) were cloned into the pFM1.2R[38] with an N-terminal FLAG/hexahistidine tag. The chimeric OMCP-mutIL-2 molecule comprises the full-length OMCP (1-152) coding sequence cloned in frame with a C-terminal FLAG/hexahistidine tag-mutant IL-2 (1-133; R38A, F42k, C125S) cloned into the pFM1.2R vector. Proteins were expressed by transient transfection into HEK293F (Life_Technologies). Supernatant was recovered at 72h and 144h post-transfection. Supernatants were supplemented with 5 mM imidazole and 0.02% sodium azide and purified by nickel-nitrilotriacetic acid (Ni-NTA) chromatography (Qiagen). Purified proteins were buffer exchanged into saline and flash frozen in liquid nitrogen. Equivalent *in vitro* and *in vivo* activity was documented for wild-type IL-2 generated in house and Teceleukin (TecinTM) available from the NCI repository (Frederick National Laboratory for Cancer Research). Thus for some experiments these two preparations of IL-2 were used interchangeably.

[0167] Wild-type IL-2 has a specific activity of $15x10^6$ IU/mg[39]. Thus, based on the molecular weight of 15.5kDa a 4.4 μM solution is equivalent to 1000 IU/μl. Based on this calculation all cytokines and construct were administered on a molar basis with 1 μl of 4.4 μM solution defined as 1000IU equivalents (IUe from here on). Such a system allows for equimolar comparison between IL-2, mutIL-2 and OMCP-mutIL-2 despite difference in molecular weight.

[0168] *Animals:* A/J (8-12 weeks) and C57BL/6J (6-9 weeks) strains of mice were purchased from the Jackson Laboratory (Bar Harbor, Maine). $NKG2D^{-/-}$ mice on the B6 background were kindly provided by Wayne Yokoyama and bred in house (Howard Hughes Institute of Medicine at Washington University in St. Louis). Animals were housed in a barrier facility in air-filtered cages and allowed free access to food and water. For some experiments A/J mice were treated with depleting concentrations of anti-Asialo-GM1 (50 μl day -2; 25 μl day -1) or control rabbit IgG (Wako Chemical Company). Animal procedures were approved by the animal studies committee of Washington University School of Medicine, St. Louis, MO.

[0169] *Tissue harvest and in vitro cultures:* Single cell suspension of splenocytes were obtained by crushing whole spleens through 70 μm cell strainers prior to RBC lysis by ACK buffer (Lonza, Walkersville, MD) and re-filtration through a 40 μm filter. Lungs were digested for 90 minutes at 37°C in 1 mg/ml collagenase II (Fisher Scientific), and 5 U/ml DNase I (Sigma-Aldridge) prior to processing in an identical fashion to spleens.

[0170] For *in vitro* cultures splenocytes from either A/J, B6, or $NKG2D^{-/-}$ mice were extracted in a sterile fashion and seeded in 12-well plates in complete media (RPMI 1640 supplemented with 10% FBS, 100 U/ml Penicillin and Streptomycin, 2 mM L-glutamine and 50 μM 2-Mercaptoethanol) at 5 million cells per ml per well. The cells were treated with increasing doses of human recombinant IL-2, mutIL-2, OMCP-mutIL-2, or OMCP for 36 hours as described in the manuscript. For some experiments bulk splenocytes were labeled with CFSE and cultured in 1000 IUe/ml of cytokine for 5 days prior to flow cytometric analysis. For NK isolation experiments bulk splenocytes were processed using either the NK cell isolation kit II or CD49b (DX5) positive magnetic bead selection (both from Miltenyi Biotech). For STAT5 phosphorylation experiments,

isolated NK cells were stimulated in increasing concentrations of IL-2 or construct at 100,000 cells/500µl for 15 minutes. For experiments evaluating the interaction of NK cells with splenic stroma, DX5 positively selected NK cells were labeled with CFSE (for identification after fixation and permeabilization) and recombined with NK depleted stromal cells. As described in the manuscript, for some studies NKG2D$^{-/-}$ NK cells were combined with wild-type splenocyte stromal cells. For other experiments, NK-depleted splenocytes from wild-type B6 mice were treated with saturating concentrations of anti-IL-2α blocking antibody (clone 3C7) or isotype control (both from Biolegend) prior to recombining with NK cells. For such competitive STAT5 phosphorylation experiments 100,000 cells were resuspended into 2 µl complete media containing 1,000 IU/ml of either wtIL2, mutIL-2 or OMCP-mut-IL-2 (freshly prepared and pre-warmed). The cells were then incubated at 37 ºC for 15 minutes

[0171] *Flow Cytometry:* All flow cytometric analysis was performed using saturating concentrations of fluorochrome-conjugated antibodies at 4°C in FACS buffer consisting of PBS with 2% FBS and 0.4% EDTA. All antibodies were anti-mouse and purchased from BD Bioscience or eBioscience and consisted of anti-CD4 (clones GK1.5 or RM4-5), anti-CD8 (clone 53-6.7), anti-CD278 (ICOS) (clone: 7E.17G9), anti-CD25 (clone PC61), anti-KLRG1 (clone 2F1), CD49b (Integrin alpha 2) (clone DX5), anti-CD3e (clone 1452C11), anti-CD45 (clone 30-F11), anti-CD69 PE (clone H1.2F3), anti-GITR (clone DTA-1), anti-Foxp3 (clone: FJK-16s) and Anti-Stat5 (clone 47/Stat5; pY694). Antibodies were conjugated to either FITC, PE, PerCP-CyTM5.5, PE-Cyanine7, APC, APC-eFluor® 780, eFluor® 450, or Alexa Fluor® 647.

[0172] Phospho-STAT5 evaluation was performed by paraformaldehyde fixation, methanol permeabilization and staining with AlexaFluor488-conjugated Anti-Stat5 (pY694) (BD Pharmingen; clone 612599). To accomplish this isolated NK cells or NK cells combined with NK-depleted splenocyte stromal cells were fixed in 2% paraformaldehyde (PFA) at 37 ºC for 10 minutes after IL-2 stimulation for 15 minutes. The cells were then washed once with ice-cold PBS and permeabilized by adding 0.5 ml/tube of 90% Methanol on ice for 1 hour. The cells were washed once with ice-cold

PBS (to remove methanol), and stained for 1 hour with anti-Stat5 (pY694) antibody at room temperature followed by one wash in PBS/0.5% fetal calf serum.

[0098] *In Vitro Cytotoxicity:* ^{51}Chromium release was conducted by incubating the target cells with 100 mCi sodium ^{51}chromate (PerkinElmer) for 1 hour. Bulk splenocytes were used as effector cells and incubated with targets at defined effector:target ratios for 4 hours at 37°C in round bottom 96 well plates. Specific lysis was expressed as (experimental release-spontaneous release)/(maximum release-spontaneous release) X100% with 0% specific lysis as lowest expressed value.

[0173] *In vivo cytokine injections:* For select experiment, the mice received intraperitoneal injections of cytokines in 200 µl volume given as ten equal doses given twice a day over a period of five days. As described above all cytokines were normalized to IUe on a molar basis. For select experiments, the mice were then sacrificed on day 6 and organs were fixed in 10% buffered formalin for histological analyses. For other experiments splenocyte and lung lymphocyte populations were analyzed flow cytometrically. For all the *in vivo* cytokine treatment experiments, animals were weighed (daily or every other day) and expressed as % change from start of cytokine therapy.

[0174] For evaluation of serum concentration wtIL-2, mutIL-2 or OMCP-mutIL-2 were labeled with Alexa Fluor® 647 (LifeTechnologies Inc.) according to manufacturer instructions. Serum was collected at times specified and concentration of cytokine determined fluoroscopically according to a standard curve.

[0175] *In vivo tumor studies:* Lewis lung carcinoma (LLC) cells were subcutaneously injected into B6 or B6 NKG2D$^{-/-}$ mice at 1 x 10^5 cells per mouse in 100 µl of sterile saline. Once visible tumors were evident, day 5 post-injection, a five day course of cytokine treatment was started as described above. Measurement of cross sectional tumor diameter was performed using calipers and tumor volume estimated as $4/3\pi r^3$. The mice were sacrificed on day 24 post injection or once they reached a maximal tumor diameter of 20mm. For NK cell depletion, mice were treated with anti-NK1.1 antibody (clone PK136) or mouse IgG isotype control (both from BioXcell) at 500 µg day -2, 250 µg day -1 and 250 µg weekly for the duration of the experiment. For lymphoma

clearance experiments A/J mice were treated with ten doses of cytokine over a period of five days as described above and on day #6 injected intravenously with YAC-1 cells that were labeled with CFSE at 5 x 10^6 cells/mouse. Mice were sacrificed 4 hours later, lungs were digested and viability of YAC-1 determined by forward and side scatter analysis of $CFSE^+$ cells.

[0176] *Statistics:* Comparison of splenic and lung-resident lymphocytes between various cytokine treatment conditions was performed by unpaired T-test with Welch's correction to account for unequal variance or unequal sample size. Tumor growth between different cytokine conditions was compared by multiple unpaired-T tests performed between various conditions at various time points using the Sidak-Bonferroni correction. Fold change in STAT5 phosphorylation was evaluated by unpaired T-test with Welch's correction in a similar fashion.

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Introduction to Examples 7-10.

[0177] Intracellular surveillance mediated by MHC class I (MHCI) is a critical host immune function and as such MHCI molecules are frequently targeted for destruction or intracellular retention by viruses [1]. Many herpesviruses encode at least one protein that prevents the cell surface expression of MHCI [1,2]. However, this immune evasion strategy renders the infected cell susceptible to NK cell-mediated lysis due to loss of inhibitory signals [3]. Viral infection also leads to cell surface display of NKG2D ligands (NKG2DLs) recognized by the activating receptor NKG2D, further predisposing the infected cell towards NK cell-mediated lysis. Therefore, viruses that target MHCI expression often also sabotage NKG2D-mediated cell responses by targeting NKG2DLs on the infected cell [4-7].

[0178] NKG2DLs are not normally expressed on the cell surface but can be induced by cellular stress [8]. The specific trigger for NKG2DL expression is not known but NKG2DLs are upregulated in response to several viral infections [9-12]. NKG2DLs comprise a large group of proteins all recognized by NKG2D, despite having low sequence identity. NKG2DLs include the MIC (A and B) and ULBP (1-6) families in humans as well as MULT1 and the RAE-1 (α-ε) and H60 (a-c) families in mice [13]. The redundancy in NKG2DLs is likely due to a combination of tissue specific expression patterns of the ligands and the need to counter viral NKG2D evasion strategies [14]. Many viruses have evolved mechanisms to inhibit the cell surface expression of NKG2DLs as a means of interfering with NKG2D surveillance of viral infection. This strategy is most apparent among β- and γ-herpesviruses, in which four murine cytomegalovirus proteins (m138, m145, m152, m155) [15-18], two human cytomegalovirus proteins (UL16, UL142) [19,20] and one Kaposi's sarcoma-associated herpesvirus protein (K5) [21] have been demonstrated to block NKG2DL surface expression. This evasion strategy is also found in RNA viruses, as hepatitis C virus NS3/4a and human immunodeficiency virus Nef proteins also block the expression of a subset of NKG2DLs [22,23]. Additionally, human cytomegalovirus, herpes simplex virus type 1 and Epstein-Barr virus each also encode at least one miRNA that prevents translation of MICB [24,25]. Similarly, JCV and BKV polyoma viruses target ULBP3 with

miRNAs [26]. However, blocking NKG2DL expression on the infected cell is an imperfect evasion strategy, since no single viral protein or miRNA has been shown to block the expression of all NKG2DLs.

[0179] Like several herpesviruses, cowpoxvirus (CPXV) also sabotages MHCI expression. CPXV expresses CPXV012 and CPXV203, two proteins that prevent TAP-mediated peptide transport and MHCI trafficking to the cell surface, respectively [27-34]. Ectromelia virus, a related orthopoxvirus, induces NKG2DL expression and NKG2D is critical for the control of ectomelia virus pathogensis [35]. Infection with another orthopoxvirus, monkeypox virus, leads to dramatic expansion of NK cells but impaired NK cell function [36]. Together this suggests that CPXV infected cells would be sensitive to NK cell-mediated lysis.

[0180] Unlike herpesviruses, CPXV does not target NKG2DLs. Instead this virus targets NKG2D directly by encoding a competitive inhibitor of NKG2DLs, orthopoxvirus MHC class I-like protein (OMCP) [37,38]. OMCP is a 152 residue protein that is secreted from infected cells and antagonizes the NKG2D-mediated killing of NKG2DL-expressing target cells [37]. OMCP also plays an important role *in vivo*, with OMCP-null CPXV attenuated in mouse models of infection (M. Sun *et al,* personal communication). OMCP binds to murine NKG2D with an affinity equal or greater than all tested murine NKG2DLs, and to human NKG2D with an affinity ~5,000-fold higher than human NKG2DLs [37-40].

[0181] Despite their divergence in sequence identity, all known host NKG2DLs share common structural features [41,42]. NKG2DLs contain an MHCI-like platform domain composed of an eight-stranded beta sheet with two helices [43-47]. The platform domain is subdivided into α1 and α2 domains, with each domain containing four beta strands and an alpha helix. Unlike MHCI, the groove between the helices of the NKG2DL platform domain is closed and therefore NKG2DLs do not bind peptides.

[0182] Like host NKG2DLs, OMCP also adopts an MHCI-like platform domain [38]. However, the platform domain of OMCP has been trimmed to have only a six-stranded beta sheet with shorter flanking helices. We termed the helix of the α1 domain H1 and the discontinuous helix of the α2 domain is termed H2a and H2b. The H2a and

H2b helices of OMCP are also rearranged to be flatter against the beta sheet and to be splayed apart from each other. These differences in the OMCP structure were hypothesized to be important for the high affinity binding of OMCP to NKG2D. However, OMCP was still expected to bind to NKG2D in the same orientation as host NKG2DLs, i.e. with the alpha helices oriented diagonally within the symmetric NKG2D binding groove.

[0183] Here we report the 2.0 Å-resolution structure of human NKG2D bound to OMCP of the Brighton Red strain of cowpoxvirus. The structure reveals a significant reorientation of OMCP in the NKG2D binding groove relative to host NKG2DLs. The interface of OMCP with NKG2D is highly complementary, buries a significantly larger surface area than host NKG2DLs, and remains continuous across the entire NKG2D binding groove. This novel binding adaptation and high affinity allows OMCP to compete with the high local concentration of membrane-associated host NKG2DLs. We further show that the mechanism of NKG2D antagonism requires OMCP to be secreted, lest it lead to NKG2D signaling.

Example 7. Structure determination of OMCP-NKG2D.

[0184] We had previously solved the structure of OMCP alone and shown that, similar to host NKG2DLs, OMCP adopts an MHCI-like platform domain [38]. Despite the overall similarity of the domain structure of OMCP to host NKG2DLs, OMCP had several notable deviations in the putative NKG2D-binding site that were hypothesized to be important for the high affinity binding of OMCP to NKG2D. To further understand the unusually high affinity of OMCP for NKG2D, we crystallized and solved the structure of OMCP bound to human NKG2D.

[0185] Initial crystallization trials with OMCP and NKG2D yielded ~30 different crystallization conditions. Subsequent data collection and molecular replacement of multiple low-resolution crystal forms all yielded similar partial solutions, with alternating sheets of OMCP-NKG2D complexes separated by undefined density. In the original structure of OMCP alone, the beta sheets packed to form a trimer with the alpha helices oriented away from the center [38]. An identical OMCP trimer formed in the OMCP-NKG2D partial solutions, with NKG2D now bound to the outward facing helices (data

not shown). In an attempt to change the lattice packing, we introduced mutations into the beta sheet of OMCP that were designed to break the trimeric interface. These mutations were on the opposite face of OMCP from the NKG2D binding site to avoid disrupting OMCP-NKG2D binding. A mutant form of OMCP (Y23D, F95D) crystallized with NKG2D in a new space group and the crystals diffracted to 2.0 Å (**Table 1**)(**FIG. 24A**).

[0186] The electron density map was continuous and unambiguous throughout all chains of the structure, with the exception of Q108 in OMCP. This residue was situated in the center of the largest loop of OMCP and unambiguous density for this residue was also absent from the structure of OMCP alone [38]. The structure of OMCP bound to NKG2D showed no major differences from our previous structure of OMCP alone, with an RMSD for all atoms of 0.8 Å. Likewise, NKG2D was also similar to previous NKG2D structures with RMSDs ranging from 0.5-0.9 Å. The β3-β4 loop of NKG2D is the only region of either OMCP or NKG2D that displayed above-average B factors. This loop is thought to be flexible and has had above average B factors in all previous NKG2D structures [48]. Interestingly, the peptide bond between S193-S194 in our NKG2D structure had a *cis* conformation not described in other NKG2D structures (**FIG. 29**).

Example 8. The interface between OMCP and NKG2D.

[0187] OMCP was hypothesized to bind to the same surface of NKG2D used by host NKG2DLs because (i) OMCP competed with host NKG2DLs for NKG2D and (ii) mutations within the NKG2DL-binding pocket of NKG2D altered OMCP binding affinity [38]. OMCP does bind NKG2D using the same concave binding pocket as host NKG2DLs (**FIG. 24A**). OMCP binds primarily using the discontinuous helices of its α2 domain, H2a and H2b. The position of the H2a and H2b helices is such that every surface exposed side chain of both helices within the binding site directly contacts NKG2D (**FIG. 24B**). Only two contacts are found outside of H2a and H2b, Ile49 and Arg66. Both of these residues are within the α1 domain but lie outside of the H1 helix.

[0188] Twelve OMCP residues contact eighteen NKG2D residues to form a mixture of bond types (**Table 2**). Three residues in each NKG2D half-site are known as core binding residues because they make contacts with all known host NKG2DLs. The

core residues of NKG2D subunit A ($NKG2D^A$) (Tyr152, Tyr199, Met184) form two hydrogen bonds and make extensive hydrophobic contacts with OMCP residues. The core residues of $NKG2D^A$ contact four OMCP residues and the most critical of these residues is Phe122. Phe122 makes multiple hydrophobic contacts with all three $NKG2D^A$ core residues, including *pi*-stacking with Tyr152. Phe122 also forms a backbone-to-sidechain hydrogen bond with Tyr152. Interestingly, OMCP is the first NKG2D ligand not to utilize all six NKG2D core-binding residues, with only Met184 and Tyr152 of NKG2D subunit B ($NKG2D^B$) contacting OMCP. $NKG2D^B$ Met184 and Tyr152 each make a single hydrogen bond and hydrophobic contacts with OMCP residues. Two OMCP residues, Trp127 and Asp132, make contacts with both NKG2D protomers. OMCP Trp127 forms a hydrogen bond to Lys150 of $NKG2D^A$ and makes several hydrophobic contacts with Leu148 of $NKG2D^B$, Lys150 and Ser151 of $NKG2D^A$. OMCP Asp132 forms a hydrogen bond with Tyr152 of $NKG2D^B$ and a salt bridge with Lys150 of $NKG2D^A$ (**FIG. 25A**).

[0189] Due to the high affinity of the OMCP-NKG2D interaction we harnessed a high throughput *in vitro* selection approach to find NKG2D-binding null mutants (**Table 3**). The results of the screen identified D132 as an important residue for disrupting NKG2D binding. We then generated the mutation D132R in attempt to completely ablate NKG2D binding. Surprisingly, the D132R mutant alone was unable to bind to NKG2D at concentrations 35-fold above the K_D (**FIG. 25B**), but did not affect binding of OMCP to FcRL5-expressing cells (**FIG. 25C**). This mutation is likely to cause significant steric clashes, as well as disrupting both interactions made by Asp132 to $NKG2D^A$ Lys150 and $NKG2D^B$ Tyr152 (**FIG. 25A**).

[0190] Previously, the 14-fold higher affinity of OMCP for human vs murine NKG2D was mapped to three amino acid substitutions in the β5'-β5 loop of NKG2D, abbreviated L2 [38]. In addition to the substitutions themselves (I182V, M184I and Q185P), the position of the loop between NKG2D orthologs differs. L2 in human NKG2D is bent towards the center of the concave binding cavity compared to L2 of murine NKG2D. Superimposition of murine NKG2D onto the human NKG2D-OMCP structure reveals that the contacts between OMCP and Met184 (mNKG2D residue I200)

in $NKG2D^B$ and between Met184 (I200) and Glu185 (P201) in $NKG2D^A$ would be altered due to the different position of the murine β5'-β5 loop (**FIG. 26A-B**). This alteration would disrupt contacts with three residues in OMCP H2a, three residues in H2b and Arg66 within the α1 domain. Of the contact residues of L2, Met184 makes the most significant contacts in both NKG2Ds (**Table 2**)(**FIG. 26C**). Critically, of the 58 NKG2D sequences available in GenBank, 54 conserve the Met184 and Glu185 found in the high affinity human NKG2D (**FIG. 26D**).

[0191] Eighteen OMCP variants have been described between different CPXV and MPXV strains [51]. In this study we have crystallized OMCP from the Brighton Red strain of CPXV which has >60% sequence identity with the highly conserved sequence of the other 17 OMCP variants, collectively termed $OMCP_{mpx}$. Of the 12 OMCP contact residues observed, 9 are identical to $OMCP_{mpx}$. Of the remaining contacts, all three are conservative hydrophobic substitutions (I49L, T118I and M135I) (**FIG. 27**). $OMCP_{mpx}$ binds to NKG2D and the substitutions in the NKG2D contact residues are unlikely to grossly affect the affinity of $OMCP_{mpx}$ for NKG2D [37].

Example 9. A novel NKG2D-binding adaptation.

[0192] Host NKG2DLs have low sequence identity but overall similar structures, with MHCI-like platform domains binding diagonally across the symmetric binding groove created by the NKG2D homodimer [13,41,52]. Host ligands contact one NKG2D half site with H1 and the S1-S2 loop, and contact the second NKG2D half site with H2b. Despite the similar MHCI-like fold, OMCP binds the NKG2D binding groove in a novel orientation, rotating ~45° relative to host NKG2DLs (**FIG. 27**). Instead of using H1 and S1-S2 loop like host ligands, OMCP has replaced these contacts with H2a. This rotation leads to the helices of OMCP being perpendicular to the NKG2D binding groove, instead of lying diagonally across it.

[0193] Two unique rearrangements of H2a and H2b make the OMCP orientation possible. The α2 helices of OMCP and host NKG2DLs are discontinuous, with the two shorter helices hinged relative to each other. For host ligands, the angle between H2a and H2b is ~90°, positioning H2a away from the NKG2D interface. In contrast, OMCP has increased the hinge angle between the helices by ~20°, leading to a α2 helix that is

flatter relative to the beta sheet of OMCP. The flattening of the α2 helix allows H2a and H2b to closely complement the concave binding groove of the NKG2D homodimer (**FIG. 24B**). The tight fit of the α2 helix for NKG2D is reflected in the high shape complementarity (0.77) and buried surface area (2,612 $Å^2$). In contrast, host NKG2DLs have shape complementarity ranging from 0.63-0.72 and buried surface areas ranging from 1,700-2,180 $Å^2$ [43,44,46].

[0194] The second unique feature of the α2 helix is the separation of H2a and H2b relative to each other. This region also contains a translation that completely separates H2a and H2b into two distinct helices. This translation is critical for NKG2D binding because it allows each helix to be directly centered on the core binding sites of each NKG2D monomer (**FIG. 27**). This creates a symmetric binding site on OMCP that recognizes the symmetric binding groove created by the NKG2D dimer. The symmetry between OMCP and NKG2D binding is in stark contrast to the canonical binding of an asymmetric host ligand to the symmetric NKG2D binding groove [52]. However, one element of asymmetry remains in the OMCP-NKG2D interaction because each NKG2D half-site recognizes an OMCP helix in a different N- to C-terminal orientation, demonstrating again the flexibility of NKG2Ds rigid adaptation recognition [41,53].

[0195] The contact sites between NKG2D and host NKG2DLs are made up of two patches centered on the core binding sites of NKG2D and H1/S1-S2 loop and H2b of NKG2DLs [41]. As a result, the interface of NKG2D with NKG2DLs is discontinuous, particularly in the center of the NKG2D binding groove (**FIG. 27**). Due to the unique orientation of OMCP, H2a and H2b make continuous contacts along the entire NKG2D binding groove (**FIG. 27**). The sidechains of OMCP Lys126, Trp127, Glu131 and Asp132 make contacts with residues in the center of the NKG2D binding groove and bridge the core binding sites on each NKG2D monomer (**FIG. 24B**). In particular, OMCP Trp127 is directed towards the center of the NKG2D dimer and makes hydrophobic contacts with residues on both NKG2D monomers, effectively closing any gaps in the binding interface.

Example 10. Signaling of NKG2D upon ligand engagement.

[0196] CPXV and MPXV-infected cells secrete OMCP, which can act as an NKG2D-antagonist [37]. This immune evasion strategy is reminiscent of cancer induced-NKG2DL shedding. Some cancer cells proteolytically cleave NKG2DLs from the cell surface using matrix metalloproteinases (MMPs), simultaneously preventing NKG2D-bearing lymphocytes from targeting the cancer cell, as well as creating soluble NKG2DLs to inhibit NKG2D in *trans*. Cell-associated NKG2DLs trigger NKG2D effector functions (**FIG. 28A**), while cancer-induced, soluble NKG2DLs block NKG2D function (**FIG. 28B**). Like shed NKG2DLs, OMCP is soluble and blocks NKG2D function in *trans* [37] (**FIG. 28C**). Unlike host NKG2DLs, OMCP binds NKG2D with a novel orientation. We therefore asked whether OMCP could serve as a NKG2D agonist in the context of the cell membrane, analogously to host NKG2D ligands. Since OMCP is a secreted protein, an artificially cell-associated OMCP was constructed by using a heterologous transmembrane domain from Thy1.1 [37] (**FIG. 28D**). To measure NKG2D-mediated cell killing, we stably transduced Ba/F3 cells with retroviral vectors expressing either the OMCP-Thy1.1 construct or host NKG2DLs. OMCP-Thy1.1-expressing target cells were killed equivalently to host NKG2DL-transduced target cells, indicating that despite its altered binding orientation, cell-associated OMCP was able to activate NKG2D signaling (**FIG. 28E**). Thus, OMCP must be secreted lest it active NKG2D-effector functions itself, despite potential loss of efficacy due to diffusion.

Discussion for Examples 7-10.

[0197] While many viruses have adopted a general mechanism of NKG2D-sabotage by trying to retain multiple host-encoded NKG2D ligands within the infected cell, CPXV and MPXV take the very different approach of targeting NKG2D directly. Since NKG2D is monomorphic, this mechanism has the significant advantage of requiring a single protein to prevent NKG2D recognition of the infected cell. The large number of sequence-divergent host NKG2DLs and their associated polymorphisms are thought to be driven by selection from pathogen-encoded NKG2DL antagonists [14]. Likewise, viral NKG2L antagonists are under selective pressure from the diverse host NKG2DLs in a continual cycle of adaptation. Due to the need to recognize multiple

NKG2DLs, NKG2D has a limited mutational space to adapt. The limited ability of NKG2D to mutate is yet another advantage of OMCP directly targeting NKG2D, instead of NKG2DLs.

[0198] Similarly to OMCP, some cancer cells shed host NKG2DLs to create their own soluble NKG2D antagonists. However, this strategy has the additional benefit of removing host NKG2DL from the surface of cancer cells. In contrast, CPXV and MPXV lack a known mechanism of blocking host NKG2DL surface expression. Secreted OMCP must then be able to compete efficiently against the high local concentration of multiple host NKG2DLs on the infected cell, as well as against diffusion away from the infected cell. One possible way to increase OMCP's ability to compete with host ligands would be to increase the avidity of OMCP by having multiple NKG2D-binding domains. However, a multimeric OMCP could crosslink NKG2D and potentially trigger NKG2D-mediated killing. Therefore, secreted OMCP must be monomeric to prevent aberrant NKG2D signaling. Thus to compensate for these deficiencies, OMCP must have the highest affinity possible to effectively compete against cell-associated host NKG2DLs [37,38]. The half-life of ligand-receptor interactions correlate well with physiological competitiveness [55]. OMCP binds human and murine NKG2D with half-lives of 348 and 54 seconds, respectively, compared to half-lives of 1.5-18 seconds for most NKG2DLs [38,44,56]. Indeed, the increased half-life for NKG2D allows OMCP to effectively antagonize NKG2D-mediated immunity in a murine infection model (M. Sun *et al,* personal communication).

[0199] To understand the molecular basis for the long half-life of OMCP for NKG2D, we previously determined the structure of OMCP alone, and here, we report the structure of OMCP bound to NKG2D. The structure of OMCP alone was grossly similar to that of host NKG2D ligands, containing an atypical MHCI-like platform domain. Host NKG2D ligands bind with the helices of their platform domains oriented diagonally within the symmetric binding groove of NKG2D. Thus it was expected that OMCP was a viral mimic of host NKG2D ligands and would interact with NKG2D analogously.

[0200] The structure of OMCP-NKG2D instead revealed a novel orientation for an NKG2D ligand in the NKG2D binding groove. Alterations within the α2 domain helix

allow OMCP to arrange its helices perpendicularly within the binding groove. This reorientation places the H2a and H2b helices directly in contact with the core binding sites of NKG2D and also forms the largest and most continuous binding interface with NKG2D. Because the forces (hydrogen bonds, van der Waals, hydrophobic interactions) that mediate protein-protein interactions are individually weak, a large, continuous interface with high shape complementary allows for a cumulatively strong interaction between proteins. This change in the binding orientation of OMCP reveals how the MHCI-like platform used by host ligands can be adapted by a pathogen to enhance NKG2D binding.

[0201] Since host NKG2DLs and OMCP have a similar MHCI-like platform, it is reasonable to wonder why no host ligand has evolved an analogous high-affinity interaction with NKG2D. One likely reason is that the host immune response must be carefully calibrated to balance the need for protection against the threat of autoimmunity. Since the expression of NKG2DLs on the cell surface signals for effector functions, even a small amount of high affinity host ligand on the cell surface could trigger an immune response, and the resulting tissue damage could be deleterious for the host. Indeed, NKG2D-expressing cells and/or aberrant expression of host NKG2DLs have been implicated in diabetes, celiac disease and rheumatoid arthritis [57-60]. Viruses are not constrained by autoimmune selective pressures. Therefore, CPXV and MPXV were free to evolve a viral NKG2DL with the highest possible affinity to maximize immune evasion potential.

[0202] Interestingly, OMCP triggers NKG2D signaling when attached to a target cell membrane, despite the novel orientation of OMCP relative to host NKG2DLs. The interaction of host NKG2DLs with the dimeric NKG2D bears broad structural similarity to the interaction between MHC molecules with their cognate T cell receptors (TCRs). In both cases, the NKG2DL/MHC lies diagonally across the surface created by the dimeric NKG2D/TCR. However, there are several examples of MHC-TCR complexes that, like OMCP-NKG2D, interact with unconventional orientations [61-65]. Several of these complexes involved autoimmune MHC-TCR complexes that were tilted or rotated outside of the normal range for MHC-TCR complexes [61,65]. While these receptors

could induce TCR signaling at high MHC concentrations, they failed to assemble characteristic immunological synapses [66]. A striking example of unconventional binding was found when an *in vitro* peptide library-MHC-TCR (H2-L^d-42F3) screen produced a p3A1-H2-L^d-42F3 complex with an interface rotated ~40° relative to other H2-L^d-42F3 complexes. This rotation places the TCR nearly parallel with the MHC peptide-binding groove and shifted the interface center almost entirely on one of the MHC α helices - an orientation strikingly similar to the interface of OMCP-NKG2D [65]. Interestingly, the p3A1-H2-L^d-42F3 complex failed to induce TCR signaling [65]. Thus, unlike OMCP/NKG2D, the orientation of MHC relative to TCR is an important factor for signaling.

[0203] OMCP-NKG2D and p3A1-H2-L^d-42F3 have opposite signaling outcomes, despite having very similar orientations. TCR signaling requires co-receptor binding to either the α2/β2 or α3 domains of MHCII or MHCI, respectively. The failure of p3A1-H2-L^d-42F3 to signal, and of other unconventional MHC-TCR complexes to form true immunological synapses, is potentially due to the inability of co-receptors to form correct quaternary structures for signaling [64,65,67]. Signaling by NKG2D is not known to require co-receptor stimulation and the majority of NKG2DLs lack the co-receptor binding α2/β2 or α3 domains of true MHC molecules. This difference in co-receptor dependency likely explains why OMCP (when attached via transmembrane) is still competent to stimulate NKG2D-signaling compared to MHC-TCR complexes with unconventional binding orientations. Further, it suggests that clustering of NKG2D on the cell surface is the major determinant of NKG2D-mediated activation.

Methods for Examples 7-10.

[0204] *Identification of NKG2D-binding null mutant D132R.* A high throughput *in vitro* selection approach based on combinatorial cell surface display was utilized to identify NKG2D-binding null mutants. The sequence of OMCP was globally mutagenized using error-prone PCR, and the mutated amplicons were spliced to a signal-less Thy1.1 cDNA via overlap extension PCR. This library of mutated OMCPs fused to unmutated Thy1.1 was cloned into the pMXs-IRES-EGFP retroviral transfer vector (kind gift of Toshio Kitamura, University of Tokyo) to generate a molecular library

for transduction into Ba/F3 cells. The transductants were then sorted for green fluorescence and anti-Thy1.1 expression to yield a cellular library whose members all had surface expression of OMCP, filtering out mutations giving frameshifts, premature stop codons, and folding-incompetent OMCP. This OMCP library was sorted for NKG2D binding using NKG2D-tetramers. Sorted cells were cloned by limiting dilution and analyzed. The retroviral cassettes of cells lacking or having reduced NKG2D-binding activity were amplified and sequenced. Utilizing this approach, we identified Asp132 as a critical residue for NKG2D binding.

[0205] *Protein expression and purification.* $OMCP_{BR}$ and human NKG2D expression constructs were previously described [38]. The (D132R) $OMCP_{BR}$ protein was prepared identically to WT $OMCP_{BR}$. (23D/95D) OMCP-NKG2D complex was reconstituted by oxidative co-refolding from purified inclusion bodies, as described previously [38]. Refolded protein was slowly diluted 10-fold with water and captured on a 5 ml HiTrap Q HP column (GE Healthcare) using a Profinia instrument (Bio-Rad). The captured protein was washed with 50 mM Tris, pH 8.5, 20 mM NaCl and bulk eluted with 50 mM Tris, pH 8.5, 250 mM NaCl. The eluted protein was then concentrated and further purified by gel filtration chromatography on a Superdex S75 column (16/60; Amersham Biosciences). Fractions containing mono-dispersed OMCP-NKG2D complex (~50 KDa) were pooled and buffer exchanged into 25mM Ammonium acetate pH 7.4.

[0206] *Crystallization, data collection and processing.* Native protein crystals were grown by hanging drop vapor diffusion at 20°C by streak seeding into a well solution containing 15% PEG 3350, 0.2M $MgCl_2$, 0.1M Bis-Tris pH 6.75. Crystals were cryoprotected with well solution containing 15% glycerol before flash freezing directly in a liquid nitrogen bath. Diffraction data were collected at the Advanced Light Source synchrotron (beamline 4.2.2). Native (23D/95D) OMCP-hNKG2D crystal diffraction data were collected at 100 K and at a wavelength of 1.00004 Å. Additional diffraction data statistics are summarized in **Table 1**. Data processing with HKL2000 [68] showed the crystals belonged to the primitive monoclinic space group $P2_1$ (space group #4). The

asymmetric unit of the crystal contained two copies of the (23D/95D) OMCP-hNKG2D complex.

[0207] *Model building and refinement.* The structures of human NKG2D (1MPU) [48] and OMCP (4FFE) [38] were used as search models for molecular replacement through Phenix [69]. Reiterative refinement and manual rebuilding were performed using Phenix and Coot [70], respectively. Both 2Fo-Fc and Fo-Fc maps were used for manual building and to place solvent molecules. The final model yielded an R_{work} of 16.6% and R_{free} of 21.4%, with 4% of all reflections set aside for free R factor cross-validation. Progress in refinement was also measured using the MOLPROBITY webserver [71]. The final Ramachandran statistics for the model were 98% favored and 0% outliers. Additional refinement statistics are summarized in **Table 1**. Images of structures were produced using the program PyMol [72].

[0208] *Structure analysis.* Analysis of the contact residues, buried surface area and shape complementarity of the OMCP-NKG2D interface were carried out using the programs Ligplot+ [73], PISA [74] and SC [75]. Structural programs as compiled by the SBGrid consortium [76]. Analysis of NKG2D conservation was performed using the ConSurf server [77-80]. GenBank numbers for species used in Consurf analysis are: Humans (30749494), Borean orangutan (21902299), Chimpanzee (57113989), Gibbon (332232684), Macaque (355785888), Green Monkey (635063485), Common marmoset (380848799), Mouse (148667521), Brown rat (149049263), Guinea Pig (348569092), Ground squirrel (532114387), Deer mouse (589967905), Naked mole rat (512868733), Prairie vole (532053033), European Shrew (505834608), Star-nosed mole (507978716), Chinese hamster (537136230), and Cat (410963826).

[0209] *Atomic coordinates.* The atomic coordinates (accession code 4PDC) have been deposited in the Protein Data Bank, Research Collaboratory for Structural Bioinformatics (Rutgers University, New Brunswick, NJ)

[0210] *In vitro NK cell killing assays.* Splenocytes from C57BL/6 mice were preactivated with 200 U/ml IL-2 for 24 hours and used as cytotoxic effectors against stably transduced Ba/F3 cell lines in standard killing assays. Target cells were carboxyfluorescein succinimidyl ester (CFSE) labeled and co-incubated with activated

splenocytes at 37°C, 5% CO2 for 4 hours at effector:target ratios of 10:1, 20:1, and 40:1. Killing percentage was determined by incorporation of the dead cell exclusion dye 7-amino-actinomycin D (7AAD) in the CFSE+ target population as assessed by flow cytometry. Percent specific lysis was calculated using the formula [(experimental dead % - background dead %) / (maximum release dead % - background dead %)] x 100. C57BL/6 mice were obtained from the National Cancer Institute (Charles River, MA). Mice were maintained under specific pathogen-free conditions and used between 8 and 12 weeks of age. Single cell suspensions of splenocytes used in killing assays were generated using standard protocols [81].

Table 1: Data collection and refinement statistics

	$OMCP_{BR}$-hNKG2D
Data collection	
Space group	$P2_1$
Cell dimensions	
a, b, c (Å)	43.3, 101.1, 91.4
α, β, γ (°)	90.0, 91.6, 90.0
Resolution (Å)	50-2.0 (2.07-2.00)
R_{sym}	11.8 (48.5)
I / σ	14.5 (3.8)
Completeness (%)	93.5 (91.5)
Redundancy	6.2 (5.3)
Refinement	
Resolution (Å)	44-2.0
Total reflections	309693
Unique reflection	50139
R_{work}	16.6% (21.0%)
R_{free}	21.4% (29.5%)
Wilson B-factor	21.62
Protein residues	791
Water molecules	524
R.M.S. deviations	
Bond lengths (Å)	0.003
Bond angles (°)	0.79

[a] As defined by PHENIX [69]

Table 2: Interface contacts between NKG2D and OMCP

NKG2D-A	OMCP	Bond type
Lys150	Asp132	Salt bridge
Lys150	Trp127	H bond
Lys150	Trp127	Φ (3)

Ser151	Lys126	H bond
Ser151	Trp127	Φ (1)
Tyr152	Phe122	H bond
Tyr152	Phe122	Φ (9)
Tyr152	Lys126	Φ (5)
Met184	Thr118	H bond
Met184	Thr119	Φ (1)
Met184	Phe122	Φ (5)
Gln185	Arg66	Φ (1)
Leu191	Phe122	Φ (1)
Tyr199	Phe122	Φ (4)
Glu201	Arg66	Salt bridge
Thr205	Arg66	H bond
NKG2D-B	**OMCP**	**Bond type**
Leu148	Trp127	Φ (1)
Ser151	Glu131	H bond
Tyr152	Asp132	H bond
Tyr152	Glu131	Φ (3)
Tyr152	Met135	Φ (5)
Ile182	Ile49	Φ (2)
Glu183	Arg142	Salt bridge
Met184	Met135	Φ (1)
Met184	Arg138	Φ (2)
Met184	Arg142	H bond
Lys186	Arg142	Φ (1)
Leu191	Met135	Φ (1)
Glu201	Arg138	Salt bridge

Hydrogen bonds (H bonds), salt bridges and carbon-to-carbon hydrophobic interactions (Φ) are shown for each contact residue. The number of hydrophobic interactions between contact residues is designated in parenthesis.

Table 3:NKG2D binding mutations identified through global

Amino Acid	Frequency of Mutation	Associated Mutations	Solvent Accessible
D132	4	D132N D132N, T31S, V68A D132G, K126N, D76V D132G, K126N, D76V	++
K126	4	K126N K126N, S71G	++

		K126N, D132G, D76V	
		K126N, D132G, D76V	
K125	2	K125E, F65C	-
		K125E, F92V	
S120	2	S120Y	-
		S120Y, E10A, N56K	
D76	2	D76V, D132G, K126N	++
		D76V, D132G, K126N	
W116	2	W116R	-
		W116R, K113Q	
R123	2	R123G, D26G, F50L	-
		R123G, D21V, F128L	
E75	1	E75D	-
S71	1	S71G, K126N	++
F92	1	F92V, K125E	+
F65	1	F65C, K125E	-
K113	1	K113Q, W116R	+
E10	1	E10A, N56K, S120Y	++
N56	1	E10A, N56K, S120Y	++
D21	1	D21V, R123G, F128L	++
F128	1	D21V, R123G, F128L	-
D26	1	D26G, F50L, R123G	++
F50	1	D26G, F50L, R123G	-
T31	1	T31S, V68A, D132N	++
V68	1	T31S, V68A, D132N	+
I30	1	I30L, L51F, L64P, M135T	-
L51	1	I30L, L51F, L64P, M135T	-
L64	1	I30L, L51F, L64P, M135T	++
M135	1	I30L, L51F, L64P, M135T	++
R67	1	R67S, L117P, T119N, F122L	+
L117	1	R67S, L117P, T119N, F122L	-
T119	1	R67S, L117P, T119N, F122L	++
F122	1	R67S, L117P, T119N, F122L	++

Mutations were sequenced from 17 clones expressing mutagenized OMCP-Thy1.1. Clones were selected for reduced binding to NKG2D tetramers. The selected clones showed variable deficits in NKG2D binding. Each clone had 1-4 mutations in the amino acid sequence of OMCP (5 clones with 1 mutation; 4 clones with 2 mutations; 6 clones with 3 mutations; 2 clones with 4 mutations). Silent mutations are not indicated. Mutations are listed in the order of frequency sequenced from the selected clones, and mutations that occurred together within individual clones are listed where applicable. Clones highlighted in grey have at least one mutation in a solvent inaccessible residue that may alter the overall stability of OMCP.

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Example 11. Individuals with poorly functioning natural killer cells are more susceptible to malignancies.

[0211] **FIG. 14A** shows that AJ and 129 are lung cancer susceptible strain of mice and B6 and C3H are lung cancer resistant strains of mice based on the larger tumor burden found in AJ and 129 mice. **FIG. 14B** shows that when NK cells from the various mouse strains were incubated with LM2 lung carcinoma cells at varying ratios, the NK cells freshly isolated from B6 and C3H mice (lung cancer resistant strains) resulted in significantly more lysis of LM2 lung carcinoma cells than the NK cells freshly isolated from AJ and 129 mice (lung cancer susceptible strains). Taken together these data show that strains of mice that are resistant to lung cancer have NK cells that more effectively lyse lung carcinoma cells. Further, susceptible strains have poorly functioning NK cells.

[0212] That data also correlates with human data. **FIG. 15** shows that a greater percentage of NK cells appear to produce TNFα in "resistant" patients versus "susceptible" patients. Further, it has been shown that tumors downregulate the lytic capacity of NK cells, even if they were highly functional before.[53] Thus, even individuals with highly functioning NK cells may benefit from therapy to enhance NK cell function.

[0213] Notably, *ex vivo* cytokine activation can reverse natural killer cell dysfuction. **FIG. 16** shows that IL-2 activated NK cells from both resistant (B6 and C3H) and susceptible (AJ and 129) mouse strains can lyse LM2 lung cancer cells. Accordingly, mouse NK Cells that did not show significant lysis of cancer cells (NK cells from 129 & AJ strains) were much more effective at lysis when treated with IL-2. NK cells from cancer-resistant strains also showed increase % of specific lysis.

Example 12. OMCP-mutIL2 mediated immunotherapy *in vivo*.

[0214] Immunoregulation of malignancies involves an intricate interplay of multiple cellular components. $CD4^+Foxp3^+$ T_{regs} have been shown in multiple models to contribute to tumor-specific tolerance and facilitate tumor growth[4,16,17]. NK cells and $CD8^+$ CTLs contribute to immunoregulation of multiple tumors, such as melanoma[12,18]. Other tumors, such as lung cancer, are controlled almost exclusively by NK cells with little contribution by the adaptive immune system[19,20] (and unpublished data AS. Krupnick). In order to test OMCP-mutIL2 mediated immunotherapy we will rely on B16 melanoma expressing the model tumor antigen ovalbumin (MO5 tumor cell line)[21]. Multiple studies have demonstrated a role for both NK cells and $CD8^+$ CTLs in controlling melanoma growth[22-24]. Thus the melanoma model offers an experimental advantage in studying OMCP-mutIL2, which can activate both types of cells (**FIG. 1E-F**). Reagents specific to this tumor, such as tetramers for the MHC Class I-restricted $CD8^+$ T cell receptor specific for the melanoma tumor associated antigen tyrosinase-related protein 2 peptide SVYDFFVWL (SEQ ID NO:3), can be readily purchased commercially (Proimmune, Sarasota, Fl.). The use of an ovalbumin-expressing cell line also offers the advantage of studying the immune response to a the highly immunogenic peptide SIINFEKL (SEQ ID NO:4) in addition to naturally occurring tumor associated antigens such as tyrosinase-related protein 2 which generally expands T cells with low avidity[25,26].

[0215] In order to perform the studies B6 mice will be injected subcutaneously with $1x10^6$ MO5 melanoma cells. One week after tumor injection mice will be divided into 4 groups (10 mice per group) and treated with ten twice a day injections of either: wild type IL2 (group #1); mutIL2 (group #2); OMCP-mutIL2 (group #3) or; saline (group #4) (**FIG. 12**). Tumor growth will be followed by daily measurements of diameter for 4 weeks, or until one of the groups develops tumors > 2cm in diameter. At that point mice in all groups will be sacrificed for analysis. In addition to tumor growth, lymphocyte infiltration of both the tumor and draining inguinal lymph node will be evaluated by flow cytometry. We will quantitate the total number and activation status of $CD4^+Foxp3^+$ Tregs (evaluated by ICOS and GITR upregulation). We will also evaluate NK cell

number and activation as measured by IFN-γ production and CD69 upregulation. Antigen-specific CTL generation will be evaluated by quantitating both $CD8^+$ T cells and $CD8^+CD44^{hi}CD62L^{low}$ effector cells (ECs) that are primarily responsible for tumor clearance[22,27,28]. Antigen specificity will be determined by identifying $CD8^+$ CTLs with T cell receptor specific for either the ovalbumin peptide SIINFEKL (SEQ ID NO:4) or melanoma specific tyrosinase-related protein 2 peptide SVYDFFVWL (SEQ ID NO:3) (both tetramers from Proimmune, Sarasota, Fl.). Tumor apoptosis will be quantitated by TUNEL staining.

[0216] Based on our *in vitro* tumor data and *in vivo* phenotypic analysis we suspect that the OMCP-mutIL2 group will demonstrate attenuation in tumor growth with high number of NK cells, antigen-specific CTLs, specifically $CD8^+$ ECs, and fewer $CD4^+Foxp3^+$ $T_{regs.}$ If this turns out to be the case we would determine the relative role for $CD8^+$ or NK CTLs by depletion experiments. Even if CTLs increase it is possible that MO5 growth will not be altered. If that turns out to be the case we would look in closer detail at the $CD4^+Foxp3^+$ T_{regs} or in the presence and activation of myeloid-derived suppressor cells in OMCP-mutIL2 treated mice. Based on melanoma data additional tumors will be tested using similar methods.

Example 13. $CD8^+$ memory T cell generation after treatment with OMCP-mutIL2 fusion construct.

[0217] Once activation through their T cell receptor, naive $CD8^+$ T cells primarily differentiate into short-lived $CD44^{hi}CD62L^{low}$ effector cells (ECs) with cytolytic potential. A portion of activated cells, however, differentiate to long-lived $CD44^{hi}CD62L^{hi}$ central memory T cells ($CD8^+$ CMs)[29-31]. $CD8^+$ CMs act as an antigen specific reservoir for cellular protection and upon restimulation differentiate into $CD8^+$ ECs with cytolytic function. The durability of $CD8^+$ CMs makes them an ideal target for *ex vivo* generation and adoptive transfer for long-term protection[31]. The possibility of generating this cell population *in vivo* offers multiple advantages over an *ex vivo* system, including establishing a polyclonal population reactive to multiple tumor associated antigens and avoidance of costs associated with donor pheresis and *ex vivo* expansion. *In vivo*

expansion of tumor antigen specific $CD8^+$ CMs could also eliminate the need for frequent pheresis and cell readministration.

[0218] High dose IL2 therapy results in activation of both $CD4^+Foxp3^+$ T_{regs} and $CD8^+$ T cells but its effect on tumor associated antigen specific $CD8^+$ CM generation is unknown. Some have demonstrated, using antibody depletion, that $CD4^+Foxp3^+T_{regs}$ interfere with tumor specific $CD8^+$ CM generation[17,32] while others, using different models, have demonstrated that $CD4^+Foxp3^+$ T_{reg} depletion impairs $CD8^+$ memory formation[33,34]. OMCP-mutIL2 creates a unique immunologic environment where $CD4^+Foxp3^+$ T_{regs} are maintained but not actively expanded (**FIG. 3**). While NKG2D is not expressed on resting $CD8^+$ T cells, it is induced on this population upon activation[35]. Thus, unlike mutIL2, OMCP-mutIL2 results in $CD8^+$ T cell proliferation at levels comparable to wild-type IL2 in NKG2D-sufficent mice (**FIG. 1E-F**). The effect of OMCP-mutIl2 on $CD8^+$ T cell memory formation, however, is unknown but is critical to decipher based on the long-term tumor specific immunity that this cell population can confer.

[0219] In order to test long-term memory formation after cytokine stimulation *in vivo* we will utilize a model of irradiated tumor cell vaccination and cytokine treatment. In order to accomplish this we will subcutaneously inject $1x10^7$ lethally irradiated (10Gy) MO5 melanoma cells into C57Bl/6 mice. The recipient mice will then be treated either regular IL2 (group #1), mutIL2 (group #2), OMCP-mutIL2 (group #3) or saline (group #4) in twice daily doses over a course of 5 days (**FIG. 13**). The mice will be sacrificed at various time points ranging from one to three months post infection (**FIG. 13**). Antigen-specific $CD8^+$ CM formation will be assessed by phenotypic analysis of splenic, peripheral lymph node, lung, and liver-resident $CD8^+CD44^{hi}CD62L^{hi}$ CMs. Antigen specificity will be determined by MHC Class I staining for either the ovalbumin peptide, SIINFEKL (SEQ ID NO:4), or melanoma specific tyrosinase-related protein 2 peptide SVYDFFVWL (SEQ ID NO:3) (both from Proimmune, Sarasota, Fl.).

[0220] In order to test the functional protection of such vaccination protocols in a separate set of experiments mice from the four groups described above will not be sacrificed for phenotypic analysis and will be reinjected with live MO5 melanoma ($1x10^6$ cells/mouse subcutaneously). Melanoma growth will be assessed by serial

measurement of tumor diameter. Contribution of $CD8^+$ T cells to any immunologic protection will be assessed by CD8-specific antibody depletion in a portion of mice (clone YTS 169.4, BioXcell Inc., West Lebanon, NH).

Example 14. Mechanism of CTL activation by OMCP-mutIL2 fusion construct.

[0221] A mechanistic understanding of the enhanced activation of effector cell function by the OMCP-mutIL2 chimera will be critical for optimizing this therapeutic agent. The interaction of the fusion protein with IL2R and NKG2D are likely to be dependent on several factors including the length of the linker peptide (**FIG. 1E-F**). Therefore, it is critical to understand the mechanism of OMCP-mutIL2 chimera mediated CTL activation in order to allow for optimization of the construct and design of future immunotherapy protocols. The two-domain chimeric protein could potentially increase the activation of NKG2D-expressing cells by three non-mutually exclusive mechanisms. First and foremost the OMCP-mutIL2 construct could increase the avidity of mutIL2 binding to targeted cells. This could lead to an increase in the number of receptors occupied and increased signaling intensity compared to mutIL2. Additionally dual binding to both NKG2D and IL2R could decrease the rate of receptor internalization and increase the duration of signaling by IL2. It is also possible that the OMCP-mutIL2 construct alters the signaling profile by the target cell by activating both the IL2 and NKG2D stimulatory pathways. These three non-mutually exclusive effects could explain the increase in activation of our construct of CTLs in an NKG2D-mediated fashion.

[0222] There are several methods for determining the avidity of a protein for a cell, either directly (radiolabeled, fluorescent) or indirectly (antigen exclusion)[38,39]. We plan to determine the avidity of wild-type IL2, mutIL2, or OMCP-mutIL2 for $CD4^+Foxp3^+$ $T_{regs,}$ NK cells, and $CD8^+$ T lymphocytes using KinExA[40]. To accomplish this we will isolate cells from splenocytes of either wild-type C57Bl/6 or $NKG2D^{-/-}$mice on a C57Bl/6 background using a magnetic bead isolation kit (Miltenyi Biotech, San Diego, Ca.). Target cells will be serially diluted by a factor of 2 in 11 falcon tubes in media containing 0.05% NaN_3. The 12th tube will contain just the media. OMCP-mutIL2 or mutIL2 alone will then be added to each tube of either wild-type or $NKG2D^{-/-}$ cells and the cells with cytokine will be rotated at 4 °C for 36 h. At the end of 36 h, the cells were centrifuged at

2400 rpm for 4 min and the free construct present in the supernatant will be measured by an anti-IL2 ELISA. The equilibrium dissociation constant (Kd) will then be calculated[41]. This approach has the advantage of measuring the avidity of cell surface molecules at physiologic densities and obviates the need for labeling, which can artificially lower the affinity of antibodies for their antigens[42,43].

[0223] The two-domain structure of the fusion protein is likely to significantly increase the half-life of the protein on the surface of NKG2D$^+$ and IL2R$^+$ cells. Any increase in surface half-life likely affects both the internalization of the bound receptors and signaling intensity and duration. To address the internalization of receptors, we will incubate each construct with the above mentioned cell types over a range of times and monitor the change in cell surface expression of IL2Rβγ and NKG2D using flow cytometry as previously described[44]. Of key interest will be the signaling profile of each construct. IL2-IL2R engagement signals through JAK-STAT pathways, while NKG2D signals through DAP10/12 pathways. While monomeric, soluble OMCP does not induce NKG2D signaling, OMCP can signal when concentrated locally on the cell surface[45]. Therefore, it is critical to determine whether the chimera is capable of inducing dual signaling through IL2R and NKG2D. IL2-mediated signaling will be assessed by Western blot for phosphorylated JAK1 and JAK3 in freshly isolated CD4+Foxp3+ T_{regs}, NK cells or CD8$^+$ T cells incubated in vitro with the construct[46,47]. NKG2D-mediated signaling will be assessed by immunoprecipitation of DAP10 or DAP12 followed by Western blotting for phosphotyrosine as previously described[48,49].

[0224] Both IL2 and OMCP interact with their cognate receptors with high affinity; the fusion of the two proteins is anticipated to greatly enhance the avidity of the chimeric construct for cells expressing both IL2R and NKG2D. As a consequence, the tethering of the construct to two cell surface receptors may lead to reduced internalization and increased duration of signaling. Combined these two phenomena represent the most likely mechanism for increased proliferation of NK cells *in vivo*. The signaling via NKG2D relies upon receptor clustering[45]. Since the construct is soluble it is possible, though unlikely, that the chimera will cluster NKG2D and induce DAP10/12 signaling. However, should DAP10/12 signaling be detected, we will then investigate

the importance of this signaling in the expansion of NK cells using cells derived from Vav1 knockout mice. Vav1 is a signal mediator downstream of DAP10[50]. Using a Vav1 knockout has the advantage of leaving NKG2D expression intact, in contrast to DAP knockouts[50]. This will remove the NKG2D signaling component while leaving the NKG2D-dependent targeting intact. A clearer understanding of the mechanism of action for OMCP-IL2 chimera dependent expansion will be crucial for further refinements of the therapeutic agent. Understanding these parameters will allow for testing of different construct designs, primarily in the length of the linker between OMCP and IL2, to calibrate the effects of the chimera.

Example 15. *In vivo* immunotherapy with IL-2, R38A/F42K IL2 or OMCP targeted IL2 constructs.

[0225] In order to determine if our construct plays a role in immunoregulation of malignancies as well as viral infections we will rely on *in vivo* models of B16 melanoma and mouse cytomegalovirus (MCMV). In one set of experiments B6 mice will be injected subcutaneously with $1x10^6$ cells of the poorly immunogenic B16 melanoma cell line. One week after tumor injection mice will be divided into 13 groups (5 mice per group) and treated with five daily injections of IL2, R38A/F42K IL2, OMCP fusion constructs or saline as described in **FIG. 18** and **Table 4**. Tumor growth will be followed by daily measurements of diameter for 4 weeks or until one of the groups develops tumors > 2cm in diameter. At that point mice in all groups will be sacrificed for analysis. In addition to tumor growth lymphocyte infiltration of both the tumor and draining inguinal lymph node will be evaluated by flow cytometry. We will quantitate the total number and activation status of $CD4^+Foxp3^+$ Tregs (expressed as % of tumor infiltrating lymphocytes and % $ICOS^+$). We will also evaluate NK cell number and activation as measured by IFN-γ production and CD69 upregulation. Tumor apoptosis will be evaluated by TUNEL staining.

Table 4: Experimental Design for Dosing for IL2, R38A/F42K IL2, OMCP-R38A/F42K IL2 or OMCP linked IL2 constructs			
Dose Cytokine	**LOW DOSE**	**INTERMEDIATE DOSE**	**HIGH DOSE**
IL2	Group 1	Group 2	Group 3
R38A/F42K IL2	Group 4	Group 5	Group 6
OMCP-wild-type IL2	Group 7	Group 8	Group 9
OMCP-R38A/F42K IL2	Group 10	Group 11	Group 12
Saline	Group 13		

[0226] In order to evaluate the therapeutic potential of IL2 in an infectious disease model, B6 mice will be infected with a sublethal dose of MCMV ($5x10^4$) particle forming units (PFUs) as previously described[29]. Day 1 post infection the mice will be divided into 13 groups (5 mice per group) and treated with five daily injections of IL2, R38A/F42K IL2, OMCP fusion constructs or saline as described in **FIG. 18** and **Table 4**. On post-infection day #6 the mice will be sacrificed and splenic and pulmonary viral load determined by standard plaque assay.

[0227] We expect that treatment with pure IL2 will have little effect on tumor growth or viral load as we expect to see preferential activation of T_{regs} over CTLs. We suspect that administration of the mutant R38A/F42K form of IL2 will result a lower tumor and viral burden compared to wild-type IL2 due to less activation of $CD4^+Foxp3^+$ Tregs. Nevertheless it is possible that despite lower levels of T_{reg} activation the tumor burden will be identical between IL2 and R38A/F42K IL2 due to decreased NK activation by the mutant form of IL2 as well. We expect OMCP IL2 construct-treated mice to have lower tumor burden compared to pure cytokine and predict that OMCP-R38A/F42K IL2 will demonstrate the best efficacy for immunotherapy with the most favorable side effect profile.

[0228] If we do not see an effect of OMCP expressing IL2 constructs we will closely evaluate our data for confounding factors such as excessive CTL death due to extreme stimulation as well as possible sequestration of CTLs in systemic organs such as the liver and lungs. If our hypothesis is supported and NK cells are activated and tumor growth ameliorated after OMCP-construct treatment we would repeat these experiments after NK depletion (using anti-NK1.1 clone PK136, mouse anti-mouse depleting antibody) and CD8 depletion (clone YTS169, rat anti-mouse $CD8^+$ T cell-

depleting antibody) (both from BioXcell, West Lebanon, NH). Based on these results future work will focus on immunotherapy in primary carcinogenesis models.

Example 16. The effects of IL-2, R38A/F42K IL2 or OMCP targeted IL2 constructs on immunosuppression after radiation exposure.

[0229] Sublethal radiation exposure is a constant risk to those involved in combat duty. In addition to the direct carcinogenic effects of radiation-induced DNA damage, sublethal irradiation results in immunologic damage due to selective death of lymphocyte subsets. $CD8^+$ T cells and $CD44^{lo}$ naïve T cells are specifically sensitive to radiation-induced death while NK cell function significantly declines after irradiation. $CD4^+25^+$ T cells as well as $CD44^{hi}$ memory-like T cells, however, have a survival advantage after radiation. Both $CD4^+25^+$ T cells and $CD8^+CD44^{hi}$ T cells can downregulate immune responses, explaining why even limited exposure to radiation can result in significant immunosuppression. Pharmacologic interventions to restore the immune system can alleviate morbidity and mortality of radiation poisoning. Surprisingly the role of IL2 in alleviating radiation-induced changes has never been studied. The low affinity IL2 receptor is expressed on bone marrow-resident hematopoietic stem cells and committed NK progenitors. NK cells, in turn, can secrete granulocyte-macrophage colony-stimulating factor (GM-CSF) upon stimulation, a cytokine that can assist with hematopoietic recovery. Based on these data in this aim we plan to test the hypothesis that IL2 or OMCP-IL2 constructs can assist with hematopoietic recovery after sublethal and lethal irradiation.

[0230] Based on previously described models of radiation-induced hematopoietic damage and recovery we will irradiate B6 mice with either sublethal 4.5 or lethal 7.5Gy from a cesium source. Within one hour of exposure mice in both radiation doses will be randomly divided into 13 groups as described in **Table 4** and treated for five days with low, intermediate or high dose IL2, R38A/F42K IL2 or OMCP expressing IL2 constructs (**FIG. 18**). A portion of the mice will be injected with saline after irradiation (group 13) (**Table 4**) and unirradiated untreated B6 mice will be included as a control as well (group 14). On day 6 hematopoietic recovery will be monitored by flow cytometric analysis of peripheral blood obtained by superficial mandibular vein sampling. The

sample will be analyzed for total number of NK cells, T cells, B cells, granulocytes, as well as monocytes and macrophages per ml of blood. Since 90% of untreated mice die 15-25 days after exposure to 7.5Gy, mice will be followed daily and survival curves in each treatment group will be compared by Kaplan-Meier analysis. Moribund mice in the 7.5Gy group will be carefully analyzed for cause of death evaluating the bone marrow, spleen and peripheral organs for both infection as well as hematopoietic failure by flow cytometry and tissue culture. Since mice in the sublethal 4.5Gy group are expected to survive long term, they will be sacrificed one month after exposure and peripheral lymphoid organs as well as bone marrow evaluated for hematopoietic recovery by flow cytometric analysis.

[0231] Radiation related DNA damage results in malignant transformation. Hematopoietic malignancies are especially prominent after radiation exposure. In order to evaluate the ability of IL2 or OMCP linked IL2 constructs to facilitate in clearing hematopoietic malignancies after radiation exposure we will treat B6 mice with sublethal exposure to 4.5Gy from a cesium source. Two days after irradiation the mice will be injected with 10^3 RMA-S lymphoma cells i.p. and three days later treated for a five day course with low, intermediate or high dose IL2, R38A/F42K IL2 or OMCP expressing IL2 constructs (**Table 4**, **FIG. 19**). Unirradiated B6 mice will be included as a control (group 14) as well. The mice will be followed for survival.

[0232] We anticipate that wild-type IL2 alone will have a negligible effect on immunorestoration since it will most likely result in preferential expansion of $CD4^+Foxp3^+$ T_{regs}, which are already preserved after irradiation. We suspect, however, that R38A/F42K IL2 as well as OMCP expressing IL2 constructs will expand the NK fraction in the peripheral blood and will contribute to broad hematopoietic recovery, albeit indirectly through secretion of homeostatic cytokines such as GM-CSF. If we detect no differences in hematopoietic recovery between IL2 and saline-treated groups, we will examine other confounding factors, such as homeostatic proliferation induced alteration of the immune system and the effect of IL2 or OMCP expressing IL2 constructs on such proliferation. While 200,000 IU of IL2 administered daily to B6 mice is not lethal, we realize that in the face of irradiation the mice might be weaker. It is thus

possible that dosing might need to be adjusted. For the "functional" part of this experiment we plan to specifically utilize the well-established model of RMA-S lymphoma challenge due to the role of NK cells in controlling hematologic malignancies. This established assay will allow us to gain rapid experimental data to advance this aim. Based on this data we would extend this aim in the future utilizing a primary carcinogenesis model as well.

Example 17. OMCP-targeted delivery of IL15 enhances CD25 upregulation.

[0233] Interleukin 15 (IL15) is a cytokine with structural similarity to IL2. Like IL2, IL15 binds to and signals through a complex composed of IL2/IL15 receptor beta chain (CD122) and the common gamma chain (gamma-C, CD132). IL15 is secreted by mononuclear phagocytes (and some other cells) following infection by viruses. IL15 regulates T and natural killer (NK) cell activation and proliferation. Survival signals that maintain memory T cells in the absence of antigen are provided by IL15. This cytokine is also implicated in NK cell development. IL-15 belongs to the four α-helix bundle family of cytokine.

[0234] OMCP was linked to the cytokine IL15 and its ability to active NK cells compared to IL15 alone was examined. NK cell activation was measured by CD25 upregulation. As demonstrated in **FIG. 21**, higher levels of CD25 are evident when IL15 is delivered by OMCP vs naked cytokine alone in equimolar doses.

Example 18. OMCP-targeted delivery of IL18 enhances NK cell activation.

[0235] OMCP was linked to WT human IL18, WT murine IL18 or mutant human IL18 (which inhibits its interaction with IL18BP) and its ability to active NK cells was examined (**FIG. 32**). Peripheral blood lymphocytes were cultured for 48 hours in 4.4 μM of either wild-type IL18 (blue), OMCP-IL18 (red) or saline (black). Activation of CD56+CD3- natural killer cells, as measured by surface CD69 expression, was superior by OMCP-IL18 compared to wild-type IL18 (**FIG. 33**). This data demonstrates that linking OMCP to IL18 also enhances NK cell activation relative to IL18 without OMCP.

Example 19. The D132R mutation in OMCP significantly decreases its NKG2D binding.

[0236] To further test the necessity of NKG2D binding in targeted delivery of IL2, we tested NK expansion and activation in the presence of mutIL2, OMCP-mutIL2, and (D132R) OMCP-mutIL2. The D132R mutation ameliorated the superiority of natural killer cell activation over cytokine alone (**FIG. 22**). Thus high affinity NKG2D binding is critical for targeted delivery and lymphocyte activation by IL2.

Example 20. OMCP-IL2 effectively treats infection caused by West Nile Virus (WNV).

[0237] The ability of various constructs of the invention to treat infection caused by West Nile Virus (WNV) was evaluated. Mice were given OMCP-IL2, the binding null mutant of OMCP, OMCP(D132R)-IL2, IL2 alone, IL2(38R/42A) alone and PBS. Upon treatment with OMCP(D132R)-IL2 and PBS all mice succumbed to infection by about day 11. Following treatment with IL2 alone, approximately 20% of mice survived until day 21. However, treatment with IL2(38R/42A) and OMCP-IL2 resulted in about 40% of mice surviving beyond 21 days (**FIG. 30A**). These results were consistently repeatable as demonstrated in **FIG. 30B**.

References for Example 11-20.

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HEADER    IMMUNE SYSTEM/VIRAL PROTEIN          17-APR-14   4PDC
TITLE     CRYSTAL STRUCTURE OF COWPOX VIRUS CPXV018 (OMCP) BOUND TO HUMAN NKG2D
COMPND    MOL_ID: 1;
COMPND   2 MOLECULE: NKG2-D TYPE II INTEGRAL MEMBRANE PROTEIN;
COMPND   3 CHAIN: A, B, C, D;
COMPND   4 FRAGMENT: UNP RESIDUES 93-215;
COMPND   5 SYNONYM: KILLER CELL LECTIN-LIKE RECEPTOR SUBFAMILY K MEMBER 1,NK
COMPND   6 CELL RECEPTOR D,NKG2-D-ACTIVATING NK RECEPTOR;
COMPND   7 ENGINEERED: YES;
COMPND   8 MOL_ID: 2;
COMPND   9 MOLECULE: CPXV018 PROTEIN;
COMPND  10 CHAIN: E, F;
COMPND  11 FRAGMENT: UNP RESIDUES 20-168;
COMPND  12 ENGINEERED: YES;
COMPND  13 MUTATION: YES
SOURCE    MOL_ID: 1;
SOURCE   2 ORGANISM_SCIENTIFIC: HOMO SAPIENS;
SOURCE   4 ORGANISM_TAXID: 9606;
SOURCE   5 GENE: KLRK1, D12S2489E, NKG2D;
SOURCE   6 EXPRESSION_SYSTEM: ESCHERICHIA COLI;
SOURCE   7 EXPRESSION_SYSTEM_TAXID: 469008;
SOURCE   8 EXPRESSION_SYSTEM_STRAIN: BL21(DE3)RIL;
SOURCE   9 EXPRESSION_SYSTEM_VECTOR_TYPE: PLASMID;
SOURCE  10 EXPRESSION_SYSTEM_PLASMID: PET21A(+);
SOURCE  11 MOL_ID: 2;
SOURCE  12 ORGANISM_SCIENTIFIC: COWPOX VIRUS;
SOURCE  13 ORGANISM_COMMON: CPV;
SOURCE  14 ORGANISM_TAXID: 10243;
SOURCE  15 GENE: CPXV018 CDS;
SOURCE  16 EXPRESSION_SYSTEM: ESCHERICHIA COLI;
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SOURCE  17 EXPRESSION_SYSTEM_TAXID: 469008;
SOURCE  18 EXPRESSION_SYSTEM_STRAIN: BL21(DE3)RIL;
SOURCE  19 EXPRESSION_SYSTEM_VECTOR_TYPE: PLASMID;
SOURCE  20 EXPRESSION_SYSTEM_PLASMID: PET21A(+)
KEYWDS    SECRETED VIRAL PROTEIN, IMMUNE EVASION, ORTHOPOXVIRUS, MHC-LIKE FOLD,
KEYWDS   2 NK CELL RECEPTOR LIGAND, STRUCTURAL GENOMICS, CENTER FOR STRUCTURAL
KEYWDS   3 GENOMICS OF INFECTIOUS DISEASES, CSGID, IMMUNE SYSTEM-VIRAL PROTEIN
KEYWDS   4 COMPLEX
EXPDTA    X-RAY DIFFRACTION
AUTHOR    E.LAZEAR,C.A.NELSON,D.H.FREMONT,CENTER FOR STRUCTURAL GENOMICS OF
AUTHOR   2 INFECTIOUS DISEASES (CSGID)
REVDAT   2   30-JUL-14 4PDC    1       JRNL
REVDAT   1   21-MAY-14 4PDC    0
JRNL        AUTH   E.LAZEAR,M.SUN,C.A.NELSON,J.A.CAMPBELL,L.N.CARAYANNOPOULOS,
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JRNL        AUTH 4 (CSGID)
JRNL        TITL   COWPOX VIRUS OMCP ANTAGONIZES NKG2D VIA AN UNEXPECTED
JRNL        TITL 2 BINDING ORIENTATION
JRNL        REF    TO BE PUBLISHED
REMARK   2 RESOLUTION.    1.99 ANGSTROMS.
REMARK   3 REFINEMENT.
REMARK   3   PROGRAM     : PHENIX (PHENIX.REFINE: 1.8.4_1496)
REMARK   3   AUTHORS     : PAUL ADAMS,PAVEL AFONINE,VINCENT CHEN,IAN
REMARK   3    REFINEMENT TARGET : ML
REMARK   3  DATA USED IN REFINEMENT.
REMARK   3   RESOLUTION RANGE HIGH (ANGSTROMS) : 1.99
REMARK   3   RESOLUTION RANGE LOW  (ANGSTROMS) : 45.67
REMARK   3   MIN(FOBS/SIGMA_FOBS)              : 1.380
REMARK   3   COMPLETENESS FOR RANGE       (%) : 92.9
REMARK   3   NUMBER OF REFLECTIONS             : 50042
REMARK   3  FIT TO DATA USED IN REFINEMENT.
REMARK   3   R VALUE     (WORKING + TEST SET) : 0.168
REMARK   3   R VALUE          (WORKING SET) : 0.166
REMARK   3   FREE R VALUE                     : 0.214
REMARK   3   FREE R VALUE TEST SET SIZE   (%) : 3.980
REMARK   3   FREE R VALUE TEST SET COUNT      : 1994
REMARK   3  FIT TO DATA USED IN REFINEMENT (IN BINS).
REMARK   3   BIN  RESOLUTION RANGE  COMPL.    NWORK NFREE   RWORK  RFREE
REMARK   3     1 45.6774 -  4.7969    1.00     3740   160  0.1646 0.1709
REMARK   3     2  4.7969 -  3.8080    1.00     3733   155  0.1289 0.1960
REMARK   3     3  3.8080 -  3.3268    1.00     3673   151  0.1493 0.1701
REMARK   3     4  3.3268 -  3.0227    0.99     3700   158  0.1688 0.2284
REMARK   3     5  3.0227 -  2.8061    0.95     3529   151  0.1864 0.2352
REMARK   3     6  2.8061 -  2.6407    0.91     3353   142  0.1826 0.2189
REMARK   3     7  2.6407 -  2.5084    0.90     3309   133  0.1790 0.2297
REMARK   3     8  2.5084 -  2.3993    0.89     3281   134  0.1744 0.2545
REMARK   3     9  2.3993 -  2.3069    0.89     3285   132  0.1778 0.2825
REMARK   3    10  2.3069 -  2.2273    0.90     3327   131  0.1764 0.2197
REMARK   3    11  2.2273 -  2.1577    0.90     3302   127  0.1777 0.2202
REMARK   3    12  2.1577 -  2.0960    0.91     3328   152  0.1834 0.2460
REMARK   3    13  2.0960 -  2.0408    0.91     3341   145  0.2098 0.2812
REMARK   3    14  2.0408 -  1.9910    0.85     3147   123  0.2098 0.2951
REMARK   3  BULK SOLVENT MODELLING.
REMARK   3   METHOD USED        : FLAT BULK SOLVENT MODEL
REMARK   3   SOLVENT RADIUS     : 1.11
REMARK   3   SHRINKAGE RADIUS   : 0.90
REMARK   3   K_SOL              : NULL
REMARK   3   B_SOL              : NULL
REMARK   3  ERROR ESTIMATES.
REMARK   3   COORDINATE ERROR (MAXIMUM-LIKELIHOOD
BASED)    : 0.230
REMARK   3   PHASE ERROR (DEGREES, MAXIMUM-LIKELIHOOD
BASED) : 20.990
REMARK   3  B VALUES.
REMARK   3   FROM WILSON PLOT          (A**2) : 21.62
REMARK   3   MEAN B VALUE      (OVERALL, A**2) : NULL
REMARK   3   OVERALL ANISOTROPIC B VALUE.
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REMARK 3 B11 (A**2) : NULL
REMARK 3 B22 (A**2) : NULL
REMARK 3 B33 (A**2) : NULL
REMARK 3 B12 (A**2) : NULL
REMARK 3 B13 (A**2) : NULL
REMARK 3 B23 (A**2) : NULL
REMARK 3 TWINNING INFORMATION.
REMARK 3 FRACTION: NULL
REMARK 3 OPERATOR: NULL
REMARK 3 DEVIATIONS FROM IDEAL VALUES.
REMARK 3 RMSD COUNT
REMARK 3 BOND : 0.003 6687
REMARK 3 ANGLE : 0.786 9030
REMARK 3 CHIRALITY : 0.031 933
REMARK 3 PLANARITY : 0.003 1150
REMARK 3 DIHEDRAL : 13.423 2426
REMARK 3 TLS DETAILS
REMARK 3 NUMBER OF TLS GROUPS : NULL
REMARK 3 NCS DETAILS
REMARK 3 NUMBER OF NCS GROUPS : NULL
REMARK 3 OTHER REFINEMENT REMARKS: NULL
REMARK 4 4PDC COMPLIES WITH FORMAT V. 3.30, 13-JUL-11
REMARK 100 THIS ENTRY HAS BEEN PROCESSED BY RCSB ON 21-APR-14.
REMARK 100 THE DEPOSITION ID IS D_1000201141.
REMARK 200 EXPERIMENTAL DETAILS
REMARK 200 EXPERIMENT TYPE : X-RAY DIFFRACTION
REMARK 200 DATE OF DATA COLLECTION : 19-OCT-10
REMARK 200 TEMPERATURE (KELVIN) : 100
REMARK 200 PH : 6.75
REMARK 200 NUMBER OF CRYSTALS USED : 1
REMARK 200 SYNCHROTRON (Y/N) : Y
REMARK 200 RADIATION SOURCE : ALS
REMARK 200 BEAMLINE : 4.2.2
REMARK 200 X-RAY GENERATOR MODEL : NULL
REMARK 200 MONOCHROMATIC OR LAUE (M/L) : M
REMARK 200 WAVELENGTH OR RANGE (A) : 1.00004
REMARK 200 MONOCHROMATOR : NULL
REMARK 200 OPTICS : NULL
REMARK 200 DETECTOR TYPE : CCD
REMARK 200 DETECTOR MANUFACTURER : NOIR-1
REMARK 200 INTENSITY-INTEGRATION SOFTWARE : HKL
REMARK 200 DATA SCALING SOFTWARE : HKL
REMARK 200 NUMBER OF UNIQUE REFLECTIONS : 50139
REMARK 200 RESOLUTION RANGE HIGH (A) : 1.991
REMARK 200 RESOLUTION RANGE LOW (A) : 50.000
REMARK 200 REJECTION CRITERIA (SIGMA(I)) : NULL
REMARK 200 OVERALL.
REMARK 200 COMPLETENESS FOR RANGE (%) : 93.5
REMARK 200 DATA REDUNDANCY : 6.200
REMARK 200 R MERGE (I) : 0.11800
REMARK 200 R SYM (I) : NULL
REMARK 200 <I/SIGMA(I)> FOR THE DATA SET : 12.7000
REMARK 200 IN THE HIGHEST RESOLUTION SHELL.
REMARK 200 HIGHEST RESOLUTION SHELL, RANGE HIGH (A) : 2.00
REMARK 200 HIGHEST RESOLUTION SHELL, RANGE LOW (A) : 2.07
REMARK 200 COMPLETENESS FOR SHELL (%) : 91.5
REMARK 200 DATA REDUNDANCY IN SHELL : 5.30
REMARK 200 R MERGE FOR SHELL (I) : 0.48500
REMARK 200 R SYM FOR SHELL (I) : NULL
REMARK 200 <I/SIGMA(I)> FOR SHELL : NULL
REMARK 200 DIFFRACTION PROTOCOL: SINGLE WAVELENGTH
REMARK 200 METHOD USED TO DETERMINE THE STRUCTURE: MOLECULAR
REPLACEMENT
REMARK 200 SOFTWARE USED: PHASER
REMARK 200 STARTING MODEL: 1MPU, 4FFE
REMARK 200 REMARK: NULL
REMARK 280 CRYSTAL
REMARK 280 SOLVENT CONTENT, VS (%): 42.94

REMARK 280 MATTHEWS COEFFICIENT, VM (ANGSTROMS**3/DA): 2.16
REMARK 280 CRYSTALLIZATION CONDITIONS: 15% PEG 3350, 0.2M MGCL2, 0.1M BIS
REMARK 280 -TRIS
REMARK 290 CRYSTALLOGRAPHIC SYMMETRY
REMARK 290 SYMMETRY OPERATORS FOR SPACE GROUP: P 1 21 1
REMARK 290 SYMOP SYMMETRY
REMARK 290 NNNMMM OPERATOR
REMARK 290 1555 X,Y,Z
REMARK 290 2555 -X,Y+1/2,-Z
REMARK 290 WHERE NNN -> OPERATOR NUMBER
REMARK 290 MMM -> TRANSLATION VECTOR
REMARK 290 CRYSTALLOGRAPHIC SYMMETRY TRANSFORMATIONS
REMARK 290 THE FOLLOWING TRANSFORMATIONS OPERATE ON THE ATOM/HETATM
REMARK 290 RECORDS IN THIS ENTRY TO PRODUCE CRYSTALLOGRAPHICALLY
REMARK 290 RELATED MOLECULES.
REMARK 290 SMTRY1 1 1.000000 0.000000 0.000000 0.00000
REMARK 290 SMTRY2 1 0.000000 1.000000 0.000000 0.00000
REMARK 290 SMTRY3 1 0.000000 0.000000 1.000000 0.00000
REMARK 290 SMTRY1 2 -1.000000 0.000000 0.000000 0.00000
REMARK 290 SMTRY2 2 0.000000 1.000000 0.000000 50.55500
REMARK 290 SMTRY3 2 0.000000 0.000000 -1.000000 0.00000
REMARK 290 REMARK: NULL
REMARK 300 BIOMOLECULE: 1, 2
REMARK 300 SEE REMARK 350 FOR THE AUTHOR PROVIDED AND/OR PROGRAM
REMARK 300 GENERATED ASSEMBLY INFORMATION FOR THE STRUCTURE IN
REMARK 300 THIS ENTRY. THE REMARK MAY ALSO PROVIDE INFORMATION ON
REMARK 300 BURIED SURFACE AREA.
REMARK 300 REMARK: THE BIOLOGICAL UNIT OF HNKG2D IS A DIMER (CHAINS A & B AND
REMARK 300 CHAINS C & D
REMARK 350 COORDINATES FOR A COMPLETE MULTIMER REPRESENTING THE KNOWN
REMARK 350 BIOLOGICALLY SIGNIFICANT OLIGOMERIZATION STATE OF THE
REMARK 350 MOLECULE CAN BE GENERATED BY APPLYING BIOMT TRANSFORMATIONS
REMARK 350 GIVEN BELOW. BOTH NON-CRYSTALLOGRAPHIC AND
REMARK 350 CRYSTALLOGRAPHIC OPERATIONS ARE GIVEN.
REMARK 350 BIOMOLECULE: 1
REMARK 350 AUTHOR DETERMINED BIOLOGICAL UNIT: TRIMERIC
REMARK 350 APPLY THE FOLLOWING TO CHAINS: A, B, E
REMARK 350 BIOMT1 1 1.000000 0.000000 0.000000 0.00000
REMARK 350 BIOMT2 1 0.000000 1.000000 0.000000 0.00000
REMARK 350 BIOMT3 1 0.000000 0.000000 1.000000 0.00000
REMARK 350 BIOMOLECULE: 2
REMARK 350 AUTHOR DETERMINED BIOLOGICAL UNIT: TRIMERIC
REMARK 350 APPLY THE FOLLOWING TO CHAINS: C, D, F
REMARK 350 BIOMT1 1 1.000000 0.000000 0.000000 0.00000
REMARK 350 BIOMT2 1 0.000000 1.000000 0.000000 0.00000
REMARK 350 BIOMT3 1 0.000000 0.000000 1.000000 0.00000
REMARK 465 MISSING RESIDUES
REMARK 465 THE FOLLOWING RESIDUES WERE NOT LOCATED IN THE
REMARK 465 EXPERIMENT. (M=MODEL NUMBER; RES=RESIDUE NAME; C=CHAIN
REMARK 465 IDENTIFIER; SSSEQ=SEQUENCE NUMBER; I=INSERTION CODE.)
REMARK 465 M RES C SSSEQI
REMARK 465 GLU B 93
REMARK 500 GEOMETRY AND STEREOCHEMISTRY
REMARK 500 SUBTOPIC: CLOSE CONTACTS IN SAME ASYMMETRIC UNIT
REMARK 500 THE FOLLOWING ATOMS ARE IN CLOSE CONTACT.
REMARK 500 ATM1 RES C SSEQI ATM2 RES C SSEQI DISTANCE
REMARK 500 O HOH F 293 O HOH F 324 2.19
REMARK 500 REMARK: NULL
REMARK 500 GEOMETRY AND STEREOCHEMISTRY
REMARK 500 SUBTOPIC: CLOSE CONTACTS
REMARK 500 THE FOLLOWING ATOMS THAT ARE RELATED BY CRYSTALLOGRAPHIC
REMARK 500 SYMMETRY ARE IN CLOSE CONTACT. AN ATOM LOCATED WITHIN 0.15
REMARK 500 ANGSTROMS OF A SYMMETRY RELATED ATOM IS ASSUMED TO BE ON A
REMARK 500 SPECIAL POSITION AND IS, THEREFORE, LISTED IN REMARK 375
REMARK 500 INSTEAD OF REMARK 500. ATOMS WITH NON-BLANK ALTERNATE
REMARK 500 LOCATION INDICATORS ARE NOT INCLUDED IN THE CALCULATIONS.
REMARK 500 DISTANCE CUTOFF:
REMARK 500 2.2 ANGSTROMS FOR CONTACTS NOT INVOLVING HYDROGEN ATOMS

REMARK 500 1.6 ANGSTROMS FOR CONTACTS INVOLVING HYDROGEN ATOMS
REMARK 500 ATM1 RES C SSEQI ATM2 RES C SSEQI SSYMOP DISTANCE
REMARK 500 O HOH C 301 O HOH D 306 1655 2.15
REMARK 500 O HOH C 318 O HOH D 306 1655 2.19
REMARK 500 REMARK: NULL
REMARK 500 GEOMETRY AND STEREOCHEMISTRY
REMARK 500 SUBTOPIC: TORSION ANGLES
REMARK 500 TORSION ANGLES OUTSIDE THE EXPECTED RAMACHANDRAN REGIONS:
REMARK 500 (M=MODEL NUMBER; RES=RESIDUE NAME; C=CHAIN IDENTIFIER;
REMARK 500 SSEQ=SEQUENCE NUMBER; I=INSERTION CODE).
REMARK 500 STANDARD TABLE:
REMARK 500 FORMAT:(10X,I3,1X,A3,1X,A1,I4,A1,4X,F7.2,3X,F7.2)
REMARK 500 EXPECTED VALUES: GJ KLEYWEGT AND TA JONES (1996). PHI/PSI-
REMARK 500 CHOLOGY: RAMACHANDRAN REVISITED. STRUCTURE 4, 1395 - 1400
REMARK 500 M RES CSSEQI PSI PHI
REMARK 500 SER A 151 -170.24 71.72
REMARK 500 THR A 162 -74.87 -58.64
REMARK 500 MET A 184 -75.63 -143.50
REMARK 500 TYR B 106 114.87 -162.70
REMARK 500 SER B 151 -171.27 67.58
REMARK 500 THR B 162 -35.85 164.34
REMARK 500 MET B 184 -59.05 -140.78
REMARK 500 SER C 151 -172.20 65.21
REMARK 500 MET C 184 -64.72 -143.36
REMARK 500 SER D 151 -170.57 74.89
REMARK 500 MET D 184 -66.96 -138.40
REMARK 500 ASN E 88 16.97 57.97
REMARK 500 THR E 104 -12.21 -141.68
REMARK 500 LYS F 35 -52.70 -131.11
REMARK 500 THR F 104 -6.09 -145.54
REMARK 500 REMARK: NULL
REMARK 525 SOLVENT
REMARK 525 THE SOLVENT MOLECULES HAVE CHAIN IDENTIFIERS THAT
REMARK 525 INDICATE THE POLYMER CHAIN WITH WHICH THEY ARE MOST
REMARK 525 CLOSELY ASSOCIATED. THE REMARK LISTS ALL THE SOLVENT
REMARK 525 MOLECULES WHICH ARE MORE THAN 5A AWAY FROM THE
REMARK 525 NEAREST POLYMER CHAIN (M = MODEL NUMBER;
REMARK 525 RES=RESIDUE NAME; C=CHAIN IDENTIFIER; SSEQ=SEQUENCE
REMARK 525 NUMBER; I=INSERTION CODE):
REMARK 525 M RES CSSEQI
REMARK 525 HOH A 385 DISTANCE = 6.57 ANGSTROMS
REMARK 525 HOH A 387 DISTANCE = 6.32 ANGSTROMS
REMARK 525 HOH F 337 DISTANCE = 5.90 ANGSTROMS
REMARK 900 RELATED ENTRIES
REMARK 900 RELATED ID: 4FFE RELATED DB: PDB
REMARK 900 4FFE IS THE STRUCTURE OF FREE COWPOX VIRUS CPXV018 (OMCP)
REMARK 900 RELATED ID: 1MPU RELATED DB: PDB
REMARK 900 1MPU IS THE STRUCTURE OF FREE HUMAN NKG2D
IMMUNORECEPTOR.
REMARK 900 RELATED ID: 1HYR RELATED DB: PDB
REMARK 900 HUMAN NKG2D IN COMPLEX WITH MIC-A
REMARK 900 RELATED ID: 1JSK RELATED DB: PDB
REMARK 900 MOUSE NKG2D IN COMPLEX WITH RAE-1BETA
REMARK 900 RELATED ID: 1KCG RELATED DB: PDB
REMARK 900 HUMAN NKG2D IN COMPLEX WITH ULBP3
REMARK 900 RELATED ID: CSGID-IDP00259 RELATED DB: TARGETTRACK
DBREF 4PDC A 93 215 UNP P26718 NKG2D_HUMAN 93 215
DBREF 4PDC B 93 215 UNP P26718 NKG2D_HUMAN 93 215
DBREF 4PDC C 93 215 UNP P26718 NKG2D_HUMAN 93 215
DBREF 4PDC D 93 215 UNP P26718 NKG2D_HUMAN 93 215
DBREF 4PDC E 1 149 UNP Q8QN43 Q8QN43_COWPX 20 168
DBREF 4PDC F 1 149 UNP Q8QN43 Q8QN43_COWPX 20 168
SEQADV 4PDC GLY E 0 UNP Q8QN43 EXPRESSION TAG
SEQADV 4PDC ASP E 23 UNP Q8QN43 TYR 42 ENGINEERED MUTATION
SEQADV 4PDC ASP E 95 UNP Q8QN43 PHE 114 ENGINEERED MUTATION
SEQADV 4PDC GLY F 0 UNP Q8QN43 EXPRESSION TAG
SEQADV 4PDC ASP F 23 UNP Q8QN43 TYR 42 ENGINEERED MUTATION
SEQADV 4PDC ASP F 95 UNP Q8QN43 PHE 114 ENGINEERED MUTATION

SEQRES 1 A 123 GLU SER TYR CYS GLY PRO CYS PRO LYS ASN TRP ILE CYS
SEQRES 2 A 123 TYR LYS ASN ASN CYS TYR GLN PHE PHE ASP GLU SER LYS
SEQRES 3 A 123 ASN TRP TYR GLU SER GLN ALA SER CYS MET SER GLN ASN
SEQRES 4 A 123 ALA SER LEU LEU LYS VAL TYR SER LYS GLU ASP GLN ASP
SEQRES 5 A 123 LEU LEU LYS LEU VAL LYS SER TYR HIS TRP MET GLY LEU
SEQRES 6 A 123 VAL HIS ILE PRO THR ASN GLY SER TRP GLN TRP GLU ASP
SEQRES 7 A 123 GLY SER ILE LEU SER PRO ASN LEU LEU THR ILE ILE GLU
SEQRES 8 A 123 MET GLN LYS GLY ASP CYS ALA LEU TYR ALA SER SER PHE
SEQRES 9 A 123 LYS GLY TYR ILE GLU ASN CYS SER THR PRO ASN THR TYR
SEQRES 10 A 123 ILE CYS MET GLN ARG THR
SEQRES 1 B 123 GLU SER TYR CYS GLY PRO CYS PRO LYS ASN TRP ILE CYS
SEQRES 2 B 123 TYR LYS ASN ASN CYS TYR GLN PHE PHE ASP GLU SER LYS
SEQRES 3 B 123 ASN TRP TYR GLU SER GLN ALA SER CYS MET SER GLN ASN
SEQRES 4 B 123 ALA SER LEU LEU LYS VAL TYR SER LYS GLU ASP GLN ASP
SEQRES 5 B 123 LEU LEU LYS LEU VAL LYS SER TYR HIS TRP MET GLY LEU
SEQRES 6 B 123 VAL HIS ILE PRO THR ASN GLY SER TRP GLN TRP GLU ASP
SEQRES 7 B 123 GLY SER ILE LEU SER PRO ASN LEU LEU THR ILE ILE GLU
SEQRES 8 B 123 MET GLN LYS GLY ASP CYS ALA LEU TYR ALA SER SER PHE
SEQRES 9 B 123 LYS GLY TYR ILE GLU ASN CYS SER THR PRO ASN THR TYR
SEQRES 10 B 123 ILE CYS MET GLN ARG THR
SEQRES 1 C 123 GLU SER TYR CYS GLY PRO CYS PRO LYS ASN TRP ILE CYS
SEQRES 2 C 123 TYR LYS ASN ASN CYS TYR GLN PHE PHE ASP GLU SER LYS
SEQRES 3 C 123 ASN TRP TYR GLU SER GLN ALA SER CYS MET SER GLN ASN
SEQRES 4 C 123 ALA SER LEU LEU LYS VAL TYR SER LYS GLU ASP GLN ASP
SEQRES 5 C 123 LEU LEU LYS LEU VAL LYS SER TYR HIS TRP MET GLY LEU
SEQRES 6 C 123 VAL HIS ILE PRO THR ASN GLY SER TRP GLN TRP GLU ASP
SEQRES 7 C 123 GLY SER ILE LEU SER PRO ASN LEU LEU THR ILE ILE GLU
SEQRES 8 C 123 MET GLN LYS GLY ASP CYS ALA LEU TYR ALA SER SER PHE
SEQRES 9 C 123 LYS GLY TYR ILE GLU ASN CYS SER THR PRO ASN THR TYR
SEQRES 10 C 123 ILE CYS MET GLN ARG THR
SEQRES 1 D 123 GLU SER TYR CYS GLY PRO CYS PRO LYS ASN TRP ILE CYS
SEQRES 2 D 123 TYR LYS ASN ASN CYS TYR GLN PHE PHE ASP GLU SER LYS
SEQRES 3 D 123 ASN TRP TYR GLU SER GLN ALA SER CYS MET SER GLN ASN
SEQRES 4 D 123 ALA SER LEU LEU LYS VAL TYR SER LYS GLU ASP GLN ASP
SEQRES 5 D 123 LEU LEU LYS LEU VAL LYS SER TYR HIS TRP MET GLY LEU
SEQRES 6 D 123 VAL HIS ILE PRO THR ASN GLY SER TRP GLN TRP GLU ASP
SEQRES 7 D 123 GLY SER ILE LEU SER PRO ASN LEU LEU THR ILE ILE GLU
SEQRES 8 D 123 MET GLN LYS GLY ASP CYS ALA LEU TYR ALA SER SER PHE
SEQRES 9 D 123 LYS GLY TYR ILE GLU ASN CYS SER THR PRO ASN THR TYR
SEQRES 10 D 123 ILE CYS MET GLN ARG THR
SEQRES 1 E 150 GLY HIS LYS LEU ALA PHE ASN PHE ASN LEU GLU ILE ASN
SEQRES 2 E 150 GLY SER ASP THR HIS SER THR VAL ASP VAL ASP LEU ASP
SEQRES 3 E 150 ASP SER GLN ILE ILE THR PHE ASP GLY LYS ASP ILE ARG
SEQRES 4 E 150 PRO THR ILE PRO PHE MET ILE GLY ASP GLU ILE PHE LEU
SEQRES 5 E 150 PRO PHE TYR LYS ASN VAL PHE SER GLU PHE PHE SER LEU
SEQRES 6 E 150 PHE ARG ARG VAL PRO THR SER THR PRO TYR GLU ASP LEU
SEQRES 7 E 150 THR TYR PHE TYR GLU CYS ASP TYR THR ASP ASN LYS SER
SEQRES 8 E 150 THR PHE ASP GLN ASP TYR LEU TYR ASN GLY GLU GLU TYR
SEQRES 9 E 150 THR VAL LYS THR GLN GLU ALA THR ASN LYS ASN MET TRP
SEQRES 10 E 150 LEU THR THR SER GLU PHE ARG LEU LYS LYS TRP PHE ASP
SEQRES 11 E 150 GLY GLU ASP CYS ILE MET HIS LEU ARG SER LEU VAL ARG
SEQRES 12 E 150 LYS MET GLU ASP SER LYS ARG
SEQRES 1 F 150 GLY HIS LYS LEU ALA PHE ASN PHE ASN LEU GLU ILE ASN
SEQRES 2 F 150 GLY SER ASP THR HIS SER THR VAL ASP VAL ASP LEU ASP
SEQRES 3 F 150 ASP SER GLN ILE ILE THR PHE ASP GLY LYS ASP ILE ARG
SEQRES 4 F 150 PRO THR ILE PRO PHE MET ILE GLY ASP GLU ILE PHE LEU
SEQRES 5 F 150 PRO PHE TYR LYS ASN VAL PHE SER GLU PHE PHE SER LEU
SEQRES 6 F 150 PHE ARG ARG VAL PRO THR SER THR PRO TYR GLU ASP LEU
SEQRES 7 F 150 THR TYR PHE TYR GLU CYS ASP TYR THR ASP ASN LYS SER
SEQRES 8 F 150 THR PHE ASP GLN ASP TYR LEU TYR ASN GLY GLU GLU TYR
SEQRES 9 F 150 THR VAL LYS THR GLN GLU ALA THR ASN LYS ASN MET TRP
SEQRES 10 F 150 LEU THR THR SER GLU PHE ARG LEU LYS LYS TRP PHE ASP
SEQRES 11 F 150 GLY GLU ASP CYS ILE MET HIS LEU ARG SER LEU VAL ARG
SEQRES 12 F 150 LYS MET GLU ASP SER LYS ARG
FORMUL 7 HOH *660(H2 O)
HELIX 1 AA1 ASN A 119 SER A 129 1 11
HELIX 2 AA2 GLN A 143 VAL A 149 5 7
HELIX 3 AA3 ASN B 119 SER B 129 1 11
HELIX 9 AA9 ILE E 41 ILE E 45 5 5
HELIX 10 AB1 ILE E 49 LEU E 64 1 16
HELIX 11 AB2 THR E 111 LYS E 126 1 16

```
HELIX   4 AA4 GLN B  143  VAL B  149  5                                   7
HELIX   5 AA5 ASN C  119  SER C  129  1                                  11
HELIX   6 AA6 GLN C  143  VAL C  149  5                                   7
HELIX   7 AA7 ASN D  119  GLN D  130  1                                  12
HELIX   8 AA8 GLN D  143  VAL D  149  5                                   7

SHEET   1 AA1 2 SER A  94  CYS A  96  0
SHEET   2 AA1 2 CYS B  96  CYS B  99 -1  O  CYS B  99   N  SER A
94

SHEET   1 AA2 4 ILE A 104  TYR A 106  0
SHEET   2 AA2 4 ASN A 109  LYS A 118 -1  O  TYR A 111   N  ILE A
104
SHEET   3 AA2 4 ASN A 207  GLN A 213 -1  O  GLN A 213   N  CYS A
110
SHEET   4 AA2 4 SER A 133  LEU A 134 -1  N  SER A 133   O  MET A
212

SHEET   1 AA3 4 HIS A 153  TRP A 154  0
SHEET   2 AA3 4 CYS A 189  ALA A 193 -1  O  TYR A 192   N  HIS A
153
SHEET   3 AA3 4 LYS A 197  GLU A 201 -1  O  GLU A 201   N  CYS A
189
SHEET   4 AA3 4 THR A 180  ILE A 182  1  N  ILE A 182   O  GLY A 198

SHEET   1 AA4 2 LEU A 157  HIS A 159  0
SHEET   2 AA4 2 TRP A 166  TRP A 168 -1  O  GLN A 167   N  VAL A
158

SHEET   1 AA5 5 ILE B 104  TYR B 106  0
SHEET   2 AA5 5 ASN B 109  LYS B 118 -1  O  TYR B 111   N  ILE B
104
SHEET   3 AA5 5 ASN B 207  ARG B 214 -1  O  ASN B 207   N  LYS B
118
SHEET   4 AA5 5 HIS B 153  HIS B 159  1  N  TRP B 154   O  THR B
208
SHEET   5 AA5 5 TRP B 166  TRP B 168 -1  O  GLN B 167   N  VAL B
158
SHEET   1 AA6 6 SER B 133  LEU B 134  0
SHEET   2 AA6 6 ASN B 207  ARG B 214 -1  O  MET B 212   N  SER B
133
SHEET   3 AA6 6 HIS B 153  HIS B 159  1  N  TRP B 154   O  THR B
208
SHEET   4 AA6 6 CYS B 189  ALA B 193 -1  O  TYR B 192   N  HIS B
153
SHEET   5 AA6 6 LYS B 197  GLU B 201 -1  O  LYS B 197   N  ALA B
193

SHEET   6 AA6 6 THR B 180  ILE B 182  1  N  ILE B 182   O  GLY B 198
SHEET   1 AA7 2 CYS C  96  CYS C  99  0
SHEET   2 AA7 2 SER D  94  CYS D  96 -1  O  SER D  94   N  CYS C
99
SHEET   1 AA8 8 SER C 133  LEU C 134  0
SHEET   2 AA8 8 ASN C 207  ARG C 214 -1  O  MET C 212   N  SER C
133
SHEET   3 AA8 8 ASN C 109  LYS C 118 -1  N  CYS C 110   O  GLN C
213
SHEET   4 AA8 8 ILE C 104  TYR C 106 -1  N  ILE C 104   O  TYR C
111
SSBOND  1 CYS A   96   CYS A  105                1555   1555  2.05
SSBOND  2 CYS A   99   CYS A  110                1555   1555  2.03
SSBOND  3 CYS A  127   CYS A  211                1555   1555  2.04
SSBOND  4 CYS A  189   CYS A  203                1555   1555  2.03
SSBOND  5 CYS B   96   CYS B  105              1555   1555  2.03
SSBOND  6 CYS B   99   CYS B  110                1555   1555  2.03
SSBOND  7 CYS B  127   CYS B  211                1555   1555  2.04
SSBOND  8 CYS B  189   CYS B  203                1555   1555  2.04
SSBOND  9 CYS C   96   CYS C  105                1555   1555  2.03

HELIX  12 AB3 ASP E  129  ASP E  146  1                                  18
HELIX  13 AB4 ILE F   41  ILE F   45  5                                5
HELIX  14 AB5 ILE F   49  LEU F   64  1                                16
HELIX  15 AB6 THR F  111  LYS F  125  1                                  15
HELIX  16 AB7 ASP F  129  ASP F  146  1                                  18
SHEET   5 AA8 8 ILE D 104  TYR D 106 -1  O  CYS D 105   N  CYS C
105
SHEET   6 AA8 8 ASN D 109  LYS D 118 -1  O  TYR D 111   N  ILE D
104
SHEET   7 AA8 8 ASN D 207  GLN D 213 -1  O  ASN D 207   N  LYS D
118
SHEET   8 AA8 8 SER D 133  LEU D 134 -1  N  SER D 133   O  MET D
212

SHEET   1 AA9 5 SER C 165  TRP C 168  0
SHEET   2 AA9 5 HIS C 153  ILE C 160 -1  N  VAL C 158   O  GLN C
167
SHEET   3 AA9 5 CYS C 189  ALA C 193 -1  O  TYR C 192   N  HIS C
153
SHEET   4 AA9 5 LYS C 197  GLU C 201 -1  O  GLU C 201   N  CYS C
189
SHEET   5 AA9 5 THR C 180  ILE C 182  1  N  ILE C 182   O  GLY C
198
SHEET   1 AB1 5 TRP D 166  TRP D 168  0
SHEET   2 AB1 5 HIS D 153  HIS D 159 -1  N  VAL D 158   O  GLN D
167
SHEET   3 AB1 5 CYS D 189  ALA D 193 -1  O  TYR D 192   N  HIS D
153
SHEET   4 AB1 5 LYS D 197  GLU D 201 -1  O  GLU D 201   N  CYS D
189
SHEET   5 AB1 5 THR D 180  ILE D 182  1  N  ILE D 182   O  GLY D
198

SHEET   1 AB2 7 ILE E  37  PRO E  39  0
SHEET   2 AB2 7 GLN E  28  PHE E  32 -1  N  THR E  31   O  ARG E
38

SHEET   3 AB2 7 ASP E  15  LEU E  24 -1  N  VAL E  22   O  ILE E  29
SHEET   4 AB2 7 HIS E   1  ASN E  12 -1  N  ALA E   4   O  ASP E  23

SHEET   5 AB2 7 TYR E  74  THR E  86 -1  O  GLU E  75   N  ILE E  11
SHEET   6 AB2 7 LYS E  89  TYR E  98 -1  O  ASP E  93   N  GLU E
82
SHEET   7 AB2 7 GLU E 101  TYR E 103 -1  O  GLU E 101   N  TYR E
98

SHEET   1 AB3 7 ILE F  37  PRO F  39  0
SHEET   2 AB3 7 SER F  27  PHE F  32 -1  N  THR F  31   O  ARG F
38
SHEET   3 AB3 7 ASP F  15  LEU F  24 -1  N  LEU F  24   O  SER F  27

SHEET   4 AB3 7 HIS F   1  ASN F  12 -1  N  ASN F  12   O  ASP F  15
SHEET   5 AB3 7 GLU F  75  THR F  86 -1  O  TYR F  81   N  PHE F   5

SHEET   6 AB3 7 LYS F  89  TYR F  98 -1  O  THR F  91   N  ASP F  84
SHEET   7 AB3 7 GLU F 101  TYR F 103 -1  O  GLU F 101   N  TYR F
98

SSBOND 11 CYS C  127   CYS C  211          1555   1555  2.03
SSBOND 12 CYS C  189   CYS C  203          1555   1555  2.04
SSBOND 13 CYS D   96   CYS D  105        1555   1555  2.04
SSBOND 14 CYS D   99   CYS D  110        1555   1555  2.03
SSBOND 15 CYS D  127   CYS D  211          1555   1555  2.04
SSBOND 16 CYS D  189   CYS D  203          1555   1555  2.04
SSBOND 17 CYS E   83   CYS E  133          1555   1555  2.06
SSBOND 18 CYS F   83   CYS F  133          1555   1555  2.06
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SSBOND  10 CYS C   99    CYS C  110                          1555   1555  2.03
CISPEP   1 GLY A   97    PRO A   98        0        1.20
CISPEP   2 SER A  194    SER A  195        0       -3.36
CISPEP   3 GLY B   97    PRO B   98        0        1.05
CISPEP   4 SER B  194    SER B  195        0       -1.59
CISPEP   5 GLY C   97    PRO C   98        0        2.40
CISPEP   6 SER C  194    SER C  195        0        1.38
CISPEP   7 GLY D   97    PRO D   98        0        0.65
CISPEP   8 SER D  194    SER D  195        0       -3.12
CRYST1   43.315  101.110   91.368  90.00  91.63  90.00 P 1 21 1     8
ORIGX1      1.000000  0.000000  0.000000        0.00000
ORIGX2      0.000000  1.000000  0.000000        0.00000
ORIGX3      0.000000  0.000000  1.000000        0.00000
SCALE1      0.023087  0.000000  0.000659        0.00000
SCALE2      0.000000  0.009890  0.000000        0.00000
SCALE3      0.000000  0.000000  0.010949        0.00000
ATOM      1  N   GLU A  93     -14.924   7.066 -22.137  1.00 59.38           N
ATOM      2  CA  GLU A  93     -14.415   6.924 -23.496  1.00 58.81           C
ATOM      3  C   GLU A  93     -15.440   6.231 -24.389  1.00 56.95           C
ATOM      4  O   GLU A  93     -16.124   5.303 -23.956  1.00 61.11           O
ATOM      5  CB  GLU A  93     -13.098   6.143 -23.497  1.00 60.00           C
ATOM      6  CG  GLU A  93     -13.220   4.711 -22.996  1.00 72.71           C
ATOM      7  CD  GLU A  93     -11.880   3.998 -22.928  1.00 80.57           C
ATOM      8  OE1 GLU A  93     -10.846   4.640 -23.211  1.00 79.10           O
ATOM      9  OE2 GLU A  93     -11.862   2.794 -22.593  1.00 85.72           O1-
ATOM     10  HA  GLU A  93     -14.242   7.805 -23.864  1.00 70.57           H
ATOM     11  HB2 GLU A  93     -12.756   6.110 -24.404  1.00 72.00           H
ATOM     12  HB3 GLU A  93     -12.464   6.603 -22.925  1.00 72.00           H
ATOM     13  HG2 GLU A  93     -13.601   4.719 -22.104  1.00 87.25           H
ATOM     14  HG3 GLU A  93     -13.794   4.213 -23.598  1.00 87.25           H
ATOM     15  N   SER A  94     -15.537   6.687 -25.634  1.00 47.51           N
ATOM     16  CA  SER A  94     -16.522   6.163 -26.571  1.00 43.60           C
ATOM     17  C   SER A  94     -15.911   5.889 -27.937  1.00 40.17           C
ATOM     18  O   SER A  94     -14.793   6.312 -28.231  1.00 42.40           O
ATOM     19  CB  SER A  94     -17.684   7.143 -26.716  1.00 50.65           C
ATOM     20  OG  SER A  94     -17.227   8.391 -27.207  1.00 53.61           O
ATOM     21  H   SER A  94     -15.038   7.306 -25.963  1.00 57.02           H
ATOM     22  HA  SER A  94     -16.874   5.328 -26.226  1.00 52.32           H
ATOM     23  HB2 SER A  94     -18.332   6.777 -27.339  1.00 60.78           H
ATOM     24  HB3 SER A  94     -18.096   7.276 -25.848  1.00 60.78           H
ATOM     25  HG  SER A  94     -17.873   8.923 -27.284  1.00 64.33           H
ATOM     26  N   TYR A  95     -16.662   5.174 -28.766  1.00 37.41           N
ATOM     27  CA  TYR A  95     -16.245   4.875 -30.126  1.00 36.16           C
ATOM     28  C   TYR A  95     -16.815   5.907 -31.089  1.00 32.15           C
ATOM     29  O   TYR A  95     -17.812   6.566 -30.789  1.00 28.55
O
ATOM     30  CB  TYR A  95     -16.696   3.473 -30.528  1.00 35.46           C
ATOM     31  CG  TYR A  95     -15.877   2.361 -29.913  1.00 39.96           C
ATOM     32  CD1 TYR A  95     -16.234   1.797 -28.694  1.00 39.91           C
ATOM     33  CD2 TYR A  95     -14.750   1.870 -30.557  1.00 39.04           C
ATOM     34  CE1 TYR A  95     -15.488   0.775 -28.135  1.00 45.29           C
ATOM     35  CE2 TYR A  95     -13.998   0.850 -30.006  1.00 44.91           C
ATOM     36  CZ  TYR A  95     -14.370   0.306 -28.795  1.00 46.64           C
ATOM     37  OH  TYR A  95     -13.617  -0.710 -28.249  1.00 43.67           O
ATOM     38  H   TYR A  95     -17.430   4.846 -28.559  1.00 44.89           H
ATOM     39  HA  TYR A  95     -15.278   4.910 -30.179  1.00 43.39           H
ATOM     40  HB2 TYR A  95     -17.617   3.350 -30.250  1.00 42.56           H
ATOM     41  HB3 TYR A  95     -16.630   3.389 -31.492  1.00 42.56           H
ATOM     42  HD1 TYR A  95     -16.988   2.111 -28.248  1.00 47.89           H
ATOM     43  HD2 TYR A  95     -14.496   2.234 -31.374  1.00 46.85           H
ATOM     44  HE1 TYR A  95     -15.737   0.407 -27.318  1.00 54.35           H
ATOM     45  HE2 TYR A  95     -13.244   0.533 -30.449  1.00 53.90           H
ATOM     46  HH  TYR A  95     -13.948  -0.951 -27.516  1.00 52.40           H
ATOM     47  N   CYS A  96     -16.167   6.043 -32.241  1.00 28.25           N
ATOM     48  CA  CYS A  96     -16.597   6.969 -33.278  1.00 23.26           C
ATOM     49  C   CYS A  96     -16.818   6.214 -34.584  1.00 27.35           C
ATOM     50  O   CYS A  96     -15.989   5.397 -34.985  1.00 25.95           O
ATOM     51  CB  CYS A  96     -15.561   8.079 -33.472  1.00 25.56           C
ATOM     52  SG  CYS A  96     -16.018   9.334 -34.695  1.00 27.03           S
ATOM     53  H   CYS A  96     -15.460   5.599 -32.448  1.00 33.90           H
ATOM     54  HA  CYS A  96     -17.437   7.378 -33.016  1.00 27.92           H
ATOM     55  HB2 CYS A  96     -15.428   8.530 -32.624  1.00 30.68           H
ATOM   6301  HB2 ALA D 125     -19.830  59.309  14.613  1.00 31.59           H
ATOM   6302  HB3 ALA D 125     -18.315  59.403  14.144  1.00 31.59           H
ATOM   6303  N   SER D 126     -17.562  59.727  11.351  1.00 25.39           N
ATOM   6304  CA  SER D 126     -16.606  60.338  10.437  1.00 25.90           C
ATOM   6305  C   SER D 126     -17.233  60.587   9.066  1.00 21.76           C
ATOM   6306  O   SER D 126     -17.156  61.693   8.535  1.00 20.77           O
ATOM   6307  CB  SER D 126     -15.363  59.460  10.298  1.00 24.59           C
ATOM   6308  OG  SER D 126     -14.403  60.072   9.456  1.00 23.90           O
ATOM   6309  H   SER D 126     -17.305  58.973  11.676  1.00 30.47           H
ATOM   6310  HA  SER D 126     -16.328  61.195  10.798  1.00 31.08           H
ATOM   6311  HB2 SER D 126     -14.973  59.325  11.175  1.00 29.51           H
ATOM   6312  HB3 SER D 126     -15.621  58.607   9.915  1.00 29.51           H
ATOM   6313  HG  SER D 126     -13.725  59.580   9.388  1.00 28.69           H
ATOM   6314  N   CYS D 127     -17.866  59.564   8.501  1.00 22.12           N
ATOM   6315  CA  CYS D 127     -18.500  59.692   7.192  1.00 22.37           C
ATOM   6316  C   CYS D 127     -19.619  60.731   7.206  1.00 23.64           C
ATOM   6317  O   CYS D 127     -19.765  61.513   6.260  1.00 23.85           O
ATOM   6318  CB  CYS D 127     -19.053  58.341   6.731  1.00 23.71           C
ATOM   6319  SG  CYS D 127     -17.786  57.091   6.427  1.00 20.25           S
ATOM   6320  H   CYS D 127     -17.943  58.784   8.855  1.00 26.54           H
ATOM   6321  HA  CYS D 127     -17.834  59.978   6.548  1.00 26.84           H
ATOM   6322  HB2 CYS D 127     -19.648  57.998   7.415  1.00 28.45           H
ATOM   6323  HB3 CYS D 127     -19.544  58.471   5.905  1.00 28.45           H
ATOM   6324  N   MET D 128     -20.406  60.737   8.277  1.00 24.97           N
ATOM   6325  CA  MET D 128     -21.524  61.668   8.398  1.00 26.23           C
ATOM   6326  C   MET D 128     -21.036  63.111   8.394  1.00 26.46           C
ATOM   6327  O   MET D 128     -21.642  63.975   7.764  1.00 29.60           O
ATOM   6328  CB  MET D 128     -22.322  61.394   9.673  1.00 27.84           C
ATOM   6329  CG  MET D 128     -23.246  60.187   9.582  1.00 42.42           C
ATOM   6330  SD  MET D 128     -24.266  59.966  11.056  1.00 63.01           S
ATOM   6331  CE  MET D 128     -25.311  61.419  10.970  1.00 61.60           C
ATOM   6332  H   MET D 128     -20.314  60.209   8.950  1.00 29.96           H
ATOM   6333  HA  MET D 128     -22.120  61.539   7.643  1.00 31.47           H
ATOM   6334  HB2 MET D 128     -21.701  61.237  10.401  1.00 33.41           H
ATOM   6335  HB3 MET D 128     -22.869  62.171   9.871  1.00 33.41           H
ATOM   6336  HG2 MET D 128     -23.839  60.301   8.823  1.00 50.90           H
ATOM   6337  HG3 MET D 128     -22.710  59.388   9.467  1.00 50.90           H
ATOM   6338  HE1 MET D 128     -25.919  61.416  11.726  1.00 73.92           H
ATOM   6339  HE2 MET D 128     -24.752  62.212  10.998  1.00 73.92           H
ATOM   6340  HE3 MET D 128     -25.814  61.398  10.141  1.00 73.92           H
ATOM   6341  N   SER D 129     -19.934  63.362   9.092  1.00 27.28           N
ATOM   6342  CA  SER D 129     -19.385  64.711   9.196  1.00 30.17           C
ATOM   6343  C   SER D 129     -18.834  65.196   7.859  1.00 28.90           C
ATOM   6344  O   SER D 129     -18.574  66.386   7.686  1.00 28.22           O
ATOM   6345  CB  SER D 129     -18.286  64.764  10.259  1.00 35.60           C
ATOM   6346  OG  SER D 129     -17.121  64.078   9.831  1.00 30.81           O
ATOM   6347  H   SER D 129     -19.482  62.766   9.517  1.00 32.74           H
ATOM   6348  HA  SER D 129     -20.092  65.318   9.466  1.00 36.20           H
ATOM   6349  HB2 SER D 129     -18.059  65.691  10.431  1.00 42.72           H
ATOM   6350  HB3 SER D 129     -18.614  64.348  11.072  1.00 42.72           H
ATOM   6351  HG  SER D 129     -17.301  63.272   9.680  1.00 36.97           H
ATOM   6352  N   GLN D 130     -18.659  64.270   6.920  1.00 27.90           N
ATOM   6353  CA  GLN D 130     -18.164  64.603   5.589  1.00 25.08           C
ATOM   6354  C   GLN D 130     -19.291  64.546   4.564  1.00 25.68           C
ATOM   6355  O   GLN D 130     -19.051  64.318   3.379  1.00 25.29           O
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ATOM 56 HB3 CYS A 96 -14.727 7.677 -33.761 1.00 30.68
H
ATOM 57 N GLY A 97 -17.937 6.497 -35.244 1.00 24.78
N
ATOM 58 CA GLY A 97 -18.277 5.840 -36.491 1.00 28.73
C
ATOM 59 C GLY A 97 -19.711 5.345 -36.494 1.00 30.42
C
ATOM 60 O GLY A 97 -20.560 5.912 -35.807 1.00 28.09
O
ATOM 61 H GLY A 97 -18.520 7.074 -34.984 1.00 29.73
H
ATOM 62 HA2 GLY A 97 -18.162 6.460 -37.228 1.00 34.47
H
ATOM 63 HA3 GLY A 97 -17.688 5.082 -36.630 1.00 34.47
H
ATOM 64 N PRO A 98 -19.994 4.281 -37.266 1.00 30.69
N
ATOM 65 CA PRO A 98 -19.033 3.536 -38.091 1.00 29.74
C
ATOM 66 C PRO A 98 -18.509 4.341 -39.280 1.00 26.22
C
ATOM 67 O PRO A 98 -19.241 5.130 -39.878 1.00 28.36
O
ATOM 68 CB PRO A 98 -19.843 2.324 -38.566 1.00 27.73
C
ATOM 69 CG PRO A 98 -21.247 2.772 -38.528 1.00 29.99
C
ATOM 70 CD PRO A 98 -21.353 3.723 -37.371 1.00 26.89
C
ATOM 71 HA PRO A 98 -18.286 3.234 -37.551 1.00 35.69
H
ATOM 72 HB2 PRO A 98 -19.581 2.088 -39.469 1.00 33.28
H
ATOM 73 HB3 PRO A 98 -19.703 1.579 -37.960 1.00 33.28
H
ATOM 74 HG2 PRO A 98 -21.466 3.222 -39.358 1.00 35.98
H
ATOM 75 HG3 PRO A 98 -21.827 2.006 -38.392 1.00 35.98
H
ATOM 76 HD2 PRO A 98 -21.993 4.424 -37.567 1.00 32.27
H
ATOM 77 HD3 PRO A 98 -21.585 3.244 -36.559 1.00 32.27
H
ATOM 78 N CYS A 99 -17.232 4.142 -39.591 1.00 22.72
N
ATOM 79 CA CYS A 99 -16.582 4.768 -40.737 1.00 27.89
C
ATOM 80 C CYS A 99 -15.575 3.793 -41.326 1.00 21.11
C
ATOM 81 O CYS A 99 -15.165 2.848 -40.653 1.00 25.21
O
ATOM 82 CB CYS A 99 -15.865 6.062 -40.337 1.00 25.67
C
ATOM 83 SG CYS A 99 -16.919 7.351 -39.649 1.00 24.92
S
ATOM 84 H CYS A 99 -16.707 3.634 -39.138 1.00 27.26
H
ATOM 85 HA CYS A 99 -17.245 4.977 -41.414 1.00 33.47
H
ATOM 86 HB2 CYS A 99 -15.194 5.847 -39.670 1.00 30.81
H
ATOM 87 HB3 CYS A 99 -15.433 6.429 -41.124 1.00 30.81
H
ATOM 88 N PRO A 100 -15.165 4.018 -42.583 1.00 24.66
N
ATOM 89 CA PRO A 100 -14.053 3.244 -43.146 1.00 24.78
C
ATOM 6356 CB GLN D 130 -17.035 63.654 5.189 1.00 27.46
C
ATOM 6357 CG GLN D 130 -15.877 63.654 6.167 1.00 29.13
C
ATOM 6358 CD GLN D 130 -14.797 62.669 5.790 1.00 26.28
C
ATOM 6359 OE1 GLN D 130 -14.110 62.843 4.786 1.00 25.42
O
ATOM 6360 NE2 GLN D 130 -14.637 61.625 6.598 1.00 26.08
N
ATOM 6361 H GLN D 130 -18.821 63.433 7.032 1.00 33.48 H
ATOM 6362 HA GLN D 130 -17.811 65.506 5.599 1.00 30.10
H
ATOM 6363 HB2 GLN D 130 -17.385 62.751 5.141 1.00 32.95
H
ATOM 6364 HB3 GLN D 130 -16.692 63.922 4.322 1.00 32.95
H
ATOM 6365 HG2 GLN D 130 -15.482 64.539 6.190 1.00 34.95
H
ATOM 6366 HG3 GLN D 130 -16.207 63.415 7.047 1.00 34.95
H
ATOM 6367 HE21 GLN D 130 -14.034 61.036 6.425 1.00 31.30
H
ATOM 6368 HE22 GLN D 130 -15.136 61.539 7.293 1.00 31.30
H
ATOM 6369 N ASN D 131 -20.515 64.766 5.035 1.00 26.26 N
ATOM 6370 CA ASN D 131 -21.699 64.750 4.182 1.00 29.68
C
ATOM 6371 C ASN D 131 -21.772 63.462 3.370 1.00 28.66 C
ATOM 6372 O ASN D 131 -21.989 63.485 2.157 1.00 26.21
O
ATOM 6373 CB ASN D 131 -21.704 65.965 3.251 1.00 33.82
C
ATOM 6374 CG ASN D 131 -23.039 66.164 2.559 1.00 43.32
C
ATOM 6375 OD1 ASN D 131 -24.084 65.767 3.074 1.00 57.86
O
ATOM 6376 ND2 ASN D 131 -23.009 66.779 1.382 1.00 51.68
N
ATOM 6377 H ASN D 131 -20.689 64.929 5.861 1.00 31.51 H
ATOM 6378 HA ASN D 131 -22.490 64.797 4.740 1.00 35.61
H
ATOM 6379 HB2 ASN D 131 -21.512 66.761 3.770 1.00 40.59
H
ATOM 6380 HB3 ASN D 131 -21.026 65.842 2.568 1.00 40.59
H
ATOM 6381 HD21 ASN D 131 -23.740 66.916 0.950 1.00 62.02
H
ATOM 6382 HD22 ASN D 131 -22.259 67.041 1.052 1.00 62.02
H
ATOM 6383 N ALA D 132 -21.587 62.341 4.058 1.00 29.65 N
ATOM 6384 CA ALA D 132 -21.549 61.035 3.420 1.00 21.47
C
ATOM 6385 C ALA D 132 -22.010 59.962 4.394 1.00 21.23 C
ATOM 6386 O ALA D 132 -22.408 60.258 5.521 1.00 20.92 O
ATOM 6387 CB ALA D 132 -20.139 60.734 2.924 1.00 25.52
C
ATOM 6388 H ALA D 132 -21.479 62.313 4.911 1.00 35.58 H
ATOM 6389 HA ALA D 132 -22.148 61.033 2.657 1.00 25.77
H

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ATOM     90  C   PRO A 100     -12.777   3.400 -42.312  1.00 27.64
C
ATOM     91  O   PRO A 100     -12.552   4.460 -41.723  1.00 21.92
O
ATOM     92  CB  PRO A 100     -13.882   3.841 -44.546  1.00 25.09
C
ATOM     93  CG  PRO A 100     -15.217   4.427 -44.874  1.00 26.97
C
ATOM     94  CD  PRO A 100     -15.757   4.935 -43.574  1.00 24.88
C
ATOM     95  HA  PRO A 100     -14.288   2.306 -43.216  1.00 29.73
H
ATOM     96  HB2 PRO A 100     -13.199   4.530 -44.527  1.00 30.11
H
ATOM     97  HB3 PRO A 100     -13.649   3.141 -45.175  1.00 30.11
H
ATOM     98  HG2 PRO A 100     -15.108   5.153 -45.507  1.00 32.37
H
ATOM     99  HG3 PRO A 100     -15.795   3.738 -45.239  1.00 32.37
H
ATOM    100  HD2 PRO A 100     -15.458   5.844 -43.415  1.00 29.86
H
ATOM    101  HD3 PRO A 100     -16.725   4.870 -43.560  1.00 29.86
H
ATOM    102  N   LYS A 101     -11.958   2.356 -42.268  1.00 25.51
N
ATOM    103  CA  LYS A 101     -10.803   2.317 -41.372  1.00 31.26
C
ATOM    104  C   LYS A 101      -9.762   3.391 -41.680  1.00 29.73
C
ATOM    105  O   LYS A 101      -9.072   3.864 -40.778  1.00 35.56
O
ATOM    106  CB  LYS A 101     -10.142   0.936 -41.429  1.00 34.82
C
ATOM    107  CG  LYS A 101     -10.941  -0.169 -40.743  1.00 42.12
C
ATOM    108  CD  LYS A 101     -10.935  -0.038 -39.222  1.00 53.27
C
ATOM    109  CE  LYS A 101      -9.570  -0.367 -38.628  1.00 64.08
C
ATOM    110  NZ  LYS A 101      -9.569  -0.299 -37.138  1.00 67.45
N1+
ATOM    111  H   LYS A 101     -12.048   1.650 -42.750  1.00 30.62
H
ATOM    112  HA  LYS A 101     -11.111   2.460 -40.464  1.00 37.51
H
ATOM    113  HB2 LYS A 101     -10.027   0.684 -42.358  1.00 41.79
H
ATOM    114  HB3 LYS A 101      -9.276   0.988 -40.994  1.00 41.79
H
ATOM    115  HG2 LYS A 101     -11.862  -0.127 -41.045  1.00 50.54
H
ATOM    116  HG3 LYS A 101     -10.554  -1.028 -40.973  1.00 50.54
H
ATOM    117  HD2 LYS A 101     -11.158   0.874 -38.979  1.00 63.92
H
ATOM    118  HD3 LYS A 101     -11.585  -0.652 -38.846  1.00 63.92
H
ATOM    119  HE2 LYS A 101      -9.319  -1.267 -38.889  1.00 76.89
H
ATOM    120  HE3 LYS A 101      -8.917   0.270 -38.959  1.00 76.89
H
ATOM    121  HZ1 LYS A 101      -8.759  -0.496 -36.825  1.00 80.94
H
ATOM    122  HZ2 LYS A 101      -9.791   0.520 -36.870  1.00 80.94
H
ATOM    123  HZ3 LYS A 101     -10.156  -0.880 -36.807  1.00 80.94
H

ATOM   6390 HB1 ALA D 132     -20.133  59.860   2.502  1.00 30.63
H
ATOM   6391 HB2 ALA D 132     -19.879  61.413   2.282  1.00 30.63
H
ATOM   6392 HB3 ALA D 132     -19.530  60.741   3.679  1.00 30.63
H

ATOM   6393  N   SER D 133     -21.960  58.712   3.950  1.00 20.34      N
ATOM   6394  CA  SER D 133     -22.241  57.581   4.818  1.00 23.44
C

ATOM   6395  C   SER D 133     -21.204  56.498   4.567  1.00 19.78      C
ATOM   6396  O   SER D 133     -20.410  56.591   3.631  1.00 21.50
O
ATOM   6397  CB  SER D 133     -23.655  57.042   4.580  1.00 25.25
C
ATOM   6398  OG  SER D 133     -23.728  56.304   3.372  1.00 29.15
O

ATOM   6399  H   SER D 133     -21.763  58.493   3.142  1.00 24.41      H
ATOM   6400  HA  SER D 133     -22.172  57.861   5.744  1.00 28.13
H
ATOM   6401  HB2 SER D 133     -23.898  56.461   5.318  1.00 30.30
H
ATOM   6402  HB3 SER D 133     -24.272  57.788   4.530  1.00 30.30
H
ATOM   6403  HG  SER D 133     -23.521  56.795   2.723  1.00 34.98
H

ATOM   6404  N   LEU D 134     -21.197  55.478   5.414  1.00 20.00      N
ATOM   6405  CA  LEU D 134     -20.356  54.318   5.176  1.00 20.07
C

ATOM   6406  C   LEU D 134     -20.763  53.669   3.859  1.00 17.40      C

ATOM   6407  O   LEU D 134     -21.874  53.883   3.376  1.00 16.70      O
ATOM   6408  CB  LEU D 134     -20.465  53.326   6.331  1.00 20.33
C
ATOM   6409  CG  LEU D 134     -19.715  53.750   7.595  1.00 21.63
C
ATOM   6410 CD1 LEU D 134     -20.135  52.914   8.797  1.00 22.51
C
ATOM   6411 CD2 LEU D 134     -18.214  53.647   7.381  1.00 18.39
C

ATOM   6412  H   LEU D 134     -21.669  55.435   6.132  1.00 23.99      H
ATOM   6413  HA  LEU D 134     -19.431  54.601   5.104  1.00 24.08
H
ATOM   6414  HB2 LEU D 134     -21.401  53.222   6.565  1.00 24.39
H
ATOM   6415  HB3 LEU D 134     -20.102  52.473   6.045  1.00 24.39
H
ATOM   6416  HG  LEU D 134     -19.925  54.677   7.789  1.00 25.96
H
ATOM   6417 HD11 LEU D 134     -19.640  53.211   9.576  1.00 27.02
H
ATOM   6418 HD12 LEU D 134     -21.087  53.030   8.944  1.00 27.02
H
ATOM   6419 HD13 LEU D 134     -19.939  51.981   8.616  1.00 27.02
H
ATOM   6420 HD21 LEU D 134     -17.760  53.920   8.194  1.00 22.07
H
ATOM   6421 HD22 LEU D 134     -17.988  52.728   7.169  1.00 22.07
H
ATOM   6422 HD23 LEU D 134     -17.959  54.228   6.648  1.00 22.07
H

ATOM   6423  N   LEU D 135     -19.852  52.894   3.279  1.00 16.34      N
```

ATOM 124 N ASN A 102 -9.648 3.770 -42.949 1.00 25.43 N
ATOM 125 CA ASN A 102 -8.650 4.749 -43.370 1.00 29.54 C
ATOM 126 C ASN A 102 -9.227 6.159 -43.532 1.00 27.18 C
ATOM 127 O ASN A 102 -8.621 7.013 -44.180 1.00 24.09 O
ATOM 128 CB ASN A 102 -7.995 4.294 -44.680 1.00 34.94 C
ATOM 129 CG ASN A 102 -9.006 3.828 -45.715 1.00 30.75 C
ATOM 130 OD1 ASN A 102 -10.215 3.951 -45.520 1.00 34.90 O
ATOM 131 ND2 ASN A 102 -8.512 3.285 -46.823 1.00 37.11 N
ATOM 132 H ASN A 102 -10.139 3.473 -43.589 1.00 30.52 H
ATOM 133 HA ASN A 102 -7.956 4.793 -42.695 1.00 35.45 H
ATOM 134 HB2 ASN A 102 -7.498 5.035 -45.060 1.00 41.92 H
ATOM 135 HB3 ASN A 102 -7.396 3.554 -44.493 1.00 41.92 H
ATOM 136 HD21 ASN A 102 -9.043 3.006 -47.439 1.00 44.53 H
ATOM 137 HD22 ASN A 102 -7.661 3.213 -46.923 1.00 44.53 H
ATOM 138 N TRP A 103 -10.392 6.399 -42.932 1.00 22.81 N
ATOM 139 CA TRP A 103 -11.038 7.712 -42.979 1.00 22.94 C
ATOM 140 C TRP A 103 -11.012 8.411 -41.623 1.00 21.34 C
ATOM 141 O TRP A 103 -10.915 7.764 -40.583 1.00 18.27 O
ATOM 142 CB TRP A 103 -12.492 7.586 -43.443 1.00 21.32 C
ATOM 143 CG TRP A 103 -12.658 7.417 -44.919 1.00 26.61 C
ATOM 144 CD1 TRP A 103 -11.883 6.664 -45.755 1.00 30.04 C
ATOM 145 CD2 TRP A 103 -13.663 8.023 -45.738 1.00 23.17 C
ATOM 146 NE1 TRP A 103 -12.351 6.759 -47.044 1.00 29.11 N
ATOM 147 CE2 TRP A 103 -13.442 7.588 -47.061 1.00 26.93 C
ATOM 148 CE3 TRP A 103 -14.731 8.887 -45.481 1.00 20.70 C
ATOM 149 CZ2 TRP A 103 -14.249 7.990 -48.123 1.00 28.53 C
ATOM 150 CZ3 TRP A 103 -15.530 9.286 -46.534 1.00 24.02 C
ATOM 151 CH2 TRP A 103 -15.285 8.837 -47.841 1.00 22.80 C
ATOM 152 H TRP A 103 -10.834 5.812 -42.486 1.00 27.37 H
ATOM 153 HA TRP A 103 -10.568 8.273 -43.616 1.00 27.52 H
ATOM 154 HB2 TRP A 103 -12.889 6.814 -43.011 1.00 25.59 H
ATOM 155 HB3 TRP A 103 -12.971 8.389 -43.183 1.00 25.59 H
ATOM 156 HD1 TRP A 103 -11.150 6.157 -45.490 1.00 36.05 H
ATOM 157 HE1 TRP A 103 -12.012 6.365 -47.729 1.00 34.93 H

ATOM 6424 CA LEU D 135 -20.103 52.208 2.015 1.00 15.50 C
ATOM 6425 C LEU D 135 -21.457 51.505 1.999 1.00 13.53 C
ATOM 6426 O LEU D 135 -21.796 50.755 2.914 1.00 17.46 O
ATOM 6427 CB LEU D 135 -18.996 51.190 1.734 1.00 18.55 C
ATOM 6428 CG LEU D 135 -19.162 50.301 0.498 1.00 20.09 C
ATOM 6429 CD1 LEU D 135 -19.189 51.135 -0.777 1.00 17.39 C
ATOM 6430 CD2 LEU D 135 -18.048 49.257 0.440 1.00 19.20 C
ATOM 6431 H LEU D 135 -19.068 52.747 3.602 1.00 19.60 H
ATOM 6432 HA LEU D 135 -20.098 52.861 1.298 1.00 18.60 H
ATOM 6433 HB2 LEU D 135 -18.163 51.674 1.627 1.00 22.27 H
ATOM 6434 HB3 LEU D 135 -18.927 50.601 2.501 1.00 22.27 H
ATOM 6435 HG LEU D 135 -20.007 49.829 0.562 1.00 24.11 H
ATOM 6436 HD11 LEU D 135 -19.295 50.543 -1.539 1.00 20.87 H
ATOM 6437 HD12 LEU D 135 -19.935 51.754 -0.733 1.00 20.87 H
ATOM 6438 HD13 LEU D 135 -18.356 51.625 -0.852 1.00 20.87 H
ATOM 6439 HD21 LEU D 135 -18.172 48.707 -0.349 1.00 23.04 H
ATOM 6440 HD22 LEU D 135 -17.192 49.712 0.395 1.00 23.04 H
ATOM 6441 HD23 LEU D 135 -18.089 48.707 1.238 1.00 23.04 H
ATOM 6442 N LYS D 136 -22.225 51.785 0.953 1.00 17.78 N
ATOM 6443 CA LYS D 136 -23.470 51.084 0.685 1.00 21.52 C
ATOM 6444 C LYS D 136 -23.326 50.350 -0.635 1.00 16.54 C
ATOM 6445 O LYS D 136 -23.061 50.967 -1.664 1.00 16.88 O
ATOM 6446 CB LYS D 136 -24.652 52.054 0.638 1.00 21.22 C
ATOM 6447 CG LYS D 136 -25.972 51.387 0.267 1.00 24.56 C
ATOM 6448 CD LYS D 136 -27.137 52.358 0.370 1.00 28.19 C
ATOM 6449 CE LYS D 136 -28.427 51.738 -0.151 1.00 28.08 C
ATOM 6450 NZ LYS D 136 -29.569 52.692 -0.091 1.00 28.58 N1+
ATOM 6451 H LYS D 136 -22.040 52.391 0.372 1.00 21.34 H
ATOM 6452 HA LYS D 136 -23.633 50.432 1.385 1.00 25.82 H
ATOM 6453 HB2 LYS D 136 -24.759 52.460 1.512 1.00 25.47 H
ATOM 6454 HB3 LYS D 136 -24.468 52.739 -0.024 1.00 25.47 H
ATOM 6455 HG2 LYS D 136 -25.923 51.067 -0.648 1.00 29.47 H
ATOM 6456 HG3 LYS D 136 -26.138 50.648 0.872 1.00 29.47 H
ATOM 6457 HD2 LYS D 136 -27.270 52.601 1.300 1.00 33.82 H

ATOM 158 HE3 TRP A 103 -14.900 9.188 -44.618 1.00 24.84
H
ATOM 159 HZ2 TRP A 103 -14.088 7.695 -48.990 1.00 34.23
H
ATOM 160 HZ3 TRP A 103 -16.243 9.861 -46.374 1.00 28.82
H
ATOM 161 HH2 TRP A 103 -15.840 9.122 -48.531 1.00 27.37
H
ATOM 162 N ILE A 104 -11.122 9.737 -41.653 1.00 15.59
N
ATOM 163 CA ILE A 104 -11.210 10.546 -40.444 1.00 17.76
C
ATOM 164 C ILE A 104 -12.621 10.491 -39.868 1.00 21.68
C
ATOM 165 O ILE A 104 -13.587 10.764 -40.577 1.00 20.98
O
ATOM 166 CB ILE A 104 -10.853 12.022 -40.718 1.00 19.18
C
ATOM 167 CG1 ILE A 104 -9.470 12.139 -41.368 1.00 22.53
C
ATOM 168 CG2 ILE A 104 -10.910 12.835 -39.425 1.00 20.64
C
ATOM 169 CD1 ILE A 104 -9.156 13.530 -41.903 1.00 18.10
C
ATOM 170 H ILE A 104 -11.147 10.199 -42.378 1.00 18.71
H
ATOM 171 HA ILE A 104 -10.594 10.201 -39.779 1.00 21.31
H
ATOM 172 HB ILE A 104 -11.510 12.384 -41.333 1.00 23.02
H
ATOM 173 HG12 ILE A 104 -8.795 11.917 -40.708 1.00 27.03
H
ATOM 174 HG13 ILE A 104 -9.421 11.518 -42.111 1.00 27.03
H
ATOM 175 HG21 ILE A 104 -10.683 13.757 -39.622 1.00 24.77
H
ATOM 176 HG22 ILE A 104 -11.808 12.785 -39.061 1.00 24.77
H
ATOM 177 HG23 ILE A 104 -10.275 12.465 -38.792 1.00 24.77
H
ATOM 178 HD11 ILE A 104 -8.270 13.523 -42.297 1.00 21.72
H
ATOM 179 HD12 ILE A 104 -9.815 13.765 -42.575 1.00 21.72
H
ATOM 180 HD13 ILE A 104 -9.189 14.164 -41.171 1.00 21.72
H
ATOM 181 N CYS A 105 -12.734 10.151 -38.587 1.00 19.34
N
ATOM 182 CA CYS A 105 -14.026 10.133 -37.909 1.00 18.07
C
ATOM 183 C CYS A 105 -14.117 11.285 -36.914 1.00 21.22
C
ATOM 184 O CYS A 105 -13.216 11.497 -36.102 1.00 21.20
O
ATOM 185 CB CYS A 105 -14.249 8.800 -37.196 1.00 23.12
C
ATOM 186 SG CYS A 105 -15.944 8.565 -36.591 1.00 26.35
S
ATOM 187 H CYS A 105 -12.073 9.926 -38.085 1.00 23.20
H
ATOM 188 HA CYS A 105 -14.731 10.246 -38.566 1.00 21.68
H
ATOM 189 HB2 CYS A 105 -14.053 8.079 -37.814 1.00 27.74
H
ATOM 190 HB3 CYS A 105 -13.653 8.750 -36.433 1.00 27.74
H
ATOM 191 N TYR A 106 -15.207 12.035 -37.000 1.00 17.94
N

ATOM 6458 HD3 LYS D 136 -26.944 53.148 -0.159 1.00 33.82
H
ATOM 6459 HE2 LYS D 136 -28.302 51.473 -1.076 1.00 33.70
H
ATOM 6460 HE3 LYS D 136 -28.650 50.965 0.391 1.00 33.70
H
ATOM 6461 HZ1 LYS D 136 -30.307 52.302 -0.401 1.00 34.29
H
ATOM 6462 HZ2 LYS D 136 -29.708 52.947 0.751 1.00 34.29
H
ATOM 6463 HZ3 LYS D 136 -29.391 53.410 -0.585 1.00 34.29
H

ATOM 6464 N VAL D 137 -23.490 49.032 -0.592 1.00 15.00 N
ATOM 6465 CA VAL D 137 -23.377 48.194 -1.777 1.00 14.80
C

ATOM 6466 C VAL D 137 -24.767 47.914 -2.328 1.00 15.82 C

ATOM 6467 O VAL D 137 -25.542 47.181 -1.714 1.00 17.01 O
ATOM 6468 CB VAL D 137 -22.661 46.870 -1.462 1.00 18.73
C
ATOM 6469 CG1 VAL D 137 -22.505 46.037 -2.723 1.00 21.27
C
ATOM 6470 CG2 VAL D 137 -21.293 47.142 -0.828 1.00 19.01
C

ATOM 6471 H VAL D 137 -23.670 48.594 0.126 1.00 18.00 H
ATOM 6472 HA VAL D 137 -22.867 48.663 -2.456 1.00 17.76
H
ATOM 6473 HB VAL D 137 -23.193 46.363 -0.829 1.00 22.47
H
ATOM 6474 HG11 VAL D 137 -22.052 45.209 -2.500 1.00 25.53
H
ATOM 6475 HG12 VAL D 137 -23.384 45.846 -3.086 1.00 25.53
H
ATOM 6476 HG13 VAL D 137 -21.981 46.537 -3.368 1.00 25.53
H
ATOM 6477 HG21 VAL D 137 -20.859 46.296 -0.638 1.00 22.82
H
ATOM 6478 HG22 VAL D 137 -20.755 47.658 -1.449 1.00 22.82
H
ATOM 6479 HG23 VAL D 137 -21.420 47.641 -0.006 1.00 22.82
H

ATOM 6480 N TYR D 138 -25.068 48.500 -3.485 1.00 15.98 N
ATOM 6481 CA TYR D 138 -26.410 48.453 -4.061 1.00 20.40
C

ATOM 6482 C TYR D 138 -26.439 47.849 -5.467 1.00 19.25 C
ATOM 6483 O TYR D 138 -27.512 47.551 -5.991 1.00 19.44
O
ATOM 6484 CB TYR D 138 -27.006 49.865 -4.106 1.00 16.40
C
ATOM 6485 CG TYR D 138 -26.405 50.758 -5.170 1.00 15.53
C
ATOM 6486 CD1 TYR D 138 -26.952 50.820 -6.446 1.00 18.12
C
ATOM 6487 CD2 TYR D 138 -25.293 51.544 -4.897 1.00 20.57
C
ATOM 6488 CE1 TYR D 138 -26.406 51.635 -7.419 1.00 18.07
C
ATOM 6489 CE2 TYR D 138 -24.742 52.366 -5.864 1.00 14.74
C
ATOM 6490 CZ TYR D 138 -25.298 52.407 -7.121 1.00 19.68
C
ATOM 6491 OH TYR D 138 -24.748 53.225 -8.080 1.00 18.98
O

ATOM 192 CA TYR A 106 -15.451 13.148 -36.097 1.00 18.87 C
ATOM 193 C TYR A 106 -16.943 13.284 -35.857 1.00 20.09 C
ATOM 194 O TYR A 106 -17.711 13.548 -36.785 1.00 17.41 O
ATOM 195 CB TYR A 106 -14.881 14.452 -36.659 1.00 17.90 C
ATOM 196 CG TYR A 106 -14.966 15.613 -35.696 1.00 17.46 C
ATOM 197 CD1 TYR A 106 -14.351 15.552 -34.452 1.00 24.97 C
ATOM 198 CD2 TYR A 106 -15.651 16.774 -36.031 1.00 21.85 C
ATOM 199 CE1 TYR A 106 -14.424 16.610 -33.562 1.00 22.33 C
ATOM 200 CE2 TYR A 106 -15.726 17.841 -35.148 1.00 20.74 C
ATOM 201 CZ TYR A 106 -15.112 17.752 -33.915 1.00 22.72 C
ATOM 202 OH TYR A 106 -15.177 18.806 -33.030 1.00 19.96 O
ATOM 203 H TYR A 106 -15.829 11.918 -37.582 1.00 21.53 H
ATOM 204 HA TYR A 106 -15.021 12.971 -35.245 1.00 22.65 H
ATOM 205 HB2 TYR A 106 -13.947 14.316 -36.880 1.00 21.49 H
ATOM 206 HB3 TYR A 106 -15.377 14.692 -37.458 1.00 21.49 H
ATOM 207 HD1 TYR A 106 -13.888 14.783 -34.209 1.00 29.97 H
ATOM 208 HD2 TYR A 106 -16.068 16.836 -36.860 1.00 26.22 H
ATOM 209 HE1 TYR A 106 -14.008 16.553 -32.732 1.00 26.79 H
ATOM 210 HE2 TYR A 106 -16.190 18.611 -35.385 1.00 24.89 H
ATOM 211 HH TYR A 106 -15.622 19.435 -33.364 1.00 23.95 H
ATOM 212 N LYS A 107 -17.336 13.091 -34.602 1.00 16.90 N
ATOM 213 CA LYS A 107 -18.732 13.154 -34.190 1.00 20.74 C
ATOM 214 C LYS A 107 -19.605 12.235 -35.048 1.00 17.68 C
ATOM 215 O LYS A 107 -20.703 12.597 -35.458 1.00 16.31 O
ATOM 216 CB LYS A 107 -19.221 14.602 -34.239 1.00 23.06 C
ATOM 217 CG LYS A 107 -18.453 15.502 -33.268 1.00 17.83 C
ATOM 218 CD LYS A 107 -18.965 16.932 -33.266 1.00 24.69 C
ATOM 219 CE LYS A 107 -18.353 17.730 -32.122 1.00 26.16 C
ATOM 220 NZ LYS A 107 -18.797 19.153 -32.118 1.00 29.75 N1+
ATOM 221 H LYS A 107 -16.797 12.917 -33.955 1.00 20.28 H
ATOM 222 HA LYS A 107 -18.800 12.851 -33.271 1.00 24.89 H
ATOM 223 HB2 LYS A 107 -19.096 14.949 -35.136 1.00 27.68 H
ATOM 224 HB3 LYS A 107 -20.160 14.629 -33.998 1.00 27.68 H
ATOM 225 HG2 LYS A 107 -18.545 15.149 -32.369 1.00 21.40 H

ATOM 6492 H TYR D 138 -24.502 48.937 -3.963 1.00 19.18 H
ATOM 6493 HA TYR D 138 -26.976 47.909 -3.492 1.00 24.48 H
ATOM 6494 HB2 TYR D 138 -27.958 49.795 -4.283 1.00 19.68 H
ATOM 6495 HB3 TYR D 138 -26.863 50.291 -3.247 1.00 19.68 H
ATOM 6496 HD1 TYR D 138 -27.696 50.301 -6.650 1.00 21.75 H
ATOM 6497 HD2 TYR D 138 -24.913 51.519 -4.049 1.00 24.68 H
ATOM 6498 HE1 TYR D 138 -26.782 51.666 -8.269 1.00 21.68 H
ATOM 6499 HE2 TYR D 138 -23.996 52.885 -5.666 1.00 17.69 H
ATOM 6500 HH TYR D 138 -25.181 53.160 -8.797 1.00 22.78 H

ATOM 6501 N SER D 139 -25.271 47.667 -6.080 1.00 18.67 N
ATOM 6502 CA SER D 139 -25.222 47.169 -7.456 1.00 20.25 C
ATOM 6503 C SER D 139 -23.873 46.574 -7.844 1.00 24.81 C
ATOM 6504 O SER D 139 -22.843 47.241 -7.753 1.00 16.53 O
ATOM 6505 CB SER D 139 -25.563 48.296 -8.428 1.00 18.66 C
ATOM 6506 OG SER D 139 -25.305 47.903 -9.763 1.00 22.13 O
ATOM 6507 H SER D 139 -24.502 47.821 -5.728 1.00 22.40 H
ATOM 6508 HA SER D 139 -25.891 46.475 -7.560 1.00 24.30 H
ATOM 6509 HB2 SER D 139 -26.504 48.515 -8.339 1.00 22.39 H
ATOM 6510 HB3 SER D 139 -25.021 49.071 -8.216 1.00 22.39 H
ATOM 6511 HG SER D 139 -25.496 48.530 -10.289 1.00 26.55 H

ATOM 6512 N LYS D 140 -23.891 45.327 -8.307 1.00 22.07 N
ATOM 6513 CA LYS D 140 -22.670 44.654 -8.737 1.00 22.87 C
ATOM 6514 C LYS D 140 -22.131 45.225 -10.041 1.00 25.49 C
ATOM 6515 O LYS D 140 -20.981 44.981 -10.396 1.00 28.27 O
ATOM 6516 CB LYS D 140 -22.907 43.153 -8.904 1.00 25.37 C
ATOM 6517 CG LYS D 140 -22.861 42.373 -7.607 1.00 28.96 C
ATOM 6518 CD LYS D 140 -22.757 40.877 -7.865 1.00 34.51 C
ATOM 6519 CE LYS D 140 -22.573 40.100 -6.570 1.00 36.49 C
ATOM 6520 NZ LYS D 140 -22.353 38.648 -6.819 1.00 49.97 N1+
ATOM 6521 H LYS D 140 -24.601 44.848 -8.383 1.00 26.49 H
ATOM 6522 HA LYS D 140 -21.990 44.774 -8.056 1.00 27.44 H
ATOM 6523 HB2 LYS D 140 -23.783 43.018 -9.299 1.00 30.45 H
ATOM 6524 HB3 LYS D 140 -22.224 42.792 -9.491 1.00 30.45 H
ATOM 6525 HG2 LYS D 140 -22.085 42.648 -7.094 1.00 34.76 H

ATOM 226 HG3 LYS A 107 -17.518 15.519 -33.524 1.00 21.40 H
ATOM 227 HD2 LYS A 107 -18.723 17.362 -34.102 1.00 29.63 H
ATOM 228 HD3 LYS A 107 -19.929 16.929 -33.155 1.00 29.63 H
ATOM 229 HE2 LYS A 107 -18.618 17.329 -31.279 1.00 31.40 H
ATOM 230 HE3 LYS A 107 -17.387 17.716 -32.208 1.00 31.40 H
ATOM 231 HZ1 LYS A 107 -18.421 19.587 -31.438 1.00 35.70 H
ATOM 232 HZ2 LYS A 107 -18.560 19.548 -32.880 1.00 35.70 H
ATOM 233 HZ3 LYS A 107 -19.682 19.195 -32.034 1.00 35.70 H
ATOM 234 N ASN A 108 -19.079 11.040 -35.303 1.00 22.60 N
ATOM 235 CA ASN A 108 -19.770 9.979 -36.040 1.00 25.82 C
ATOM 236 C ASN A 108 -20.056 10.310 -37.506 1.00 27.70 C
ATOM 237 O ASN A 108 -20.822 9.609 -38.164 1.00 25.85 O
ATOM 238 CB ASN A 108 -21.069 9.606 -35.324 1.00 25.22 C
ATOM 239 CG ASN A 108 -20.816 8.947 -33.984 1.00 29.09 C
ATOM 240 OD1 ASN A 108 -19.803 8.274 -33.796 1.00 25.84 O
ATOM 241 ND2 ASN A 108 -21.733 9.139 -33.043 1.00 32.94 N
ATOM 242 H ASN A 108 -18.290 10.810 -35.050 1.00 27.12 H
ATOM 243 HA ASN A 108 -19.204 9.191 -36.033 1.00 30.98 H
ATOM 244 HB2 ASN A 108 -21.590 10.410 -35.172 1.00 30.27 H
ATOM 245 HB3 ASN A 108 -21.569 8.984 -35.876 1.00 30.27 H
ATOM 246 HD21 ASN A 108 -21.632 8.784 -32.266 1.00 39.52 H
ATOM 247 HD22 ASN A 108 -22.427 9.617 -33.210 1.00 39.52 H
ATOM 248 N ASN A 109 -19.429 11.369 -38.013 1.00 18.88 N
ATOM 249 CA ASN A 109 -19.347 11.605 -39.450 1.00 16.87 C
ATOM 250 C ASN A 109 -17.968 11.166 -39.936 1.00 20.87 C
ATOM 251 O ASN A 109 -17.001 11.227 -39.174 1.00 18.96 O
ATOM 252 CB ASN A 109 -19.587 13.078 -39.786 1.00 18.38 C
ATOM 253 CG ASN A 109 -21.004 13.525 -39.487 1.00 25.45 C
ATOM 254 OD1 ASN A 109 -21.960 12.779 -39.697 1.00 23.05 O
ATOM 255 ND2 ASN A 109 -21.145 14.749 -38.994 1.00 21.26 N
ATOM 256 H ASN A 109 -19.038 11.971 -37.539 1.00 22.66 H
ATOM 257 HA ASN A 109 -20.019 11.072 -39.905 1.00 20.25 H
ATOM 258 HB2 ASN A 109 -18.983 13.625 -39.259 1.00 22.05 H
ATOM 259 HB3 ASN A 109 -19.422 13.218 -40.731 1.00 22.05 H

ATOM 6526 HG3 LYS D 140 -23.673 42.539 -7.103 1.00 34.76 H
ATOM 6527 HD2 LYS D 140 -23.571 40.568 -8.292 1.00 41.41 H
ATOM 6528 HD3 LYS D 140 -21.992 40.703 -8.435 1.00 41.41 H
ATOM 6529 HE2 LYS D 140 -21.801 40.447 -6.097 1.00 43.79 H
ATOM 6530 HE3 LYS D 140 -23.370 40.196 -6.025 1.00 43.79 H
ATOM 6531 HZ1 LYS D 140 -22.249 38.220 -6.046 1.00 59.97 H
ATOM 6532 HZ2 LYS D 140 -23.051 38.304 -7.249 1.00 59.97 H
ATOM 6533 HZ3 LYS D 140 -21.622 38.532 -7.314 1.00 59.97 H
ATOM 6534 N GLU D 141 -22.959 45.974 -10.758 1.00 21.06 N
ATOM 6535 CA GLU D 141 -22.523 46.596 -12.001 1.00 23.91 C
ATOM 6536 C GLU D 141 -21.994 48.009 -11.753 1.00 24.83 C
ATOM 6537 O GLU D 141 -20.867 48.325 -12.135 1.00 23.48 O
ATOM 6538 CB GLU D 141 -23.666 46.614 -13.015 1.00 31.80 C
ATOM 6539 CG GLU D 141 -23.913 45.254 -13.656 1.00 35.80 C
ATOM 6540 CD GLU D 141 -25.007 45.285 -14.707 1.00 40.22 C
ATOM 6541 OE1 GLU D 141 -26.098 45.818 -14.415 1.00 42.25 O
ATOM 6542 OE2 GLU D 141 -24.775 44.777 -15.825 1.00 36.77 O1-
ATOM 6543 H GLU D 141 -23.776 46.138 -10.547 1.00 25.27 H
ATOM 6544 HA GLU D 141 -21.800 46.070 -12.378 1.00 28.69 H
ATOM 6545 HB2 GLU D 141 -24.482 46.886 -12.566 1.00 38.16 H
ATOM 6546 HB3 GLU D 141 -23.451 47.243 -13.722 1.00 38.16 H
ATOM 6547 HG2 GLU D 141 -23.096 44.954 -14.084 1.00 42.96 H
ATOM 6548 HG3 GLU D 141 -24.178 44.624 -12.968 1.00 42.96 H
ATOM 6549 N ASP D 142 -22.795 48.851 -11.106 1.00 22.91 N
ATOM 6550 CA ASP D 142 -22.382 50.226 -10.809 1.00 21.81 C
ATOM 6551 C ASP D 142 -21.179 50.272 -9.870 1.00 17.14 C
ATOM 6552 O ASP D 142 -20.484 51.284 -9.793 1.00 18.60 O
ATOM 6553 CB ASP D 142 -23.534 51.015 -10.182 1.00 23.08 C
ATOM 6554 CG ASP D 142 -24.591 51.429 -11.192 1.00 29.65 C
ATOM 6555 OD1 ASP D 142 -24.549 50.952 -12.347 1.00 32.81 O
ATOM 6556 OD2 ASP D 142 -25.474 52.232 -10.819 1.00 29.12 O1-
ATOM 6557 H ASP D 142 -23.584 48.654 -10.827 1.00 27.49 H
ATOM 6558 HA ASP D 142 -22.133 50.666 -11.637 1.00 26.17 H
ATOM 6559 HB2 ASP D 142 -23.963 50.465 -9.508 1.00 27.70 H

ATOM 260 HD21 ASN A 109 -21.929 15.050 -38.808 1.00 25.51 H
ATOM 261 HD22 ASN A 109 -20.453 15.242 -38.862 1.00 25.51 H
ATOM 262 N CYS A 110 -17.878 10.721 -41.188 1.00 16.93 N
ATOM 263 CA CYS A 110 -16.608 10.264 -41.760 1.00 16.78 C
ATOM 264 C CYS A 110 -16.142 11.205 -42.866 1.00 19.88 C
ATOM 265 O CYS A 110 -16.951 11.666 -43.665 1.00 18.76 O
ATOM 266 CB CYS A 110 -16.748 8.846 -42.312 1.00 23.56 C
ATOM 267 SG CYS A 110 -17.888 7.805 -41.378 1.00 24.98 S
ATOM 268 H CYS A 110 -18.543 10.673 -41.732 1.00 20.32 H
ATOM 269 HA CYS A 110 -15.931 10.253 -41.065 1.00 20.14 H
ATOM 270 HB2 CYS A 110 -17.074 8.898 -43.224 1.00 28.27 H
ATOM 271 HB3 CYS A 110 -15.878 8.419 -42.297 1.00 28.27 H
ATOM 272 N TYR A 111 -14.842 11.489 -42.904 1.00 14.28 N
ATOM 273 CA TYR A 111 -14.262 12.364 -43.921 1.00 17.86 C
ATOM 274 C TYR A 111 -12.987 11.787 -44.505 1.00 17.19 C
ATOM 275 O TYR A 111 -12.298 10.990 -43.866 1.00 20.29 O
ATOM 276 CB TYR A 111 -13.932 13.740 -43.342 1.00 15.15 C
ATOM 277 CG TYR A 111 -15.080 14.434 -42.669 1.00 16.62 C
ATOM 278 CD1 TYR A 111 -15.332 14.246 -41.317 1.00 16.48 C
ATOM 279 CD2 TYR A 111 -15.907 15.292 -43.381 1.00 18.87 C
ATOM 280 CE1 TYR A 111 -16.382 14.887 -40.694 1.00 16.82 C
ATOM 281 CE2 TYR A 111 -16.956 15.935 -42.770 1.00 19.83 C
ATOM 282 CZ TYR A 111 -17.191 15.730 -41.425 1.00 18.41 C
ATOM 283 OH TYR A 111 -18.242 16.373 -40.816 1.00 19.61 O
ATOM 284 H TYR A 111 -14.266 11.182 -42.343 1.00 17.13 H
ATOM 285 HA TYR A 111 -14.901 12.482 -44.642 1.00 21.43 H
ATOM 286 HB2 TYR A 111 -13.226 13.638 -42.685 1.00 18.18 H
ATOM 287 HB3 TYR A 111 -13.625 14.313 -44.063 1.00 18.18 H
ATOM 288 HD1 TYR A 111 -14.786 13.677 -40.825 1.00 19.77 H
ATOM 289 HD2 TYR A 111 -15.751 15.431 -44.287 1.00 22.65 H
ATOM 290 HE1 TYR A 111 -16.543 14.750 -39.788 1.00 20.19 H
ATOM 291 HE2 TYR A 111 -17.505 16.505 -43.259 1.00 23.79 H
ATOM 292 HH TYR A 111 -18.275 16.163 -40.004 1.00 23.53 H
ATOM 293 N GLN A 112 -12.659 12.214 -45.716 1.00 18.48 N

ATOM 6560 HB3 ASP D 142 -23.179 51.821 -9.774 1.00 27.70 H

ATOM 6561 N GLN D 143 -20.951 49.180 -9.149 1.00 17.82 N
ATOM 6562 CA GLN D 143 -19.869 49.108 -8.173 1.00 20.33 C

ATOM 6563 C GLN D 143 -19.029 47.858 -8.395 1.00 17.41 C
ATOM 6564 O GLN D 143 -18.528 47.255 -7.444 1.00 16.39 O
ATOM 6565 CB GLN D 143 -20.433 49.119 -6.754 1.00 16.84 C
ATOM 6566 CG GLN D 143 -21.350 50.301 -6.464 1.00 19.15 C
ATOM 6567 CD GLN D 143 -21.996 50.201 -5.100 1.00 15.77 C
ATOM 6568 OE1 GLN D 143 -22.746 49.264 -4.827 1.00 18.59 O
ATOM 6569 NE2 GLN D 143 -21.696 51.156 -4.229 1.00 14.45 N

ATOM 6570 H GLN D 143 -21.414 48.458 -9.208 1.00 21.39 H
ATOM 6571 HA GLN D 143 -19.294 49.882 -8.276 1.00 24.40 H
ATOM 6572 HB2 GLN D 143 -20.944 48.306 -6.615 1.00 20.21 H
ATOM 6573 HB3 GLN D 143 -19.695 49.155 -6.125 1.00 20.21 H
ATOM 6574 HG2 GLN D 143 -20.832 51.120 -6.493 1.00 22.98 H
ATOM 6575 HG3 GLN D 143 -22.054 50.327 -7.130 1.00 22.98 H
ATOM 6576 HE21 GLN D 143 -22.039 51.141 -3.440 1.00 17.34 H
ATOM 6577 HE22 GLN D 143 -21.159 51.789 -4.453 1.00 17.34 H

ATOM 6578 N ASP D 144 -18.880 47.478 -9.659 1.00 18.01 N
ATOM 6579 CA ASP D 144 -18.187 46.248 -10.016 1.00 19.97 C

ATOM 6580 C ASP D 144 -16.735 46.242 -9.540 1.00 19.34 C
ATOM 6581 O ASP D 144 -16.177 45.186 -9.256 1.00 20.61 O
ATOM 6582 CB ASP D 144 -18.247 46.025 -11.534 1.00 22.96 C
ATOM 6583 CG ASP D 144 -17.787 47.234 -12.330 1.00 26.02 C
ATOM 6584 OD1 ASP D 144 -17.622 48.322 -11.741 1.00 22.89 O
ATOM 6585 OD2 ASP D 144 -17.611 47.097 -13.558 1.00 29.55 O1-
ATOM 6586 H ASP D 144 -19.175 47.921 -10.335 1.00 21.62 H
ATOM 6587 HA ASP D 144 -18.639 45.503 -9.590 1.00 23.97 H
ATOM 6588 HB2 ASP D 144 -17.672 45.278 -11.765 1.00 27.56 H
ATOM 6589 HB3 ASP D 144 -19.162 45.830 -11.788 1.00 27.56 H

ATOM 6590 N LEU D 145 -16.128 47.417 -9.434 1.00 17.08 N
ATOM 6591 CA LEU D 145 -14.718 47.487 -9.074 1.00 21.64 C

ATOM 6592 C LEU D 145 -14.485 47.240 -7.581 1.00 19.33 C

ATOM 6593 O LEU D 145 -13.340 47.192 -7.132 1.00 18.18 O

ATOM 294 CA GLN A 112 -11.331 11.972 -46.254 1.00 20.70 C
ATOM 295 C GLN A 112 -10.973 13.053 -47.256 1.00 20.13 C
ATOM 296 O GLN A 112 -11.806 13.479 -48.055 1.00 20.24 O
ATOM 297 CB GLN A 112 -11.233 10.591 -46.905 1.00 24.04 C
ATOM 298 CG GLN A 112 -9.818 10.232 -47.369 1.00 23.23 C
ATOM 299 CD GLN A 112 -8.771 10.400 -46.272 1.00 29.49 C
ATOM 300 OE1 GLN A 112 -8.311 11.511 -45.994 1.00 31.23 O
ATOM 301 NE2 GLN A 112 -8.392 9.296 -45.645 1.00 30.50 N
ATOM 302 H GLN A 112 -13.184 12.644 -46.244 1.00 22.17 H
ATOM 303 HA GLN A 112 -10.687 12.008 -45.530 1.00 24.84 H
ATOM 304 HB2 GLN A 112 -11.513 9.921 -46.262 1.00 28.85 H
ATOM 305 HB3 GLN A 112 -11.815 10.567 -47.680 1.00 28.85 H
ATOM 306 HG2 GLN A 112 -9.806 9.306 -47.655 1.00 27.88 H
ATOM 307 HG3 GLN A 112 -9.573 10.811 -48.108 1.00 27.88 H
ATOM 308 HE21 GLN A 112 -7.804 9.338 -45.018 1.00 36.60 H
ATOM 309 HE22 GLN A 112 -8.733 8.538 -45.864 1.00 36.60 H
ATOM 310 N PHE A 113 -9.722 13.492 -47.189 1.00 18.31 N
ATOM 311 CA PHE A 113 -9.211 14.536 -48.062 1.00 22.45 C
ATOM 312 C PHE A 113 -8.399 13.908 -49.187 1.00 18.61 C
ATOM 313 O PHE A 113 -7.556 13.051 -48.936 1.00 23.89 O
ATOM 314 CB PHE A 113 -8.360 15.523 -47.259 1.00 23.17 C
ATOM 315 CG PHE A 113 -9.135 16.272 -46.211 1.00 24.24 C
ATOM 316 CD1 PHE A 113 -9.569 15.633 -45.060 1.00 29.05 C
ATOM 317 CD2 PHE A 113 -9.431 17.615 -46.375 1.00 27.58 C
ATOM 318 CE1 PHE A 113 -10.287 16.317 -44.096 1.00 26.86 C
ATOM 319 CE2 PHE A 113 -10.149 18.306 -45.412 1.00 28.41 C
ATOM 320 CZ PHE A 113 -10.574 17.655 -44.272 1.00 30.18 C
ATOM 321 H PHE A 113 -9.138 13.192 -46.634 1.00 21.97 H
ATOM 322 HA PHE A 113 -9.954 15.021 -48.454 1.00 26.94 H
ATOM 323 HB2 PHE A 113 -7.651 15.034 -46.812 1.00 27.81 H
ATOM 324 HB3 PHE A 113 -7.977 16.174 -47.868 1.00 27.81 H
ATOM 325 HD1 PHE A 113 -9.379 14.731 -44.936 1.00 34.86 H
ATOM 326 HD2 PHE A 113 -9.147 18.058 -47.142 1.00 33.09 H
ATOM 327 HE1 PHE A 113 -10.572 15.877 -43.328 1.00 32.23 H
ATOM 6594 CB LEU D 145 -14.139 48.835 -9.498 1.00 22.74 C
ATOM 6595 CG LEU D 145 -14.106 49.032 -11.021 1.00 27.25 C
ATOM 6596 CD1 LEU D 145 -13.556 50.397 -11.374 1.00 29.85 C
ATOM 6597 CD2 LEU D 145 -13.283 47.949 -11.725 1.00 30.04 C
ATOM 6598 H LEU D 145 -16.504 48.179 -9.563 1.00 20.50 H
ATOM 6599 HA LEU D 145 -14.240 46.798 -9.562 1.00 25.97 H
ATOM 6600 HB2 LEU D 145 -14.683 49.543 -9.118 1.00 27.29 H
ATOM 6601 HB3 LEU D 145 -13.230 48.905 -9.168 1.00 27.29 H
ATOM 6602 HG LEU D 145 -15.013 48.982 -11.361 1.00 32.69 H
ATOM 6603 HD11 LEU D 145 -13.546 50.493 -12.339 1.00 35.82 H
ATOM 6604 HD12 LEU D 145 -14.123 51.077 -10.979 1.00 35.82 H
ATOM 6605 HD13 LEU D 145 -12.654 50.474 -11.024 1.00 35.82 H
ATOM 6606 HD21 LEU D 145 -13.293 48.117 -12.680 1.00 36.04 H
ATOM 6607 HD22 LEU D 145 -12.372 47.979 -11.392 1.00 36.04 H
ATOM 6608 HD23 LEU D 145 -13.676 47.082 -11.537 1.00 36.04 H
ATOM 6609 N LEU D 146 -15.561 47.059 -6.818 1.00 14.34 N
ATOM 6610 CA LEU D 146 -15.431 46.629 -5.427 1.00 15.08 C
ATOM 6611 C LEU D 146 -14.819 45.229 -5.369 1.00 15.01 C
ATOM 6612 O LEU D 146 -14.308 44.808 -4.332 1.00 16.15 O
ATOM 6613 CB LEU D 146 -16.784 46.644 -4.710 1.00 19.54 C
ATOM 6614 CG LEU D 146 -17.430 48.005 -4.436 1.00 17.93 C
ATOM 6615 CD1 LEU D 146 -18.798 47.820 -3.797 1.00 17.26 C
ATOM 6616 CD2 LEU D 146 -16.545 48.849 -3.537 1.00 18.06 C
ATOM 6617 H LEU D 146 -16.372 47.177 -7.079 1.00 17.21 H
ATOM 6618 HA LEU D 146 -14.836 47.238 -4.961 1.00 18.10 H
ATOM 6619 HB2 LEU D 146 -17.413 46.135 -5.246 1.00 23.45 H
ATOM 6620 HB3 LEU D 146 -16.673 46.206 -3.851 1.00 23.45 H
ATOM 6621 HG LEU D 146 -17.548 48.477 -5.275 1.00 21.51 H
ATOM 6622 HD11 LEU D 146 -19.189 48.692 -3.632 1.00 20.71 H
ATOM 6623 HD12 LEU D 146 -19.362 47.312 -4.400 1.00 20.71 H
ATOM 6624 HD13 LEU D 146 -18.692 47.340 -2.960 1.00 20.71 H
ATOM 6625 HD21 LEU D 146 -16.977 49.703 -3.381 1.00 21.67 H
ATOM 6626 HD22 LEU D 146 -16.416 48.384 -2.695 1.00 21.67 H
ATOM 6627 HD23 LEU D 146 -15.689 48.986 -3.974 1.00 21.67 H

ATOM 328 HE2 PHE A 113 -10.342 19.208 -45.533 1.00 34.10
H
ATOM 329 HZ PHE A 113 -11.055 18.118 -43.624 1.00 36.22
H
ATOM 330 N PHE A 114 -8.669 14.324 -50.420 1.00 16.59
N
ATOM 331 CA PHE A 114 -7.977 13.782 -51.589 1.00 20.44
C
ATOM 332 C PHE A 114 -7.120 14.850 -52.250 1.00 23.27
C
ATOM 333 O PHE A 114 -7.637 15.860 -52.728 1.00 21.65
O
ATOM 334 CB PHE A 114 -8.987 13.208 -52.582 1.00 23.69
C
ATOM 335 CG PHE A 114 -9.683 11.983 -52.077 1.00 18.44
C
ATOM 336 CD1 PHE A 114 -10.811 12.092 -51.285 1.00 22.02
C
ATOM 337 CD2 PHE A 114 -9.190 10.723 -52.366 1.00 25.83
C
ATOM 338 CE1 PHE A 114 -11.447 10.964 -50.805 1.00 26.42
C
ATOM 339 CE2 PHE A 114 -9.821 9.592 -51.890 1.00 23.08
C
ATOM 340 CZ PHE A 114 -10.949 9.712 -51.107 1.00 25.76
C
ATOM 341 H PHE A 114 -9.255 14.925 -50.610 1.00 19.91
H
ATOM 342 HA PHE A 114 -7.393 13.062 -51.305 1.00 24.52
H
ATOM 343 HB2 PHE A 114 -9.662 13.880 -52.767 1.00 28.43
H
ATOM 344 HB3 PHE A 114 -8.524 12.972 -53.401 1.00 28.43
H
ATOM 345 HD1 PHE A 114 -11.149 12.933 -51.079 1.00 26.43
H
ATOM 346 HD2 PHE A 114 -8.428 10.637 -52.893 1.00 31.00
H
ATOM 347 HE1 PHE A 114 -12.209 11.047 -50.278 1.00 31.70
H
ATOM 348 HE2 PHE A 114 -9.485 8.749 -52.095 1.00 27.69
H
ATOM 349 HZ PHE A 114 -11.377 8.951 -50.787 1.00 30.91
H
ATOM 350 N ASP A 115 -5.810 14.617 -52.275 1.00 21.39
N
ATOM 351 CA ASP A 115 -4.861 15.629 -52.727 1.00 28.87
C
ATOM 352 C ASP A 115 -4.607 15.563 -54.233 1.00 29.39
C
ATOM 353 O ASP A 115 -3.870 16.383 -54.778 1.00 29.44
O
ATOM 354 CB ASP A 115 -3.541 15.496 -51.959 1.00 30.80
C
ATOM 355 CG ASP A 115 -2.889 14.136 -52.135 1.00 36.31
C
ATOM 356 OD1 ASP A 115 -3.559 13.199 -52.615 1.00 34.47
O
ATOM 357 OD2 ASP A 115 -1.698 14.005 -51.780 1.00 46.52
O1-
ATOM 358 H ASP A 115 -5.444 13.877 -52.034 1.00 25.67
H
ATOM 359 HA ASP A 115 -5.228 16.505 -52.530 1.00 34.65
H
ATOM 360 HB2 ASP A 115 -2.921 16.169 -52.278 1.00 36.95
H
ATOM 361 HB3 ASP A 115 -3.713 15.625 -51.013 1.00 36.95
H

ATOM 6628 N LYS D 147 -14.872 44.513 -6.490 1.00 14.65 N
ATOM 6629 CA LYS D 147 -14.213 43.214 -6.620 1.00 17.93
C
ATOM 6630 C LYS D 147 -12.713 43.325 -6.339 1.00 15.43 C
ATOM 6631 O LYS D 147 -12.098 42.393 -5.821 1.00 16.29 O
ATOM 6632 CB LYS D 147 -14.423 42.649 -8.031 1.00 22.58
C
ATOM 6633 CG LYS D 147 -13.517 43.312 -9.070 1.00 45.24
C
ATOM 6634 CD LYS D 147 -13.950 43.075 -10.516 1.00 79.42
C
ATOM 6635 CE LYS D 147 -13.696 44.304 -11.398 1.00 90.15
C
ATOM 6636 NZ LYS D 147 -12.667 44.084 -12.457 1.00103.84
N1+
ATOM 6637 H LYS D 147 -15.290 44.761 -7.199 1.00 17.58 H
ATOM 6638 HA LYS D 147 -14.598 42.593 -5.982 1.00 21.51
H
ATOM 6639 HB2 LYS D 147 -14.228 41.699 -8.024 1.00 27.09
H
ATOM 6640 HB3 LYS D 147 -15.344 42.796 -8.298 1.00 27.09
H
ATOM 6641 HG2 LYS D 147 -13.514 44.269 -8.915 1.00 54.29
H
ATOM 6642 HG3 LYS D 147 -12.618 42.961 -8.969 1.00 54.29
H
ATOM 6643 HD2 LYS D 147 -13.447 42.331 -10.882 1.00 95.30
H
ATOM 6644 HD3 LYS D 147 -14.900 42.879 -10.536 1.00 95.30
H
ATOM 6645 HE2 LYS D 147 -14.526 44.550 -11.837 1.00108.18
H
ATOM 6646 HE3 LYS D 147 -13.392 45.034 -10.836 1.00108.18
H
ATOM 6647 HZ1 LYS D 147 -12.923 43.424 -12.998 1.00124.61
H
ATOM 6648 HZ2 LYS D 147 -12.561 44.826 -12.937 1.00124.61
H
ATOM 6649 HZ3 LYS D 147 -11.889 43.866 -12.085 1.00124.61
H

ATOM 6650 N LEU D 148 -12.136 44.472 -6.685 1.00 14.11 N
ATOM 6651 CA LEU D 148 -10.686 44.663 -6.635 1.00 14.27
C
ATOM 6652 C LEU D 148 -10.199 45.320 -5.346 1.00 14.62 C
ATOM 6653 O LEU D 148 -9.001 45.581 -5.189 1.00 17.22 O
ATOM 6654 CB LEU D 148 -10.235 45.508 -7.827 1.00 14.41
C
ATOM 6655 CG LEU D 148 -10.319 44.864 -9.212 1.00 21.00
C
ATOM 6656 CD1 LEU D 148 -9.959 45.879 -10.272 1.00 22.02
C
ATOM 6657 CD2 LEU D 148 -9.408 43.651 -9.311 1.00 24.34
C
ATOM 6658 H LEU D 148 -12.567 45.165 -6.956 1.00 16.94 H
ATOM 6659 HA LEU D 148 -10.256 43.797 -6.706 1.00 17.12
H
ATOM 6660 HB2 LEU D 148 -10.780 46.309 -7.852 1.00 17.29
H
ATOM 6661 HB3 LEU D 148 -9.308 45.758 -7.685 1.00 17.29
H

ATOM 362 N GLU A 116 -5.226 14.596 -54.903 1.00 28.73
N
ATOM 363 CA GLU A 116 -5.170 14.520 -56.362 1.00 33.21
C
ATOM 364 C GLU A 116 -6.288 15.378 -56.938 1.00 33.91
C
ATOM 365 O GLU A 116 -7.466 15.116 -56.699 1.00 38.64
O
ATOM 366 CB GLU A 116 -5.287 13.075 -56.860 1.00 37.54
C
ATOM 367 CG GLU A 116 -6.251 12.196 -56.072 1.00 39.66
C
ATOM 368 CD GLU A 116 -5.606 11.573 -54.842 1.00 41.78
C
ATOM 369 OE1 GLU A 116 -4.525 10.959 -54.979 1.00 47.28
O
ATOM 370 OE2 GLU A 116 -6.177 11.707 -53.737 1.00 32.41
O1-
ATOM 371 H GLU A 116 -5.687 13.969 -54.536 1.00 34.48
H
ATOM 372 HA GLU A 116 -4.323 14.880 -56.669 1.00 39.85
H
ATOM 373 HB2 GLU A 116 -5.592 13.090 -57.781 1.00 45.05
H
ATOM 374 HB3 GLU A 116 -4.411 12.662 -56.815 1.00 45.05
H
ATOM 375 HG2 GLU A 116 -7.001 12.735 -55.777 1.00 47.60
H
ATOM 376 HG3 GLU A 116 -6.563 11.477 -56.643 1.00 47.60
H
ATOM 377 N SER A 117 -5.915 16.408 -57.690 1.00 24.41
N
ATOM 378 CA SER A 117 -6.878 17.401 -58.140 1.00 29.40
C
ATOM 379 C SER A 117 -7.682 16.920 -59.344 1.00 31.91
C
ATOM 380 O SER A 117 -7.135 16.366 -60.296 1.00 31.79
O
ATOM 381 CB SER A 117 -6.169 18.715 -58.475 1.00 29.88
C
ATOM 382 OG SER A 117 -5.324 18.570 -59.597 1.00 37.03
O
ATOM 383 H SER A 117 -5.109 16.553 -57.953 1.00 29.30
H
ATOM 384 HA SER A 117 -7.502 17.578 -57.419 1.00 35.28
H
ATOM 385 HB2 SER A 117 -6.836 19.392 -58.669 1.00 35.86
H
ATOM 386 HB3 SER A 117 -5.634 18.987 -57.712 1.00 35.86
H
ATOM 387 HG SER A 117 -4.943 19.299 -59.767 1.00 44.43
H
ATOM 388 N LYS A 118 -8.992 17.136 -59.276 1.00 27.54
N
ATOM 389 CA LYS A 118 -9.912 16.776 -60.348 1.00 27.36
C
ATOM 390 C LYS A 118 -10.967 17.859 -60.482 1.00 25.25
C
ATOM 391 O LYS A 118 -11.153 18.661 -59.564 1.00 21.89
O
ATOM 392 CB LYS A 118 -10.586 15.433 -60.070 1.00 24.18
C
ATOM 393 CG LYS A 118 -9.635 14.268 -59.906 1.00 30.02
C
ATOM 394 CD LYS A 118 -10.378 12.951 -60.041 1.00 32.21
C
ATOM 395 CE LYS A 118 -9.457 11.767 -59.823 1.00 34.89
C

ATOM 6662 HG LEU D 148 -11.230 44.571 -9.371 1.00 25.20
H
ATOM 6663 HD11 LEU D 148 -10.016 45.457 -11.144 1.00 26.42
H
ATOM 6664 HD12 LEU D 148 -10.580 46.622 -10.222 1.00 26.42
H
ATOM 6665 HD13 LEU D 148 -9.054 46.192 -10.115 1.00 26.42
H
ATOM 6666 HD21 LEU D 148 -9.487 43.270 -10.199 1.00 29.20
H
ATOM 6667 HD22 LEU D 148 -8.493 43.930 -9.151 1.00 29.20
H
ATOM 6668 HD23 LEU D 148 -9.677 42.999 -8.645 1.00 29.20
H

ATOM 6669 N VAL D 149 -11.114 45.590 -4.424 1.00 18.94 N
ATOM 6670 CA VAL D 149 -10.744 46.245 -3.176 1.00 18.09
C

ATOM 6671 C VAL D 149 -9.970 45.299 -2.268 1.00 14.58 C

ATOM 6672 O VAL D 149 -10.466 44.240 -1.876 1.00 14.09 O
ATOM 6673 CB VAL D 149 -11.983 46.778 -2.430 1.00 19.00
C
ATOM 6674 CG1 VAL D 149 -11.624 47.240 -1.013 1.00 15.72
C
ATOM 6675 CG2 VAL D 149 -12.601 47.914 -3.214 1.00 15.52
C

ATOM 6676 H VAL D 149 -11.951 45.406 -4.495 1.00 22.73 H
ATOM 6677 HA VAL D 149 -10.170 47.001 -3.377 1.00 21.71
H
ATOM 6678 HB VAL D 149 -12.640 46.068 -2.359 1.00 22.80
H
ATOM 6679 HG11 VAL D 149 -12.426 47.568 -0.576 1.00 18.87
H
ATOM 6680 HG12 VAL D 149 -11.261 46.489 -0.519 1.00 18.87
H
ATOM 6681 HG13 VAL D 149 -10.964 47.949 -1.070 1.00 18.87
H
ATOM 6682 HG21 VAL D 149 -13.379 48.240 -2.736 1.00 18.62
H
ATOM 6683 HG22 VAL D 149 -11.947 48.624 -3.309 1.00 18.62
H
ATOM 6684 HG23 VAL D 149 -12.863 47.587 -4.089 1.00 18.62
H

ATOM 6685 N LYS D 150 -8.748 45.704 -1.934 1.00 11.38 N

ATOM 6686 CA LYS D 150 -7.897 44.949 -1.021 1.00 13.03 C

ATOM 6687 C LYS D 150 -8.243 45.267 0.428 1.00 12.12 C

ATOM 6688 O LYS D 150 -8.703 46.366 0.733 1.00 11.51 O

ATOM 6689 CB LYS D 150 -6.421 45.270 -1.290 1.00 15.75 C
ATOM 6690 CG LYS D 150 -5.427 44.415 -0.510 1.00 18.85
C

ATOM 6691 CD LYS D 150 -4.028 45.031 -0.525 1.00 25.97 C

ATOM 6692 CE LYS D 150 -2.999 44.123 -1.170 1.00 28.15 C
ATOM 6693 NZ LYS D 150 -2.862 42.800 -0.512 1.00 27.44
N1+

ATOM 6694 H LYS D 150 -8.384 46.425 -2.228 1.00 13.65 H

ATOM 6695 HA LYS D 150 -8.034 43.999 -1.166 1.00 15.63 H

ATOM 396 NZ LYS A 118 -9.058 11.664 -58.403 1.00 38.04 N1+
ATOM 397 H LYS A 118 -9.381 17.499 -58.600 1.00 33.04 H
ATOM 398 HA LYS A 118 -9.427 16.712 -61.185 1.00 32.84 H
ATOM 399 HB2 LYS A 118 -11.100 15.508 -59.252 1.00 29.02 H
ATOM 400 HB3 LYS A 118 -11.178 15.225 -60.810 1.00 29.02 H
ATOM 401 HG2 LYS A 118 -8.953 14.308 -60.595 1.00 36.02 H
ATOM 402 HG3 LYS A 118 -9.230 14.303 -59.025 1.00 36.02 H
ATOM 403 HD2 LYS A 118 -11.085 12.913 -59.378 1.00 38.65 H
ATOM 404 HD3 LYS A 118 -10.752 12.885 -60.934 1.00 38.65 H
ATOM 405 HE2 LYS A 118 -9.918 10.950 -60.071 1.00 41.87 H
ATOM 406 HE3 LYS A 118 -8.656 11.879 -60.358 1.00 41.87 H
ATOM 407 HZ1 LYS A 118 -9.779 11.559 -57.891 1.00 45.64 H
ATOM 408 HZ2 LYS A 118 -8.518 10.966 -58.288 1.00 45.64 H
ATOM 409 HZ3 LYS A 118 -8.631 12.404 -58.152 1.00 45.64 H
ATOM 410 N ASN A 119 -11.664 17.885 -61.612 1.00 23.33 N
ATOM 411 CA ASN A 119 -12.769 18.818 -61.770 1.00 22.32 C
ATOM 412 C ASN A 119 -13.904 18.370 -60.861 1.00 18.79 C
ATOM 413 O ASN A 119 -13.846 17.281 -60.292 1.00 20.16 O
ATOM 414 CB ASN A 119 -13.213 18.920 -63.235 1.00 26.91 C
ATOM 415 CG ASN A 119 -13.744 17.612 -63.795 1.00 27.14 C
ATOM 416 OD1 ASN A 119 -14.413 16.842 -63.110 1.00 23.11 O
ATOM 417 ND2 ASN A 119 -13.453 17.366 -65.066 1.00 29.78 N
ATOM 418 H ASN A 119 -11.520 17.380 -62.293 1.00 27.99 H
ATOM 419 HA ASN A 119 -12.483 19.699 -61.481 1.00 26.78 H
ATOM 420 HB2 ASN A 119 -13.919 19.582 -63.304 1.00 32.29 H
ATOM 421 HB3 ASN A 119 -12.454 19.189 -63.775 1.00 32.29 H
ATOM 422 HD21 ASN A 119 -13.728 16.641 -65.437 1.00 35.74 H
ATOM 423 HD22 ASN A 119 -12.990 17.932 -65.518 1.00 35.74 H
ATOM 424 N TRP A 120 -14.925 19.204 -60.713 1.00 19.00 N
ATOM 425 CA TRP A 120 -15.991 18.921 -59.760 1.00 20.49 C
ATOM 426 C TRP A 120 -16.696 17.599 -60.061 1.00 22.80 C
ATOM 427 O TRP A 120 -16.990 16.822 -59.150 1.00 19.34 O
ATOM 428 CB TRP A 120 -17.014 20.055 -59.746 1.00 21.71 C
ATOM 429 CG TRP A 120 -18.043 19.878 -58.679 1.00 20.57 C

ATOM 6696 HB2 LYS D 150 -6.243 45.139 -2.234 1.00 18.90 H
ATOM 6697 HB3 LYS D 150 -6.259 46.197 -1.054 1.00 18.90 H
ATOM 6698 HG2 LYS D 150 -5.719 44.345 0.412 1.00 22.62 H
ATOM 6699 HG3 LYS D 150 -5.376 43.535 -0.914 1.00 22.62 H
ATOM 6700 HD2 LYS D 150 -4.053 45.861 -1.027 1.00 31.17 H
ATOM 6701 HD3 LYS D 150 -3.748 45.203 0.388 1.00 31.17 H
ATOM 6702 HE2 LYS D 150 -3.254 43.968 -2.093 1.00 33.78 H
ATOM 6703 HE3 LYS D 150 -2.133 44.560 -1.137 1.00 33.78 H
ATOM 6704 HZ1 LYS D 150 -3.639 42.367 -0.535 1.00 32.92 H
ATOM 6705 HZ2 LYS D 150 -2.246 42.314 -0.932 1.00 32.92 H
ATOM 6706 HZ3 LYS D 150 -2.616 42.907 0.337 1.00 32.92 H

ATOM 6707 N SER D 151 -8.011 44.299 1.308 1.00 9.93 N
ATOM 6708 CA SER D 151 -8.161 44.483 2.751 1.00 17.48 C
ATOM 6709 C SER D 151 -9.629 44.513 3.165 1.00 15.32 C
ATOM 6710 O SER D 151 -10.520 44.226 2.361 1.00 11.83 O
ATOM 6711 CB SER D 151 -7.461 45.765 3.220 1.00 14.44 C
ATOM 6712 OG SER D 151 -7.316 45.776 4.629 1.00 15.79 O
ATOM 6713 H SER D 151 -7.760 43.506 1.090 1.00 11.92 H
ATOM 6714 HA SER D 151 -7.742 43.735 3.205 1.00 20.98 H
ATOM 6715 HB2 SER D 151 -6.582 45.812 2.812 1.00 17.33 H
ATOM 6716 HB3 SER D 151 -7.993 46.531 2.952 1.00 17.33 H
ATOM 6717 HG SER D 151 -6.857 45.117 4.875 1.00 18.95 H

ATOM 6718 N TYR D 152 -9.849 44.872 4.428 1.00 14.15 N
ATOM 6719 CA TYR D 152 -11.134 44.731 5.099 1.00 14.23 C
ATOM 6720 C TYR D 152 -11.546 46.065 5.719 1.00 15.88 C
ATOM 6721 O TYR D 152 -10.765 46.681 6.436 1.00 15.07 O
ATOM 6722 CB TYR D 152 -11.037 43.620 6.152 1.00 14.66 C
ATOM 6723 CG TYR D 152 -10.793 42.275 5.507 1.00 14.16 C
ATOM 6724 CD1 TYR D 152 -9.544 41.942 4.993 1.00 16.37 C
ATOM 6725 CD2 TYR D 152 -11.819 41.354 5.375 1.00 12.96 C
ATOM 6726 CE1 TYR D 152 -9.327 40.728 4.372 1.00 16.79 C
ATOM 6727 CE2 TYR D 152 -11.611 40.138 4.758 1.00 17.09 C
ATOM 6728 CZ TYR D 152 -10.365 39.830 4.257 1.00 15.39 C
ATOM 6729 OH TYR D 152 -10.164 38.616 3.641 1.00 19.34 O

ATOM 430 CD1 TRP A 120 -17.954 20.290 -57.382 1.00 20.10 C
ATOM 431 CD2 TRP A 120 -19.313 19.229 -58.808 1.00 20.41 C
ATOM 432 NE1 TRP A 120 -19.092 19.944 -56.696 1.00 18.87 N
ATOM 433 CE2 TRP A 120 -19.942 19.290 -57.548 1.00 21.17 C
ATOM 434 CE3 TRP A 120 -19.978 18.602 -59.865 1.00 22.60 C
ATOM 435 CZ2 TRP A 120 -21.205 18.749 -57.316 1.00 22.12 C
ATOM 436 CZ3 TRP A 120 -21.230 18.065 -59.635 1.00 20.75 C
ATOM 437 CH2 TRP A 120 -21.832 18.142 -58.371 1.00 28.09 C
ATOM 438 H TRP A 120 -15.025 19.938 -61.149 1.00 22.80 H
ATOM 439 HA TRP A 120 -15.606 18.856 -58.872 1.00 24.58 H
ATOM 440 HB2 TRP A 120 -16.555 20.894 -59.586 1.00 26.06 H
ATOM 441 HB3 TRP A 120 -17.470 20.082 -60.602 1.00 26.06 H
ATOM 442 HD1 TRP A 120 -17.230 20.744 -57.017 1.00 24.12 H
ATOM 443 HE1 TRP A 120 -19.246 20.110 -55.866 1.00 22.64 H
ATOM 444 HE3 TRP A 120 -19.585 18.546 -60.706 1.00 27.12 H
ATOM 445 HZ2 TRP A 120 -21.607 18.799 -56.479 1.00 26.54 H
ATOM 446 HZ3 TRP A 120 -21.683 17.647 -60.331 1.00 24.90 H
ATOM 447 HH2 TRP A 120 -22.677 17.774 -58.246 1.00 33.71 H
ATOM 448 N TYR A 121 -16.960 17.346 -61.339 1.00 21.32 N
ATOM 449 CA TYR A 121 -17.709 16.158 -61.743 1.00 25.07 C
ATOM 450 C TYR A 121 -16.927 14.885 -61.415 1.00 20.81 C
ATOM 451 O TYR A 121 -17.473 13.937 -60.848 1.00 21.52 O
ATOM 452 CB TYR A 121 -18.037 16.221 -63.238 1.00 23.23 C
ATOM 453 CG TYR A 121 -18.622 17.550 -63.662 1.00 26.15 C
ATOM 454 CD1 TYR A 121 -19.935 17.885 -63.353 1.00 33.80 C
ATOM 455 CD2 TYR A 121 -17.859 18.473 -64.363 1.00 24.99 C
ATOM 456 CE1 TYR A 121 -20.471 19.105 -63.734 1.00 30.23 C
ATOM 457 CE2 TYR A 121 -18.386 19.693 -64.748 1.00 33.24 C
ATOM 458 CZ TYR A 121 -19.689 20.003 -64.431 1.00 29.90 C
ATOM 459 OH TYR A 121 -20.210 21.217 -64.815 1.00 39.68 O
ATOM 460 H TYR A 121 -16.717 17.848 -61.993 1.00 25.59 H
ATOM 461 HA TYR A 121 -18.546 16.130 -61.254 1.00 30.08 H
ATOM 462 HB2 TYR A 121 -17.222 16.079 -63.745 1.00 27.87 H
ATOM 463 HB3 TYR A 121 -18.683 15.529 -63.448 1.00 27.87 H

ATOM 6730 H TYR D 152 -9.243 45.214 4.934 1.00 16.98 H
ATOM 6731 HA TYR D 152 -11.809 44.477 4.449 1.00 17.08 H
ATOM 6732 HB2 TYR D 152 -10.298 43.809 6.751 1.00 17.59 H
ATOM 6733 HB3 TYR D 152 -11.870 43.574 6.647 1.00 17.59 H
ATOM 6734 HD1 TYR D 152 -8.845 42.551 5.062 1.00 19.64 H
ATOM 6735 HD2 TYR D 152 -12.664 41.561 5.704 1.00 15.55 H
ATOM 6736 HE1 TYR D 152 -8.486 40.518 4.035 1.00 20.15 H
ATOM 6737 HE2 TYR D 152 -12.309 39.529 4.679 1.00 20.50 H
ATOM 6738 HH TYR D 152 -10.877 38.172 3.641 1.00 23.21 H

ATOM 6739 N HIS D 153 -12.762 46.519 5.418 1.00 15.60 N

ATOM 6740 CA HIS D 153 -13.195 47.868 5.791 1.00 14.87 C

ATOM 6741 C HIS D 153 -14.638 47.906 6.274 1.00 15.50 C

ATOM 6742 O HIS D 153 -15.492 47.185 5.761 1.00 15.53 O

ATOM 6743 CB HIS D 153 -13.048 48.819 4.603 1.00 14.96 C
ATOM 6744 CG HIS D 153 -11.822 48.574 3.783 1.00 17.33 C
ATOM 6745 ND1 HIS D 153 -10.655 49.285 3.958 1.00 14.80 N
ATOM 6746 CD2 HIS D 153 -11.579 47.690 2.786 1.00 15.17 C

ATOM 6747 CE1 HIS D 153 -9.747 48.853 3.100 1.00 17.80 C
ATOM 6748 NE2 HIS D 153 -10.283 47.885 2.377 1.00 14.81 N

ATOM 6749 H HIS D 153 -13.358 46.064 4.996 1.00 18.72 H

ATOM 6750 HA HIS D 153 -12.630 48.194 6.509 1.00 17.84 H
ATOM 6751 HB2 HIS D 153 -13.819 48.715 4.023 1.00 17.95 H
ATOM 6752 HB3 HIS D 153 -13.007 49.730 4.935 1.00 17.95 H
ATOM 6753 HD1 HIS D 153 -10.537 49.914 4.533 1.00 17.76 H
ATOM 6754 HD2 HIS D 153 -12.179 47.069 2.441 1.00 18.21 H

ATOM 6755 HE1 HIS D 153 -8.879 49.175 3.020 1.00 21.36 H

ATOM 6756 HE2 HIS D 153 -9.884 47.448 1.753 1.00 17.77 H

ATOM 6757 N TRP D 154 -14.911 48.764 7.251 1.00 14.83 N
ATOM 6758 CA TRP D 154 -16.280 48.975 7.703 1.00 18.59 C

ATOM 6759 C TRP D 154 -17.160 49.471 6.558 1.00 16.71 C

ATOM 6760 O TRP D 154 -16.792 50.405 5.843 1.00 15.23 O
ATOM 6761 CB TRP D 154 -16.340 49.994 8.849 1.00 20.54 C
ATOM 6762 CG TRP D 154 -15.871 49.510 10.190 1.00 19.81 C
ATOM 6763 CD1 TRP D 154 -14.965 50.126 11.007 1.00 23.78 C

ATOM 464 HD1 TYR A 121 -20.462 17.281 -62.882 1.00 40.56
H
ATOM 465 HD2 TYR A 121 -16.978 18.268 -64.578 1.00 29.99
H
ATOM 466 HE1 TYR A 121 -21.351 19.317 -63.521 1.00 36.27
H
ATOM 467 HE2 TYR A 121 -17.862 20.301 -65.218 1.00 39.89
H
ATOM 468 HH TYR A 121 -21.008 21.280 -64.562 1.00 47.62
H
ATOM 469 N GLU A 122 -15.645 14.883 -61.760 1.00 20.76
N
ATOM 470 CA GLU A 122 -14.760 13.767 -61.449 1.00 22.88
C
ATOM 471 C GLU A 122 -14.653 13.563 -59.938 1.00 22.74
C
ATOM 472 O GLU A 122 -14.647 12.432 -59.451 1.00 21.61
O
ATOM 473 CB GLU A 122 -13.374 14.011 -62.049 1.00 30.20
C
ATOM 474 CG GLU A 122 -13.320 13.954 -63.575 1.00 37.52
C
ATOM 475 CD GLU A 122 -11.969 14.386 -64.136 1.00 47.14
C
ATOM 476 OE1 GLU A 122 -11.248 15.152 -63.458 1.00 45.66
O
ATOM 477 OE2 GLU A 122 -11.625 13.956 -65.257 1.00 59.27
O1-
ATOM 478 H GLU A 122 -15.258 15.525 -62.180 1.00 24.92
H
ATOM 479 HA GLU A 122 -15.121 12.956 -61.839 1.00 27.46
H
ATOM 480 HB2 GLU A 122 -13.070 14.891 -61.777 1.00 36.24
H
ATOM 481 HB3 GLU A 122 -12.766 13.337 -61.708 1.00 36.24
H
ATOM 482 HG2 GLU A 122 -13.487 13.042 -63.863 1.00 45.03
H
ATOM 483 HG3 GLU A 122 -13.998 14.545 -63.937 1.00 45.03
H
ATOM 484 N SER A 123 -14.565 14.666 -59.202 1.00 22.30
N
ATOM 485 CA SER A 123 -14.528 14.613 -57.745 1.00 20.93
C
ATOM 486 C SER A 123 -15.806 13.978 -57.214 1.00 20.42
C
ATOM 487 O SER A 123 -15.762 13.104 -56.344 1.00 18.79
O
ATOM 488 CB SER A 123 -14.345 16.015 -57.155 1.00 20.25
C
ATOM 489 OG SER A 123 -13.110 16.585 -57.557 1.00 15.46
O
ATOM 490 H SER A 123 -14.526 15.463 -59.524 1.00 26.76
H
ATOM 491 HA SER A 123 -13.778 14.066 -57.465 1.00 25.12
H
ATOM 492 HB2 SER A 123 -15.069 16.583 -57.463 1.00 24.31
H
ATOM 493 HB3 SER A 123 -14.363 15.953 -56.187 1.00 24.31
H
ATOM 494 HG SER A 123 -13.080 16.645 -58.395 1.00 18.56
H
ATOM 495 N GLN A 124 -16.941 14.421 -57.749 1.00 19.50
N
ATOM 496 CA GLN A 124 -18.241 13.880 -57.365 1.00 18.56
C
ATOM 497 C GLN A 124 -18.300 12.380 -57.618 1.00 21.42
C
ATOM 6764 CD2 TRP D 154 -16.298 48.331 10.886 1.00 21.11
C
ATOM 6765 NE1 TRP D 154 -14.798 49.402 12.160 1.00 23.26
N
ATOM 6766 CE2 TRP D 154 -15.602 48.295 12.112 1.00 23.65
C
ATOM 6767 CE3 TRP D 154 -17.194 47.300 10.591 1.00 19.42
C
ATOM 6768 CZ2 TRP D 154 -15.774 47.269 13.040 1.00 25.29
C
ATOM 6769 CZ3 TRP D 154 -17.362 46.281 11.514 1.00 22.46
C
ATOM 6770 CH2 TRP D 154 -16.657 46.275 12.723 1.00 25.53
C
ATOM 6771 H TRP D 154 -14.324 49.234 7.667 1.00 17.80 H
ATOM 6772 HA TRP D 154 -16.644 48.135 8.024 1.00 22.30
H
ATOM 6773 HB2 TRP D 154 -15.789 50.756 8.609 1.00 24.65
H
ATOM 6774 HB3 TRP D 154 -17.260 50.283 8.952 1.00 24.65
H
ATOM 6775 HD1 TRP D 154 -14.527 50.922 10.811 1.00 28.53
H
ATOM 6776 HE1 TRP D 154 -14.270 49.609 12.808 1.00 27.92
H
ATOM 6777 HE3 TRP D 154 -17.667 47.298 9.790 1.00 23.30
H
ATOM 6778 HZ2 TRP D 154 -15.305 47.261 13.843 1.00 30.35
H
ATOM 6779 HZ3 TRP D 154 -17.957 45.591 11.329 1.00 26.95
H
ATOM 6780 HH2 TRP D 154 -16.791 45.577 13.323 1.00 30.63
H
ATOM 6781 N MET D 155 -18.321 48.845 6.392 1.00 16.33 N
ATOM 6782 CA MET D 155 -19.362 49.379 5.519 1.00 14.51
C
ATOM 6783 C MET D 155 -20.595 49.713 6.361 1.00 17.12 C
ATOM 6784 O MET D 155 -20.603 49.497 7.573 1.00 19.71
O
ATOM 6785 CB MET D 155 -19.704 48.392 4.397 1.00 15.94
C
ATOM 6786 CG MET D 155 -19.896 46.957 4.840 1.00 16.64
C
ATOM 6787 SD MET D 155 -20.468 45.915 3.480 1.00 19.78
S
ATOM 6788 CE MET D 155 -20.186 44.291 4.179 1.00 21.22
C
ATOM 6789 H MET D 155 -18.533 48.105 6.776 1.00 19.60 H
ATOM 6790 HA MET D 155 -19.035 50.194 5.107 1.00 17.42
H
ATOM 6791 HB2 MET D 155 -20.528 48.680 3.974 1.00 19.13
H
ATOM 6792 HB3 MET D 155 -18.984 48.403 3.747 1.00 19.13
H
ATOM 6793 HG2 MET D 155 -19.050 46.605 5.158 1.00 19.97
H
ATOM 6794 HG3 MET D 155 -20.560 46.927 5.547 1.00 19.97
H
ATOM 6795 HE1 MET D 155 -20.458 43.619 3.535 1.00 25.46
H
ATOM 6796 HE2 MET D 155 -19.242 44.194 4.381 1.00 25.46
H
ATOM 6797 HE3 MET D 155 -20.709 44.202 4.992 1.00 25.46
H

ATOM 498 O GLN A 124 -18.736 11.612 -56.758 1.00 18.75 O
ATOM 499 CB GLN A 124 -19.363 14.585 -58.134 1.00 22.37 C
ATOM 500 CG GLN A 124 -20.744 13.971 -57.944 1.00 25.68 C
ATOM 501 CD GLN A 124 -21.805 14.643 -58.800 1.00 30.60 C
ATOM 502 OE1 GLN A 124 -21.672 14.729 -60.023 1.00 32.60 O
ATOM 503 NE2 GLN A 124 -22.862 15.130 -58.159 1.00 27.20 N
ATOM 504 H GLN A 124 -16.985 15.041 -58.344 1.00 23.40 H
ATOM 505 HA GLN A 124 -18.382 14.033 -56.418 1.00 22.27 H
ATOM 506 HB2 GLN A 124 -19.408 15.508 -57.839 1.00 26.84 H
ATOM 507 HB3 GLN A 124 -19.156 14.555 -59.082 1.00 26.84 H
ATOM 508 HG2 GLN A 124 -20.710 13.033 -58.189 1.00 30.82 H
ATOM 509 HG3 GLN A 124 -21.006 14.062 -57.014 1.00 30.82 H
ATOM 510 HE21 GLN A 124 -23.489 15.520 -58.599 1.00 32.63 H
ATOM 511 HE22 GLN A 124 -22.918 15.055 -57.305 1.00 32.63 H
ATOM 512 N ALA A 125 -17.868 11.972 -58.807 1.00 21.97 N
ATOM 513 CA ALA A 125 -17.868 10.561 -59.176 1.00 20.84 C
ATOM 514 C ALA A 125 -16.946 9.762 -58.260 1.00 21.56 C
ATOM 515 O ALA A 125 -17.233 8.613 -57.929 1.00 23.96 O
ATOM 516 CB ALA A 125 -17.448 10.394 -60.623 1.00 22.81 C
ATOM 517 H ALA A 125 -17.569 12.494 -59.420 1.00 26.37 H
ATOM 518 HA ALA A 125 -18.767 10.208 -59.081 1.00 25.01 H
ATOM 519 HB1 ALA A 125 -17.455 9.450 -60.846 1.00 27.37 H
ATOM 520 HB2 ALA A 125 -18.072 10.873 -61.190 1.00 27.37 H
ATOM 521 HB3 ALA A 125 -16.554 10.754 -60.735 1.00 27.37 H
ATOM 522 N SER A 126 -15.841 10.380 -57.850 1.00 19.66 N
ATOM 523 CA SER A 126 -14.891 9.726 -56.960 1.00 21.36 C
ATOM 524 C SER A 126 -15.526 9.424 -55.597 1.00 20.78 C
ATOM 525 O SER A 126 -15.400 8.316 -55.079 1.00 20.50 O
ATOM 526 CB SER A 126 -13.644 10.595 -56.782 1.00 21.76 C
ATOM 527 OG SER A 126 -12.641 9.910 -56.052 1.00 22.07 O
ATOM 528 H SER A 126 -15.619 11.180 -58.074 1.00 23.59 H
ATOM 529 HA SER A 126 -14.615 8.884 -57.355 1.00 25.64 H
ATOM 530 HB2 SER A 126 -13.294 10.826 -57.657 1.00 26.11 H
ATOM 531 HB3 SER A 126 -13.888 11.401 -56.301 1.00 26.11 H

ATOM 6798 N GLY D 156 -21.629 50.248 5.719 1.00 19.69 N
ATOM 6799 CA GLY D 156 -22.778 50.784 6.429 1.00 20.08 C
ATOM 6800 C GLY D 156 -23.884 49.782 6.697 1.00 27.40 C
ATOM 6801 O GLY D 156 -25.047 50.157 6.856 1.00 25.15 O
ATOM 6802 H GLY D 156 -21.686 50.313 4.863 1.00 23.63 H
ATOM 6803 HA2 GLY D 156 -22.484 51.139 7.282 1.00 24.09 H
ATOM 6804 HA3 GLY D 156 -23.155 51.514 5.913 1.00 24.09 H
ATOM 6805 N LEU D 157 -23.523 48.505 6.755 1.00 22.24 N
ATOM 6806 CA LEU D 157 -24.486 47.457 7.038 1.00 24.99 C
ATOM 6807 C LEU D 157 -24.748 47.391 8.542 1.00 32.61 C
ATOM 6808 O LEU D 157 -23.816 47.402 9.348 1.00 32.90 O
ATOM 6809 CB LEU D 157 -23.981 46.116 6.506 1.00 27.86 C
ATOM 6810 CG LEU D 157 -25.030 45.102 6.053 1.00 31.65 C
ATOM 6811 CD1 LEU D 157 -25.857 45.622 4.884 1.00 33.53 C
ATOM 6812 CD2 LEU D 157 -24.345 43.799 5.675 1.00 34.82 C
ATOM 6813 H LEU D 157 -22.720 48.221 6.632 1.00 26.69 H
ATOM 6814 HA LEU D 157 -25.323 47.663 6.594 1.00 29.98 H
ATOM 6815 HB2 LEU D 157 -23.408 46.293 5.743 1.00 33.43 H
ATOM 6816 HB3 LEU D 157 -23.459 45.693 7.205 1.00 33.43 H
ATOM 6817 HG LEU D 157 -25.633 44.921 6.790 1.00 37.98 H
ATOM 6818 HD11 LEU D 157 -26.507 44.947 4.632 1.00 40.23 H
ATOM 6819 HD12 LEU D 157 -26.312 46.434 5.156 1.00 40.23 H
ATOM 6820 HD13 LEU D 157 -25.266 45.808 4.137 1.00 40.23 H
ATOM 6821 HD21 LEU D 157 -25.017 43.161 5.389 1.00 41.79 H
ATOM 6822 HD22 LEU D 157 -23.720 43.968 4.953 1.00 41.79 H
ATOM 6823 HD23 LEU D 157 -23.871 43.456 6.449 1.00 41.79 H
ATOM 6824 N VAL D 158 -26.026 47.342 8.902 1.00 33.79 N
ATOM 6825 CA VAL D 158 -26.462 47.376 10.293 1.00 34.56 C
ATOM 6826 C VAL D 158 -27.282 46.133 10.623 1.00 40.45 C
ATOM 6827 O VAL D 158 -28.183 45.762 9.871 1.00 38.74 O
ATOM 6828 CB VAL D 158 -27.307 48.635 10.579 1.00 31.82 C
ATOM 6829 CG1 VAL D 158 -27.896 48.591 11.984 1.00 45.90 C
ATOM 6830 CG2 VAL D 158 -26.472 49.890 10.392 1.00 35.55 C
ATOM 6831 H VAL D 158 -26.677 47.288 8.342 1.00 40.54 H

ATOM 532 HG SER A 126 -11.965 10.401 -55.964 1.00 26.49 H
ATOM 533 N CYS A 127 -16.208 10.408 -55.018 1.00 17.68 N
ATOM 534 CA CYS A 127 -16.855 10.214 -53.722 1.00 20.49 C
ATOM 535 C CYS A 127 -17.995 9.206 -53.839 1.00 20.57 C
ATOM 536 O CYS A 127 -18.171 8.348 -52.973 1.00 19.87 O
ATOM 537 CB CYS A 127 -17.379 11.542 -53.174 1.00 18.87 C
ATOM 538 SG CYS A 127 -16.086 12.764 -52.854 1.00 19.71 S
ATOM 539 H CYS A 127 -16.312 11.193 -55.352 1.00 21.21 H
ATOM 540 HA CYS A 127 -16.206 9.863 -53.092 1.00 24.59 H
ATOM 541 HB2 CYS A 127 -17.995 11.925 -53.818 1.00 22.65 H
ATOM 542 HB3 CYS A 127 -17.842 11.374 -52.337 1.00 22.65 H
ATOM 543 N MET A 128 -18.765 9.315 -54.918 1.00 17.80 N
ATOM 544 CA MET A 128 -19.856 8.382 -55.179 1.00 25.06 C
ATOM 545 C MET A 128 -19.319 6.961 -55.283 1.00 22.86 C
ATOM 546 O MET A 128 -19.956 6.008 -54.835 1.00 25.41 O
ATOM 547 CB MET A 128 -20.593 8.754 -56.464 1.00 28.91 C
ATOM 548 CG MET A 128 -22.085 8.970 -56.280 1.00 40.17 C
ATOM 549 SD MET A 128 -22.957 9.136 -57.850 1.00 65.50 S
ATOM 550 CE MET A 128 -22.156 10.582 -58.544 1.00 43.48 C
ATOM 551 H MET A 128 -18.675 9.925 -55.518 1.00 21.37 H
ATOM 552 HA MET A 128 -20.490 8.426 -54.447 1.00 30.08 H
ATOM 553 HB2 MET A 128 -20.216 9.577 -56.812 1.00 34.70 H
ATOM 554 HB3 MET A 128 -20.474 8.040 -57.110 1.00 34.70 H
ATOM 555 HG2 MET A 128 -22.459 8.210 -55.808 1.00 48.20 H
ATOM 556 HG3 MET A 128 -22.227 9.782 -55.769 1.00 48.20 H
ATOM 557 HE1 MET A 128 -22.549 10.776 -59.410 1.00 52.17 H
ATOM 558 HE2 MET A 128 -22.288 11.334 -57.945 1.00 52.17 H
ATOM 559 HE3 MET A 128 -21.208 10.401 -58.644 1.00 52.17 H
ATOM 560 N SER A 129 -18.133 6.833 -55.865 1.00 22.61 N
ATOM 561 CA SER A 129 -17.491 5.535 -56.033 1.00 26.16 C
ATOM 562 C SER A 129 -17.085 4.913 -54.697 1.00 25.71 C
ATOM 563 O SER A 129 -16.695 3.745 -54.645 1.00 24.09 O
ATOM 564 CB SER A 129 -16.261 5.674 -56.935 1.00 25.52 C
ATOM 565 OG SER A 129 -15.546 4.455 -57.022 1.00 33.82 O

ATOM 6832 HA VAL D 158 -25.685 47.392 10.873 1.00 41.47 H
ATOM 6833 HB VAL D 158 -28.043 48.669 9.948 1.00 38.18 H
ATOM 6834 HG11 VAL D 158 -28.419 49.394 12.131 1.00 55.08 H
ATOM 6835 HG12 VAL D 158 -28.461 47.807 12.064 1.00 55.08 H
ATOM 6836 HG13 VAL D 158 -27.172 48.545 12.628 1.00 55.08 H
ATOM 6837 HG21 VAL D 158 -27.024 50.666 10.577 1.00 42.66 H
ATOM 6838 HG22 VAL D 158 -25.721 49.863 11.006 1.00 42.66 H
ATOM 6839 HG23 VAL D 158 -26.151 49.922 9.477 1.00 42.66 H

ATOM 6840 N HIS D 159 -26.974 45.501 11.751 1.00 42.21 N
ATOM 6841 CA HIS D 159 -27.698 44.309 12.176 1.00 47.51 C

ATOM 6842 C HIS D 159 -28.905 44.685 13.029 1.00 56.08 C

ATOM 6843 O HIS D 159 -28.829 45.584 13.867 1.00 51.08 O
ATOM 6844 CB HIS D 159 -26.785 43.370 12.962 1.00 48.52 C
ATOM 6845 CG HIS D 159 -27.304 41.969 13.065 1.00 50.74 C
ATOM 6846 ND1 HIS D 159 -26.815 41.062 13.981 1.00 52.54 N
ATOM 6847 CD2 HIS D 159 -28.266 41.318 12.369 1.00 56.93 C
ATOM 6848 CE1 HIS D 159 -27.454 39.914 13.845 1.00 63.50 C
ATOM 6849 NE2 HIS D 159 -28.340 40.043 12.874 1.00 64.61 N

ATOM 6850 H HIS D 159 -26.348 45.743 12.289 1.00 50.65 H
ATOM 6851 HA HIS D 159 -28.018 43.835 11.392 1.00 57.02 H
ATOM 6852 HB2 HIS D 159 -25.920 43.334 12.524 1.00 58.23 H
ATOM 6853 HB3 HIS D 159 -26.683 43.715 13.863 1.00 58.23 H
ATOM 6854 HD1 HIS D 159 -26.191 41.219 14.552 1.00 63.05 H
ATOM 6855 HD2 HIS D 159 -28.781 41.669 11.679 1.00 68.31 H
ATOM 6856 HE1 HIS D 159 -27.305 39.145 14.347 1.00 76.20 H
ATOM 6857 HE2 HIS D 159 -28.875 39.427 12.601 1.00 77.54 H

ATOM 6858 N ILE D 160 -30.011 43.984 12.807 1.00 60.19 N
ATOM 6859 CA ILE D 160 -31.243 44.209 13.553 1.00 72.28 C

ATOM 6860 C ILE D 160 -31.530 43.001 14.446 1.00 84.70 C

ATOM 6861 O ILE D 160 -31.991 41.970 13.955 1.00 84.61 O
ATOM 6862 CB ILE D 160 -32.433 44.447 12.609 1.00 73.35 C
ATOM 6863 CG1 ILE D 160 -32.142 45.623 11.674 1.00 59.74 C
ATOM 6864 CG2 ILE D 160 -33.694 44.725 13.407 1.00 85.05 C
ATOM 6865 CD1 ILE D 160 -33.047 45.674 10.476 1.00 64.40 C

ATOM 566 H SER A 129 -17.673 7.491 -56.175 1.00 27.13
H
ATOM 567 HA SER A 129 -18.113 4.930 -56.467 1.00 31.39
H
ATOM 568 HB2 SER A 129 -16.551 5.932 -57.824 1.00 30.62
H
ATOM 569 HB3 SER A 129 -15.677 6.355 -56.567 1.00 30.62
H
ATOM 570 HG SER A 129 -16.039 3.855 -57.341 1.00 40.59
H
ATOM 571 N GLN A 130 -17.171 5.694 -53.623 1.00 20.18
N
ATOM 572 CA GLN A 130 -16.753 5.233 -52.303 1.00 22.43
C
ATOM 573 C GLN A 130 -17.916 5.241 -51.317 1.00 24.16
C
ATOM 574 O GLN A 130 -17.715 5.372 -50.111 1.00 27.76
O
ATOM 575 CB GLN A 130 -15.612 6.103 -51.779 1.00 23.18
C
ATOM 576 CG GLN A 130 -14.386 6.095 -52.674 1.00 25.86
C
ATOM 577 CD GLN A 130 -13.321 7.067 -52.215 1.00 22.81
C
ATOM 578 OE1 GLN A 130 -12.837 6.988 -51.087 1.00 19.87
O
ATOM 579 NE2 GLN A 130 -12.951 7.993 -53.091 1.00 20.58
N
ATOM 580 H GLN A 130 -17.470 6.500 -53.634 1.00 24.21
H
ATOM 581 HA GLN A 130 -16.427 4.322 -52.375 1.00 26.92
H
ATOM 582 HB2 GLN A 130 -15.923 7.019 -51.709 1.00 27.81
H
ATOM 583 HB3 GLN A 130 -15.345 5.778 -50.905 1.00 27.81
H
ATOM 584 HG2 GLN A 130 -14.001 5.205 -52.674 1.00 31.04
H
ATOM 585 HG3 GLN A 130 -14.650 6.342 -53.574 1.00 31.04
H
ATOM 586 HE21 GLN A 130 -12.349 8.569 -52.879 1.00 24.70
H
ATOM 587 HE22 GLN A 130 -13.313 8.016 -53.871 1.00 24.70
H
ATOM 588 N ASN A 131 -19.127 5.083 -51.839 1.00 23.03
N
ATOM 589 CA ASN A 131 -20.331 5.118 -51.016 1.00 28.97
C
ATOM 590 C ASN A 131 -20.370 6.396 -50.190 1.00 27.25
C
ATOM 591 O ASN A 131 -20.655 6.375 -48.992 1.00 24.85
O
ATOM 592 CB ASN A 131 -20.396 3.890 -50.104 1.00 30.97
C
ATOM 593 CG ASN A 131 -21.744 3.736 -49.429 1.00 34.40
C
ATOM 594 OD1 ASN A 131 -22.772 4.158 -49.962 1.00 38.37
O
ATOM 595 ND2 ASN A 131 -21.745 3.139 -48.241 1.00 40.30
N
ATOM 596 H ASN A 131 -19.280 4.953 -52.676 1.00 27.63
H
ATOM 597 HA ASN A 131 -21.111 5.107 -51.593 1.00 34.76
H
ATOM 598 HB2 ASN A 131 -20.232 3.093 -50.633 1.00 37.17
H
ATOM 599 HB3 ASN A 131 -19.721 3.973 -49.413 1.00 37.17
H

ATOM 6866 H ILE D 160 -30.074 43.361 12.218 1.00 72.23 H
ATOM 6867 HA ILE D 160 -31.139 44.990 14.119 1.00 86.74
H
ATOM 6868 HB ILE D 160 -32.571 43.650 12.074 1.00 88.02
H
ATOM 6869 HG12 ILE D 160 -32.255 46.450 12.168 1.00 71.69
H
ATOM 6870 HG13 ILE D 160 -31.229 45.551 11.355 1.00 71.69
H
ATOM 6871 HG21 ILE D 160 -33.883 43.961 13.974 1.00102.06
H
ATOM 6872 HG22 ILE D 160 -33.555 45.516 13.952 1.00102.06
H
ATOM 6873 HG23 ILE D 160 -34.430 44.872 12.793 1.00102.06
H
ATOM 6874 HD11 ILE D 160 -32.806 46.440 9.932 1.00 77.27
H
ATOM 6875 HD12 ILE D 160 -32.939 44.857 9.964 1.00 77.27
H
ATOM 6876 HD13 ILE D 160 -33.965 45.757 10.778 1.00 77.27
H
ATOM 6877 N PRO D 161 -31.256 43.117 15.758 1.00 91.91
N
ATOM 6878 CA PRO D 161 -31.459 41.971 16.655 1.00100.89
C
ATOM 6879 C PRO D 161 -32.918 41.531 16.773 1.00107.68
C
ATOM 6880 O PRO D 161 -33.184 40.448 17.295 1.00110.28
O
ATOM 6881 CB PRO D 161 -30.946 42.484 18.008 1.00104.17
C
ATOM 6882 CG PRO D 161 -30.073 43.643 17.685 1.00 92.23
C
ATOM 6883 CD PRO D 161 -30.672 44.267 16.470 1.00 90.01
C
ATOM 6884 HA PRO D 161 -30.917 41.218 16.370 1.00121.07
H
ATOM 6885 HB2 PRO D 161 -31.696 42.763 18.557 1.00125.00
H
ATOM 6886 HB3 PRO D 161 -30.439 41.786 18.451 1.00125.00
H
ATOM 6887 HG2 PRO D 161 -30.073 44.268 18.426 1.00110.68
H
ATOM 6888 HG3 PRO D 161 -29.173 43.331 17.500 1.00110.68
H
ATOM 6889 HD2 PRO D 161 -31.365 44.898 16.720 1.00108.01
H
ATOM 6890 HD3 PRO D 161 -29.984 44.687 15.930 1.00108.01
H
ATOM 6891 N THR D 162 -33.845 42.358 16.298 1.00107.82
N
ATOM 6892 CA THR D 162 -35.265 42.042 16.398 1.00113.32
C
ATOM 6893 C THR D 162 -35.606 40.838 15.526 1.00113.82
C
ATOM 6894 O THR D 162 -36.327 39.935 15.953 1.00117.27
O
ATOM 6895 CB THR D 162 -36.158 43.231 15.977 1.00116.05
C
ATOM 6896 OG1 THR D 162 -36.171 43.348 14.549 1.00118.64
O
ATOM 6897 CG2 THR D 162 -35.669 44.537 16.597 1.00119.38
C
ATOM 6898 H THR D 162 -33.677 43.109 15.914 1.00129.39
H
ATOM 6899 HA THR D 162 -35.476 41.818 17.318 1.00135.98
H

ATOM 600 HD21 ASN A 131 -22.485 3.028 -47.817 1.00 48.35
H
ATOM 601 HD22 ASN A 131 -21.006 2.864 -47.897 1.00 48.35
H
ATOM 602 N ALA A 132 -20.066 7.510 -50.846 1.00 25.64
N
ATOM 603 CA ALA A 132 -19.980 8.800 -50.181 1.00 21.88
C
ATOM 604 C ALA A 132 -20.378 9.915 -51.139 1.00 21.78
C
ATOM 605 O ALA A 132 -20.768 9.663 -52.277 1.00 22.40
O
ATOM 606 CB ALA A 132 -18.570 9.026 -49.656 1.00 20.15
C
ATOM 607 H ALA A 132 -19.903 7.543 -51.690 1.00 30.77
H
ATOM 608 HA ALA A 132 -20.591 8.813 -49.428 1.00 26.25
H
ATOM 609 HB1 ALA A 132 -18.531 9.890 -49.217 1.00 24.18
H
ATOM 610 HB2 ALA A 132 -18.352 8.323 -49.025 1.00 24.18
H
ATOM 611 HB3 ALA A 132 -17.949 9.006 -50.401 1.00 24.18
H
ATOM 612 N SER A 133 -20.270 11.151 -50.672 1.00 18.84
N
ATOM 613 CA SER A 133 -20.529 12.309 -51.509 1.00 21.81
C
ATOM 614 C SER A 133 -19.499 13.378 -51.190 1.00 19.07
C
ATOM 615 O SER A 133 -18.693 13.211 -50.276 1.00 17.95
O
ATOM 616 CB SER A 133 -21.945 12.833 -51.281 1.00 25.17
C
ATOM 617 OG SER A 133 -22.071 13.372 -49.979 1.00 30.73
O
ATOM 618 H SER A 133 -20.045 11.346 -49.865 1.00 22.61
H
ATOM 619 HA SER A 133 -20.438 12.061 -52.442 1.00 26.18
H
ATOM 620 HB2 SER A 133 -22.134 13.528 -51.931 1.00 30.20
H
ATOM 621 HB3 SER A 133 -22.574 12.102 -51.384 1.00 30.20
H
ATOM 622 HG SER A 133 -21.908 12.780 -49.406 1.00 36.88
H
ATOM 623 N LEU A 134 -19.516 14.469 -51.947 1.00 18.66
N
ATOM 624 CA LEU A 134 -18.644 15.594 -51.646 1.00 18.37
C
ATOM 625 C LEU A 134 -19.076 16.218 -50.327 1.00 17.90
C
ATOM 626 O LEU A 134 -20.216 16.046 -49.898 1.00 17.30
O
ATOM 627 CB LEU A 134 -18.675 16.627 -52.772 1.00 17.75
C
ATOM 628 CG LEU A 134 -17.977 16.210 -54.067 1.00 16.83
C
ATOM 629 CD1 LEU A 134 -18.320 17.168 -55.192 1.00 18.55
C
ATOM 630 CD2 LEU A 134 -16.469 16.142 -53.878 1.00 18.53
C
ATOM 631 H LEU A 134 -20.019 14.581 -52.635 1.00 22.40
H
ATOM 632 HA LEU A 134 -17.733 15.276 -51.549 1.00 22.05
H
ATOM 633 HB2 LEU A 134 -19.601 16.817 -52.988 1.00 21.31
H
ATOM 6900 HB THR D 162 -37.063 43.072 16.288 1.00139.27
H
ATOM 6901 HG1 THR D 162 -36.656 43.994 14.318 1.00142.36
H
ATOM 6902 HG21 THR D 162 -36.242 45.270 16.321 1.00143.26
H
ATOM 6903 HG22 THR D 162 -35.687 44.471 17.565 1.00143.26
H
ATOM 6904 HG23 THR D 162 -34.761 44.721 16.310 1.00143.26
H
ATOM 6905 N ASN D 163 -35.079 40.834 14.305 1.00109.79
N
ATOM 6906 CA ASN D 163 -35.341 39.764 13.348 1.00106.91
C
ATOM 6907 C ASN D 163 -34.070 39.304 12.634 1.00 99.24
C
ATOM 6908 O ASN D 163 -34.132 38.638 11.599 1.00 96.09
O
ATOM 6909 CB ASN D 163 -36.389 40.223 12.329 1.00110.79
C
ATOM 6910 CG ASN D 163 -36.099 41.606 11.774 1.00109.36
C
ATOM 6911 OD1 ASN D 163 -34.944 41.980 11.575 1.00 98.35
O
ATOM 6912 ND2 ASN D 163 -37.154 42.377 11.533 1.00116.08
N
ATOM 6913 H ASN D 163 -34.559 41.449 14.003 1.00131.75
H
ATOM 6914 HA ASN D 163 -35.705 39.001 13.824 1.00128.29
H
ATOM 6915 HB2 ASN D 163 -36.404 39.599 11.587 1.00132.95
H
ATOM 6916 HB3 ASN D 163 -37.258 40.249 12.759 1.00132.95
H
ATOM 6917 HD21 ASN D 163 -37.044 43.170 11.218 1.00139.29
H
ATOM 6918 HD22 ASN D 163 -37.947 42.084 11.692 1.00139.29
H
ATOM 6919 N GLY D 164 -32.918 39.661 13.195 1.00 96.98
N
ATOM 6920 CA GLY D 164 -31.634 39.227 12.670 1.00 87.96
C
ATOM 6921 C GLY D 164 -31.365 39.684 11.248 1.00 79.64
C
ATOM 6922 O GLY D 164 -30.536 39.102 10.548 1.00 69.70
O
ATOM 6923 H GLY D 164 -32.856 40.162 13.892 1.00116.37
H
ATOM 6924 HA2 GLY D 164 -30.926 39.570 13.237 1.00105.56
H
ATOM 6925 HA3 GLY D 164 -31.595 38.258 12.689 1.00105.56
H
ATOM 6926 N SER D 165 -32.062 40.732 10.822 1.00 81.83
N
ATOM 6927 CA SER D 165 -31.935 41.238 9.460 1.00 71.12
C
ATOM 6928 C SER D 165 -30.735 42.170 9.313 1.00 57.71 C
ATOM 6929 O SER D 165 -30.340 42.844 10.265 1.00 55.24
O
ATOM 6930 CB SER D 165 -33.213 41.973 9.050 1.00 73.02
C
ATOM 6931 OG SER D 165 -33.077 42.556 7.766 1.00 71.30
O
ATOM 6932 H SER D 165 -32.620 41.171 11.307 1.00 98.19
H
ATOM 6933 HA SER D 165 -31.810 40.491 8.855 1.00 85.34
H

ATOM 634 HB3 LEU A 134 -18.243 17.436 -52.457 1.00 21.31 H
ATOM 635 HG LEU A 134 -18.287 15.327 -54.322 1.00 20.20 H
ATOM 636 HD11 LEU A 134 -18.028 18.060 -54.946 1.00 22.26 H
ATOM 637 HD12 LEU A 134 -17.866 16.882 -56.000 1.00 22.26 H
ATOM 638 HD13 LEU A 134 -19.280 17.161 -55.331 1.00 22.26 H
ATOM 639 HD21 LEU A 134 -16.266 15.491 -53.188 1.00 22.24 H
ATOM 640 HD22 LEU A 134 -16.058 15.876 -54.716 1.00 22.24 H
ATOM 641 HD23 LEU A 134 -16.144 17.017 -53.613 1.00 22.24 H
ATOM 642 N LEU A 135 -18.157 16.926 -49.681 1.00 15.27 N
ATOM 643 CA LEU A 135 -18.428 17.543 -48.386 1.00 14.24 C
ATOM 644 C LEU A 135 -19.756 18.295 -48.351 1.00 13.72 C
ATOM 645 O LEU A 135 -20.021 19.141 -49.207 1.00 14.87 O
ATOM 646 CB LEU A 135 -17.299 18.503 -48.018 1.00 11.92 C
ATOM 647 CG LEU A 135 -17.524 19.369 -46.773 1.00 13.80 C
ATOM 648 CD1 LEU A 135 -17.707 18.499 -45.536 1.00 16.19 C
ATOM 649 CD2 LEU A 135 -16.366 20.340 -46.586 1.00 15.37 C
ATOM 650 H LEU A 135 -17.361 17.065 -49.975 1.00 18.33 H
ATOM 651 HA LEU A 135 -18.461 16.848 -47.710 1.00 17.09 H
ATOM 652 HB2 LEU A 135 -16.495 17.982 -47.865 1.00 14.30 H
ATOM 653 HB3 LEU A 135 -17.156 19.104 -48.765 1.00 14.30 H
ATOM 654 HG LEU A 135 -18.333 19.889 -46.894 1.00 16.56 H
ATOM 655 HD11 LEU A 135 -17.846 19.072 -44.766 1.00 19.43 H
ATOM 656 HD12 LEU A 135 -18.477 17.924 -45.666 1.00 19.43 H
ATOM 657 HD13 LEU A 135 -16.910 17.961 -45.409 1.00 19.43 H
ATOM 658 HD21 LEU A 135 -16.529 20.877 -45.795 1.00 18.45 H
ATOM 659 HD22 LEU A 135 -15.545 19.835 -46.480 1.00 18.45 H
ATOM 660 HD23 LEU A 135 -16.305 20.912 -47.367 1.00 18.45 H
ATOM 661 N LYS A 136 -20.583 17.967 -47.359 1.00 11.97 N
ATOM 662 CA LYS A 136 -21.789 18.732 -47.064 1.00 19.27 C
ATOM 663 C LYS A 136 -21.649 19.428 -45.714 1.00 16.87 C
ATOM 664 O LYS A 136 -21.409 18.784 -44.691 1.00 16.35 O
ATOM 665 CB LYS A 136 -23.029 17.836 -47.062 1.00 20.92 C
ATOM 666 CG LYS A 136 -24.294 18.572 -46.624 1.00 23.85 C
ATOM 667 CD LYS A 136 -25.542 17.721 -46.767 1.00 27.86 C

ATOM 6934 HB2 SER D 165 -33.948 41.341 9.033 1.00 87.63 H
ATOM 6935 HB3 SER D 165 -33.394 42.674 9.696 1.00 87.63 H
ATOM 6936 HG SER D 165 -33.785 42.955 7.555 1.00 85.56 H

ATOM 6937 N TRP D 166 -30.159 42.193 8.114 1.00 41.62 N
ATOM 6938 CA TRP D 166 -29.122 43.161 7.768 1.00 41.01 C

ATOM 6939 C TRP D 166 -29.709 44.238 6.867 1.00 35.15 C

ATOM 6940 O TRP D 166 -30.344 43.933 5.858 1.00 33.29 O
ATOM 6941 CB TRP D 166 -27.942 42.481 7.067 1.00 31.04 C
ATOM 6942 CG TRP D 166 -27.138 41.590 7.958 1.00 32.96 C
ATOM 6943 CD1 TRP D 166 -27.222 40.232 8.050 1.00 39.24 C
ATOM 6944 CD2 TRP D 166 -26.124 41.993 8.889 1.00 33.27 C
ATOM 6945 NE1 TRP D 166 -26.324 39.763 8.979 1.00 36.80 N
ATOM 6946 CE2 TRP D 166 -25.639 40.824 9.509 1.00 32.66 C
ATOM 6947 CE3 TRP D 166 -25.582 43.227 9.257 1.00 32.29 C
ATOM 6948 CZ2 TRP D 166 -24.637 40.854 10.475 1.00 31.08 C
ATOM 6949 CZ3 TRP D 166 -24.586 43.254 10.217 1.00 29.48 C
ATOM 6950 CH2 TRP D 166 -24.125 42.074 10.815 1.00 29.86 C

ATOM 6951 H TRP D 166 -30.355 41.652 7.476 1.00 49.94 H
ATOM 6952 HA TRP D 166 -28.795 43.584 8.577 1.00 49.21 H
ATOM 6953 HB2 TRP D 166 -28.282 41.940 6.337 1.00 37.24 H
ATOM 6954 HB3 TRP D 166 -27.349 43.165 6.720 1.00 37.24 H
ATOM 6955 HD1 TRP D 166 -27.803 39.700 7.556 1.00 47.09 H
ATOM 6956 HE1 TRP D 166 -26.212 38.938 9.194 1.00 44.16 H
ATOM 6957 HE3 TRP D 166 -25.883 44.014 8.865 1.00 38.74 H
ATOM 6958 HZ2 TRP D 166 -24.328 40.072 10.873 1.00 37.29 H
ATOM 6959 HZ3 TRP D 166 -24.218 44.069 10.470 1.00 35.37 H
ATOM 6960 HH2 TRP D 166 -23.455 42.123 11.457 1.00 35.83 H

ATOM 6961 N GLN D 167 -29.503 45.497 7.238 1.00 34.74 N
ATOM 6962 CA GLN D 167 -29.909 46.611 6.392 1.00 36.36 C

ATOM 6963 C GLN D 167 -28.873 47.728 6.465 1.00 32.14 C
ATOM 6964 O GLN D 167 -27.979 47.711 7.315 1.00 28.97 O
ATOM 6965 CB GLN D 167 -31.294 47.127 6.800 1.00 43.23 C
ATOM 6966 CG GLN D 167 -31.323 47.983 8.059 1.00 42.74 C
ATOM 6967 CD GLN D 167 -32.719 48.487 8.383 1.00 45.63 C

ATOM 668 CE LYS A 136 -26.766 18.475 -46.263 1.00 36.34 C
ATOM 669 NZ LYS A 136 -28.041 17.844 -46.689 1.00 34.12 N1+
ATOM 670 H LYS A 136 -20.463 17.295 -46.836 1.00 14.37 H
ATOM 671 HA LYS A 136 -21.908 19.412 -47.745 1.00 23.12 H
ATOM 672 HB2 LYS A 136 -23.176 17.498 -47.959 1.00 25.11 H
ATOM 673 HB3 LYS A 136 -22.885 17.099 -46.448 1.00 25.11 H
ATOM 674 HG2 LYS A 136 -24.207 18.824 -45.691 1.00 28.62 H
ATOM 675 HG3 LYS A 136 -24.406 19.364 -47.172 1.00 28.62 H
ATOM 676 HD2 LYS A 136 -25.679 17.503 -47.702 1.00 33.44 H
ATOM 677 HD3 LYS A 136 -25.443 16.912 -46.241 1.00 33.44 H
ATOM 678 HE2 LYS A 136 -26.749 18.494 -45.294 1.00 43.61 H
ATOM 679 HE3 LYS A 136 -26.746 19.379 -46.614 1.00 43.61 H
ATOM 680 HZ1 LYS A 136 -28.730 18.312 -46.377 1.00 40.94 H
ATOM 681 HZ2 LYS A 136 -28.086 17.820 -47.577 1.00 40.94 H
ATOM 682 HZ3 LYS A 136 -28.088 17.013 -46.374 1.00 40.94 H
ATOM 683 N VAL A 137 -21.807 20.746 -45.726 1.00 17.32 N
ATOM 684 CA VAL A 137 -21.728 21.552 -44.516 1.00 16.33 C
ATOM 685 C VAL A 137 -23.137 21.792 -43.974 1.00 18.35 C
ATOM 686 O VAL A 137 -23.930 22.488 -44.603 1.00 20.87 O
ATOM 687 CB VAL A 137 -21.028 22.895 -44.788 1.00 17.82 C
ATOM 688 CG1 VAL A 137 -20.955 23.732 -43.518 1.00 22.96 C
ATOM 689 CG2 VAL A 137 -19.627 22.656 -45.354 1.00 18.45 C
ATOM 690 H VAL A 137 -21.964 21.205 -46.436 1.00 20.78 H
ATOM 691 HA VAL A 137 -21.220 21.073 -43.843 1.00 19.60 H
ATOM 692 HB VAL A 137 -21.539 23.391 -45.447 1.00 21.39 H
ATOM 693 HG11 VAL A 137 -20.510 24.571 -43.719 1.00 27.55 H
ATOM 694 HG12 VAL A 137 -21.856 23.903 -43.201 1.00 27.55 H
ATOM 695 HG13 VAL A 137 -20.454 23.244 -42.847 1.00 27.55 H
ATOM 696 HG21 VAL A 137 -19.203 23.513 -45.519 1.00 22.14 H
ATOM 697 HG22 VAL A 137 -19.109 22.148 -44.711 1.00 22.14 H
ATOM 698 HG23 VAL A 137 -19.703 22.159 -46.184 1.00 22.14 H
ATOM 699 N TYR A 138 -23.437 21.220 -42.810 1.00 19.32 N
ATOM 700 CA TYR A 138 -24.792 21.266 -42.259 1.00 24.49 C
ATOM 701 C TYR A 138 -24.832 21.797 -40.830 1.00 24.58 C
ATOM 6968 OE1 GLN D 167 -33.717 47.883 7.991 1.00 48.25 O
ATOM 6969 NE2 GLN D 167 -32.795 49.599 9.102 1.00 46.85 N
ATOM 6970 H GLN D 167 -29.130 45.732 7.976 1.00 41.69 H
ATOM 6971 HA GLN D 167 -29.960 46.308 5.472 1.00 43.63 H
ATOM 6972 HB2 GLN D 167 -31.649 47.663 6.074 1.00 51.88 H
ATOM 6973 HB3 GLN D 167 -31.874 46.364 6.953 1.00 51.88 H
ATOM 6974 HG2 GLN D 167 -31.012 47.454 8.810 1.00 51.28 H
ATOM 6975 HG3 GLN D 167 -30.747 48.753 7.932 1.00 51.28 H
ATOM 6976 HE21 GLN D 167 -33.563 49.925 9.312 1.00 56.22 H
ATOM 6977 HE22 GLN D 167 -32.076 49.994 9.360 1.00 56.22 H
ATOM 6978 N TRP D 168 -28.992 48.694 5.561 1.00 29.94 N
ATOM 6979 CA TRP D 168 -28.064 49.813 5.524 1.00 27.82 C
ATOM 6980 C TRP D 168 -28.475 50.864 6.546 1.00 33.11 C
ATOM 6981 O TRP D 168 -29.618 50.874 7.009 1.00 32.83 O
ATOM 6982 CB TRP D 168 -28.007 50.400 4.117 1.00 27.85 C
ATOM 6983 CG TRP D 168 -27.611 49.378 3.104 1.00 29.12 C
ATOM 6984 CD1 TRP D 168 -28.412 48.801 2.163 1.00 27.50 C
ATOM 6985 CD2 TRP D 168 -26.317 48.788 2.946 1.00 22.83 C
ATOM 6986 NE1 TRP D 168 -27.694 47.894 1.423 1.00 27.86 N
ATOM 6987 CE2 TRP D 168 -26.404 47.868 1.882 1.00 21.96 C
ATOM 6988 CE3 TRP D 168 -25.090 48.953 3.596 1.00 24.25 C
ATOM 6989 CZ2 TRP D 168 -25.312 47.116 1.454 1.00 18.62 C
ATOM 6990 CZ3 TRP D 168 -24.008 48.207 3.169 1.00 21.72 C
ATOM 6991 CH2 TRP D 168 -24.127 47.296 2.111 1.00 18.99 C
ATOM 6992 H TRP D 168 -29.604 48.723 4.958 1.00 35.93 H
ATOM 6993 HA TRP D 168 -27.176 49.498 5.755 1.00 33.38 H
ATOM 6994 HB2 TRP D 168 -28.884 50.740 3.877 1.00 33.42 H
ATOM 6995 HB3 TRP D 168 -27.354 51.116 4.096 1.00 33.42 H
ATOM 6996 HD1 TRP D 168 -29.313 48.995 2.041 1.00 33.00 H
ATOM 6997 HE1 TRP D 168 -28.004 47.421 0.775 1.00 33.44 H
ATOM 6998 HE3 TRP D 168 -25.004 49.554 4.301 1.00 29.10 H
ATOM 6999 HZ2 TRP D 168 -25.387 46.512 0.750 1.00 22.35 H
ATOM 7000 HZ3 TRP D 168 -23.188 48.308 3.595 1.00 26.06 H
ATOM 7001 HH2 TRP D 168 -23.381 46.810 1.845 1.00 22.79 H

ATOM 702 O TYR A 138 -25.909 22.078 -40.302 1.00 22.30
O
ATOM 703 CB TYR A 138 -25.423 19.871 -42.295 1.00 21.46
C
ATOM 704 CG TYR A 138 -24.849 18.919 -41.271 1.00 22.69
C
ATOM 705 CD1 TYR A 138 -23.689 18.203 -41.533 1.00 21.21
C
ATOM 706 CD2 TYR A 138 -25.463 18.742 -40.037 1.00 22.66
C
ATOM 707 CE1 TYR A 138 -23.160 17.331 -40.598 1.00 19.74
C
ATOM 708 CE2 TYR A 138 -24.940 17.874 -39.095 1.00 23.87
C
ATOM 709 CZ TYR A 138 -23.788 17.172 -39.380 1.00 23.25
C
ATOM 710 OH TYR A 138 -23.263 16.308 -38.446 1.00 19.45
O
ATOM 711 H TYR A 138 -22.873 20.797 -42.318 1.00 23.18
H
ATOM 712 HA TYR A 138 -25.334 21.853 -42.809 1.00 29.39
H
ATOM 713 HB2 TYR A 138 -26.374 19.954 -42.123 1.00 25.75
H
ATOM 714 HB3 TYR A 138 -25.279 19.485 -43.173 1.00 25.75
H
ATOM 715 HD1 TYR A 138 -23.263 18.308 -42.353 1.00 25.45
H
ATOM 716 HD2 TYR A 138 -26.239 19.214 -39.842 1.00 27.20
H
ATOM 717 HE1 TYR A 138 -22.383 16.857 -40.788 1.00 23.69
H
ATOM 718 HE2 TYR A 138 -25.363 17.766 -38.274 1.00 28.64
H
ATOM 719 HH TYR A 138 -23.740 16.308 -37.755 1.00 23.34
H
ATOM 720 N SER A 139 -23.668 21.933 -40.202 1.00 16.32
N
ATOM 721 CA SER A 139 -23.620 22.342 -38.802 1.00 22.45
C
ATOM 722 C SER A 139 -22.280 22.946 -38.399 1.00 21.92
C
ATOM 723 O SER A 139 -21.243 22.310 -38.547 1.00 20.19
O
ATOM 724 CB SER A 139 -23.922 21.142 -37.908 1.00 20.56
C
ATOM 725 OG SER A 139 -23.630 21.435 -36.555 1.00 23.25
O
ATOM 726 H SER A 139 -22.899 21.796 -40.560 1.00 19.58
H
ATOM 727 HA SER A 139 -24.306 23.010 -38.646 1.00 26.94
H
ATOM 728 HB2 SER A 139 -24.862 20.918 -37.987 1.00 24.67
H
ATOM 729 HB3 SER A 139 -23.377 20.391 -38.193 1.00 24.67
H
ATOM 730 HG SER A 139 -23.799 20.768 -36.073 1.00 27.89
H
ATOM 731 N LYS A 140 -22.304 24.164 -37.869 1.00 21.91
N
ATOM 732 CA LYS A 140 -21.074 24.803 -37.417 1.00 22.19
C
ATOM 733 C LYS A 140 -20.566 24.160 -36.132 1.00 22.96
C
ATOM 734 O LYS A 140 -19.382 24.240 -35.823 1.00 23.93
O
ATOM 735 CB LYS A 140 -21.280 26.304 -37.215 1.00 25.51
C

ATOM 7002 N GLU D 169 -27.541 51.742 6.905 1.00 32.76 N
ATOM 7003 CA GLU D 169 -27.781 52.721 7.962 1.00 34.47
C
ATOM 7004 C GLU D 169 -28.861 53.734 7.566 1.00 29.80 C
ATOM 7005 O GLU D 169 -29.420 54.412 8.425 1.00 39.17
O
ATOM 7006 CB GLU D 169 -26.473 53.442 8.329 1.00 36.50
C
ATOM 7007 CG GLU D 169 -25.907 54.339 7.239 1.00 37.04
C
ATOM 7008 CD GLU D 169 -24.412 54.619 7.405 1.00 37.98
C
ATOM 7009 OE1 GLU D 169 -23.995 55.125 8.473 1.00 34.25
O
ATOM 7010 OE2 GLU D 169 -23.651 54.335 6.457 1.00 31.91
O1-
ATOM 7011 H GLU D 169 -26.759 51.790 6.551 1.00 39.31 H
ATOM 7012 HA GLU D 169 -28.091 52.254 8.753 1.00 41.37
H
ATOM 7013 HB2 GLU D 169 -26.634 53.996 9.109 1.00 43.80
H
ATOM 7014 HB3 GLU D 169 -25.800 52.775 8.537 1.00 43.80
H
ATOM 7015 HG2 GLU D 169 -26.036 53.909 6.379 1.00 44.45
H
ATOM 7016 HG3 GLU D 169 -26.374 55.189 7.256 1.00 44.45
H
ATOM 7017 N ASP D 170 -29.163 53.822 6.273 1.00 30.55 N
ATOM 7018 CA ASP D 170 -30.212 54.719 5.789 1.00 31.25
C
ATOM 7019 C ASP D 170 -31.587 54.053 5.821 1.00 31.67 C
ATOM 7020 O ASP D 170 -32.580 54.645 5.407 1.00 37.31 O
ATOM 7021 CB ASP D 170 -29.900 55.192 4.366 1.00 25.76
C
ATOM 7022 CG ASP D 170 -30.035 54.083 3.334 1.00 29.56
C
ATOM 7023 OD1 ASP D 170 -30.204 52.907 3.720 1.00 30.98
O
ATOM 7024 OD2 ASP D 170 -29.959 54.387 2.127 1.00 27.01
O1-
ATOM 7025 H ASP D 170 -28.774 53.372 5.652 1.00 36.66 H
ATOM 7026 HA ASP D 170 -30.246 55.501 6.362 1.00 37.50
H
ATOM 7027 HB2 ASP D 170 -30.517 55.901 4.127 1.00 30.92
H
ATOM 7028 HB3 ASP D 170 -28.988 55.521 4.335 1.00 30.92
H
ATOM 7029 N GLY D 171 -31.629 52.808 6.286 1.00 31.62 N
ATOM 7030 CA GLY D 171 -32.877 52.081 6.423 1.00 31.76
C
ATOM 7031 C GLY D 171 -33.213 51.178 5.248 1.00 32.34 C
ATOM 7032 O GLY D 171 -34.017 50.259 5.393 1.00 36.75 O
ATOM 7033 H GLY D 171 -30.937 52.361 6.531 1.00 37.95 H
ATOM 7034 HA2 GLY D 171 -32.836 51.532 7.221 1.00 38.11
H
ATOM 7035 HA3 GLY D 171 -33.603 52.715 6.531 1.00 38.11
H

ATOM 736 CG LYS A 140 -21.119 27.111 -38.497 1.00 26.71
C
ATOM 737 CD LYS A 140 -21.243 28.605 -38.258 1.00 29.71
C
ATOM 738 CE LYS A 140 -20.959 29.383 -39.534 1.00 30.52
C
ATOM 739 NZ LYS A 140 -21.099 30.852 -39.352 1.00 46.50
N1+
ATOM 740 H LYS A 140 -23.013 24.638 -37.760 1.00 26.29
H
ATOM 741 HA LYS A 140 -20.392 24.686 -38.097 1.00 26.63
H
ATOM 742 HB2 LYS A 140 -22.177 26.456 -36.877 1.00 30.61
H
ATOM 743 HB3 LYS A 140 -20.627 26.628 -36.574 1.00 30.61
H
ATOM 744 HG2 LYS A 140 -20.242 26.938 -38.873 1.00 32.06
H
ATOM 745 HG3 LYS A 140 -21.809 26.848 -39.126 1.00 32.06
H
ATOM 746 HD2 LYS A 140 -22.145 28.811 -37.969 1.00 35.66
H
ATOM 747 HD3 LYS A 140 -20.601 28.877 -37.584 1.00 35.66
H
ATOM 748 HE2 LYS A 140 -20.049 29.201 -39.819 1.00 36.62
H
ATOM 749 HE3 LYS A 140 -21.584 29.104 -40.220 1.00 36.62
H
ATOM 750 HZ1 LYS A 140 -20.925 31.271 -40.118 1.00 55.80
H
ATOM 751 HZ2 LYS A 140 -21.928 31.049 -39.097 1.00 55.80
H
ATOM 752 HZ3 LYS A 140 -20.529 31.138 -38.731 1.00 55.80
H
ATOM 753 N GLU A 141 -21.459 23.513 -35.390 1.00 22.30
N
ATOM 754 CA GLU A 141 -21.065 22.818 -34.170 1.00 22.51
C
ATOM 755 C GLU A 141 -20.504 21.427 -34.473 1.00 23.38
C
ATOM 756 O GLU A 141 -19.397 21.093 -34.048 1.00 20.37
O
ATOM 757 CB GLU A 141 -22.250 22.705 -33.215 1.00 27.68
C
ATOM 758 CG GLU A 141 -21.925 22.006 -31.910 1.00 37.33
C
ATOM 759 CD GLU A 141 -23.137 21.869 -31.013 1.00 48.81
C
ATOM 760 OE1 GLU A 141 -23.280 22.685 -30.079 1.00 53.50
O
ATOM 761 OE2 GLU A 141 -23.950 20.947 -31.241 1.00 51.65
O1-
ATOM 762 H GLU A 141 -22.298 23.461 -35.571 1.00 26.77
H
ATOM 763 HA GLU A 141 -20.370 23.330 -33.727 1.00 27.01
H
ATOM 764 HB2 GLU A 141 -22.565 23.598 -33.003 1.00 33.21
H
ATOM 765 HB3 GLU A 141 -22.956 22.203 -33.652 1.00 33.21
H
ATOM 766 HG2 GLU A 141 -21.589 21.116 -32.101 1.00 44.80
H
ATOM 767 HG3 GLU A 141 -21.254 22.520 -31.433 1.00 44.80
H
ATOM 768 N ASP A 142 -21.273 20.619 -35.200 1.00 22.34
N
ATOM 769 CA ASP A 142 -20.873 19.244 -35.515 1.00 21.81
C

ATOM 7036 N SER D 172 -32.609 51.426 4.088 1.00 29.62 N
ATOM 7037 CA SER D 172 -32.938 50.654 2.888 1.00 31.61
C

ATOM 7038 C SER D 172 -32.552 49.188 3.061 1.00 30.37 C
ATOM 7039 O SER D 172 -31.747 48.846 3.927 1.00 33.60
O
ATOM 7040 CB SER D 172 -32.246 51.240 1.650 1.00 33.37
C
ATOM 7041 OG SER D 172 -30.837 51.125 1.737 1.00 30.18
O

ATOM 7042 H SER D 172 -32.009 52.031 3.968 1.00 35.54 H
ATOM 7043 HA SER D 172 -33.895 50.696 2.742 1.00 37.93
H
ATOM 7044 HB2 SER D 172 -32.552 50.761 0.864 1.00 40.04
H
ATOM 7045 HB3 SER D 172 -32.479 52.179 1.576 1.00 40.04
H
ATOM 7046 HG SER D 172 -30.619 50.316 1.800 1.00 36.22
H

ATOM 7047 N ILE D 173 -33.139 48.325 2.236 1.00 34.65 N

ATOM 7048 CA ILE D 173 -32.919 46.889 2.352 1.00 35.81 C

ATOM 7049 C ILE D 173 -31.672 46.444 1.600 1.00 32.48 C

ATOM 7050 O ILE D 173 -31.201 47.117 0.676 1.00 25.43 O

ATOM 7051 CB ILE D 173 -34.131 46.073 1.827 1.00 36.56 C
ATOM 7052 CG1 ILE D 173 -34.365 46.330 0.332 1.00 38.02
C
ATOM 7053 CG2 ILE D 173 -35.382 46.407 2.633 1.00 43.13
C
ATOM 7054 CD1 ILE D 173 -35.348 45.372 -0.303 1.00 40.93
C

ATOM 7055 H ILE D 173 -33.671 48.548 1.598 1.00 41.58 H

ATOM 7056 HA ILE D 173 -32.796 46.667 3.289 1.00 42.97 H

ATOM 7057 HB ILE D 173 -33.936 45.130 1.945 1.00 43.88 H
ATOM 7058 HG12 ILE D 173 -34.713 47.229 0.220 1.00 45.63
H
ATOM 7059 HG13 ILE D 173 -33.521 46.243 -0.137 1.00 45.63
H
ATOM 7060 HG21 ILE D 173 -36.126 45.888 2.289 1.00 51.76
H
ATOM 7061 HG22 ILE D 173 -35.225 46.186 3.564 1.00 51.76
H
ATOM 7062 HG23 ILE D 173 -35.570 47.355 2.544 1.00 51.76
H
ATOM 7063 HD11 ILE D 173 -35.444 45.595 -1.242 1.00 49.11
H
ATOM 7064 HD12 ILE D 173 -35.010 44.467 -0.211 1.00 49.11
H
ATOM 7065 HD13 ILE D 173 -36.203 45.453 0.147 1.00 49.11
H

ATOM 7066 N LEU D 174 -31.153 45.293 2.007 1.00 31.77 N
ATOM 7067 CA LEU D 174 -30.037 44.657 1.330 1.00 27.52
C

ATOM 7068 C LEU D 174 -30.557 43.827 0.166 1.00 25.72 C

ATOM 7069 O LEU D 174 -31.252 42.838 0.374 1.00 30.63 O

ATOM 770 C ASP A 142 -19.649 19.185 -36.433 1.00 18.46 C
ATOM 771 O ASP A 142 -18.949 18.171 -36.480 1.00 19.90 O
ATOM 772 CB ASP A 142 -22.029 18.486 -36.178 1.00 21.93 C
ATOM 773 CG ASP A 142 -23.054 17.966 -35.180 1.00 25.65 C
ATOM 774 OD1 ASP A 142 -23.061 18.415 -34.015 1.00 31.16 O
ATOM 775 OD2 ASP A 142 -23.865 17.101 -35.576 1.00 29.49 O1-
ATOM 776 H ASP A 142 -22.037 20.843 -35.526 1.00 26.80 H
ATOM 777 HA ASP A 142 -20.649 18.786 -34.690 1.00 26.17 H
ATOM 778 HB2 ASP A 142 -22.485 19.082 -36.792 1.00 26.32 H
ATOM 779 HB3 ASP A 142 -21.670 17.725 -36.661 1.00 26.32 H
ATOM 780 N GLN A 143 -19.407 20.265 -37.169 1.00 17.54 N
ATOM 781 CA GLN A 143 -18.302 20.325 -38.124 1.00 18.55 C
ATOM 782 C GLN A 143 -17.408 21.528 -37.839 1.00 21.09 C
ATOM 783 O GLN A 143 -16.838 22.123 -38.756 1.00 15.66 O
ATOM 784 CB GLN A 143 -18.842 20.393 -39.553 1.00 17.56 C
ATOM 785 CG GLN A 143 -19.803 19.267 -39.896 1.00 20.23 C
ATOM 786 CD GLN A 143 -20.459 19.445 -41.251 1.00 20.71 C
ATOM 787 OE1 GLN A 143 -21.171 20.425 -41.486 1.00 19.03 O
ATOM 788 NE2 GLN A 143 -20.225 18.496 -42.152 1.00 18.38 N
ATOM 789 H GLN A 143 -19.874 20.986 -37.134 1.00 21.05 H
ATOM 790 HA GLN A 143 -17.765 19.521 -38.041 1.00 22.26 H
ATOM 791 HB2 GLN A 143 -19.314 21.232 -39.670 1.00 21.08 H
ATOM 792 HB3 GLN A 143 -18.096 20.345 -40.172 1.00 21.08 H
ATOM 793 HG2 GLN A 143 -19.315 18.428 -39.907 1.00 24.27 H
ATOM 794 HG3 GLN A 143 -20.503 19.234 -39.226 1.00 24.27 H
ATOM 795 HE21 GLN A 143 -20.574 18.552 -42.935 1.00 22.06 H
ATOM 796 HE22 GLN A 143 -19.724 17.827 -41.950 1.00 22.06 H
ATOM 797 N ASP A 144 -17.288 21.876 -36.561 1.00 17.64 N
ATOM 798 CA ASP A 144 -16.568 23.078 -36.157 1.00 19.87 C
ATOM 799 C ASP A 144 -15.114 23.071 -36.621 1.00 19.55 C
ATOM 800 O ASP A 144 -14.547 24.122 -36.920 1.00 19.43 O
ATOM 801 CB ASP A 144 -16.632 23.247 -34.636 1.00 21.16 C
ATOM 802 CG ASP A 144 -16.132 22.027 -33.882 1.00 25.44 C
ATOM 803 OD1 ASP A 144 -16.127 20.917 -34.455 1.00 24.83 O

ATOM 7070 CB LEU D 174 -29.257 43.784 2.312 1.00 31.85 C
ATOM 7071 CG LEU D 174 -28.071 42.986 1.764 1.00 33.37 C
ATOM 7072 CD1 LEU D 174 -27.043 43.905 1.129 1.00 26.92 C
ATOM 7073 CD2 LEU D 174 -27.441 42.169 2.880 1.00 26.89 C
ATOM 7074 H LEU D 174 -31.438 44.853 2.688 1.00 38.12 H
ATOM 7075 HA LEU D 174 -29.440 45.337 0.980 1.00 33.02 H
ATOM 7076 HB2 LEU D 174 -28.912 44.357 3.015 1.00 38.22 H
ATOM 7077 HB3 LEU D 174 -29.874 43.144 2.700 1.00 38.22 H
ATOM 7078 HG LEU D 174 -28.389 42.372 1.084 1.00 40.04 H
ATOM 7079 HD11 LEU D 174 -26.307 43.370 0.793 1.00 32.31 H
ATOM 7080 HD12 LEU D 174 -27.461 44.389 0.400 1.00 32.31 H
ATOM 7081 HD13 LEU D 174 -26.721 44.528 1.799 1.00 32.31 H
ATOM 7082 HD21 LEU D 174 -26.692 41.669 2.521 1.00 32.27 H
ATOM 7083 HD22 LEU D 174 -27.134 42.771 3.577 1.00 32.27 H
ATOM 7084 HD23 LEU D 174 -28.105 41.559 3.239 1.00 32.27 H
ATOM 7085 N SER D 175 -30.242 44.239 -1.058 1.00 27.73 N
ATOM 7086 CA SER D 175 -30.653 43.479 -2.231 1.00 23.91 C
ATOM 7087 C SER D 175 -30.187 42.029 -2.083 1.00 28.76 C
ATOM 7088 O SER D 175 -28.991 41.786 -1.925 1.00 27.41 O
ATOM 7089 CB SER D 175 -30.077 44.098 -3.505 1.00 26.73 C
ATOM 7090 OG SER D 175 -30.445 43.344 -4.648 1.00 22.87 O
ATOM 7091 H SER D 175 -29.793 44.951 -1.234 1.00 33.27 H
ATOM 7092 HA SER D 175 -31.620 43.485 -2.297 1.00 28.69 H
ATOM 7093 HB2 SER D 175 -30.419 45.000 -3.600 1.00 32.07 H
ATOM 7094 HB3 SER D 175 -29.110 44.116 -3.438 1.00 32.07 H
ATOM 7095 HG SER D 175 -30.123 43.694 -5.340 1.00 27.44 H
ATOM 7096 N PRO D 176 -31.127 41.063 -2.098 1.00 25.88 N
ATOM 7097 CA PRO D 176 -30.728 39.659 -1.923 1.00 27.19 C
ATOM 7098 C PRO D 176 -29.657 39.204 -2.916 1.00 26.97 C
ATOM 7099 O PRO D 176 -29.693 39.601 -4.079 1.00 27.85 O
ATOM 7100 CB PRO D 176 -32.035 38.891 -2.155 1.00 23.99 C
ATOM 7101 CG PRO D 176 -33.107 39.860 -1.828 1.00 25.30 C
ATOM 7102 CD PRO D 176 -32.588 41.204 -2.234 1.00 25.95 C
ATOM 7103 HA PRO D 176 -30.418 39.504 -1.017 1.00 32.63 H

ATOM 804 OD2 ASP A 144 -15.753 22.181 -32.702 1.00 30.53
O1-
ATOM 805 H ASP A 144 -17.618 21.429 -35.904 1.00 21.16
H
ATOM 806 HA ASP A 144 -17.001 23.848 -36.558 1.00 23.85
H
ATOM 807 HB2 ASP A 144 -16.081 24.004 -34.380 1.00 25.40
H
ATOM 808 HB3 ASP A 144 -17.552 23.405 -34.374 1.00 25.40
H
ATOM 809 N LEU A 145 -14.516 21.891 -36.711 1.00 17.05
N
ATOM 810 CA LEU A 145 -13.098 21.807 -37.047 1.00 17.13
C
ATOM 811 C LEU A 145 -12.832 22.091 -38.531 1.00 17.51
C
ATOM 812 O LEU A 145 -11.681 22.142 -38.963 1.00 18.01
O
ATOM 813 CB LEU A 145 -12.549 20.442 -36.639 1.00 22.72
C
ATOM 814 CG LEU A 145 -12.526 20.245 -35.115 1.00 27.83
C
ATOM 815 CD1 LEU A 145 -12.087 18.841 -34.761 1.00 30.89
C
ATOM 816 CD2 LEU A 145 -11.610 21.254 -34.415 1.00 26.54
C
ATOM 817 H LEU A 145 -14.900 21.132 -36.585 1.00 20.46
H
ATOM 818 HA LEU A 145 -12.621 22.478 -36.533 1.00 20.56
H
ATOM 819 HB2 LEU A 145 -13.109 19.748 -37.023 1.00 27.26
H
ATOM 820 HB3 LEU A 145 -11.641 20.355 -36.967 1.00 27.26
H
ATOM 821 HG LEU A 145 -13.424 20.371 -34.770 1.00 33.39
H
ATOM 822 HD11 LEU A 145 -12.082 18.746 -33.795 1.00 37.07
H
ATOM 823 HD12 LEU A 145 -12.709 18.208 -35.152 1.00 37.07
H
ATOM 824 HD13 LEU A 145 -11.196 18.691 -35.113 1.00 37.07
H
ATOM 825 HD21 LEU A 145 -11.630 21.089 -33.459 1.00 31.85
H
ATOM 826 HD22 LEU A 145 -10.706 21.145 -34.750 1.00 31.85
H
ATOM 827 HD23 LEU A 145 -11.927 22.151 -34.602 1.00 31.85
H
ATOM 828 N LEU A 146 -13.892 22.317 -39.300 1.00 14.54
N
ATOM 829 CA LEU A 146 -13.741 22.812 -40.663 1.00 17.73
C
ATOM 830 C LEU A 146 -13.100 24.200 -40.661 1.00 13.72
C
ATOM 831 O LEU A 146 -12.574 24.650 -41.679 1.00 14.63
O
ATOM 832 CB LEU A 146 -15.093 22.857 -41.382 1.00 16.27
C
ATOM 833 CG LEU A 146 -15.734 21.525 -41.770 1.00 19.70
C
ATOM 834 CD1 LEU A 146 -17.090 21.764 -42.414 1.00 16.79
C
ATOM 835 CD2 LEU A 146 -14.839 20.740 -42.715 1.00 17.92
C
ATOM 836 H LEU A 146 -14.708 22.193 -39.057 1.00 17.45
H
ATOM 837 HA LEU A 146 -13.158 22.212 -41.155 1.00 21.28
H

ATOM 7104 HB2 PRO D 176 -32.092 38.614 -3.082 1.00 28.78
H
ATOM 7105 HB3 PRO D 176 -32.073 38.123 -1.563 1.00 28.78
H
ATOM 7106 HG2 PRO D 176 -33.907 39.638 -2.330 1.00 30.36
H
ATOM 7107 HG3 PRO D 176 -33.285 39.837 -0.875 1.00 30.36
H
ATOM 7108 HD2 PRO D 176 -32.825 41.393 -3.155 1.00 31.14
H
ATOM 7109 HD3 PRO D 176 -32.919 41.889 -1.633 1.00 31.14
H

ATOM 7110 N ASN D 177 -28.715 38.392 -2.442 1.00 24.96 N
ATOM 7111 CA ASN D 177 -27.667 37.810 -3.280 1.00 24.54
C

ATOM 7112 C ASN D 177 -26.704 38.844 -3.866 1.00 29.77 C
ATOM 7113 O ASN D 177 -26.083 38.603 -4.900 1.00 33.58
O
ATOM 7114 CB ASN D 177 -28.291 36.990 -4.415 1.00 30.08
C
ATOM 7115 CG ASN D 177 -29.188 35.884 -3.905 1.00 29.31
C
ATOM 7116 OD1 ASN D 177 -30.398 35.883 -4.142 1.00 27.98
O
ATOM 7117 ND2 ASN D 177 -28.598 34.933 -3.193 1.00 30.03
N

ATOM 7118 H ASN D 177 -28.660 38.158 -1.616 1.00 29.95 H
ATOM 7119 HA ASN D 177 -27.144 37.202 -2.735 1.00 29.44
H
ATOM 7120 HB2 ASN D 177 -28.825 37.576 -4.974 1.00 36.09
H
ATOM 7121 HB3 ASN D 177 -27.583 36.585 -4.940 1.00 36.09
H
ATOM 7122 HD21 ASN D 177 -29.062 34.281 -2.879 1.00 36.03
H
ATOM 7123 HD22 ASN D 177 -27.752 34.969 -3.046 1.00 36.03
H

ATOM 7124 N LEU D 178 -26.577 39.988 -3.202 1.00 29.98 N
ATOM 7125 CA LEU D 178 -25.592 40.989 -3.594 1.00 25.52
C

ATOM 7126 C LEU D 178 -24.290 40.721 -2.851 1.00 26.67 C

ATOM 7127 O LEU D 178 -23.228 40.588 -3.463 1.00 28.33 O
ATOM 7128 CB LEU D 178 -26.098 42.400 -3.295 1.00 26.47
C
ATOM 7129 CG LEU D 178 -25.654 43.482 -4.281 1.00 26.81
C
ATOM 7130 CD1 LEU D 178 -26.117 44.846 -3.805 1.00 26.04
C
ATOM 7131 CD2 LEU D 178 -24.150 43.470 -4.484 1.00 28.87
C

ATOM 7132 H LEU D 178 -27.051 40.209 -2.520 1.00 35.97 H
ATOM 7133 HA LEU D 178 -25.423 40.919 -4.546 1.00 30.62
H
ATOM 7134 HB2 LEU D 178 -27.068 42.385 -3.298 1.00 31.77
H
ATOM 7135 HB3 LEU D 178 -25.781 42.659 -2.416 1.00 31.77
H
ATOM 7136 HG LEU D 178 -26.070 43.312 -5.141 1.00 32.18
H
ATOM 7137 HD11 LEU D 178 -25.727 45.025 -2.934 1.00 31.25
H

ATOM 838 HB2 LEU A 146 -15.723 23.318 -40.806 1.00 19.52
H
ATOM 839 HB3 LEU A 146 -14.980 23.366 -42.200 1.00 19.52
H
ATOM 840 HG LEU A 146 -15.869 20.992 -40.971 1.00 23.64
H
ATOM 841 HD11 LEU A 146 -17.481 20.909 -42.653 1.00 20.15
H
ATOM 842 HD12 LEU A 146 -17.663 22.224 -41.782 1.00 20.15
H
ATOM 843 HD13 LEU A 146 -16.970 22.307 -43.209 1.00 20.15
H
ATOM 844 HD21 LEU A 146 -15.275 19.903 -42.940 1.00 21.50
H
ATOM 845 HD22 LEU A 146 -14.692 21.264 -43.518 1.00 21.50
H
ATOM 846 HD23 LEU A 146 -13.992 20.565 -42.275 1.00 21.50
H
ATOM 847 N LYS A 147 -13.140 24.875 -39.517 1.00 15.29
N
ATOM 848 CA LYS A 147 -12.485 26.173 -39.360 1.00 18.16
C
ATOM 849 C LYS A 147 -10.973 26.053 -39.545 1.00 16.32
C
ATOM 850 O LYS A 147 -10.321 26.979 -40.029 1.00 15.57
O
ATOM 851 CB LYS A 147 -12.798 26.763 -37.981 1.00 22.56
C
ATOM 852 CG LYS A 147 -12.018 28.031 -37.645 1.00 33.54
C
ATOM 853 CD LYS A 147 -12.430 28.588 -36.287 1.00 49.30
C
ATOM 854 CE LYS A 147 -11.588 29.796 -35.894 1.00 57.42
C
ATOM 855 NZ LYS A 147 -11.760 30.941 -36.829 1.00 59.81
N1+
ATOM 856 H LYS A 147 -13.544 24.601 -38.808 1.00 18.35
H
ATOM 857 HA LYS A 147 -12.824 26.783 -40.034 1.00 21.79
H
ATOM 858 HB2 LYS A 147 -13.742 26.980 -37.943 1.00 27.07
H
ATOM 859 HB3 LYS A 147 -12.587 26.100 -37.305 1.00 27.07
H
ATOM 860 HG2 LYS A 147 -11.070 27.826 -37.616 1.00 40.24
H
ATOM 861 HG3 LYS A 147 -12.197 28.705 -38.318 1.00 40.24
H
ATOM 862 HD2 LYS A 147 -13.359 28.864 -36.324 1.00 59.16
H
ATOM 863 HD3 LYS A 147 -12.310 27.902 -35.612 1.00 59.16
H
ATOM 864 HE2 LYS A 147 -11.851 30.089 -35.008 1.00 68.91
H
ATOM 865 HE3 LYS A 147 -10.652 29.543 -35.897 1.00 68.91
H
ATOM 866 HZ1 LYS A 147 -11.255 31.626 -36.567 1.00 71.78
H
ATOM 867 HZ2 LYS A 147 -11.519 30.701 -37.652 1.00 71.78
H
ATOM 868 HZ3 LYS A 147 -12.612 31.199 -36.841 1.00 71.78
H
ATOM 869 N LEU A 148 -10.426 24.903 -39.166 1.00 13.11
N
ATOM 870 CA LEU A 148 -8.984 24.680 -39.204 1.00 13.14
C
ATOM 871 C LEU A 148 -8.491 24.075 -40.519 1.00 13.81
C

ATOM 7138 HD12 LEU D 178 -25.826 45.518 -4.442 1.00 31.25
H
ATOM 7139 HD13 LEU D 178 -27.085 44.847 -3.741 1.00 31.25
H
ATOM 7140 HD21 LEU D 178 -23.910 44.168 -5.113 1.00 34.64
H
ATOM 7141 HD22 LEU D 178 -23.716 43.630 -3.631 1.00 34.64
H
ATOM 7142 HD23 LEU D 178 -23.885 42.605 -4.833 1.00 34.64
H

ATOM 7143 N LEU D 179 -24.389 40.630 -1.528 1.00 19.13 N
ATOM 7144 CA LEU D 179 -23.244 40.332 -0.679 1.00 21.55
C

ATOM 7145 C LEU D 179 -23.321 38.920 -0.113 1.00 28.27 C

ATOM 7146 O LEU D 179 -24.408 38.392 0.125 1.00 25.28 O
ATOM 7147 CB LEU D 179 -23.155 41.335 0.469 1.00 22.39
C
ATOM 7148 CG LEU D 179 -22.856 42.788 0.096 1.00 22.47
C
ATOM 7149 CD1 LEU D 179 -22.901 43.661 1.336 1.00 24.98
C
ATOM 7150 CD2 LEU D 179 -21.504 42.910 -0.586 1.00 23.45
C

ATOM 7151 H LEU D 179 -25.123 40.739 -1.093 1.00 22.95 H
ATOM 7152 HA LEU D 179 -22.432 40.403 -1.205 1.00 25.86
H
ATOM 7153 HB2 LEU D 179 -24.003 41.329 0.941 1.00 26.87
H
ATOM 7154 HB3 LEU D 179 -22.453 41.043 1.071 1.00 26.87
H
ATOM 7155 HG LEU D 179 -23.535 43.104 -0.521 1.00 26.97
H
ATOM 7156 HD11 LEU D 179 -22.710 44.577 1.083 1.00 29.97
H
ATOM 7157 HD12 LEU D 179 -23.786 43.604 1.729 1.00 29.97
H
ATOM 7158 HD13 LEU D 179 -22.237 43.346 1.968 1.00 29.97
H
ATOM 7159 HD21 LEU D 179 -21.346 43.840 -0.809 1.00 28.13
H
ATOM 7160 HD22 LEU D 179 -20.816 42.593 0.020 1.00 28.13
H
ATOM 7161 HD23 LEU D 179 -21.508 42.372 -1.393 1.00 28.13
H

ATOM 7162 N THR D 180 -22.153 38.316 0.088 1.00 19.72 N
ATOM 7163 CA THR D 180 -22.040 37.069 0.827 1.00 19.71
C

ATOM 7164 C THR D 180 -21.583 37.388 2.242 1.00 23.17 C
ATOM 7165 O THR D 180 -20.446 37.813 2.455 1.00 23.15
O
ATOM 7166 CB THR D 180 -21.059 36.099 0.154 1.00 23.54
C
ATOM 7167 OG1 THR D 180 -21.581 35.709 -1.122 1.00 25.00
O
ATOM 7168 CG2 THR D 180 -20.847 34.854 1.006 1.00 24.90
C

ATOM 7169 H THR D 180 -21.401 38.616 -0.201 1.00 23.66 H
ATOM 7170 HA THR D 180 -22.910 36.642 0.875 1.00 23.65
H
ATOM 7171 HB THR D 180 -20.203 36.538 0.032 1.00 28.24
H

ATOM 872 O LEU A 148 -7.296 23.812 -40.667 1.00 17.85 O
ATOM 873 CB LEU A 148 -8.568 23.765 -38.052 1.00 15.95 C
ATOM 874 CG LEU A 148 -8.725 24.317 -36.634 1.00 20.41 C
ATOM 875 CD1 LEU A 148 -8.325 23.250 -35.630 1.00 17.28 C
ATOM 876 CD2 LEU A 148 -7.903 25.578 -36.435 1.00 21.97 C
ATOM 877 H LEU A 148 -10.875 24.228 -38.879 1.00 15.73 H
ATOM 878 HA LEU A 148 -8.534 25.531 -39.084 1.00 15.77 H
ATOM 879 HB2 LEU A 148 -9.099 22.954 -38.103 1.00 19.14 H
ATOM 880 HB3 LEU A 148 -7.631 23.540 -38.169 1.00 19.14 H
ATOM 881 HG LEU A 148 -9.657 24.538 -36.482 1.00 24.49 H
ATOM 882 HD11 LEU A 148 -8.427 23.607 -34.733 1.00 20.73 H
ATOM 883 HD12 LEU A 148 -8.898 22.477 -35.746 1.00 20.73 H
ATOM 884 HD13 LEU A 148 -7.400 23.003 -35.784 1.00 20.73 H
ATOM 885 HD21 LEU A 148 -8.028 25.897 -35.527 1.00 26.36 H
ATOM 886 HD22 LEU A 148 -6.967 25.372 -36.587 1.00 26.36 H
ATOM 887 HD23 LEU A 148 -8.200 26.252 -37.066 1.00 26.36 H
ATOM 888 N VAL A 149 -9.396 23.849 -41.467 1.00 14.39 N
ATOM 889 CA VAL A 149 -9.009 23.240 -42.738 1.00 13.95 C
ATOM 890 C VAL A 149 -8.252 24.220 -43.624 1.00 15.01 C
ATOM 891 O VAL A 149 -8.734 25.307 -43.936 1.00 13.43 O
ATOM 892 CB VAL A 149 -10.234 22.703 -43.505 1.00 13.62 C
ATOM 893 CG1 VAL A 149 -9.869 22.333 -44.945 1.00 18.07 C
ATOM 894 CG2 VAL A 149 -10.796 21.498 -42.787 1.00 13.27 C
ATOM 895 H VAL A 149 -10.233 24.036 -41.401 1.00 17.27 H
ATOM 896 HA VAL A 149 -8.422 22.490 -42.557 1.00 16.74 H
ATOM 897 HB VAL A 149 -10.920 23.388 -43.532 1.00 16.34 H
ATOM 898 HG11 VAL A 149 -10.661 22.000 -45.396 1.00 21.68 H
ATOM 899 HG12 VAL A 149 -9.537 23.123 -45.400 1.00 21.68 H
ATOM 900 HG13 VAL A 149 -9.184 21.646 -44.930 1.00 21.68 H
ATOM 901 HG21 VAL A 149 -11.566 21.169 -43.278 1.00 15.93 H
ATOM 902 HG22 VAL A 149 -10.113 20.811 -42.742 1.00 15.93 H
ATOM 903 HG23 VAL A 149 -11.062 21.760 -41.892 1.00 15.93 H
ATOM 904 N LYS A 150 -7.063 23.797 -44.032 1.00 13.03 N
ATOM 905 CA LYS A 150 -6.189 24.572 -44.898 1.00 14.72 C
ATOM 7172 HG1 THR D 180 -21.682 36.386 -1.610 1.00 30.00 H
ATOM 7173 HG21 THR D 180 -20.225 34.253 0.566 1.00 29.88 H
ATOM 7174 HG22 THR D 180 -20.486 35.102 1.872 1.00 29.88 H
ATOM 7175 HG23 THR D 180 -21.691 34.394 1.137 1.00 29.88 H

ATOM 7176 N ILE D 181 -22.478 37.187 3.204 1.00 22.44 N
ATOM 7177 CA ILE D 181 -22.186 37.469 4.602 1.00 23.18 C
ATOM 7178 C ILE D 181 -21.541 36.264 5.269 1.00 25.41 C
ATOM 7179 O ILE D 181 -22.102 35.168 5.252 1.00 23.82 O
ATOM 7180 CB ILE D 181 -23.459 37.851 5.386 1.00 25.11 C
ATOM 7181 CG1 ILE D 181 -24.171 39.037 4.725 1.00 25.99 C
ATOM 7182 CG2 ILE D 181 -23.116 38.174 6.841 1.00 32.01 C
ATOM 7183 CD1 ILE D 181 -23.360 40.323 4.695 1.00 29.24 C

ATOM 7184 H ILE D 181 -23.271 36.883 3.069 1.00 26.93 H
ATOM 7185 HA ILE D 181 -21.565 38.212 4.654 1.00 27.81 H
ATOM 7186 HB ILE D 181 -24.062 37.091 5.377 1.00 30.13 H
ATOM 7187 HG12 ILE D 181 -24.382 38.800 3.809 1.00 31.19 H
ATOM 7188 HG13 ILE D 181 -24.990 39.218 5.213 1.00 31.19 H
ATOM 7189 HG21 ILE D 181 -23.930 38.411 7.312 1.00 38.41 H
ATOM 7190 HG22 ILE D 181 -22.711 37.393 7.250 1.00 38.41 H
ATOM 7191 HG23 ILE D 181 -22.494 38.918 6.861 1.00 38.41 H
ATOM 7192 HD11 ILE D 181 -23.883 41.016 4.262 1.00 35.08 H
ATOM 7193 HD12 ILE D 181 -23.151 40.586 5.605 1.00 35.08 H
ATOM 7194 HD13 ILE D 181 -22.541 40.168 4.198 1.00 35.08 H

ATOM 7195 N ILE D 182 -20.375 36.484 5.873 1.00 23.72 N
ATOM 7196 CA ILE D 182 -19.615 35.416 6.521 1.00 22.37 C
ATOM 7197 C ILE D 182 -19.531 35.640 8.024 1.00 22.69 C
ATOM 7198 O ILE D 182 -19.146 36.717 8.478 1.00 17.58 O
ATOM 7199 CB ILE D 182 -18.184 35.315 5.950 1.00 20.91 C
ATOM 7200 CG1 ILE D 182 -18.233 35.144 4.428 1.00 19.30 C
ATOM 7201 CG2 ILE D 182 -17.422 34.159 6.609 1.00 18.99 C
ATOM 7202 CD1 ILE D 182 -16.890 35.250 3.753 1.00 20.70 C

ATOM 7203 H ILE D 182 -19.997 37.255 5.922 1.00 28.47 H
ATOM 7204 HA ILE D 182 -20.062 34.569 6.366 1.00 26.85 H
ATOM 7205 HB ILE D 182 -17.716 36.141 6.149 1.00 25.09 H

ATOM 906 C LYS A 150 -6.493 24.295 -46.366 1.00 13.85 C
ATOM 907 O LYS A 150 -6.988 23.224 -46.705 1.00 15.19 O
ATOM 908 CB LYS A 150 -4.730 24.229 -44.589 1.00 17.03 C
ATOM 909 CG LYS A 150 -3.696 25.097 -45.282 1.00 16.21 C
ATOM 910 CD LYS A 150 -2.302 24.647 -44.880 1.00 15.63 C
ATOM 911 CE LYS A 150 -1.224 25.608 -45.344 1.00 20.81 C
ATOM 912 NZ LYS A 150 0.121 25.154 -44.907 1.00 24.83 N1+
ATOM 913 H LYS A 150 -6.729 23.036 -43.810 1.00 15.64 H
ATOM 914 HA LYS A 150 -6.324 25.518 -44.730 1.00 17.66 H
ATOM 915 HB2 LYS A 150 -4.590 24.317 -43.633 1.00 20.44 H
ATOM 916 HB3 LYS A 150 -4.567 23.312 -44.857 1.00 20.44 H
ATOM 917 HG2 LYS A 150 -3.786 25.006 -46.243 1.00 19.45 H
ATOM 918 HG3 LYS A 150 -3.813 26.021 -45.013 1.00 19.45 H
ATOM 919 HD2 LYS A 150 -2.255 24.587 -43.913 1.00 18.76 H
ATOM 920 HD3 LYS A 150 -2.122 23.780 -45.276 1.00 18.76 H
ATOM 921 HE2 LYS A 150 -1.230 25.654 -46.313 1.00 24.98 H
ATOM 922 HE3 LYS A 150 -1.389 26.484 -44.964 1.00 24.98 H
ATOM 923 HZ1 LYS A 150 0.296 24.350 -45.246 1.00 29.79 H
ATOM 924 HZ2 LYS A 150 0.741 25.728 -45.186 1.00 29.79 H
ATOM 925 HZ3 LYS A 150 0.151 25.106 -44.018 1.00 29.79 H
ATOM 926 N SER A 151 -6.191 25.271 -47.219 1.00 11.64 N
ATOM 927 CA SER A 151 -6.340 25.146 -48.669 1.00 12.00 C
ATOM 928 C SER A 151 -7.809 25.150 -49.090 1.00 15.77 C
ATOM 929 O SER A 151 -8.698 25.423 -48.283 1.00 13.47 O
ATOM 930 CB SER A 151 -5.657 23.875 -49.185 1.00 15.08 C
ATOM 931 OG SER A 151 -5.545 23.900 -50.600 1.00 18.05 O
ATOM 932 H SER A 151 -5.889 26.038 -46.975 1.00 13.97 H
ATOM 933 HA SER A 151 -5.910 25.905 -49.092 1.00 14.40 H
ATOM 934 HB2 SER A 151 -4.769 23.815 -48.800 1.00 18.09 H
ATOM 935 HB3 SER A 151 -6.184 23.104 -48.924 1.00 18.09 H
ATOM 936 HG SER A 151 -5.169 23.200 -50.871 1.00 21.66 H
ATOM 937 N TYR A 152 -8.034 24.838 -50.363 1.00 15.37 N
ATOM 938 CA TYR A 152 -9.332 24.985 -51.015 1.00 14.25 C
ATOM 939 C TYR A 152 -9.729 23.674 -51.687 1.00 16.05 C
ATOM 7206 HG12 ILE D 182 -18.598 34.269 4.225 1.00 23.16 H
ATOM 7207 HG13 ILE D 182 -18.805 35.833 4.056 1.00 23.16 H
ATOM 7208 HG21 ILE D 182 -16.528 34.116 6.235 1.00 22.78 H
ATOM 7209 HG22 ILE D 182 -17.373 34.318 7.565 1.00 22.78 H
ATOM 7210 HG23 ILE D 182 -17.894 33.330 6.435 1.00 22.78 H
ATOM 7211 HD11 ILE D 182 -17.007 35.131 2.797 1.00 24.84 H
ATOM 7212 HD12 ILE D 182 -16.513 36.125 3.934 1.00 24.84 H
ATOM 7213 HD13 ILE D 182 -16.305 34.559 4.103 1.00 24.84 H
ATOM 7214 N GLU D 183 -19.895 34.615 8.789 1.00 24.20 N
ATOM 7215 CA GLU D 183 -19.788 34.661 10.241 1.00 26.38 C
ATOM 7216 C GLU D 183 -18.337 34.472 10.651 1.00 31.18 C
ATOM 7217 O GLU D 183 -17.673 33.538 10.205 1.00 29.96 O
ATOM 7218 CB GLU D 183 -20.662 33.587 10.888 1.00 35.36 C
ATOM 7219 CG GLU D 183 -22.150 33.765 10.648 1.00 46.80 C
ATOM 7220 CD GLU D 183 -22.982 32.679 11.304 1.00 73.69 C
ATOM 7221 OE1 GLU D 183 -22.398 31.680 11.776 1.00 79.19 O
ATOM 7222 OE2 GLU D 183 -24.222 32.825 11.351 1.00 81.50 O1-
ATOM 7223 H GLU D 183 -20.210 33.874 8.486 1.00 29.04 H
ATOM 7224 HA GLU D 183 -20.085 35.529 10.557 1.00 31.66 H
ATOM 7225 HB2 GLU D 183 -20.407 32.722 10.531 1.00 42.43 H
ATOM 7226 HB3 GLU D 183 -20.514 33.602 11.847 1.00 42.43 H
ATOM 7227 HG2 GLU D 183 -22.430 34.619 11.013 1.00 56.15 H
ATOM 7228 HG3 GLU D 183 -22.322 33.739 9.694 1.00 56.15 H
ATOM 7229 N MET D 184 -17.846 35.363 11.502 1.00 30.31 N
ATOM 7230 CA MET D 184 -16.458 35.313 11.938 1.00 29.78 C
ATOM 7231 C MET D 184 -16.376 35.603 13.430 1.00 35.79 C
ATOM 7232 O MET D 184 -16.026 34.731 14.229 1.00 37.59 O
ATOM 7233 CB MET D 184 -15.621 36.315 11.147 1.00 27.05 C
ATOM 7234 CG MET D 184 -14.138 36.253 11.442 1.00 26.53 C
ATOM 7235 SD MET D 184 -13.261 37.651 10.735 1.00 30.02 S
ATOM 7236 CE MET D 184 -13.846 38.985 11.783 1.00 31.51 C
ATOM 7237 H MET D 184 -18.299 36.010 11.843 1.00 36.37 H
ATOM 7238 HA MET D 184 -16.104 34.426 11.768 1.00 35.73 H
ATOM 7239 HB2 MET D 184 -15.741 36.142 10.200 1.00 32.46 H

ATOM 940 O TYR A 152 -8.929 23.071 -52.401 1.00 15.60
O
ATOM 941 CB TYR A 152 -9.270 26.138 -52.025 1.00 15.37
C
ATOM 942 CG TYR A 152 -8.986 27.455 -51.343 1.00 16.48
C
ATOM 943 CD1 TYR A 152 -7.721 27.747 -50.853 1.00 14.01
C
ATOM 944 CD2 TYR A 152 -9.991 28.393 -51.161 1.00 18.15
C
ATOM 945 CE1 TYR A 152 -7.464 28.935 -50.202 1.00 15.58
C
ATOM 946 CE2 TYR A 152 -9.745 29.584 -50.511 1.00 16.03
C
ATOM 947 CZ TYR A 152 -8.480 29.850 -50.032 1.00 17.68
C
ATOM 948 OH TYR A 152 -8.237 31.038 -49.385 1.00 16.49
O
ATOM 949 H TYR A 152 -7.428 24.528 -50.888 1.00 18.44
H
ATOM 950 HA TYR A 152 -10.003 25.200 -50.348 1.00 17.09
H
ATOM 951 HB2 TYR A 152 -8.560 25.967 -52.663 1.00 18.44
H
ATOM 952 HB3 TYR A 152 -10.123 26.210 -52.482 1.00 18.44
H
ATOM 953 HD1 TYR A 152 -7.036 27.127 -50.958 1.00 16.82
H
ATOM 954 HD2 TYR A 152 -10.847 28.212 -51.474 1.00 21.78
H
ATOM 955 HE1 TYR A 152 -6.611 29.117 -49.879 1.00 18.70
H
ATOM 956 HE2 TYR A 152 -10.428 30.204 -50.396 1.00 19.23
H
ATOM 957 HH TYR A 152 -8.940 31.496 -49.353 1.00 19.79
H
ATOM 958 N HIS A 153 -10.959 23.228 -51.441 1.00 16.84
N
ATOM 959 CA HIS A 153 -11.394 21.895 -51.859 1.00 17.66
C
ATOM 960 C HIS A 153 -12.829 21.891 -52.367 1.00 16.44
C
ATOM 961 O HIS A 153 -13.682 22.586 -51.821 1.00 13.76
O
ATOM 962 CB HIS A 153 -11.271 20.913 -50.690 1.00 13.32
C
ATOM 963 CG HIS A 153 -10.048 21.124 -49.856 1.00 19.37
C
ATOM 964 ND1 HIS A 153 -8.865 20.454 -50.086 1.00 19.53
N
ATOM 965 CD2 HIS A 153 -9.819 21.941 -48.801 1.00 16.93
C
ATOM 966 CE1 HIS A 153 -7.963 20.843 -49.203 1.00 16.06
C
ATOM 967 NE2 HIS A 153 -8.516 21.746 -48.413 1.00 15.08
N
ATOM 968 H HIS A 153 -11.565 23.680 -51.031 1.00 20.20
H
ATOM 969 HA HIS A 153 -10.819 21.584 -52.576 1.00 21.19
H
ATOM 970 HB2 HIS A 153 -12.044 21.015 -50.113 1.00 15.98
H
ATOM 971 HB3 HIS A 153 -11.239 20.010 -51.041 1.00 15.98
H
ATOM 972 HD1 HIS A 153 -8.736 19.870 -50.705 1.00 23.43
H
ATOM 973 HD2 HIS A 153 -10.430 22.523 -48.411 1.00 20.31
H

ATOM 7240 HB3 MET D 184 -15.927 37.211 11.357 1.00 32.46
H
ATOM 7241 HG2 MET D 184 -14.002 36.265 12.403 1.00 31.83
H
ATOM 7242 HG3 MET D 184 -13.770 35.441 11.062 1.00 31.83
H
ATOM 7243 HE1 MET D 184 -13.435 39.816 11.496 1.00 37.82
H
ATOM 7244 HE2 MET D 184 -14.811 39.049 11.703 1.00 37.82
H
ATOM 7245 HE3 MET D 184 -13.602 38.795 12.702 1.00 37.82
H
ATOM 7246 N GLN D 185 -16.705 36.837 13.791 1.00 33.99
N
ATOM 7247 CA GLN D 185 -16.777 37.246 15.185 1.00 37.58
C
ATOM 7248 C GLN D 185 -18.202 37.678 15.488 1.00 40.84
C
ATOM 7249 O GLN D 185 -18.821 38.383 14.691 1.00 36.32
O
ATOM 7250 CB GLN D 185 -15.797 38.383 15.470 1.00 40.17
C
ATOM 7251 CG GLN D 185 -15.634 38.706 16.944 1.00 46.92
C
ATOM 7252 CD GLN D 185 -14.883 37.625 17.695 1.00 55.70
C
ATOM 7253 OE1 GLN D 185 -13.773 37.249 17.317 1.00 53.14
O
ATOM 7254 NE2 GLN D 185 -15.487 37.116 18.763 1.00 59.98
N
ATOM 7255 H GLN D 185 -16.894 37.467 13.236 1.00 40.79
H
ATOM 7256 HA GLN D 185 -16.554 36.495 15.756 1.00 45.09
H
ATOM 7257 HB2 GLN D 185 -14.925 38.137 15.124 1.00 48.21
H
ATOM 7258 HB3 GLN D 185 -16.111 39.185 15.025 1.00 48.21
H
ATOM 7259 HG2 GLN D 185 -15.139 39.535 17.034 1.00 56.30
H
ATOM 7260 HG3 GLN D 185 -16.512 38.797 17.347 1.00 56.30
H
ATOM 7261 HE21 GLN D 185 -15.101 36.500 19.222 1.00 71.97
H
ATOM 7262 HE22 GLN D 185 -16.264 37.402 18.995 1.00 71.97
H
ATOM 7263 N LYS D 186 -18.723 37.242 16.631 1.00 46.47
N
ATOM 7264 CA LYS D 186 -20.057 37.639 17.061 1.00 45.40
C
ATOM 7265 C LYS D 186 -20.143 39.158 17.171 1.00 39.69
C
ATOM 7266 O LYS D 186 -19.414 39.777 17.947 1.00 41.64
O
ATOM 7267 CB LYS D 186 -20.405 36.981 18.398 1.00 51.52
C
ATOM 7268 CG LYS D 186 -20.680 35.489 18.289 1.00 65.11
C
ATOM 7269 CD LYS D 186 -19.861 34.683 19.288 1.00 84.25
C
ATOM 7270 CE LYS D 186 -20.168 33.195 19.180 1.00 86.61
C
ATOM 7271 NZ LYS D 186 -18.935 32.360 19.163 1.00 76.57
N1+
ATOM 7272 H LYS D 186 -18.321 36.712 17.176 1.00 55.77
H
ATOM 7273 HA LYS D 186 -20.705 37.346 16.402 1.00 54.47
H

ATOM 974 HE1 HIS A 153 -7.087 20.535 -49.149 1.00 19.27
H
ATOM 975 HE2 HIS A 153 -8.124 22.146 -47.760 1.00 18.09
H
ATOM 976 N TRP A 154 -13.094 21.106 -53.409 1.00 16.17
N
ATOM 977 CA TRP A 154 -14.461 20.939 -53.897 1.00 16.21
C
ATOM 978 C TRP A 154 -15.351 20.404 -52.787 1.00 14.86
C
ATOM 979 O TRP A 154 -14.984 19.458 -52.093 1.00 13.34
O
ATOM 980 CB TRP A 154 -14.523 19.976 -55.092 1.00 15.43
C
ATOM 981 CG TRP A 154 -14.018 20.527 -56.390 1.00 17.31
C
ATOM 982 CD1 TRP A 154 -13.089 19.957 -57.210 1.00 18.38
C
ATOM 983 CD2 TRP A 154 -14.421 21.746 -57.029 1.00 22.30
C
ATOM 984 NE1 TRP A 154 -12.884 20.744 -58.317 1.00 20.02
N
ATOM 985 CE2 TRP A 154 -13.687 21.850 -58.230 1.00 22.60
C
ATOM 986 CE3 TRP A 154 -15.326 22.761 -56.702 1.00 18.30
C
ATOM 987 CZ2 TRP A 154 -13.831 22.927 -59.104 1.00 22.55
C
ATOM 988 CZ3 TRP A 154 -15.464 23.831 -57.568 1.00 19.05
C
ATOM 989 CH2 TRP A 154 -14.723 23.904 -58.757 1.00 23.40
C
ATOM 990 H TRP A 154 -12.504 20.661 -53.848 1.00 19.40
H
ATOM 991 HA TRP A 154 -14.808 21.799 -54.179 1.00 19.45
H
ATOM 992 HB2 TRP A 154 -13.992 19.192 -54.882 1.00 18.52
H
ATOM 993 HB3 TRP A 154 -15.447 19.714 -55.226 1.00 18.52
H
ATOM 994 HD1 TRP A 154 -12.657 19.150 -57.044 1.00 22.06
H
ATOM 995 HE1 TRP A 154 -12.338 20.572 -58.959 1.00 24.02
H
ATOM 996 HE3 TRP A 154 -15.821 22.720 -55.916 1.00 21.96
H
ATOM 997 HZ2 TRP A 154 -13.339 22.979 -59.891 1.00 27.07
H
ATOM 998 HZ3 TRP A 154 -16.064 24.511 -57.361 1.00 22.86
H
ATOM 999 HH2 TRP A 154 -14.838 24.635 -59.321 1.00 28.08
H
ATOM 1000 N MET A 155 -16.514 21.022 -52.612 1.00 17.17
N
ATOM 1001 CA MET A 155 -17.553 20.465 -51.758 1.00 15.84
C
ATOM 1002 C MET A 155 -18.796 20.242 -52.615 1.00 16.30
C
ATOM 1003 O MET A 155 -18.784 20.513 -53.816 1.00 19.47
O
ATOM 1004 CB MET A 155 -17.852 21.382 -50.569 1.00 15.20
C
ATOM 1005 CG MET A 155 -18.223 22.801 -50.940 1.00 12.06
C
ATOM 1006 SD MET A 155 -18.683 23.761 -49.486 1.00 15.98
S
ATOM 1007 CE MET A 155 -18.393 25.415 -50.109 1.00 15.70
C

ATOM 7274 HB2 LYS D 186 -19.662 37.103 19.010 1.00 61.82
H
ATOM 7275 HB3 LYS D 186 -21.200 37.405 18.758 1.00 61.82
H
ATOM 7276 HG2 LYS D 186 -21.619 35.325 18.466 1.00 78.14
H
ATOM 7277 HG3 LYS D 186 -20.450 35.188 17.397 1.00 78.14
H
ATOM 7278 HD2 LYS D 186 -18.917 34.814 19.108 1.00101.10
H
ATOM 7279 HD3 LYS D 186 -20.076 34.975 20.188 1.00101.10
H
ATOM 7280 HE2 LYS D 186 -20.703 32.926 19.943 1.00103.94
H
ATOM 7281 HE3 LYS D 186 -20.654 33.031 18.357 1.00103.94
H
ATOM 7282 HZ1 LYS D 186 -19.151 31.500 19.100 1.00 91.88
H
ATOM 7283 HZ2 LYS D 186 -18.426 32.583 18.467 1.00 91.88
H
ATOM 7284 HZ3 LYS D 186 -18.471 32.488 19.912 1.00 91.88
H
ATOM 7285 N GLY D 187 -21.027 39.755 16.379 1.00 38.31
N
ATOM 7286 CA GLY D 187 -21.164 41.200 16.353 1.00 35.66
C
ATOM 7287 C GLY D 187 -22.311 41.654 15.477 1.00 29.40
C
ATOM 7288 O GLY D 187 -22.977 40.839 14.843 1.00 28.79
O
ATOM 7289 H GLY D 187 -21.560 39.342 15.845 1.00 45.97
H
ATOM 7290 HA2 GLY D 187 -21.318 41.526 17.254 1.00 42.79
H
ATOM 7291 HA3 GLY D 187 -20.345 41.596 16.018 1.00 42.79
H
ATOM 7292 N ASP D 188 -22.528 42.966 15.435 1.00 30.44
N
ATOM 7293 CA ASP D 188 -23.660 43.549 14.722 1.00 29.39
C
ATOM 7294 C ASP D 188 -23.208 44.460 13.580 1.00 29.72
C
ATOM 7295 O ASP D 188 -24.003 45.223 13.031 1.00 31.13
O
ATOM 7296 CB ASP D 188 -24.540 44.327 15.705 1.00 37.77
C
ATOM 7297 CG ASP D 188 -25.117 43.439 16.801 1.00 39.59
C
ATOM 7298 OD1 ASP D 188 -25.551 42.311 16.485 1.00 40.77
O
ATOM 7299 OD2 ASP D 188 -25.127 43.863 17.977 1.00 38.82
O1-
ATOM 7300 H ASP D 188 -22.025 43.548 15.819 1.00 36.53
H
ATOM 7301 HA ASP D 188 -24.195 42.835 14.341 1.00 35.27
H
ATOM 7302 HB2 ASP D 188 -24.007 45.019 16.128 1.00 45.33
H
ATOM 7303 HB3 ASP D 188 -25.280 44.726 15.221 1.00 45.33
H
ATOM 7304 N CYS D 189 -21.928 44.372 13.230 1.00 29.33
N
ATOM 7305 CA CYS D 189 -21.362 45.161 12.140 1.00 27.86
C
ATOM 7306 C CYS D 189 -20.576 44.256 11.195 1.00 25.45
C
ATOM 7307 O CYS D 189 -20.198 43.145 11.568 1.00 23.49
O

ATOM 1008 H MET A 155 -16.726 21.770 -52.980 1.00 20.60 H
ATOM 1009 HA MET A 155 -17.252 19.612 -51.410 1.00 19.01 H
ATOM 1010 HB2 MET A 155 -18.592 21.006 -50.068 1.00 18.23 H
ATOM 1011 HB3 MET A 155 -17.064 21.423 -50.005 1.00 18.23 H
ATOM 1012 HG2 MET A 155 -17.463 23.231 -51.362 1.00 14.47 H
ATOM 1013 HG3 MET A 155 -18.980 22.785 -51.547 1.00 14.47 H
ATOM 1014 HE1 MET A 155 -18.606 26.056 -49.412 1.00 18.84 H
ATOM 1015 HE2 MET A 155 -17.461 25.498 -50.362 1.00 18.84 H
ATOM 1016 HE3 MET A 155 -18.961 25.565 -50.881 1.00 18.84 H
ATOM 1017 N GLY A 156 -19.859 19.739 -52.000 1.00 16.55 N
ATOM 1018 CA GLY A 156 -21.008 19.259 -52.744 1.00 17.95 C
ATOM 1019 C GLY A 156 -22.078 20.285 -53.069 1.00 23.68 C
ATOM 1020 O GLY A 156 -23.217 19.911 -53.339 1.00 23.71 O
ATOM 1021 H GLY A 156 -19.937 19.667 -51.147 1.00 19.86 H
ATOM 1022 HA2 GLY A 156 -20.698 18.882 -53.582 1.00 21.54 H
ATOM 1023 HA3 GLY A 156 -21.428 18.546 -52.237 1.00 21.54 H
ATOM 1024 N LEU A 157 -21.732 21.569 -53.048 1.00 20.60 N
ATOM 1025 CA LEU A 157 -22.694 22.607 -53.407 1.00 26.74 C
ATOM 1026 C LEU A 157 -22.917 22.621 -54.914 1.00 32.20 C
ATOM 1027 O LEU A 157 -21.984 22.421 -55.695 1.00 30.50 O
ATOM 1028 CB LEU A 157 -22.230 23.992 -52.945 1.00 23.22 C
ATOM 1029 CG LEU A 157 -22.516 24.455 -51.512 1.00 27.17 C
ATOM 1030 CD1 LEU A 157 -22.148 25.924 -51.377 1.00 29.03 C
ATOM 1031 CD2 LEU A 157 -23.963 24.244 -51.093 1.00 26.60 C
ATOM 1032 H LEU A 157 -20.953 21.864 -52.831 1.00 24.72 H
ATOM 1033 HA LEU A 157 -23.543 22.415 -52.978 1.00 32.08 H
ATOM 1034 HB2 LEU A 157 -21.268 24.030 -53.059 1.00 27.87 H
ATOM 1035 HB3 LEU A 157 -22.639 24.647 -53.532 1.00 27.87 H
ATOM 1036 HG LEU A 157 -21.954 23.951 -50.903 1.00 32.60 H
ATOM 1037 HD11 LEU A 157 -22.331 26.212 -50.469 1.00 34.83 H
ATOM 1038 HD12 LEU A 157 -21.205 26.033 -51.576 1.00 34.83 H
ATOM 1039 HD13 LEU A 157 -22.681 26.440 -52.002 1.00 34.83 H
ATOM 1040 HD21 LEU A 157 -24.076 24.556 -50.181 1.00 31.92 H
ATOM 1041 HD22 LEU A 157 -24.540 24.747 -51.689 1.00 31.92 H

ATOM 7308 CB CYS D 189 -20.468 46.272 12.692 1.00 28.54 C
ATOM 7309 SG CYS D 189 -21.349 47.483 13.716 1.00 29.86 S
ATOM 7310 H CYS D 189 -21.358 43.854 13.613 1.00 35.19 H
ATOM 7311 HA CYS D 189 -22.082 45.573 11.637 1.00 33.43 H
ATOM 7312 HB2 CYS D 189 -19.773 45.872 13.238 1.00 34.24 H
ATOM 7313 HB3 CYS D 189 -20.067 46.749 11.948 1.00 34.24 H

ATOM 7314 N ALA D 190 -20.337 44.731 9.975 1.00 22.91 N
ATOM 7315 CA ALA D 190 -19.680 43.915 8.960 1.00 22.33 C

ATOM 7316 C ALA D 190 -18.577 44.667 8.221 1.00 20.44 C

ATOM 7317 O ALA D 190 -18.711 45.845 7.890 1.00 20.09 O
ATOM 7318 CB ALA D 190 -20.702 43.395 7.971 1.00 21.39 C

ATOM 7319 H ALA D 190 -20.546 45.522 9.710 1.00 27.50 H
ATOM 7320 HA ALA D 190 -19.273 43.149 9.394 1.00 26.80 H
ATOM 7321 HB1 ALA D 190 -20.250 42.855 7.304 1.00 25.67 H
ATOM 7322 HB2 ALA D 190 -21.355 42.856 8.446 1.00 25.67 H
ATOM 7323 HB3 ALA D 190 -21.141 44.148 7.545 1.00 25.67 H

ATOM 7324 N LEU D 191 -17.484 43.959 7.972 1.00 17.46 N
ATOM 7325 CA LEU D 191 -16.381 44.479 7.183 1.00 17.75 C

ATOM 7326 C LEU D 191 -16.573 44.087 5.727 1.00 15.67 C

ATOM 7327 O LEU D 191 -16.806 42.915 5.429 1.00 16.92 O
ATOM 7328 CB LEU D 191 -15.052 43.935 7.699 1.00 15.85 C
ATOM 7329 CG LEU D 191 -14.674 44.331 9.125 1.00 17.91 C
ATOM 7330 CD1 LEU D 191 -13.616 43.387 9.665 1.00 17.38 C
ATOM 7331 CD2 LEU D 191 -14.181 45.770 9.157 1.00 16.48 C

ATOM 7332 H LEU D 191 -17.356 43.157 8.256 1.00 20.95 H
ATOM 7333 HA LEU D 191 -16.364 45.447 7.244 1.00 21.30 H
ATOM 7334 HB2 LEU D 191 -15.087 42.966 7.668 1.00 19.03 H
ATOM 7335 HB3 LEU D 191 -14.346 44.251 7.115 1.00 19.03 H
ATOM 7336 HG LEU D 191 -15.458 44.265 9.693 1.00 21.50 H
ATOM 7337 HD11 LEU D 191 -13.388 43.652 10.569 1.00 20.86 H
ATOM 7338 HD12 LEU D 191 -13.969 42.483 9.664 1.00 20.86 H
ATOM 7339 HD13 LEU D 191 -12.830 43.436 9.097 1.00 20.86 H
ATOM 7340 HD21 LEU D 191 -13.946 46.003 10.069 1.00 19.78 H
ATOM 7341 HD22 LEU D 191 -13.402 45.850 8.584 1.00 19.78 H

ATOM 1042 HD23 LEU A 157 -24.173 23.299 -51.148 1.00 31.92 H
ATOM 1043 N VAL A 158 -24.164 22.860 -55.306 1.00 35.94 N
ATOM 1044 CA VAL A 158 -24.554 22.891 -56.709 1.00 35.15 C
ATOM 1045 C VAL A 158 -25.361 24.154 -56.983 1.00 41.48 C
ATOM 1046 O VAL A 158 -26.272 24.493 -56.226 1.00 36.73 O
ATOM 1047 CB VAL A 158 -25.393 21.662 -57.097 1.00 38.21 C
ATOM 1048 CG1 VAL A 158 -25.423 21.504 -58.607 1.00 49.98 C
ATOM 1049 CG2 VAL A 158 -24.839 20.401 -56.443 1.00 39.33 C
ATOM 1050 H VAL A 158 -24.816 23.011 -54.765 1.00 43.13 H
ATOM 1051 HA VAL A 158 -23.759 22.908 -57.265 1.00 42.18 H
ATOM 1052 HB VAL A 158 -26.303 21.787 -56.788 1.00 45.85 H
ATOM 1053 HG11 VAL A 158 -25.955 20.725 -58.832 1.00 59.98 H
ATOM 1054 HG12 VAL A 158 -25.816 22.299 -58.999 1.00 59.98 H
ATOM 1055 HG13 VAL A 158 -24.515 21.389 -58.930 1.00 59.98 H
ATOM 1056 HG21 VAL A 158 -25.386 19.644 -56.704 1.00 47.20 H
ATOM 1057 HG22 VAL A 158 -23.925 20.267 -56.739 1.00 47.20 H
ATOM 1058 HG23 VAL A 158 -24.863 20.510 -55.479 1.00 47.20 H
ATOM 1059 N HIS A 159 -25.018 24.849 -58.062 1.00 40.87 N
ATOM 1060 CA HIS A 159 -25.710 26.078 -58.427 1.00 49.33 C
ATOM 1061 C HIS A 159 -26.895 25.782 -59.331 1.00 56.17 C
ATOM 1062 O HIS A 159 -26.738 25.178 -60.390 1.00 50.22 O
ATOM 1063 CB HIS A 159 -24.759 27.046 -59.131 1.00 49.48 C
ATOM 1064 CG HIS A 159 -25.285 28.444 -59.229 1.00 56.01 C
ATOM 1065 ND1 HIS A 159 -24.876 29.324 -60.207 1.00 66.11 N
ATOM 1066 CD2 HIS A 159 -26.184 29.115 -58.470 1.00 57.64 C
ATOM 1067 CE1 HIS A 159 -25.502 30.477 -60.048 1.00 76.90 C
ATOM 1068 NE2 HIS A 159 -26.301 30.377 -59.001 1.00 68.99 N
ATOM 1069 H HIS A 159 -24.386 24.629 -58.601 1.00 49.05 H
ATOM 1070 HA HIS A 159 -26.041 26.509 -57.624 1.00 59.20 H
ATOM 1071 HB2 HIS A 159 -23.924 27.077 -58.639 1.00 59.38 H
ATOM 1072 HB3 HIS A 159 -24.598 26.726 -60.032 1.00 59.38 H
ATOM 1073 HD1 HIS A 159 -24.304 29.150 -60.825 1.00 79.33 H
ATOM 1074 HD2 HIS A 159 -26.637 28.784 -57.729 1.00 69.17 H
ATOM 1075 HE1 HIS A 159 -25.397 31.231 -60.582 1.00 92.28 H
ATOM 7342 HD23 LEU D 191 -14.888 46.353 8.838 1.00 19.78 H
ATOM 7343 N TYR D 192 -16.495 45.052 4.819 1.00 15.37 N
ATOM 7344 CA TYR D 192 -16.479 44.714 3.406 1.00 13.02 C
ATOM 7345 C TYR D 192 -15.140 44.117 3.025 1.00 16.84 C
ATOM 7346 O TYR D 192 -14.100 44.556 3.500 1.00 13.73 O
ATOM 7347 CB TYR D 192 -16.737 45.919 2.500 1.00 14.04 C
ATOM 7348 CG TYR D 192 -16.606 45.490 1.060 1.00 15.73 C
ATOM 7349 CD1 TYR D 192 -17.668 44.878 0.411 1.00 15.86 C
ATOM 7350 CD2 TYR D 192 -15.399 45.615 0.376 1.00 15.68 C
ATOM 7351 CE1 TYR D 192 -17.553 44.440 -0.884 1.00 16.16 C
ATOM 7352 CE2 TYR D 192 -15.272 45.172 -0.928 1.00 16.99 C
ATOM 7353 CZ TYR D 192 -16.358 44.585 -1.552 1.00 18.72 C
ATOM 7354 OH TYR D 192 -16.257 44.134 -2.845 1.00 20.02 O
ATOM 7355 H TYR D 192 -16.451 45.893 4.992 1.00 18.45 H
ATOM 7356 HA TYR D 192 -17.166 44.052 3.231 1.00 15.62 H
ATOM 7357 HB2 TYR D 192 -17.637 46.252 2.645 1.00 16.85 H
ATOM 7358 HB3 TYR D 192 -16.082 46.611 2.680 1.00 16.85 H
ATOM 7359 HD1 TYR D 192 -18.477 44.774 0.858 1.00 19.03 H
ATOM 7360 HD2 TYR D 192 -14.670 46.006 0.800 1.00 18.82 H
ATOM 7361 HE1 TYR D 192 -18.279 44.042 -1.308 1.00 19.40 H
ATOM 7362 HE2 TYR D 192 -14.466 45.270 -1.381 1.00 20.39 H
ATOM 7363 HH TYR D 192 -15.484 44.279 -3.140 1.00 24.03 H
ATOM 7364 N ALA D 193 -15.174 43.130 2.136 1.00 16.16 N
ATOM 7365 CA ALA D 193 -13.962 42.620 1.512 1.00 15.91 C
ATOM 7366 C ALA D 193 -14.293 41.994 0.167 1.00 17.11 C
ATOM 7367 O ALA D 193 -15.458 41.709 -0.137 1.00 14.31 O
ATOM 7368 CB ALA D 193 -13.279 41.614 2.413 1.00 17.57 C
ATOM 7369 H ALA D 193 -15.894 42.736 1.876 1.00 19.39 H
ATOM 7370 HA ALA D 193 -13.349 43.356 1.360 1.00 19.09 H
ATOM 7371 HB1 ALA D 193 -12.476 41.292 1.974 1.00 21.09 H
ATOM 7372 HB2 ALA D 193 -13.047 42.047 3.250 1.00 21.09 H
ATOM 7373 HB3 ALA D 193 -13.885 40.876 2.578 1.00 21.09 H
ATOM 7374 N SER D 194 -13.261 41.795 -0.642 1.00 13.16 N
ATOM 7375 CA SER D 194 -13.424 41.159 -1.940 1.00 19.38 C

ATOM 1076 HE2 HIS A 159 -26.811 31.000 -58.701 1.00 82.79
H
ATOM 1077 N ILE A 160 -28.078 26.209 -58.904 1.00 63.42
N
ATOM 1078 CA ILE A 160 -29.278 26.111 -59.725 1.00 74.82
C
ATOM 1079 C ILE A 160 -29.379 27.349 -60.618 1.00 81.75
C
ATOM 1080 O ILE A 160 -29.585 28.452 -60.113 1.00 78.84
O
ATOM 1081 CB ILE A 160 -30.549 25.992 -58.859 1.00 74.40
C
ATOM 1082 CG1 ILE A 160 -30.450 24.786 -57.917 1.00 65.58
C
ATOM 1083 CG2 ILE A 160 -31.790 25.885 -59.736 1.00 81.67
C
ATOM 1084 CD1 ILE A 160 -30.357 23.442 -58.622 1.00 62.63
C
ATOM 1085 H ILE A 160 -28.213 26.565 -58.132 1.00 76.11
H
ATOM 1086 HA ILE A 160 -29.219 25.326 -60.292 1.00 89.78
H
ATOM 1087 HB ILE A 160 -30.626 26.794 -58.319 1.00 89.28
H
ATOM 1088 HG12 ILE A 160 -29.657 24.886 -57.368 1.00 78.70
H
ATOM 1089 HG13 ILE A 160 -31.238 24.768 -57.352 1.00 78.70
H
ATOM 1090 HG21 ILE A 160 -32.573 25.811 -59.168 1.00 98.00
H
ATOM 1091 HG22 ILE A 160 -31.856 26.680 -60.288 1.00 98.00
H
ATOM 1092 HG23 ILE A 160 -31.713 25.097 -60.297 1.00 98.00
H
ATOM 1093 HD11 ILE A 160 -30.298 22.740 -57.955 1.00 75.15
H
ATOM 1094 HD12 ILE A 160 -31.150 23.316 -59.166 1.00 75.15
H
ATOM 1095 HD13 ILE A 160 -29.565 23.434 -59.182 1.00 75.15
H
ATOM 1096 N PRO A 161 -29.227 27.178 -61.946 1.00 91.79
N
ATOM 1097 CA PRO A 161 -29.299 28.358 -62.819 1.00 98.12
C
ATOM 1098 C PRO A 161 -30.683 29.003 -62.824 1.00100.10
C
ATOM 1099 O PRO A 161 -30.811 30.182 -63.157 1.00100.43
O
ATOM 1100 CB PRO A 161 -28.959 27.797 -64.208 1.00103.41
C
ATOM 1101 CG PRO A 161 -28.314 26.477 -63.957 1.00 98.76
C
ATOM 1102 CD PRO A 161 -28.948 25.953 -62.715 1.00 93.32
C
ATOM 1103 HA PRO A 161 -28.634 29.015 -62.561 1.00117.74
H
ATOM 1104 HB2 PRO A 161 -29.774 27.687 -64.723 1.00124.09
H
ATOM 1105 HB3 PRO A 161 -28.346 28.398 -64.660 1.00124.09
H
ATOM 1106 HG2 PRO A 161 -28.485 25.884 -64.705 1.00118.52
H
ATOM 1107 HG3 PRO A 161 -27.360 26.600 -63.829 1.00118.52
H
ATOM 1108 HD2 PRO A 161 -29.774 25.489 -62.925 1.00111.99
H
ATOM 1109 HD3 PRO A 161 -28.330 25.383 -62.232 1.00111.99
H

ATOM 7376 C SER D 194 -13.783 39.688 -1.736 1.00 15.86 C
ATOM 7377 O SER D 194 -13.257 39.081 -0.811 1.00 17.79
O
ATOM 7378 CB SER D 194 -12.134 41.288 -2.759 1.00 16.87
C
ATOM 7379 OG SER D 194 -12.254 40.631 -4.006 1.00 19.40
O

ATOM 7380 H SER D 194 -12.452 42.020 -0.461 1.00 15.79 H
ATOM 7381 HA SER D 194 -14.144 41.590 -2.427 1.00 23.26
H
ATOM 7382 HB2 SER D 194 -11.953 42.228 -2.914 1.00 20.25
H
ATOM 7383 HB3 SER D 194 -11.404 40.888 -2.261 1.00 20.25
H
ATOM 7384 HG SER D 194 -11.540 40.711 -4.442 1.00 23.28
H

ATOM 7385 N SER D 195 -14.655 39.097 -2.558 1.00 16.08 N
ATOM 7386 CA SER D 195 -15.382 39.753 -3.644 1.00 19.93
C

ATOM 7387 C SER D 195 -16.864 39.846 -3.286 1.00 18.77 C
ATOM 7388 O SER D 195 -17.570 38.835 -3.271 1.00 17.62
O
ATOM 7389 CB SER D 195 -15.212 38.984 -4.953 1.00 17.02
C
ATOM 7390 OG SER D 195 -15.833 39.680 -6.022 1.00 21.30
O

ATOM 7391 H SER D 195 -14.851 38.262 -2.497 1.00 19.30 H
ATOM 7392 HA SER D 195 -15.037 40.652 -3.768 1.00 23.92
H
ATOM 7393 HB2 SER D 195 -14.266 38.888 -5.144 1.00 20.43
H
ATOM 7394 HB3 SER D 195 -15.623 38.110 -4.863 1.00 20.43
H
ATOM 7395 HG SER D 195 -15.736 39.252 -6.738 1.00 25.57
H

ATOM 7396 N PHE D 196 -17.323 41.062 -3.010 1.00 16.50 N
ATOM 7397 CA PHE D 196 -18.681 41.297 -2.521 1.00 18.66
C

ATOM 7398 C PHE D 196 -18.989 40.392 -1.338 1.00 16.83 C
ATOM 7399 O PHE D 196 -19.992 39.680 -1.320 1.00 17.38
O
ATOM 7400 CB PHE D 196 -19.699 41.099 -3.646 1.00 16.78
C
ATOM 7401 CG PHE D 196 -19.660 42.189 -4.674 1.00 18.16
C
ATOM 7402 CD1 PHE D 196 -18.851 42.083 -5.789 1.00 19.31
C
ATOM 7403 CD2 PHE D 196 -20.415 43.336 -4.509 1.00 23.49
C
ATOM 7404 CE1 PHE D 196 -18.805 43.095 -6.725 1.00 21.60
C
ATOM 7405 CE2 PHE D 196 -20.372 44.349 -5.443 1.00 21.99
C
ATOM 7406 CZ PHE D 196 -19.567 44.230 -6.549 1.00 21.26
C

ATOM 7407 H PHE D 196 -16.860 41.782 -3.098 1.00 19.80 H
ATOM 7408 HA PHE D 196 -18.750 42.215 -2.218 1.00 22.39
H
ATOM 7409 HB2 PHE D 196 -19.513 40.259 -4.095 1.00 20.13
H

ATOM 1110 N THR A 162 -31.699 28.227 -62.458 1.00100.32
N
ATOM 1111 CA THR A 162 -33.074 28.712 -62.425 1.00102.58
C
ATOM 1112 C THR A 162 -33.221 29.911 -61.488 1.00 98.89
C
ATOM 1113 O THR A 162 -33.339 31.051 -61.940 1.00100.64
O
ATOM 1114 CB THR A 162 -34.048 27.597 -61.978 1.00103.40
C
ATOM 1115 OG1 THR A 162 -33.897 26.454 -62.828 1.00102.81
O
ATOM 1116 CG2 THR A 162 -35.492 28.078 -62.034 1.00106.25
C
ATOM 1117 H THR A 162 -31.616 27.405 -62.222 1.00120.38
H
ATOM 1118 HA THR A 162 -33.331 28.995 -63.316 1.00123.09
H
ATOM 1119 HB THR A 162 -33.847 27.345 -61.063 1.00124.08
H
ATOM 1120 HG1 THR A 162 -34.066 26.664 -63.624 1.00123.38
H
ATOM 1121 HG21 THR A 162 -36.089 27.368 -61.751 1.00127.50
H
ATOM 1122 HG22 THR A 162 -35.610 28.842 -61.447 1.00127.50
H
ATOM 1123 HG23 THR A 162 -35.719 28.339 -62.940 1.00127.50
H
ATOM 1124 N ASN A 163 -33.204 29.643 -60.185 1.00 94.97
N
ATOM 1125 CA ASN A 163 -33.435 30.674 -59.178 1.00 91.11
C
ATOM 1126 C ASN A 163 -32.140 31.232 -58.589 1.00 85.58
C
ATOM 1127 O ASN A 163 -32.171 32.030 -57.651 1.00 80.37
O
ATOM 1128 CB ASN A 163 -34.319 30.117 -58.057 1.00 85.28
C
ATOM 1129 CG ASN A 163 -33.748 28.858 -57.431 1.00 81.50
C
ATOM 1130 OD1 ASN A 163 -32.899 28.188 -58.018 1.00 80.62
O
ATOM 1131 ND2 ASN A 163 -34.221 28.525 -56.236 1.00 76.73
N
ATOM 1132 H ASN A 163 -33.060 28.862 -59.856 1.00113.96
H
ATOM 1133 HA ASN A 163 -33.912 31.411 -59.591 1.00109.34
H
ATOM 1134 HB2 ASN A 163 -34.404 30.787 -57.360 1.00102.34
H
ATOM 1135 HB3 ASN A 163 -35.192 29.903 -58.420 1.00102.34
H
ATOM 1136 HD21 ASN A 163 -33.930 27.820 -55.839 1.00 92.07
H
ATOM 1137 HD22 ASN A 163 -34.819 29.015 -55.858 1.00 92.07
H
ATOM 1138 N GLY A 164 -31.005 30.815 -59.141 1.00 84.69
N
ATOM 1139 CA GLY A 164 -29.712 31.301 -58.690 1.00 79.34
C
ATOM 1140 C GLY A 164 -29.381 30.898 -57.264 1.00 74.41
C
ATOM 1141 O GLY A 164 -28.510 31.495 -56.630 1.00 68.03
O
ATOM 1142 H GLY A 164 -30.959 30.245 -59.784 1.00101.63
H
ATOM 1143 HA2 GLY A 164 -29.019 30.953 -59.273 1.00 95.20
H
ATOM 7410 HB3 PHE D 196 -20.590 41.080 -3.264 1.00 20.13
H
ATOM 7411 HD1 PHE D 196 -18.334 41.320 -5.911 1.00 23.17
H
ATOM 7412 HD2 PHE D 196 -20.960 43.423 -3.761 1.00 28.18
H
ATOM 7413 HE1 PHE D 196 -18.261 43.011 -7.475 1.00 25.93
H
ATOM 7414 HE2 PHE D 196 -20.888 45.114 -5.323 1.00 26.39
H
ATOM 7415 HZ PHE D 196 -19.540 44.911 -7.181 1.00 25.51
H

ATOM 7416 N LYS D 197 -18.103 40.436 -0.351 1.00 14.08 N
ATOM 7417 CA LYS D 197 -18.266 39.684 0.880 1.00 14.96
C

ATOM 7418 C LYS D 197 -18.416 40.637 2.051 1.00 18.83 C

ATOM 7419 O LYS D 197 -17.959 41.781 2.004 1.00 17.01 O
ATOM 7420 CB LYS D 197 -17.076 38.744 1.114 1.00 17.88
C
ATOM 7421 CG LYS D 197 -17.105 37.490 0.254 1.00 16.95
C
ATOM 7422 CD LYS D 197 -15.837 36.661 0.414 1.00 18.84
C
ATOM 7423 CE LYS D 197 -15.895 35.393 -0.433 1.00 17.58
C
ATOM 7424 NZ LYS D 197 -14.589 34.675 -0.468 1.00 18.73
N1+

ATOM 7425 H LYS D 197 -17.383 40.906 -0.373 1.00 16.90 H
ATOM 7426 HA LYS D 197 -19.071 39.146 0.822 1.00 17.95
H
ATOM 7427 HB2 LYS D 197 -16.256 39.222 0.913 1.00 21.45
H
ATOM 7428 HB3 LYS D 197 -17.075 38.466 2.043 1.00 21.45
H
ATOM 7429 HG2 LYS D 197 -17.860 36.941 0.517 1.00 20.35
H
ATOM 7430 HG3 LYS D 197 -17.184 37.744 -0.678 1.00 20.35
H
ATOM 7431 HD2 LYS D 197 -15.073 37.185 0.128 1.00 22.61
H
ATOM 7432 HD3 LYS D 197 -15.738 36.402 1.344 1.00 22.61
H
ATOM 7433 HE2 LYS D 197 -16.559 34.792 -0.061 1.00 21.10
H
ATOM 7434 HE3 LYS D 197 -16.132 35.630 -1.343 1.00 21.10
H
ATOM 7435 HZ1 LYS D 197 -14.658 33.943 -0.969 1.00 22.47
H
ATOM 7436 HZ2 LYS D 197 -13.961 35.204 -0.812 1.00 22.47
H
ATOM 7437 HZ3 LYS D 197 -14.350 34.440 0.356 1.00 22.47
H

ATOM 7438 N GLY D 198 -19.080 40.155 3.094 1.00 20.04 N
ATOM 7439 CA GLY D 198 -19.195 40.872 4.344 1.00 19.36
C

ATOM 7440 C GLY D 198 -18.810 39.944 5.473 1.00 16.53 C

ATOM 7441 O GLY D 198 -19.383 38.868 5.610 1.00 23.62 O

ATOM 7442 H GLY D 198 -19.482 39.394 3.096 1.00 24.05 H
ATOM 7443 HA2 GLY D 198 -18.603 41.640 4.346 1.00 23.23
H

ATOM 1144 HA3 GLY A 164 -29.698 32.269 -58.744 1.00 95.20
H
ATOM 1145 N SER A 165 -30.073 29.880 -56.761 1.00 71.84
N
ATOM 1146 CA SER A 165 -29.858 29.399 -55.402 1.00 60.50
C
ATOM 1147 C SER A 165 -28.787 28.313 -55.373 1.00 53.12
C
ATOM 1148 O SER A 165 -28.365 27.818 -56.418 1.00 52.63
O
ATOM 1149 CB SER A 165 -31.163 28.861 -54.811 1.00 63.49
C
ATOM 1150 OG SER A 165 -31.594 27.699 -55.498 1.00 66.50
O
ATOM 1151 H SER A 165 -30.679 29.448 -57.192 1.00 86.21
H
ATOM 1152 HA SER A 165 -29.556 30.135 -54.847 1.00 72.59
H
ATOM 1153 HB2 SER A 165 -31.018 28.639 -53.878 1.00 76.19
H
ATOM 1154 HB3 SER A 165 -31.848 29.544 -54.886 1.00 76.19
H
ATOM 1155 HG SER A 165 -31.724 27.876 -56.309 1.00 79.80
H
ATOM 1156 N TRP A 166 -28.355 27.956 -54.167 1.00 44.12
N
ATOM 1157 CA TRP A 166 -27.377 26.893 -53.971 1.00 38.56
C
ATOM 1158 C TRP A 166 -27.987 25.748 -53.173 1.00 36.68
C
ATOM 1159 O TRP A 166 -28.722 25.969 -52.211 1.00 33.26
O
ATOM 1160 CB TRP A 166 -26.135 27.424 -53.250 1.00 32.81
C
ATOM 1161 CG TRP A 166 -25.290 28.347 -54.080 1.00 38.99
C
ATOM 1162 CD1 TRP A 166 -25.364 29.709 -54.125 1.00 41.82
C
ATOM 1163 CD2 TRP A 166 -24.237 27.973 -54.978 1.00 38.51
C
ATOM 1164 NE1 TRP A 166 -24.424 30.207 -54.996 1.00 39.58
N
ATOM 1165 CE2 TRP A 166 -23.720 29.162 -55.533 1.00 36.70
C
ATOM 1166 CE3 TRP A 166 -23.682 26.751 -55.366 1.00 35.41
C
ATOM 1167 CZ2 TRP A 166 -22.678 29.163 -56.458 1.00 35.25
C
ATOM 1168 CZ3 TRP A 166 -22.646 26.753 -56.282 1.00 32.08
C
ATOM 1169 CH2 TRP A 166 -22.154 27.952 -56.817 1.00 33.54
C
ATOM 1170 H TRP A 166 -28.620 28.321 -53.435 1.00 52.94
H
ATOM 1171 HA TRP A 166 -27.102 26.548 -54.835 1.00 46.28
H
ATOM 1172 HB2 TRP A 166 -26.418 27.912 -52.461 1.00 39.37
H
ATOM 1173 HB3 TRP A 166 -25.581 26.672 -52.989 1.00 39.37
H
ATOM 1174 HD1 TRP A 166 -25.964 30.226 -53.637 1.00 50.18
H
ATOM 1175 HE1 TRP A 166 -24.300 31.039 -55.177 1.00 47.49
H
ATOM 1176 HE3 TRP A 166 -24.003 25.951 -55.015 1.00 42.49
H
ATOM 1177 HZ2 TRP A 166 -22.348 29.956 -56.813 1.00 42.30
H

ATOM 7444 HA3 GLY D 198 -20.108 41.172 4.476 1.00 23.23
H
ATOM 7445 N TYR D 199 -17.821 40.349 6.262 1.00 15.37 N
ATOM 7446 CA TYR D 199 -17.404 39.590 7.436 1.00 16.35
C
ATOM 7447 C TYR D 199 -17.961 40.233 8.696 1.00 19.39 C
ATOM 7448 O TYR D 199 -17.670 41.391 8.988 1.00 22.65 O
ATOM 7449 CB TYR D 199 -15.879 39.512 7.523 1.00 21.01
C
ATOM 7450 CG TYR D 199 -15.236 38.665 6.450 1.00 15.07
C
ATOM 7451 CD1 TYR D 199 -15.126 39.129 5.146 1.00 19.90
C
ATOM 7452 CD2 TYR D 199 -14.730 37.408 6.742 1.00 17.60
C
ATOM 7453 CE1 TYR D 199 -14.536 38.361 4.162 1.00 14.62
C
ATOM 7454 CE2 TYR D 199 -14.134 36.631 5.763 1.00 18.84
C
ATOM 7455 CZ TYR D 199 -14.039 37.115 4.476 1.00 15.72
C
ATOM 7456 OH TYR D 199 -13.448 36.351 3.498 1.00 18.51
O
ATOM 7457 H TYR D 199 -17.370 41.070 6.137 1.00 18.44 H
ATOM 7458 HA TYR D 199 -17.753 38.687 7.375 1.00 19.62
H
ATOM 7459 HB2 TYR D 199 -15.517 40.409 7.447 1.00 25.22
H
ATOM 7460 HB3 TYR D 199 -15.636 39.133 8.383 1.00 25.22
H
ATOM 7461 HD1 TYR D 199 -15.459 39.970 4.930 1.00 23.88
H
ATOM 7462 HD2 TYR D 199 -14.792 37.081 7.611 1.00 21.12
H
ATOM 7463 HE1 TYR D 199 -14.470 38.685 3.293 1.00 17.55
H
ATOM 7464 HE2 TYR D 199 -13.799 35.789 5.973 1.00 22.61
H
ATOM 7465 HH TYR D 199 -13.459 36.762 2.766 1.00 22.22
H
ATOM 7466 N ILE D 200 -18.760 39.478 9.443 1.00 24.76 N
ATOM 7467 CA ILE D 200 -19.354 39.983 10.674 1.00 23.61
C
ATOM 7468 C ILE D 200 -18.272 40.156 11.733 1.00 26.05 C
ATOM 7469 O ILE D 200 -17.486 39.242 11.981 1.00 24.51 O
ATOM 7470 CB ILE D 200 -20.449 39.045 11.204 1.00 25.21
C
ATOM 7471 CG1 ILE D 200 -21.472 38.752 10.102 1.00 25.80
C
ATOM 7472 CG2 ILE D 200 -21.132 39.664 12.427 1.00 27.37
C
ATOM 7473 CD1 ILE D 200 -22.495 37.695 10.470 1.00 32.98
C
ATOM 7474 H ILE D 200 -18.974 38.667 9.257 1.00 29.71 H
ATOM 7475 HA ILE D 200 -19.753 40.850 10.504 1.00 28.33
H
ATOM 7476 HB ILE D 200 -20.037 38.209 11.472 1.00 30.25
H
ATOM 7477 HG12 ILE D 200 -21.953 39.569 9.898 1.00 30.95
H

ATOM 1178 HZ3 TRP A 166 -22.270 25.946 -56.548 1.00 38.50
H
ATOM 1179 HH2 TRP A 166 -21.457 27.923 -57.432 1.00 40.24
H
ATOM 1180 N GLN A 167 -27.678 24.524 -53.583 1.00 31.80
N
ATOM 1181 CA GLN A 167 -28.116 23.343 -52.859 1.00 37.87
C
ATOM 1182 C GLN A 167 -27.035 22.268 -52.901 1.00 26.79
C
ATOM 1183 O GLN A 167 -26.107 22.337 -53.706 1.00 25.74
O
ATOM 1184 CB GLN A 167 -29.425 22.807 -53.444 1.00 40.72
C
ATOM 1185 CG GLN A 167 -29.394 22.600 -54.947 1.00 46.08
C
ATOM 1186 CD GLN A 167 -30.494 21.674 -55.428 1.00 45.10
C
ATOM 1187 OE1 GLN A 167 -30.226 20.635 -56.033 1.00 47.82
O
ATOM 1188 NE2 GLN A 167 -31.737 22.046 -55.162 1.00 41.89
N
ATOM 1189 H GLN A 167 -27.212 24.352 -54.285 1.00 38.17
H
ATOM 1190 HA GLN A 167 -28.273 23.578 -51.932 1.00 45.44
H
ATOM 1191 HB2 GLN A 167 -29.623 21.952 -53.032 1.00 48.87
H
ATOM 1192 HB3 GLN A 167 -30.135 23.438 -53.248 1.00 48.87
H
ATOM 1193 HG2 GLN A 167 -29.507 23.457 -55.387 1.00 55.29
H
ATOM 1194 HG3 GLN A 167 -28.541 22.209 -55.195 1.00 55.29
H
ATOM 1195 HE21 GLN A 167 -32.397 21.555 -55.414 1.00 50.26
H
ATOM 1196 HE22 GLN A 167 -31.885 22.779 -54.737 1.00 50.26
H
ATOM 1197 N TRP A 168 -27.159 21.284 -52.019 1.00 29.00
N
ATOM 1198 CA TRP A 168 -26.234 20.160 -51.988 1.00 25.20
C
ATOM 1199 C TRP A 168 -26.642 19.126 -53.024 1.00 33.37
C
ATOM 1200 O TRP A 168 -27.778 19.137 -53.500 1.00 26.70
O
ATOM 1201 CB TRP A 168 -26.194 19.554 -50.590 1.00 25.54
C
ATOM 1202 CG TRP A 168 -25.774 20.563 -49.587 1.00 26.46
C
ATOM 1203 CD1 TRP A 168 -26.564 21.196 -48.677 1.00 29.23
C
ATOM 1204 CD2 TRP A 168 -24.458 21.094 -49.417 1.00 24.51
C
ATOM 1205 NE1 TRP A 168 -25.818 22.082 -47.938 1.00 25.79
N
ATOM 1206 CE2 TRP A 168 -24.520 22.038 -48.376 1.00 20.96
C
ATOM 1207 CE3 TRP A 168 -23.231 20.858 -50.044 1.00 20.74
C
ATOM 1208 CZ2 TRP A 168 -23.402 22.746 -47.944 1.00 18.61
C
ATOM 1209 CZ3 TRP A 168 -22.122 21.558 -49.613 1.00 18.82
C
ATOM 1210 CH2 TRP A 168 -22.215 22.493 -48.573 1.00 19.65
C
ATOM 1211 H TRP A 168 -27.777 21.244 -51.423 1.00 34.80
H
ATOM 7478 HG13 ILE D 200 -21.000 38.443 9.313 1.00 30.95
H
ATOM 7479 HG21 ILE D 200 -21.818 39.058 12.745 1.00 32.84
H
ATOM 7480 HG22 ILE D 200 -20.468 39.807 13.119 1.00 32.84
H
ATOM 7481 HG23 ILE D 200 -21.530 40.511 12.170 1.00 32.84
H
ATOM 7482 HD11 ILE D 200 -23.102 37.570 9.724 1.00 39.58
H
ATOM 7483 HD12 ILE D 200 -22.034 36.864 10.665 1.00 39.58
H
ATOM 7484 HD13 ILE D 200 -22.988 37.992 11.251 1.00 39.58
H
ATOM 7485 N GLU D 201 -18.251 41.329 12.359 1.00 25.97
N
ATOM 7486 CA GLU D 201 -17.193 41.698 13.295 1.00 27.39
C
ATOM 7487 C GLU D 201 -17.754 42.496 14.470 1.00 26.93
C
ATOM 7488 O GLU D 201 -18.775 43.171 14.345 1.00 25.15
O
ATOM 7489 CB GLU D 201 -16.114 42.507 12.562 1.00 22.39
C
ATOM 7490 CG GLU D 201 -15.018 43.107 13.435 1.00 30.66
C
ATOM 7491 CD GLU D 201 -14.139 42.058 14.079 1.00 34.67
C
ATOM 7492 OE1 GLU D 201 -12.954 41.963 13.696 1.00 37.53
O
ATOM 7493 OE2 GLU D 201 -14.628 41.333 14.970 1.00 42.28
O1-
ATOM 7494 H GLU D 201 -18.849 41.939 12.256 1.00 31.16
H
ATOM 7495 HA GLU D 201 -16.782 40.892 13.645 1.00 32.87
H
ATOM 7496 HB2 GLU D 201 -15.683 41.926 11.916 1.00 26.87
H
ATOM 7497 HB3 GLU D 201 -16.546 43.241 12.097 1.00 26.87
H
ATOM 7498 HG2 GLU D 201 -14.454 43.675 12.887 1.00 36.80
H
ATOM 7499 HG3 GLU D 201 -15.428 43.629 14.142 1.00 36.80
H
ATOM 7500 N ASN D 202 -17.082 42.406 15.611 1.00 31.13
N
ATOM 7501 CA ASN D 202 -17.415 43.226 16.767 1.00 31.58
C
ATOM 7502 C ASN D 202 -17.351 44.709 16.409 1.00 28.02
C
ATOM 7503 O ASN D 202 -16.326 45.199 15.934 1.00 27.55
O
ATOM 7504 CB ASN D 202 -16.463 42.920 17.926 1.00 33.82
C
ATOM 7505 CG ASN D 202 -16.877 43.595 19.223 1.00 40.88
C
ATOM 7506 OD1 ASN D 202 -17.685 44.526 19.228 1.00 37.61
O
ATOM 7507 ND2 ASN D 202 -16.317 43.129 20.332 1.00 46.74
N
ATOM 7508 H ASN D 202 -16.421 41.870 15.742 1.00 37.35
H
ATOM 7509 HA ASN D 202 -18.318 43.022 17.055 1.00 37.89
H
ATOM 7510 HB2 ASN D 202 -16.449 41.962 18.078 1.00 40.59
H
ATOM 7511 HB3 ASN D 202 -15.574 43.232 17.695 1.00 40.59
H

ATOM 1212 HA TRP A 168 -25.343 20.474 -52.207 1.00 30.24
H
ATOM 1213 HB2 TRP A 168 -27.078 19.235 -50.351 1.00 30.65
H
ATOM 1214 HB3 TRP A 168 -25.556 18.823 -50.573 1.00 30.65
H
ATOM 1215 HD1 TRP A 168 -27.476 21.048 -48.569 1.00 35.07
H
ATOM 1216 HE1 TRP A 168 -26.116 22.582 -47.306 1.00 30.95
H
ATOM 1217 HE3 TRP A 168 -23.162 20.241 -50.736 1.00 24.89
H
ATOM 1218 HZ2 TRP A 168 -23.459 23.364 -47.251 1.00 22.33
H
ATOM 1219 HZ3 TRP A 168 -21.300 21.410 -50.023 1.00 22.59
H
ATOM 1220 HH2 TRP A 168 -21.451 22.949 -48.303 1.00 23.58
H
ATOM 1221 N GLU A 169 -25.718 18.238 -53.379 1.00 30.13
N
ATOM 1222 CA GLU A 169 -25.959 17.297 -54.468 1.00 31.20
C
ATOM 1223 C GLU A 169 -27.056 16.293 -54.122 1.00 30.15
C
ATOM 1224 O GLU A 169 -27.646 15.685 -55.013 1.00 35.52
O
ATOM 1225 CB GLU A 169 -24.668 16.564 -54.842 1.00 34.22
C
ATOM 1226 CG GLU A 169 -24.055 15.756 -53.726 1.00 30.07
C
ATOM 1227 CD GLU A 169 -22.585 15.446 -53.980 1.00 32.91
C
ATOM 1228 OE1 GLU A 169 -22.224 15.153 -55.140 1.00 30.13
O
ATOM 1229 OE2 GLU A 169 -21.789 15.504 -53.021 1.00 27.40
O1-
ATOM 1230 H GLU A 169 -24.947 18.160 -53.007 1.00 36.15
H
ATOM 1231 HA GLU A 169 -26.252 17.794 -55.248 1.00 37.44
H
ATOM 1232 HB2 GLU A 169 -24.858 15.957 -55.574 1.00 41.07
H
ATOM 1233 HB3 GLU A 169 -24.011 17.219 -55.125 1.00 41.07
H
ATOM 1234 HG2 GLU A 169 -24.119 16.257 -52.898 1.00 36.08
H
ATOM 1235 HG3 GLU A 169 -24.531 14.914 -53.644 1.00 36.08
H
ATOM 1236 N ASP A 170 -27.342 16.132 -52.834 1.00 31.34
N
ATOM 1237 CA ASP A 170 -28.442 15.270 -52.412 1.00 30.16
C
ATOM 1238 C ASP A 170 -29.781 15.998 -52.539 1.00 31.43
C
ATOM 1239 O ASP A 170 -30.818 15.485 -52.124 1.00 29.59
O
ATOM 1240 CB ASP A 170 -28.229 14.785 -50.974 1.00 32.21
C
ATOM 1241 CG ASP A 170 -28.404 15.887 -49.939 1.00 31.98
C
ATOM 1242 OD1 ASP A 170 -28.531 17.071 -50.314 1.00 33.58
O
ATOM 1243 OD2 ASP A 170 -28.398 15.562 -48.733 1.00 27.25
O1-
ATOM 1244 H ASP A 170 -26.918 16.508 -52.187 1.00 37.61
H
ATOM 1245 HA ASP A 170 -28.470 14.491 -52.989 1.00 36.19
H

ATOM 7512 HD21 ASN D 202 -16.516 43.476 21.094 1.00 56.09
H
ATOM 7513 HD22 ASN D 202 -15.754 42.479 20.290 1.00 56.09
H
ATOM 7514 N CYS D 203 -18.448 45.418 16.648 1.00 31.67
N
ATOM 7515 CA CYS D 203 -18.552 46.823 16.270 1.00 32.67
C
ATOM 7516 C CYS D 203 -17.468 47.680 16.919 1.00 30.69
C
ATOM 7517 O CYS D 203 -17.086 48.716 16.382 1.00 28.93
O
ATOM 7518 CB CYS D 203 -19.932 47.370 16.639 1.00 28.67
C
ATOM 7519 SG CYS D 203 -21.284 46.744 15.612 1.00 35.00
S
ATOM 7520 H CYS D 203 -19.152 45.107 17.032 1.00 38.00
H
ATOM 7521 HA CYS D 203 -18.451 46.896 15.308 1.00 39.21
H
ATOM 7522 HB2 CYS D 203 -20.125 47.130 17.559 1.00 34.41
H
ATOM 7523 HB3 CYS D 203 -19.917 48.336 16.550 1.00 34.41
H
ATOM 7524 N SER D 204 -16.966 47.234 18.066 1.00 29.38
N
ATOM 7525 CA SER D 204 -16.014 48.019 18.843 1.00 30.77
C
ATOM 7526 C SER D 204 -14.590 47.917 18.316 1.00 28.07
C
ATOM 7527 O SER D 204 -13.735 48.720 18.680 1.00 28.24
O
ATOM 7528 CB SER D 204 -16.041 47.577 20.308 1.00 33.15
C
ATOM 7529 OG SER D 204 -17.311 47.822 20.885 1.00 37.66
O
ATOM 7530 H SER D 204 -17.163 46.474 18.418 1.00 35.26
H
ATOM 7531 HA SER D 204 -16.277 48.952 18.809 1.00 36.93
H
ATOM 7532 HB2 SER D 204 -15.851 46.627 20.355 1.00 39.78
H
ATOM 7533 HB3 SER D 204 -15.370 48.075 20.800 1.00 39.78
H
ATOM 7534 HG SER D 204 -17.314 47.576 21.688 1.00 45.19
H
ATOM 7535 N THR D 205 -14.331 46.924 17.472 1.00 31.36
N
ATOM 7536 CA THR D 205 -12.979 46.684 16.975 1.00 30.91
C
ATOM 7537 C THR D 205 -12.561 47.749 15.956 1.00 29.01
C
ATOM 7538 O THR D 205 -13.268 47.974 14.975 1.00 28.55
O
ATOM 7539 CB THR D 205 -12.869 45.296 16.324 1.00 34.84
C
ATOM 7540 OG1 THR D 205 -13.239 44.290 17.277 1.00 35.51
O
ATOM 7541 CG2 THR D 205 -11.447 45.032 15.835 1.00 30.24
C
ATOM 7542 H THR D 205 -14.920 46.375 17.171 1.00 37.63
H
ATOM 7543 HA THR D 205 -12.357 46.719 17.719 1.00 37.09
H
ATOM 7544 HB THR D 205 -13.467 45.251 15.562 1.00 41.81
H
ATOM 7545 HG1 THR D 205 -13.181 43.529 16.928 1.00 42.61
H

ATOM 1246 HB2 ASP A 170 -28.874 14.087 -50.779 1.00 38.65
H
ATOM 1247 HB3 ASP A 170 -27.328 14.435 -50.890 1.00 38.65
H
ATOM 1248 N GLY A 171 -29.741 17.204 -53.098 1.00 35.35
N
ATOM 1249 CA GLY A 171 -30.939 17.987 -53.336 1.00 37.34
C
ATOM 1250 C GLY A 171 -31.329 18.850 -52.152 1.00 34.83
C
ATOM 1251 O GLY A 171 -32.126 19.779 -52.294 1.00 36.63
O
ATOM 1252 H GLY A 171 -29.017 17.594 -53.351 1.00 42.42
H
ATOM 1253 HA2 GLY A 171 -30.798 18.565 -54.102 1.00 44.81
H
ATOM 1254 HA3 GLY A 171 -31.678 17.390 -53.535 1.00 44.81
H
ATOM 1255 N SER A 172 -30.760 18.555 -50.987 1.00 33.06
N
ATOM 1256 CA SER A 172 -31.137 19.238 -49.752 1.00 34.83
C
ATOM 1257 C SER A 172 -30.789 20.720 -49.789 1.00 39.00
C
ATOM 1258 O SER A 172 -30.003 21.170 -50.623 1.00 36.04
O
ATOM 1259 CB SER A 172 -30.454 18.589 -48.551 1.00 37.68
C
ATOM 1260 OG SER A 172 -29.067 18.869 -48.560 1.00 31.69
O
ATOM 1261 H SER A 172 -30.149 17.959 -50.883 1.00 39.68
H
ATOM 1262 HA SER A 172 -32.096 19.160 -49.630 1.00 41.80
H
ATOM 1263 HB2 SER A 172 -30.844 18.943 -47.736 1.00 45.22
H
ATOM 1264 HB3 SER A 172 -30.584 17.629 -48.593 1.00 45.22
H
ATOM 1265 HG SER A 172 -28.718 18.569 -49.263 1.00 38.03
H
ATOM 1266 N ILE A 173 -31.374 21.467 -48.859 1.00 40.76
N
ATOM 1267 CA ILE A 173 -31.214 22.915 -48.809 1.00 44.21
C
ATOM 1268 C ILE A 173 -29.943 23.328 -48.070 1.00 35.14
C
ATOM 1269 O ILE A 173 -29.563 22.716 -47.069 1.00 35.11
O
ATOM 1270 CB ILE A 173 -32.431 23.587 -48.128 1.00 50.72
C
ATOM 1271 CG1 ILE A 173 -32.642 23.026 -46.711 1.00 49.11
C
ATOM 1272 CG2 ILE A 173 -33.678 23.388 -48.982 1.00 62.02
C
ATOM 1273 CD1 ILE A 173 -33.764 23.689 -45.932 1.00 53.43
C
ATOM 1274 H ILE A 173 -31.876 21.153 -48.236 1.00 48.91
H
ATOM 1275 HA ILE A 173 -31.154 23.254 -49.716 1.00 53.05
H
ATOM 1276 HB ILE A 173 -32.256 24.538 -48.058 1.00 60.86
H
ATOM 1277 HG12 ILE A 173 -32.849 22.081 -46.779 1.00 58.93
H
ATOM 1278 HG13 ILE A 173 -31.822 23.145 -46.205 1.00 58.93
H
ATOM 1279 HG21 ILE A 173 -34.431 23.814 -48.543 1.00 74.42
H

ATOM 7546 HG21 THR D 205 -11.394 44.154 15.428 1.00 36.29
H
ATOM 7547 HG22 THR D 205 -11.193 45.700 15.179 1.00 36.29
H
ATOM 7548 HG23 THR D 205 -10.827 45.072 16.580 1.00 36.29
H
ATOM 7549 N PRO D 206 -11.413 48.410 16.184 1.00 24.70
N
ATOM 7550 CA PRO D 206 -10.936 49.381 15.192 1.00 29.16
C
ATOM 7551 C PRO D 206 -10.597 48.762 13.834 1.00 29.75
C
ATOM 7552 O PRO D 206 -9.898 47.749 13.760 1.00 25.31
O
ATOM 7553 CB PRO D 206 -9.674 49.960 15.845 1.00 31.51
C
ATOM 7554 CG PRO D 206 -9.855 49.738 17.291 1.00 28.53
C
ATOM 7555 CD PRO D 206 -10.598 48.444 17.410 1.00 34.12
C
ATOM 7556 HA PRO D 206 -11.589 50.088 15.070 1.00 34.99
H
ATOM 7557 HB2 PRO D 206 -8.892 49.488 15.520 1.00 37.81
H
ATOM 7558 HB3 PRO D 206 -9.610 50.908 15.648 1.00 37.81
H
ATOM 7559 HG2 PRO D 206 -8.988 49.676 17.721 1.00 34.23
H
ATOM 7560 HG3 PRO D 206 -10.372 50.466 17.669 1.00 34.23
H
ATOM 7561 HD2 PRO D 206 -9.978 47.698 17.426 1.00 40.94
H
ATOM 7562 HD3 PRO D 206 -11.167 48.452 18.195 1.00 40.94
H
ATOM 7563 N ASN D 207 -11.101 49.384 12.772 1.00 27.98
N
ATOM 7564 CA ASN D 207 -10.802 48.982 11.404 1.00 25.19
C
ATOM 7565 C ASN D 207 -10.805 50.193 10.486 1.00 22.66
C
ATOM 7566 O ASN D 207 -11.386 51.228 10.813 1.00 22.52
O
ATOM 7567 CB ASN D 207 -11.816 47.951 10.899 1.00 21.57
C
ATOM 7568 CG ASN D 207 -11.586 46.572 11.476 1.00 23.31
C
ATOM 7569 OD1 ASN D 207 -12.271 46.152 12.410 1.00 30.03
O
ATOM 7570 ND2 ASN D 207 -10.620 45.858 10.922 1.00 21.76
N
ATOM 7571 H ASN D 207 -11.631 50.060 12.822 1.00 33.58
H
ATOM 7572 HA ASN D 207 -9.919 48.579 11.374 1.00 30.23
H
ATOM 7573 HB2 ASN D 207 -12.708 48.237 11.150 1.00 25.88
H
ATOM 7574 HB3 ASN D 207 -11.748 47.888 9.933 1.00 25.88
H
ATOM 7575 HD21 ASN D 207 -10.448 45.067 11.213 1.00 26.11
H
ATOM 7576 HD22 ASN D 207 -10.163 46.185 10.270 1.00 26.11
H

ATOM 7577 N THR D 208 -10.153 50.066 9.337 1.00 21.73 N
ATOM 7578 CA THR D 208 -10.243 51.086 8.302 1.00 17.49
C

ATOM 7579 C THR D 208 -11.686 51.128 7.807 1.00 18.74 C

ATOM 1280 HG22 ILE A 173 -33.532 23.790 -49.852 1.00 74.42 H
ATOM 1281 HG23 ILE A 173 -33.845 22.438 -49.079 1.00 74.42 H
ATOM 1282 HD11 ILE A 173 -33.826 23.276 -45.056 1.00 64.11 H
ATOM 1283 HD12 ILE A 173 -33.568 24.634 -45.840 1.00 64.11 H
ATOM 1284 HD13 ILE A 173 -34.596 23.568 -46.415 1.00 64.11 H
ATOM 1285 N LEU A 174 -29.284 24.363 -48.579 1.00 36.19 N
ATOM 1286 CA LEU A 174 -28.194 25.002 -47.854 1.00 33.01 C
ATOM 1287 C LEU A 174 -28.785 25.874 -46.762 1.00 25.23 C
ATOM 1288 O LEU A 174 -29.378 26.910 -47.051 1.00 35.07 O
ATOM 1289 CB LEU A 174 -27.317 25.839 -48.788 1.00 28.79 C
ATOM 1290 CG LEU A 174 -26.268 26.722 -48.096 1.00 30.47 C
ATOM 1291 CD1 LEU A 174 -25.235 25.873 -47.369 1.00 28.59 C
ATOM 1292 CD2 LEU A 174 -25.593 27.650 -49.086 1.00 23.68 C
ATOM 1293 H LEU A 174 -29.449 24.715 -49.346 1.00 43.42 H
ATOM 1294 HA LEU A 174 -27.640 24.322 -47.438 1.00 39.62 H
ATOM 1295 HB2 LEU A 174 -26.843 25.238 -49.385 1.00 34.54 H
ATOM 1296 HB3 LEU A 174 -27.892 26.422 -49.307 1.00 34.54 H
ATOM 1297 HG LEU A 174 -26.715 27.273 -47.434 1.00 36.57 H
ATOM 1298 HD11 LEU A 174 -24.589 26.458 -46.944 1.00 34.31 H
ATOM 1299 HD12 LEU A 174 -25.685 25.334 -46.699 1.00 34.31 H
ATOM 1300 HD13 LEU A 174 -24.790 25.299 -48.012 1.00 34.31 H
ATOM 1301 HD21 LEU A 174 -24.939 28.191 -48.616 1.00 28.42 H
ATOM 1302 HD22 LEU A 174 -25.154 27.119 -49.768 1.00 28.42 H
ATOM 1303 HD23 LEU A 174 -26.265 28.221 -49.492 1.00 28.42 H
ATOM 1304 N SER A 175 -28.630 25.450 -45.513 1.00 30.51 N
ATOM 1305 CA SER A 175 -29.152 26.205 -44.382 1.00 30.76 C
ATOM 1306 C SER A 175 -28.581 27.619 -44.380 1.00 30.60 C
ATOM 1307 O SER A 175 -27.416 27.820 -44.727 1.00 29.98 O
ATOM 1308 CB SER A 175 -28.819 25.511 -43.063 1.00 29.16 C
ATOM 1309 OG SER A 175 -29.013 24.111 -43.155 1.00 41.38 O
ATOM 1310 H SER A 175 -28.224 24.724 -45.293 1.00 36.61 H
ATOM 1311 HA SER A 175 -30.117 26.267 -44.458 1.00 36.91 H
ATOM 1312 HB2 SER A 175 -27.891 25.686 -42.842 1.00 35.00 H
ATOM 1313 HB3 SER A 175 -29.396 25.863 -42.368 1.00 35.00 H
ATOM 7580 O THR D 208 -12.457 50.211 8.075 1.00 15.97 O
ATOM 7581 CB THR D 208 -9.287 50.797 7.138 1.00 18.70 C
ATOM 7582 OG1 THR D 208 -9.593 49.516 6.576 1.00 17.72 O
ATOM 7583 CG2 THR D 208 -7.842 50.802 7.622 1.00 23.48 C
ATOM 7584 H THR D 208 -9.652 49.398 9.132 1.00 26.07 H
ATOM 7585 HA THR D 208 -10.019 51.952 8.678 1.00 20.99 H
ATOM 7586 HB THR D 208 -9.386 51.482 6.458 1.00 22.43 H
ATOM 7587 HG1 THR D 208 -9.072 49.351 5.937 1.00 21.26 H
ATOM 7588 HG21 THR D 208 -7.244 50.618 6.881 1.00 28.17 H
ATOM 7589 HG22 THR D 208 -7.622 51.668 7.999 1.00 28.17 H
ATOM 7590 HG23 THR D 208 -7.719 50.121 8.303 1.00 28.17 H
ATOM 7591 N TYR D 209 -12.065 52.188 7.099 1.00 18.19 N
ATOM 7592 CA TYR D 209 -13.438 52.291 6.614 1.00 18.43 C
ATOM 7593 C TYR D 209 -13.528 53.013 5.280 1.00 18.76 C
ATOM 7594 O TYR D 209 -12.606 53.722 4.865 1.00 18.98 O
ATOM 7595 CB TYR D 209 -14.322 52.995 7.651 1.00 18.49 C
ATOM 7596 CG TYR D 209 -13.825 54.355 8.083 1.00 19.96 C
ATOM 7597 CD1 TYR D 209 -12.821 54.477 9.032 1.00 23.84 C
ATOM 7598 CD2 TYR D 209 -14.367 55.516 7.550 1.00 21.18 C
ATOM 7599 CE1 TYR D 209 -12.364 55.717 9.433 1.00 23.52 C
ATOM 7600 CE2 TYR D 209 -13.918 56.763 7.947 1.00 23.67 C
ATOM 7601 CZ TYR D 209 -12.914 56.856 8.887 1.00 25.34 C
ATOM 7602 OH TYR D 209 -12.459 58.091 9.288 1.00 25.68 O
ATOM 7603 H TYR D 209 -11.557 52.849 6.888 1.00 21.83 H
ATOM 7604 HA TYR D 209 -13.789 51.396 6.487 1.00 22.12 H
ATOM 7605 HB2 TYR D 209 -15.209 53.112 7.275 1.00 22.19 H
ATOM 7606 HB3 TYR D 209 -14.375 52.437 8.443 1.00 22.19 H
ATOM 7607 HD1 TYR D 209 -12.446 53.711 9.401 1.00 28.60 H
ATOM 7608 HD2 TYR D 209 -15.043 55.455 6.914 1.00 25.42 H
ATOM 7609 HE1 TYR D 209 -11.688 55.783 10.068 1.00 28.22 H
ATOM 7610 HE2 TYR D 209 -14.288 57.533 7.579 1.00 28.40 H
ATOM 7611 HH TYR D 209 -11.853 58.001 9.862 1.00 30.82 H
ATOM 7612 N ILE D 210 -14.657 52.805 4.615 1.00 17.13 N
ATOM 7613 CA ILE D 210 -14.930 53.405 3.322 1.00 15.89 C

ATOM 1314 HG SER A 175 -28.825 23.746 -42.422 1.00 49.66
H
ATOM 1315 N PRO A 176 -29.399 28.608 -43.989 1.00 27.59
N
ATOM 1316 CA PRO A 176 -28.904 29.986 -43.961 1.00 27.04
C
ATOM 1317 C PRO A 176 -27.802 30.194 -42.923 1.00 27.52
C
ATOM 1318 O PRO A 176 -27.783 29.514 -41.898 1.00 28.41
O
ATOM 1319 CB PRO A 176 -30.154 30.800 -43.603 1.00 27.57
C
ATOM 1320 CG PRO A 176 -31.030 29.849 -42.883 1.00 31.89
C
ATOM 1321 CD PRO A 176 -30.791 28.510 -43.515 1.00 24.67
C
ATOM 1322 HA PRO A 176 -28.583 30.252 -44.837 1.00 32.45
H
ATOM 1323 HB2 PRO A 176 -29.908 31.544 -43.030 1.00 33.08
H
ATOM 1324 HB3 PRO A 176 -30.583 31.117 -44.414 1.00 33.08
H
ATOM 1325 HG2 PRO A 176 -30.787 29.831 -41.944 1.00 38.27
H
ATOM 1326 HG3 PRO A 176 -31.957 30.116 -42.990 1.00 38.27
H
ATOM 1327 HD2 PRO A 176 -30.876 27.804 -42.856 1.00 29.60
H
ATOM 1328 HD3 PRO A 176 -31.394 28.376 -44.262 1.00 29.60
H
ATOM 1329 N ASN A 177 -26.890 31.117 -43.213 1.00 26.69
N
ATOM 1330 CA ASN A 177 -25.849 31.524 -42.273 1.00 28.90
C
ATOM 1331 C ASN A 177 -24.926 30.384 -41.861 1.00 30.53
C
ATOM 1332 O ASN A 177 -24.475 30.324 -40.719 1.00 37.62
O
ATOM 1333 CB ASN A 177 -26.488 32.149 -41.034 1.00 32.10
C
ATOM 1334 CG ASN A 177 -27.336 33.353 -41.374 1.00 27.74
C
ATOM 1335 OD1 ASN A 177 -26.880 34.275 -42.050 1.00 29.89
O
ATOM 1336 ND2 ASN A 177 -28.585 33.345 -40.927 1.00 27.40
N
ATOM 1337 H ASN A 177 -26.853 31.532 -43.965 1.00 32.03
H
ATOM 1338 HA ASN A 177 -25.302 32.204 -42.696 1.00 34.68
H
ATOM 1339 HB2 ASN A 177 -27.057 31.492 -40.604 1.00 38.52
H
ATOM 1340 HB3 ASN A 177 -25.789 32.435 -40.426 1.00 38.52
H
ATOM 1341 HD21 ASN A 177 -29.106 34.008 -41.095 1.00 32.88
H
ATOM 1342 HD22 ASN A 177 -28.873 32.676 -40.469 1.00 32.88
H
ATOM 1343 N LEU A 178 -24.646 29.488 -42.802 1.00 23.55
N
ATOM 1344 CA LEU A 178 -23.682 28.417 -42.587 1.00 26.07
C
ATOM 1345 C LEU A 178 -22.392 28.718 -43.335 1.00 25.37
C
ATOM 1346 O LEU A 178 -21.299 28.646 -42.771 1.00 26.43
O
ATOM 1347 CB LEU A 178 -24.243 27.071 -43.052 1.00 27.18
C

ATOM 7614 C ILE D 210 -16.147 54.297 3.433 1.00 16.38 C

ATOM 7615 O ILE D 210 -17.221 53.836 3.825 1.00 16.32 O

ATOM 7616 CB ILE D 210 -15.183 52.337 2.244 1.00 15.95 C
ATOM 7617 CG1 ILE D 210 -13.990 51.379 2.155 1.00 22.22
C
ATOM 7618 CG2 ILE D 210 -15.457 52.997 0.902 1.00 16.76
C
ATOM 7619 CD1 ILE D 210 -14.247 50.150 1.290 1.00 22.46
C

ATOM 7620 H ILE D 210 -15.296 52.307 4.902 1.00 20.56 H

ATOM 7621 HA ILE D 210 -14.173 53.947 3.049 1.00 19.06 H

ATOM 7622 HB ILE D 210 -15.967 51.826 2.498 1.00 19.13 H
ATOM 7623 HG12 ILE D 210 -13.235 51.856 1.775 1.00 26.67
H
ATOM 7624 HG13 ILE D 210 -13.769 51.072 3.048 1.00 26.67
H
ATOM 7625 HG21 ILE D 210 -15.614 52.308 0.238 1.00 20.12
H
ATOM 7626 HG22 ILE D 210 -16.240 53.563 0.983 1.00 20.12
H
ATOM 7627 HG23 ILE D 210 -14.687 53.531 0.650 1.00 20.12
H
ATOM 7628 HD11 ILE D 210 -13.451 49.596 1.284 1.00 26.95
H
ATOM 7629 HD12 ILE D 210 -14.993 49.653 1.662 1.00 26.95
H
ATOM 7630 HD13 ILE D 210 -14.458 50.438 0.388 1.00 26.95
H

ATOM 7631 N CYS D 211 -15.976 55.568 3.085 1.00 14.23 N
ATOM 7632 CA CYS D 211 -17.094 56.494 3.006 1.00 16.85
C

ATOM 7633 C CYS D 211 -17.596 56.584 1.574 1.00 18.03 C
ATOM 7634 O CYS D 211 -16.827 56.422 0.622 1.00 15.29
O
ATOM 7635 CB CYS D 211 -16.693 57.878 3.515 1.00 21.08
C
ATOM 7636 SG CYS D 211 -16.320 57.907 5.274 1.00 27.03
S

ATOM 7637 H CYS D 211 -15.216 55.919 2.888 1.00 17.07 H
ATOM 7638 HA CYS D 211 -17.819 56.166 3.561 1.00 20.22
H
ATOM 7639 HB2 CYS D 211 -15.901 58.171 3.037 1.00 25.30
H
ATOM 7640 HB3 CYS D 211 -17.423 58.496 3.354 1.00 25.30
H

ATOM 7641 N MET D 212 -18.892 56.843 1.434 1.00 17.13 N
ATOM 7642 CA MET D 212 -19.522 56.931 0.127 1.00 20.63
C

ATOM 7643 C MET D 212 -20.557 58.047 0.075 1.00 21.00 C
ATOM 7644 O MET D 212 -21.345 58.230 1.007 1.00 20.37
O
ATOM 7645 CB MET D 212 -20.182 55.597 -0.230 1.00 18.86
C
ATOM 7646 CG MET D 212 -21.001 55.619 -1.511 1.00 20.28
C
ATOM 7647 SD MET D 212 -21.817 54.042 -1.811 1.00 22.14
S

ATOM 1348 CG LEU A 178 -24.863 26.136 -42.012 1.00 31.75 C
ATOM 1349 CD1 LEU A 178 -25.286 24.847 -42.694 1.00 32.44 C
ATOM 1350 CD2 LEU A 178 -23.906 25.830 -40.869 1.00 27.31 C
ATOM 1351 H LEU A 178 -25.006 29.479 -43.583 1.00 28.26 H
ATOM 1352 HA LEU A 178 -23.478 28.353 -41.641 1.00 31.28 H
ATOM 1353 HB2 LEU A 178 -24.931 27.249 -43.712 1.00 32.62 H
ATOM 1354 HB3 LEU A 178 -23.522 26.579 -43.475 1.00 32.62 H
ATOM 1355 HG LEU A 178 -25.655 26.555 -41.639 1.00 38.10 H
ATOM 1356 HD11 LEU A 178 -25.679 24.255 -42.034 1.00 38.93 H
ATOM 1357 HD12 LEU A 178 -25.937 25.054 -43.383 1.00 38.93 H
ATOM 1358 HD13 LEU A 178 -24.505 24.430 -43.091 1.00 38.93 H
ATOM 1359 HD21 LEU A 178 -24.345 25.236 -40.240 1.00 32.77 H
ATOM 1360 HD22 LEU A 178 -23.113 25.403 -41.228 1.00 32.77 H
ATOM 1361 HD23 LEU A 178 -23.665 26.660 -40.428 1.00 32.77 H
ATOM 1362 N LEU A 179 -22.536 29.044 -44.614 1.00 21.47 N
ATOM 1363 CA LEU A 179 -21.403 29.358 -45.471 1.00 22.73 C
ATOM 1364 C LEU A 179 -21.496 30.785 -45.977 1.00 24.99 C
ATOM 1365 O LEU A 179 -22.580 31.279 -46.292 1.00 21.88 O
ATOM 1366 CB LEU A 179 -21.340 28.399 -46.660 1.00 20.75 C
ATOM 1367 CG LEU A 179 -21.094 26.923 -46.352 1.00 20.55 C
ATOM 1368 CD1 LEU A 179 -21.138 26.111 -47.637 1.00 23.59 C
ATOM 1369 CD2 LEU A 179 -19.764 26.739 -45.650 1.00 20.81 C
ATOM 1370 H LEU A 179 -23.295 29.090 -45.015 1.00 25.76 H
ATOM 1371 HA LEU A 179 -20.582 29.267 -44.963 1.00 27.27 H
ATOM 1372 HB2 LEU A 179 -22.182 28.454 -47.137 1.00 24.90 H
ATOM 1373 HB3 LEU A 179 -20.623 28.691 -47.245 1.00 24.90 H
ATOM 1374 HG LEU A 179 -21.795 26.598 -45.764 1.00 24.66 H
ATOM 1375 HD11 LEU A 179 -20.980 25.178 -47.426 1.00 28.30 H
ATOM 1376 HD12 LEU A 179 -22.011 26.216 -48.047 1.00 28.30 H
ATOM 1377 HD13 LEU A 179 -20.449 26.436 -48.238 1.00 28.30 H
ATOM 1378 HD21 LEU A 179 -19.632 25.796 -45.465 1.00 24.97 H
ATOM 1379 HD22 LEU A 179 -19.055 27.066 -46.226 1.00 24.97 H
ATOM 1380 HD23 LEU A 179 -19.773 27.241 -44.820 1.00 24.97 H
ATOM 1381 N THR A 180 -20.347 31.443 -46.038 1.00 21.26 N

ATOM 7648 CE MET D 212 -22.962 54.507 -3.108 1.00 27.72 C
ATOM 7649 H MET D 212 -19.432 56.974 2.090 1.00 20.55 H
ATOM 7650 HA MET D 212 -18.838 57.110 -0.538 1.00 24.76 H
ATOM 7651 HB2 MET D 212 -19.488 54.927 -0.336 1.00 22.63 H
ATOM 7652 HB3 MET D 212 -20.774 55.341 0.494 1.00 22.63 H
ATOM 7653 HG2 MET D 212 -21.684 56.305 -1.441 1.00 24.34 H
ATOM 7654 HG3 MET D 212 -20.415 55.805 -2.262 1.00 24.34 H
ATOM 7655 HE1 MET D 212 -23.477 53.728 -3.368 1.00 33.26 H
ATOM 7656 HE2 MET D 212 -23.554 55.199 -2.773 1.00 33.26 H
ATOM 7657 HE3 MET D 212 -22.459 54.841 -3.867 1.00 33.26 H
ATOM 7658 N GLN D 213 -20.540 58.781 -1.031 1.00 16.69 N
ATOM 7659 CA GLN D 213 -21.591 59.731 -1.354 1.00 22.03 C
ATOM 7660 C GLN D 213 -22.309 59.236 -2.599 1.00 22.94 C
ATOM 7661 O GLN D 213 -21.704 59.102 -3.664 1.00 20.77 O
ATOM 7662 CB GLN D 213 -21.026 61.135 -1.587 1.00 18.19 C
ATOM 7663 CG GLN D 213 -20.428 61.794 -0.357 1.00 25.42 C
ATOM 7664 CD GLN D 213 -19.984 63.221 -0.629 1.00 27.60 C
ATOM 7665 OE1 GLN D 213 -19.786 63.611 -1.781 1.00 28.10 O
ATOM 7666 NE2 GLN D 213 -19.833 64.008 0.431 1.00 28.85 N
ATOM 7667 H GLN D 213 -19.916 58.744 -1.622 1.00 20.02 H
ATOM 7668 HA GLN D 213 -22.229 59.771 -0.624 1.00 26.43 H
ATOM 7669 HB2 GLN D 213 -20.328 61.080 -2.258 1.00 21.83 H
ATOM 7670 HB3 GLN D 213 -21.741 61.707 -1.908 1.00 21.83 H
ATOM 7671 HG2 GLN D 213 -21.095 61.815 0.348 1.00 30.50 H
ATOM 7672 HG3 GLN D 213 -19.654 61.287 -0.069 1.00 30.50 H
ATOM 7673 HE21 GLN D 213 -19.583 64.825 0.328 1.00 34.62 H
ATOM 7674 HE22 GLN D 213 -19.985 63.701 1.220 1.00 34.62 H
ATOM 7675 N ARG D 214 -23.594 58.939 -2.457 1.00 25.52 N
ATOM 7676 CA ARG D 214 -24.407 58.541 -3.592 1.00 32.54 C
ATOM 7677 C ARG D 214 -24.815 59.790 -4.356 1.00 40.12 C
ATOM 7678 O ARG D 214 -25.017 60.850 -3.763 1.00 43.97 O
ATOM 7679 CB ARG D 214 -25.639 57.758 -3.136 1.00 30.59 C
ATOM 7680 CG ARG D 214 -26.467 57.167 -4.271 1.00 32.12 C
ATOM 7681 CD ARG D 214 -25.894 55.846 -4.775 1.00 28.20 C

ATOM 1382 CA THR A 180 -20.231 32.721 -46.711 1.00 19.84
C
ATOM 1383 C THR A 180 -19.779 32.441 -48.136 1.00 21.52
C
ATOM 1384 O THR A 180 -18.640 32.036 -48.366 1.00 23.27
O
ATOM 1385 CB THR A 180 -19.238 33.651 -45.993 1.00 24.67
C
ATOM 1386 OG1 THR A 180 -19.714 33.921 -44.669 1.00 25.74
O
ATOM 1387 CG2 THR A 180 -19.074 34.963 -46.744 1.00 25.66
C
ATOM 1388 H THR A 180 -19.612 31.164 -45.691 1.00 25.51
H
ATOM 1389 HA THR A 180 -21.098 33.155 -46.740 1.00 23.81
H
ATOM 1390 HB THR A 180 -18.372 33.218 -45.942 1.00 29.61
H
ATOM 1391 HG1 THR A 180 -19.784 33.203 -44.237 1.00 30.89
H
ATOM 1392 HG21 THR A 180 -18.445 35.535 -46.276 1.00 30.80
H
ATOM 1393 HG22 THR A 180 -18.741 34.793 -47.639 1.00 30.80
H
ATOM 1394 HG23 THR A 180 -19.928 35.418 -46.806 1.00 30.80
H
ATOM 1395 N ILE A 181 -20.683 32.633 -49.089 1.00 22.03
N
ATOM 1396 CA ILE A 181 -20.372 32.385 -50.490 1.00 21.98
C
ATOM 1397 C ILE A 181 -19.733 33.621 -51.100 1.00 25.54
C
ATOM 1398 O ILE A 181 -20.283 34.720 -51.025 1.00 23.45
O
ATOM 1399 CB ILE A 181 -21.623 31.998 -51.297 1.00 25.31
C
ATOM 1400 CG1 ILE A 181 -22.295 30.767 -50.684 1.00 27.58
C
ATOM 1401 CG2 ILE A 181 -21.257 31.731 -52.759 1.00 29.37
C
ATOM 1402 CD1 ILE A 181 -21.409 29.523 -50.619 1.00 25.67
C
ATOM 1403 H ILE A 181 -21.487 32.906 -48.950 1.00 26.43
H
ATOM 1404 HA ILE A 181 -19.736 31.655 -50.550 1.00 26.37
H
ATOM 1405 HB ILE A 181 -22.249 32.738 -51.267 1.00 30.37
H
ATOM 1406 HG12 ILE A 181 -22.567 30.982 -49.778 1.00 33.09
H
ATOM 1407 HG13 ILE A 181 -23.076 30.544 -51.215 1.00 33.09
H
ATOM 1408 HG21 ILE A 181 -22.061 31.489 -53.246 1.00 35.24
H
ATOM 1409 HG22 ILE A 181 -20.869 32.534 -53.139 1.00 35.24
H
ATOM 1410 HG23 ILE A 181 -20.617 31.003 -52.796 1.00 35.24
H
ATOM 1411 HD11 ILE A 181 -21.913 28.797 -50.219 1.00 30.81
H
ATOM 1412 HD12 ILE A 181 -21.138 29.282 -51.519 1.00 30.81
H
ATOM 1413 HD13 ILE A 181 -20.628 29.720 -50.079 1.00 30.81
H
ATOM 1414 N ILE A 182 -18.567 33.418 -51.706 1.00 21.72
N
ATOM 1415 CA ILE A 182 -17.765 34.497 -52.261 1.00 20.53
C

ATOM 7682 NE ARG D 214 -26.798 55.208 -5.732 1.00 27.38
N
ATOM 7683 CZ ARG D 214 -26.767 55.390 -7.050 1.00 28.78
C
ATOM 7684 NH1 ARG D 214 -25.862 56.189 -7.606 1.00 27.43
N1+
ATOM 7685 NH2 ARG D 214 -27.649 54.766 -7.819 1.00 26.83
N
ATOM 7686 H ARG D 214 -24.019 58.961 -1.710 1.00 30.63
H
ATOM 7687 HA ARG D 214 -23.885 57.976 -4.183 1.00 39.04
H
ATOM 7688 HB2 ARG D 214 -25.349 57.025 -2.571 1.00 36.70
H
ATOM 7689 HB3 ARG D 214 -26.215 58.352 -2.630 1.00 36.70
H
ATOM 7690 HG2 ARG D 214 -27.369 57.004 -3.954 1.00 38.54
H
ATOM 7691 HG3 ARG D 214 -26.481 57.793 -5.012 1.00 38.54
H
ATOM 7692 HD2 ARG D 214 -25.047 56.011 -5.220 1.00 33.84
H
ATOM 7693 HD3 ARG D 214 -25.768 55.243 -4.026 1.00 33.84
H
ATOM 7694 HE ARG D 214 -27.395 54.674 -5.418 1.00 32.85
H
ATOM 7695 HH11 ARG D 214 -25.290 56.599 -7.113 1.00 32.91
H
ATOM 7696 HH12 ARG D 214 -25.851 56.297 -8.459 1.00 32.91
H
ATOM 7697 HH21 ARG D 214 -28.235 54.245 -7.466 1.00 32.19
H
ATOM 7698 HH22 ARG D 214 -27.629 54.875 -8.672 1.00 32.19
H

ATOM 7699 N THR D 215 -24.923 59.656 -5.672 1.00 49.40 N
ATOM 7700 CA THR D 215 -25.345 60.749 -6.538 1.00 47.09
C

ATOM 7701 C THR D 215 -26.665 61.379 -6.091 1.00 38.12 C
ATOM 7702 O THR D 215 -27.251 62.193 -6.808 1.00 43.45
O
ATOM 7703 CB THR D 215 -25.504 60.261 -7.984 1.00 43.89
C
ATOM 7704 OG1 THR D 215 -24.958 58.940 -8.113 1.00 51.06
O
ATOM 7705 CG2 THR D 215 -24.794 61.194 -8.917 1.00 44.94
C

ATOM 7706 H THR D 215 -24.753 58.927 -6.095 1.00 59.28 H
ATOM 7707 HA THR D 215 -24.664 61.440 -6.528 1.00 56.50
H
ATOM 7708 HB THR D 215 -26.445 60.247 -8.220 1.00 52.66
H
ATOM 7709 HG1 THR D 215 -25.043 58.670 -8.903 1.00 61.28
H
ATOM 7710 HG21 THR D 215 -25.168 62.086 -8.841 1.00 53.93
H
ATOM 7711 HG22 THR D 215 -23.850 61.228 -8.697 1.00 53.93
H
ATOM 7712 HG23 THR D 215 -24.893 60.887 -9.832 1.00 53.93
H

TER 7713 THR D 215

ATOM 7714 N GLY E 0 -1.565 40.227 -65.921 1.00 24.87 N

ATOM 7715 CA GLY E 0 -1.695 39.502 -64.623 1.00 25.57 C

ATOM 1416 C ILE A 182 -17.654 34.340 -53.767 1.00 23.40
C
ATOM 1417 O ILE A 182 -17.226 33.296 -54.256 1.00 22.37
O
ATOM 1418 CB ILE A 182 -16.346 34.515 -51.649 1.00 20.38
C
ATOM 1419 CG1 ILE A 182 -16.430 34.684 -50.132 1.00 20.79
C
ATOM 1420 CG2 ILE A 182 -15.494 35.626 -52.271 1.00 21.86
C
ATOM 1421 CD1 ILE A 182 -15.132 34.434 -49.414 1.00 22.03
C
ATOM 1422 H ILE A 182 -18.211 32.641 -51.808 1.00 26.06
H
ATOM 1423 HA ILE A 182 -18.192 35.347 -52.072 1.00 24.63
H
ATOM 1424 HB ILE A 182 -15.922 33.664 -51.838 1.00 24.45
H
ATOM 1425 HG12 ILE A 182 -16.706 35.593 -49.934 1.00 24.95
H
ATOM 1426 HG13 ILE A 182 -17.085 34.059 -49.784 1.00 24.95
H
ATOM 1427 HG21 ILE A 182 -14.613 35.611 -51.867 1.00 26.24
H
ATOM 1428 HG22 ILE A 182 -15.424 35.472 -53.226 1.00 26.24
H
ATOM 1429 HG23 ILE A 182 -15.921 36.481 -52.104 1.00 26.24
H
ATOM 1430 HD11 ILE A 182 -15.269 34.561 -48.462 1.00 26.43
H
ATOM 1431 HD12 ILE A 182 -14.845 33.524 -49.589 1.00 26.43
H
ATOM 1432 HD13 ILE A 182 -14.466 35.060 -49.740 1.00 26.43
H
ATOM 1433 N GLU A 183 -18.035 35.379 -54.500 1.00 21.68
N
ATOM 1434 CA GLU A 183 -17.855 35.391 -55.943 1.00 27.56
C
ATOM 1435 C GLU A 183 -16.373 35.527 -56.271 1.00 29.48
C
ATOM 1436 O GLU A 183 -15.667 36.337 -55.670 1.00 31.01
O
ATOM 1437 CB GLU A 183 -18.648 36.533 -56.582 1.00 39.38
C
ATOM 1438 CG GLU A 183 -20.154 36.416 -56.407 1.00 45.85
C
ATOM 1439 CD GLU A 183 -20.911 37.550 -57.074 1.00 71.49
C
ATOM 1440 OE1 GLU A 183 -20.297 38.607 -57.336 1.00 65.31
O
ATOM 1441 OE2 GLU A 183 -22.120 37.382 -57.340 1.00 84.35
O1-
ATOM 1442 H GLU A 183 -18.402 36.090 -54.184 1.00 26.02
H
ATOM 1443 HA GLU A 183 -18.174 34.553 -56.314 1.00 33.07
H
ATOM 1444 HB2 GLU A 183 -18.368 37.370 -56.180 1.00 47.25
H
ATOM 1445 HB3 GLU A 183 -18.461 36.548 -57.534 1.00 47.25
H
ATOM 1446 HG2 GLU A 183 -20.454 35.582 -56.802 1.00 55.02
H
ATOM 1447 HG3 GLU A 183 -20.364 36.430 -55.461 1.00 55.02
H
ATOM 1448 N MET A 184 -15.908 34.723 -57.219 1.00 27.36
N
ATOM 1449 CA MET A 184 -14.520 34.765 -57.655 1.00 30.39
C
ATOM 7716 C GLY E 0 -2.109 40.445 -63.512 1.00 23.21 C
ATOM 7717 O GLY E 0 -2.318 41.635 -63.745 1.00 21.52 O
ATOM 7718 H1 GLY E 0 -2.226 39.984 -66.465 1.00 29.85 H
ATOM 7719 H2 GLY E 0 -1.608 41.105 -65.776 1.00 29.85 H
ATOM 7720 H3 GLY E 0 -0.783 40.027 -66.296 1.00 29.85 H
ATOM 7721 HA2 GLY E 0 -2.363 38.803 -64.704 1.00 30.68 H
ATOM 7722 HA3 GLY E 0 -0.846 39.096 -64.388 1.00 30.68 H
ATOM 7723 N HIS E 1 -2.229 39.916 -62.300 1.00 20.53 N
ATOM 7724 CA HIS E 1 -2.640 40.720 -61.155 1.00 19.68 C
ATOM 7725 C HIS E 1 -1.777 40.422 -59.946 1.00 18.24 C
ATOM 7726 O HIS E 1 -1.189 39.348 -59.847 1.00 15.98 O
ATOM 7727 CB HIS E 1 -4.111 40.469 -60.821 1.00 19.17 C
ATOM 7728 CG HIS E 1 -5.048 40.824 -61.931 1.00 22.06 C
ATOM 7729 ND1 HIS E 1 -5.356 42.128 -62.255 1.00 23.79 N
ATOM 7730 CD2 HIS E 1 -5.744 40.047 -62.794 1.00 22.57 C
ATOM 7731 CE1 HIS E 1 -6.202 42.139 -63.270 1.00 22.50 C
ATOM 7732 NE2 HIS E 1 -6.454 40.889 -63.614 1.00 22.56 N
ATOM 7733 H HIS E 1 -2.078 39.090 -62.113 1.00 24.63 H
ATOM 7734 HA HIS E 1 -2.537 41.660 -61.374 1.00 23.61 H
ATOM 7735 HB2 HIS E 1 -4.231 39.528 -60.622 1.00 23.00 H
ATOM 7736 HB3 HIS E 1 -4.352 41.003 -60.047 1.00 23.00 H
ATOM 7737 HD1 HIS E 1 -5.045 42.826 -61.859 1.00 28.55 H
ATOM 7738 HD2 HIS E 1 -5.743 39.118 -62.823 1.00 27.08 H
ATOM 7739 HE1 HIS E 1 -6.559 42.897 -63.672 1.00 27.00 H
ATOM 7740 HE2 HIS E 1 -6.977 40.642 -64.251 1.00 27.08 H
ATOM 7741 N LYS E 2 -1.704 41.383 -59.031 1.00 18.21 N
ATOM 7742 CA LYS E 2 -0.948 41.206 -57.804 1.00 17.86 C
ATOM 7743 C LYS E 2 -1.636 41.890 -56.629 1.00 19.00 C
ATOM 7744 O LYS E 2 -2.239 42.957 -56.769 1.00 19.28 O
ATOM 7745 CB LYS E 2 0.478 41.736 -57.970 1.00 23.19 C
ATOM 7746 CG LYS E 2 0.564 43.187 -58.389 1.00 27.11 C
ATOM 7747 CD LYS E 2 1.980 43.554 -58.803 1.00 34.68 C
ATOM 7748 CE LYS E 2 2.079 45.021 -59.188 1.00 38.27 C
ATOM 7749 NZ LYS E 2 3.461 45.403 -59.589 1.00 38.97
N1+

ATOM 1450 C MET A 184 -14.461 34.514 -59.154 1.00 36.58
C
ATOM 1451 O MET A 184 -14.269 35.441 -59.942 1.00 34.99
O
ATOM 1452 CB MET A 184 -13.684 33.732 -56.895 1.00 28.20
C
ATOM 1453 CG MET A 184 -12.200 33.780 -57.213 1.00 26.40
C
ATOM 1454 SD MET A 184 -11.300 32.412 -56.469 1.00 27.32
S
ATOM 1455 CE MET A 184 -11.827 31.057 -57.524 1.00 31.27
C
ATOM 1456 H MET A 184 -16.384 34.136 -57.631 1.00 32.83
H
ATOM 1457 HA MET A 184 -14.155 35.644 -57.466 1.00 36.47
H
ATOM 1458 HB2 MET A 184 -13.788 33.887 -55.943 1.00 33.85
H
ATOM 1459 HB3 MET A 184 -14.006 32.845 -57.120 1.00 33.85
H
ATOM 1460 HG2 MET A 184 -12.080 33.732 -58.175 1.00 31.68
H
ATOM 1461 HG3 MET A 184 -11.828 34.607 -56.871 1.00 31.68
H
ATOM 1462 HE1 MET A 184 -11.402 30.239 -57.223 1.00 37.53
H
ATOM 1463 HE2 MET A 184 -12.791 30.969 -57.468 1.00 37.53
H
ATOM 1464 HE3 MET A 184 -11.565 31.248 -58.439 1.00 37.53
H
ATOM 1465 N GLN A 185 -14.639 33.253 -59.535 1.00 34.02
N
ATOM 1466 CA GLN A 185 -14.708 32.865 -60.935 1.00 39.99
C
ATOM 1467 C GLN A 185 -16.136 32.439 -61.257 1.00 36.81
C
ATOM 1468 O GLN A 185 -16.749 31.687 -60.498 1.00 32.57
O
ATOM 1469 CB GLN A 185 -13.724 31.732 -61.230 1.00 31.78
C
ATOM 1470 CG GLN A 185 -13.525 31.454 -62.708 1.00 37.09
C
ATOM 1471 CD GLN A 185 -12.853 32.606 -63.427 1.00 49.35
C
ATOM 1472 OE1 GLN A 185 -11.834 33.129 -62.972 1.00 44.78
O
ATOM 1473 NE2 GLN A 185 -13.427 33.014 -64.554 1.00 50.69
N
ATOM 1474 H GLN A 185 -14.723 32.593 -58.990 1.00 40.83
H
ATOM 1475 HA GLN A 185 -14.480 33.624 -61.494 1.00 47.99
H
ATOM 1476 HB2 GLN A 185 -12.860 31.964 -60.855 1.00 38.14
H
ATOM 1477 HB3 GLN A 185 -14.053 30.918 -60.818 1.00 38.14
H
ATOM 1478 HG2 GLN A 185 -12.966 30.668 -62.810 1.00 44.51
H
ATOM 1479 HG3 GLN A 185 -14.390 31.304 -63.121 1.00 44.51
H
ATOM 1480 HE21 GLN A 185 -13.084 33.665 -64.999 1.00 60.83
H
ATOM 1481 HE22 GLN A 185 -14.141 32.629 -64.837 1.00 60.83
H
ATOM 1482 N LYS A 186 -16.669 32.933 -62.370 1.00 41.91
N
ATOM 1483 CA LYS A 186 -18.026 32.585 -62.779 1.00 44.77
C

ATOM 7750 H LYS E 2 -2.086 42.150 -59.100 1.00 21.85 H

ATOM 7751 HA LYS E 2 -0.891 40.259 -57.605 1.00 21.44 H

ATOM 7752 HB2 LYS E 2 0.943 41.647 -57.123 1.00 27.83 H

ATOM 7753 HB3 LYS E 2 0.929 41.208 -58.647 1.00 27.83 H

ATOM 7754 HG2 LYS E 2 -0.024 43.338 -59.145 1.00 32.53 H

ATOM 7755 HG3 LYS E 2 0.307 43.752 -57.644 1.00 32.53 H

ATOM 7756 HD2 LYS E 2 2.584 43.392 -58.061 1.00 41.61 H

ATOM 7757 HD3 LYS E 2 2.239 43.020 -59.570 1.00 41.61 H

ATOM 7758 HE2 LYS E 2 1.489 45.194 -59.937 1.00 45.93 H

ATOM 7759 HE3 LYS E 2 1.824 45.567 -58.428 1.00 45.93 H

ATOM 7760 HZ1 LYS E 2 4.024 45.259 -58.915 1.00 46.77 H

ATOM 7761 HZ2 LYS E 2 3.719 44.919 -60.290 1.00 46.77 H

ATOM 7762 HZ3 LYS E 2 3.487 46.265 -59.808 1.00 46.77 H

ATOM 7763 N LEU E 3 -1.558 41.235 -55.477 1.00 15.59 N

ATOM 7764 CA LEU E 3 -2.079 41.766 -54.229 1.00 13.41 C

ATOM 7765 C LEU E 3 -0.905 41.903 -53.273 1.00 13.12 C

ATOM 7766 O LEU E 3 -0.228 40.922 -52.981 1.00 12.97 O

ATOM 7767 CB LEU E 3 -3.160 40.847 -53.661 1.00 14.06 C

ATOM 7768 CG LEU E 3 -3.893 41.275 -52.390 1.00 12.36 C

ATOM 7769 CD1 LEU E 3 -4.662 42.573 -52.590 1.00 15.83 C

ATOM 7770 CD2 LEU E 3 -4.825 40.167 -51.968 1.00 11.74 C

ATOM 7771 H LEU E 3 -1.197 40.458 -55.394 1.00 18.71 H

ATOM 7772 HA LEU E 3 -2.463 42.644 -54.380 1.00 16.10 H

ATOM 7773 HB2 LEU E 3 -3.835 40.727 -54.346 1.00 16.87 H

ATOM 7774 HB3 LEU E 3 -2.748 39.990 -53.471 1.00 16.87 H

ATOM 7775 HG LEU E 3 -3.246 41.413 -51.681 1.00 14.83 H
ATOM 7776 HD11 LEU E 3 -5.110 42.805 -51.761 1.00 18.99
H
ATOM 7777 HD12 LEU E 3 -4.039 43.274 -52.837 1.00 18.99
H
ATOM 7778 HD13 LEU E 3 -5.315 42.447 -53.296 1.00 18.99
H
ATOM 7779 HD21 LEU E 3 -5.291 40.437 -51.162 1.00 14.08
H
ATOM 7780 HD22 LEU E 3 -5.462 40.003 -52.680 1.00 14.08
H
ATOM 7781 HD23 LEU E 3 -4.305 39.366 -51.798 1.00 14.08
H

ATOM 7782 N ALA E 4 -0.654 43.124 -52.813 1.00 14.08 N

ATOM 7783 CA ALA E 4 0.497 43.406 -51.961 1.00 13.44 C

ATOM 1484 C LYS A 186 -18.149 31.085 -63.028 1.00 32.82
C
ATOM 1485 O LYS A 186 -17.492 30.537 -63.913 1.00 41.23
O
ATOM 1486 CB LYS A 186 -18.427 33.361 -64.033 1.00 55.29
C
ATOM 1487 CG LYS A 186 -18.429 34.868 -63.851 1.00 69.71
C
ATOM 1488 CD LYS A 186 -18.935 35.578 -65.096 1.00 87.98
C
ATOM 1489 CE LYS A 186 -18.822 37.087 -64.961 1.00 90.78
C
ATOM 1490 NZ LYS A 186 -17.407 37.529 -64.823 1.00 89.35
N1+
ATOM 1491 H LYS A 186 -16.266 33.470 -62.907 1.00 50.30
H
ATOM 1492 HA LYS A 186 -18.642 32.823 -62.068 1.00 53.72
H
ATOM 1493 HB2 LYS A 186 -17.802 33.150 -64.744 1.00 66.35
H
ATOM 1494 HB3 LYS A 186 -19.323 33.093 -64.293 1.00 66.35
H
ATOM 1495 HG2 LYS A 186 -19.012 35.100 -63.110 1.00 83.65
H
ATOM 1496 HG3 LYS A 186 -17.525 35.171 -63.674 1.00 83.65
H
ATOM 1497 HD2 LYS A 186 -18.406 35.301 -65.860 1.00105.57
H
ATOM 1498 HD3 LYS A 186 -19.869 35.354 -65.235 1.00105.57
H
ATOM 1499 HE2 LYS A 186 -19.194 37.507 -65.753 1.00108.94
H
ATOM 1500 HE3 LYS A 186 -19.307 37.374 -64.172 1.00108.94
H
ATOM 1501 HZ1 LYS A 186 -16.940 37.281 -65.540 1.00107.22
H
ATOM 1502 HZ2 LYS A 186 -17.371 38.415 -64.747 1.00107.22
H
ATOM 1503 HZ3 LYS A 186 -17.043 37.160 -64.100 1.00107.22
H
ATOM 1504 N GLY A 187 -18.991 30.427 -62.239 1.00 31.79
N
ATOM 1505 CA GLY A 187 -19.178 28.993 -62.350 1.00 33.62
C
ATOM 1506 C GLY A 187 -20.338 28.512 -61.506 1.00 28.83
C
ATOM 1507 O GLY A 187 -20.967 29.303 -60.803 1.00 31.67
O
ATOM 1508 H GLY A 187 -19.468 30.795 -61.626 1.00 38.15
H
ATOM 1509 HA2 GLY A 187 -19.350 28.758 -63.276 1.00 40.35
H
ATOM 1510 HA3 GLY A 187 -18.373 28.536 -62.060 1.00 40.35
H
ATOM 1511 N ASP A 188 -20.613 27.211 -61.571 1.00 26.78
N
ATOM 1512 CA ASP A 188 -21.741 26.613 -60.860 1.00 29.71
C
ATOM 1513 C ASP A 188 -21.302 25.691 -59.721 1.00 27.78
C
ATOM 1514 O ASP A 188 -22.110 24.929 -59.185 1.00 26.36
O
ATOM 1515 CB ASP A 188 -22.617 25.840 -61.843 1.00 34.87
C
ATOM 1516 CG ASP A 188 -23.227 26.735 -62.901 1.00 39.70
C
ATOM 1517 OD1 ASP A 188 -23.676 27.848 -62.551 1.00 38.40
O

ATOM 7784 C ALA E 4 0.060 43.927 -50.597 1.00 17.16 C

ATOM 7785 O ALA E 4 -0.878 44.720 -50.492 1.00 16.57 O

ATOM 7786 CB ALA E 4 1.416 44.405 -52.632 1.00 18.34 C

ATOM 7787 H ALA E 4 -1.140 43.813 -52.981 1.00 16.90 H

ATOM 7788 HA ALA E 4 0.995 42.586 -51.822 1.00 16.13 H

ATOM 7789 HB1 ALA E 4 2.172 44.578 -52.050 1.00 22.01 H

ATOM 7790 HB2 ALA E 4 1.723 44.035 -53.474 1.00 22.01 H

ATOM 7791 HB3 ALA E 4 0.925 45.227 -52.791 1.00 22.01 H

ATOM 7792 N PHE E 5 0.753 43.463 -49.563 1.00 15.63 N

ATOM 7793 CA PHE E 5 0.549 43.919 -48.195 1.00 13.64 C

ATOM 7794 C PHE E 5 1.836 44.553 -47.690 1.00 14.46 C

ATOM 7795 O PHE E 5 2.882 43.911 -47.705 1.00 13.48 O

ATOM 7796 CB PHE E 5 0.153 42.757 -47.285 1.00 12.69 C

ATOM 7797 CG PHE E 5 -1.145 42.107 -47.655 1.00 12.18 C
ATOM 7798 CD1 PHE E 5 -1.202 41.174 -48.674 1.00 13.36
C
ATOM 7799 CD2 PHE E 5 -2.305 42.415 -46.970 1.00 13.02
C
ATOM 7800 CE1 PHE E 5 -2.394 40.571 -49.012 1.00 16.36
C
ATOM 7801 CE2 PHE E 5 -3.500 41.813 -47.302 1.00 13.36
C

ATOM 7802 CZ PHE E 5 -3.545 40.890 -48.324 1.00 16.42 C

ATOM 7803 H PHE E 5 1.366 42.864 -49.633 1.00 18.75 H

ATOM 7804 HA PHE E 5 -0.156 44.585 -48.174 1.00 16.37 H

ATOM 7805 HB2 PHE E 5 0.845 42.079 -47.327 1.00 15.23 H

ATOM 7806 HB3 PHE E 5 0.070 43.087 -46.377 1.00 15.23 H
ATOM 7807 HD1 PHE E 5 -0.429 40.956 -49.142 1.00 16.03
H
ATOM 7808 HD2 PHE E 5 -2.280 43.038 -46.280 1.00 15.63
H
ATOM 7809 HE1 PHE E 5 -2.422 39.947 -49.701 1.00 19.63
H
ATOM 7810 HE2 PHE E 5 -4.276 42.030 -46.837 1.00 16.03
H

ATOM 7811 HZ PHE E 5 -4.350 40.483 -48.550 1.00 19.70 H

ATOM 7812 N ASN E 6 1.761 45.806 -47.252 1.00 14.65 N

ATOM 7813 CA ASN E 6 2.928 46.501 -46.714 1.00 15.88 C

ATOM 7814 C ASN E 6 2.745 46.820 -45.232 1.00 16.33 C

ATOM 7815 O ASN E 6 2.007 47.736 -44.871 1.00 15.03 O

ATOM 7816 CB ASN E 6 3.201 47.786 -47.499 1.00 19.07 C

ATOM 7817 CG ASN E 6 4.557 48.391 -47.170 1.00 26.15 C

ATOM 1518 OD2 ASP A 188 -23.248 26.332 -64.083 1.00 40.40
O1-
ATOM 1519 H ASP A 188 -20.154 26.645 -62.028 1.00 32.14
H
ATOM 1520 HA ASP A 188 -22.280 27.322 -60.476 1.00 35.65
H
ATOM 1521 HB2 ASP A 188 -22.077 25.170 -62.291 1.00 41.85
H
ATOM 1522 HB3 ASP A 188 -23.340 25.413 -61.357 1.00 41.85
H
ATOM 1523 N CYS A 189 -20.027 25.772 -59.349 1.00 25.17
N
ATOM 1524 CA CYS A 189 -19.485 24.978 -58.248 1.00 21.30
C
ATOM 1525 C CYS A 189 -18.739 25.877 -57.264 1.00 22.52
C
ATOM 1526 O CYS A 189 -18.363 27.001 -57.605 1.00 24.18
O
ATOM 1527 CB CYS A 189 -18.546 23.887 -58.776 1.00 24.76
C
ATOM 1528 SG CYS A 189 -19.310 22.735 -59.952 1.00 29.58
S
ATOM 1529 H CYS A 189 -19.448 26.286 -59.723 1.00 30.21
H
ATOM 1530 HA CYS A 189 -20.214 24.548 -57.774 1.00 25.56
H
ATOM 1531 HB2 CYS A 189 -17.799 24.312 -59.224 1.00 29.72
H
ATOM 1532 HB3 CYS A 189 -18.222 23.367 -58.024 1.00 29.72
H
ATOM 1533 N ALA A 190 -18.520 25.374 -56.053 1.00 21.28
N
ATOM 1534 CA ALA A 190 -17.838 26.140 -55.015 1.00 21.57
C
ATOM 1535 C ALA A 190 -16.767 25.316 -54.311 1.00 18.66
C
ATOM 1536 O ALA A 190 -16.936 24.118 -54.073 1.00 17.27
O
ATOM 1537 CB ALA A 190 -18.838 26.661 -54.007 1.00 20.73
C
ATOM 1538 H ALA A 190 -18.759 24.585 -55.805 1.00 25.54
H
ATOM 1539 HA ALA A 190 -17.403 26.904 -55.425 1.00 25.89
H
ATOM 1540 HB1 ALA A 190 -18.366 27.166 -53.327 1.00 24.88
H
ATOM 1541 HB2 ALA A 190 -19.476 27.232 -54.462 1.00 24.88
H
ATOM 1542 HB3 ALA A 190 -19.298 25.909 -53.602 1.00 24.88
H
ATOM 1543 N LEU A 191 -15.664 25.981 -53.984 1.00 20.48
N
ATOM 1544 CA LEU A 191 -14.578 25.382 -53.216 1.00 18.02
C
ATOM 1545 C LEU A 191 -14.722 25.748 -51.745 1.00 17.63
C
ATOM 1546 O LEU A 191 -14.852 26.927 -51.421 1.00 16.65
O
ATOM 1547 CB LEU A 191 -13.226 25.869 -53.737 1.00 15.13
C
ATOM 1548 CG LEU A 191 -12.856 25.493 -55.171 1.00 21.15
C
ATOM 1549 CD1 LEU A 191 -11.760 26.409 -55.687 1.00 23.95
C
ATOM 1550 CD2 LEU A 191 -12.414 24.040 -55.236 1.00 19.16
C
ATOM 1551 H LEU A 191 -15.518 26.800 -54.200 1.00 24.57
H

ATOM 7818 OD1 ASN E 6 4.646 49.449 -46.550 1.00 33.75
O
ATOM 7819 ND2 ASN E 6 5.622 47.706 -47.572 1.00 23.45
N

ATOM 7820 H ASN E 6 1.042 46.279 -47.255 1.00 17.58 H

ATOM 7821 HA ASN E 6 3.704 45.926 -46.802 1.00 19.05 H

ATOM 7822 HB2 ASN E 6 3.181 47.588 -48.448 1.00 22.89 H

ATOM 7823 HB3 ASN E 6 2.519 48.441 -47.282 1.00 22.89 H
ATOM 7824 HD21 ASN E 6 6.412 48.005 -47.411 1.00 28.14
H
ATOM 7825 HD22 ASN E 6 5.522 46.963 -47.994 1.00 28.14
H

ATOM 7826 N PHE E 7 3.411 46.041 -44.385 1.00 13.46 N

ATOM 7827 CA PHE E 7 3.355 46.228 -42.942 1.00 16.36 C

ATOM 7828 C PHE E 7 4.478 47.139 -42.488 1.00 15.66 C

ATOM 7829 O PHE E 7 5.634 46.909 -42.829 1.00 14.02 O

ATOM 7830 CB PHE E 7 3.464 44.888 -42.217 1.00 14.45 C

ATOM 7831 CG PHE E 7 2.371 43.929 -42.549 1.00 13.89 C
ATOM 7832 CD1 PHE E 7 2.434 43.159 -43.700 1.00 13.75
C
ATOM 7833 CD2 PHE E 7 1.285 43.779 -41.705 1.00 13.24
C

ATOM 7834 CE1 PHE E 7 1.425 42.267 -44.007 1.00 13.98 C

ATOM 7835 CE2 PHE E 7 0.270 42.887 -42.009 1.00 16.30 C

ATOM 7836 CZ PHE E 7 0.342 42.131 -43.161 1.00 16.68 C

ATOM 7837 H PHE E 7 3.912 45.386 -44.628 1.00 16.16 H

ATOM 7838 HA PHE E 7 2.509 46.639 -42.702 1.00 19.63 H

ATOM 7839 HB2 PHE E 7 4.307 44.472 -42.456 1.00 17.33 H

ATOM 7840 HB3 PHE E 7 3.437 45.048 -41.260 1.00 17.33 H
ATOM 7841 HD1 PHE E 7 3.160 43.248 -44.274 1.00 16.50
H
ATOM 7842 HD2 PHE E 7 1.232 44.289 -40.928 1.00 15.89
H

ATOM 7843 HE1 PHE E 7 1.474 41.757 -44.784 1.00 16.77 H
ATOM 7844 HE2 PHE E 7 -0.457 42.796 -41.437 1.00 19.56
H

ATOM 7845 HZ PHE E 7 -0.337 41.530 -43.367 1.00 20.02 H

ATOM 7846 N ASN E 8 4.139 48.165 -41.715 1.00 18.72 N

ATOM 7847 CA ASN E 8 5.147 49.064 -41.166 1.00 17.71 C

ATOM 7848 C ASN E 8 4.955 49.290 -39.675 1.00 18.89 C

ATOM 7849 O ASN E 8 3.850 49.591 -39.218 1.00 16.16 O

ATOM 7850 CB ASN E 8 5.124 50.406 -41.893 1.00 17.97 C

ATOM 7851 CG ASN E 8 6.231 51.331 -41.433 1.00 21.21 C

ATOM 1552 HA LEU A 191 -14.613 24.416 -53.300 1.00 21.63 H
ATOM 1553 HB2 LEU A 191 -13.213 26.837 -53.683 1.00 18.15 H
ATOM 1554 HB3 LEU A 191 -12.533 25.509 -53.160 1.00 18.15 H
ATOM 1555 HG LEU A 191 -13.634 25.600 -55.741 1.00 25.38 H
ATOM 1556 HD11 LEU A 191 -11.540 26.155 -56.597 1.00 28.74 H
ATOM 1557 HD12 LEU A 191 -12.079 27.324 -55.667 1.00 28.74 H
ATOM 1558 HD13 LEU A 191 -10.979 26.317 -55.119 1.00 28.74 H
ATOM 1559 HD21 LEU A 191 -12.183 23.821 -56.153 1.00 22.99 H
ATOM 1560 HD22 LEU A 191 -11.641 23.919 -54.663 1.00 22.99 H
ATOM 1561 HD23 LEU A 191 -13.142 23.475 -54.934 1.00 22.99 H
ATOM 1562 N TYR A 192 -14.703 24.757 -50.855 1.00 15.23 N
ATOM 1563 CA TYR A 192 -14.718 25.056 -49.430 1.00 14.68 C
ATOM 1564 C TYR A 192 -13.365 25.597 -48.980 1.00 17.40 C
ATOM 1565 O TYR A 192 -12.324 25.129 -49.427 1.00 12.57 O
ATOM 1566 CB TYR A 192 -15.055 23.831 -48.568 1.00 16.60 C
ATOM 1567 CG TYR A 192 -14.916 24.199 -47.115 1.00 16.87 C
ATOM 1568 CD1 TYR A 192 -15.948 24.847 -46.450 1.00 14.23 C
ATOM 1569 CD2 TYR A 192 -13.724 23.981 -46.428 1.00 17.91 C
ATOM 1570 CE1 TYR A 192 -15.817 25.235 -45.140 1.00 15.45 C
ATOM 1571 CE2 TYR A 192 -13.584 24.368 -45.111 1.00 16.81 C
ATOM 1572 CZ TYR A 192 -14.637 24.997 -44.473 1.00 17.95 C
ATOM 1573 OH TYR A 192 -14.514 25.401 -43.164 1.00 18.94 O
ATOM 1574 H TYR A 192 -14.683 23.919 -51.048 1.00 18.28 H
ATOM 1575 HA TYR A 192 -15.386 25.737 -49.257 1.00 17.62 H
ATOM 1576 HB2 TYR A 192 -15.970 23.556 -48.734 1.00 19.92 H
ATOM 1577 HB3 TYR A 192 -14.437 23.110 -48.768 1.00 19.92 H
ATOM 1578 HD1 TYR A 192 -16.745 25.017 -46.898 1.00 17.07 H
ATOM 1579 HD2 TYR A 192 -13.015 23.564 -46.861 1.00 21.49 H
ATOM 1580 HE1 TYR A 192 -16.521 25.660 -44.706 1.00 18.54 H
ATOM 1581 HE2 TYR A 192 -12.788 24.210 -44.657 1.00 20.17 H
ATOM 1582 HH TYR A 192 -13.753 25.200 -42.872 1.00 22.72 H
ATOM 1583 N ALA A 193 -13.392 26.573 -48.078 1.00 14.04 N
ATOM 1584 CA ALA A 193 -12.184 27.021 -47.395 1.00 14.46 C
ATOM 1585 C ALA A 193 -12.528 27.614 -46.037 1.00 14.85 C

ATOM 7852 OD1 ASN E 8 7.411 51.033 -41.604 1.00 24.65 O
ATOM 7853 ND2 ASN E 8 5.856 52.462 -40.850 1.00 23.34 N
ATOM 7854 H ASN E 8 3.332 48.362 -41.493 1.00 22.47 H
ATOM 7855 HA ASN E 8 6.023 48.669 -41.297 1.00 21.25 H
ATOM 7856 HB2 ASN E 8 5.236 50.253 -42.845 1.00 21.57 H
ATOM 7857 HB3 ASN E 8 4.275 50.844 -41.724 1.00 21.57 H
ATOM 7858 HD21 ASN E 8 6.449 53.019 -40.572 1.00 28.01 H
ATOM 7859 HD22 ASN E 8 5.020 52.638 -40.751 1.00 28.01 H
ATOM 7860 N LEU E 9 6.043 49.124 -38.928 1.00 15.50 N
ATOM 7861 CA LEU E 9 6.083 49.460 -37.513 1.00 16.76 C
ATOM 7862 C LEU E 9 7.182 50.492 -37.294 1.00 19.62 C
ATOM 7863 O LEU E 9 8.365 50.183 -37.428 1.00 18.29 O
ATOM 7864 CB LEU E 9 6.330 48.214 -36.656 1.00 17.53 C
ATOM 7865 CG LEU E 9 6.418 48.451 -35.145 1.00 16.67 C
ATOM 7866 CD1 LEU E 9 5.120 49.012 -34.599 1.00 22.09 C
ATOM 7867 CD2 LEU E 9 6.781 47.164 -34.417 1.00 17.22 C
ATOM 7868 H LEU E 9 6.786 48.811 -39.228 1.00 18.60 H
ATOM 7869 HA LEU E 9 5.236 49.851 -37.249 1.00 20.12 H
ATOM 7870 HB2 LEU E 9 5.605 47.589 -36.809 1.00 21.03 H
ATOM 7871 HB3 LEU E 9 7.167 47.812 -36.935 1.00 21.03 H
ATOM 7872 HG LEU E 9 7.119 49.099 -34.970 1.00 20.00 H
ATOM 7873 HD11 LEU E 9 5.213 49.149 -33.644 1.00 26.51 H
ATOM 7874 HD12 LEU E 9 4.933 49.857 -35.038 1.00 26.51 H
ATOM 7875 HD13 LEU E 9 4.405 48.381 -34.776 1.00 26.51 H
ATOM 7876 HD21 LEU E 9 6.830 47.343 -33.465 1.00 20.67 H
ATOM 7877 HD22 LEU E 9 6.098 46.498 -34.594 1.00 20.67 H
ATOM 7878 HD23 LEU E 9 7.641 46.851 -34.740 1.00 20.67 H
ATOM 7879 N GLU E 10 6.781 51.720 -36.979 1.00 18.79 N
ATOM 7880 CA GLU E 10 7.726 52.814 -36.766 1.00 25.42 C
ATOM 7881 C GLU E 10 7.809 53.176 -35.290 1.00 25.51 C
ATOM 7882 O GLU E 10 6.822 53.608 -34.700 1.00 24.74 O
ATOM 7883 CB GLU E 10 7.320 54.046 -37.582 1.00 23.36 C
ATOM 7884 CG GLU E 10 8.326 55.197 -37.512 1.00 31.78 C
ATOM 7885 CD GLU E 10 7.883 56.420 -38.300 1.00 32.30 C

ATOM 1586 O ALA A 193 -13.669 28.005 -45.784 1.00 16.32 O
ATOM 1587 CB ALA A 193 -11.440 28.029 -48.233 1.00 16.01 C
ATOM 1588 H ALA A 193 -14.103 26.995 -47.843 1.00 16.85 H
ATOM 1589 HA ALA A 193 -11.600 26.260 -47.251 1.00 17.35 H
ATOM 1590 HB1 ALA A 193 -10.644 28.309 -47.756 1.00 19.22 H
ATOM 1591 HB2 ALA A 193 -11.194 27.617 -49.076 1.00 19.22 H
ATOM 1592 HB3 ALA A 193 -12.017 28.792 -48.393 1.00 19.22 H
ATOM 1593 N SER A 194 -11.534 27.675 -45.162 1.00 13.15 N
ATOM 1594 CA SER A 194 -11.726 28.278 -43.857 1.00 12.99 C
ATOM 1595 C SER A 194 -11.964 29.777 -44.025 1.00 15.13 C
ATOM 1596 O SER A 194 -11.387 30.378 -44.930 1.00 16.35 O
ATOM 1597 CB SER A 194 -10.507 28.029 -42.963 1.00 15.47 C
ATOM 1598 OG SER A 194 -10.547 28.856 -41.815 1.00 15.91 O
ATOM 1599 H SER A 194 -10.741 27.374 -45.301 1.00 15.78 H
ATOM 1600 HA SER A 194 -12.505 27.888 -43.431 1.00 15.59 H
ATOM 1601 HB2 SER A 194 -10.506 27.100 -42.684 1.00 18.57 H
ATOM 1602 HB3 SER A 194 -9.701 28.226 -43.466 1.00 18.57 H
ATOM 1603 HG SER A 194 -9.875 28.710 -41.333 1.00 19.09 H
ATOM 1604 N SER A 195 -12.803 30.394 -43.191 1.00 13.88 N
ATOM 1605 CA SER A 195 -13.586 29.735 -42.148 1.00 14.38 C
ATOM 1606 C SER A 195 -15.056 29.686 -42.571 1.00 18.17 C
ATOM 1607 O SER A 195 -15.731 30.717 -42.606 1.00 15.70 O
ATOM 1608 CB SER A 195 -13.442 30.477 -40.821 1.00 15.67 C
ATOM 1609 OG SER A 195 -14.164 29.810 -39.798 1.00 20.71 O
ATOM 1610 H SER A 195 -12.941 31.242 -43.215 1.00 16.65 H
ATOM 1611 HA SER A 195 -13.268 28.826 -42.029 1.00 17.26 H
ATOM 1612 HB2 SER A 195 -12.503 30.510 -40.577 1.00 18.81 H
ATOM 1613 HB3 SER A 195 -13.791 31.376 -40.922 1.00 18.81 H
ATOM 1614 HG SER A 195 -14.080 30.224 -39.071 1.00 24.86 H
ATOM 1615 N PHE A 196 -15.542 28.492 -42.898 1.00 14.12 N
ATOM 1616 CA PHE A 196 -16.912 28.314 -43.376 1.00 16.50 C
ATOM 1617 C PHE A 196 -17.212 29.262 -44.530 1.00 16.82 C
ATOM 1618 O PHE A 196 -18.205 29.992 -44.522 1.00 15.43 O
ATOM 1619 CB PHE A 196 -17.909 28.514 -42.233 1.00 19.48 C
ATOM 7886 OE1 GLU E 10 6.687 56.775 -38.234 1.00 36.09 O
ATOM 7887 OE2 GLU E 10 8.732 57.026 -38.988 1.00 36.34 O1-
ATOM 7888 H GLU E 10 5.958 51.949 -36.880 1.00 22.55 H
ATOM 7889 HA GLU E 10 8.608 52.534 -37.059 1.00 30.51 H
ATOM 7890 HB2 GLU E 10 7.230 53.788 -38.512 1.00 28.04 H
ATOM 7891 HB3 GLU E 10 6.471 54.375 -37.248 1.00 28.04 H
ATOM 7892 HG2 GLU E 10 8.438 55.462 -36.586 1.00 38.14 H
ATOM 7893 HG3 GLU E 10 9.174 54.897 -37.876 1.00 38.14 H
ATOM 7894 N ILE E 11 8.988 52.981 -34.703 1.00 28.61 N
ATOM 7895 CA ILE E 11 9.253 53.384 -33.326 1.00 25.78 C
ATOM 7896 C ILE E 11 10.184 54.588 -33.321 1.00 24.72 C
ATOM 7897 O ILE E 11 11.389 54.450 -33.528 1.00 24.06 O
ATOM 7898 CB ILE E 11 9.891 52.248 -32.498 1.00 31.17 C
ATOM 7899 CG1 ILE E 11 9.015 50.995 -32.536 1.00 30.05 C
ATOM 7900 CG2 ILE E 11 10.114 52.692 -31.056 1.00 30.83 C
ATOM 7901 CD1 ILE E 11 9.421 50.004 -33.599 1.00 30.44 C
ATOM 7902 H ILE E 11 9.662 52.612 -35.089 1.00 34.34 H
ATOM 7903 HA ILE E 11 8.420 53.640 -32.900 1.00 30.94 H
ATOM 7904 HB ILE E 11 10.752 52.031 -32.888 1.00 37.40 H
ATOM 7905 HG12 ILE E 11 9.070 50.548 -31.677 1.00 36.06 H
ATOM 7906 HG13 ILE E 11 8.098 51.259 -32.712 1.00 36.06 H
ATOM 7907 HG21 ILE E 11 10.515 51.962 -30.560 1.00 37.00 H
ATOM 7908 HG22 ILE E 11 10.706 53.461 -31.051 1.00 37.00 H
ATOM 7909 HG23 ILE E 11 9.259 52.930 -30.664 1.00 37.00 H
ATOM 7910 HD11 ILE E 11 8.824 49.240 -33.563 1.00 36.53 H
ATOM 7911 HD12 ILE E 11 9.361 50.431 -34.468 1.00 36.53 H
ATOM 7912 HD13 ILE E 11 10.334 49.719 -33.432 1.00 36.53 H
ATOM 7913 N ASN E 12 9.610 55.765 -33.095 1.00 26.17 N
ATOM 7914 CA ASN E 12 10.364 57.010 -33.023 1.00 30.19 C
ATOM 7915 C ASN E 12 10.274 57.565 -31.611 1.00 33.21 C
ATOM 7916 O ASN E 12 9.309 58.238 -31.259 1.00 28.03 O
ATOM 7917 CB ASN E 12 9.830 58.023 -34.042 1.00 28.09 C
ATOM 7918 CG ASN E 12 10.710 59.256 -34.166 1.00 34.34 C
ATOM 7919 OD1 ASN E 12 11.388 59.657 -33.218 1.00 28.23 O

ATOM 1620 CG PHE A 196 -17.900 27.392 -41.233 1.00 20.88 C
ATOM 1621 CD1 PHE A 196 -17.045 27.420 -40.146 1.00 19.36 C
ATOM 1622 CD2 PHE A 196 -18.734 26.300 -41.395 1.00 21.00 C
ATOM 1623 CE1 PHE A 196 -17.028 26.381 -39.233 1.00 22.54 C
ATOM 1624 CE2 PHE A 196 -18.722 25.259 -40.489 1.00 24.48 C
ATOM 1625 CZ PHE A 196 -17.868 25.297 -39.409 1.00 23.71 C
ATOM 1626 H PHE A 196 -15.093 27.760 -42.851 1.00 16.94 H
ATOM 1627 HA PHE A 196 -17.014 27.407 -43.703 1.00 19.80 H
ATOM 1628 HB2 PHE A 196 -17.689 29.334 -41.763 1.00 23.38 H
ATOM 1629 HB3 PHE A 196 -18.803 28.576 -42.603 1.00 23.38 H
ATOM 1630 HD1 PHE A 196 -16.476 28.146 -40.027 1.00 23.23 H
ATOM 1631 HD2 PHE A 196 -19.310 26.267 -42.125 1.00 25.20 H
ATOM 1632 HE1 PHE A 196 -16.451 26.410 -38.504 1.00 27.05 H
ATOM 1633 HE2 PHE A 196 -19.290 24.532 -40.608 1.00 29.38 H
ATOM 1634 HZ PHE A 196 -17.862 24.598 -38.795 1.00 28.45 H
ATOM 1635 N LYS A 197 -16.328 29.240 -45.519 1.00 12.88 N
ATOM 1636 CA LYS A 197 -16.488 30.028 -46.726 1.00 14.65 C
ATOM 1637 C LYS A 197 -16.602 29.102 -47.924 1.00 20.06 C
ATOM 1638 O LYS A 197 -16.201 27.937 -47.864 1.00 15.47 O
ATOM 1639 CB LYS A 197 -15.316 30.995 -46.902 1.00 17.78 C
ATOM 1640 CG LYS A 197 -15.280 32.100 -45.858 1.00 18.13 C
ATOM 1641 CD LYS A 197 -14.046 32.976 -45.998 1.00 21.25 C
ATOM 1642 CE LYS A 197 -14.128 34.170 -45.061 1.00 21.78 C
ATOM 1643 NZ LYS A 197 -12.877 34.972 -45.042 1.00 22.18 N1+
ATOM 1644 H LYS A 197 -15.612 28.764 -45.511 1.00 15.45 H
ATOM 1645 HA LYS A 197 -17.305 30.547 -46.664 1.00 17.58 H
ATOM 1646 HB2 LYS A 197 -14.486 30.497 -46.837 1.00 21.34 H
ATOM 1647 HB3 LYS A 197 -15.382 31.413 -47.775 1.00 21.34 H
ATOM 1648 HG2 LYS A 197 -16.063 32.662 -45.962 1.00 21.75 H
ATOM 1649 HG3 LYS A 197 -15.269 31.702 -44.973 1.00 21.75 H
ATOM 1650 HD2 LYS A 197 -13.257 32.461 -45.770 1.00 25.49 H
ATOM 1651 HD3 LYS A 197 -13.985 33.305 -46.908 1.00 25.49 H
ATOM 1652 HE2 LYS A 197 -14.851 34.749 -45.349 1.00 26.13 H
ATOM 1653 HE3 LYS A 197 -14.295 33.854 -44.159 1.00 26.13 H

ATOM 7920 ND2 ASN E 12 10.701 59.869 -35.347 1.00 37.26 N
ATOM 7921 H ASN E 12 8.765 55.869 -32.977 1.00 31.41 H
ATOM 7922 HA ASN E 12 11.297 56.834 -33.225 1.00 36.22 H
ATOM 7923 HB2 ASN E 12 9.784 57.599 -34.914 1.00 33.71 H
ATOM 7924 HB3 ASN E 12 8.947 58.312 -33.766 1.00 33.71 H
ATOM 7925 HD21 ASN E 12 11.181 60.571 -35.471 1.00 44.71 H
ATOM 7926 HD22 ASN E 12 10.214 59.562 -35.986 1.00 44.71 H

ATOM 7927 N GLY E 13 11.280 57.273 -30.797 1.00 33.39 N
ATOM 7928 CA GLY E 13 11.269 57.704 -29.414 1.00 37.75 C
ATOM 7929 C GLY E 13 10.163 57.015 -28.639 1.00 37.43 C
ATOM 7930 O GLY E 13 10.112 55.786 -28.582 1.00 37.21 O
ATOM 7931 H GLY E 13 11.979 56.827 -31.024 1.00 40.07 H
ATOM 7932 HA2 GLY E 13 12.120 57.492 -28.998 1.00 45.30 H
ATOM 7933 HA3 GLY E 13 11.130 58.663 -29.371 1.00 45.30 H

ATOM 7934 N SER E 14 9.260 57.809 -28.068 1.00 44.23 N
ATOM 7935 CA SER E 14 8.265 57.294 -27.129 1.00 48.10 C
ATOM 7936 C SER E 14 6.947 56.870 -27.780 1.00 45.20 C
ATOM 7937 O SER E 14 6.185 56.108 -27.185 1.00 44.70 O
ATOM 7938 CB SER E 14 7.978 58.343 -26.052 1.00 44.32 C
ATOM 7939 OG SER E 14 7.497 59.546 -26.627 1.00 49.63 O
ATOM 7940 H SER E 14 9.201 58.655 -28.209 1.00 53.08 H
ATOM 7941 HA SER E 14 8.635 56.514 -26.686 1.00 57.72 H
ATOM 7942 HB2 SER E 14 7.309 57.995 -25.444 1.00 53.18 H
ATOM 7943 HB3 SER E 14 8.799 58.531 -25.570 1.00 53.18 H
ATOM 7944 HG SER E 14 7.345 60.111 -26.024 1.00 59.56 H

ATOM 7945 N ASP E 15 6.670 57.358 -28.986 1.00 47.04 N
ATOM 7946 CA ASP E 15 5.445 56.970 -29.683 1.00 51.32 C
ATOM 7947 C ASP E 15 5.751 55.979 -30.804 1.00 46.88 C
ATOM 7948 O ASP E 15 6.834 55.997 -31.394 1.00 42.45 O
ATOM 7949 CB ASP E 15 4.707 58.201 -30.229 1.00 55.08 C
ATOM 7950 CG ASP E 15 5.515 58.970 -31.250 1.00 56.39 C
ATOM 7951 OD1 ASP E 15 6.755 58.979 -31.140 1.00 57.41 O
ATOM 7952 OD2 ASP E 15 4.907 59.575 -32.160 1.00 64.51 O1-
ATOM 7953 H ASP E 15 7.168 57.909 -29.420 1.00 56.44 H

ATOM 1654 HZ1 LYS A 197 -12.703 35.282 -45.858 1.00 26.61 H
ATOM 1655 HZ2 LYS A 197 -12.965 35.659 -44.484 1.00 26.61 H
ATOM 1656 HZ3 LYS A 197 -12.196 34.466 -44.774 1.00 26.61 H
ATOM 1657 N GLY A 198 -17.172 29.632 -49.001 1.00 21.19 N
ATOM 1658 CA GLY A 198 -17.291 28.916 -50.256 1.00 20.02 C
ATOM 1659 C GLY A 198 -16.977 29.862 -51.394 1.00 18.77 C
ATOM 1660 O GLY A 198 -17.644 30.880 -51.561 1.00 21.65 O
ATOM 1661 H GLY A 198 -17.505 30.424 -49.026 1.00 25.43 H
ATOM 1662 HA2 GLY A 198 -16.667 28.173 -50.278 1.00 24.02 H
ATOM 1663 HA3 GLY A 198 -18.193 28.577 -50.364 1.00 24.02 H
ATOM 1664 N TYR A 199 -15.942 29.535 -52.160 1.00 17.44 N
ATOM 1665 CA TYR A 199 -15.521 30.351 -53.289 1.00 16.54 C
ATOM 1666 C TYR A 199 -16.048 29.768 -54.591 1.00 23.54 C
ATOM 1667 O TYR A 199 -15.735 28.630 -54.944 1.00 19.00 O
ATOM 1668 CB TYR A 199 -13.997 30.446 -53.349 1.00 17.44 C
ATOM 1669 CG TYR A 199 -13.376 31.238 -52.222 1.00 14.05 C
ATOM 1670 CD1 TYR A 199 -13.236 30.689 -50.958 1.00 15.06 C
ATOM 1671 CD2 TYR A 199 -12.912 32.529 -52.432 1.00 17.40 C
ATOM 1672 CE1 TYR A 199 -12.663 31.410 -49.926 1.00 17.88 C
ATOM 1673 CE2 TYR A 199 -12.332 33.255 -51.409 1.00 15.39 C
ATOM 1674 CZ TYR A 199 -12.213 32.690 -50.156 1.00 15.83 C
ATOM 1675 OH TYR A 199 -11.637 33.406 -49.131 1.00 18.67 O
ATOM 1676 H TYR A 199 -15.461 28.832 -52.043 1.00 20.93 H
ATOM 1677 HA TYR A 199 -15.878 31.247 -53.189 1.00 19.84 H
ATOM 1678 HB2 TYR A 199 -13.629 29.549 -53.316 1.00 20.92 H
ATOM 1679 HB3 TYR A 199 -13.745 30.872 -54.183 1.00 20.92 H
ATOM 1680 HD1 TYR A 199 -13.541 29.825 -50.798 1.00 18.08 H
ATOM 1681 HD2 TYR A 199 -12.992 32.912 -53.275 1.00 20.88 H
ATOM 1682 HE1 TYR A 199 -12.579 31.030 -49.082 1.00 21.46 H
ATOM 1683 HE2 TYR A 199 -12.029 34.120 -51.564 1.00 18.47 H
ATOM 1684 HH TYR A 199 -11.626 32.945 -48.429 1.00 22.40 H
ATOM 1685 N ILE A 200 -16.841 30.552 -55.309 1.00 22.64 N
ATOM 1686 CA ILE A 200 -17.424 30.090 -56.558 1.00 23.49 C
ATOM 1687 C ILE A 200 -16.323 29.921 -57.600 1.00 24.43 C

ATOM 7954 HA ASP E 15 4.855 56.529 -29.052 1.00 61.58 H
ATOM 7955 HB2 ASP E 15 3.884 57.913 -30.654 1.00 66.10 H
ATOM 7956 HB3 ASP E 15 4.507 58.801 -29.493 1.00 66.10 H

ATOM 7957 N THR E 16 4.790 55.100 -31.069 1.00 40.99 N

ATOM 7958 CA THR E 16 4.933 54.071 -32.088 1.00 35.68 C

ATOM 7959 C THR E 16 3.735 54.097 -33.026 1.00 38.72 C

ATOM 7960 O THR E 16 2.618 54.422 -32.613 1.00 33.45 O

ATOM 7961 CB THR E 16 5.068 52.671 -31.464 1.00 38.05 C
ATOM 7962 OG1 THR E 16 3.910 52.381 -30.674 1.00 48.80 O
ATOM 7963 CG2 THR E 16 6.302 52.596 -30.585 1.00 39.99 C

ATOM 7964 H THR E 16 4.032 55.080 -30.662 1.00 49.19 H

ATOM 7965 HA THR E 16 5.731 54.249 -32.611 1.00 42.82 H

ATOM 7966 HB THR E 16 5.153 52.009 -32.168 1.00 45.66 H
ATOM 7967 HG1 THR E 16 3.980 51.618 -30.331 1.00 58.56 H
ATOM 7968 HG21 THR E 16 6.378 51.711 -30.196 1.00 47.99 H
ATOM 7969 HG22 THR E 16 7.095 52.779 -31.112 1.00 47.99 H
ATOM 7970 HG23 THR E 16 6.240 53.250 -29.871 1.00 47.99 H

ATOM 7971 N HIS E 17 3.974 53.758 -34.290 1.00 31.94 N

ATOM 7972 CA HIS E 17 2.917 53.737 -35.295 1.00 33.04 C

ATOM 7973 C HIS E 17 2.903 52.408 -36.036 1.00 25.75 C

ATOM 7974 O HIS E 17 3.919 51.976 -36.579 1.00 21.85 O

ATOM 7975 CB HIS E 17 3.093 54.890 -36.284 1.00 33.14 C

ATOM 7976 CG HIS E 17 3.093 56.242 -35.639 1.00 43.36 C

ATOM 7977 ND1 HIS E 17 4.224 56.801 -35.083 1.00 49.33 N

ATOM 7978 CD2 HIS E 17 2.098 57.141 -35.454 1.00 48.56 C

ATOM 7979 CE1 HIS E 17 3.926 57.989 -34.587 1.00 47.74 C

ATOM 7980 NE2 HIS E 17 2.643 58.219 -34.799 1.00 51.13 N

ATOM 7981 H HIS E 17 4.747 53.533 -34.592 1.00 38.33 H

ATOM 7982 HA HIS E 17 2.059 53.846 -34.855 1.00 39.65 H

ATOM 7983 HB2 HIS E 17 3.940 54.781 -36.744 1.00 39.77 H

ATOM 7984 HB3 HIS E 17 2.365 54.867 -36.924 1.00 39.77 H

ATOM 7985 HD1 HIS E 17 5.001 56.435 -35.063 1.00 59.20 H

ATOM 7986 HD2 HIS E 17 1.213 57.048 -35.722 1.00 58.27 H

ATOM 7987 HE1 HIS E 17 4.519 58.565 -34.161 1.00 57.28 H

ATOM 1688 O ILE A 200 -15.491 30.808 -57.790 1.00 21.73
O
ATOM 1689 CB ILE A 200 -18.499 31.059 -57.068 1.00 24.34
C
ATOM 1690 CG1 ILE A 200 -19.571 31.263 -55.989 1.00 24.68
C
ATOM 1691 CG2 ILE A 200 -19.121 30.526 -58.354 1.00 27.39
C
ATOM 1692 CD1 ILE A 200 -20.587 32.342 -56.308 1.00 32.82
C
ATOM 1693 H ILE A 200 -17.058 31.356 -55.094 1.00 27.17
H
ATOM 1694 HA ILE A 200 -17.840 29.226 -56.415 1.00 28.19
H
ATOM 1695 HB ILE A 200 -18.082 31.915 -57.257 1.00 29.21
H
ATOM 1696 HG12 ILE A 200 -20.054 30.430 -55.870 1.00 29.61
H
ATOM 1697 HG13 ILE A 200 -19.133 31.508 -55.158 1.00 29.61
H
ATOM 1698 HG21 ILE A 200 -19.797 31.151 -58.660 1.00 32.86
H
ATOM 1699 HG22 ILE A 200 -18.427 30.433 -59.025 1.00 32.86
H
ATOM 1700 HG23 ILE A 200 -19.525 29.663 -58.174 1.00 32.86
H
ATOM 1701 HD11 ILE A 200 -21.223 32.403 -55.578 1.00 39.38
H
ATOM 1702 HD12 ILE A 200 -20.125 33.188 -56.417 1.00 39.38
H
ATOM 1703 HD13 ILE A 200 -21.048 32.108 -57.129 1.00 39.38
H
ATOM 1704 N GLU A 201 -16.330 28.769 -58.264 1.00 22.73
N
ATOM 1705 CA GLU A 201 -15.255 28.388 -59.169 1.00 24.00
C
ATOM 1706 C GLU A 201 -15.800 27.657 -60.392 1.00 25.50
C
ATOM 1707 O GLU A 201 -16.887 27.076 -60.350 1.00 22.40
O
ATOM 1708 CB GLU A 201 -14.244 27.508 -58.425 1.00 23.12
C
ATOM 1709 CG GLU A 201 -13.104 26.959 -59.269 1.00 25.67
C
ATOM 1710 CD GLU A 201 -12.274 28.048 -59.917 1.00 31.64
C
ATOM 1711 OE1 GLU A 201 -11.116 28.247 -59.490 1.00 34.45
O
ATOM 1712 OE2 GLU A 201 -12.777 28.700 -60.856 1.00 31.63
O1-
ATOM 1713 H GLU A 201 -16.957 28.184 -58.206 1.00 27.27
H
ATOM 1714 HA GLU A 201 -14.797 29.186 -59.473 1.00 28.80
H
ATOM 1715 HB2 GLU A 201 -13.849 28.032 -57.710 1.00 27.75
H
ATOM 1716 HB3 GLU A 201 -14.716 26.750 -58.047 1.00 27.75
H
ATOM 1717 HG2 GLU A 201 -12.518 26.432 -58.704 1.00 30.81
H
ATOM 1718 HG3 GLU A 201 -13.472 26.404 -59.974 1.00 30.81
H
ATOM 1719 N ASN A 202 -15.040 27.709 -61.480 1.00 26.48
N
ATOM 1720 CA ASN A 202 -15.344 26.948 -62.684 1.00 25.56
C
ATOM 1721 C ASN A 202 -15.316 25.452 -62.389 1.00 24.34
C

ATOM 7988 HE2 HIS E 17 2.218 58.929 -34.565 1.00 61.35 H

ATOM 7989 N SER E 18 1.744 51.762 -36.039 1.00 18.75 N

ATOM 7990 CA SER E 18 1.548 50.514 -36.761 1.00 18.70 C

ATOM 7991 C SER E 18 0.600 50.766 -37.917 1.00 22.66 C

ATOM 7992 O SER E 18 -0.503 51.269 -37.710 1.00 22.11 O

ATOM 7993 CB SER E 18 0.987 49.434 -35.839 1.00 21.15 C
ATOM 7994 OG SER E 18 1.713 49.382 -34.625 1.00 25.66
O

ATOM 7995 H SER E 18 1.042 52.032 -35.621 1.00 22.50 H

ATOM 7996 HA SER E 18 2.396 50.207 -37.118 1.00 22.43 H
ATOM 7997 HB2 SER E 18 0.059 49.637 -35.643 1.00 25.38
H
ATOM 7998 HB3 SER E 18 1.052 48.574 -36.283 1.00 25.38
H
ATOM 7999 HG SER E 18 1.396 48.785 -34.125 1.00 30.79
H

ATOM 8000 N THR E 19 1.029 50.431 -39.131 1.00 16.84 N

ATOM 8001 CA THR E 19 0.194 50.639 -40.306 1.00 18.45 C

ATOM 8002 C THR E 19 0.315 49.485 -41.295 1.00 15.64 C

ATOM 8003 O THR E 19 1.355 48.834 -41.386 1.00 15.74 O

ATOM 8004 CB THR E 19 0.553 51.957 -41.024 1.00 19.60 C
ATOM 8005 OG1 THR E 19 1.853 51.848 -41.611 1.00 27.97
O
ATOM 8006 CG2 THR E 19 0.540 53.128 -40.050 1.00 25.33
C

ATOM 8007 H THR E 19 1.798 50.084 -39.299 1.00 20.21 H
ATOM 8008 HA THR E 19 -0.733 50.696 -40.025 1.00 22.14
H
ATOM 8009 HB THR E 19 -0.100 52.132 -41.720 1.00 23.52
H
ATOM 8010 HG1 THR E 19 2.425 51.696 -41.015 1.00 33.57
H
ATOM 8011 HG21 THR E 19 0.766 53.948 -40.514 1.00 30.39
H
ATOM 8012 HG22 THR E 19 -0.342 53.221 -39.657 1.00 30.39
H
ATOM 8013 HG23 THR E 19 1.186 52.977 -39.342 1.00 30.39
H

ATOM 8014 N VAL E 20 -0.767 49.227 -42.020 1.00 13.81 N

ATOM 8015 CA VAL E 20 -0.733 48.293 -43.138 1.00 13.33 C

ATOM 8016 C VAL E 20 -1.448 48.899 -44.341 1.00 17.42 C

ATOM 8017 O VAL E 20 -2.502 49.514 -44.192 1.00 15.32 O

ATOM 8018 CB VAL E 20 -1.387 46.947 -42.794 1.00 13.54 C
ATOM 8019 CG1 VAL E 20 -1.103 45.934 -43.893 1.00 12.41
C
ATOM 8020 CG2 VAL E 20 -0.887 46.429 -41.450 1.00 15.63
C

ATOM 8021 H VAL E 20 -1.538 49.583 -41.884 1.00 16.57 H

ATOM 1722 O ASN A 202 -14.295 24.914 -61.967 1.00 26.28 O
ATOM 1723 CB ASN A 202 -14.343 27.294 -63.788 1.00 29.63 C
ATOM 1724 CG ASN A 202 -14.689 26.660 -65.123 1.00 31.70 C
ATOM 1725 OD1 ASN A 202 -15.292 25.589 -65.187 1.00 30.51 O
ATOM 1726 ND2 ASN A 202 -14.297 27.323 -66.203 1.00 38.46 N
ATOM 1727 H ASN A 202 -14.328 28.187 -61.546 1.00 31.77 H
ATOM 1728 HA ASN A 202 -16.234 27.180 -62.994 1.00 30.67 H
ATOM 1729 HB2 ASN A 202 -14.329 28.256 -63.910 1.00 35.55 H
ATOM 1730 HB3 ASN A 202 -13.464 26.980 -63.526 1.00 35.55 H
ATOM 1731 HD21 ASN A 202 -14.466 27.009 -66.985 1.00 46.15 H
ATOM 1732 HD22 ASN A 202 -13.873 28.067 -66.121 1.00 46.15 H
ATOM 1733 N CYS A 203 -16.440 24.785 -62.627 1.00 28.75 N
ATOM 1734 CA CYS A 203 -16.574 23.364 -62.325 1.00 25.56 C
ATOM 1735 C CYS A 203 -15.508 22.513 -63.014 1.00 26.17 C
ATOM 1736 O CYS A 203 -15.174 21.430 -62.539 1.00 23.90 O
ATOM 1737 CB CYS A 203 -17.967 22.874 -62.726 1.00 25.82 C
ATOM 1738 SG CYS A 203 -19.313 23.627 -61.778 1.00 33.04 S
ATOM 1739 H CYS A 203 -17.148 25.136 -62.966 1.00 34.50 H
ATOM 1740 HA CYS A 203 -16.479 23.238 -61.368 1.00 30.67 H
ATOM 1741 HB2 CYS A 203 -18.112 23.081 -63.663 1.00 30.99 H
ATOM 1742 HB3 CYS A 203 -18.011 21.914 -62.592 1.00 30.99 H
ATOM 1743 N SER A 204 -14.962 23.015 -64.118 1.00 26.58 N
ATOM 1744 CA SER A 204 -14.011 22.250 -64.918 1.00 28.83 C
ATOM 1745 C SER A 204 -12.568 22.426 -64.464 1.00 29.48 C
ATOM 1746 O SER A 204 -11.670 21.765 -64.980 1.00 30.84 O
ATOM 1747 CB SER A 204 -14.130 22.646 -66.391 1.00 34.76 C
ATOM 1748 OG SER A 204 -15.399 22.282 -66.905 1.00 36.78 O
ATOM 1749 H SER A 204 -15.127 23.801 -64.426 1.00 31.89 H
ATOM 1750 HA SER A 204 -14.230 21.308 -64.847 1.00 34.60 H
ATOM 1751 HB2 SER A 204 -14.020 23.607 -66.470 1.00 41.72 H
ATOM 1752 HB3 SER A 204 -13.440 22.190 -66.898 1.00 41.72 H
ATOM 1753 HG SER A 204 -15.456 22.503 -67.713 1.00 44.13 H
ATOM 1754 N THR A 205 -12.342 23.313 -63.501 1.00 30.18 N
ATOM 1755 CA THR A 205 -10.991 23.564 -63.010 1.00 31.93 C

ATOM 8022 HA VAL E 20 0.190 48.127 -43.386 1.00 16.00 H
ATOM 8023 HB VAL E 20 -2.348 47.066 -42.734 1.00 16.24 H
ATOM 8024 HG11 VAL E 20 -1.522 45.091 -43.660 1.00 14.89 H
ATOM 8025 HG12 VAL E 20 -1.466 46.266 -44.729 1.00 14.89 H
ATOM 8026 HG13 VAL E 20 -0.144 45.816 -43.972 1.00 14.89 H
ATOM 8027 HG21 VAL E 20 -1.316 45.580 -41.260 1.00 18.75 H
ATOM 8028 HG22 VAL E 20 0.075 46.311 -41.496 1.00 18.75 H
ATOM 8029 HG23 VAL E 20 -1.109 47.074 -40.761 1.00 18.75 H

ATOM 8030 N ASP E 21 -0.848 48.729 -45.518 1.00 15.97 N
ATOM 8031 CA ASP E 21 -1.440 49.125 -46.794 1.00 21.15 C
ATOM 8032 C ASP E 21 -1.657 47.896 -47.664 1.00 18.26 C
ATOM 8033 O ASP E 21 -0.754 47.072 -47.817 1.00 17.18 O
ATOM 8034 CB ASP E 21 -0.544 50.116 -47.543 1.00 22.93 C
ATOM 8035 CG ASP E 21 -0.289 51.386 -46.761 1.00 24.35 C
ATOM 8036 OD1 ASP E 21 -1.220 51.871 -46.088 1.00 25.88 O1-
ATOM 8037 OD2 ASP E 21 0.849 51.897 -46.822 1.00 27.99 O

ATOM 8038 H ASP E 21 -0.070 48.373 -45.604 1.00 19.17 H
ATOM 8039 HA ASP E 21 -2.300 49.546 -46.635 1.00 25.38 H
ATOM 8040 HB2 ASP E 21 0.312 49.696 -47.720 1.00 27.51 H
ATOM 8041 HB3 ASP E 21 -0.973 50.360 -48.378 1.00 27.51 H

ATOM 8042 N VAL E 22 -2.853 47.775 -48.230 1.00 15.73 N
ATOM 8043 CA VAL E 22 -3.147 46.699 -49.170 1.00 16.91 C
ATOM 8044 C VAL E 22 -3.314 47.289 -50.559 1.00 18.18 C
ATOM 8045 O VAL E 22 -4.196 48.120 -50.785 1.00 18.14 O
ATOM 8046 CB VAL E 22 -4.411 45.929 -48.787 1.00 13.15 C
ATOM 8047 CG1 VAL E 22 -4.570 44.701 -49.670 1.00 18.48 C
ATOM 8048 CG2 VAL E 22 -4.362 45.523 -47.319 1.00 14.73 C

ATOM 8049 H VAL E 22 -3.514 48.305 -48.086 1.00 18.88 H
ATOM 8050 HA VAL E 22 -2.403 46.077 -49.189 1.00 20.29 H
ATOM 8051 HB VAL E 22 -5.184 46.499 -48.919 1.00 15.79 H
ATOM 8052 HG11 VAL E 22 -5.376 44.228 -49.411 1.00 22.17 H
ATOM 8053 HG12 VAL E 22 -4.635 44.985 -50.595 1.00 22.17 H
ATOM 8054 HG13 VAL E 22 -3.797 44.127 -49.554 1.00 22.17 H
ATOM 8055 HG21 VAL E 22 -5.172 45.036 -47.099 1.00 17.68 H

ATOM 1756 C THR A 205 -10.595 22.490 -62.002 1.00 26.32 C
ATOM 1757 O THR A 205 -11.300 22.280 -61.017 1.00 27.11 O
ATOM 1758 CB THR A 205 -10.880 24.953 -62.354 1.00 30.33 C
ATOM 1759 OG1 THR A 205 -11.195 25.962 -63.322 1.00 32.74 O
ATOM 1760 CG2 THR A 205 -9.473 25.195 -61.822 1.00 28.31 C
ATOM 1761 H THR A 205 -12.951 23.783 -63.117 1.00 36.22 H
ATOM 1762 HA THR A 205 -10.369 23.528 -63.753 1.00 38.32 H
ATOM 1763 HB THR A 205 -11.503 25.011 -61.613 1.00 36.40 H
ATOM 1764 HG1 THR A 205 -10.660 25.917 -63.968 1.00 39.29 H
ATOM 1765 HG21 THR A 205 -9.420 26.073 -61.413 1.00 33.97 H
ATOM 1766 HG22 THR A 205 -9.250 24.524 -61.158 1.00 33.97 H
ATOM 1767 HG23 THR A 205 -8.831 25.146 -62.547 1.00 33.97 H
ATOM 1768 N PRO A 206 -9.462 21.808 -62.235 1.00 25.18 N
ATOM 1769 CA PRO A 206 -9.108 20.744 -61.290 1.00 27.92 C
ATOM 1770 C PRO A 206 -8.728 21.285 -59.913 1.00 27.31 C
ATOM 1771 O PRO A 206 -8.020 22.285 -59.806 1.00 24.19 O
ATOM 1772 CB PRO A 206 -7.918 20.051 -61.963 1.00 27.16 C
ATOM 1773 CG PRO A 206 -7.340 21.073 -62.876 1.00 35.92 C
ATOM 1774 CD PRO A 206 -8.479 21.937 -63.326 1.00 32.59 C
ATOM 1775 HA PRO A 206 -9.839 20.113 -61.199 1.00 33.50 H
ATOM 1776 HB2 PRO A 206 -7.271 19.786 -61.290 1.00 32.59 H
ATOM 1777 HB3 PRO A 206 -8.229 19.280 -62.463 1.00 32.59 H
ATOM 1778 HG2 PRO A 206 -6.683 21.600 -62.396 1.00 43.11 H
ATOM 1779 HG3 PRO A 206 -6.930 20.631 -63.636 1.00 43.11 H
ATOM 1780 HD2 PRO A 206 -8.189 22.859 -63.411 1.00 39.11 H
ATOM 1781 HD3 PRO A 206 -8.850 21.602 -64.157 1.00 39.11 H
ATOM 1782 N ASN A 207 -9.223 20.624 -58.873 1.00 24.26 N
ATOM 1783 CA ASN A 207 -8.923 20.983 -57.492 1.00 25.76 C
ATOM 1784 C ASN A 207 -8.955 19.741 -56.616 1.00 23.33 C
ATOM 1785 O ASN A 207 -9.560 18.734 -56.988 1.00 20.60 O
ATOM 1786 CB ASN A 207 -9.927 22.010 -56.957 1.00 23.82 C
ATOM 1787 CG ASN A 207 -9.620 23.423 -57.405 1.00 27.43 C
ATOM 1788 OD1 ASN A 207 -8.771 24.097 -56.822 1.00 28.42 O
ATOM 1789 ND2 ASN A 207 -10.327 23.889 -58.430 1.00 23.94 N
ATOM 8056 HG22 VAL E 22 -3.587 44.958 -47.173 1.00 17.68 H
ATOM 8057 HG23 VAL E 22 -4.298 46.322 -46.773 1.00 17.68 H

ATOM 8058 N ASP E 23 -2.464 46.854 -51.482 1.00 15.34 N

ATOM 8059 CA ASP E 23 -2.482 47.357 -52.849 1.00 19.21 C

ATOM 8060 C ASP E 23 -2.905 46.259 -53.817 1.00 19.78 C

ATOM 8061 O ASP E 23 -2.353 45.158 -53.794 1.00 18.41 O

ATOM 8062 CB ASP E 23 -1.103 47.894 -53.253 1.00 21.71 C
ATOM 8063 CG ASP E 23 -0.614 49.015 -52.347 1.00 27.17 C
ATOM 8064 OD1 ASP E 23 -1.453 49.705 -51.735 1.00 25.29 O
ATOM 8065 OD2 ASP E 23 0.618 49.212 -52.256 1.00 37.02 O1-

ATOM 8066 H ASP E 23 -1.859 46.260 -51.339 1.00 18.40 H

ATOM 8067 HA ASP E 23 -3.122 48.083 -52.914 1.00 23.05 H
ATOM 8068 HB2 ASP E 23 -0.458 47.171 -53.209 1.00 26.06 H
ATOM 8069 HB3 ASP E 23 -1.152 48.240 -54.157 1.00 26.06 H

ATOM 8070 N LEU E 24 -3.888 46.567 -54.659 1.00 16.92 N

ATOM 8071 CA LEU E 24 -4.251 45.703 -55.777 1.00 17.78 C

ATOM 8072 C LEU E 24 -3.735 46.318 -57.072 1.00 20.26 C

ATOM 8073 O LEU E 24 -4.165 47.398 -57.462 1.00 21.27 O

ATOM 8074 CB LEU E 24 -5.768 45.506 -55.844 1.00 17.65 C
ATOM 8075 CG LEU E 24 -6.282 44.629 -56.988 1.00 20.38 C
ATOM 8076 CD1 LEU E 24 -5.743 43.211 -56.874 1.00 20.35 C
ATOM 8077 CD2 LEU E 24 -7.803 44.623 -57.009 1.00 21.16 C

ATOM 8078 H LEU E 24 -4.365 47.280 -54.603 1.00 20.30 H

ATOM 8079 HA LEU E 24 -3.835 44.834 -55.662 1.00 21.34 H
ATOM 8080 HB2 LEU E 24 -6.060 45.098 -55.014 1.00 21.18 H
ATOM 8081 HB3 LEU E 24 -6.184 46.377 -55.938 1.00 21.18 H
ATOM 8082 HG LEU E 24 -5.973 44.999 -57.831 1.00 24.45 H
ATOM 8083 HD11 LEU E 24 -6.087 42.683 -57.612 1.00 24.42 H
ATOM 8084 HD12 LEU E 24 -4.774 43.237 -56.909 1.00 24.42 H
ATOM 8085 HD13 LEU E 24 -6.034 42.830 -56.031 1.00 24.42 H
ATOM 8086 HD21 LEU E 24 -8.106 44.062 -57.740 1.00 25.39 H
ATOM 8087 HD22 LEU E 24 -8.128 44.271 -56.165 1.00 25.39 H
ATOM 8088 HD23 LEU E 24 -8.120 45.531 -57.134 1.00 25.39 H

ATOM 8089 N ASP E 25 -2.807 45.630 -57.729 1.00 19.76 N

ATOM 1790 H ASN A 207 -9.749 19.947 -58.944 1.00 29.12
H
ATOM 1791 HA ASN A 207 -8.034 21.369 -57.444 1.00 30.91
H
ATOM 1792 HB2 ASN A 207 -10.813 21.780 -57.276 1.00 28.58
H
ATOM 1793 HB3 ASN A 207 -9.909 21.993 -55.987 1.00 28.58
H
ATOM 1794 HD21 ASN A 207 -10.189 24.687 -58.721 1.00 28.73
H
ATOM 1795 HD22 ASN A 207 -10.923 23.393 -58.803 1.00 28.73
H
ATOM 1796 N THR A 208 -8.312 19.815 -55.454 1.00 22.57
N
ATOM 1797 CA THR A 208 -8.444 18.773 -54.443 1.00 19.78
C
ATOM 1798 C THR A 208 -9.888 18.768 -53.954 1.00 16.39
C
ATOM 1799 O THR A 208 -10.620 19.723 -54.195 1.00 15.26
O
ATOM 1800 CB THR A 208 -7.479 18.998 -53.260 1.00 20.25
C
ATOM 1801 OG1 THR A 208 -7.743 20.271 -52.655 1.00 17.10
O
ATOM 1802 CG2 THR A 208 -6.032 18.957 -53.738 1.00 20.83
C
ATOM 1803 H THR A 208 -7.792 20.461 -55.227 1.00 27.08
H
ATOM 1804 HA THR A 208 -8.249 17.909 -54.840 1.00 23.73
H
ATOM 1805 HB THR A 208 -7.605 18.296 -52.603 1.00 24.30
H
ATOM 1806 HG1 THR A 208 -7.219 20.397 -52.010 1.00 20.52
H
ATOM 1807 HG21 THR A 208 -5.432 19.099 -52.989 1.00 24.99
H
ATOM 1808 HG22 THR A 208 -5.839 18.094 -54.137 1.00 24.99
H
ATOM 1809 HG23 THR A 208 -5.881 19.650 -54.399 1.00 24.99
H
ATOM 1810 N TYR A 209 -10.303 17.702 -53.277 1.00 16.05
N
ATOM 1811 CA TYR A 209 -11.692 17.583 -52.843 1.00 17.55
C
ATOM 1812 C TYR A 209 -11.836 16.812 -51.533 1.00 16.31
C
ATOM 1813 O TYR A 209 -10.928 16.090 -51.112 1.00 16.24
O
ATOM 1814 CB TYR A 209 -12.534 16.920 -53.941 1.00 17.25
C
ATOM 1815 CG TYR A 209 -12.030 15.571 -54.393 1.00 14.62
C
ATOM 1816 CD1 TYR A 209 -10.964 15.467 -55.276 1.00 19.20
C
ATOM 1817 CD2 TYR A 209 -12.633 14.401 -53.955 1.00 18.23
C
ATOM 1818 CE1 TYR A 209 -10.499 14.234 -55.695 1.00 22.13
C
ATOM 1819 CE2 TYR A 209 -12.175 13.160 -54.372 1.00 21.56
C
ATOM 1820 CZ TYR A 209 -11.107 13.085 -55.243 1.00 22.08
C
ATOM 1821 OH TYR A 209 -10.644 11.857 -55.664 1.00 21.65
O
ATOM 1822 H TYR A 209 -9.804 17.037 -53.057 1.00 19.26
H
ATOM 1823 HA TYR A 209 -12.048 18.474 -52.698 1.00 21.06
H

ATOM 8090 CA ASP E 25 -2.193 46.137 -58.953 1.00 22.73 C

ATOM 8091 C ASP E 25 -1.618 47.542 -58.756 1.00 27.17 C

ATOM 8092 O ASP E 25 -1.913 48.462 -59.520 1.00 23.98 O

ATOM 8093 CB ASP E 25 -3.211 46.124 -60.095 1.00 21.06 C
ATOM 8094 CG ASP E 25 -3.666 44.718 -60.449 1.00 22.08
C
ATOM 8095 OD1 ASP E 25 -2.862 43.783 -60.271 1.00 20.88
O
ATOM 8096 OD2 ASP E 25 -4.820 44.541 -60.895 1.00 23.06
O1-

ATOM 8097 H ASP E 25 -2.513 44.860 -57.485 1.00 23.71 H

ATOM 8098 HA ASP E 25 -1.462 45.550 -59.201 1.00 27.28 H
ATOM 8099 HB2 ASP E 25 -3.992 46.636 -59.830 1.00 25.27
H
ATOM 8100 HB3 ASP E 25 -2.807 46.518 -60.884 1.00 25.27
H

ATOM 8101 N ASP E 26 -0.796 47.691 -57.720 1.00 25.96 N

ATOM 8102 CA ASP E 26 -0.129 48.958 -57.415 1.00 32.50 C

ATOM 8103 C ASP E 26 -1.125 50.097 -57.208 1.00 32.04 C

ATOM 8104 O ASP E 26 -0.835 51.257 -57.508 1.00 30.72 O

ATOM 8105 CB ASP E 26 0.862 49.324 -58.527 1.00 34.94 C
ATOM 8106 CG ASP E 26 2.007 48.334 -58.635 1.00 43.04
C
ATOM 8107 OD1 ASP E 26 2.488 47.863 -57.580 1.00 38.49
O
ATOM 8108 OD2 ASP E 26 2.426 48.024 -59.773 1.00 45.93
O1-

ATOM 8109 H ASP E 26 -0.603 47.061 -57.168 1.00 31.15 H

ATOM 8110 HA ASP E 26 0.375 48.854 -56.593 1.00 39.00 H
ATOM 8111 HB2 ASP E 26 0.394 49.337 -59.377 1.00 41.93
H
ATOM 8112 HB3 ASP E 26 1.237 50.199 -58.341 1.00 41.93
H

ATOM 8113 N SER E 27 -2.300 49.749 -56.696 1.00 27.41 N
ATOM 8114 CA SER E 27 -3.304 50.730 -56.305 1.00 26.12
C

ATOM 8115 C SER E 27 -3.839 50.370 -54.923 1.00 25.00 C

ATOM 8116 O SER E 27 -4.302 49.252 -54.707 1.00 22.30 O
ATOM 8117 CB SER E 27 -4.438 50.781 -57.328 1.00 27.19
C
ATOM 8118 OG SER E 27 -5.564 51.464 -56.803 1.00 35.60
O

ATOM 8119 H SER E 27 -2.544 48.935 -56.562 1.00 32.89 H
ATOM 8120 HA SER E 27 -2.895 51.608 -56.257 1.00 31.34
H
ATOM 8121 HB2 SER E 27 -4.128 51.247 -58.120 1.00 32.63
H
ATOM 8122 HB3 SER E 27 -4.697 49.874 -57.556 1.00 32.63
H
ATOM 8123 HG SER E 27 -6.179 51.484 -57.375 1.00 42.72
H

ATOM 1824 HB2 TYR A 209 -13.437 16.800 -53.608 1.00 20.70 H
ATOM 1825 HB3 TYR A 209 -12.547 17.504 -54.716 1.00 20.70 H
ATOM 1826 HD1 TYR A 209 -10.548 16.240 -55.582 1.00 23.04 H
ATOM 1827 HD2 TYR A 209 -13.351 14.449 -53.366 1.00 21.87 H
ATOM 1828 HE1 TYR A 209 -9.780 14.182 -56.283 1.00 26.56 H
ATOM 1829 HE2 TYR A 209 -12.585 12.383 -54.067 1.00 25.87 H
ATOM 1830 HH TYR A 209 -9.994 11.959 -56.187 1.00 25.99 H
ATOM 1831 N ILE A 210 -12.986 16.991 -50.892 1.00 14.44 N
ATOM 1832 CA ILE A 210 -13.276 16.355 -49.617 1.00 13.02 C
ATOM 1833 C ILE A 210 -14.502 15.475 -49.750 1.00 14.98 C
ATOM 1834 O ILE A 210 -15.563 15.937 -50.175 1.00 15.19 O
ATOM 1835 CB ILE A 210 -13.520 17.394 -48.506 1.00 15.09 C
ATOM 1836 CG1 ILE A 210 -12.293 18.294 -48.337 1.00 18.45 C
ATOM 1837 CG2 ILE A 210 -13.860 16.695 -47.190 1.00 15.58 C
ATOM 1838 CD1 ILE A 210 -12.516 19.483 -47.404 1.00 16.93 C
ATOM 1839 H ILE A 210 -13.625 17.487 -51.184 1.00 17.32 H
ATOM 1840 HA ILE A 210 -12.526 15.798 -49.356 1.00 15.62 H
ATOM 1841 HB ILE A 210 -14.274 17.948 -48.763 1.00 18.10 H
ATOM 1842 HG12 ILE A 210 -11.566 17.764 -47.974 1.00 22.14 H
ATOM 1843 HG13 ILE A 210 -12.042 18.643 -49.207 1.00 22.14 H
ATOM 1844 HG21 ILE A 210 -14.010 17.366 -46.506 1.00 18.70 H
ATOM 1845 HG22 ILE A 210 -14.662 16.164 -47.313 1.00 18.70 H
ATOM 1846 HG23 ILE A 210 -13.119 16.123 -46.936 1.00 18.70 H
ATOM 1847 HD11 ILE A 210 -11.697 20.000 -47.351 1.00 20.32 H
ATOM 1848 HD12 ILE A 210 -13.232 20.033 -47.758 1.00 20.32 H
ATOM 1849 HD13 ILE A 210 -12.756 19.153 -46.524 1.00 20.32 H
ATOM 1850 N CYS A 211 -14.352 14.207 -49.383 1.00 13.79 N
ATOM 1851 CA CYS A 211 -15.472 13.276 -49.363 1.00 18.54 C
ATOM 1852 C CYS A 211 -15.996 13.147 -47.940 1.00 18.83 C
ATOM 1853 O CYS A 211 -15.243 13.306 -46.976 1.00 15.68 O
ATOM 1854 CB CYS A 211 -15.057 11.909 -49.912 1.00 19.87 C
ATOM 1855 SG CYS A 211 -14.655 11.923 -51.673 1.00 23.90 S
ATOM 1856 H CYS A 211 -13.604 13.859 -49.139 1.00 16.55 H
ATOM 1857 HA CYS A 211 -16.186 13.623 -49.920 1.00 22.25 H

ATOM 8124 N GLN E 28 -3.763 51.311 -53.985 1.00 20.78 N
ATOM 8125 CA GLN E 28 -4.183 51.043 -52.614 1.00 21.26 C
ATOM 8126 C GLN E 28 -5.695 50.879 -52.532 1.00 20.87 C
ATOM 8127 O GLN E 28 -6.443 51.709 -53.055 1.00 18.20 O
ATOM 8128 CB GLN E 28 -3.725 52.167 -51.683 1.00 22.63 C
ATOM 8129 CG GLN E 28 -3.899 51.850 -50.211 1.00 23.18 C
ATOM 8130 CD GLN E 28 -3.629 53.049 -49.326 1.00 23.30 C
ATOM 8131 OE1 GLN E 28 -4.462 53.945 -49.208 1.00 29.76 O
ATOM 8132 NE2 GLN E 28 -2.458 53.076 -48.708 1.00 25.07 N
ATOM 8133 H GLN E 28 -3.472 52.109 -54.117 1.00 24.94 H
ATOM 8134 HA GLN E 28 -3.774 50.217 -52.313 1.00 25.51 H
ATOM 8135 HB2 GLN E 28 -2.784 52.339 -51.840 1.00 27.15 H
ATOM 8136 HB3 GLN E 28 -4.242 52.964 -51.878 1.00 27.15 H
ATOM 8137 HG2 GLN E 28 -4.812 51.561 -50.054 1.00 27.82 H
ATOM 8138 HG3 GLN E 28 -3.279 51.147 -49.962 1.00 27.82 H
ATOM 8139 HE21 GLN E 28 -2.257 53.736 -48.194 1.00 30.08 H
ATOM 8140 HE22 GLN E 28 -1.897 52.433 -48.820 1.00 30.08 H
ATOM 8141 N ILE E 29 -6.137 49.807 -51.873 1.00 16.99 N
ATOM 8142 CA ILE E 29 -7.560 49.506 -51.751 1.00 18.10 C
ATOM 8143 C ILE E 29 -8.009 49.446 -50.291 1.00 17.82 C
ATOM 8144 O ILE E 29 -9.179 49.671 -49.990 1.00 16.96 O
ATOM 8145 CB ILE E 29 -7.919 48.170 -52.445 1.00 17.51 C
ATOM 8146 CG1 ILE E 29 -7.158 46.996 -51.819 1.00 18.43 C
ATOM 8147 CG2 ILE E 29 -7.625 48.259 -53.938 1.00 21.63 C
ATOM 8148 CD1 ILE E 29 -7.710 45.630 -52.204 1.00 14.47 C
ATOM 8149 H ILE E 29 -5.626 49.235 -51.484 1.00 20.39 H
ATOM 8150 HA ILE E 29 -8.065 50.211 -52.186 1.00 21.72 H
ATOM 8151 HB ILE E 29 -8.869 48.012 -52.331 1.00 21.02 H
ATOM 8152 HG12 ILE E 29 -6.233 47.034 -52.108 1.00 22.12 H
ATOM 8153 HG13 ILE E 29 -7.204 47.074 -50.853 1.00 22.12 H
ATOM 8154 HG21 ILE E 29 -7.855 47.415 -54.356 1.00 25.95 H
ATOM 8155 HG22 ILE E 29 -8.155 48.974 -54.322 1.00 25.95 H
ATOM 8156 HG23 ILE E 29 -6.681 48.443 -54.063 1.00 25.95 H
ATOM 8157 HD11 ILE E 29 -7.179 44.943 -51.771 1.00 17.36 H

ATOM 1858 HB2 CYS A 211 -14.272 11.605 -49.431 1.00 23.84
H
ATOM 1859 HB3 CYS A 211 -15.787 11.284 -49.779 1.00 23.84
H
ATOM 1860 N MET A 212 -17.290 12.865 -47.821 1.00 16.73
N
ATOM 1861 CA MET A 212 -17.952 12.779 -46.527 1.00 19.25
C
ATOM 1862 C MET A 212 -19.005 11.671 -46.513 1.00 21.41
C
ATOM 1863 O MET A 212 -19.713 11.464 -47.500 1.00 24.33
O
ATOM 1864 CB MET A 212 -18.598 14.124 -46.181 1.00 15.50
C
ATOM 1865 CG MET A 212 -19.443 14.128 -44.912 1.00 19.16
C
ATOM 1866 SD MET A 212 -20.263 15.719 -44.644 1.00 21.71
S
ATOM 1867 CE MET A 212 -21.410 15.313 -43.333 1.00 26.47
C
ATOM 1868 H MET A 212 -17.813 12.717 -48.487 1.00 20.08
H
ATOM 1869 HA MET A 212 -17.286 12.586 -45.848 1.00 23.10
H
ATOM 1870 HB2 MET A 212 -17.896 14.783 -46.066 1.00 18.61
H
ATOM 1871 HB3 MET A 212 -19.174 14.388 -46.916 1.00 18.61
H
ATOM 1872 HG2 MET A 212 -20.127 13.444 -44.983 1.00 22.99
H
ATOM 1873 HG3 MET A 212 -18.871 13.951 -44.148 1.00 22.99
H
ATOM 1874 HE1 MET A 212 -21.917 16.107 -43.101 1.00 31.76
H
ATOM 1875 HE2 MET A 212 -22.009 14.616 -43.643 1.00 31.76
H
ATOM 1876 HE3 MET A 212 -20.910 15.002 -42.562 1.00 31.76
H
ATOM 1877 N GLN A 213 -19.090 10.969 -45.385 1.00 18.51
N
ATOM 1878 CA GLN A 213 -20.142 9.985 -45.123 1.00 26.68
C
ATOM 1879 C GLN A 213 -20.849 10.345 -43.823 1.00 25.55
C
ATOM 1880 O GLN A 213 -20.203 10.470 -42.781 1.00 22.83
O
ATOM 1881 CB GLN A 213 -19.567 8.571 -45.017 1.00 26.14
C
ATOM 1882 CG GLN A 213 -19.588 7.762 -46.297 1.00 36.07
C
ATOM 1883 CD GLN A 213 -19.101 6.337 -46.080 1.00 35.95
C
ATOM 1884 OE1 GLN A 213 -19.049 5.856 -44.949 1.00 38.02
O
ATOM 1885 NE2 GLN A 213 -18.738 5.658 -47.164 1.00 33.49
N
ATOM 1886 H GLN A 213 -18.531 11.047 -44.735 1.00 22.21
H
ATOM 1887 HA GLN A 213 -20.790 10.003 -45.844 1.00 32.01
H
ATOM 1888 HB2 GLN A 213 -18.643 8.636 -44.729 1.00 31.37
H
ATOM 1889 HB3 GLN A 213 -20.079 8.081 -44.354 1.00 31.37
H
ATOM 1890 HG2 GLN A 213 -20.497 7.722 -46.634 1.00 43.28
H
ATOM 1891 HG3 GLN A 213 -19.008 8.184 -46.950 1.00 43.28
H

ATOM 8158 HD12 ILE E 29 -8.632 45.570 -51.911 1.00 17.36
H
ATOM 8159 HD13 ILE E 29 -7.660 45.530 -53.167 1.00 17.36
H

ATOM 8160 N ILE E 30 -7.077 49.137 -49.395 1.00 16.02 N

ATOM 8161 CA ILE E 30 -7.363 49.058 -47.965 1.00 15.82 C

ATOM 8162 C ILE E 30 -6.210 49.679 -47.184 1.00 16.69 C

ATOM 8163 O ILE E 30 -5.058 49.618 -47.614 1.00 18.17 O

ATOM 8164 CB ILE E 30 -7.569 47.595 -47.501 1.00 16.57 C

ATOM 8165 CG1 ILE E 30 -8.733 46.939 -48.247 1.00 15.95 C

ATOM 8166 CG2 ILE E 30 -7.827 47.525 -46.004 1.00 17.26 C

ATOM 8167 CD1 ILE E 30 -8.751 45.428 -48.111 1.00 16.72 C

ATOM 8168 H ILE E 30 -6.258 48.966 -49.593 1.00 19.23 H

ATOM 8169 HA ILE E 30 -8.170 49.558 -47.769 1.00 18.99 H

ATOM 8170 HB ILE E 30 -6.761 47.096 -47.696 1.00 19.88 H
ATOM 8171 HG12 ILE E 30 -9.568 47.280 -47.890 1.00 19.14
H
ATOM 8172 HG13 ILE E 30 -8.664 47.153 -49.190 1.00 19.14
H
ATOM 8173 HG21 ILE E 30 -7.952 46.598 -45.749 1.00 20.72
H
ATOM 8174 HG22 ILE E 30 -7.065 47.899 -45.535 1.00 20.72
H
ATOM 8175 HG23 ILE E 30 -8.626 48.036 -45.798 1.00 20.72
H
ATOM 8176 HD11 ILE E 30 -9.509 45.076 -48.603 1.00 20.06
H
ATOM 8177 HD12 ILE E 30 -7.925 45.069 -48.473 1.00 20.06
H
ATOM 8178 HD13 ILE E 30 -8.829 45.196 -47.172 1.00 20.06
H

ATOM 8179 N THR E 31 -6.519 50.278 -46.039 1.00 16.82 N
ATOM 8180 CA THR E 31 -5.482 50.768 -45.141 1.00 15.25
C

ATOM 8181 C THR E 31 -5.893 50.529 -43.693 1.00 15.57 C

ATOM 8182 O THR E 31 -7.079 50.454 -43.371 1.00 17.03 O
ATOM 8183 CB THR E 31 -5.179 52.269 -45.372 1.00 20.77
C
ATOM 8184 OG1 THR E 31 -3.995 52.640 -44.653 1.00 24.59
O
ATOM 8185 CG2 THR E 31 -6.341 53.143 -44.936 1.00 22.38
C

ATOM 8186 H THR E 31 -7.322 50.414 -45.761 1.00 20.18 H
ATOM 8187 HA THR E 31 -4.665 50.271 -45.304 1.00 18.30
H
ATOM 8188 HB THR E 31 -5.032 52.418 -46.320 1.00 24.93
H
ATOM 8189 HG1 THR E 31 -3.342 52.184 -44.919 1.00 29.51
H
ATOM 8190 HG21 THR E 31 -6.130 54.077 -45.090 1.00 26.85
H
ATOM 8191 HG22 THR E 31 -7.137 52.913 -45.441 1.00 26.85
H

ATOM 1892 HE21 GLN A 213 -18.786 6.028 -47.939 1.00 40.19
H
ATOM 1893 HE22 GLN A 213 -18.456 4.849 -47.090 1.00 40.19
H
ATOM 1894 N ARG A 214 -22.169 10.497 -43.875 1.00 30.78
N
ATOM 1895 CA ARG A 214 -22.922 10.975 -42.717 1.00 39.00
C
ATOM 1896 C ARG A 214 -23.600 9.833 -41.967 1.00 50.04
C
ATOM 1897 O ARG A 214 -23.446 9.709 -40.749 1.00 47.20
O
ATOM 1898 CB ARG A 214 -23.958 12.010 -43.156 1.00 48.11
C
ATOM 1899 CG ARG A 214 -24.524 12.838 -42.013 1.00 41.27
C
ATOM 1900 CD ARG A 214 -24.916 14.231 -42.480 1.00 41.95
C
ATOM 1901 NE ARG A 214 -25.794 14.187 -43.648 1.00 45.75
N
ATOM 1902 CZ ARG A 214 -26.622 15.164 -44.006 1.00 46.72
C
ATOM 1903 NH1 ARG A 214 -26.706 16.278 -43.285 1.00 46.09
N
ATOM 1904 NH2 ARG A 214 -27.378 15.022 -45.084 1.00 46.67
N
ATOM 1905 H ARG A 214 -22.653 10.331 -44.566 1.00 36.93
H
ATOM 1906 HA ARG A 214 -22.310 11.410 -42.104 1.00 46.80
H
ATOM 1907 HB2 ARG A 214 -23.543 12.619 -43.786 1.00 57.73
H
ATOM 1908 HB3 ARG A 214 -24.698 11.550 -43.582 1.00 57.73
H
ATOM 1909 HG2 ARG A 214 -25.315 12.401 -41.661 1.00 49.52
H
ATOM 1910 HG3 ARG A 214 -23.852 12.928 -41.319 1.00 49.52
H
ATOM 1911 HD2 ARG A 214 -25.387 14.686 -41.765 1.00 50.35
H
ATOM 1912 HD3 ARG A 214 -24.116 14.723 -42.721 1.00 50.35
H
ATOM 1913 HE ARG A 214 -25.774 13.480 -44.137 1.00 54.90
H
ATOM 1914 HH11 ARG A 214 -26.219 16.374 -42.584 1.00 55.31
H
ATOM 1915 HH12 ARG A 214 -27.246 16.904 -43.523 1.00 55.31
H
ATOM 1916 HH21 ARG A 214 -27.328 14.302 -45.553 1.00 56.01
H
ATOM 1917 HH22 ARG A 214 -27.916 15.651 -45.318 1.00 56.01
H
ATOM 1918 N THR A 215 -24.349 9.007 -42.691 1.00 58.90
N
ATOM 1919 CA THR A 215 -24.978 7.827 -42.103 1.00 68.61
C
ATOM 1920 C THR A 215 -25.559 6.955 -43.210 1.00 64.97
C
ATOM 1921 O THR A 215 -26.049 7.466 -44.216 1.00 62.09
O
ATOM 1922 CB THR A 215 -26.083 8.217 -41.083 1.00 70.62
C
ATOM 1923 OG1 THR A 215 -25.689 7.809 -39.767 1.00 63.52
O
ATOM 1924 CG2 THR A 215 -27.433 7.574 -41.417 1.00 62.01
C
ATOM 1925 H THR A 215 -24.510 9.108 -43.530 1.00 70.68
H
ATOM 8192 HG23 THR E 31 -6.518 53.012 -43.991 1.00 26.85
H
ATOM 8193 N PHE E 32 -4.890 50.416 -42.831 1.00 15.94 N
ATOM 8194 CA PHE E 32 -5.070 50.053 -41.431 1.00 16.83
C
ATOM 8195 C PHE E 32 -4.106 50.905 -40.613 1.00 18.16 C
ATOM 8196 O PHE E 32 -2.923 50.965 -40.937 1.00 14.88 O
ATOM 8197 CB PHE E 32 -4.811 48.553 -41.239 1.00 12.85
C
ATOM 8198 CG PHE E 32 -4.831 48.096 -39.805 1.00 15.97
C
ATOM 8199 CD1 PHE E 32 -6.027 47.872 -39.151 1.00 15.86
C
ATOM 8200 CD2 PHE E 32 -3.646 47.864 -39.121 1.00 17.02
C
ATOM 8201 CE1 PHE E 32 -6.045 47.442 -37.834 1.00 20.56
C
ATOM 8202 CE2 PHE E 32 -3.658 47.430 -37.807 1.00 16.71
C
ATOM 8203 CZ PHE E 32 -4.858 47.220 -37.163 1.00 21.71 C
ATOM 8204 H PHE E 32 -4.067 50.549 -43.042 1.00 19.12 H
ATOM 8205 HA PHE E 32 -5.978 50.252 -41.154 1.00 20.19
H
ATOM 8206 HB2 PHE E 32 -5.494 48.056 -41.716 1.00 15.42
H
ATOM 8207 HB3 PHE E 32 -3.937 48.339 -41.603 1.00 15.42
H
ATOM 8208 HD1 PHE E 32 -6.829 48.021 -39.597 1.00 19.03
H
ATOM 8209 HD2 PHE E 32 -2.834 48.004 -39.551 1.00 20.42
H
ATOM 8210 HE1 PHE E 32 -6.857 47.300 -37.402 1.00 24.68
H
ATOM 8211 HE2 PHE E 32 -2.856 47.284 -37.358 1.00 20.05
H
ATOM 8212 HZ PHE E 32 -4.868 46.931 -36.279 1.00 26.05 H
ATOM 8213 N ASP E 33 -4.611 51.580 -39.580 1.00 21.77 N
ATOM 8214 CA ASP E 33 -3.809 52.557 -38.833 1.00 24.90 C
ATOM 8215 C ASP E 33 -3.354 52.053 -37.464 1.00 26.03 C
ATOM 8216 O ASP E 33 -2.901 52.838 -36.628 1.00 24.42 O
ATOM 8217 CB ASP E 33 -4.596 53.866 -38.656 1.00 23.77 C
ATOM 8218 CG ASP E 33 -5.878 53.692 -37.849 1.00 27.99
C
ATOM 8219 OD1 ASP E 33 -6.013 52.697 -37.102 1.00 26.15
O
ATOM 8220 OD2 ASP E 33 -6.762 54.571 -37.959 1.00 30.81
O1-
ATOM 8221 H ASP E 33 -5.415 51.492 -39.290 1.00 26.13 H
ATOM 8222 HA ASP E 33 -3.013 52.761 -39.348 1.00 29.88 H
ATOM 8223 HB2 ASP E 33 -4.036 54.509 -38.194 1.00 28.52
H
ATOM 8224 HB3 ASP E 33 -4.838 54.207 -39.531 1.00 28.52
H
ATOM 8225 N GLY E 34 -3.480 50.750 -37.238 1.00 21.69 N

ATOM 1926 HA THR A 215 -24.304 7.310 -41.635 1.00 82.33
H
ATOM 1927 HB THR A 215 -26.198 9.180 -41.094 1.00 84.75
H
ATOM 1928 HG1 THR A 215 -26.283 8.018 -39.211 1.00 76.23
H
ATOM 1929 HG21 THR A 215 -27.350 6.608 -41.411 1.00 74.41
H
ATOM 1930 HG22 THR A 215 -28.097 7.839 -40.761 1.00 74.41
H
ATOM 1931 HG23 THR A 215 -27.727 7.860 -42.296 1.00 74.41
H
TER 1932 THR A 215
ATOM 1933 N SER B 94 -17.256 -1.068 -39.057 1.00 38.91
N
ATOM 1934 CA SER B 94 -16.499 -1.068 -37.812 1.00 42.58
C
ATOM 1935 C SER B 94 -16.281 0.359 -37.313 1.00 42.15
C
ATOM 1936 O SER B 94 -16.626 1.322 -37.999 1.00 37.44
O
ATOM 1937 CB SER B 94 -15.156 -1.775 -37.999 1.00 45.61
C
ATOM 1938 OG SER B 94 -14.385 -1.141 -39.004 1.00 54.06
O
ATOM 1939 HA SER B 94 -17.001 -1.549 -37.136 1.00 51.10
H
ATOM 1940 HB2 SER B 94 -14.667 -1.748 -37.162 1.00 54.73
H
ATOM 1941 HB3 SER B 94 -15.318 -2.695 -38.259 1.00 54.73
H
ATOM 1942 HG SER B 94 -14.237 -0.342 -38.791 1.00 64.88
H
ATOM 1943 N TYR B 95 -15.698 0.478 -36.122 1.00 37.34
N
ATOM 1944 CA TYR B 95 -15.564 1.760 -35.437 1.00 35.53
C
ATOM 1945 C TYR B 95 -14.114 2.137 -35.164 1.00 36.30
C
ATOM 1946 O TYR B 95 -13.233 1.279 -35.095 1.00 36.50
O
ATOM 1947 CB TYR B 95 -16.332 1.732 -34.113 1.00 34.25
C
ATOM 1948 CG TYR B 95 -17.832 1.686 -34.273 1.00 32.06
C
ATOM 1949 CD1 TYR B 95 -18.476 0.505 -34.615 1.00 35.96
C
ATOM 1950 CD2 TYR B 95 -18.604 2.822 -34.078 1.00 33.01
C
ATOM 1951 CE1 TYR B 95 -19.848 0.458 -34.761 1.00 34.20
C
ATOM 1952 CE2 TYR B 95 -19.976 2.784 -34.220 1.00 40.01
C
ATOM 1953 CZ TYR B 95 -20.593 1.601 -34.563 1.00 39.11
C
ATOM 1954 OH TYR B 95 -21.960 1.564 -34.706 1.00 42.00
O
ATOM 1955 H TYR B 95 -15.367 -0.183 -35.682 1.00 44.80
H
ATOM 1956 HA TYR B 95 -15.953 2.454 -35.992 1.00 42.63
H
ATOM 1957 HB2 TYR B 95 -16.063 0.945 -33.614 1.00 41.11
H
ATOM 1958 HB3 TYR B 95 -16.113 2.531 -33.608 1.00 41.11
H
ATOM 1959 HD1 TYR B 95 -17.975 -0.267 -34.749 1.00 43.16
H
ATOM 1960 HD2 TYR B 95 -18.191 3.622 -33.847 1.00 39.62

ATOM 8226 CA GLY E 34 -3.124 50.158 -35.963 1.00 25.18 C

ATOM 8227 C GLY E 34 -4.353 49.841 -35.137 1.00 24.85 C

ATOM 8228 O GLY E 34 -4.330 48.938 -34.301 1.00 24.27 O

ATOM 8229 H GLY E 34 -3.772 50.184 -37.816 1.00 26.03 H
ATOM 8230 HA2 GLY E 34 -2.629 49.338 -36.111 1.00 30.22
H
ATOM 8231 HA3 GLY E 34 -2.564 50.773 -35.463 1.00 30.22
H
ATOM 8232 N LYS E 35 -5.429 50.583 -35.381 1.00 24.67 N

ATOM 8233 CA LYS E 35 -6.686 50.404 -34.661 1.00 27.22 C

ATOM 8234 C LYS E 35 -7.814 50.034 -35.616 1.00 26.78 C

ATOM 8235 O LYS E 35 -8.439 48.984 -35.477 1.00 29.19 O

ATOM 8236 CB LYS E 35 -7.049 51.681 -33.898 1.00 30.19 C

ATOM 8237 CG LYS E 35 -8.397 51.631 -33.184 1.00 33.78 C

ATOM 8238 CD LYS E 35 -8.744 52.972 -32.557 1.00 33.80 C
ATOM 8239 CE LYS E 35 -10.123 52.940 -31.915 1.00 41.60
C
ATOM 8240 NZ LYS E 35 -10.580 54.294 -31.489 1.00 39.39
N1+

ATOM 8241 H LYS E 35 -5.456 51.209 -35.970 1.00 29.61 H

ATOM 8242 HA LYS E 35 -6.585 49.685 -34.018 1.00 32.67 H
ATOM 8243 HB2 LYS E 35 -6.367 51.847 -33.228 1.00 36.23
H
ATOM 8244 HB3 LYS E 35 -7.076 52.421 -34.525 1.00 36.23
H
ATOM 8245 HG2 LYS E 35 -9.090 51.406 -33.824 1.00 40.53
H
ATOM 8246 HG3 LYS E 35 -8.362 50.966 -32.479 1.00 40.53
H
ATOM 8247 HD2 LYS E 35 -8.093 53.184 -31.870 1.00 40.56
H
ATOM 8248 HD3 LYS E 35 -8.744 53.657 -33.244 1.00 40.56
H
ATOM 8249 HE2 LYS E 35 -10.763 52.594 -32.555 1.00 49.92
H
ATOM 8250 HE3 LYS E 35 -10.094 52.371 -31.130 1.00 49.92
H
ATOM 8251 HZ1 LYS E 35 -10.621 54.837 -32.193 1.00 47.26
H
ATOM 8252 HZ2 LYS E 35 -11.387 54.240 -31.118 1.00 47.26
H
ATOM 8253 HZ3 LYS E 35 -10.011 54.634 -30.895 1.00 47.26
H

ATOM 8254 N ASP E 36 -8.070 50.912 -36.581 1.00 26.84 N

ATOM 8255 CA ASP E 36 -9.188 50.744 -37.498 1.00 25.99 C

ATOM 8256 C ASP E 36 -8.724 50.409 -38.907 1.00 22.89 C

ATOM 8257 O ASP E 36 -7.639 50.805 -39.332 1.00 21.76 O
ATOM 8258 CB ASP E 36 -10.043 52.011 -37.524 1.00 31.28
C
ATOM 8259 CG ASP E 36 -10.676 52.313 -36.178 1.00 34.69
C
ATOM 8260 OD1 ASP E 36 -11.667 51.640 -35.823 1.00 35.73

H
ATOM 1961 HE1 TYR B 95 -20.267 -0.339 -34.991 1.00 41.04
H
ATOM 1962 HE2 TYR B 95 -20.482 3.554 -34.088 1.00 48.01
H
ATOM 1963 HH TYR B 95 -22.285 2.324 -34.558 1.00 50.40
H
ATOM 1964 N CYS B 96 -13.888 3.438 -35.010 1.00 30.02
N
ATOM 1965 CA CYS B 96 -12.593 3.973 -34.613 1.00 34.28
C
ATOM 1966 C CYS B 96 -12.642 4.321 -33.129 1.00 32.78
C
ATOM 1967 O CYS B 96 -13.603 4.937 -32.669 1.00 31.30
O
ATOM 1968 CB CYS B 96 -12.247 5.206 -35.453 1.00 31.86
C
ATOM 1969 SG CYS B 96 -10.576 5.848 -35.221 1.00 33.72
S
ATOM 1970 H CYS B 96 -14.485 4.044 -35.133 1.00 36.02
H
ATOM 1971 HA CYS B 96 -11.907 3.302 -34.752 1.00 41.13
H
ATOM 1972 HB2 CYS B 96 -12.345 4.977 -36.391 1.00 38.23
H
ATOM 1973 HB3 CYS B 96 -12.867 5.917 -35.227 1.00 38.23
H
ATOM 1974 N GLY B 97 -11.618 3.918 -32.381 1.00 33.09
N
ATOM 1975 CA GLY B 97 -11.554 4.204 -30.957 1.00 31.22
C
ATOM 1976 C GLY B 97 -11.135 2.998 -30.132 1.00 35.55
C
ATOM 1977 O GLY B 97 -10.551 2.054 -30.663 1.00 39.96
O
ATOM 1978 H GLY B 97 -10.944 3.474 -32.680 1.00 39.71
H
ATOM 1979 HA2 GLY B 97 -10.917 4.918 -30.800 1.00 37.46
H
ATOM 1980 HA3 GLY B 97 -12.426 4.497 -30.648 1.00 37.46
H
ATOM 1981 N PRO B 98 -11.429 3.019 -28.821 1.00 38.20
N
ATOM 1982 CA PRO B 98 -12.139 4.096 -28.120 1.00 36.03
C
ATOM 1983 C PRO B 98 -11.312 5.373 -27.973 1.00 35.11
C
ATOM 1984 O PRO B 98 -10.086 5.318 -27.863 1.00 34.34
O
ATOM 1985 CB PRO B 98 -12.439 3.480 -26.749 1.00 43.03
C
ATOM 1986 CG PRO B 98 -11.379 2.466 -26.551 1.00 44.90
C
ATOM 1987 CD PRO B 98 -11.075 1.914 -27.912 1.00 43.35
C
ATOM 1988 HA PRO B 98 -12.973 4.301 -28.570 1.00 43.23
H
ATOM 1989 HB2 PRO B 98 -12.392 4.165 -26.065 1.00 51.64
H
ATOM 1990 HB3 PRO B 98 -13.315 3.064 -26.761 1.00 51.64
H
ATOM 1991 HG2 PRO B 98 -10.593 2.888 -26.172 1.00 53.88
H
ATOM 1992 HG3 PRO B 98 -11.706 1.765 -25.965 1.00 53.88
H
ATOM 1993 HD2 PRO B 98 -10.131 1.703 -27.988 1.00 52.02
H
ATOM 1994 HD3 PRO B 98 -11.628 1.138 -28.093 1.00 52.02
O
ATOM 8261 OD2 ASP E 36 -10.185 53.223 -35.478 1.00 37.15
O1-
ATOM 8262 H ASP E 36 -7.604 51.621 -36.726 1.00 32.21 H
ATOM 8263 HA ASP E 36 -9.744 50.014 -37.185 1.00 31.19 H
ATOM 8264 HB2 ASP E 36 -9.485 52.766 -37.769 1.00 37.54
H
ATOM 8265 HB3 ASP E 36 -10.756 51.900 -38.173 1.00 37.54
H
ATOM 8266 N ILE E 37 -9.559 49.663 -39.619 1.00 20.05 N
ATOM 8267 CA ILE E 37 -9.321 49.351 -41.018 1.00 19.38 C
ATOM 8268 C ILE E 37 -10.347 50.116 -41.835 1.00 18.03 C
ATOM 8269 O ILE E 37 -11.438 50.406 -41.347 1.00 16.80 O
ATOM 8270 CB ILE E 37 -9.424 47.836 -41.289 1.00 17.86 C
ATOM 8271 CG1 ILE E 37 -8.817 47.486 -42.648 1.00 17.25 C
ATOM 8272 CG2 ILE E 37 -10.872 47.365 -41.198 1.00 20.70
C
ATOM 8273 CD1 ILE E 37 -8.468 46.019 -42.783 1.00 17.20 C
ATOM 8274 H ILE E 37 -10.283 49.319 -39.307 1.00 24.06 H
ATOM 8275 HA ILE E 37 -8.435 49.652 -41.273 1.00 23.26 H
ATOM 8276 HB ILE E 37 -8.915 47.374 -40.605 1.00 21.43 H
ATOM 8277 HG12 ILE E 37 -9.455 47.707 -43.344 1.00 20.70
H
ATOM 8278 HG13 ILE E 37 -8.002 47.999 -42.770 1.00 20.70
H
ATOM 8279 HG21 ILE E 37 -10.905 46.411 -41.372 1.00 24.84
H
ATOM 8280 HG22 ILE E 37 -11.209 47.550 -40.307 1.00 24.84
H
ATOM 8281 HG23 ILE E 37 -11.401 47.841 -41.858 1.00 24.84
H
ATOM 8282 HD11 ILE E 37 -8.090 45.864 -43.663 1.00 20.64
H
ATOM 8283 HD12 ILE E 37 -7.823 45.784 -42.099 1.00 20.64
H
ATOM 8284 HD13 ILE E 37 -9.275 45.492 -42.673 1.00 20.64
H
ATOM 8285 N ARG E 38 -10.007 50.450 -43.072 1.00 17.17
N
ATOM 8286 CA ARG E 38 -10.945 51.180 -43.913 1.00 18.63
C
ATOM 8287 C ARG E 38 -10.678 50.981 -45.400 1.00 15.53
C
ATOM 8288 O ARG E 38 -9.529 50.822 -45.817 1.00 13.55 O
ATOM 8289 CB ARG E 38 -10.905 52.672 -43.576 1.00 21.12
C
ATOM 8290 CG ARG E 38 -9.612 53.367 -43.935 1.00 24.59
C
ATOM 8291 CD ARG E 38 -9.632 54.826 -43.497 1.00 34.01
C
ATOM 8292 NE ARG E 38 -8.473 55.561 -44.000 1.00 36.68
N
ATOM 8293 CZ ARG E 38 -8.437 56.219 -45.156 1.00 39.43
C
ATOM 8294 NH1 ARG E 38 -9.501 56.252 -45.953 1.00 38.87

H
ATOM 1995 N CYS B 99 -11.999 6.510 -27.991 1.00 28.31
N
ATOM 1996 CA CYS B 99 -11.382 7.814 -27.782 1.00 31.04
C
ATOM 1997 C CYS B 99 -12.176 8.587 -26.750 1.00 29.57
C
ATOM 1998 O CYS B 99 -13.297 8.207 -26.419 1.00 34.43
O
ATOM 1999 CB CYS B 99 -11.330 8.620 -29.080 1.00 22.49
C
ATOM 2000 SG CYS B 99 -10.222 7.973 -30.330 1.00 25.81
S
ATOM 2001 H CYS B 99 -12.847 6.552 -28.127 1.00 33.97
H
ATOM 2002 HA CYS B 99 -10.477 7.697 -27.453 1.00 37.25
H
ATOM 2003 HB2 CYS B 99 -12.220 8.645 -29.464 1.00 26.99
H
ATOM 2004 HB3 CYS B 99 -11.040 9.522 -28.872 1.00 26.99
H
ATOM 2005 N PRO B 100 -11.599 9.682 -26.237 1.00 32.75
N
ATOM 2006 CA PRO B 100 -12.421 10.607 -25.458 1.00 27.02
C
ATOM 2007 C PRO B 100 -13.576 11.111 -26.308 1.00 29.55
C
ATOM 2008 O PRO B 100 -13.455 11.152 -27.535 1.00 23.90
O
ATOM 2009 CB PRO B 100 -11.450 11.733 -25.099 1.00 26.53
C
ATOM 2010 CG PRO B 100 -10.094 11.101 -25.168 1.00 24.03
C
ATOM 2011 CD PRO B 100 -10.181 10.084 -26.262 1.00 29.20
C
ATOM 2012 HA PRO B 100 -12.756 10.184 -24.652 1.00 32.42
H
ATOM 2013 HB2 PRO B 100 -11.528 12.452 -25.745 1.00 31.83
H
ATOM 2014 HB3 PRO B 100 -11.635 12.053 -24.202 1.00 31.83
H
ATOM 2015 HG2 PRO B 100 -9.431 11.776 -25.381 1.00 28.84
H
ATOM 2016 HG3 PRO B 100 -9.890 10.676 -24.321 1.00 28.84
H
ATOM 2017 HD2 PRO B 100 -9.957 10.486 -27.116 1.00 35.04
H
ATOM 2018 HD3 PRO B 100 -9.610 9.325 -26.064 1.00 35.04
H
ATOM 2019 N LYS B 101 -14.678 11.479 -25.668 1.00 32.78
N
ATOM 2020 CA LYS B 101 -15.875 11.896 -26.387 1.00 39.36
C
ATOM 2021 C LYS B 101 -15.597 13.072 -27.325 1.00 32.37
C
ATOM 2022 O LYS B 101 -14.877 14.005 -26.970 1.00 30.08
O
ATOM 2023 CB LYS B 101 -16.984 12.266 -25.396 1.00 44.44
C
ATOM 2024 CG LYS B 101 -18.332 12.570 -26.041 1.00 61.82
C
ATOM 2025 CD LYS B 101 -18.865 11.378 -26.824 1.00 74.76
C
ATOM 2026 CE LYS B 101 -20.227 11.667 -27.429 1.00100.45
C
ATOM 2027 NZ LYS B 101 -20.686 10.552 -28.301 1.00117.51
N1+
ATOM 2028 H LYS B 101 -14.760 11.497 -24.812 1.00 39.34
N1+
ATOM 8295 NH2 ARG E 38 -7.330 56.851 -45.519 1.00 39.19
N

ATOM 8296 H ARG E 38 -9.253 50.270 -43.444 1.00 20.60 H
ATOM 8297 HA ARG E 38 -11.842 50.859 -43.729 1.00 22.36
H
ATOM 8298 HB2 ARG E 38 -11.621 53.117 -44.056 1.00 25.34
H
ATOM 8299 HB3 ARG E 38 -11.040 52.777 -42.621 1.00 25.34
H
ATOM 8300 HG2 ARG E 38 -8.874 52.925 -43.487 1.00 29.50
H
ATOM 8301 HG3 ARG E 38 -9.488 53.339 -44.896 1.00 29.50
H
ATOM 8302 HD2 ARG E 38 -10.433 55.252 -43.841 1.00 40.81
H
ATOM 8303 HD3 ARG E 38 -9.621 54.869 -42.528 1.00 40.81
H
ATOM 8304 HE ARG E 38 -7.764 55.568 -43.514 1.00 44.02
H
ATOM 8305 HH11 ARG E 38 -10.222 55.844 -45.724 1.00 46.64
H
ATOM 8306 HH12 ARG E 38 -9.467 56.681 -46.698 1.00 46.64
H
ATOM 8307 HH21 ARG E 38 -6.639 56.834 -45.008 1.00 47.03
H
ATOM 8308 HH22 ARG E 38 -7.304 57.279 -46.264 1.00 47.03
H
ATOM 8309 N PRO E 39 -11.746 50.991 -46.210 1.00 16.34
N
ATOM 8310 CA PRO E 39 -11.558 50.928 -47.660 1.00 17.96
C
ATOM 8311 C PRO E 39 -11.021 52.249 -48.203 1.00 17.79
C
ATOM 8312 O PRO E 39 -11.322 53.300 -47.639 1.00 17.56
O
ATOM 8313 CB PRO E 39 -12.968 50.636 -48.183 1.00 16.77
C
ATOM 8314 CG PRO E 39 -13.872 51.230 -47.161 1.00 25.13
C
ATOM 8315 CD PRO E 39 -13.172 51.069 -45.840 1.00 16.34
C
ATOM 8316 HA PRO E 39 -10.961 50.203 -47.900 1.00 21.55
H
ATOM 8317 HB2 PRO E 39 -13.095 51.063 -49.045 1.00 20.12
H
ATOM 8318 HB3 PRO E 39 -13.103 49.678 -48.249 1.00 20.12
H
ATOM 8319 HG2 PRO E 39 -14.013 52.169 -47.360 1.00 30.16
H
ATOM 8320 HG3 PRO E 39 -14.716 50.753 -47.159 1.00 30.16
H
ATOM 8321 HD2 PRO E 39 -13.332 51.842 -45.276 1.00 19.60
H
ATOM 8322 HD3 PRO E 39 -13.453 50.249 -45.406 1.00 19.60
H

ATOM 8323 N THR E 40 -10.224 52.189 -49.267 1.00 16.36 N
ATOM 8324 CA THR E 40 -9.672 53.389 -49.895 1.00 18.13
C

ATOM 8325 C THR E 40 -9.954 53.377 -51.393 1.00 18.97 C

ATOM 8326 O THR E 40 -9.306 54.076 -52.169 1.00 26.46 O
ATOM 8327 CB THR E 40 -8.149 53.511 -49.662 1.00 19.81
C
ATOM 8328 OG1 THR E 40 -7.473 52.405 -50.272 1.00 21.82

H
ATOM 2029 HA LYS B 101 -16.192 11.153 -26.926 1.00 47.24
H
ATOM 2030 HB2 LYS B 101 -17.111 11.525 -24.782 1.00 53.33
H
ATOM 2031 HB3 LYS B 101 -16.709 13.054 -24.903 1.00 53.33
H
ATOM 2032 HG2 LYS B 101 -18.975 12.790 -25.348 1.00 74.18
H
ATOM 2033 HG3 LYS B 101 -18.232 13.315 -26.654 1.00 74.18
H
ATOM 2034 HD2 LYS B 101 -18.251 11.169 -27.546 1.00 89.71
H
ATOM 2035 HD3 LYS B 101 -18.953 10.617 -26.228 1.00 89.71
H
ATOM 2036 HE2 LYS B 101 -20.876 11.782 -26.716 1.00120.53
H
ATOM 2037 HE3 LYS B 101 -20.174 12.472 -27.967 1.00120.53
H
ATOM 2038 HZ1 LYS B 101 -21.485 10.743 -28.644 1.00141.01
H
ATOM 2039 HZ2 LYS B 101 -20.108 10.429 -28.967 1.00141.01
H
ATOM 2040 HZ3 LYS B 101 -20.747 9.800 -27.828 1.00141.01
H
ATOM 2041 N ASN B 102 -16.163 12.996 -28.527 1.00 30.16
N
ATOM 2042 CA ASN B 102 -16.115 14.077 -29.514 1.00 31.24
C
ATOM 2043 C ASN B 102 -14.712 14.442 -30.002 1.00 27.87
C
ATOM 2044 O ASN B 102 -14.519 15.491 -30.613 1.00 26.23
O
ATOM 2045 CB ASN B 102 -16.798 15.329 -28.954 1.00 34.75
C
ATOM 2046 CG ASN B 102 -18.292 15.143 -28.774 1.00 42.54
C
ATOM 2047 OD1 ASN B 102 -18.922 14.366 -29.491 1.00 45.19
O
ATOM 2048 ND2 ASN B 102 -18.866 15.857 -27.814 1.00 46.35
N
ATOM 2049 H ASN B 102 -16.596 12.306 -28.804 1.00 36.19
H
ATOM 2050 HA ASN B 102 -16.623 13.797 -30.292 1.00 37.49
H
ATOM 2051 HB2 ASN B 102 -16.414 15.538 -28.088 1.00 41.70
H
ATOM 2052 HB3 ASN B 102 -16.659 16.067 -29.567 1.00 41.70
H
ATOM 2053 HD21 ASN B 102 -19.712 15.786 -27.673 1.00 55.63
H
ATOM 2054 HD22 ASN B 102 -18.394 16.391 -27.333 1.00 55.63
H
ATOM 2055 N TRP B 103 -13.737 13.577 -29.751 1.00 23.28
N
ATOM 2056 CA TRP B 103 -12.410 13.762 -30.328 1.00 23.16
C
ATOM 2057 C TRP B 103 -12.392 13.237 -31.763 1.00 23.53
C
ATOM 2058 O TRP B 103 -13.233 12.419 -32.140 1.00 22.63
O
ATOM 2059 CB TRP B 103 -11.343 13.049 -29.491 1.00 21.69
C
ATOM 2060 CG TRP B 103 -10.963 13.783 -28.236 1.00 23.99
C
ATOM 2061 CD1 TRP B 103 -11.760 14.599 -27.485 1.00 23.75
C
ATOM 2062 CD2 TRP B 103 -9.679 13.777 -27.595 1.00 20.75
O
ATOM 8329 CG2 THR E 40 -7.832 53.535 -48.171 1.00 20.16
C
ATOM 8330 H THR E 40 -9.985 51.456 -49.649 1.00 19.64 H
ATOM 8331 HA THR E 40 -10.098 54.172 -49.514 1.00 21.76
H
ATOM 8332 HB THR E 40 -7.829 54.338 -50.055 1.00 23.77
H
ATOM 8333 HG1 THR E 40 -7.623 52.397 -51.098 1.00 26.18
H
ATOM 8334 HG21 THR E 40 -6.874 53.611 -48.037 1.00 24.19
H
ATOM 8335 HG22 THR E 40 -8.270 54.292 -47.752 1.00 24.19
H
ATOM 8336 HG23 THR E 40 -8.145 52.718 -47.752 1.00 24.19
H
ATOM 8337 N ILE E 41 -10.930 52.569 -51.783 1.00 21.52 N
ATOM 8338 CA ILE E 41 -11.361 52.471 -53.166 1.00 21.60 C
ATOM 8339 C ILE E 41 -12.865 52.188 -53.133 1.00 21.26 C
ATOM 8340 O ILE E 41 -13.332 51.475 -52.245 1.00 20.35 O
ATOM 8341 CB ILE E 41 -10.587 51.364 -53.925 1.00 22.21 C
ATOM 8342 CG1 ILE E 41 -10.776 51.488 -55.437 1.00 27.01
C
ATOM 8343 CG2 ILE E 41 -11.002 49.983 -53.443 1.00 22.35
C
ATOM 8344 CD1 ILE E 41 -10.107 52.705 -56.037 1.00 23.85
C
ATOM 8345 H ILE E 41 -11.368 52.055 -51.251 1.00 25.82 H
ATOM 8346 HA ILE E 41 -11.214 53.318 -53.616 1.00 25.92 H
ATOM 8347 HB ILE E 41 -9.642 51.476 -53.733 1.00 26.65 H
ATOM 8348 HG12 ILE E 41 -10.401 50.702 -55.865 1.00 32.41
H
ATOM 8349 HG13 ILE E 41 -11.725 51.546 -55.630 1.00 32.41
H
ATOM 8350 HG21 ILE E 41 -10.501 49.313 -53.936 1.00 26.82
H
ATOM 8351 HG22 ILE E 41 -10.811 49.908 -52.495 1.00 26.82
H
ATOM 8352 HG23 ILE E 41 -11.952 49.867 -53.600 1.00 26.82
H
ATOM 8353 HD11 ILE E 41 -10.271 52.716 -56.993 1.00 28.62
H
ATOM 8354 HD12 ILE E 41 -10.479 53.503 -55.629 1.00 28.62
H
ATOM 8355 HD13 ILE E 41 -9.154 52.659 -55.864 1.00 28.62
H
ATOM 8356 N PRO E 42 -13.636 52.768 -54.072 1.00 23.49
N
ATOM 8357 CA PRO E 42 -15.093 52.589 -54.005 1.00 24.92
C
ATOM 8358 C PRO E 42 -15.578 51.136 -53.948 1.00 23.20
C
ATOM 8359 O PRO E 42 -16.532 50.858 -53.219 1.00 22.70
O
ATOM 8360 CB PRO E 42 -15.575 53.260 -55.294 1.00 31.54
C
ATOM 8361 CG PRO E 42 -14.576 54.332 -55.538 1.00 29.15
C
ATOM 8362 CD PRO E 42 -13.256 53.771 -55.086 1.00 24.13

C
ATOM 2063 NE1 TRP B 103 -11.054 15.094 -26.413 1.00 20.78
N
ATOM 2064 CE2 TRP B 103 -9.775 14.606 -26.459 1.00 20.29
C
ATOM 2065 CE3 TRP B 103 -8.461 13.150 -27.871 1.00 21.26
C
ATOM 2066 CZ2 TRP B 103 -8.699 14.823 -25.600 1.00 21.46
C
ATOM 2067 CZ3 TRP B 103 -7.394 13.365 -27.015 1.00 25.01
C
ATOM 2068 CH2 TRP B 103 -7.521 14.195 -25.893 1.00 17.81
C
ATOM 2069 H TRP B 103 -13.815 12.881 -29.253 1.00 27.94
H
ATOM 2070 HA TRP B 103 -12.198 14.708 -30.348 1.00 27.79
H
ATOM 2071 HB2 TRP B 103 -11.680 12.176 -29.233 1.00 26.03
H
ATOM 2072 HB3 TRP B 103 -10.542 12.946 -30.028 1.00 26.03
H
ATOM 2073 HD1 TRP B 103 -12.652 14.789 -27.670 1.00 28.50
H
ATOM 2074 HE1 TRP B 103 -11.365 15.626 -25.813 1.00 24.94
H
ATOM 2075 HE3 TRP B 103 -8.370 12.597 -28.613 1.00 25.51
H
ATOM 2076 HZ2 TRP B 103 -8.781 15.373 -24.854 1.00 25.75
H
ATOM 2077 HZ3 TRP B 103 -6.578 12.953 -27.188 1.00 30.01
H
ATOM 2078 HH2 TRP B 103 -6.787 14.323 -25.336 1.00 21.37
H
ATOM 2079 N ILE B 104 -11.452 13.725 -32.566 1.00 17.20
N
ATOM 2080 CA ILE B 104 -11.198 13.133 -33.873 1.00 21.24
C
ATOM 2081 C ILE B 104 -10.616 11.753 -33.647 1.00 24.16
C
ATOM 2082 O ILE B 104 -9.835 11.559 -32.719 1.00 23.98
O
ATOM 2083 CB ILE B 104 -10.215 13.966 -34.726 1.00 21.34
C
ATOM 2084 CG1 ILE B 104 -10.796 15.348 -35.026 1.00 22.32
C
ATOM 2085 CG2 ILE B 104 -9.876 13.230 -36.033 1.00 24.29
C
ATOM 2086 CD1 ILE B 104 -9.849 16.253 -35.781 1.00 28.99
C
ATOM 2087 H ILE B 104 -10.949 14.396 -32.377 1.00 20.64
H
ATOM 2088 HA ILE B 104 -12.032 13.044 -34.359 1.00 25.48
H
ATOM 2089 HB ILE B 104 -9.395 14.083 -34.221 1.00 25.61
H
ATOM 2090 HG12 ILE B 104 -11.597 15.241 -35.564 1.00 26.78
H
ATOM 2091 HG13 ILE B 104 -11.018 15.783 -34.188 1.00 26.78
H
ATOM 2092 HG21 ILE B 104 -9.259 13.772 -36.550 1.00 29.15
H
ATOM 2093 HG22 ILE B 104 -9.467 12.377 -35.818 1.00 29.15
H
ATOM 2094 HG23 ILE B 104 -10.693 13.088 -36.536 1.00 29.15
H
ATOM 2095 HD11 ILE B 104 -10.283 17.107 -35.934 1.00 34.79
H
ATOM 2096 HD12 ILE B 104 -9.046 16.381 -35.252 1.00 34.79
C
ATOM 8363 HA PRO E 42 -15.451 53.072 -53.245 1.00 29.90
H
ATOM 8364 HB2 PRO E 42 -15.577 52.617 -56.020 1.00 37.85
H
ATOM 8365 HB3 PRO E 42 -16.460 53.635 -55.159 1.00 37.85
H
ATOM 8366 HG2 PRO E 42 -14.551 54.544 -56.484 1.00 34.98
H
ATOM 8367 HG3 PRO E 42 -14.809 55.118 -55.019 1.00 34.98
H
ATOM 8368 HD2 PRO E 42 -12.799 53.346 -55.828 1.00 28.96
H
ATOM 8369 HD3 PRO E 42 -12.713 54.468 -54.685 1.00 28.96
H

ATOM 8370 N PHE E 43 -14.949 50.224 -54.683 1.00 22.14 N
ATOM 8371 CA PHE E 43 -15.479 48.865 -54.768 1.00 22.57
C

ATOM 8372 C PHE E 43 -15.282 48.081 -53.469 1.00 19.70 C
ATOM 8373 O PHE E 43 -15.809 46.981 -53.327 1.00 22.95
O
ATOM 8374 CB PHE E 43 -14.863 48.109 -55.963 1.00 22.95
C
ATOM 8375 CG PHE E 43 -13.453 47.620 -55.747 1.00 22.38
C
ATOM 8376 CD1 PHE E 43 -13.203 46.454 -55.040 1.00 20.54
C
ATOM 8377 CD2 PHE E 43 -12.382 48.296 -56.303 1.00 22.45
C
ATOM 8378 CE1 PHE E 43 -11.912 45.996 -54.859 1.00 21.86
C
ATOM 8379 CE2 PHE E 43 -11.085 47.839 -56.127 1.00 25.06
C
ATOM 8380 CZ PHE E 43 -10.852 46.686 -55.403 1.00 20.17
C

ATOM 8381 H PHE E 43 -14.228 50.361 -55.133 1.00 26.57 H
ATOM 8382 HA PHE E 43 -16.434 48.922 -54.926 1.00 27.09
H
ATOM 8383 HB2 PHE E 43 -15.415 47.335 -56.156 1.00 27.54
H
ATOM 8384 HB3 PHE E 43 -14.854 48.702 -56.731 1.00 27.54
H
ATOM 8385 HD1 PHE E 43 -13.913 45.984 -54.667 1.00 24.65
H
ATOM 8386 HD2 PHE E 43 -12.532 49.074 -56.789 1.00 26.94
H
ATOM 8387 HE1 PHE E 43 -11.759 45.218 -54.372 1.00 26.23
H
ATOM 8388 HE2 PHE E 43 -10.372 48.309 -56.496 1.00 30.07
H

ATOM 8389 HZ PHE E 43 -9.983 46.378 -55.283 1.00 24.21 H

ATOM 8390 N MET E 44 -14.556 48.657 -52.513 1.00 23.05 N
ATOM 8391 CA MET E 44 -14.353 48.017 -51.212 1.00 21.06
C

ATOM 8392 C MET E 44 -15.333 48.520 -50.151 1.00 22.24 C
ATOM 8393 O MET E 44 -15.417 47.962 -49.059 1.00 19.63
O
ATOM 8394 CB MET E 44 -12.917 48.239 -50.730 1.00 19.76
C
ATOM 8395 CG MET E 44 -11.878 47.391 -51.456 1.00 21.55
C
ATOM 8396 SD MET E 44 -12.224 45.620 -51.414 1.00 21.18

H
ATOM 2097 HD13 ILE B 104 -9.624 15.839 -36.628 1.00 34.79
H
ATOM 2098 N CYS B 105 -11.001 10.800 -34.489 1.00 22.22
N
ATOM 2099 CA CYS B 105 -10.421 9.462 -34.455 1.00 24.13
C
ATOM 2100 C CYS B 105 -9.930 9.120 -35.853 1.00 25.68
C
ATOM 2101 O CYS B 105 -10.660 9.288 -36.830 1.00 25.12
O
ATOM 2102 CB CYS B 105 -11.440 8.433 -33.962 1.00 25.61
C
ATOM 2103 SG CYS B 105 -10.702 6.857 -33.461 1.00 33.63
S
ATOM 2104 H CYS B 105 -11.602 10.904 -35.096 1.00 26.67
H
ATOM 2105 HA CYS B 105 -9.661 9.455 -33.852 1.00 28.95
H
ATOM 2106 HB2 CYS B 105 -11.908 8.799 -33.195 1.00 30.73
H
ATOM 2107 HB3 CYS B 105 -12.071 8.251 -34.676 1.00 30.73
H
ATOM 2108 N TYR B 106 -8.689 8.653 -35.949 1.00 22.66
N
ATOM 2109 CA TYR B 106 -8.061 8.421 -37.245 1.00 21.90
C
ATOM 2110 C TYR B 106 -6.840 7.512 -37.140 1.00 29.80
C
ATOM 2111 O TYR B 106 -5.832 7.876 -36.531 1.00 19.08
O
ATOM 2112 CB TYR B 106 -7.656 9.754 -37.874 1.00 22.79
C
ATOM 2113 CG TYR B 106 -7.090 9.639 -39.271 1.00 21.75
C
ATOM 2114 CD1 TYR B 106 -7.886 9.228 -40.333 1.00 23.00
C
ATOM 2115 CD2 TYR B 106 -5.766 9.961 -39.532 1.00 22.30
C
ATOM 2116 CE1 TYR B 106 -7.375 9.131 -41.614 1.00 22.33
C
ATOM 2117 CE2 TYR B 106 -5.247 9.871 -40.811 1.00 23.29
C
ATOM 2118 CZ TYR B 106 -6.056 9.455 -41.846 1.00 24.28
C
ATOM 2119 OH TYR B 106 -5.543 9.363 -43.116 1.00 28.23
O
ATOM 2120 H TYR B 106 -8.188 8.462 -35.277 1.00 27.19
H
ATOM 2121 HA TYR B 106 -8.703 7.995 -37.834 1.00 26.28
H
ATOM 2122 HB2 TYR B 106 -8.438 10.326 -37.919 1.00 27.35
H
ATOM 2123 HB3 TYR B 106 -6.980 10.168 -37.315 1.00 27.35
H
ATOM 2124 HD1 TYR B 106 -8.777 9.010 -40.179 1.00 27.60
H
ATOM 2125 HD2 TYR B 106 -5.218 10.244 -38.836 1.00 26.77
H
ATOM 2126 HE1 TYR B 106 -7.919 8.852 -42.315 1.00 26.80
H
ATOM 2127 HE2 TYR B 106 -4.357 10.087 -40.970 1.00 27.94
H
ATOM 2128 HH TYR B 106 -4.733 9.588 -43.115 1.00 33.88
H
ATOM 2129 N LYS B 107 -6.944 6.335 -37.750 1.00 26.75
N
ATOM 2130 CA LYS B 107 -5.852 5.367 -37.787 1.00 26.22
S
ATOM 8397 CE MET E 44 -12.382 45.323 -49.660 1.00 17.95
C

ATOM 8398 H MET E 44 -14.167 49.420 -52.592 1.00 27.65 H
ATOM 8399 HA MET E 44 -14.480 47.061 -51.318 1.00 25.27
H
ATOM 8400 HB2 MET E 44 -12.685 49.171 -50.866 1.00 23.72
H
ATOM 8401 HB3 MET E 44 -12.869 48.023 -49.786 1.00 23.72
H
ATOM 8402 HG2 MET E 44 -11.846 47.665 -52.386 1.00 25.86
H
ATOM 8403 HG3 MET E 44 -11.013 47.534 -51.041 1.00 25.86
H
ATOM 8404 HE1 MET E 44 -12.572 44.383 -49.515 1.00 21.55
H
ATOM 8405 HE2 MET E 44 -11.550 45.564 -49.223 1.00 21.55
H
ATOM 8406 HE3 MET E 44 -13.107 45.865 -49.312 1.00 21.55
H

ATOM 8407 N ILE E 45 -16.073 49.575 -50.467 1.00 27.83 N

ATOM 8408 CA ILE E 45 -17.051 50.108 -49.527 1.00 22.95 C

ATOM 8409 C ILE E 45 -18.164 49.096 -49.288 1.00 21.71 C

ATOM 8410 O ILE E 45 -18.742 48.560 -50.231 1.00 21.43 O

ATOM 8411 CB ILE E 45 -17.634 51.442 -50.029 1.00 24.78 C
ATOM 8412 CG1 ILE E 45 -16.560 52.530 -49.916 1.00 25.65
C
ATOM 8413 CG2 ILE E 45 -18.877 51.838 -49.221 1.00 32.38
C
ATOM 8414 CD1 ILE E 45 -16.940 53.868 -50.511 1.00 38.64
C

ATOM 8415 H ILE E 45 -16.029 49.999 -51.214 1.00 33.40 H

ATOM 8416 HA ILE E 45 -16.612 50.275 -48.678 1.00 27.54 H

ATOM 8417 HB ILE E 45 -17.884 51.344 -50.961 1.00 29.73 H
ATOM 8418 HG12 ILE E 45 -16.363 52.672 -48.977 1.00 30.78
H
ATOM 8419 HG13 ILE E 45 -15.761 52.223 -50.372 1.00 30.78
H
ATOM 8420 HG21 ILE E 45 -19.219 52.680 -49.561 1.00 38.86
H
ATOM 8421 HG22 ILE E 45 -19.549 51.145 -49.316 1.00 38.86
H
ATOM 8422 HG23 ILE E 45 -18.630 51.934 -48.288 1.00 38.86
H
ATOM 8423 HD11 ILE E 45 -16.202 54.487 -50.392 1.00 46.36
H
ATOM 8424 HD12 ILE E 45 -17.125 53.752 -51.456 1.00 46.36
H
ATOM 8425 HD13 ILE E 45 -17.729 54.203 -50.057 1.00 46.36
H

ATOM 8426 N GLY E 46 -18.445 48.832 -48.015 1.00 19.01 N
ATOM 8427 CA GLY E 46 -19.499 47.909 -47.638 1.00 26.57
C

ATOM 8428 C GLY E 46 -19.056 46.457 -47.589 1.00 28.55 C

ATOM 8429 O GLY E 46 -19.844 45.577 -47.242 1.00 27.44 O
ATOM 8430 H GLY E 46 -18.032 49.181 -47.346 1.00 22.81 H

```
C
ATOM  2131  C   LYS B 107      -5.272   5.107 -36.397  1.00 26.74
C
ATOM  2132  O   LYS B 107      -4.095   5.360 -36.145  1.00 26.52
O
ATOM  2133  CB  LYS B 107      -4.763   5.846 -38.749  1.00 24.14
C
ATOM  2134  CG  LYS B 107      -5.256   5.963 -40.189  1.00 25.22
C
ATOM  2135  CD  LYS B 107      -4.169   6.410 -41.147  1.00 30.82
C
ATOM  2136  CE  LYS B 107      -4.650   6.327 -42.592  1.00 28.59
C
ATOM  2137  NZ  LYS B 107      -3.633   6.838 -43.557  1.00 32.24
N1+
ATOM  2138  H   LYS B 107      -7.653   6.068 -38.157  1.00 32.10
H
ATOM  2139  HA  LYS B 107      -6.195   4.525 -38.126  1.00 31.46
H
ATOM  2140  HB2 LYS B 107      -4.453   6.721 -38.466  1.00 28.97
H
ATOM  2141  HB3 LYS B 107      -4.027   5.214 -38.734  1.00 28.97
H
ATOM  2142  HG2 LYS B 107      -5.578   5.097 -40.483  1.00 30.27
H
ATOM  2143  HG3 LYS B 107      -5.974   6.614 -40.224  1.00 30.27
H
ATOM  2144  HD2 LYS B 107      -3.930   7.331 -40.957  1.00 36.98
H
ATOM  2145  HD3 LYS B 107      -3.395   5.834 -41.049  1.00 36.98
H
ATOM  2146  HE2 LYS B 107      -4.836   5.401 -42.812  1.00 34.30
H
ATOM  2147  HE3 LYS B 107      -5.453   6.861 -42.690  1.00 34.30
H
ATOM  2148  HZ1 LYS B 107      -3.448   7.690 -43.381  1.00 38.69
H
ATOM  2149  HZ2 LYS B 107      -2.885   6.360 -43.491  1.00 38.69
H
ATOM  2150  HZ3 LYS B 107      -3.944   6.775 -44.388  1.00 38.69
H
ATOM  2151  N   ASN B 108      -6.125   4.609 -35.505  1.00 28.96
N
ATOM  2152  CA  ASN B 108      -5.729   4.193 -34.160  1.00 35.20
C
ATOM  2153  C   ASN B 108      -5.175   5.334 -33.306  1.00 33.16
C
ATOM  2154  O   ASN B 108      -4.472   5.094 -32.324  1.00 35.70
O
ATOM  2155  CB  ASN B 108      -4.701   3.058 -34.243  1.00 34.00
C
ATOM  2156  CG  ASN B 108      -5.251   1.820 -34.927  1.00 38.47
C
ATOM  2157  OD1 ASN B 108      -6.448   1.540 -34.861  1.00 40.72
O
ATOM  2158  ND2 ASN B 108      -4.377   1.071 -35.589  1.00 50.98
N
ATOM  2159  H   ASN B 108      -6.964   4.500 -35.660  1.00 34.75
H
ATOM  2160  HA  ASN B 108      -6.512   3.844 -33.705  1.00 42.24
H
ATOM  2161  HB2 ASN B 108      -3.932   3.364 -34.749  1.00 40.80
H
ATOM  2162  HB3 ASN B 108      -4.430   2.810 -33.345  1.00 40.80
H
ATOM  2163 HD21 ASN B 108      -4.640   0.359 -35.993  1.00 61.17
H
ATOM  2164 HD22 ASN B 108      -3.548   1.298 -35.613  1.00 61.17
ATOM  8431  HA2 GLY E  46     -19.837  48.152 -46.762  1.00 31.88
H
ATOM  8432  HA3 GLY E  46     -20.228  47.981 -48.274  1.00 31.88
H

ATOM  8433  N   ASP E  47     -17.800  46.196 -47.936  1.00 25.13           N
ATOM  8434  CA  ASP E  47     -17.279  44.834 -47.895  1.00 20.13
C

ATOM  8435  C   ASP E  47     -17.364  44.271 -46.477  1.00 19.36           C

ATOM  8436  O   ASP E  47     -16.968  44.931 -45.520  1.00 23.09           O
ATOM  8437  CB  ASP E  47     -15.838  44.793 -48.394  1.00 23.01
C
ATOM  8438  CG  ASP E  47     -15.165  43.465 -48.107  1.00 25.88
C
ATOM  8439  OD1 ASP E  47     -15.541  42.456 -48.738  1.00 25.43
O
ATOM  8440  OD2 ASP E  47     -14.260  43.431 -47.248  1.00 29.08
O1-

ATOM  8441  H   ASP E  47     -17.231  46.786 -48.198  1.00 30.15           H
ATOM  8442  HA  ASP E  47     -17.816  44.271 -48.475  1.00 24.15
H
ATOM  8443  HB2 ASP E  47     -15.831  44.933 -49.354  1.00 27.62
H
ATOM  8444  HB3 ASP E  47     -15.329  45.490 -47.952  1.00 27.62
H

ATOM  8445  N   GLU E  48     -17.891  43.056 -46.351  1.00 16.14           N
ATOM  8446  CA  GLU E  48     -18.090  42.431 -45.044  1.00 21.48
C

ATOM  8447  C   GLU E  48     -17.292  41.133 -44.913  1.00 17.74           C
ATOM  8448  O   GLU E  48     -17.473  40.382 -43.958  1.00 20.31
O
ATOM  8449  CB  GLU E  48     -19.587  42.164 -44.805  1.00 22.20
C
ATOM  8450  CG  GLU E  48     -20.255  41.340 -45.897  1.00 25.85
C
ATOM  8451  CD  GLU E  48     -21.750  41.133 -45.672  1.00 29.32
C
ATOM  8452  OE1 GLU E  48     -22.447  40.770 -46.643  1.00 34.96
O
ATOM  8453  OE2 GLU E  48     -22.226  41.325 -44.535  1.00 26.64
O1-

ATOM  8454  H   GLU E  48     -18.143  42.568 -47.012  1.00 19.37           H
ATOM  8455  HA  GLU E  48     -17.783  43.040 -44.354  1.00 25.77
H
ATOM  8456  HB2 GLU E  48     -19.688  41.684 -43.969  1.00 26.64
H
ATOM  8457  HB3 GLU E  48     -20.050  43.015 -44.753  1.00 26.64
H
ATOM  8458  HG2 GLU E  48     -20.141  41.793 -46.747  1.00 31.02
H
ATOM  8459  HG3 GLU E  48     -19.836  40.466 -45.931  1.00 31.02
H

ATOM  8460  N   ILE E  49     -16.399  40.887 -45.867  1.00 20.94           N

ATOM  8461  CA  ILE E  49     -15.620  39.649 -45.906  1.00 18.17           C

ATOM  8462  C   ILE E  49     -14.134  39.889 -45.647  1.00 17.63           C

ATOM  8463  O   ILE E  49     -13.544  39.294 -44.747  1.00 20.44           O
ATOM  8464  CB  ILE E  49     -15.778  38.951 -47.266  1.00 21.61           C
```

H
ATOM 2165 N ASN B 109 -5.499 6.570 -33.679 1.00 26.48
N
ATOM 2166 CA ASN B 109 -5.125 7.739 -32.888 1.00 25.08
C
ATOM 2167 C ASN B 109 -6.311 8.665 -32.655 1.00 23.92
C
ATOM 2168 O ASN B 109 -7.165 8.828 -33.526 1.00 25.78
O
ATOM 2169 CB ASN B 109 -3.994 8.508 -33.571 1.00 25.68
C
ATOM 2170 CG ASN B 109 -2.706 7.718 -33.624 1.00 28.52
C
ATOM 2171 OD1 ASN B 109 -2.107 7.550 -34.686 1.00 29.25
O
ATOM 2172 ND2 ASN B 109 -2.278 7.221 -32.474 1.00 28.60
N
ATOM 2173 H ASN B 109 -5.940 6.759 -34.393 1.00 31.78
H
ATOM 2174 HA ASN B 109 -4.804 7.442 -32.022 1.00 30.10
H
ATOM 2175 HB2 ASN B 109 -4.257 8.715 -34.482 1.00 30.82
H
ATOM 2176 HB3 ASN B 109 -3.825 9.326 -33.079 1.00 30.82
H
ATOM 2177 HD21 ASN B 109 -1.551 6.763 -32.448 1.00 34.32
H
ATOM 2178 HD22 ASN B 109 -2.728 7.355 -31.753 1.00 34.32
H
ATOM 2179 N CYS B 110 -6.355 9.262 -31.467 1.00 21.75
N
ATOM 2180 CA CYS B 110 -7.381 10.236 -31.115 1.00 19.96
C
ATOM 2181 C CYS B 110 -6.754 11.621 -31.065 1.00 20.85
C
ATOM 2182 O CYS B 110 -5.632 11.768 -30.591 1.00 18.06
O
ATOM 2183 CB CYS B 110 -8.015 9.899 -29.766 1.00 23.36
C
ATOM 2184 SG CYS B 110 -8.365 8.144 -29.523 1.00 28.07
S
ATOM 2185 H CYS B 110 -5.789 9.116 -30.836 1.00 26.10
H
ATOM 2186 HA CYS B 110 -8.076 10.235 -31.792 1.00 23.95
H
ATOM 2187 HB2 CYS B 110 -7.411 10.180 -29.061 1.00 28.03
H
ATOM 2188 HB3 CYS B 110 -8.854 10.380 -29.689 1.00 28.03
H
ATOM 2189 N TYR B 111 -7.475 12.626 -31.554 1.00 18.22
N
ATOM 2190 CA TYR B 111 -6.973 13.997 -31.572 1.00 16.26
C
ATOM 2191 C TYR B 111 -8.020 14.998 -31.110 1.00 18.87
C
ATOM 2192 O TYR B 111 -9.212 14.830 -31.370 1.00 17.84
O
ATOM 2193 CB TYR B 111 -6.517 14.392 -32.977 1.00 16.69
C
ATOM 2194 CG TYR B 111 -5.434 13.532 -33.571 1.00 17.24
C
ATOM 2195 CD1 TYR B 111 -4.095 13.773 -33.292 1.00 20.23
C
ATOM 2196 CD2 TYR B 111 -5.747 12.493 -34.436 1.00 19.87
C
ATOM 2197 CE1 TYR B 111 -3.102 12.992 -33.843 1.00 17.86
C
ATOM 2198 CE2 TYR B 111 -4.763 11.710 -34.994 1.00 19.29
ATOM 8465 CG1 ILE E 49 -17.244 38.564 -47.486 1.00 23.02
C
ATOM 8466 CG2 ILE E 49 -14.893 37.713 -47.346 1.00 20.19
C
ATOM 8467 CD1 ILE E 49 -17.580 38.261 -48.922 1.00 30.12
C
ATOM 8468 H ILE E 49 -16.222 41.428 -46.512 1.00 25.13 H
ATOM 8469 HA ILE E 49 -15.950 39.048 -45.220 1.00 21.81 H
ATOM 8470 HB ILE E 49 -15.512 39.569 -47.965 1.00 25.94 H
ATOM 8471 HG12 ILE E 49 -17.442 37.773 -46.961 1.00 27.63
H
ATOM 8472 HG13 ILE E 49 -17.808 39.299 -47.198 1.00 27.63
H
ATOM 8473 HG21 ILE E 49 -15.014 37.295 -48.213 1.00 24.23
H
ATOM 8474 HG22 ILE E 49 -13.967 37.979 -47.233 1.00 24.23
H
ATOM 8475 HG23 ILE E 49 -15.149 37.096 -46.643 1.00 24.23
H
ATOM 8476 HD11 ILE E 49 -18.519 38.026 -48.983 1.00 36.14
H
ATOM 8477 HD12 ILE E 49 -17.400 39.047 -49.461 1.00 36.14
H
ATOM 8478 HD13 ILE E 49 -17.033 37.519 -49.224 1.00 36.14
H
ATOM 8479 N PHE E 50 -13.528 40.757 -46.443 1.00 14.54 N
ATOM 8480 CA PHE E 50 -12.085 40.946 -46.383 1.00 17.11
C
ATOM 8481 C PHE E 50 -11.662 41.946 -45.309 1.00 16.26 C
ATOM 8482 O PHE E 50 -10.690 41.706 -44.593 1.00 13.97
O
ATOM 8483 CB PHE E 50 -11.576 41.369 -47.758 1.00 15.93
C
ATOM 8484 CG PHE E 50 -11.833 40.337 -48.816 1.00 17.08
C
ATOM 8485 CD1 PHE E 50 -10.955 39.286 -49.001 1.00 17.90
C
ATOM 8486 CD2 PHE E 50 -12.980 40.391 -49.591 1.00 20.60
C
ATOM 8487 CE1 PHE E 50 -11.200 38.319 -49.958 1.00 19.37
C
ATOM 8488 CE2 PHE E 50 -13.230 39.428 -50.552 1.00 20.80
C
ATOM 8489 CZ PHE E 50 -12.342 38.391 -50.733 1.00 20.26
C
ATOM 8490 H PHE E 50 -13.927 41.248 -47.026 1.00 17.44 H
ATOM 8491 HA PHE E 50 -11.672 40.095 -46.167 1.00 20.53
H
ATOM 8492 HB2 PHE E 50 -12.024 42.187 -48.023 1.00 19.11
H
ATOM 8493 HB3 PHE E 50 -10.618 41.515 -47.709 1.00 19.11
H
ATOM 8494 HD1 PHE E 50 -10.186 39.232 -48.480 1.00 21.48
H
ATOM 8495 HD2 PHE E 50 -13.584 41.088 -49.472 1.00 24.72
H
ATOM 8496 HE1 PHE E 50 -10.598 37.621 -50.081 1.00 23.24
H
ATOM 8497 HE2 PHE E 50 -13.999 39.479 -51.073 1.00 24.96
H
ATOM 8498 HZ PHE E 50 -12.507 37.744 -51.381 1.00 24.31

C
ATOM 2199 CZ TYR B 111 -3.443 11.962 -34.696 1.00 19.83
C
ATOM 2200 OH TYR B 111 -2.463 11.177 -35.251 1.00 21.43
O
ATOM 2201 H TYR B 111 -8.264 12.539 -31.884 1.00 21.87
H
ATOM 2202 HA TYR B 111 -6.209 14.064 -30.977 1.00 19.51
H
ATOM 2203 HB2 TYR B 111 -7.282 14.349 -33.571 1.00 20.03
H
ATOM 2204 HB3 TYR B 111 -6.181 15.302 -32.947 1.00 20.03
H
ATOM 2205 HD1 TYR B 111 -3.865 14.467 -32.717 1.00 24.28
H
ATOM 2206 HD2 TYR B 111 -6.638 12.321 -34.639 1.00 23.85
H
ATOM 2207 HE1 TYR B 111 -2.210 13.160 -33.644 1.00 21.44
H
ATOM 2208 HE2 TYR B 111 -4.988 11.013 -35.568 1.00 23.14
H
ATOM 2209 HH TYR B 111 -2.809 10.593 -35.746 1.00 25.72
H
ATOM 2210 N GLN B 112 -7.573 16.055 -30.444 1.00 16.37
N
ATOM 2211 CA GLN B 112 -8.440 17.199 -30.183 1.00 18.53
C
ATOM 2212 C GLN B 112 -7.660 18.496 -30.315 1.00 18.90
C
ATOM 2213 O GLN B 112 -6.506 18.591 -29.890 1.00 13.32
O
ATOM 2214 CB GLN B 112 -9.083 17.104 -28.798 1.00 18.31
C
ATOM 2215 CG GLN B 112 -10.016 18.266 -28.458 1.00 20.42
C
ATOM 2216 CD GLN B 112 -11.205 18.373 -29.402 1.00 22.22
C
ATOM 2217 OE1 GLN B 112 -11.057 18.710 -30.575 1.00 23.60
O
ATOM 2218 NE2 GLN B 112 -12.395 18.088 -28.886 1.00 27.09
N
ATOM 2219 H GLN B 112 -6.775 16.136 -30.133 1.00 19.65
H
ATOM 2220 HA GLN B 112 -9.152 17.210 -30.842 1.00 22.24
H
ATOM 2221 HB2 GLN B 112 -9.601 16.285 -28.751 1.00 21.98
H
ATOM 2222 HB3 GLN B 112 -8.380 17.085 -28.130 1.00 21.98
H
ATOM 2223 HG2 GLN B 112 -10.359 18.142 -27.559 1.00 24.51
H
ATOM 2224 HG3 GLN B 112 -9.517 19.096 -28.511 1.00 24.51
H
ATOM 2225 HE21 GLN B 112 -13.099 18.134 -29.378 1.00 32.51
H
ATOM 2226 HE22 GLN B 112 -12.462 17.858 -28.060 1.00 32.51
H
ATOM 2227 N PHE B 113 -8.309 19.484 -30.923 1.00 17.31
N
ATOM 2228 CA PHE B 113 -7.731 20.801 -31.141 1.00 18.02
C
ATOM 2229 C PHE B 113 -8.352 21.798 -30.178 1.00 19.91
C
ATOM 2230 O PHE B 113 -9.508 22.181 -30.346 1.00 25.64
O
ATOM 2231 CB PHE B 113 -7.961 21.259 -32.583 1.00 16.63
C
ATOM 2232 CG PHE B 113 -7.265 20.414 -33.612 1.00 20.32
H
ATOM 8499 N LEU E 51 -12.392 43.050 -45.180 1.00 16.41 N
ATOM 8500 CA LEU E 51 -12.055 44.057 -44.177 1.00 16.35
C
ATOM 8501 C LEU E 51 -12.009 43.470 -42.757 1.00 15.68 C
ATOM 8502 O LEU E 51 -11.023 43.665 -42.044 1.00 14.16 O
ATOM 8503 CB LEU E 51 -13.045 45.228 -44.226 1.00 17.16
C
ATOM 8504 CG LEU E 51 -13.007 46.120 -45.473 1.00 18.54
C
ATOM 8505 CD1 LEU E 51 -14.064 47.212 -45.365 1.00 24.77
C
ATOM 8506 CD2 LEU E 51 -11.630 46.737 -45.699 1.00 22.00
C
ATOM 8507 H LEU E 51 -13.082 43.240 -45.657 1.00 19.69 H
ATOM 8508 HA LEU E 51 -11.174 44.410 -44.377 1.00 19.62
H
ATOM 8509 HB2 LEU E 51 -13.943 44.866 -44.161 1.00 20.59
H
ATOM 8510 HB3 LEU E 51 -12.875 45.799 -43.461 1.00 20.59
H
ATOM 8511 HG LEU E 51 -13.219 45.579 -46.250 1.00 22.25
H
ATOM 8512 HD11 LEU E 51 -14.027 47.767 -46.160 1.00 29.72
H
ATOM 8513 HD12 LEU E 51 -14.938 46.799 -45.290 1.00 29.72
H
ATOM 8514 HD13 LEU E 51 -13.883 47.749 -44.578 1.00 29.72
H
ATOM 8515 HD21 LEU E 51 -11.659 47.289 -46.496 1.00 26.40
H
ATOM 8516 HD22 LEU E 51 -11.398 47.278 -44.929 1.00 26.40
H
ATOM 8517 HD23 LEU E 51 -10.981 46.025 -45.812 1.00 26.40
H
ATOM 8518 N PRO E 52 -13.065 42.750 -42.337 1.00 15.67
N
ATOM 8519 CA PRO E 52 -13.023 42.226 -40.962 1.00 16.66
C
ATOM 8520 C PRO E 52 -11.952 41.159 -40.777 1.00 15.48
C
ATOM 8521 O PRO E 52 -11.369 41.065 -39.700 1.00 15.44
O
ATOM 8522 CB PRO E 52 -14.425 41.638 -40.758 1.00 19.47
C
ATOM 8523 CG PRO E 52 -14.947 41.399 -42.123 1.00 23.22
C
ATOM 8524 CD PRO E 52 -14.344 42.450 -43.001 1.00 19.17
C
ATOM 8525 HA PRO E 52 -12.878 42.946 -40.328 1.00 19.99
H
ATOM 8526 HB2 PRO E 52 -14.362 40.806 -40.264 1.00 23.36
H
ATOM 8527 HB3 PRO E 52 -14.982 42.277 -40.285 1.00 23.36
H
ATOM 8528 HG2 PRO E 52 -14.680 40.515 -42.421 1.00 27.86
H
ATOM 8529 HG3 PRO E 52 -15.914 41.477 -42.117 1.00 27.86
H
ATOM 8530 HD2 PRO E 52 -14.189 42.099 -43.892 1.00 23.00
H
ATOM 8531 HD3 PRO E 52 -14.908 43.239 -43.021 1.00 23.00
H
ATOM 8532 N PHE E 53 -11.697 40.378 -41.822 1.00 13.56 N

C
ATOM 2233 CD1 PHE B 113 -7.730 19.144 -33.920 1.00 23.50
C
ATOM 2234 CD2 PHE B 113 -6.158 20.898 -34.285 1.00 20.35
C
ATOM 2235 CE1 PHE B 113 -7.092 18.371 -34.870 1.00 25.58
C
ATOM 2236 CE2 PHE B 113 -5.515 20.128 -35.235 1.00 24.89
C
ATOM 2237 CZ PHE B 113 -5.984 18.863 -35.529 1.00 28.96
C
ATOM 2238 H PHE B 113 -9.110 19.410 -31.227 1.00 20.77
H
ATOM 2239 HA PHE B 113 -6.775 20.767 -30.977 1.00 21.62
H
ATOM 2240 HB2 PHE B 113 -8.913 21.230 -32.770 1.00 19.95
H
ATOM 2241 HB3 PHE B 113 -7.636 22.168 -32.677 1.00 19.95
H
ATOM 2242 HD1 PHE B 113 -8.475 18.807 -33.478 1.00 28.20
H
ATOM 2243 HD2 PHE B 113 -5.837 21.749 -34.090 1.00 24.42
H
ATOM 2244 HE1 PHE B 113 -7.410 17.519 -35.066 1.00 30.70
H
ATOM 2245 HE2 PHE B 113 -4.769 20.463 -35.678 1.00 29.86
H
ATOM 2246 HZ PHE B 113 -5.554 18.344 -36.170 1.00 34.75
H
ATOM 2247 N PHE B 114 -7.589 22.215 -29.173 1.00 18.14
N
ATOM 2248 CA PHE B 114 -8.090 23.146 -28.167 1.00 16.48
C
ATOM 2249 C PHE B 114 -7.775 24.587 -28.554 1.00 19.56
C
ATOM 2250 O PHE B 114 -6.611 24.962 -28.675 1.00 18.71
O
ATOM 2251 CB PHE B 114 -7.496 22.821 -26.799 1.00 19.55
C
ATOM 2252 CG PHE B 114 -7.961 21.508 -26.237 1.00 21.13
C
ATOM 2253 CD1 PHE B 114 -7.233 20.352 -26.450 1.00 21.85
C
ATOM 2254 CD2 PHE B 114 -9.132 21.429 -25.501 1.00 27.16
C
ATOM 2255 CE1 PHE B 114 -7.658 19.140 -25.935 1.00 21.25
C
ATOM 2256 CE2 PHE B 114 -9.564 20.218 -24.984 1.00 27.33
C
ATOM 2257 CZ PHE B 114 -8.824 19.074 -25.202 1.00 22.66
C
ATOM 2258 H PHE B 114 -6.773 21.972 -29.050 1.00 21.76
H
ATOM 2259 HA PHE B 114 -9.054 23.056 -28.105 1.00 19.78
H
ATOM 2260 HB2 PHE B 114 -6.530 22.785 -26.878 1.00 23.47
H
ATOM 2261 HB3 PHE B 114 -7.750 23.518 -26.174 1.00 23.47
H
ATOM 2262 HD1 PHE B 114 -6.445 20.391 -26.942 1.00 26.22
H
ATOM 2263 HD2 PHE B 114 -9.633 22.198 -25.351 1.00 32.60
H
ATOM 2264 HE1 PHE B 114 -7.158 18.370 -26.084 1.00 25.50
H
ATOM 2265 HE2 PHE B 114 -10.351 20.176 -24.490 1.00 32.79
H
ATOM 2266 HZ PHE B 114 -9.111 18.260 -24.856 1.00 27.20

ATOM 8533 CA PHE E 53 -10.656 39.358 -41.790 1.00 17.24
C
ATOM 8534 C PHE E 53 -9.283 40.010 -41.632 1.00 14.01 C
ATOM 8535 O PHE E 53 -8.506 39.630 -40.757 1.00 13.44 O
ATOM 8536 CB PHE E 53 -10.709 38.506 -43.064 1.00 16.33
C
ATOM 8537 CG PHE E 53 -9.659 37.431 -43.128 1.00 15.12
C
ATOM 8538 CD1 PHE E 53 -9.837 36.229 -42.465 1.00 17.88
C
ATOM 8539 CD2 PHE E 53 -8.505 37.614 -43.867 1.00 12.71
C
ATOM 8540 CE1 PHE E 53 -8.878 35.234 -42.530 1.00 14.56
C
ATOM 8541 CE2 PHE E 53 -7.540 36.622 -43.934 1.00 14.02
C
ATOM 8542 CZ PHE E 53 -7.729 35.432 -43.263 1.00 13.27 C
ATOM 8543 H PHE E 53 -12.120 40.419 -42.570 1.00 16.27 H
ATOM 8544 HA PHE E 53 -10.804 38.775 -41.030 1.00 20.68
H
ATOM 8545 HB2 PHE E 53 -11.577 38.076 -43.115 1.00 19.60
H
ATOM 8546 HB3 PHE E 53 -10.585 39.086 -43.832 1.00 19.60
H
ATOM 8547 HD1 PHE E 53 -10.611 36.089 -41.967 1.00 21.46
H
ATOM 8548 HD2 PHE E 53 -8.372 38.416 -44.320 1.00 15.25
H
ATOM 8549 HE1 PHE E 53 -9.008 34.433 -42.076 1.00 17.48
H
ATOM 8550 HE2 PHE E 53 -6.766 36.759 -44.431 1.00 16.83
H
ATOM 8551 HZ PHE E 53 -7.083 34.764 -43.307 1.00 15.93 H
ATOM 8552 N TYR E 54 -8.997 41.002 -42.470 1.00 12.77 N
ATOM 8553 CA TYR E 54 -7.711 41.685 -42.426 1.00 13.18 C
ATOM 8554 C TYR E 54 -7.531 42.456 -41.122 1.00 14.10 C
ATOM 8555 O TYR E 54 -6.416 42.550 -40.606 1.00 12.95 O
ATOM 8556 CB TYR E 54 -7.557 42.641 -43.614 1.00 13.17 C
ATOM 8557 CG TYR E 54 -7.431 41.959 -44.968 1.00 15.46
C
ATOM 8558 CD1 TYR E 54 -6.845 40.702 -45.094 1.00 12.49
C
ATOM 8559 CD2 TYR E 54 -7.897 42.581 -46.121 1.00 14.64
C
ATOM 8560 CE1 TYR E 54 -6.735 40.083 -46.336 1.00 15.66
C
ATOM 8561 CE2 TYR E 54 -7.789 41.974 -47.361 1.00 14.01
C
ATOM 8562 CZ TYR E 54 -7.212 40.726 -47.462 1.00 13.86 C
ATOM 8563 OH TYR E 54 -7.117 40.130 -48.694 1.00 15.59
O
ATOM 8564 H TYR E 54 -9.532 41.298 -43.074 1.00 15.33 H
ATOM 8565 HA TYR E 54 -7.003 41.024 -42.481 1.00 15.81 H
ATOM 8566 HB2 TYR E 54 -8.335 43.219 -43.649 1.00 15.80

H
ATOM 2267 N ASP B 115 -8.820 25.391 -28.738 1.00 19.34
N
ATOM 2268 CA ASP B 115 -8.666 26.759 -29.234 1.00 22.18
C
ATOM 2269 C ASP B 115 -8.421 27.778 -28.121 1.00 22.24
C
ATOM 2270 O ASP B 115 -8.374 28.983 -28.375 1.00 23.21
O
ATOM 2271 CB ASP B 115 -9.896 27.172 -30.053 1.00 28.95
C
ATOM 2272 CG ASP B 115 -11.204 26.959 -29.310 1.00 30.69
C
ATOM 2273 OD1 ASP B 115 -11.201 26.953 -28.060 1.00 36.27
O
ATOM 2274 OD2 ASP B 115 -12.244 26.800 -29.985 1.00 43.50
O1-
ATOM 2275 H ASP B 115 -9.636 25.167 -28.582 1.00 23.21
H
ATOM 2276 HA ASP B 115 -7.898 26.786 -29.826 1.00 26.62
H
ATOM 2277 HB2 ASP B 115 -9.827 28.115 -30.272 1.00 34.74
H
ATOM 2278 HB3 ASP B 115 -9.925 26.645 -30.866 1.00 34.74
H
ATOM 2279 N GLU B 116 -8.267 27.295 -26.892 1.00 21.76
N
ATOM 2280 CA GLU B 116 -7.861 28.151 -25.782 1.00 25.37
C
ATOM 2281 C GLU B 116 -6.344 28.309 -25.771 1.00 26.04
C
ATOM 2282 O GLU B 116 -5.610 27.323 -25.778 1.00 26.31
O
ATOM 2283 CB GLU B 116 -8.340 27.578 -24.447 1.00 30.28
C
ATOM 2284 CG GLU B 116 -9.811 27.839 -24.153 1.00 43.86
C
ATOM 2285 CD GLU B 116 -10.256 27.250 -22.827 1.00 59.80
C
ATOM 2286 OE1 GLU B 116 -9.383 26.828 -22.037 1.00 55.77
O
ATOM 2287 OE2 GLU B 116 -11.480 27.208 -22.576 1.00 69.76
O1-
ATOM 2288 H GLU B 116 -8.391 26.473 -26.674 1.00 26.11
H
ATOM 2289 HA GLU B 116 -8.256 29.029 -25.895 1.00 30.45
H
ATOM 2290 HB2 GLU B 116 -8.205 26.618 -24.453 1.00 36.34
H
ATOM 2291 HB3 GLU B 116 -7.820 27.978 -23.732 1.00 36.34
H
ATOM 2292 HG2 GLU B 116 -9.963 28.796 -24.123 1.00 52.63
H
ATOM 2293 HG3 GLU B 116 -10.349 27.439 -24.855 1.00 52.63
H
ATOM 2294 N SER B 117 -5.878 29.551 -25.757 1.00 24.25
N
ATOM 2295 CA SER B 117 -4.446 29.825 -25.766 1.00 24.22
C
ATOM 2296 C SER B 117 -3.832 29.548 -24.401 1.00 24.91
C
ATOM 2297 O SER B 117 -4.271 30.095 -23.390 1.00 25.88
O
ATOM 2298 CB SER B 117 -4.179 31.275 -26.178 1.00 25.72
C
ATOM 2299 OG SER B 117 -4.568 31.501 -27.519 1.00 35.43
O
ATOM 2300 H SER B 117 -6.371 30.256 -25.743 1.00 29.10
H
ATOM 8567 HB3 TYR E 54 -6.759 43.176 -43.480 1.00 15.80
H
ATOM 8568 HD1 TYR E 54 -6.526 40.267 -44.336 1.00 14.99
H
ATOM 8569 HD2 TYR E 54 -8.290 43.421 -46.058 1.00 17.56
H
ATOM 8570 HE1 TYR E 54 -6.345 39.241 -46.407 1.00 18.79
H
ATOM 8571 HE2 TYR E 54 -8.111 42.403 -48.120 1.00 16.81
H
ATOM 8572 HH TYR E 54 -7.445 40.632 -49.283 1.00 18.71
H
ATOM 8573 N LYS E 55 -8.612 43.018 -40.592 1.00 11.71 N
ATOM 8574 CA LYS E 55 -8.514 43.757 -39.335 1.00 15.22 C
ATOM 8575 C LYS E 55 -7.955 42.845 -38.248 1.00 13.95 C
ATOM 8576 O LYS E 55 -7.113 43.257 -37.454 1.00 16.50 O
ATOM 8577 CB LYS E 55 -9.871 44.321 -38.913 1.00 16.70 C
ATOM 8578 CG LYS E 55 -9.803 45.205 -37.669 1.00 20.44 C
ATOM 8579 CD LYS E 55 -11.158 45.809 -37.335 1.00 27.75
C
ATOM 8580 CE LYS E 55 -11.074 46.749 -36.141 1.00 30.79
C
ATOM 8581 NZ LYS E 55 -12.385 47.406 -35.858 1.00 31.93
N1+
ATOM 8582 H LYS E 55 -9.401 42.989 -40.931 1.00 14.05 H
ATOM 8583 HA LYS E 55 -7.902 44.500 -39.451 1.00 18.27 H
ATOM 8584 HB2 LYS E 55 -10.227 44.857 -39.639 1.00 20.04
H
ATOM 8585 HB3 LYS E 55 -10.471 43.584 -38.722 1.00 20.04
H
ATOM 8586 HG2 LYS E 55 -9.515 44.671 -36.912 1.00 24.53
H
ATOM 8587 HG3 LYS E 55 -9.178 45.930 -37.825 1.00 24.53
H
ATOM 8588 HD2 LYS E 55 -11.479 46.315 -38.098 1.00 33.29
H
ATOM 8589 HD3 LYS E 55 -11.780 45.098 -37.118 1.00 33.29
H
ATOM 8590 HE2 LYS E 55 -10.812 46.244 -35.355 1.00 36.95
H
ATOM 8591 HE3 LYS E 55 -10.421 47.443 -36.326 1.00 36.95
H
ATOM 8592 HZ1 LYS E 55 -12.308 47.949 -35.157 1.00 38.32
H
ATOM 8593 HZ2 LYS E 55 -12.645 47.881 -36.565 1.00 38.32
H
ATOM 8594 HZ3 LYS E 55 -13.001 46.790 -35.681 1.00 38.32
H
ATOM 8595 N ASN E 56 -8.406 41.596 -38.236 1.00 12.27 N
ATOM 8596 CA ASN E 56 -7.924 40.627 -37.264 1.00 13.08
C
ATOM 8597 C ASN E 56 -6.491 40.185 -37.546 1.00 15.68 C
ATOM 8598 O ASN E 56 -5.659 40.159 -36.642 1.00 13.45 O
ATOM 8599 CB ASN E 56 -8.843 39.404 -37.234 1.00 20.81
C
ATOM 8600 CG ASN E 56 -10.166 39.686 -36.549 1.00 25.65

H
ATOM 2301 HA SER B 117 -4.017 29.244 -26.413 1.00 29.07
H
ATOM 2302 HB2 SER B 117 -4.687 31.865 -25.599 1.00 30.86
H
ATOM 2303 HB3 SER B 117 -3.231 31.458 -26.089 1.00 30.86
H
ATOM 2304 HG SER B 117 -4.416 32.299 -27.731 1.00 42.52
H
ATOM 2305 N LYS B 118 -2.815 28.692 -24.384 1.00 17.66
N
ATOM 2306 CA LYS B 118 -2.093 28.355 -23.163 1.00 23.06
C
ATOM 2307 C LYS B 118 -0.612 28.252 -23.478 1.00 21.34
C
ATOM 2308 O LYS B 118 -0.238 27.982 -24.623 1.00 18.83
O
ATOM 2309 CB LYS B 118 -2.597 27.035 -22.571 1.00 22.84
C
ATOM 2310 CG LYS B 118 -4.060 27.046 -22.162 1.00 24.02
C
ATOM 2311 CD LYS B 118 -4.473 25.704 -21.567 1.00 26.42
C
ATOM 2312 CE LYS B 118 -5.958 25.669 -21.232 1.00 32.25
C
ATOM 2313 NZ LYS B 118 -6.343 26.770 -20.307 1.00 35.19
N1+
ATOM 2314 H LYS B 118 -2.518 28.286 -25.082 1.00 21.19
H
ATOM 2315 HA LYS B 118 -2.222 29.057 -22.506 1.00 27.68
H
ATOM 2316 HB2 LYS B 118 -2.481 26.335 -23.231 1.00 27.41
H
ATOM 2317 HB3 LYS B 118 -2.072 26.830 -21.781 1.00 27.41
H
ATOM 2318 HG2 LYS B 118 -4.202 27.733 -21.492 1.00 28.83
H
ATOM 2319 HG3 LYS B 118 -4.611 27.216 -22.942 1.00 28.83
H
ATOM 2320 HD2 LYS B 118 -4.290 25.000 -22.209 1.00 31.70
H
ATOM 2321 HD3 LYS B 118 -3.974 25.550 -20.749 1.00 31.70
H
ATOM 2322 HE2 LYS B 118 -6.471 25.767 -22.049 1.00 38.70
H
ATOM 2323 HE3 LYS B 118 -6.168 24.825 -20.803 1.00 38.70
H
ATOM 2324 HZ1 LYS B 118 -5.888 26.700 -19.545 1.00 42.23
H
ATOM 2325 HZ2 LYS B 118 -6.164 27.557 -20.680 1.00 42.23
H
ATOM 2326 HZ3 LYS B 118 -7.214 26.726 -20.129 1.00 42.23
H
ATOM 2327 N ASN B 119 0.236 28.473 -22.478 1.00 16.27
N
ATOM 2328 CA ASN B 119 1.659 28.241 -22.668 1.00 20.30
C
ATOM 2329 C ASN B 119 1.878 26.738 -22.763 1.00 16.48
C
ATOM 2330 O ASN B 119 0.946 25.951 -22.569 1.00 17.62
O
ATOM 2331 CB ASN B 119 2.499 28.869 -21.542 1.00 19.64
C
ATOM 2332 CG ASN B 119 2.262 28.228 -20.183 1.00 20.65
C
ATOM 2333 OD1 ASN B 119 2.498 27.035 -19.986 1.00 17.21
O
ATOM 2334 ND2 ASN B 119 1.823 29.036 -19.224 1.00 20.04
C
ATOM 8601 OD1 ASN E 56 -10.228 40.453 -35.587 1.00 32.51
O
ATOM 8602 ND2 ASN E 56 -11.234 39.066 -37.040 1.00 27.48
N

ATOM 8603 H ASN E 56 -8.993 41.285 -38.782 1.00 14.72 H
ATOM 8604 HA ASN E 56 -7.941 41.032 -36.383 1.00 15.70
H
ATOM 8605 HB2 ASN E 56 -9.029 39.126 -38.145 1.00 24.97
H
ATOM 8606 HB3 ASN E 56 -8.402 38.687 -36.752 1.00 24.97
H
ATOM 8607 HD21 ASN E 56 -12.007 39.194 -36.685 1.00 32.98
H
ATOM 8608 HD22 ASN E 56 -11.152 38.536 -37.712 1.00 32.98
H

ATOM 8609 N VAL E 57 -6.209 39.830 -38.795 1.00 12.98 N

ATOM 8610 CA VAL E 57 -4.869 39.403 -39.172 1.00 11.78 C

ATOM 8611 C VAL E 57 -3.849 40.512 -38.932 1.00 10.70 C

ATOM 8612 O VAL E 57 -2.742 40.250 -38.470 1.00 12.79 O

ATOM 8613 CB VAL E 57 -4.811 38.970 -40.651 1.00 15.00 C
ATOM 8614 CG1 VAL E 57 -3.373 38.701 -41.085 1.00 13.02
C
ATOM 8615 CG2 VAL E 57 -5.665 37.734 -40.867 1.00 11.75
C

ATOM 8616 H VAL E 57 -6.776 39.828 -39.441 1.00 15.57 H

ATOM 8617 HA VAL E 57 -4.616 38.641 -38.627 1.00 14.14 H

ATOM 8618 HB VAL E 57 -5.166 39.682 -41.205 1.00 18.00 H
ATOM 8619 HG11 VAL E 57 -3.369 38.432 -42.016 1.00 15.62
H
ATOM 8620 HG12 VAL E 57 -2.853 39.513 -40.972 1.00 15.62
H
ATOM 8621 HG13 VAL E 57 -3.004 37.993 -40.533 1.00 15.62
H
ATOM 8622 HG21 VAL E 57 -5.617 37.476 -41.801 1.00 14.10
H
ATOM 8623 HG22 VAL E 57 -5.327 37.016 -40.308 1.00 14.10
H
ATOM 8624 HG23 VAL E 57 -6.582 37.938 -40.626 1.00 14.10
H

ATOM 8625 N PHE E 58 -4.216 41.746 -39.259 1.00 12.71 N
ATOM 8626 CA PHE E 58 -3.288 42.862 -39.119 1.00 12.91
C

ATOM 8627 C PHE E 58 -3.030 43.177 -37.645 1.00 15.14 C

ATOM 8628 O PHE E 58 -1.881 43.346 -37.236 1.00 12.36 O
ATOM 8629 CB PHE E 58 -3.814 44.103 -39.851 1.00 10.07
C
ATOM 8630 CG PHE E 58 -3.890 43.946 -41.352 1.00 13.18
C
ATOM 8631 CD1 PHE E 58 -3.394 42.810 -41.982 1.00 13.27
C
ATOM 8632 CD2 PHE E 58 -4.463 44.938 -42.135 1.00 15.09
C
ATOM 8633 CE1 PHE E 58 -3.470 42.667 -43.360 1.00 14.15
C
ATOM 8634 CE2 PHE E 58 -4.542 44.799 -43.518 1.00 14.94

N
ATOM 2335 H ASN B 119 0.016 28.753 -21.695 1.00 19.52
H
ATOM 2336 HA ASN B 119 1.936 28.639 -23.508 1.00 24.36
H
ATOM 2337 HB2 ASN B 119 3.439 28.769 -21.759 1.00 23.57
H
ATOM 2338 HB3 ASN B 119 2.275 29.810 -21.471 1.00 23.57
H
ATOM 2339 HD21 ASN B 119 1.673 28.726 -18.436 1.00 24.05
H
ATOM 2340 HD22 ASN B 119 1.691 29.869 -19.391 1.00 24.05
H
ATOM 2341 N TRP B 120 3.102 26.333 -23.067 1.00 15.24
N
ATOM 2342 CA TRP B 120 3.362 24.930 -23.348 1.00 16.04
C
ATOM 2343 C TRP B 120 3.052 24.039 -22.148 1.00 19.13
C
ATOM 2344 O TRP B 120 2.588 22.909 -22.313 1.00 15.63
O
ATOM 2345 CB TRP B 120 4.813 24.733 -23.779 1.00 16.87
C
ATOM 2346 CG TRP B 120 5.085 23.340 -24.242 1.00 15.71
C
ATOM 2347 CD1 TRP B 120 5.006 22.874 -25.520 1.00 15.03
C
ATOM 2348 CD2 TRP B 120 5.465 22.226 -23.431 1.00 19.26
C
ATOM 2349 NE1 TRP B 120 5.318 21.540 -25.558 1.00 16.56
N
ATOM 2350 CE2 TRP B 120 5.604 21.116 -24.288 1.00 19.91
C
ATOM 2351 CE3 TRP B 120 5.703 22.059 -22.064 1.00 20.14
C
ATOM 2352 CZ2 TRP B 120 5.972 19.856 -23.823 1.00 20.45
C
ATOM 2353 CZ3 TRP B 120 6.068 20.807 -21.604 1.00 24.00
C
ATOM 2354 CH2 TRP B 120 6.199 19.721 -22.482 1.00 20.10
C
ATOM 2355 H TRP B 120 3.792 26.844 -23.117 1.00 18.29
H
ATOM 2356 HA TRP B 120 2.793 24.648 -24.082 1.00 19.25
H
ATOM 2357 HB2 TRP B 120 5.012 25.338 -24.510 1.00 20.25
H
ATOM 2358 HB3 TRP B 120 5.395 24.918 -23.025 1.00 20.25
H
ATOM 2359 HD1 TRP B 120 4.775 23.387 -26.261 1.00 18.03
H
ATOM 2360 HE1 TRP B 120 5.332 21.049 -26.264 1.00 19.88
H
ATOM 2361 HE3 TRP B 120 5.618 22.775 -21.476 1.00 24.16
H
ATOM 2362 HZ2 TRP B 120 6.060 19.134 -24.403 1.00 24.54
H
ATOM 2363 HZ3 TRP B 120 6.230 20.683 -20.697 1.00 28.80
H
ATOM 2364 HH2 TRP B 120 6.446 18.891 -22.144 1.00 24.12
H
ATOM 2365 N TYR B 121 3.297 24.553 -20.946 1.00 20.90
N
ATOM 2366 CA TYR B 121 3.179 23.750 -19.733 1.00 19.53
C
ATOM 2367 C TYR B 121 1.735 23.563 -19.268 1.00 17.33
C
ATOM 2368 O TYR B 121 1.386 22.498 -18.763 1.00 20.12
C
ATOM 8635 CZ PHE E 58 -4.045 43.664 -44.127 1.00 15.54 C
ATOM 8636 H PHE E 58 -4.991 41.964 -39.561 1.00 15.25 H
ATOM 8637 HA PHE E 58 -2.441 42.616 -39.523 1.00 15.49
H
ATOM 8638 HB2 PHE E 58 -4.708 44.300 -39.529 1.00 12.09
H
ATOM 8639 HB3 PHE E 58 -3.226 44.850 -39.662 1.00 12.09
H
ATOM 8640 HD1 PHE E 58 -3.008 42.135 -41.471 1.00 15.93
H
ATOM 8641 HD2 PHE E 58 -4.801 45.703 -41.731 1.00 18.11
H
ATOM 8642 HE1 PHE E 58 -3.134 41.902 -43.768 1.00 16.98
H
ATOM 8643 HE2 PHE E 58 -4.928 45.471 -44.032 1.00 17.92
H
ATOM 8644 HZ PHE E 58 -4.095 43.571 -45.051 1.00 18.65 H
ATOM 8645 N SER E 59 -4.088 43.250 -36.844 1.00 12.44 N
ATOM 8646 CA SER E 59 -3.935 43.540 -35.418 1.00 15.47
C
ATOM 8647 C SER E 59 -3.058 42.488 -34.743 1.00 15.91 C
ATOM 8648 O SER E 59 -2.148 42.820 -33.978 1.00 14.84 O
ATOM 8649 CB SER E 59 -5.299 43.608 -34.727 1.00 19.05
C
ATOM 8650 OG SER E 59 -6.086 44.656 -35.260 1.00 26.66
O
ATOM 8651 H SER E 59 -4.902 43.137 -37.098 1.00 14.93 H
ATOM 8652 HA SER E 59 -3.503 44.402 -35.315 1.00 18.56
H
ATOM 8653 HB2 SER E 59 -5.763 42.766 -34.860 1.00 22.86
H
ATOM 8654 HB3 SER E 59 -5.165 43.766 -33.779 1.00 22.86
H
ATOM 8655 HG SER E 59 -6.211 44.532 -36.082 1.00 31.99
H
ATOM 8656 N GLU E 60 -3.325 41.221 -35.046 1.00 14.24 N
ATOM 8657 CA GLU E 60 -2.553 40.120 -34.483 1.00 16.08
C
ATOM 8658 C GLU E 60 -1.097 40.145 -34.956 1.00 14.22 C
ATOM 8659 O GLU E 60 -0.192 39.806 -34.197 1.00 18.48 O
ATOM 8660 CB GLU E 60 -3.198 38.780 -34.844 1.00 19.87
C
ATOM 8661 CG GLU E 60 -4.571 38.559 -34.219 1.00 27.96
C
ATOM 8662 CD GLU E 60 -4.514 38.305 -32.722 1.00 41.64
C
ATOM 8663 OE1 GLU E 60 -3.399 38.165 -32.175 1.00 41.26
O
ATOM 8664 OE2 GLU E 60 -5.592 38.243 -32.090 1.00 50.70
O1-
ATOM 8665 H GLU E 60 -3.952 40.972 -35.579 1.00 17.09 H
ATOM 8666 HA GLU E 60 -2.553 40.199 -33.517 1.00 19.30
H
ATOM 8667 HB2 GLU E 60 -3.302 38.734 -35.808 1.00 23.84
H
ATOM 8668 HB3 GLU E 60 -2.618 38.064 -34.543 1.00 23.84

O
ATOM 2369 CB TYR B 121 4.006 24.375 -18.612 1.00 20.76
C
ATOM 2370 CG TYR B 121 5.479 24.438 -18.945 1.00 27.57
C
ATOM 2371 CD1 TYR B 121 6.266 23.294 -18.909 1.00 26.72
C
ATOM 2372 CD2 TYR B 121 6.077 25.635 -19.312 1.00 22.00
C
ATOM 2373 CE1 TYR B 121 7.607 23.343 -19.222 1.00 27.02
C
ATOM 2374 CE2 TYR B 121 7.416 25.693 -19.623 1.00 29.21
C
ATOM 2375 CZ TYR B 121 8.175 24.544 -19.578 1.00 30.61
C
ATOM 2376 OH TYR B 121 9.511 24.599 -19.891 1.00 42.90
O
ATOM 2377 H TYR B 121 3.533 25.368 -20.805 1.00 25.08
H
ATOM 2378 HA TYR B 121 3.545 22.869 -19.911 1.00 23.43
H
ATOM 2379 HB2 TYR B 121 3.694 25.280 -18.455 1.00 24.91
H
ATOM 2380 HB3 TYR B 121 3.902 23.843 -17.807 1.00 24.91
H
ATOM 2381 HD1 TYR B 121 5.882 22.481 -18.670 1.00 32.06
H
ATOM 2382 HD2 TYR B 121 5.565 26.411 -19.344 1.00 26.41
H
ATOM 2383 HE1 TYR B 121 8.124 22.570 -19.192 1.00 32.42
H
ATOM 2384 HE2 TYR B 121 7.805 26.502 -19.866 1.00 35.05
H
ATOM 2385 HH TYR B 121 9.728 25.386 -20.088 1.00 51.48
H
ATOM 2386 N GLU B 122 0.899 24.586 -19.418 1.00 19.17
N
ATOM 2387 CA GLU B 122 -0.514 24.422 -19.074 1.00 20.84
C
ATOM 2388 C GLU B 122 -1.187 23.598 -20.161 1.00 20.40
C
ATOM 2389 O GLU B 122 -2.164 22.904 -19.895 1.00 23.74
O
ATOM 2390 CB GLU B 122 -1.240 25.765 -18.887 1.00 25.11
C
ATOM 2391 CG GLU B 122 -0.550 26.974 -19.475 1.00 30.11
C
ATOM 2392 CD GLU B 122 -1.378 28.248 -19.377 1.00 32.89
C
ATOM 2393 OE1 GLU B 122 -2.424 28.235 -18.687 1.00 36.08
O
ATOM 2394 OE2 GLU B 122 -0.975 29.264 -19.988 1.00 26.01
O1-
ATOM 2395 H GLU B 122 1.114 25.366 -19.709 1.00 23.01
H
ATOM 2396 HA GLU B 122 -0.580 23.929 -18.241 1.00 25.00
H
ATOM 2397 HB2 GLU B 122 -2.114 25.699 -19.303 1.00 30.13
H
ATOM 2398 HB3 GLU B 122 -1.346 25.925 -17.937 1.00 30.13
H
ATOM 2399 HG2 GLU B 122 0.283 27.123 -19.000 1.00 36.13
H
ATOM 2400 HG3 GLU B 122 -0.369 26.807 -20.414 1.00 36.13
H
ATOM 2401 N SER B 123 -0.657 23.676 -21.382 1.00 17.88
N
ATOM 2402 CA SER B 123 -1.132 22.838 -22.477 1.00 18.47
H
ATOM 8669 HG2 GLU E 60 -5.114 39.348 -34.367 1.00 33.56
H
ATOM 8670 HG3 GLU E 60 -4.986 37.788 -34.637 1.00 33.56
H

ATOM 8671 N PHE E 61 -0.873 40.545 -36.206 1.00 15.60 N

ATOM 8672 CA PHE E 61 0.484 40.651 -36.745 1.00 14.83 C

ATOM 8673 C PHE E 61 1.364 41.506 -35.841 1.00 13.77 C

ATOM 8674 O PHE E 61 2.510 41.154 -35.556 1.00 15.86 O

ATOM 8675 CB PHE E 61 0.466 41.242 -38.161 1.00 13.27 C
ATOM 8676 CG PHE E 61 1.838 41.467 -38.745 1.00 10.38
C
ATOM 8677 CD1 PHE E 61 2.456 40.482 -39.495 1.00 10.57
C
ATOM 8678 CD2 PHE E 61 2.506 42.668 -38.548 1.00 12.22
C
ATOM 8679 CE1 PHE E 61 3.722 40.689 -40.033 1.00 13.44
C
ATOM 8680 CE2 PHE E 61 3.764 42.881 -39.087 1.00 12.04
C

ATOM 8681 CZ PHE E 61 4.372 41.889 -39.825 1.00 12.36 C

ATOM 8682 H PHE E 61 -1.491 40.762 -36.764 1.00 18.72 H

ATOM 8683 HA PHE E 61 0.875 39.764 -36.795 1.00 17.79 H
ATOM 8684 HB2 PHE E 61 -0.010 40.634 -38.748 1.00 15.92
H
ATOM 8685 HB3 PHE E 61 0.011 42.099 -38.136 1.00 15.92
H
ATOM 8686 HD1 PHE E 61 2.022 39.671 -39.635 1.00 12.69
H
ATOM 8687 HD2 PHE E 61 2.102 43.341 -38.049 1.00 14.66
H
ATOM 8688 HE1 PHE E 61 4.129 40.019 -40.534 1.00 16.13
H
ATOM 8689 HE2 PHE E 61 4.201 43.689 -38.944 1.00 14.45
H

ATOM 8690 HZ PHE E 61 5.217 42.029 -40.187 1.00 14.83 H

ATOM 8691 N PHE E 62 0.821 42.630 -35.385 1.00 13.88 N

ATOM 8692 CA PHE E 62 1.579 43.544 -34.541 1.00 15.96 C

ATOM 8693 C PHE E 62 1.603 43.105 -33.079 1.00 14.71 C

ATOM 8694 O PHE E 62 2.630 43.211 -32.414 1.00 11.05 O

ATOM 8695 CB PHE E 62 1.008 44.956 -34.649 1.00 16.31 C
ATOM 8696 CG PHE E 62 1.245 45.598 -35.986 1.00 16.94
C
ATOM 8697 CD1 PHE E 62 2.509 46.039 -36.340 1.00 16.08
C
ATOM 8698 CD2 PHE E 62 0.207 45.758 -36.888 1.00 13.45
C
ATOM 8699 CE1 PHE E 62 2.734 46.631 -37.569 1.00 16.16
C
ATOM 8700 CE2 PHE E 62 0.424 46.349 -38.117 1.00 15.64
C

ATOM 8701 CZ PHE E 62 1.691 46.784 -38.459 1.00 17.68 C
ATOM 8702 H PHE E 62 0.017 42.886 -35.551 1.00 16.66 H

C
ATOM 2403 C SER B 123 -0.844 21.374 -22.160 1.00 17.37
C
ATOM 2404 O SER B 123 -1.706 20.515 -22.321 1.00 17.15
O
ATOM 2405 CB SER B 123 -0.472 23.230 -23.805 1.00 17.79
C
ATOM 2406 OG SER B 123 -0.916 24.501 -24.251 1.00 16.72
O
ATOM 2407 H SER B 123 -0.019 24.209 -21.600 1.00 21.45
H
ATOM 2408 HA SER B 123 -2.091 22.946 -22.571 1.00 22.17
H
ATOM 2409 HB2 SER B 123 0.490 23.261 -23.680 1.00 21.34
H
ATOM 2410 HB3 SER B 123 -0.697 22.567 -24.475 1.00 21.34
H
ATOM 2411 HG SER B 123 -0.727 25.088 -23.681 1.00 20.06
H
ATOM 2412 N GLN B 124 0.376 21.105 -21.709 1.00 17.12
N
ATOM 2413 CA GLN B 124 0.765 19.765 -21.286 1.00 19.26
C
ATOM 2414 C GLN B 124 -0.119 19.251 -20.156 1.00 17.95
C
ATOM 2415 O GLN B 124 -0.516 18.086 -20.153 1.00 18.47
O
ATOM 2416 CB GLN B 124 2.225 19.751 -20.831 1.00 19.97
C
ATOM 2417 CG GLN B 124 2.631 18.463 -20.125 1.00 20.40
C
ATOM 2418 CD GLN B 124 4.098 18.437 -19.763 1.00 25.03
C
ATOM 2419 OE1 GLN B 124 4.522 19.090 -18.811 1.00 29.00
O
ATOM 2420 NE2 GLN B 124 4.884 17.686 -20.523 1.00 22.34
N
ATOM 2421 H GLN B 124 1.004 21.688 -21.639 1.00 20.54
H
ATOM 2422 HA GLN B 124 0.678 19.158 -22.037 1.00 23.11
H
ATOM 2423 HB2 GLN B 124 2.797 19.856 -21.607 1.00 23.97
H
ATOM 2424 HB3 GLN B 124 2.369 20.485 -20.214 1.00 23.97
H
ATOM 2425 HG2 GLN B 124 2.118 18.376 -19.307 1.00 24.48
H
ATOM 2426 HG3 GLN B 124 2.452 17.711 -20.711 1.00 24.48
H
ATOM 2427 HE21 GLN B 124 5.726 17.639 -20.356 1.00 26.81
H
ATOM 2428 HE22 GLN B 124 4.551 17.246 -21.183 1.00 26.81
H
ATOM 2429 N ALA B 125 -0.397 20.118 -19.186 1.00 19.16
N
ATOM 2430 CA ALA B 125 -1.234 19.754 -18.050 1.00 21.66
C
ATOM 2431 C ALA B 125 -2.650 19.437 -18.513 1.00 22.92
C
ATOM 2432 O ALA B 125 -3.292 18.528 -17.996 1.00 22.29
O
ATOM 2433 CB ALA B 125 -1.251 20.873 -17.021 1.00 21.65
C
ATOM 2434 H ALA B 125 -0.111 20.928 -19.164 1.00 23.00
H
ATOM 2435 HA ALA B 125 -0.870 18.961 -17.627 1.00 26.00
H
ATOM 2436 HB1 ALA B 125 -1.813 20.609 -16.276 1.00 25.98

ATOM 8703 HA PHE E 62 2.496 43.571 -34.856 1.00 19.16 H
ATOM 8704 HB2 PHE E 62 0.049 44.918 -34.503 1.00 19.58
H
ATOM 8705 HB3 PHE E 62 1.422 45.515 -33.973 1.00 19.58
H
ATOM 8706 HD1 PHE E 62 3.214 45.937 -35.743 1.00 19.30
H
ATOM 8707 HD2 PHE E 62 -0.647 45.467 -36.663 1.00 16.15
H
ATOM 8708 HE1 PHE E 62 3.587 46.923 -37.795 1.00 19.39
H
ATOM 8709 HE2 PHE E 62 -0.281 46.451 -38.715 1.00 18.77
H

ATOM 8710 HZ PHE E 62 1.839 47.182 -39.287 1.00 21.21 H

ATOM 8711 N SER E 63 0.479 42.603 -32.580 1.00 14.62 N

ATOM 8712 CA SER E 63 0.375 42.269 -31.163 1.00 17.58 C

ATOM 8713 C SER E 63 1.149 40.993 -30.833 1.00 18.25 C

ATOM 8714 O SER E 63 1.469 40.744 -29.675 1.00 15.30 O
ATOM 8715 CB SER E 63 -1.092 42.124 -30.749 1.00 21.93
C
ATOM 8716 OG SER E 63 -1.698 41.011 -31.375 1.00 26.07
O

ATOM 8717 H SER E 63 -0.233 42.446 -33.036 1.00 17.54 H

ATOM 8718 HA SER E 63 0.760 42.992 -30.643 1.00 21.09 H
ATOM 8719 HB2 SER E 63 -1.136 42.007 -29.787 1.00 26.31
H
ATOM 8720 HB3 SER E 63 -1.571 42.928 -31.006 1.00 26.31
H
ATOM 8721 HG SER E 63 -2.501 40.948 -31.136 1.00 31.29
H

ATOM 8722 N LEU E 64 1.453 40.196 -31.854 1.00 15.25 N

ATOM 8723 CA LEU E 64 2.259 38.989 -31.684 1.00 16.15 C

ATOM 8724 C LEU E 64 3.760 39.284 -31.762 1.00 18.76 C

ATOM 8725 O LEU E 64 4.583 38.437 -31.411 1.00 13.28 O

ATOM 8726 CB LEU E 64 1.895 37.948 -32.745 1.00 18.37 C

ATOM 8727 CG LEU E 64 0.535 37.263 -32.613 1.00 26.98 C
ATOM 8728 CD1 LEU E 64 0.210 36.496 -33.888 1.00 24.22
C
ATOM 8729 CD2 LEU E 64 0.517 36.335 -31.413 1.00 22.89
C

ATOM 8730 H LEU E 64 1.201 40.334 -32.665 1.00 18.30 H

ATOM 8731 HA LEU E 64 2.074 38.606 -30.813 1.00 19.38 H
ATOM 8732 HB2 LEU E 64 1.912 38.384 -33.612 1.00 22.05
H
ATOM 8733 HB3 LEU E 64 2.569 37.251 -32.725 1.00 22.05
H
ATOM 8734 HG LEU E 64 -0.150 37.938 -32.483 1.00 32.37
H
ATOM 8735 HD11 LEU E 64 -0.655 36.069 -33.787 1.00 29.07
H
ATOM 8736 HD12 LEU E 64 0.187 37.118 -34.633 1.00 29.07

H
ATOM 2437 HB2 ALA B 125 -0.345 21.032 -16.712 1.00 25.98
H
ATOM 2438 HB3 ALA B 125 -1.605 21.676 -17.434 1.00 25.98
H
ATOM 2439 N SER B 126 -3.129 20.199 -19.491 1.00 19.48
N
ATOM 2440 CA SER B 126 -4.467 20.008 -20.035 1.00 22.96
C
ATOM 2441 C SER B 126 -4.622 18.638 -20.696 1.00 24.30
C
ATOM 2442 O SER B 126 -5.617 17.945 -20.474 1.00 23.17
O
ATOM 2443 CB SER B 126 -4.790 21.113 -21.042 1.00 21.51
C
ATOM 2444 OG SER B 126 -6.033 20.874 -21.679 1.00 26.37
O
ATOM 2445 H SER B 126 -2.692 20.841 -19.861 1.00 23.37
H
ATOM 2446 HA SER B 126 -5.111 20.065 -19.311 1.00 27.56
H
ATOM 2447 HB2 SER B 126 -4.833 21.962 -20.575 1.00 25.81
H
ATOM 2448 HB3 SER B 126 -4.091 21.140 -21.714 1.00 25.81
H
ATOM 2449 HG SER B 126 -6.197 21.488 -22.228 1.00 31.64
H
ATOM 2450 N CYS B 127 -3.646 18.251 -21.511 1.00 19.38
N
ATOM 2451 CA CYS B 127 -3.696 16.956 -22.182 1.00 17.72
C
ATOM 2452 C CYS B 127 -3.596 15.833 -21.158 1.00 23.86
C
ATOM 2453 O CYS B 127 -4.292 14.824 -21.262 1.00 24.87
O
ATOM 2454 CB CYS B 127 -2.574 16.829 -23.215 1.00 16.67
C
ATOM 2455 SG CYS B 127 -2.664 18.028 -24.573 1.00 18.01
S
ATOM 2456 H CYS B 127 -2.946 18.717 -21.692 1.00 23.26
H
ATOM 2457 HA CYS B 127 -4.544 16.869 -22.644 1.00 21.26
H
ATOM 2458 HB2 CYS B 127 -1.724 16.956 -22.766 1.00 20.01
H
ATOM 2459 HB3 CYS B 127 -2.610 15.941 -23.603 1.00 20.01
H
ATOM 2460 N MET B 128 -2.728 16.014 -20.169 1.00 21.99
N
ATOM 2461 CA MET B 128 -2.562 15.018 -19.119 1.00 30.30
C
ATOM 2462 C MET B 128 -3.878 14.767 -18.387 1.00 27.68
C
ATOM 2463 O MET B 128 -4.261 13.620 -18.166 1.00 33.94
O
ATOM 2464 CB MET B 128 -1.491 15.452 -18.115 1.00 27.20
C
ATOM 2465 CG MET B 128 -1.259 14.418 -17.019 1.00 33.45
C
ATOM 2466 SD MET B 128 -0.009 14.851 -15.796 1.00 47.54
S
ATOM 2467 CE MET B 128 -0.094 13.355 -14.801 1.00 39.77
C
ATOM 2468 H MET B 128 -2.224 16.706 -20.083 1.00 26.39
H
ATOM 2469 HA MET B 128 -2.267 14.187 -19.523 1.00 36.36
H
ATOM 2470 HB2 MET B 128 -0.652 15.585 -18.584 1.00 32.64
H
ATOM 8737 HD13 LEU E 64 0.895 35.827 -34.037 1.00 29.07
H
ATOM 8738 HD21 LEU E 64 -0.355 35.915 -31.353 1.00 27.46
H
ATOM 8739 HD22 LEU E 64 1.203 35.660 -31.526 1.00 27.46
H
ATOM 8740 HD23 LEU E 64 0.691 36.853 -30.611 1.00 27.46
H

ATOM 8741 N PHE E 65 4.118 40.475 -32.233 1.00 16.54 N

ATOM 8742 CA PHE E 65 5.526 40.845 -32.337 1.00 16.39 C

ATOM 8743 C PHE E 65 6.045 41.265 -30.970 1.00 18.01 C

ATOM 8744 O PHE E 65 5.574 42.242 -30.391 1.00 17.22 O

ATOM 8745 CB PHE E 65 5.726 41.971 -33.354 1.00 14.80 C
ATOM 8746 CG PHE E 65 7.166 42.375 -33.535 1.00 14.42
C
ATOM 8747 CD1 PHE E 65 8.128 41.434 -33.870 1.00 16.17
C
ATOM 8748 CD2 PHE E 65 7.554 43.693 -33.380 1.00 15.24
C
ATOM 8749 CE1 PHE E 65 9.454 41.805 -34.040 1.00 14.97
C
ATOM 8750 CE2 PHE E 65 8.876 44.070 -33.549 1.00 14.62
C

ATOM 8751 CZ PHE E 65 9.824 43.127 -33.876 1.00 16.09 C

ATOM 8752 H PHE E 65 3.569 41.082 -32.497 1.00 19.85 H

ATOM 8753 HA PHE E 65 6.038 40.075 -32.632 1.00 19.67 H
ATOM 8754 HB2 PHE E 65 5.390 41.678 -34.216 1.00 17.76
H
ATOM 8755 HB3 PHE E 65 5.234 42.752 -33.057 1.00 17.76
H
ATOM 8756 HD1 PHE E 65 7.883 40.544 -33.979 1.00 19.41
H
ATOM 8757 HD2 PHE E 65 6.919 44.335 -33.157 1.00 18.29
H
ATOM 8758 HE1 PHE E 65 10.092 41.166 -34.262 1.00 17.96
H
ATOM 8759 HE2 PHE E 65 9.124 44.959 -33.439 1.00 17.55
H
ATOM 8760 HZ PHE E 65 10.712 43.379 -33.991 1.00 19.31
H

ATOM 8761 N ARG E 66 7.018 40.520 -30.459 1.00 18.88 N
ATOM 8762 CA ARG E 66 7.536 40.756 -29.118 1.00 20.69
C

ATOM 8763 C ARG E 66 8.694 41.748 -29.143 1.00 18.93 C

ATOM 8764 O ARG E 66 9.834 41.401 -28.836 1.00 16.41 O
ATOM 8765 CB ARG E 66 7.968 39.434 -28.484 1.00 25.21
C
ATOM 8766 CG ARG E 66 6.879 38.373 -28.539 1.00 29.70
C
ATOM 8767 CD ARG E 66 7.008 37.358 -27.421 1.00 35.51
C
ATOM 8768 NE ARG E 66 8.129 36.441 -27.606 1.00 45.62
N
ATOM 8769 CZ ARG E 66 8.038 35.247 -28.185 1.00 49.30
C
ATOM 8770 NH1 ARG E 66 6.876 34.804 -28.652 1.00 48.42

H
ATOM 2471 HB3 MET B 128 -1.770 16.279 -17.692 1.00 32.64
H
ATOM 2472 HG2 MET B 128 -2.094 14.281 -16.545 1.00 40.14
H
ATOM 2473 HG3 MET B 128 -0.983 13.587 -17.435 1.00 40.14
H
ATOM 2474 HE1 MET B 128 -0.994 13.260 -14.451 1.00 47.73
H
ATOM 2475 HE2 MET B 128 0.126 12.593 -15.359 1.00 47.73
H
ATOM 2476 HE3 MET B 128 0.540 13.426 -14.071 1.00 47.73
H
ATOM 2477 N SER B 129 -4.573 15.842 -18.029 1.00 29.26
N
ATOM 2478 CA SER B 129 -5.795 15.737 -17.233 1.00 32.80
C
ATOM 2479 C SER B 129 -6.901 14.984 -17.968 1.00 29.82
C
ATOM 2480 O SER B 129 -7.932 14.658 -17.381 1.00 30.42
O
ATOM 2481 CB SER B 129 -6.296 17.127 -16.839 1.00 32.72
C
ATOM 2482 OG SER B 129 -6.872 17.799 -17.945 1.00 38.37
O
ATOM 2483 H SER B 129 -4.358 16.649 -18.235 1.00 35.11
H
ATOM 2484 HA SER B 129 -5.596 15.250 -16.418 1.00 39.36
H
ATOM 2485 HB2 SER B 129 -6.966 17.034 -16.144 1.00 39.26
H
ATOM 2486 HB3 SER B 129 -5.548 17.649 -16.509 1.00 39.26
H
ATOM 2487 HG SER B 129 -6.302 17.888 -18.556 1.00 46.05
H
ATOM 2488 N GLN B 130 -6.682 14.717 -19.251 1.00 32.61
N
ATOM 2489 CA GLN B 130 -7.630 13.962 -20.059 1.00 32.51
C
ATOM 2490 C GLN B 130 -7.007 12.648 -20.517 1.00 30.71
C
ATOM 2491 O GLN B 130 -7.402 12.083 -21.536 1.00 31.54
O
ATOM 2492 CB GLN B 130 -8.082 14.801 -21.255 1.00 34.47
C
ATOM 2493 CG GLN B 130 -8.648 16.155 -20.845 1.00 35.04
C
ATOM 2494 CD GLN B 130 -8.999 17.038 -22.023 1.00 35.73
C
ATOM 2495 OE1 GLN B 130 -9.762 16.647 -22.906 1.00 32.33
O
ATOM 2496 NE2 GLN B 130 -8.442 18.245 -22.040 1.00 42.10
N
ATOM 2497 H GLN B 130 -5.981 14.966 -19.681 1.00 39.14
H
ATOM 2498 HA GLN B 130 -8.411 13.755 -19.523 1.00 39.01
H
ATOM 2499 HB2 GLN B 130 -7.322 14.957 -21.837 1.00 41.37
H
ATOM 2500 HB3 GLN B 130 -8.774 14.319 -21.735 1.00 41.37
H
ATOM 2501 HG2 GLN B 130 -9.456 16.015 -20.327 1.00 42.05
H
ATOM 2502 HG3 GLN B 130 -7.988 16.622 -20.309 1.00 42.05
H
ATOM 2503 HE21 GLN B 130 -8.608 18.786 -22.687 1.00 50.53
H
ATOM 2504 HE22 GLN B 130 -7.915 18.484 -21.404 1.00 50.53
N1+
ATOM 8771 NH2 ARG E 66 9.117 34.488 -28.298 1.00 50.83
N

ATOM 8772 H ARG E 66 7.397 39.868 -30.872 1.00 22.66 H
ATOM 8773 HA ARG E 66 6.831 41.134 -28.570 1.00 24.83
H
ATOM 8774 HB2 ARG E 66 8.743 39.094 -28.958 1.00 30.25
H
ATOM 8775 HB3 ARG E 66 8.190 39.588 -27.552 1.00 30.25
H
ATOM 8776 HG2 ARG E 66 6.013 38.803 -28.458 1.00 35.64
H
ATOM 8777 HG3 ARG E 66 6.939 37.901 -29.384 1.00 35.64
H
ATOM 8778 HD2 ARG E 66 7.142 37.828 -26.583 1.00 42.61
H
ATOM 8779 HD3 ARG E 66 6.195 36.831 -27.378 1.00 42.61
H
ATOM 8780 HE ARG E 66 8.901 36.691 -27.322 1.00 54.74
H
ATOM 8781 HH11 ARG E 66 6.170 35.290 -28.581 1.00 58.11
H
ATOM 8782 HH12 ARG E 66 6.829 34.030 -29.025 1.00 58.11
H
ATOM 8783 HH21 ARG E 66 9.873 34.768 -27.999 1.00 60.99
H
ATOM 8784 HH22 ARG E 66 9.062 33.716 -28.674 1.00 60.99
H

ATOM 8785 N ARG E 67 8.380 42.984 -29.513 1.00 18.67 N
ATOM 8786 CA ARG E 67 9.361 44.059 -29.578 1.00 20.20
C

ATOM 8787 C ARG E 67 10.020 44.281 -28.218 1.00 21.69 C

ATOM 8788 O ARG E 67 9.332 44.366 -27.204 1.00 17.08 O
ATOM 8789 CB ARG E 67 8.685 45.349 -30.057 1.00 21.97
C
ATOM 8790 CG ARG E 67 9.601 46.559 -30.135 1.00 27.90
C
ATOM 8791 CD ARG E 67 8.884 47.772 -30.720 1.00 40.95
C
ATOM 8792 NE ARG E 67 8.218 48.579 -29.698 1.00 59.70
N
ATOM 8793 CZ ARG E 67 6.960 48.412 -29.296 1.00 72.67
C
ATOM 8794 NH1 ARG E 67 6.199 47.460 -29.821 1.00 75.12
N1+
ATOM 8795 NH2 ARG E 67 6.457 49.206 -28.360 1.00 72.00
N

ATOM 8796 H ARG E 67 7.587 43.230 -29.736 1.00 22.41 H
ATOM 8797 HA ARG E 67 10.053 43.823 -30.216 1.00 24.24
H
ATOM 8798 HB2 ARG E 67 8.323 45.197 -30.944 1.00 26.37
H
ATOM 8799 HB3 ARG E 67 7.964 45.566 -29.444 1.00 26.37
H
ATOM 8800 HG2 ARG E 67 9.906 46.787 -29.243 1.00 33.48
H
ATOM 8801 HG3 ARG E 67 10.358 46.350 -30.705 1.00 33.48
H
ATOM 8802 HD2 ARG E 67 9.532 48.335 -31.172 1.00 49.14
H
ATOM 8803 HD3 ARG E 67 8.211 47.468 -31.349 1.00 49.14
H
ATOM 8804 HE ARG E 67 8.673 49.208 -29.328 1.00 71.64

H
ATOM 2505 N ASN B 131 -6.032 12.168 -19.750 1.00 31.89
N
ATOM 2506 CA ASN B 131 -5.372 10.896 -20.028 1.00 35.86
C
ATOM 2507 C ASN B 131 -4.770 10.869 -21.431 1.00 35.32
C
ATOM 2508 O ASN B 131 -4.818 9.852 -22.125 1.00 31.56
O
ATOM 2509 CB ASN B 131 -6.358 9.740 -19.852 1.00 44.38
C
ATOM 2510 CG ASN B 131 -5.665 8.403 -19.679 1.00 65.46
C
ATOM 2511 OD1 ASN B 131 -5.153 8.093 -18.604 1.00 82.44
O
ATOM 2512 ND2 ASN B 131 -5.648 7.603 -20.737 1.00 73.37
N
ATOM 2513 H ASN B 131 -5.730 12.567 -19.050 1.00 38.26
H
ATOM 2514 HA ASN B 131 -4.650 10.772 -19.392 1.00 43.03
H
ATOM 2515 HB2 ASN B 131 -6.899 9.903 -19.063 1.00 53.26
H
ATOM 2516 HB3 ASN B 131 -6.925 9.685 -20.638 1.00 53.26
H
ATOM 2517 HD21 ASN B 131 -5.267 6.833 -20.689 1.00 88.04
H
ATOM 2518 HD22 ASN B 131 -6.019 7.853 -21.472 1.00 88.04
H
ATOM 2519 N ALA B 132 -4.206 12.001 -21.838 1.00 25.52
N
ATOM 2520 CA ALA B 132 -3.593 12.132 -23.153 1.00 27.44
C
ATOM 2521 C ALA B 132 -2.264 12.868 -23.050 1.00 26.46
C
ATOM 2522 O ALA B 132 -1.802 13.178 -21.954 1.00 24.84
O
ATOM 2523 CB ALA B 132 -4.533 12.860 -24.100 1.00 24.28
C
ATOM 2524 H ALA B 132 -4.166 12.717 -21.364 1.00 30.62
H
ATOM 2525 HA ALA B 132 -3.422 11.248 -23.515 1.00 32.93
H
ATOM 2526 HB1 ALA B 132 -4.107 12.937 -24.969 1.00 29.14
H
ATOM 2527 HB2 ALA B 132 -5.356 12.353 -24.179 1.00 29.14
H
ATOM 2528 HB3 ALA B 132 -4.719 13.742 -23.743 1.00 29.14
H
ATOM 2529 N SER B 133 -1.657 13.137 -24.201 1.00 21.19
N
ATOM 2530 CA SER B 133 -0.426 13.913 -24.270 1.00 20.84
C
ATOM 2531 C SER B 133 -0.540 14.942 -25.383 1.00 21.20
C
ATOM 2532 O SER B 133 -1.480 14.903 -26.177 1.00 19.82
O
ATOM 2533 CB SER B 133 0.776 13.001 -24.514 1.00 26.77
C
ATOM 2534 OG SER B 133 0.841 11.979 -23.535 1.00 32.82
O
ATOM 2535 H SER B 133 -1.944 12.875 -24.968 1.00 25.43
H
ATOM 2536 HA SER B 133 -0.292 14.381 -23.431 1.00 25.01
H
ATOM 2537 HB2 SER B 133 0.691 12.594 -25.390 1.00 32.13
H
ATOM 2538 HB3 SER B 133 1.588 13.530 -24.472 1.00 32.13
H
ATOM 8805 HH11 ARG E 67 6.518 46.941 -30.429 1.00 90.15
H
ATOM 8806 HH12 ARG E 67 5.388 47.361 -29.554 1.00 90.15
H
ATOM 8807 HH21 ARG E 67 6.944 49.825 -28.014 1.00 86.40
H
ATOM 8808 HH22 ARG E 67 5.645 49.101 -28.097 1.00 86.40
H

ATOM 8809 N VAL E 68 11.348 44.362 -28.193 1.00 22.03 N
ATOM 8810 CA VAL E 68 12.059 44.659 -26.953 1.00 20.34
C

ATOM 8811 C VAL E 68 12.343 46.156 -26.894 1.00 22.74 C

ATOM 8812 O VAL E 68 12.682 46.762 -27.912 1.00 25.42 O
ATOM 8813 CB VAL E 68 13.384 43.867 -26.823 1.00 27.96
C
ATOM 8814 CG1 VAL E 68 13.108 42.374 -26.817 1.00 30.54
C
ATOM 8815 CG2 VAL E 68 14.361 44.220 -27.936 1.00 28.18
C

ATOM 8816 H VAL E 68 11.858 44.250 -28.877 1.00 26.44 H
ATOM 8817 HA VAL E 68 11.494 44.428 -26.199 1.00 24.41
H
ATOM 8818 HB VAL E 68 13.803 44.095 -25.978 1.00 33.55
H
ATOM 8819 HG11 VAL E 68 13.950 41.899 -26.735 1.00 36.65
H
ATOM 8820 HG12 VAL E 68 12.534 42.163 -26.064 1.00 36.65
H
ATOM 8821 HG13 VAL E 68 12.670 42.131 -27.647 1.00 36.65
H
ATOM 8822 HG21 VAL E 68 15.174 43.705 -27.818 1.00 33.82
H
ATOM 8823 HG22 VAL E 68 13.954 44.008 -28.791 1.00 33.82
H
ATOM 8824 HG23 VAL E 68 14.560 45.169 -27.891 1.00 33.82
H

ATOM 8825 N PRO E 69 12.187 46.769 -25.710 1.00 21.06 N
ATOM 8826 CA PRO E 69 12.539 48.190 -25.618 1.00 24.69
C

ATOM 8827 C PRO E 69 14.021 48.401 -25.907 1.00 22.26 C
ATOM 8828 O PRO E 69 14.823 47.522 -25.593 1.00 19.66
O
ATOM 8829 CB PRO E 69 12.198 48.553 -24.168 1.00 20.34
C
ATOM 8830 CG PRO E 69 11.276 47.473 -23.698 1.00 22.90
C
ATOM 8831 CD PRO E 69 11.689 46.241 -24.428 1.00 24.19
C
ATOM 8832 HA PRO E 69 12.002 48.721 -26.227 1.00 29.63
H
ATOM 8833 HB2 PRO E 69 13.009 48.566 -23.636 1.00 24.40
H
ATOM 8834 HB3 PRO E 69 11.756 49.416 -24.142 1.00 24.40
H
ATOM 8835 HG2 PRO E 69 11.377 47.353 -22.741 1.00 27.48
H
ATOM 8836 HG3 PRO E 69 10.361 47.709 -23.918 1.00 27.48
H
ATOM 8837 HD2 PRO E 69 12.400 45.786 -23.949 1.00 29.03
H
ATOM 8838 HD3 PRO E 69 10.926 45.661 -24.573 1.00 29.03

```
H
ATOM  2539  HG  SER B 133      0.914  12.318 -22.770  1.00 39.39
H
ATOM  2540  N   LEU B 134      0.404  15.873 -25.431  1.00 18.46
N
ATOM  2541  CA  LEU B 134      0.479  16.796 -26.550  1.00 18.04
C
ATOM  2542  C   LEU B 134      0.794  15.995 -27.806  1.00 21.00
C
ATOM  2543  O   LEU B 134      1.303  14.877 -27.723  1.00 18.42
O
ATOM  2544  CB  LEU B 134      1.540  17.869 -26.311  1.00 20.17
C
ATOM  2545  CG  LEU B 134      1.167  18.973 -25.319  1.00 19.25
C
ATOM  2546  CD1 LEU B 134      2.400  19.780 -24.937  1.00 19.48
C
ATOM  2547  CD2 LEU B 134      0.096  19.889 -25.898  1.00 16.17
C
ATOM  2548  H   LEU B 134      1.010  15.990 -24.831  1.00 22.15
H
ATOM  2549  HA  LEU B 134     -0.379  17.231 -26.669  1.00 21.65
H
ATOM  2550  HB2 LEU B 134      2.341  17.437 -25.976  1.00 24.20
H
ATOM  2551  HB3 LEU B 134      1.736  18.298 -27.159  1.00 24.20
H
ATOM  2552  HG  LEU B 134      0.812  18.567 -24.513  1.00 23.10
H
ATOM  2553 HD11 LEU B 134      2.142  20.472 -24.308  1.00 23.37
H
ATOM  2554 HD12 LEU B 134      3.050  19.187 -24.528  1.00 23.37
H
ATOM  2555 HD13 LEU B 134      2.775  20.181 -25.736  1.00 23.37
H
ATOM  2556 HD21 LEU B 134     -0.117  20.576 -25.247  1.00 19.40
H
ATOM  2557 HD22 LEU B 134      0.435  20.297 -26.710  1.00 19.40
H
ATOM  2558 HD23 LEU B 134     -0.695  19.363 -26.097  1.00 19.40
H
ATOM  2559  N   LEU B 135      0.486  16.570 -28.963  1.00 15.70
N
ATOM  2560  CA  LEU B 135      0.693  15.894 -30.236  1.00 15.71
C
ATOM  2561  C   LEU B 135      2.099  15.320 -30.370  1.00 16.68
C
ATOM  2562  O   LEU B 135      3.084  16.020 -30.142  1.00 15.25
O
ATOM  2563  CB  LEU B 135      0.430  16.862 -31.388  1.00 13.32
C
ATOM  2564  CG  LEU B 135      0.715  16.342 -32.793  1.00 13.52
C
ATOM  2565  CD1 LEU B 135     -0.220  15.193 -33.142  1.00 16.61
C
ATOM  2566  CD2 LEU B 135      0.582  17.468 -33.796  1.00 13.74
C
ATOM  2567  H   LEU B 135      0.152  17.359 -29.037  1.00 18.84
H
ATOM  2568  HA  LEU B 135      0.062  15.161 -30.310  1.00 18.85
H
ATOM  2569  HB2 LEU B 135     -0.505  17.120 -31.360  1.00 15.99
H
ATOM  2570  HB3 LEU B 135      0.983  17.648 -31.255  1.00 15.99
H
ATOM  2571  HG  LEU B 135      1.626  16.011 -32.831  1.00 16.22
H
ATOM  2572 HD11 LEU B 135     -0.017  14.882 -34.038  1.00 19.93
H
ATOM  8839  N   THR E  70     14.370  49.538 -26.499  1.00 24.37      N
ATOM  8840  CA  THR E  70     15.756  49.821 -26.866  1.00 29.94
C
ATOM  8841  C   THR E  70     16.152  51.237 -26.484  1.00 29.58      C
ATOM  8842  O   THR E  70     15.305  52.123 -26.385  1.00 29.43      O
ATOM  8843  CB  THR E  70     15.997  49.653 -28.383  1.00 31.13
C
ATOM  8844  OG1 THR E  70     15.358  50.722 -29.092  1.00 33.21
O
ATOM  8845  CG2 THR E  70     15.456  48.325 -28.879  1.00 33.64
C
ATOM  8846  H   THR E  70     13.820  50.168 -26.701  1.00 29.24      H
ATOM  8847  HA  THR E  70     16.341  49.205 -26.396  1.00 35.92
H
ATOM  8848  HB  THR E  70     16.951  49.677 -28.560  1.00 37.36
H
ATOM  8849  HG1 THR E  70     15.486  50.636 -29.918  1.00 39.85
H
ATOM  8850 HG21 THR E  70     15.615  48.237 -29.832  1.00 40.36
H
ATOM  8851 HG22 THR E  70     15.895  47.594 -28.417  1.00 40.36
H
ATOM  8852 HG23 THR E  70     14.501  48.274 -28.713  1.00 40.36
H
ATOM  8853  N   SER E  71     17.447  51.439 -26.274  1.00 28.05      N
ATOM  8854  CA  SER E  71     17.991  52.775 -26.086  1.00 33.59
C
ATOM  8855  C   SER E  71     18.133  53.456 -27.445  1.00 32.14      C
ATOM  8856  O   SER E  71     18.290  54.673 -27.528  1.00 34.41      O
ATOM  8857  CB  SER E  71     19.339  52.713 -25.369  1.00 30.01
C
ATOM  8858  OG  SER E  71     20.249  51.897 -26.084  1.00 38.73
O
ATOM  8859  H   SER E  71     18.036  50.813 -26.236  1.00 33.66      H
ATOM  8860  HA  SER E  71     17.379  53.298 -25.543  1.00 40.31
H
ATOM  8861  HB2 SER E  71     19.703  53.610 -25.303  1.00 36.01
H
ATOM  8862  HB3 SER E  71     19.209  52.342 -24.483  1.00 36.01
H
ATOM  8863  HG  SER E  71     20.986  51.869 -25.682  1.00 46.48
H
ATOM  8864  N   THR E  72     18.084  52.655 -28.507  1.00 29.50      N
ATOM  8865  CA  THR E  72     18.097  53.166 -29.873  1.00 29.84
C
ATOM  8866  C   THR E  72     16.844  54.008 -30.118  1.00 28.11      C
ATOM  8867  O   THR E  72     15.733  53.480 -30.080  1.00 28.11      O
ATOM  8868  CB  THR E  72     18.157  52.014 -30.900  1.00 32.89
C
ATOM  8869  OG1 THR E  72     19.282  51.168 -30.614  1.00 37.51
O
ATOM  8870  CG2 THR E  72     18.275  52.554 -32.320  1.00 35.87
C
ATOM  8871  H   THR E  72     18.043  51.797 -28.459  1.00 35.40      H
ATOM  8872  HA  THR E  72     18.875  53.730 -30.000  1.00 35.81
```

H
ATOM 2573 HD12 LEU B 135 -0.087 14.474 -32.504 1.00 19.93
H
ATOM 2574 HD13 LEU B 135 -1.136 15.508 -33.099 1.00 19.93
H
ATOM 2575 HD21 LEU B 135 0.765 17.123 -34.684 1.00 16.49
H
ATOM 2576 HD22 LEU B 135 -0.321 17.820 -33.758 1.00 16.49
H
ATOM 2577 HD23 LEU B 135 1.219 18.165 -33.574 1.00 16.49
H
ATOM 2578 N LYS B 136 2.178 14.042 -30.735 1.00 16.35
N
ATOM 2579 CA LYS B 136 3.437 13.426 -31.139 1.00 16.55
C
ATOM 2580 C LYS B 136 3.381 13.084 -32.624 1.00 17.63
C
ATOM 2581 O LYS B 136 2.532 12.309 -33.055 1.00 21.03
O
ATOM 2582 CB LYS B 136 3.728 12.163 -30.323 1.00 19.40
C
ATOM 2583 CG LYS B 136 4.973 11.413 -30.793 1.00 19.92
C
ATOM 2584 CD LYS B 136 5.200 10.114 -30.027 1.00 27.62
C
ATOM 2585 CE LYS B 136 6.484 9.429 -30.494 1.00 26.76
C
ATOM 2586 NZ LYS B 136 6.768 8.164 -29.765 1.00 29.82
N1+
ATOM 2587 H LYS B 136 1.507 13.505 -30.757 1.00 19.62
H
ATOM 2588 HA LYS B 136 4.162 14.054 -30.998 1.00 19.86
H
ATOM 2589 HB2 LYS B 136 3.863 12.413 -29.395 1.00 23.28
H
ATOM 2590 HB3 LYS B 136 2.972 11.560 -30.396 1.00 23.28
H
ATOM 2591 HG2 LYS B 136 4.875 11.194 -31.733 1.00 23.90
H
ATOM 2592 HG3 LYS B 136 5.751 11.978 -30.663 1.00 23.90
H
ATOM 2593 HD2 LYS B 136 5.283 10.307 -29.080 1.00 33.15
H
ATOM 2594 HD3 LYS B 136 4.457 9.511 -30.186 1.00 33.15
H
ATOM 2595 HE2 LYS B 136 6.403 9.219 -31.437 1.00 32.11
H
ATOM 2596 HE3 LYS B 136 7.231 10.031 -30.351 1.00 32.11
H
ATOM 2597 HZ1 LYS B 136 6.101 7.588 -29.885 1.00 35.78
H
ATOM 2598 HZ2 LYS B 136 7.522 7.802 -30.069 1.00 35.78
H
ATOM 2599 HZ3 LYS B 136 6.856 8.328 -28.895 1.00 35.78
H
ATOM 2600 N VAL B 137 4.281 13.676 -33.401 1.00 17.20
N
ATOM 2601 CA VAL B 137 4.399 13.367 -34.822 1.00 17.92
C
ATOM 2602 C VAL B 137 5.388 12.221 -34.998 1.00 22.09
C
ATOM 2603 O VAL B 137 6.556 12.346 -34.630 1.00 20.93
O
ATOM 2604 CB VAL B 137 4.868 14.590 -35.643 1.00 23.08
C
ATOM 2605 CG1 VAL B 137 5.015 14.234 -37.124 1.00 22.11
C
ATOM 2606 CG2 VAL B 137 3.896 15.744 -35.477 1.00 15.93
H
ATOM 8873 HB THR E 72 17.342 51.491 -30.841 1.00 39.47
H
ATOM 8874 HG1 THR E 72 19.318 50.540 -31.171 1.00 45.01
H
ATOM 8875 HG21 THR E 72 18.312 51.820 -32.952 1.00 43.05
H
ATOM 8876 HG22 THR E 72 17.507 53.110 -32.527 1.00 43.05
H
ATOM 8877 HG23 THR E 72 19.082 53.086 -32.406 1.00 43.05
H

ATOM 8878 N PRO E 73 17.014 55.318 -30.378 1.00 33.46 N
ATOM 8879 CA PRO E 73 15.854 56.220 -30.408 1.00 32.41
C

ATOM 8880 C PRO E 73 14.911 56.022 -31.595 1.00 26.60 C
ATOM 8881 O PRO E 73 13.739 56.379 -31.482 1.00 30.39
O
ATOM 8882 CB PRO E 73 16.497 57.609 -30.470 1.00 29.80
C
ATOM 8883 CG PRO E 73 17.797 57.390 -31.135 1.00 29.20
C
ATOM 8884 CD PRO E 73 18.267 56.028 -30.697 1.00 34.72
C
ATOM 8885 HA PRO E 73 15.349 56.141 -29.584 1.00 38.89
H
ATOM 8886 HB2 PRO E 73 15.939 58.206 -30.993 1.00 35.76
H
ATOM 8887 HB3 PRO E 73 16.623 57.953 -29.572 1.00 35.76
H
ATOM 8888 HG2 PRO E 73 17.677 57.415 -32.097 1.00 35.04
H
ATOM 8889 HG3 PRO E 73 18.425 58.073 -30.852 1.00 35.04
H
ATOM 8890 HD2 PRO E 73 18.732 55.582 -31.422 1.00 41.67
H
ATOM 8891 HD3 PRO E 73 18.824 56.101 -29.907 1.00 41.67
H

ATOM 8892 N TYR E 74 15.402 55.472 -32.703 1.00 27.41 N
ATOM 8893 CA TYR E 74 14.567 55.297 -33.890 1.00 22.57
C

ATOM 8894 C TYR E 74 14.741 53.922 -34.522 1.00 23.86 C

ATOM 8895 O TYR E 74 15.859 53.493 -34.810 1.00 23.15 O
ATOM 8896 CB TYR E 74 14.878 56.382 -34.925 1.00 23.62
C
ATOM 8897 CG TYR E 74 13.905 56.415 -36.084 1.00 23.55
C
ATOM 8898 CD1 TYR E 74 14.120 55.645 -37.221 1.00 21.50
C
ATOM 8899 CD2 TYR E 74 12.770 57.211 -36.038 1.00 23.88
C
ATOM 8900 CE1 TYR E 74 13.232 55.673 -38.283 1.00 25.17
C
ATOM 8901 CE2 TYR E 74 11.875 57.244 -37.094 1.00 27.31
C
ATOM 8902 CZ TYR E 74 12.112 56.473 -38.214 1.00 25.37
C
ATOM 8903 OH TYR E 74 11.224 56.503 -39.265 1.00 28.87
O

ATOM 8904 H TYR E 74 16.211 55.193 -32.794 1.00 32.90 H
ATOM 8905 HA TYR E 74 13.636 55.390 -33.633 1.00 27.09
H
ATOM 8906 HB2 TYR E 74 14.849 57.247 -34.489 1.00 28.34

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C
ATOM  2607  H   VAL B 137      4.842  14.268 -33.126  1.00 20.64
H
ATOM  2608  HA  VAL B 137      3.537  13.082 -35.162  1.00 21.51
H
ATOM  2609  HB  VAL B 137      5.734  14.878 -35.316  1.00 27.69
H
ATOM  2610 HG11 VAL B 137      5.309  15.020 -37.610  1.00 26.53
H
ATOM  2611 HG12 VAL B 137      5.670  13.525 -37.214  1.00 26.53
H
ATOM  2612 HG13 VAL B 137      4.156  13.937 -37.464  1.00 26.53
H
ATOM  2613 HG21 VAL B 137      4.210  16.499 -36.000  1.00 19.12
H
ATOM  2614 HG22 VAL B 137      3.021  15.467 -35.789  1.00 19.12
H
ATOM  2615 HG23 VAL B 137      3.852  15.987 -34.539  1.00 19.12
H
ATOM  2616  N   TYR B 138      4.915  11.113 -35.563  1.00 20.52
N
ATOM  2617  CA  TYR B 138      5.748   9.928 -35.754  1.00 25.30
C
ATOM  2618  C   TYR B 138      5.614   9.342 -37.163  1.00 26.25
C
ATOM  2619  O   TYR B 138      6.481   8.587 -37.601  1.00 27.44
O
ATOM  2620  CB  TYR B 138      5.393   8.861 -34.713  1.00 26.97
C
ATOM  2621  CG  TYR B 138      4.047   8.217 -34.940  1.00 23.68
C
ATOM  2622  CD1 TYR B 138      2.886   8.797 -34.451  1.00 23.08
C
ATOM  2623  CD2 TYR B 138      3.938   7.028 -35.650  1.00 27.12
C
ATOM  2624  CE1 TYR B 138      1.654   8.212 -34.661  1.00 25.34
C
ATOM  2625  CE2 TYR B 138      2.709   6.437 -35.867  1.00 26.65
C
ATOM  2626  CZ  TYR B 138      1.572   7.033 -35.371  1.00 28.22
C
ATOM  2627  OH  TYR B 138      0.347   6.447 -35.581  1.00 30.35
O
ATOM  2628  H   TYR B 138      4.108  11.021 -35.847  1.00 24.63
H
ATOM  2629  HA  TYR B 138      6.676  10.175 -35.623  1.00 30.36
H
ATOM  2630  HB2 TYR B 138      6.066   8.163 -34.740  1.00 32.36
H
ATOM  2631  HB3 TYR B 138      5.381   9.273 -33.835  1.00 32.36
H
ATOM  2632  HD1 TYR B 138      2.939   9.593 -33.974  1.00 27.70
H
ATOM  2633  HD2 TYR B 138      4.705   6.626 -35.988  1.00 32.54
H
ATOM  2634  HE1 TYR B 138      0.883   8.612 -34.327  1.00 30.41
H
ATOM  2635  HE2 TYR B 138      2.650   5.641 -36.344  1.00 31.98
H
ATOM  2636  HH  TYR B 138     -0.257   6.909 -35.225  1.00 36.42
H
ATOM  2637  N   SER B 139      4.538   9.689 -37.870  1.00 26.36
N
ATOM  2638  CA  SER B 139      4.288   9.139 -39.207  1.00 27.55
C
ATOM  2639  C   SER B 139      3.526  10.099 -40.119  1.00 23.78
C
ATOM  2640  O   SER B 139      2.379  10.447 -39.841  1.00 22.07
H
ATOM  8907 HB3 TYR E  74     15.765  56.225 -35.286  1.00 28.34
H
ATOM  8908 HD1 TYR E  74     14.875  55.105 -37.271  1.00 25.80
H
ATOM  8909 HD2 TYR E  74     12.608  57.732 -35.286  1.00 28.65
H
ATOM  8910 HE1 TYR E  74     13.390  55.153 -39.038  1.00 30.20
H
ATOM  8911 HE2 TYR E  74     11.119  57.784 -37.050  1.00 32.77
H
ATOM  8912 HH  TYR E  74     10.592  57.028 -39.092  1.00 34.65
H

ATOM  8913  N   GLU E  75     13.616  53.243 -34.736  1.00 23.34      N
ATOM  8914  CA  GLU E  75     13.590  51.973 -35.452  1.00 22.00
C

ATOM  8915  C   GLU E  75     12.361  51.911 -36.345  1.00 22.18      C

ATOM  8916  O   GLU E  75     11.232  52.031 -35.868  1.00 22.80      O
ATOM  8917  CB  GLU E  75     13.585  50.783 -34.486  1.00 22.49
C
ATOM  8918  CG  GLU E  75     14.930  50.477 -33.863  1.00 25.87
C
ATOM  8919  CD  GLU E  75     15.016  49.060 -33.322  1.00 31.04
C
ATOM  8920  OE1 GLU E  75     14.083  48.630 -32.606  1.00 23.10
O
ATOM  8921  OE2 GLU E  75     16.021  48.375 -33.619  1.00 30.63
O1-

ATOM  8922  H   GLU E  75     12.841  53.503 -34.469  1.00 28.00      H
ATOM  8923  HA  GLU E  75     14.378  51.906 -36.013  1.00 26.40
H
ATOM  8924  HB2 GLU E  75     12.962  50.971 -33.766  1.00 26.99
H
ATOM  8925  HB3 GLU E  75     13.297  49.993 -34.970  1.00 26.99
H
ATOM  8926  HG2 GLU E  75     15.621  50.584 -34.535  1.00 31.05
H
ATOM  8927  HG3 GLU E  75     15.084  51.090 -33.127  1.00 31.05
H

ATOM  8928  N   ASP E  76     12.598  51.733 -37.641  1.00 18.47      N
ATOM  8929  CA  ASP E  76     11.532  51.564 -38.616  1.00 21.95
C

ATOM  8930  C   ASP E  76     11.628  50.178 -39.234  1.00 16.59      C

ATOM  8931  O   ASP E  76     12.632  49.831 -39.851  1.00 16.66      O
ATOM  8932  CB  ASP E  76     11.610  52.637 -39.701  1.00 19.62
C
ATOM  8933  CG  ASP E  76     10.424  52.599 -40.638  1.00 25.99
C
ATOM  8934  OD1 ASP E  76      9.322  53.005 -40.215  1.00 30.46
O
ATOM  8935  OD2 ASP E  76     10.590  52.164 -41.797  1.00 34.44
O1-

ATOM  8936  H   ASP E  76     13.386  51.706 -37.984  1.00 22.16      H
ATOM  8937  HA  ASP E  76     10.674  51.641 -38.171  1.00 26.34
H
ATOM  8938  HB2 ASP E  76     11.634  53.511 -39.282  1.00 23.54
H
ATOM  8939  HB3 ASP E  76     12.413  52.498 -40.227  1.00 23.54
H
ATOM  8940  N   LEU E  77     10.574  49.392 -39.056  1.00 15.41      N
```

O
ATOM 2641 CB SER B 139 3.507 7.826 -39.099 1.00 25.84
C
ATOM 2642 OG SER B 139 3.173 7.324 -40.386 1.00 25.64
O
ATOM 2643 H SER B 139 3.936 10.241 -37.600 1.00 31.64
H
ATOM 2644 HA SER B 139 5.140 8.944 -39.628 1.00 33.05
H
ATOM 2645 HB2 SER B 139 4.054 7.171 -38.638 1.00 31.01
H
ATOM 2646 HB3 SER B 139 2.690 7.985 -38.601 1.00 31.01
H
ATOM 2647 HG SER B 139 3.872 7.181 -40.829 1.00 30.77
H
ATOM 2648 N LYS B 140 4.161 10.507 -41.215 1.00 23.74
N
ATOM 2649 CA LYS B 140 3.520 11.383 -42.190 1.00 25.13
C
ATOM 2650 C LYS B 140 2.262 10.751 -42.772 1.00 27.27
C
ATOM 2651 O LYS B 140 1.310 11.446 -43.124 1.00 23.60
O
ATOM 2652 CB LYS B 140 4.479 11.725 -43.332 1.00 33.45
C
ATOM 2653 CG LYS B 140 5.508 12.792 -43.013 1.00 30.77
C
ATOM 2654 CD LYS B 140 6.309 13.145 -44.257 1.00 35.69
C
ATOM 2655 CE LYS B 140 7.517 13.999 -43.925 1.00 38.62
C
ATOM 2656 NZ LYS B 140 7.166 15.412 -43.646 1.00 40.07
N1+
ATOM 2657 H LYS B 140 4.968 10.290 -41.417 1.00 28.48
H
ATOM 2658 HA LYS B 140 3.265 12.211 -41.753 1.00 30.15
H
ATOM 2659 HB2 LYS B 140 4.961 10.921 -43.581 1.00 40.14
H
ATOM 2660 HB3 LYS B 140 3.959 12.039 -44.088 1.00 40.14
H
ATOM 2661 HG2 LYS B 140 5.058 13.592 -42.699 1.00 36.92
H
ATOM 2662 HG3 LYS B 140 6.119 12.460 -42.337 1.00 36.92
H
ATOM 2663 HD2 LYS B 140 6.621 12.329 -44.678 1.00 42.82
H
ATOM 2664 HD3 LYS B 140 5.745 13.643 -44.869 1.00 42.82
H
ATOM 2665 HE2 LYS B 140 7.953 13.637 -43.138 1.00 46.34
H
ATOM 2666 HE3 LYS B 140 8.129 13.985 -44.678 1.00 46.34
H
ATOM 2667 HZ1 LYS B 140 7.902 15.876 -43.456 1.00 48.08
H
ATOM 2668 HZ2 LYS B 140 6.771 15.773 -44.357 1.00 48.08
H
ATOM 2669 HZ3 LYS B 140 6.610 15.455 -42.952 1.00 48.08
H
ATOM 2670 N GLU B 141 2.267 9.427 -42.874 1.00 25.00
N
ATOM 2671 CA GLU B 141 1.193 8.708 -43.544 1.00 27.84
C
ATOM 2672 C GLU B 141 0.014 8.489 -42.607 1.00 25.06
C
ATOM 2673 O GLU B 141 -1.123 8.813 -42.942 1.00 27.37
O
ATOM 2674 CB GLU B 141 1.700 7.367 -44.078 1.00 34.11

ATOM 8941 CA LEU E 77 10.537 48.025 -39.553 1.00 16.17
C
ATOM 8942 C LEU E 77 9.455 47.893 -40.609 1.00 15.56 C
ATOM 8943 O LEU E 77 8.319 48.306 -40.388 1.00 17.25 O
ATOM 8944 CB LEU E 77 10.286 47.048 -38.405 1.00 15.28
C
ATOM 8945 CG LEU E 77 11.389 46.987 -37.350 1.00 16.96
C
ATOM 8946 CD1 LEU E 77 10.879 46.320 -36.093 1.00 21.16
C
ATOM 8947 CD2 LEU E 77 12.592 46.234 -37.902 1.00 19.76
C
ATOM 8948 H LEU E 77 9.858 49.631 -38.643 1.00 18.50 H
ATOM 8949 HA LEU E 77 11.390 47.807 -39.960 1.00 19.40
H
ATOM 8950 HB2 LEU E 77 9.466 47.305 -37.955 1.00 18.34
H
ATOM 8951 HB3 LEU E 77 10.188 46.157 -38.775 1.00 18.34
H
ATOM 8952 HG LEU E 77 11.669 47.888 -37.126 1.00 20.35
H
ATOM 8953 HD11 LEU E 77 11.594 46.292 -35.438 1.00 25.39
H
ATOM 8954 HD12 LEU E 77 10.131 46.831 -35.746 1.00 25.39
H
ATOM 8955 HD13 LEU E 77 10.593 45.418 -36.309 1.00 25.39
H
ATOM 8956 HD21 LEU E 77 13.284 46.203 -37.223 1.00 23.72
H
ATOM 8957 HD22 LEU E 77 12.319 45.333 -38.138 1.00 23.72
H
ATOM 8958 HD23 LEU E 77 12.921 46.697 -38.689 1.00 23.72
H
ATOM 8959 N THR E 78 9.813 47.329 -41.759 1.00 14.27 N
ATOM 8960 CA THR E 78 8.840 47.089 -42.818 1.00 14.26 C
ATOM 8961 C THR E 78 8.861 45.634 -43.248 1.00 14.87 C
ATOM 8962 O THR E 78 9.922 45.020 -43.355 1.00 12.85 O
ATOM 8963 CB THR E 78 9.100 47.973 -44.050 1.00 15.27 C
ATOM 8964 OG1 THR E 78 9.102 49.353 -43.665 1.00 19.62
O
ATOM 8965 CG2 THR E 78 8.035 47.754 -45.113 1.00 15.91
C
ATOM 8966 H THR E 78 10.612 47.075 -41.950 1.00 17.12 H
ATOM 8967 HA THR E 78 7.952 47.292 -42.484 1.00 17.11 H
ATOM 8968 HB THR E 78 9.962 47.746 -44.431 1.00 18.32 H
ATOM 8969 HG1 THR E 78 9.704 49.491 -43.096 1.00 23.54
H
ATOM 8970 HG21 THR E 78 8.213 48.317 -45.882 1.00 19.09
H
ATOM 8971 HG22 THR E 78 8.035 46.826 -45.396 1.00 19.09
H
ATOM 8972 HG23 THR E 78 7.160 47.974 -44.757 1.00 19.09
H
ATOM 8973 N TYR E 79 7.670 45.095 -43.484 1.00 13.27 N
ATOM 8974 CA TYR E 79 7.514 43.775 -44.072 1.00 14.20 C

C
ATOM 2675 CG GLU B 141 2.769 7.490 -45.160 1.00 36.43
C
ATOM 2676 CD GLU B 141 4.098 8.026 -44.638 1.00 46.40
C
ATOM 2677 OE1 GLU B 141 4.499 7.656 -43.512 1.00 42.36
O
ATOM 2678 OE2 GLU B 141 4.740 8.824 -45.356 1.00 49.27
O1-
ATOM 2679 H GLU B 141 2.886 8.919 -42.561 1.00 30.00
H
ATOM 2680 HA GLU B 141 0.883 9.233 -44.298 1.00 33.41
H
ATOM 2681 HB2 GLU B 141 2.082 6.864 -43.342 1.00 40.93
H
ATOM 2682 HB3 GLU B 141 0.952 6.879 -44.455 1.00 40.93
H
ATOM 2683 HG2 GLU B 141 2.932 6.613 -45.543 1.00 43.71
H
ATOM 2684 HG3 GLU B 141 2.452 8.097 -45.847 1.00 43.71
H
ATOM 2685 N ASP B 142 0.290 7.943 -41.429 1.00 28.26
N
ATOM 2686 CA ASP B 142 -0.758 7.684 -40.452 1.00 24.57
C
ATOM 2687 C ASP B 142 -1.332 8.975 -39.892 1.00 20.54
C
ATOM 2688 O ASP B 142 -2.446 8.987 -39.375 1.00 22.29
O
ATOM 2689 CB ASP B 142 -0.226 6.820 -39.310 1.00 25.59
C
ATOM 2690 CG ASP B 142 0.030 5.390 -39.737 1.00 31.43
C
ATOM 2691 OD1 ASP B 142 -0.408 5.011 -40.844 1.00 33.75
O
ATOM 2692 OD2 ASP B 142 0.658 4.641 -38.960 1.00 36.61
O1-
ATOM 2693 H ASP B 142 1.077 7.713 -41.171 1.00 33.91
H
ATOM 2694 HA ASP B 142 -1.479 7.199 -40.884 1.00 29.48
H
ATOM 2695 HB2 ASP B 142 0.612 7.194 -38.994 1.00 30.71
H
ATOM 2696 HB3 ASP B 142 -0.877 6.807 -38.592 1.00 30.71
H
ATOM 2697 N GLN B 143 -0.567 10.057 -39.996 1.00 21.57
N
ATOM 2698 CA GLN B 143 -1.007 11.352 -39.489 1.00 22.32
C
ATOM 2699 C GLN B 143 -1.076 12.372 -40.617 1.00 21.14
C
ATOM 2700 O GLN B 143 -0.821 13.555 -40.412 1.00 19.64
O
ATOM 2701 CB GLN B 143 -0.069 11.831 -38.383 1.00 16.49
C
ATOM 2702 CG GLN B 143 0.132 10.792 -37.295 1.00 21.19
C
ATOM 2703 CD GLN B 143 1.050 11.269 -36.196 1.00 21.57
C
ATOM 2704 OE1 GLN B 143 2.263 11.355 -36.384 1.00 19.08
O
ATOM 2705 NE2 GLN B 143 0.478 11.581 -35.039 1.00 19.58
N
ATOM 2706 H GLN B 143 0.213 10.068 -40.356 1.00 25.88
H
ATOM 2707 HA GLN B 143 -1.896 11.260 -39.112 1.00 26.78
H
ATOM 2708 HB2 GLN B 143 0.798 12.032 -38.769 1.00 19.78
ATOM 8975 C TYR E 79 6.573 43.872 -45.256 1.00 14.36 C
ATOM 8976 O TYR E 79 5.421 44.279 -45.111 1.00 13.68 O
ATOM 8977 CB TYR E 79 6.982 42.777 -43.049 1.00 13.72 C
ATOM 8978 CG TYR E 79 6.699 41.404 -43.618 1.00 14.03
C
ATOM 8979 CD1 TYR E 79 7.700 40.665 -44.239 1.00 15.69
C
ATOM 8980 CD2 TYR E 79 5.438 40.835 -43.512 1.00 13.78
C
ATOM 8981 CE1 TYR E 79 7.447 39.401 -44.750 1.00 15.27
C
ATOM 8982 CE2 TYR E 79 5.177 39.579 -44.016 1.00 12.76
C
ATOM 8983 CZ TYR E 79 6.182 38.865 -44.635 1.00 15.58 C
ATOM 8984 OH TYR E 79 5.914 37.609 -45.136 1.00 14.38
O
ATOM 8985 H TYR E 79 6.924 45.484 -43.308 1.00 15.93 H
ATOM 8986 HA TYR E 79 8.375 43.460 -44.390 1.00 17.04 H
ATOM 8987 HB2 TYR E 79 7.638 42.675 -42.342 1.00 16.47
H
ATOM 8988 HB3 TYR E 79 6.153 43.120 -42.681 1.00 16.47
H
ATOM 8989 HD1 TYR E 79 8.553 41.027 -44.317 1.00 18.83
H
ATOM 8990 HD2 TYR E 79 4.756 41.311 -43.096 1.00 16.54
H
ATOM 8991 HE1 TYR E 79 8.124 38.920 -45.167 1.00 18.32
H
ATOM 8992 HE2 TYR E 79 4.325 39.215 -43.940 1.00 15.31
H
ATOM 8993 HH TYR E 79 6.606 37.285 -45.484 1.00 17.25 H
ATOM 8994 N PHE E 80 7.078 43.501 -46.426 1.00 13.15 N
ATOM 8995 CA PHE E 80 6.317 43.575 -47.664 1.00 14.24 C
ATOM 8996 C PHE E 80 6.024 42.162 -48.125 1.00 16.30 C
ATOM 8997 O PHE E 80 6.934 41.349 -48.213 1.00 15.43 O
ATOM 8998 CB PHE E 80 7.102 44.352 -48.722 1.00 17.01 C
ATOM 8999 CG PHE E 80 6.447 44.383 -50.071 1.00 19.40
C
ATOM 9000 CD1 PHE E 80 5.421 45.272 -50.337 1.00 18.32
C
ATOM 9001 CD2 PHE E 80 6.877 43.541 -51.084 1.00 19.37
C
ATOM 9002 CE1 PHE E 80 4.824 45.310 -51.585 1.00 23.34
C
ATOM 9003 CE2 PHE E 80 6.285 43.574 -52.334 1.00 18.06
C
ATOM 9004 CZ PHE E 80 5.259 44.459 -52.585 1.00 18.37 C
ATOM 9005 H PHE E 80 7.876 43.197 -46.529 1.00 15.78 H
ATOM 9006 HA PHE E 80 5.476 44.031 -47.504 1.00 17.09 H
ATOM 9007 HB2 PHE E 80 7.206 45.269 -48.422 1.00 20.41
H
ATOM 9008 HB3 PHE E 80 7.975 43.941 -48.827 1.00 20.41

H
ATOM 2709 HB3 GLN B 143 -0.443 12.626 -37.974 1.00 19.78
H
ATOM 2710 HG2 GLN B 143 -0.727 10.581 -36.897 1.00 25.43
H
ATOM 2711 HG3 GLN B 143 0.521 9.995 -37.686 1.00 25.43
H
ATOM 2712 HE21 GLN B 143 0.960 11.858 -34.382 1.00 23.50
H
ATOM 2713 HE22 GLN B 143 -0.374 11.507 -34.946 1.00 23.50
H
ATOM 2714 N ASP B 144 -1.441 11.906 -41.808 1.00 23.98
N
ATOM 2715 CA ASP B 144 -1.449 12.764 -42.986 1.00 24.23
C
ATOM 2716 C ASP B 144 -2.493 13.879 -42.881 1.00 22.36
C
ATOM 2717 O ASP B 144 -2.389 14.881 -43.582 1.00 21.23
O
ATOM 2718 CB ASP B 144 -1.678 11.933 -44.256 1.00 28.70
C
ATOM 2719 CG ASP B 144 -2.948 11.106 -44.203 1.00 27.60
C
ATOM 2720 OD1 ASP B 144 -3.543 10.979 -43.113 1.00 24.37
O
ATOM 2721 OD2 ASP B 144 -3.344 10.567 -45.258 1.00 40.47
O1-
ATOM 2722 H ASP B 144 -1.689 11.096 -41.960 1.00 28.78
H
ATOM 2723 HA ASP B 144 -0.579 13.185 -43.065 1.00 29.08
H
ATOM 2724 HB2 ASP B 144 -1.742 12.532 -45.016 1.00 34.44
H
ATOM 2725 HB3 ASP B 144 -0.930 11.326 -44.374 1.00 34.44
H
ATOM 2726 N LEU B 145 -3.477 13.728 -41.996 1.00 19.04
N
ATOM 2727 CA LEU B 145 -4.471 14.785 -41.804 1.00 22.41
C
ATOM 2728 C LEU B 145 -3.812 16.062 -41.284 1.00 23.21
C
ATOM 2729 O LEU B 145 -4.353 17.157 -41.440 1.00 16.02
O
ATOM 2730 CB LEU B 145 -5.590 14.338 -40.849 1.00 23.82
C
ATOM 2731 CG LEU B 145 -5.318 14.061 -39.362 1.00 27.11
C
ATOM 2732 CD1 LEU B 145 -5.111 15.321 -38.530 1.00 36.24
C
ATOM 2733 CD2 LEU B 145 -6.485 13.274 -38.783 1.00 26.90
C
ATOM 2734 H LEU B 145 -3.591 13.034 -41.501 1.00 22.85
H
ATOM 2735 HA LEU B 145 -4.878 14.990 -42.661 1.00 26.90
H
ATOM 2736 HB2 LEU B 145 -6.276 15.024 -40.873 1.00 28.59
H
ATOM 2737 HB3 LEU B 145 -5.962 13.519 -41.211 1.00 28.59
H
ATOM 2738 HG LEU B 145 -4.520 13.515 -39.283 1.00 32.54
H
ATOM 2739 HD11 LEU B 145 -4.946 15.068 -37.609 1.00 43.49
H
ATOM 2740 HD12 LEU B 145 -4.349 15.809 -38.881 1.00 43.49
H
ATOM 2741 HD13 LEU B 145 -5.909 15.870 -38.585 1.00 43.49
H
ATOM 2742 HD21 LEU B 145 -6.571 12.437 -39.266 1.00 32.28
H
ATOM 9009 HD1 PHE E 80 5.125 45.846 -49.668 1.00 21.98
H
ATOM 9010 HD2 PHE E 80 7.569 42.942 -50.920 1.00 23.25
H
ATOM 9011 HE1 PHE E 80 4.131 45.908 -51.751 1.00 28.00
H
ATOM 9012 HE2 PHE E 80 6.579 43.000 -53.004 1.00 21.67
H
ATOM 9013 HZ PHE E 80 4.858 44.482 -53.424 1.00 22.04 H
ATOM 9014 N TYR E 81 4.751 41.864 -48.376 1.00 13.87 N
ATOM 9015 CA TYR E 81 4.354 40.551 -48.870 1.00 15.55 C
ATOM 9016 C TYR E 81 3.404 40.698 -50.049 1.00 17.93 C
ATOM 9017 O TYR E 81 2.378 41.378 -49.952 1.00 14.45 O
ATOM 9018 CB TYR E 81 3.696 39.715 -47.768 1.00 13.17 C
ATOM 9019 CG TYR E 81 3.300 38.345 -48.261 1.00 15.78
C
ATOM 9020 CD1 TYR E 81 4.237 37.324 -48.352 1.00 19.61
C
ATOM 9021 CD2 TYR E 81 1.998 38.077 -48.663 1.00 18.88
C
ATOM 9022 CE1 TYR E 81 3.887 36.072 -48.816 1.00 19.41
C
ATOM 9023 CE2 TYR E 81 1.640 36.827 -49.130 1.00 17.69
C
ATOM 9024 CZ TYR E 81 2.586 35.829 -49.203 1.00 17.85 C
ATOM 9025 OH TYR E 81 2.237 34.580 -49.670 1.00 17.84
O
ATOM 9026 H TYR E 81 4.095 42.409 -48.267 1.00 16.64 H
ATOM 9027 HA TYR E 81 5.143 40.076 -49.177 1.00 18.66 H
ATOM 9028 HB2 TYR E 81 4.322 39.604 -47.036 1.00 15.81
H
ATOM 9029 HB3 TYR E 81 2.897 40.169 -47.459 1.00 15.81
H
ATOM 9030 HD1 TYR E 81 5.115 37.485 -48.092 1.00 23.54
H
ATOM 9031 HD2 TYR E 81 1.357 38.749 -48.615 1.00 22.66
H
ATOM 9032 HE1 TYR E 81 4.525 35.397 -48.868 1.00 23.29
H
ATOM 9033 HE2 TYR E 81 0.763 36.660 -49.392 1.00 21.22
H
ATOM 9034 HH TYR E 81 1.421 34.566 -49.870 1.00 21.41 H
ATOM 9035 N GLU E 82 3.755 40.055 -51.159 1.00 15.98 N
ATOM 9036 CA GLU E 82 3.003 40.184 -52.399 1.00 14.65 C
ATOM 9037 C GLU E 82 2.789 38.829 -53.047 1.00 14.84 C
ATOM 9038 O GLU E 82 3.732 38.055 -53.188 1.00 17.94 O
ATOM 9039 CB GLU E 82 3.737 41.109 -53.373 1.00 18.04 C
ATOM 9040 CG GLU E 82 3.018 41.338 -54.689 1.00 16.30
C
ATOM 9041 CD GLU E 82 3.879 42.074 -55.695 1.00 22.72
C
ATOM 9042 OE1 GLU E 82 4.616 41.397 -56.440 1.00 20.02

H
ATOM 2743 HD22 LEU B 145 -6.313 13.100 -37.845 1.00 32.28
H
ATOM 2744 HD23 LEU B 145 -7.296 13.797 -38.880 1.00 32.28
H
ATOM 2745 N LEU B 146 -2.641 15.917 -40.669 1.00 18.69
N
ATOM 2746 CA LEU B 146 -1.906 17.067 -40.147 1.00 20.59
C
ATOM 2747 C LEU B 146 -1.461 18.011 -41.261 1.00 22.13
C
ATOM 2748 O LEU B 146 -1.050 19.139 -40.994 1.00 20.52
O
ATOM 2749 CB LEU B 146 -0.687 16.603 -39.346 1.00 17.78
C
ATOM 2750 CG LEU B 146 -0.968 15.902 -38.018 1.00 17.50
C
ATOM 2751 CD1 LEU B 146 0.325 15.414 -37.395 1.00 17.27
C
ATOM 2752 CD2 LEU B 146 -1.696 16.837 -37.055 1.00 20.64
C
ATOM 2753 H LEU B 146 -2.250 15.162 -40.542 1.00 22.42
H
ATOM 2754 HA LEU B 146 -2.485 17.564 -39.548 1.00 24.71
H
ATOM 2755 HB2 LEU B 146 -0.181 15.984 -39.896 1.00 21.34
H
ATOM 2756 HB3 LEU B 146 -0.140 17.380 -39.151 1.00 21.34
H
ATOM 2757 HG LEU B 146 -1.536 15.132 -38.178 1.00 21.00
H
ATOM 2758 HD11 LEU B 146 0.123 14.973 -36.555 1.00 20.72
H
ATOM 2759 HD12 LEU B 146 0.751 14.789 -38.003 1.00 20.72
H
ATOM 2760 HD13 LEU B 146 0.907 16.174 -37.239 1.00 20.72
H
ATOM 2761 HD21 LEU B 146 -1.861 16.367 -36.223 1.00 24.77
H
ATOM 2762 HD22 LEU B 146 -1.142 17.615 -36.892 1.00 24.77
H
ATOM 2763 HD23 LEU B 146 -2.538 17.108 -37.455 1.00 24.77
H
ATOM 2764 N LYS B 147 -1.546 17.549 -42.505 1.00 18.08
N
ATOM 2765 CA LYS B 147 -1.162 18.363 -43.656 1.00 21.55
C
ATOM 2766 C LYS B 147 -2.100 19.543 -43.918 1.00 18.51
C
ATOM 2767 O LYS B 147 -1.684 20.547 -44.493 1.00 21.96
O
ATOM 2768 CB LYS B 147 -1.098 17.501 -44.915 1.00 21.16
C
ATOM 2769 CG LYS B 147 0.074 16.547 -44.957 1.00 30.69
C
ATOM 2770 CD LYS B 147 0.195 15.878 -46.321 1.00 36.31
C
ATOM 2771 CE LYS B 147 -0.442 14.498 -46.326 1.00 47.69
C
ATOM 2772 NZ LYS B 147 -0.373 13.845 -47.665 1.00 54.63
N1+
ATOM 2773 H LYS B 147 -1.824 16.762 -42.711 1.00 21.70
H
ATOM 2774 HA LYS B 147 -0.275 18.723 -43.499 1.00 25.85
H
ATOM 2775 HB2 LYS B 147 -1.910 16.973 -44.972 1.00 25.39
H
ATOM 2776 HB3 LYS B 147 -1.032 18.084 -45.688 1.00 25.39

O
ATOM 9043 OE2 GLU E 82 3.824 43.322 -55.736 1.00 20.27
O1-

ATOM 9044 H GLU E 82 4.434 39.531 -51.219 1.00 19.17 H

ATOM 9045 HA GLU E 82 2.134 40.571 -52.208 1.00 17.57 H
ATOM 9046 HB2 GLU E 82 3.857 41.974 -52.949 1.00 21.64
H
ATOM 9047 HB3 GLU E 82 4.604 40.722 -53.575 1.00 21.64
H
ATOM 9048 HG2 GLU E 82 2.774 40.481 -55.071 1.00 19.56
H
ATOM 9049 HG3 GLU E 82 2.223 41.870 -54.527 1.00 19.56
H

ATOM 9050 N CYS E 83 1.547 38.545 -53.433 1.00 15.34 N

ATOM 9051 CA CYS E 83 1.264 37.378 -54.257 1.00 12.96 C

ATOM 9052 C CYS E 83 0.843 37.867 -55.639 1.00 19.15 C

ATOM 9053 O CYS E 83 0.264 38.947 -55.785 1.00 15.77 O

ATOM 9054 CB CYS E 83 0.197 36.477 -53.621 1.00 16.84 C
ATOM 9055 SG CYS E 83 -1.483 37.137 -53.496 1.00 23.13
S

ATOM 9056 H CYS E 83 0.854 39.012 -53.230 1.00 18.41 H

ATOM 9057 HA CYS E 83 2.076 36.857 -54.357 1.00 15.56 H
ATOM 9058 HB2 CYS E 83 0.144 35.661 -54.142 1.00 20.21
H
ATOM 9059 HB3 CYS E 83 0.486 36.260 -52.720 1.00 20.21
H

ATOM 9060 N ASP E 84 1.163 37.066 -56.648 1.00 17.04 N

ATOM 9061 CA ASP E 84 0.974 37.441 -58.041 1.00 17.78 C

ATOM 9062 C ASP E 84 0.295 36.299 -58.783 1.00 19.08 C

ATOM 9063 O ASP E 84 0.770 35.164 -58.744 1.00 16.97 O

ATOM 9064 CB ASP E 84 2.325 37.778 -58.678 1.00 20.88 C
ATOM 9065 CG ASP E 84 2.208 38.205 -60.131 1.00 25.61
C
ATOM 9066 OD1 ASP E 84 1.845 37.363 -60.982 1.00 20.93
O
ATOM 9067 OD2 ASP E 84 2.505 39.382 -60.423 1.00 20.27
O1-

ATOM 9068 H ASP E 84 1.500 36.281 -56.547 1.00 20.45 H

ATOM 9069 HA ASP E 84 0.405 38.224 -58.092 1.00 21.34 H
ATOM 9070 HB2 ASP E 84 2.734 38.506 -58.184 1.00 25.05
H
ATOM 9071 HB3 ASP E 84 2.895 36.993 -58.642 1.00 25.05
H

ATOM 9072 N TYR E 85 -0.824 36.598 -59.437 1.00 18.50 N

ATOM 9073 CA TYR E 85 -1.525 35.609 -60.252 1.00 19.06 C

ATOM 9074 C TYR E 85 -1.499 36.041 -61.713 1.00 20.41 C

ATOM 9075 O TYR E 85 -2.219 36.955 -62.124 1.00 20.32 O
ATOM 9076 CB TYR E 85 -2.960 35.422 -59.768 1.00 18.28 C

H
ATOM 2777 HG2 LYS B 147 0.893 17.037 -44.784 1.00 36.83
H
ATOM 2778 HG3 LYS B 147 -0.052 15.855 -44.289 1.00 36.83
H
ATOM 2779 HD2 LYS B 147 -0.255 16.423 -46.986 1.00 43.57
H
ATOM 2780 HD3 LYS B 147 1.134 15.780 -46.547 1.00 43.57
H
ATOM 2781 HE2 LYS B 147 0.023 13.931 -45.691 1.00 57.23
H
ATOM 2782 HE3 LYS B 147 -1.376 14.579 -46.078 1.00 57.23
H
ATOM 2783 HZ1 LYS B 147 0.476 13.753 -47.915 1.00 65.55
H
ATOM 2784 HZ2 LYS B 147 -0.754 13.042 -47.632 1.00 65.55
H
ATOM 2785 HZ3 LYS B 147 -0.799 14.343 -48.268 1.00 65.55
H
ATOM 2786 N LEU B 148 -3.362 19.420 -43.518 1.00 18.78
N
ATOM 2787 CA LEU B 148 -4.353 20.450 -43.829 1.00 22.97
C
ATOM 2788 C LEU B 148 -4.868 21.167 -42.585 1.00 14.82
C
ATOM 2789 O LEU B 148 -6.011 21.617 -42.541 1.00 14.64
O
ATOM 2790 CB LEU B 148 -5.517 19.832 -44.607 1.00 26.00
C
ATOM 2791 CG LEU B 148 -5.160 19.380 -46.029 1.00 31.59
C
ATOM 2792 CD1 LEU B 148 -6.356 18.716 -46.679 1.00 33.85
C
ATOM 2793 CD2 LEU B 148 -4.670 20.547 -46.891 1.00 31.17
C
ATOM 2794 H LEU B 148 -3.670 18.755 -43.068 1.00 22.53
H
ATOM 2795 HA LEU B 148 -3.939 21.115 -44.401 1.00 27.56
H
ATOM 2796 HB2 LEU B 148 -5.837 19.055 -44.123 1.00 31.20
H
ATOM 2797 HB3 LEU B 148 -6.228 20.489 -44.677 1.00 31.20
H
ATOM 2798 HG LEU B 148 -4.446 18.725 -45.980 1.00 37.91
H
ATOM 2799 HD11 LEU B 148 -6.113 18.437 -47.575 1.00 40.61
H
ATOM 2800 HD12 LEU B 148 -6.614 17.944 -46.150 1.00 40.61
H
ATOM 2801 HD13 LEU B 148 -7.088 19.351 -46.716 1.00 40.61
H
ATOM 2802 HD21 LEU B 148 -3.878 20.931 -46.481 1.00 37.40
H
ATOM 2803 HD22 LEU B 148 -4.456 20.216 -47.778 1.00 37.40
H
ATOM 2804 HD23 LEU B 148 -5.371 21.215 -46.946 1.00 37.40
H
ATOM 2805 N VAL B 149 -4.000 21.295 -41.587 1.00 21.37
N
ATOM 2806 CA VAL B 149 -4.324 22.025 -40.365 1.00 16.00
C
ATOM 2807 C VAL B 149 -3.814 23.459 -40.465 1.00 15.16
C
ATOM 2808 O VAL B 149 -2.619 23.685 -40.651 1.00 17.77
O
ATOM 2809 CB VAL B 149 -3.708 21.343 -39.130 1.00 15.06
C
ATOM 2810 CG1 VAL B 149 -4.064 22.100 -37.853 1.00 19.91

ATOM 9077 CG TYR E 85 -3.596 34.138 -60.246 1.00 18.94
C
ATOM 9078 CD1 TYR E 85 -3.038 32.910 -59.929 1.00 19.95
C
ATOM 9079 CD2 TYR E 85 -4.760 34.154 -61.002 1.00 23.18
C
ATOM 9080 CE1 TYR E 85 -3.613 31.733 -60.354 1.00 20.65
C
ATOM 9081 CE2 TYR E 85 -5.345 32.979 -61.430 1.00 25.96
C

ATOM 9082 CZ TYR E 85 -4.767 31.772 -61.099 1.00 23.05 C
ATOM 9083 OH TYR E 85 -5.337 30.594 -61.524 1.00 26.20
O

ATOM 9084 H TYR E 85 -1.201 37.371 -59.426 1.00 22.20 H

ATOM 9085 HA TYR E 85 -1.068 34.757 -60.180 1.00 22.87 H
ATOM 9086 HB2 TYR E 85 -2.965 35.412 -58.798 1.00 21.94
H
ATOM 9087 HB3 TYR E 85 -3.499 36.160 -60.093 1.00 21.94
H
ATOM 9088 HD1 TYR E 85 -2.259 32.880 -59.422 1.00 23.94
H
ATOM 9089 HD2 TYR E 85 -5.152 34.968 -61.222 1.00 27.82
H
ATOM 9090 HE1 TYR E 85 -3.226 30.917 -60.134 1.00 24.78
H
ATOM 9091 HE2 TYR E 85 -6.124 33.002 -61.937 1.00 31.15
H
ATOM 9092 HH TYR E 85 -6.033 30.755 -61.966 1.00 31.44
H

ATOM 9093 N THR E 86 -0.648 35.368 -62.481 1.00 21.39 N
ATOM 9094 CA THR E 86 -0.390 35.705 -63.874 1.00 20.93
C

ATOM 9095 C THR E 86 -0.293 34.414 -64.674 1.00 21.34 C

ATOM 9096 O THR E 86 0.496 33.532 -64.334 1.00 19.84 O

ATOM 9097 CB THR E 86 0.921 36.515 -64.029 1.00 22.67 C
ATOM 9098 OG1 THR E 86 0.862 37.696 -63.217 1.00 24.63
O
ATOM 9099 CG2 THR E 86 1.149 36.917 -65.478 1.00 23.65
C

ATOM 9100 H THR E 86 -0.196 34.690 -62.206 1.00 25.66 H
ATOM 9101 HA THR E 86 -1.125 36.233 -64.223 1.00 25.12
H

ATOM 9102 HB THR E 86 1.670 35.969 -63.744 1.00 27.20 H
ATOM 9103 HG1 THR E 86 0.765 37.485 -62.410 1.00 29.56
H
ATOM 9104 HG21 THR E 86 1.973 37.423 -65.555 1.00 28.38
H
ATOM 9105 HG22 THR E 86 1.212 36.126 -66.035 1.00 28.38
H
ATOM 9106 HG23 THR E 86 0.412 37.466 -65.790 1.00 28.38
H

ATOM 9107 N ASP E 87 -1.096 34.300 -65.727 1.00 22.89 N

ATOM 9108 CA ASP E 87 -1.097 33.101 -66.563 1.00 23.19 C

ATOM 9109 C ASP E 87 -1.404 31.876 -65.703 1.00 26.71 C
ATOM 9110 O ASP E 87 -0.771 30.830 -65.835 1.00 23.26 O

C
ATOM 2811 CG2 VAL B 149 -4.179 19.899 -39.037 1.00 22.08
C
ATOM 2812 H VAL B 149 -3.206 20.964 -41.594 1.00 25.65
H
ATOM 2813 HA VAL B 149 -5.287 22.050 -40.252 1.00 19.19
H
ATOM 2814 HB VAL B 149 -2.742 21.340 -39.219 1.00 18.07
H
ATOM 2815 HG11 VAL B 149 -3.662 21.646 -37.096 1.00 23.89
H
ATOM 2816 HG12 VAL B 149 -3.721 23.005 -37.917 1.00 23.89
H
ATOM 2817 HG13 VAL B 149 -5.028 22.118 -37.755 1.00 23.89
H
ATOM 2818 HG21 VAL B 149 -3.781 19.488 -38.254 1.00 26.49
H
ATOM 2819 HG22 VAL B 149 -5.146 19.886 -38.963 1.00 26.49
H
ATOM 2820 HG23 VAL B 149 -3.902 19.425 -39.837 1.00 26.49
H
ATOM 2821 N LYS B 150 -4.723 24.422 -40.354 1.00 13.81
N
ATOM 2822 CA LYS B 150 -4.346 25.833 -40.340 1.00 15.89
C
ATOM 2823 C LYS B 150 -3.784 26.238 -38.987 1.00 14.81
C
ATOM 2824 O LYS B 150 -3.953 25.531 -37.996 1.00 17.84
O
ATOM 2825 CB LYS B 150 -5.542 26.729 -40.663 1.00 19.83
C
ATOM 2826 CG LYS B 150 -5.939 26.780 -42.121 1.00 18.05
C
ATOM 2827 CD LYS B 150 -6.947 27.893 -42.372 1.00 16.00
C
ATOM 2828 CE LYS B 150 -6.287 29.264 -42.452 1.00 20.31
C
ATOM 2829 NZ LYS B 150 -5.422 29.408 -43.661 1.00 20.83
N1+
ATOM 2830 H LYS B 150 -5.569 24.285 -40.285 1.00 16.58
H
ATOM 2831 HA LYS B 150 -3.663 25.986 -41.011 1.00 19.07
H
ATOM 2832 HB2 LYS B 150 -6.310 26.409 -40.163 1.00 23.79
H
ATOM 2833 HB3 LYS B 150 -5.331 27.634 -40.386 1.00 23.79
H
ATOM 2834 HG2 LYS B 150 -5.153 26.952 -42.662 1.00 21.66
H
ATOM 2835 HG3 LYS B 150 -6.346 25.937 -42.373 1.00 21.66
H
ATOM 2836 HD2 LYS B 150 -7.400 27.728 -43.214 1.00 19.21
H
ATOM 2837 HD3 LYS B 150 -7.589 27.910 -41.645 1.00 19.21
H
ATOM 2838 HE2 LYS B 150 -6.976 29.946 -42.491 1.00 24.37
H
ATOM 2839 HE3 LYS B 150 -5.732 29.395 -41.667 1.00 24.37
H
ATOM 2840 HZ1 LYS B 150 -5.053 30.217 -43.676 1.00 25.00
H
ATOM 2841 HZ2 LYS B 150 -4.776 28.796 -43.647 1.00 25.00
H
ATOM 2842 HZ3 LYS B 150 -5.908 29.297 -44.398 1.00 25.00
H
ATOM 2843 N SER B 151 -3.129 27.394 -38.963 1.00 16.36
N
ATOM 2844 CA SER B 151 -2.654 28.008 -37.729 1.00 15.93

ATOM 9111 CB ASP E 87 0.252 32.946 -67.275 1.00 25.03 C
ATOM 9112 CG ASP E 87 0.247 31.838 -68.316 1.00 28.16
C
ATOM 9113 OD1 ASP E 87 -0.798 31.626 -68.965 1.00 24.41
O
ATOM 9114 OD2 ASP E 87 1.295 31.180 -68.478 1.00 26.54
O1-

ATOM 9115 H ASP E 87 -1.653 34.904 -65.981 1.00 27.47 H

ATOM 9116 HA ASP E 87 -1.789 33.181 -67.237 1.00 27.83 H
ATOM 9117 HB2 ASP E 87 0.469 33.778 -67.725 1.00 30.03
H
ATOM 9118 HB3 ASP E 87 0.934 32.737 -66.618 1.00 30.03
H

ATOM 9119 N ASN E 88 -2.372 32.032 -64.803 1.00 29.28 N
ATOM 9120 CA ASN E 88 -2.802 30.961 -63.906 1.00 25.51
C

ATOM 9121 C ASN E 88 -1.681 30.405 -63.031 1.00 23.64 C

ATOM 9122 O ASN E 88 -1.812 29.322 -62.465 1.00 24.76 O
ATOM 9123 CB ASN E 88 -3.430 29.821 -64.709 1.00 29.13
C
ATOM 9124 CG ASN E 88 -4.619 30.277 -65.532 1.00 35.20
C
ATOM 9125 OD1 ASN E 88 -4.620 30.161 -66.757 1.00 40.38
O
ATOM 9126 ND2 ASN E 88 -5.637 30.804 -64.860 1.00 37.30
N

ATOM 9127 H ASN E 88 -2.804 32.767 -64.690 1.00 35.13 H
ATOM 9128 HA ASN E 88 -3.486 31.313 -63.314 1.00 30.61
H
ATOM 9129 HB2 ASN E 88 -2.766 29.457 -65.316 1.00 34.96
H
ATOM 9130 HB3 ASN E 88 -3.735 29.133 -64.097 1.00 34.96
H
ATOM 9131 HD21 ASN E 88 -6.335 31.078 -65.282 1.00 44.76
H
ATOM 9132 HD22 ASN E 88 -5.599 30.871 -64.004 1.00 44.76
H

ATOM 9133 N LYS E 89 -0.585 31.150 -62.920 1.00 20.99 N

ATOM 9134 CA LYS E 89 0.543 30.745 -62.087 1.00 22.61 C

ATOM 9135 C LYS E 89 0.681 31.653 -60.868 1.00 18.77 C

ATOM 9136 O LYS E 89 0.632 32.882 -60.978 1.00 17.15 O

ATOM 9137 CB LYS E 89 1.835 30.748 -62.902 1.00 24.56 C

ATOM 9138 CG LYS E 89 1.924 29.593 -63.887 1.00 35.41 C

ATOM 9139 CD LYS E 89 3.119 29.732 -64.818 1.00 45.55 C

ATOM 9140 CE LYS E 89 3.242 28.527 -65.737 1.00 46.80 C
ATOM 9141 NZ LYS E 89 1.975 28.255 -66.473 1.00 49.89
N1+

ATOM 9142 H LYS E 89 -0.469 31.902 -63.320 1.00 25.19 H

ATOM 9143 HA LYS E 89 0.391 29.841 -61.770 1.00 27.14 H
ATOM 9144 HB2 LYS E 89 1.888 31.575 -63.406 1.00 29.48

C
ATOM 2845 C SER B 151 -1.536 27.201 -37.075 1.00 14.66
C
ATOM 2846 O SER B 151 -1.004 26.253 -37.656 1.00 15.81
O
ATOM 2847 CB SER B 151 -3.817 28.195 -36.746 1.00 16.71
C
ATOM 2848 OG SER B 151 -3.442 29.042 -35.672 1.00 18.88
O
ATOM 2849 H SER B 151 -2.944 27.853 -39.666 1.00 19.63
H
ATOM 2850 HA SER B 151 -2.300 28.887 -37.937 1.00 19.12
H
ATOM 2851 HB2 SER B 151 -4.566 28.593 -37.215 1.00 20.05
H
ATOM 2852 HB3 SER B 151 -4.071 27.329 -36.390 1.00 20.05
H
ATOM 2853 HG SER B 151 -4.087 29.136 -35.142 1.00 22.66
H
ATOM 2854 N TYR B 152 -1.184 27.604 -35.862 1.00 13.42
N
ATOM 2855 CA TYR B 152 -0.041 27.051 -35.150 1.00 12.43
C
ATOM 2856 C TYR B 152 -0.498 26.485 -33.816 1.00 12.59
C
ATOM 2857 O TYR B 152 -1.349 27.075 -33.152 1.00 14.90
O
ATOM 2858 CB TYR B 152 1.015 28.128 -34.925 1.00 11.01
C
ATOM 2859 CG TYR B 152 1.401 28.904 -36.165 1.00 14.74
C
ATOM 2860 CD1 TYR B 152 1.697 28.254 -37.356 1.00 14.53
C
ATOM 2861 CD2 TYR B 152 1.476 30.291 -36.140 1.00 16.11
C
ATOM 2862 CE1 TYR B 152 2.063 28.964 -38.488 1.00 19.24
C
ATOM 2863 CE2 TYR B 152 1.837 31.011 -37.265 1.00 13.65
C
ATOM 2864 CZ TYR B 152 2.132 30.343 -38.436 1.00 18.79
C
ATOM 2865 OH TYR B 152 2.492 31.058 -39.558 1.00 16.60
O
ATOM 2866 H TYR B 152 -1.602 28.212 -35.420 1.00 16.10
H
ATOM 2867 HA TYR B 152 0.353 26.334 -35.672 1.00 14.92
H
ATOM 2868 HB2 TYR B 152 0.676 28.764 -34.276 1.00 13.21
H
ATOM 2869 HB3 TYR B 152 1.818 27.708 -34.581 1.00 13.21
H
ATOM 2870 HD1 TYR B 152 1.656 27.325 -37.393 1.00 17.43
H
ATOM 2871 HD2 TYR B 152 1.283 30.744 -35.351 1.00 19.33
H
ATOM 2872 HE1 TYR B 152 2.259 28.516 -39.278 1.00 23.09
H
ATOM 2873 HE2 TYR B 152 1.884 31.939 -37.231 1.00 16.38
H
ATOM 2874 HH TYR B 152 2.493 31.880 -39.386 1.00 19.92
H
ATOM 2875 N HIS B 153 0.066 25.347 -33.423 1.00 12.19
N
ATOM 2876 CA HIS B 153 -0.389 24.651 -32.228 1.00 14.36
C
ATOM 2877 C HIS B 153 0.758 23.957 -31.495 1.00 13.41
C
ATOM 2878 O HIS B 153 1.626 23.342 -32.118 1.00 12.89
H
ATOM 9145 HB3 LYS E 89 2.590 30.682 -62.296 1.00 29.48
H
ATOM 9146 HG2 LYS E 89 2.018 28.762 -63.396 1.00 42.50
H
ATOM 9147 HG3 LYS E 89 1.120 29.573 -64.428 1.00 42.50
H
ATOM 9148 HD2 LYS E 89 3.008 30.524 -65.367 1.00 54.66
H
ATOM 9149 HD3 LYS E 89 3.930 29.799 -64.291 1.00 54.66
H
ATOM 9150 HE2 LYS E 89 3.941 28.695 -66.389 1.00 56.16
H
ATOM 9151 HE3 LYS E 89 3.459 27.744 -65.207 1.00 56.16
H
ATOM 9152 HZ1 LYS E 89 1.755 28.959 -66.971 1.00 59.87
H
ATOM 9153 HZ2 LYS E 89 2.077 27.546 -67.001 1.00 59.87
H
ATOM 9154 HZ3 LYS E 89 1.317 28.093 -65.895 1.00 59.87
H

ATOM 9155 N SER E 90 0.843 31.024 -59.709 1.00 16.33 N

ATOM 9156 CA SER E 90 0.971 31.729 -58.442 1.00 17.73 C

ATOM 9157 C SER E 90 2.439 31.908 -58.084 1.00 18.63 C

ATOM 9158 O SER E 90 3.171 30.928 -57.975 1.00 17.42 O

ATOM 9159 CB SER E 90 0.257 30.961 -57.328 1.00 17.54 C
ATOM 9160 OG SER E 90 -1.103 30.730 -57.645 1.00 20.05
O

ATOM 9161 H SER E 90 0.883 30.169 -59.631 1.00 19.60 H

ATOM 9162 HA SER E 90 0.565 32.607 -58.518 1.00 21.27 H
ATOM 9163 HB2 SER E 90 0.699 30.107 -57.203 1.00 21.05
H
ATOM 9164 HB3 SER E 90 0.305 31.479 -56.509 1.00 21.05
H
ATOM 9165 HG SER E 90 -1.501 31.461 -57.755 1.00 24.06
H

ATOM 9166 N THR E 91 2.864 33.157 -57.912 1.00 17.55 N

ATOM 9167 CA THR E 91 4.222 33.455 -57.473 1.00 14.99 C

ATOM 9168 C THR E 91 4.178 34.462 -56.329 1.00 20.38 C

ATOM 9169 O THR E 91 3.207 35.208 -56.177 1.00 19.44 O

ATOM 9170 CB THR E 91 5.096 34.001 -58.621 1.00 18.36 C
ATOM 9171 OG1 THR E 91 4.482 35.159 -59.191 1.00 17.75
O
ATOM 9172 CG2 THR E 91 5.280 32.946 -59.702 1.00 21.31
C

ATOM 9173 H THR E 91 2.379 33.855 -58.045 1.00 21.06 H

ATOM 9174 HA THR E 91 4.634 32.641 -57.142 1.00 17.98 H

ATOM 9175 HB THR E 91 5.971 34.239 -58.274 1.00 22.03 H
ATOM 9176 HG1 THR E 91 4.394 35.756 -58.607 1.00 21.30
H
ATOM 9177 HG21 THR E 91 5.830 33.299 -60.419 1.00 25.58
H
ATOM 9178 HG22 THR E 91 5.712 32.161 -59.329 1.00 25.58

O
ATOM 2879 CB HIS B 153 -1.464 23.627 -32.601 1.00 15.15
C
ATOM 2880 CG HIS B 153 -2.473 24.146 -33.578 1.00 14.40
C
ATOM 2881 ND1 HIS B 153 -3.664 24.719 -33.187 1.00 12.28
N
ATOM 2882 CD2 HIS B 153 -2.459 24.195 -34.932 1.00 15.15
C
ATOM 2883 CE1 HIS B 153 -4.344 25.088 -34.257 1.00 14.83
C
ATOM 2884 NE2 HIS B 153 -3.635 24.783 -35.329 1.00 14.05
N
ATOM 2885 H HIS B 153 0.714 24.958 -33.833 1.00 14.63
H
ATOM 2886 HA HIS B 153 -0.787 25.294 -31.621 1.00 17.23
H
ATOM 2887 HB2 HIS B 153 -1.035 22.854 -32.999 1.00 18.18
H
ATOM 2888 HB3 HIS B 153 -1.937 23.364 -31.796 1.00 18.18
H
ATOM 2889 HD1 HIS B 153 -3.926 24.816 -32.373 1.00 14.73
H
ATOM 2890 HD2 HIS B 153 -1.781 23.885 -35.488 1.00 18.18
H
ATOM 2891 HE1 HIS B 153 -5.180 25.496 -34.257 1.00 17.79
H
ATOM 2892 HE2 HIS B 153 -3.871 24.928 -36.143 1.00 16.86
H
ATOM 2893 N TRP B 154 0.757 24.065 -30.169 1.00 14.83
N
ATOM 2894 CA TRP B 154 1.722 23.341 -29.353 1.00 15.59
C
ATOM 2895 C TRP B 154 1.638 21.838 -29.612 1.00 15.56
C
ATOM 2896 O TRP B 154 0.546 21.257 -29.644 1.00 12.57
O
ATOM 2897 CB TRP B 154 1.497 23.599 -27.860 1.00 17.58
C
ATOM 2898 CG TRP B 154 1.962 24.933 -27.340 1.00 16.06
C
ATOM 2899 CD1 TRP B 154 1.230 25.821 -26.606 1.00 18.33
C
ATOM 2900 CD2 TRP B 154 3.265 25.515 -27.489 1.00 12.92
C
ATOM 2901 NE1 TRP B 154 1.993 26.922 -26.293 1.00 15.98
N
ATOM 2902 CE2 TRP B 154 3.244 26.760 -26.825 1.00 16.75
C
ATOM 2903 CE3 TRP B 154 4.441 25.112 -28.125 1.00 14.07
C
ATOM 2904 CZ2 TRP B 154 4.357 27.600 -26.777 1.00 16.96
C
ATOM 2905 CZ3 TRP B 154 5.543 25.946 -28.075 1.00 13.07
C
ATOM 2906 CH2 TRP B 154 5.493 27.176 -27.407 1.00 16.27
C
ATOM 2907 H TRP B 154 0.208 24.551 -29.720 1.00 17.80
H
ATOM 2908 HA TRP B 154 2.617 23.638 -29.580 1.00 18.71
H
ATOM 2909 HB2 TRP B 154 0.546 23.535 -27.681 1.00 21.10
H
ATOM 2910 HB3 TRP B 154 1.966 22.914 -27.359 1.00 21.10
H
ATOM 2911 HD1 TRP B 154 0.345 25.698 -26.350 1.00 22.00
H
ATOM 2912 HE1 TRP B 154 1.726 27.602 -25.839 1.00 19.17
H
ATOM 9179 HG23 THR E 91 4.417 32.689 -60.064 1.00 25.58
H
ATOM 9180 N PHE E 92 5.232 34.465 -55.523 1.00 17.07 N
ATOM 9181 CA PHE E 92 5.250 35.231 -54.287 1.00 19.25 C
ATOM 9182 C PHE E 92 6.563 35.971 -54.119 1.00 24.03 C
ATOM 9183 O PHE E 92 7.601 35.561 -54.641 1.00 20.37 O
ATOM 9184 CB PHE E 92 5.015 34.308 -53.091 1.00 18.30 C
ATOM 9185 CG PHE E 92 3.758 33.502 -53.192 1.00 20.97
C
ATOM 9186 CD1 PHE E 92 2.557 34.006 -52.722 1.00 19.39
C
ATOM 9187 CD2 PHE E 92 3.773 32.244 -53.771 1.00 24.13
C
ATOM 9188 CE1 PHE E 92 1.397 33.266 -52.819 1.00 18.89
C
ATOM 9189 CE2 PHE E 92 2.616 31.498 -53.871 1.00 17.65
C
ATOM 9190 CZ PHE E 92 1.426 32.010 -53.395 1.00 24.23 C
ATOM 9191 H PHE E 92 5.957 34.027 -55.672 1.00 20.48 H
ATOM 9192 HA PHE E 92 4.535 35.885 -54.308 1.00 23.10 H
ATOM 9193 HB2 PHE E 92 5.760 33.690 -53.022 1.00 21.96
H
ATOM 9194 HB3 PHE E 92 4.959 34.846 -52.287 1.00 21.96
H
ATOM 9195 HD1 PHE E 92 2.533 34.850 -52.333 1.00 23.27
H
ATOM 9196 HD2 PHE E 92 4.573 31.895 -54.092 1.00 28.95
H
ATOM 9197 HE1 PHE E 92 0.596 33.612 -52.498 1.00 22.66
H
ATOM 9198 HE2 PHE E 92 2.638 30.653 -54.259 1.00 21.19
H
ATOM 9199 HZ PHE E 92 0.644 31.510 -53.461 1.00 29.08 H
ATOM 9200 N ASP E 93 6.497 37.065 -53.374 1.00 20.31 N
ATOM 9201 CA ASP E 93 7.647 37.915 -53.135 1.00 22.87 C
ATOM 9202 C ASP E 93 7.507 38.528 -51.752 1.00 21.59 C
ATOM 9203 O ASP E 93 6.409 38.918 -51.354 1.00 20.77 O
ATOM 9204 CB ASP E 93 7.743 39.002 -54.211 1.00 24.57 C
ATOM 9205 CG ASP E 93 8.998 39.840 -54.085 1.00 32.86
C
ATOM 9206 OD1 ASP E 93 9.991 39.332 -53.526 1.00 32.28
O1-
ATOM 9207 OD2 ASP E 93 8.994 41.002 -54.550 1.00 30.92
O
ATOM 9208 H ASP E 93 5.779 37.340 -52.989 1.00 24.37 H
ATOM 9209 HA ASP E 93 8.458 37.382 -53.158 1.00 27.44 H
ATOM 9210 HB2 ASP E 93 7.748 38.582 -55.085 1.00 29.48
H
ATOM 9211 HB3 ASP E 93 6.978 39.594 -54.131 1.00 29.48
H
ATOM 9212 N GLN E 94 8.601 38.592 -51.005 1.00 21.93 N

H
ATOM 2913 HE3 TRP B 154 4.484 24.295 -28.568 1.00 16.88
H
ATOM 2914 HZ2 TRP B 154 4.325 28.418 -26.337 1.00 20.35
H
ATOM 2915 HZ3 TRP B 154 6.332 25.686 -28.493 1.00 15.69
H
ATOM 2916 HH2 TRP B 154 6.249 27.717 -27.393 1.00 19.52
H
ATOM 2917 N MET B 155 2.802 21.229 -29.810 1.00 9.94
N
ATOM 2918 CA MET B 155 2.946 19.779 -29.802 1.00 14.74
C
ATOM 2919 C MET B 155 3.944 19.396 -28.711 1.00 16.06
C
ATOM 2920 O MET B 155 4.555 20.265 -28.092 1.00 15.26
O
ATOM 2921 CB MET B 155 3.401 19.261 -31.167 1.00 14.63
C
ATOM 2922 CG MET B 155 4.639 19.948 -31.731 1.00 14.92
C
ATOM 2923 SD MET B 155 5.043 19.295 -33.366 1.00 14.73
S
ATOM 2924 CE MET B 155 6.245 20.481 -33.946 1.00 14.31
C
ATOM 2925 H MET B 155 3.541 21.645 -29.955 1.00 11.93
H
ATOM 2926 HA MET B 155 2.086 19.377 -29.600 1.00 17.69
H
ATOM 2927 HB2 MET B 155 3.601 18.315 -31.088 1.00 17.56
H
ATOM 2928 HB3 MET B 155 2.680 19.389 -31.803 1.00 17.56
H
ATOM 2929 HG2 MET B 155 4.470 20.900 -31.814 1.00 17.90
H
ATOM 2930 HG3 MET B 155 5.393 19.789 -31.142 1.00 17.90
H
ATOM 2931 HE1 MET B 155 6.539 20.224 -34.834 1.00 17.17
H
ATOM 2932 HE2 MET B 155 5.834 21.359 -33.973 1.00 17.17
H
ATOM 2933 HE3 MET B 155 7.000 20.487 -33.337 1.00 17.17
H
ATOM 2934 N GLY B 156 4.118 18.098 -28.488 1.00 16.14
N
ATOM 2935 CA GLY B 156 4.866 17.615 -27.341 1.00 17.15
C
ATOM 2936 C GLY B 156 6.372 17.566 -27.518 1.00 20.32
C
ATOM 2937 O GLY B 156 7.040 16.765 -26.871 1.00 22.44
O
ATOM 2938 H GLY B 156 3.809 17.474 -28.993 1.00 19.37
H
ATOM 2939 HA2 GLY B 156 4.674 18.186 -26.580 1.00 20.58
H
ATOM 2940 HA3 GLY B 156 4.563 16.719 -27.125 1.00 20.58
H
ATOM 2941 N LEU B 157 6.907 18.425 -28.379 1.00 19.69
N
ATOM 2942 CA LEU B 157 8.338 18.436 -28.667 1.00 18.90
C
ATOM 2943 C LEU B 157 9.056 19.485 -27.826 1.00 26.50
C
ATOM 2944 O LEU B 157 8.641 20.647 -27.784 1.00 20.35
O
ATOM 2945 CB LEU B 157 8.575 18.704 -30.151 1.00 21.54
C
ATOM 2946 CG LEU B 157 9.956 18.345 -30.698 1.00 24.32
C
ATOM 9213 CA GLN E 94 8.567 39.269 -49.718 1.00 21.60 C
ATOM 9214 C GLN E 94 9.897 39.936 -49.420 1.00 25.96 C
ATOM 9215 O GLN E 94 10.960 39.425 -49.778 1.00 22.95 O
ATOM 9216 CB GLN E 94 8.184 38.298 -48.590 1.00 18.61 C
ATOM 9217 CG GLN E 94 9.153 37.149 -48.353 1.00 22.48
C
ATOM 9218 CD GLN E 94 8.735 36.253 -47.190 1.00 31.39
C
ATOM 9219 OE1 GLN E 94 7.596 36.309 -46.716 1.00 22.85
O
ATOM 9220 NE2 GLN E 94 9.662 35.422 -46.724 1.00 33.95
N
ATOM 9221 H GLN E 94 9.365 38.258 -51.217 1.00 26.32 H
ATOM 9222 HA GLN E 94 7.890 39.963 -49.750 1.00 25.92 H
ATOM 9223 HB2 GLN E 94 8.120 38.800 -47.762 1.00 22.33
H
ATOM 9224 HB3 GLN E 94 7.320 37.910 -48.799 1.00 22.33
H
ATOM 9225 HG2 GLN E 94 9.197 36.603 -49.153 1.00 26.97
H
ATOM 9226 HG3 GLN E 94 10.030 37.513 -48.151 1.00 26.97
H
ATOM 9227 HE21 GLN E 94 9.478 34.895 -46.070 1.00 40.74
H
ATOM 9228 HE22 GLN E 94 10.446 35.411 -47.078 1.00 40.74
H
ATOM 9229 N ASP E 95 9.812 41.095 -48.774 1.00 19.56 N
ATOM 9230 CA ASP E 95 10.979 41.896 -48.435 1.00 23.21
C
ATOM 9231 C ASP E 95 10.903 42.330 -46.983 1.00 20.85 C
ATOM 9232 O ASP E 95 9.814 42.501 -46.431 1.00 16.26 O
ATOM 9233 CB ASP E 95 11.077 43.129 -49.338 1.00 22.27
C
ATOM 9234 CG ASP E 95 11.333 42.774 -50.787 1.00 29.57
C
ATOM 9235 OD1 ASP E 95 12.132 41.848 -51.043 1.00 35.45
O
ATOM 9236 OD2 ASP E 95 10.733 43.425 -51.668 1.00 31.38
O1-
ATOM 9237 H ASP E 95 9.070 41.446 -48.517 1.00 23.47 H
ATOM 9238 HA ASP E 95 11.781 41.364 -48.554 1.00 27.85
H
ATOM 9239 HB2 ASP E 95 10.242 43.621 -49.293 1.00 26.72
H
ATOM 9240 HB3 ASP E 95 11.808 43.687 -49.032 1.00 26.72
H
ATOM 9241 N TYR E 96 12.072 42.504 -46.380 1.00 15.26 N
ATOM 9242 CA TYR E 96 12.200 43.027 -45.028 1.00 16.09
C
ATOM 9243 C TYR E 96 13.083 44.268 -45.060 1.00 18.85 C
ATOM 9244 O TYR E 96 14.186 44.218 -45.609 1.00 18.14 O
ATOM 9245 CB TYR E 96 12.814 41.990 -44.091 1.00 17.29
C
ATOM 9246 CG TYR E 96 12.171 40.625 -44.131 1.00 19.72

C
ATOM 2947 CD1 LEU B 157 10.180 16.839 -30.673 1.00 23.00
C
ATOM 2948 CD2 LEU B 157 10.107 18.882 -32.106 1.00 21.66
C
ATOM 2949 H LEU B 157 6.459 19.017 -28.813 1.00 23.63
H
ATOM 2950 HA LEU B 157 8.713 17.567 -28.453 1.00 22.67
H
ATOM 2951 HB2 LEU B 157 7.924 18.195 -30.659 1.00 25.85
H
ATOM 2952 HB3 LEU B 157 8.440 19.651 -30.313 1.00 25.85
H
ATOM 2953 HG LEU B 157 10.635 18.760 -30.143 1.00 29.18
H
ATOM 2954 HD11 LEU B 157 11.063 16.646 -31.026 1.00 27.60
H
ATOM 2955 HD12 LEU B 157 10.114 16.526 -29.757 1.00 27.60
H
ATOM 2956 HD13 LEU B 157 9.504 16.411 -31.220 1.00 27.60
H
ATOM 2957 HD21 LEU B 157 10.986 18.647 -32.441 1.00 25.99
H
ATOM 2958 HD22 LEU B 157 9.422 18.488 -32.669 1.00 25.99
H
ATOM 2959 HD23 LEU B 157 10.006 19.847 -32.088 1.00 25.99
H
ATOM 2960 N VAL B 158 10.131 19.072 -27.160 1.00 22.65
N
ATOM 2961 CA VAL B 158 10.884 19.968 -26.289 1.00 21.67
C
ATOM 2962 C VAL B 158 12.384 19.821 -26.504 1.00 23.85
C
ATOM 2963 O VAL B 158 12.879 18.732 -26.798 1.00 21.21
O
ATOM 2964 CB VAL B 158 10.560 19.711 -24.804 1.00 27.43
C
ATOM 2965 CG1 VAL B 158 9.115 20.099 -24.502 1.00 26.57
C
ATOM 2966 CG2 VAL B 158 10.814 18.253 -24.446 1.00 29.47
C
ATOM 2967 H VAL B 158 10.447 18.273 -27.197 1.00 27.18
H
ATOM 2968 HA VAL B 158 10.641 20.885 -26.494 1.00 26.01
H
ATOM 2969 HB VAL B 158 11.139 20.261 -24.254 1.00 32.92
H
ATOM 2970 HG11 VAL B 158 8.933 19.929 -23.565 1.00 31.88
H
ATOM 2971 HG12 VAL B 158 8.995 21.041 -24.698 1.00 31.88
H
ATOM 2972 HG13 VAL B 158 8.524 19.567 -25.056 1.00 31.88
H
ATOM 2973 HG21 VAL B 158 10.602 18.117 -23.509 1.00 35.36
H
ATOM 2974 HG22 VAL B 158 10.249 17.689 -24.998 1.00 35.36
H
ATOM 2975 HG23 VAL B 158 11.747 18.046 -24.608 1.00 35.36
H
ATOM 2976 N HIS B 159 13.096 20.933 -26.357 1.00 22.33
N
ATOM 2977 CA HIS B 159 14.541 20.959 -26.523 1.00 29.47
C
ATOM 2978 C HIS B 159 15.215 20.956 -25.158 1.00 41.69
C
ATOM 2979 O HIS B 159 14.926 21.802 -24.315 1.00 37.55
O
ATOM 2980 CB HIS B 159 14.961 22.189 -27.327 1.00 33.99
C
ATOM 9247 CD1 TYR E 96 12.520 39.700 -45.108 1.00 19.79
C
ATOM 9248 CD2 TYR E 96 11.234 40.250 -43.177 1.00 18.62
C
ATOM 9249 CE1 TYR E 96 11.944 38.446 -45.140 1.00 22.85
C
ATOM 9250 CE2 TYR E 96 10.652 38.999 -43.201 1.00 20.70
C
ATOM 9251 CZ TYR E 96 11.012 38.099 -44.185 1.00 20.85
C
ATOM 9252 OH TYR E 96 10.437 36.849 -44.213 1.00 24.95
O
ATOM 9253 H TYR E 96 12.828 42.319 -46.746 1.00 18.31 H
ATOM 9254 HA TYR E 96 11.326 43.275 -44.688 1.00 19.31
H
ATOM 9255 HB2 TYR E 96 13.749 41.879 -44.325 1.00 20.75
H
ATOM 9256 HB3 TYR E 96 12.745 42.318 -43.181 1.00 20.75
H
ATOM 9257 HD1 TYR E 96 13.149 39.930 -45.753 1.00 23.75
H
ATOM 9258 HD2 TYR E 96 10.992 40.855 -42.513 1.00 22.34
H
ATOM 9259 HE1 TYR E 96 12.184 37.838 -45.801 1.00 27.42
H
ATOM 9260 HE2 TYR E 96 10.024 38.762 -42.558 1.00 24.84
H
ATOM 9261 HH TYR E 96 9.891 36.770 -43.580 1.00 29.94 H
ATOM 9262 N LEU E 97 12.606 45.365 -44.474 1.00 14.66 N
ATOM 9263 CA LEU E 97 13.385 46.602 -44.404 1.00 20.71
C
ATOM 9264 C LEU E 97 13.605 47.025 -42.961 1.00 17.15 C
ATOM 9265 O LEU E 97 12.681 46.998 -42.143 1.00 15.93 O
ATOM 9266 CB LEU E 97 12.698 47.752 -45.151 1.00 18.74
C
ATOM 9267 CG LEU E 97 12.170 47.515 -46.563 1.00 24.83
C
ATOM 9268 CD1 LEU E 97 11.391 48.729 -47.041 1.00 31.08
C
ATOM 9269 CD2 LEU E 97 13.316 47.219 -47.496 1.00 24.75
C
ATOM 9270 H LEU E 97 11.831 45.420 -44.106 1.00 17.60 H
ATOM 9271 HA LEU E 97 14.253 46.453 -44.811 1.00 24.85
H
ATOM 9272 HB2 LEU E 97 11.942 48.039 -44.617 1.00 22.48
H
ATOM 9273 HB3 LEU E 97 13.334 48.482 -45.212 1.00 22.48
H
ATOM 9274 HG LEU E 97 11.574 46.750 -46.559 1.00 29.80
H
ATOM 9275 HD11 LEU E 97 11.064 48.560 -47.938 1.00 37.30
H
ATOM 9276 HD12 LEU E 97 10.645 48.881 -46.440 1.00 37.30
H
ATOM 9277 HD13 LEU E 97 11.979 49.500 -47.043 1.00 37.30
H
ATOM 9278 HD21 LEU E 97 12.965 47.071 -48.388 1.00 29.70
H
ATOM 9279 HD22 LEU E 97 13.923 47.976 -47.500 1.00 29.70
H
ATOM 9280 HD23 LEU E 97 13.778 46.425 -47.186 1.00 29.70

C
ATOM 2981 CG HIS B 159 16.430 22.259 -27.601 1.00 41.87
C
ATOM 2982 ND1 HIS B 159 17.272 23.120 -26.929 1.00 45.71
N
ATOM 2983 CD2 HIS B 159 17.207 21.576 -28.474 1.00 42.10
C
ATOM 2984 CE1 HIS B 159 18.505 22.962 -27.377 1.00 52.16
C
ATOM 2985 NE2 HIS B 159 18.492 22.032 -28.314 1.00 50.26
N
ATOM 2986 H HIS B 159 12.757 21.698 -26.158 1.00 26.80
H
ATOM 2987 HA HIS B 159 14.824 20.167 -27.006 1.00 35.36
H
ATOM 2988 HB2 HIS B 159 14.501 22.177 -28.180 1.00 40.79
H
ATOM 2989 HB3 HIS B 159 14.714 22.985 -26.831 1.00 40.79
H
ATOM 2990 HD1 HIS B 159 17.033 23.672 -26.315 1.00 54.85
H
ATOM 2991 HD2 HIS B 159 16.923 20.920 -29.070 1.00 50.52
H
ATOM 2992 HE1 HIS B 159 19.255 23.428 -27.083 1.00 62.60
H
ATOM 2993 HE2 HIS B 159 19.178 21.757 -28.754 1.00 60.31
H
ATOM 2994 N ILE B 160 16.102 19.991 -24.944 1.00 47.95
N
ATOM 2995 CA ILE B 160 16.840 19.885 -23.692 1.00 58.27
C
ATOM 2996 C ILE B 160 18.248 20.455 -23.880 1.00 66.09
C
ATOM 2997 O ILE B 160 19.148 19.743 -24.324 1.00 70.94
O
ATOM 2998 CB ILE B 160 16.936 18.419 -23.208 1.00 63.95
C
ATOM 2999 CG1 ILE B 160 15.588 17.704 -23.348 1.00 56.29
C
ATOM 3000 CG2 ILE B 160 17.414 18.368 -21.768 1.00 67.71
C
ATOM 3001 CD1 ILE B 160 14.461 18.326 -22.545 1.00 48.29
C
ATOM 3002 H ILE B 160 16.295 19.377 -25.514 1.00 57.54
H
ATOM 3003 HA ILE B 160 16.389 20.404 -23.007 1.00 69.92
H
ATOM 3004 HB ILE B 160 17.585 17.958 -23.761 1.00 76.73
H
ATOM 3005 HG12 ILE B 160 15.326 17.717 -24.282 1.00 67.54
H
ATOM 3006 HG13 ILE B 160 15.690 16.787 -23.050 1.00 67.54
H
ATOM 3007 HG21 ILE B 160 17.467 17.442 -21.486 1.00 81.25
H
ATOM 3008 HG22 ILE B 160 18.290 18.782 -21.712 1.00 81.25
H
ATOM 3009 HG23 ILE B 160 16.784 18.849 -21.209 1.00 81.25
H
ATOM 3010 HD11 ILE B 160 13.650 17.815 -22.691 1.00 57.95
H
ATOM 3011 HD12 ILE B 160 14.698 18.311 -21.605 1.00 57.95
H
ATOM 3012 HD13 ILE B 160 14.332 19.242 -22.839 1.00 57.95
H
ATOM 3013 N PRO B 161 18.448 21.748 -23.558 1.00 69.70
N
ATOM 3014 CA PRO B 161 19.784 22.316 -23.778 1.00 73.07
H

ATOM 9281 N TYR E 98 14.840 47.417 -42.665 1.00 15.72 N
ATOM 9282 CA TYR E 98 15.182 48.046 -41.401 1.00 18.67
C

ATOM 9283 C TYR E 98 15.675 49.456 -41.704 1.00 22.10 C

ATOM 9284 O TYR E 98 16.701 49.630 -42.363 1.00 18.15 O
ATOM 9285 CB TYR E 98 16.247 47.242 -40.655 1.00 19.19
C
ATOM 9286 CG TYR E 98 16.571 47.797 -39.287 1.00 23.54
C
ATOM 9287 CD1 TYR E 98 17.573 48.742 -39.119 1.00 25.80
C
ATOM 9288 CD2 TYR E 98 15.864 47.387 -38.165 1.00 22.25
C
ATOM 9289 CE1 TYR E 98 17.866 49.257 -37.872 1.00 24.47
C
ATOM 9290 CE2 TYR E 98 16.153 47.895 -36.913 1.00 22.72
C
ATOM 9291 CZ TYR E 98 17.154 48.829 -36.774 1.00 26.85
C
ATOM 9292 OH TYR E 98 17.446 49.337 -35.533 1.00 29.33
O

ATOM 9293 H TYR E 98 15.511 47.325 -43.196 1.00 18.86 H
ATOM 9294 HA TYR E 98 14.392 48.107 -40.843 1.00 22.40
H
ATOM 9295 HB2 TYR E 98 15.930 46.333 -40.540 1.00 23.03
H
ATOM 9296 HB3 TYR E 98 17.064 47.243 -41.177 1.00 23.03
H
ATOM 9297 HD1 TYR E 98 18.056 49.032 -39.859 1.00 30.96
H
ATOM 9298 HD2 TYR E 98 15.187 46.755 -38.256 1.00 26.70
H
ATOM 9299 HE1 TYR E 98 18.543 49.887 -37.774 1.00 29.36
H
ATOM 9300 HE2 TYR E 98 15.674 47.609 -36.169 1.00 27.26
H
ATOM 9301 HH TYR E 98 16.941 48.995 -34.956 1.00 35.20
H

ATOM 9302 N ASN E 99 14.934 50.454 -41.232 1.00 19.00 N
ATOM 9303 CA ASN E 99 15.201 51.846 -41.579 1.00 17.34
C

ATOM 9304 C ASN E 99 15.317 52.027 -43.095 1.00 24.69 C

ATOM 9305 O ASN E 99 16.193 52.735 -43.589 1.00 20.15 O
ATOM 9306 CB ASN E 99 16.465 52.334 -40.868 1.00 18.40
C
ATOM 9307 CG ASN E 99 16.290 52.391 -39.355 1.00 18.42
C
ATOM 9308 OD1 ASN E 99 15.170 52.483 -38.856 1.00 19.63
O
ATOM 9309 ND2 ASN E 99 17.393 52.334 -38.623 1.00 23.08
N

ATOM 9310 H ASN E 99 14.263 50.350 -40.704 1.00 22.81 H
ATOM 9311 HA ASN E 99 14.460 52.391 -41.272 1.00 20.80
H
ATOM 9312 HB2 ASN E 99 17.195 51.726 -41.064 1.00 22.08
H
ATOM 9313 HB3 ASN E 99 16.681 53.226 -41.180 1.00 22.08
H
ATOM 9314 HD21 ASN E 99 17.342 52.363 -37.765 1.00 27.69

C
ATOM 3015 C PRO B 161 20.833 21.764 -22.813 1.00 80.56
C
ATOM 3016 O PRO B 161 20.862 22.147 -21.644 1.00 84.37
O
ATOM 3017 CB PRO B 161 19.570 23.817 -23.556 1.00 69.03
C
ATOM 3018 CG PRO B 161 18.392 23.902 -22.659 1.00 63.55
C
ATOM 3019 CD PRO B 161 17.503 22.758 -23.048 1.00 60.94
C
ATOM 3020 HA PRO B 161 20.072 22.162 -24.692 1.00 87.68
H
ATOM 3021 HB2 PRO B 161 20.354 24.200 -23.132 1.00 82.83
H
ATOM 3022 HB3 PRO B 161 19.390 24.251 -24.404 1.00 82.83
H
ATOM 3023 HG2 PRO B 161 18.678 23.814 -21.737 1.00 76.25
H
ATOM 3024 HG3 PRO B 161 17.939 24.749 -22.798 1.00 76.25
H
ATOM 3025 HD2 PRO B 161 17.031 22.417 -22.272 1.00 73.12
H
ATOM 3026 HD3 PRO B 161 16.888 23.029 -23.748 1.00 73.12
H
ATOM 3027 N THR B 162 21.679 20.880 -23.334 1.00 82.80
N
ATOM 3028 CA THR B 162 22.732 20.185 -22.591 1.00 89.98
C
ATOM 3029 C THR B 162 23.165 19.019 -23.470 1.00 91.72
C
ATOM 3030 O THR B 162 24.340 18.653 -23.513 1.00 95.85
O
ATOM 3031 CB THR B 162 22.284 19.660 -21.201 1.00 95.35
C
ATOM 3032 OG1 THR B 162 23.364 18.945 -20.585 1.00 96.68
O
ATOM 3033 CG2 THR B 162 21.080 18.741 -21.324 1.00 98.91
C
ATOM 3034 H THR B 162 21.661 20.654 -24.164 1.00 99.36
H
ATOM 3035 HA THR B 162 23.490 20.778 -22.468 1.00107.98
H
ATOM 3036 HB THR B 162 22.037 20.412 -20.640 1.00114.42
H
ATOM 3037 HG1 THR B 162 23.588 18.294 -21.066 1.00116.01
H
ATOM 3038 HG21 THR B 162 20.815 18.424 -20.446 1.00118.69
H
ATOM 3039 HG22 THR B 162 20.337 19.220 -21.724 1.00118.69
H
ATOM 3040 HG23 THR B 162 21.301 17.979 -21.881 1.00118.69
H
ATOM 3041 N ASN B 163 22.186 18.447 -24.166 1.00 91.10
N
ATOM 3042 CA ASN B 163 22.418 17.423 -25.177 1.00 91.71
C
ATOM 3043 C ASN B 163 22.143 17.982 -26.573 1.00 82.79
C
ATOM 3044 O ASN B 163 22.538 17.393 -27.580 1.00 78.88
O
ATOM 3045 CB ASN B 163 21.543 16.190 -24.907 1.00 94.16
C
ATOM 3046 CG ASN B 163 20.053 16.513 -24.865 1.00 93.87
C
ATOM 3047 OD1 ASN B 163 19.539 17.272 -25.687 1.00 91.61
O
ATOM 3048 ND2 ASN B 163 19.353 15.925 -23.900 1.00 94.10
H
ATOM 9315 HD22 ASN E 99 18.161 52.269 -39.006 1.00 27.69
H
ATOM 9316 N GLY E 100 14.419 51.373 -43.825 1.00 19.11
N
ATOM 9317 CA GLY E 100 14.309 51.561 -45.260 1.00 22.08
C
ATOM 9318 C GLY E 100 15.283 50.739 -46.080 1.00 25.95
C
ATOM 9319 O GLY E 100 15.210 50.742 -47.308 1.00 24.82
O
ATOM 9320 H GLY E 100 13.856 50.807 -43.505 1.00 22.93
H
ATOM 9321 HA2 GLY E 100 13.410 51.329 -45.541 1.00 26.49
H
ATOM 9322 HA3 GLY E 100 14.457 52.497 -45.467 1.00 26.49
H
ATOM 9323 N GLU E 101 16.189 50.032 -45.410 1.00 23.34
N
ATOM 9324 CA GLU E 101 17.208 49.242 -46.095 1.00 21.40
C
ATOM 9325 C GLU E 101 16.874 47.756 -46.068 1.00 25.31
C
ATOM 9326 O GLU E 101 16.667 47.178 -44.996 1.00 20.68
O
ATOM 9327 CB GLU E 101 18.576 49.483 -45.457 1.00 28.51
C
ATOM 9328 CG GLU E 101 19.701 48.678 -46.079 1.00 36.34
C
ATOM 9329 CD GLU E 101 21.060 49.064 -45.529 1.00 50.28
C
ATOM 9330 OE1 GLU E 101 21.512 50.198 -45.804 1.00 53.61
O
ATOM 9331 OE2 GLU E 101 21.673 48.237 -44.819 1.00 56.44
O1-
ATOM 9332 H GLU E 101 16.236 49.993 -44.552 1.00 28.01
H
ATOM 9333 HA GLU E 101 17.255 49.522 -47.022 1.00 25.68
H
ATOM 9334 HB2 GLU E 101 18.800 50.422 -45.548 1.00 34.21
H
ATOM 9335 HB3 GLU E 101 18.528 49.247 -44.518 1.00 34.21
H
ATOM 9336 HG2 GLU E 101 19.558 47.737 -45.893 1.00 43.61
H
ATOM 9337 HG3 GLU E 101 19.709 48.831 -47.037 1.00 43.61
H
ATOM 9338 N GLU E 102 16.828 47.141 -47.248 1.00 19.84
N
ATOM 9339 CA GLU E 102 16.530 45.717 -47.360 1.00 21.48
C
ATOM 9340 C GLU E 102 17.575 44.873 -46.653 1.00 22.97
C
ATOM 9341 O GLU E 102 18.764 45.180 -46.681 1.00 23.40
O
ATOM 9342 CB GLU E 102 16.447 45.279 -48.826 1.00 28.87
C
ATOM 9343 CG GLU E 102 15.053 45.320 -49.420 1.00 34.38
C
ATOM 9344 CD GLU E 102 14.891 44.382 -50.604 1.00 39.93
C
ATOM 9345 OE1 GLU E 102 14.841 43.150 -50.386 1.00 41.37
O
ATOM 9346 OE2 GLU E 102 14.807 44.875 -51.749 1.00 49.33
O1-
ATOM 9347 H GLU E 102 16.968 47.529 -48.003 1.00 23.81
H
ATOM 9348 HA GLU E 102 15.671 45.541 -46.945 1.00 25.78

N
ATOM 3049 H ASN B 163 21.354 18.643 -24.066 1.00109.32
H
ATOM 3050 HA ASN B 163 23.347 17.147 -25.141 1.00110.05
H
ATOM 3051 HB2 ASN B 163 21.688 15.540 -25.612 1.00112.99
H
ATOM 3052 HB3 ASN B 163 21.791 15.810 -24.050 1.00112.99
H
ATOM 3053 HD21 ASN B 163 18.509 16.073 -23.831 1.00112.92
H
ATOM 3054 HD22 ASN B 163 19.744 15.398 -23.345 1.00112.92
H
ATOM 3055 N GLY B 164 21.463 19.124 -26.622 1.00 81.60
N
ATOM 3056 CA GLY B 164 21.145 19.781 -27.877 1.00 76.23
C
ATOM 3057 C GLY B 164 20.312 18.905 -28.793 1.00 73.18
C
ATOM 3058 O GLY B 164 20.669 18.689 -29.951 1.00 76.11
O
ATOM 3059 H GLY B 164 21.172 19.542 -25.929 1.00 97.92
H
ATOM 3060 HA2 GLY B 164 20.652 20.597 -27.700 1.00 91.48
H
ATOM 3061 HA3 GLY B 164 21.967 20.012 -28.338 1.00 91.48
H
ATOM 3062 N SER B 165 19.200 18.399 -28.269 1.00 64.95
N
ATOM 3063 CA SER B 165 18.326 17.518 -29.031 1.00 57.43
C
ATOM 3064 C SER B 165 16.861 17.810 -28.744 1.00 45.57
C
ATOM 3065 O SER B 165 16.511 18.287 -27.663 1.00 44.26
O
ATOM 3066 CB SER B 165 18.635 16.056 -28.711 1.00 62.72
C
ATOM 3067 OG SER B 165 18.321 15.754 -27.362 1.00 67.74
O
ATOM 3068 H SER B 165 18.928 18.554 -27.468 1.00 77.94
H
ATOM 3069 HA SER B 165 18.481 17.659 -29.978 1.00 68.91
H
ATOM 3070 HB2 SER B 165 18.106 15.488 -29.292 1.00 75.26
H
ATOM 3071 HB3 SER B 165 19.580 15.894 -28.859 1.00 75.26
H
ATOM 3072 HG SER B 165 17.505 15.890 -27.219 1.00 81.29
H
ATOM 3073 N TRP B 166 16.012 17.515 -29.723 1.00 40.98
N
ATOM 3074 CA TRP B 166 14.569 17.656 -29.572 1.00 34.55
C
ATOM 3075 C TRP B 166 13.945 16.298 -29.288 1.00 31.08
C
ATOM 3076 O TRP B 166 14.212 15.330 -29.999 1.00 34.34
O
ATOM 3077 CB TRP B 166 13.953 18.265 -30.830 1.00 30.13
C
ATOM 3078 CG TRP B 166 14.302 19.703 -31.041 1.00 30.81
C
ATOM 3079 CD1 TRP B 166 15.354 20.196 -31.756 1.00 36.26
C
ATOM 3080 CD2 TRP B 166 13.591 20.841 -30.538 1.00 28.21
C
ATOM 3081 NE1 TRP B 166 15.344 21.569 -31.726 1.00 34.03
N
ATOM 3082 CE2 TRP B 166 14.272 21.990 -30.984 1.00 27.63
H
ATOM 9349 HB2 GLU E 102 17.009 45.865 -49.357 1.00 34.65
H
ATOM 9350 HB3 GLU E 102 16.769 44.367 -48.896 1.00 34.65
H
ATOM 9351 HG2 GLU E 102 14.413 45.059 -48.740 1.00 41.25
H
ATOM 9352 HG3 GLU E 102 14.866 46.222 -49.724 1.00 41.25
H
ATOM 9353 N TYR E 103 17.121 43.797 -46.025 1.00 21.26
N
ATOM 9354 CA TYR E 103 18.031 42.827 -45.444 1.00 20.13
C
ATOM 9355 C TYR E 103 17.377 41.454 -45.470 1.00 20.08
C
ATOM 9356 O TYR E 103 16.155 41.338 -45.607 1.00 18.12
O
ATOM 9357 CB TYR E 103 18.430 43.236 -44.021 1.00 21.72
C
ATOM 9358 CG TYR E 103 17.330 43.173 -42.978 1.00 21.02
C
ATOM 9359 CD1 TYR E 103 16.273 44.078 -42.985 1.00 21.46
C
ATOM 9360 CD2 TYR E 103 17.374 42.232 -41.961 1.00 19.71
C
ATOM 9361 CE1 TYR E 103 15.279 44.024 -42.020 1.00 14.20
C
ATOM 9362 CE2 TYR E 103 16.388 42.171 -40.994 1.00 15.96
C
ATOM 9363 CZ TYR E 103 15.344 43.065 -41.029 1.00 14.97
C
ATOM 9364 OH TYR E 103 14.370 43.002 -40.059 1.00 13.45
O
ATOM 9365 H TYR E 103 16.289 43.607 -45.923 1.00 25.51
H
ATOM 9366 HA TYR E 103 18.837 42.786 -45.982 1.00 24.15
H
ATOM 9367 HB2 TYR E 103 19.144 42.651 -43.724 1.00 26.06
H
ATOM 9368 HB3 TYR E 103 18.752 44.151 -44.046 1.00 26.06
H
ATOM 9369 HD1 TYR E 103 16.226 44.722 -43.654 1.00 25.75
H
ATOM 9370 HD2 TYR E 103 18.076 41.623 -41.935 1.00 23.65
H
ATOM 9371 HE1 TYR E 103 14.573 44.630 -42.040 1.00 17.04
H
ATOM 9372 HE2 TYR E 103 16.430 41.528 -40.324 1.00 19.15
H
ATOM 9373 HH TYR E 103 14.536 42.375 -39.526 1.00 16.14
H
ATOM 9374 N THR E 104 18.199 40.415 -45.378 1.00 18.46
N
ATOM 9375 CA THR E 104 17.706 39.043 -45.423 1.00 21.91
C
ATOM 9376 C THR E 104 18.453 38.129 -44.461 1.00 20.34
C
ATOM 9377 O THR E 104 18.024 37.003 -44.211 1.00 22.09
O
ATOM 9378 CB THR E 104 17.830 38.452 -46.844 1.00 22.12
C
ATOM 9379 OG1 THR E 104 19.214 38.270 -47.169 1.00 23.24
O
ATOM 9380 CG2 THR E 104 17.185 39.369 -47.872 1.00 25.29
C
ATOM 9381 H THR E 104 19.052 40.478 -45.288 1.00 22.15
H
ATOM 9382 HA THR E 104 16.768 39.037 -45.176 1.00 26.30

C
ATOM 3083 CE3 TRP B 166 12.446 20.999 -29.751 1.00 23.82
C
ATOM 3084 CZ2 TRP B 166 13.846 23.280 -30.671 1.00 27.91
C
ATOM 3085 CZ3 TRP B 166 12.024 22.281 -29.440 1.00 24.12
C
ATOM 3086 CH2 TRP B 166 12.722 23.405 -29.901 1.00 25.08
C
ATOM 3087 H TRP B 166 16.252 17.226 -30.496 1.00 49.18
H
ATOM 3088 HA TRP B 166 14.379 18.243 -28.824 1.00 41.46
H
ATOM 3089 HB2 TRP B 166 14.265 17.769 -31.603 1.00 36.16
H
ATOM 3090 HB3 TRP B 166 12.987 18.201 -30.767 1.00 36.16
H
ATOM 3091 HD1 TRP B 166 15.987 19.677 -32.198 1.00 43.51
H
ATOM 3092 HE1 TRP B 166 15.918 22.081 -32.111 1.00 40.83
H
ATOM 3093 HE3 TRP B 166 11.977 20.257 -29.442 1.00 28.59
H
ATOM 3094 HZ2 TRP B 166 14.308 24.028 -30.975 1.00 33.49
H
ATOM 3095 HZ3 TRP B 166 11.263 22.398 -28.918 1.00 28.94
H
ATOM 3096 HH2 TRP B 166 12.416 24.254 -29.676 1.00 30.10
H
ATOM 3097 N GLN B 167 13.119 16.225 -28.250 1.00 27.39
N
ATOM 3098 CA GLN B 167 12.485 14.965 -27.879 1.00 30.85
C
ATOM 3099 C GLN B 167 11.020 15.147 -27.492 1.00 26.83
C
ATOM 3100 O GLN B 167 10.604 16.219 -27.048 1.00 24.25
O
ATOM 3101 CB GLN B 167 13.248 14.306 -26.729 1.00 31.47
C
ATOM 3102 CG GLN B 167 13.319 15.142 -25.462 1.00 39.54
C
ATOM 3103 CD GLN B 167 13.995 14.409 -24.315 1.00 47.76
C
ATOM 3104 OE1 GLN B 167 13.559 14.498 -23.168 1.00 47.44
O
ATOM 3105 NE2 GLN B 167 15.066 13.683 -24.618 1.00 48.92
N
ATOM 3106 H GLN B 167 12.910 16.889 -27.745 1.00 32.87
H
ATOM 3107 HA GLN B 167 12.517 14.364 -28.639 1.00 37.02
H
ATOM 3108 HB2 GLN B 167 12.811 13.469 -26.505 1.00 37.76
H
ATOM 3109 HB3 GLN B 167 14.157 14.132 -27.018 1.00 37.76
H
ATOM 3110 HG2 GLN B 167 13.827 15.949 -25.644 1.00 47.45
H
ATOM 3111 HG3 GLN B 167 12.419 15.371 -25.183 1.00 47.45
H
ATOM 3112 HE21 GLN B 167 15.482 13.251 -24.002 1.00 58.70
H
ATOM 3113 HE22 GLN B 167 15.344 13.645 -25.431 1.00 58.70
H
ATOM 3114 N TRP B 168 10.249 14.079 -27.668 1.00 23.01
N
ATOM 3115 CA TRP B 168 8.838 14.077 -27.318 1.00 26.18
C
ATOM 3116 C TRP B 168 8.659 13.855 -25.826 1.00 24.45
H
ATOM 9383 HB THR E 104 17.377 37.595 -46.875 1.00 26.55
H
ATOM 9384 HG1 THR E 104 19.287 37.948 -47.941 1.00 27.89
H
ATOM 9385 HG21 THR E 104 17.271 38.985 -48.758 1.00 30.35
H
ATOM 9386 HG22 THR E 104 16.244 39.485 -47.668 1.00 30.35
H
ATOM 9387 HG23 THR E 104 17.620 40.236 -47.860 1.00 30.35
H

ATOM 9388 N VAL E 105 19.570 38.612 -43.925 1.00 23.32 N
ATOM 9389 CA VAL E 105 20.446 37.784 -43.105 1.00 21.10
C

ATOM 9390 C VAL E 105 20.199 37.994 -41.613 1.00 24.91 C
ATOM 9391 O VAL E 105 20.247 39.116 -41.110 1.00 23.61
O
ATOM 9392 CB VAL E 105 21.928 38.072 -43.414 1.00 26.35
C
ATOM 9393 CG1 VAL E 105 22.838 37.197 -42.560 1.00 25.25
C
ATOM 9394 CG2 VAL E 105 22.214 37.842 -44.892 1.00 28.02
C

ATOM 9395 H VAL E 105 19.844 39.421 -44.023 1.00 27.98 H
ATOM 9396 HA VAL E 105 20.275 36.850 -43.307 1.00 25.32
H
ATOM 9397 HB VAL E 105 22.121 39.000 -43.210 1.00 31.62
H
ATOM 9398 HG11 VAL E 105 23.762 37.400 -42.775 1.00 30.30
H
ATOM 9399 HG12 VAL E 105 22.667 37.385 -41.624 1.00 30.30
H
ATOM 9400 HG13 VAL E 105 22.649 36.265 -42.751 1.00 30.30
H
ATOM 9401 HG21 VAL E 105 23.150 38.028 -45.064 1.00 33.63
H
ATOM 9402 HG22 VAL E 105 22.014 36.918 -45.111 1.00 33.63
H
ATOM 9403 HG23 VAL E 105 21.655 38.435 -45.417 1.00 33.63
H

ATOM 9404 N LYS E 106 19.944 36.892 -40.916 1.00 28.46 N
ATOM 9405 CA LYS E 106 19.775 36.896 -39.469 1.00 32.57
C

ATOM 9406 C LYS E 106 21.133 36.835 -38.787 1.00 31.99 C
ATOM 9407 O LYS E 106 21.998 36.062 -39.198 1.00 30.22
O
ATOM 9408 CB LYS E 106 18.914 35.706 -39.033 1.00 33.52
C
ATOM 9409 CG LYS E 106 18.726 35.569 -37.528 1.00 37.03
C
ATOM 9410 CD LYS E 106 18.189 34.196 -37.165 1.00 45.30
C
ATOM 9411 CE LYS E 106 17.955 34.067 -35.665 1.00 57.12
C
ATOM 9412 NZ LYS E 106 19.210 34.241 -34.879 1.00 54.38
N1+

ATOM 9413 H LYS E 106 19.862 36.112 -41.269 1.00 34.15 H
ATOM 9414 HA LYS E 106 19.330 37.714 -39.198 1.00 39.08
H
ATOM 9415 HB2 LYS E 106 18.035 35.799 -39.431 1.00 40.22
H
ATOM 9416 HB3 LYS E 106 19.331 34.890 -39.351 1.00 40.22

C
ATOM 3117 O TRP B 168 9.611 13.512 -25.128 1.00 28.38
O
ATOM 3118 CB TRP B 168 8.100 13.000 -28.108 1.00 25.30
C
ATOM 3119 CG TRP B 168 8.224 13.197 -29.577 1.00 26.32
C
ATOM 3120 CD1 TRP B 168 8.994 12.476 -30.439 1.00 25.09
C
ATOM 3121 CD2 TRP B 168 7.571 14.198 -30.361 1.00 22.02
C
ATOM 3122 NE1 TRP B 168 8.856 12.963 -31.716 1.00 23.33
N
ATOM 3123 CE2 TRP B 168 7.985 14.020 -31.694 1.00 23.22
C
ATOM 3124 CE3 TRP B 168 6.670 15.228 -30.064 1.00 25.48
C
ATOM 3125 CZ2 TRP B 168 7.532 14.832 -32.731 1.00 20.73
C
ATOM 3126 CZ3 TRP B 168 6.220 16.029 -31.093 1.00 20.54
C
ATOM 3127 CH2 TRP B 168 6.653 15.829 -32.410 1.00 19.21
C
ATOM 3128 H TRP B 168 10.527 13.334 -27.995 1.00 27.61
H
ATOM 3129 HA TRP B 168 8.452 14.937 -27.544 1.00 31.42
H
ATOM 3130 HB2 TRP B 168 8.473 12.133 -27.888 1.00 30.36
H
ATOM 3131 HB3 TRP B 168 7.158 13.027 -27.879 1.00 30.36
H
ATOM 3132 HD1 TRP B 168 9.534 11.758 -30.198 1.00 30.11
H
ATOM 3133 HE1 TRP B 168 9.250 12.653 -32.415 1.00 28.00
H
ATOM 3134 HE3 TRP B 168 6.379 15.367 -29.192 1.00 30.57
H
ATOM 3135 HZ2 TRP B 168 7.815 14.701 -33.607 1.00 24.88
H
ATOM 3136 HZ3 TRP B 168 5.622 16.717 -30.909 1.00 24.65
H
ATOM 3137 HH2 TRP B 168 6.332 16.385 -33.082 1.00 23.05
H
ATOM 3138 N GLU B 169 7.440 14.052 -25.341 1.00 23.03
N
ATOM 3139 CA GLU B 169 7.144 13.867 -23.922 1.00 27.07
C
ATOM 3140 C GLU B 169 7.491 12.466 -23.430 1.00 28.35
C
ATOM 3141 O GLU B 169 7.865 12.291 -22.271 1.00 29.75
O
ATOM 3142 CB GLU B 169 5.670 14.146 -23.646 1.00 26.09
C
ATOM 3143 CG GLU B 169 5.303 15.611 -23.690 1.00 25.97
C
ATOM 3144 CD GLU B 169 3.812 15.826 -23.565 1.00 24.50
C
ATOM 3145 OE1 GLU B 169 3.374 16.389 -22.542 1.00 25.81
O
ATOM 3146 OE2 GLU B 169 3.078 15.423 -24.491 1.00 26.86
O1-
ATOM 3147 H GLU B 169 6.762 14.294 -25.812 1.00 27.63
H
ATOM 3148 HA GLU B 169 7.669 14.501 -23.408 1.00 32.48
H
ATOM 3149 HB2 GLU B 169 5.135 13.687 -24.312 1.00 31.30
H
ATOM 3150 HB3 GLU B 169 5.450 13.813 -22.762 1.00 31.30
H
ATOM 9417 HG2 LYS E 106 19.581 35.689 -37.086 1.00 44.43
H
ATOM 9418 HG3 LYS E 106 18.092 36.236 -37.222 1.00 44.43
H
ATOM 9419 HD2 LYS E 106 17.343 34.054 -37.618 1.00 54.35
H
ATOM 9420 HD3 LYS E 106 18.831 33.520 -37.432 1.00 54.35
H
ATOM 9421 HE2 LYS E 106 17.325 34.748 -35.382 1.00 68.55
H
ATOM 9422 HE3 LYS E 106 17.600 33.184 -35.475 1.00 68.55
H
ATOM 9423 HZ1 LYS E 106 19.805 33.622 -35.116 1.00 65.26
H
ATOM 9424 HZ2 LYS E 106 19.554 35.047 -35.031 1.00 65.26
H
ATOM 9425 HZ3 LYS E 106 19.038 34.159 -34.010 1.00 65.26
H
ATOM 9426 N THR E 107 21.315 37.652 -37.752 1.00 30.36
N
ATOM 9427 CA THR E 107 22.519 37.598 -36.926 1.00 39.31
C
ATOM 9428 C THR E 107 22.178 36.947 -35.588 1.00 41.69
C
ATOM 9429 O THR E 107 21.024 36.604 -35.336 1.00 35.99
O
ATOM 9430 CB THR E 107 23.125 38.998 -36.691 1.00 36.74
C
ATOM 9431 OG1 THR E 107 22.180 39.833 -36.013 1.00 34.87
O
ATOM 9432 CG2 THR E 107 23.513 39.643 -38.017 1.00 37.13
C
ATOM 9433 H THR E 107 20.751 38.253 -37.505 1.00 36.43
H
ATOM 9434 HA THR E 107 23.185 37.050 -37.369 1.00 47.17
H
ATOM 9435 HB THR E 107 23.925 38.913 -36.149 1.00 44.09
H
ATOM 9436 HG1 THR E 107 22.509 40.595 -35.885 1.00 41.85
H
ATOM 9437 HG21 THR E 107 23.893 40.521 -37.860 1.00 44.55
H
ATOM 9438 HG22 THR E 107 24.169 39.093 -38.474 1.00 44.55
H
ATOM 9439 HG23 THR E 107 22.730 39.735 -38.582 1.00 44.55
H
ATOM 9440 N GLN E 108 23.180 36.784 -34.731 1.00 41.22
N
ATOM 9441 CA GLN E 108 23.017 36.001 -33.511 1.00 51.91
C
ATOM 9442 C GLN E 108 22.373 36.798 -32.379 1.00 44.49
C
ATOM 9443 O GLN E 108 21.587 36.256 -31.602 1.00 43.27
O
ATOM 9444 CB GLN E 108 24.372 35.461 -33.049 1.00 68.26
C
ATOM 9445 CG GLN E 108 24.287 34.140 -32.303 1.00 83.56
C
ATOM 9446 CD GLN E 108 23.781 33.007 -33.179 1.00 91.50
C
ATOM 9447 OE1 GLN E 108 23.967 33.017 -34.397 1.00 89.80
O
ATOM 9448 NE2 GLN E 108 23.130 32.028 -32.563 1.00 95.77
N
ATOM 9449 H GLN E 108 23.966 37.116 -34.833 1.00 49.46
H
ATOM 9450 HA GLN E 108 22.444 35.241 -33.701 1.00 62.30

H
ATOM 3151 HG2 GLU B 169 5.737 16.071 -22.954 1.00 31.17
H
ATOM 3152 HG3 GLU B 169 5.593 15.987 -24.536 1.00 31.17
H
ATOM 3153 N ASP B 170 7.365 11.472 -24.307 1.00 30.20
N
ATOM 3154 CA ASP B 170 7.651 10.088 -23.935 1.00 31.21
C
ATOM 3155 C ASP B 170 9.145 9.779 -24.005 1.00 30.44
C
ATOM 3156 O ASP B 170 9.549 8.620 -23.930 1.00 33.82
O
ATOM 3157 CB ASP B 170 6.872 9.111 -24.827 1.00 31.14
C
ATOM 3158 CG ASP B 170 7.274 9.188 -26.297 1.00 28.80
C
ATOM 3159 OD1 ASP B 170 8.297 9.822 -26.629 1.00 28.18
O
ATOM 3160 OD2 ASP B 170 6.557 8.594 -27.131 1.00 33.86
O1-
ATOM 3161 H ASP B 170 7.116 11.573 -25.124 1.00 36.24
H
ATOM 3162 HA ASP B 170 7.363 9.946 -23.020 1.00 37.45
H
ATOM 3163 HB2 ASP B 170 7.036 8.206 -24.520 1.00 37.37
H
ATOM 3164 HB3 ASP B 170 5.926 9.315 -24.766 1.00 37.37
H
ATOM 3165 N GLY B 171 9.959 10.816 -24.173 1.00 28.28
N
ATOM 3166 CA GLY B 171 11.402 10.665 -24.161 1.00 30.98
C
ATOM 3167 C GLY B 171 11.999 10.269 -25.498 1.00 29.68
C
ATOM 3168 O GLY B 171 13.213 10.362 -25.688 1.00 36.65
O
ATOM 3169 H GLY B 171 9.693 11.625 -24.296 1.00 33.93
H
ATOM 3170 HA2 GLY B 171 11.806 11.503 -23.887 1.00 37.17
H
ATOM 3171 HA3 GLY B 171 11.644 9.987 -23.511 1.00 37.17
H
ATOM 3172 N SER B 172 11.159 9.829 -26.428 1.00 28.25
N
ATOM 3173 CA SER B 172 11.644 9.397 -27.733 1.00 32.36
C
ATOM 3174 C SER B 172 12.201 10.584 -28.513 1.00 30.64
C
ATOM 3175 O SER B 172 11.694 11.699 -28.417 1.00 29.69
O
ATOM 3176 CB SER B 172 10.531 8.712 -28.527 1.00 30.14
C
ATOM 3177 OG SER B 172 9.494 9.620 -28.857 1.00 32.10
O
ATOM 3178 H SER B 172 10.307 9.770 -26.329 1.00 33.90
H
ATOM 3179 HA SER B 172 12.362 8.757 -27.607 1.00 38.83
H
ATOM 3180 HB2 SER B 172 10.906 8.353 -29.346 1.00 36.17
H
ATOM 3181 HB3 SER B 172 10.160 7.994 -27.991 1.00 36.17
H
ATOM 3182 HG SER B 172 9.158 9.939 -28.157 1.00 38.52
H
ATOM 3183 N ILE B 173 13.257 10.336 -29.274 1.00 33.34
N
ATOM 3184 CA ILE B 173 13.897 11.382 -30.055 1.00 36.79
H
ATOM 9451 HB2 GLN E 108 24.936 35.327 -33.827 1.00 81.91
H
ATOM 9452 HB3 GLN E 108 24.781 36.111 -32.456 1.00 81.91
H
ATOM 9453 HG2 GLN E 108 25.171 33.900 -31.982 1.00100.27
H
ATOM 9454 HG3 GLN E 108 23.677 34.238 -31.555 1.00100.27
H
ATOM 9455 HE21 GLN E 108 22.823 31.364 -33.016 1.00114.92
H
ATOM 9456 HE22 GLN E 108 23.014 32.058 -31.711 1.00114.92
H
ATOM 9457 N GLU E 109 22.717 38.078 -32.288 1.00 45.66
N
ATOM 9458 CA GLU E 109 22.231 38.935 -31.207 1.00 42.78
C
ATOM 9459 C GLU E 109 20.706 39.053 -31.196 1.00 40.26
C
ATOM 9460 O GLU E 109 20.050 38.976 -32.238 1.00 31.16
O
ATOM 9461 CB GLU E 109 22.860 40.332 -31.304 1.00 42.62
C
ATOM 9462 CG GLU E 109 22.975 40.884 -32.724 1.00 52.37
C
ATOM 9463 CD GLU E 109 23.398 42.343 -32.764 1.00 59.49
C
ATOM 9464 OE1 GLU E 109 23.528 42.964 -31.686 1.00 62.06
O
ATOM 9465 OE2 GLU E 109 23.602 42.868 -33.881 1.00 51.48
O1-
ATOM 9466 H GLU E 109 23.234 38.481 -32.845 1.00 54.80
H
ATOM 9467 HA GLU E 109 22.502 38.548 -30.359 1.00 51.33
H
ATOM 9468 HB2 GLU E 109 22.317 40.952 -30.791 1.00 51.15
H
ATOM 9469 HB3 GLU E 109 23.754 40.296 -30.929 1.00 51.15
H
ATOM 9470 HG2 GLU E 109 23.638 40.367 -33.209 1.00 62.84
H
ATOM 9471 HG3 GLU E 109 22.113 40.810 -33.161 1.00 62.84
H
ATOM 9472 N ALA E 110 20.150 39.233 -30.001 1.00 41.90 N
ATOM 9473 CA ALA E 110 18.712 39.410 -29.837 1.00 33.67
C
ATOM 9474 C ALA E 110 18.339 40.867 -30.069 1.00 35.94 C
ATOM 9475 O ALA E 110 18.587 41.730 -29.225 1.00 34.30
O
ATOM 9476 CB ALA E 110 18.270 38.958 -28.455 1.00 41.21
C
ATOM 9477 H ALA E 110 20.590 39.258 -29.263 1.00 50.29 H
ATOM 9478 HA ALA E 110 18.247 38.869 -30.495 1.00 40.41
H
ATOM 9479 HB1 ALA E 110 17.312 39.086 -28.372 1.00 49.45
H
ATOM 9480 HB2 ALA E 110 18.490 38.020 -28.344 1.00 49.45
H
ATOM 9481 HB3 ALA E 110 18.734 39.488 -27.787 1.00 49.45
H
ATOM 9482 N THR E 111 17.745 41.129 -31.226 1.00 23.46
N
ATOM 9483 CA THR E 111 17.372 42.476 -31.620 1.00 23.33
C
ATOM 9484 C THR E 111 15.999 42.480 -32.272 1.00 19.12

C
ATOM 3185 C ILE B 173 13.052 11.692 -31.284 1.00 34.73
C
ATOM 3186 O ILE B 173 12.329 10.831 -31.782 1.00 35.37
O
ATOM 3187 CB ILE B 173 15.328 10.966 -30.480 1.00 41.45
C
ATOM 3188 CG1 ILE B 173 16.111 12.158 -31.044 1.00 45.90
C
ATOM 3189 CG2 ILE B 173 15.285 9.821 -31.487 1.00 41.81
C
ATOM 3190 CD1 ILE B 173 16.543 13.160 -29.995 1.00 47.62
C
ATOM 3191 H ILE B 173 13.625 9.563 -29.357 1.00 40.01
H
ATOM 3192 HA ILE B 173 13.961 12.187 -29.518 1.00 44.15
H
ATOM 3193 HB ILE B 173 15.794 10.650 -29.690 1.00 49.74
H
ATOM 3194 HG12 ILE B 173 16.910 11.826 -31.483 1.00 55.09
H
ATOM 3195 HG13 ILE B 173 15.553 12.623 -31.686 1.00 55.09
H
ATOM 3196 HG21 ILE B 173 16.193 9.584 -31.734 1.00 50.17
H
ATOM 3197 HG22 ILE B 173 14.843 9.060 -31.081 1.00 50.17
H
ATOM 3198 HG23 ILE B 173 14.794 10.110 -32.272 1.00 50.17
H
ATOM 3199 HD11 ILE B 173 17.029 13.879 -30.428 1.00 57.15
H
ATOM 3200 HD12 ILE B 173 15.755 13.513 -29.553 1.00 57.15
H
ATOM 3201 HD13 ILE B 173 17.114 12.715 -29.350 1.00 57.15
H
ATOM 3202 N LEU B 174 13.137 12.929 -31.760 1.00 35.60
N
ATOM 3203 CA LEU B 174 12.474 13.322 -32.997 1.00 31.48
C
ATOM 3204 C LEU B 174 13.053 12.550 -34.174 1.00 35.42
C
ATOM 3205 O LEU B 174 14.217 12.734 -34.531 1.00 33.32
O
ATOM 3206 CB LEU B 174 12.623 14.826 -33.230 1.00 26.55
C
ATOM 3207 CG LEU B 174 12.246 15.348 -34.619 1.00 31.49
C
ATOM 3208 CD1 LEU B 174 10.787 15.050 -34.937 1.00 27.57
C
ATOM 3209 CD2 LEU B 174 12.528 16.840 -34.714 1.00 29.29
C
ATOM 3210 H LEU B 174 13.576 13.564 -31.382 1.00 42.72
H
ATOM 3211 HA LEU B 174 11.528 13.116 -32.933 1.00 37.78
H
ATOM 3212 HB2 LEU B 174 12.063 15.289 -32.588 1.00 31.86
H
ATOM 3213 HB3 LEU B 174 13.551 15.065 -33.077 1.00 31.86
H
ATOM 3214 HG LEU B 174 12.793 14.899 -35.282 1.00 37.79
H
ATOM 3215 HD11 LEU B 174 10.581 15.392 -35.821 1.00 33.08
H
ATOM 3216 HD12 LEU B 174 10.649 14.090 -34.913 1.00 33.08
H
ATOM 3217 HD13 LEU B 174 10.225 15.482 -34.275 1.00 33.08
H
ATOM 3218 HD21 LEU B 174 12.283 17.151 -35.599 1.00 35.15
C
ATOM 9485 O THR E 111 15.517 41.447 -32.737 1.00 17.50
O
ATOM 9486 CB THR E 111 18.375 43.062 -32.609 1.00 21.03
C
ATOM 9487 OG1 THR E 111 18.395 42.245 -33.786 1.00 19.06
O
ATOM 9488 CG2 THR E 111 19.769 43.117 -31.995 1.00 30.25
C
ATOM 9489 H THR E 111 17.546 40.530 -31.811 1.00 28.16
H
ATOM 9490 HA THR E 111 17.342 43.047 -30.837 1.00 28.00
H
ATOM 9491 HB THR E 111 18.107 43.963 -32.846 1.00 25.24
H
ATOM 9492 HG1 THR E 111 18.944 42.555 -34.341 1.00 22.88
H
ATOM 9493 HG21 THR E 111 20.397 43.491 -32.633 1.00 36.30
H
ATOM 9494 HG22 THR E 111 19.759 43.673 -31.200 1.00 36.30
H
ATOM 9495 HG23 THR E 111 20.060 42.225 -31.753 1.00 36.30
H
ATOM 9496 N ASN E 112 15.383 43.653 -32.322 1.00 18.03
N
ATOM 9497 CA ASN E 112 14.118 43.813 -33.014 1.00 18.86
C
ATOM 9498 C ASN E 112 14.283 43.492 -34.496 1.00 18.90
C
ATOM 9499 O ASN E 112 13.396 42.909 -35.116 1.00 15.74
O
ATOM 9500 CB ASN E 112 13.581 45.231 -32.820 1.00 19.71
C
ATOM 9501 CG ASN E 112 13.143 45.494 -31.389 1.00 24.98
C
ATOM 9502 OD1 ASN E 112 12.646 44.597 -30.710 1.00 22.68
O
ATOM 9503 ND2 ASN E 112 13.331 46.723 -30.923 1.00 22.07
N
ATOM 9504 H ASN E 112 15.680 44.375 -31.960 1.00 21.63
H
ATOM 9505 HA ASN E 112 13.472 43.192 -32.642 1.00 22.63
H
ATOM 9506 HB2 ASN E 112 14.278 45.867 -33.044 1.00 23.65
H
ATOM 9507 HB3 ASN E 112 12.813 45.361 -33.399 1.00 23.65
H
ATOM 9508 HD21 ASN E 112 13.098 46.918 -30.118 1.00 26.49
H
ATOM 9509 HD22 ASN E 112 13.684 47.325 -31.426 1.00 26.49
H

ATOM 9510 N LYS E 113 15.439 43.854 -35.047 1.00 16.41 N
ATOM 9511 CA LYS E 113 15.739 43.600 -36.451 1.00 15.65
C

ATOM 9512 C LYS E 113 15.712 42.103 -36.766 1.00 16.82 C
ATOM 9513 O LYS E 113 15.106 41.673 -37.751 1.00 16.67
O
ATOM 9514 CB LYS E 113 17.102 44.193 -36.806 1.00 20.54
C
ATOM 9515 CG LYS E 113 17.454 44.125 -38.276 1.00 20.47
C
ATOM 9516 CD LYS E 113 18.816 44.753 -38.539 1.00 22.73
C
ATOM 9517 CE LYS E 113 19.154 44.754 -40.019 1.00 24.48
C
ATOM 9518 NZ LYS E 113 20.513 45.300 -40.281 1.00 26.06

H
ATOM 3219 HD22 LEU B 174 12.004 17.303 -34.043 1.00 35.15
H
ATOM 3220 HD23 LEU B 174 13.474 16.992 -34.560 1.00 35.15
H
ATOM 3221 N SER B 175 12.242 11.686 -34.776 1.00 36.01
N
ATOM 3222 CA SER B 175 12.703 10.894 -35.911 1.00 38.08
C
ATOM 3223 C SER B 175 12.978 11.796 -37.114 1.00 39.53
C
ATOM 3224 O SER B 175 12.257 12.771 -37.345 1.00 35.10
O
ATOM 3225 CB SER B 175 11.679 9.818 -36.277 1.00 34.05
C
ATOM 3226 OG SER B 175 11.435 8.952 -35.181 1.00 46.41
O
ATOM 3227 H SER B 175 11.426 11.540 -34.548 1.00 43.22
H
ATOM 3228 HA SER B 175 13.532 10.451 -35.672 1.00 45.70
H
ATOM 3229 HB2 SER B 175 10.847 10.248 -36.530 1.00 40.86
H
ATOM 3230 HB3 SER B 175 12.022 9.297 -37.020 1.00 40.86
H
ATOM 3231 HG SER B 175 10.872 8.368 -35.397 1.00 55.69
H
ATOM 3232 N PRO B 176 14.024 11.475 -37.890 1.00 37.56
N
ATOM 3233 CA PRO B 176 14.394 12.331 -39.020 1.00 40.19
C
ATOM 3234 C PRO B 176 13.366 12.306 -40.148 1.00 39.31
C
ATOM 3235 O PRO B 176 12.536 11.398 -40.204 1.00 39.37
O
ATOM 3236 CB PRO B 176 15.725 11.738 -39.482 1.00 42.21
C
ATOM 3237 CG PRO B 176 15.663 10.317 -39.076 1.00 48.89
C
ATOM 3238 CD PRO B 176 14.882 10.281 -37.799 1.00 40.78
C
ATOM 3239 HA PRO B 176 14.530 13.245 -38.724 1.00 48.23
H
ATOM 3240 HB2 PRO B 176 15.803 11.818 -40.446 1.00 50.65
H
ATOM 3241 HB3 PRO B 176 16.459 12.192 -39.038 1.00 50.65
H
ATOM 3242 HG2 PRO B 176 15.212 9.803 -39.764 1.00 58.67
H
ATOM 3243 HG3 PRO B 176 16.562 9.981 -38.934 1.00 58.67
H
ATOM 3244 HD2 PRO B 176 14.341 9.477 -37.757 1.00 48.94
H
ATOM 3245 HD3 PRO B 176 15.478 10.350 -37.037 1.00 48.94
H
ATOM 3246 N ASN B 177 13.423 13.307 -41.022 1.00 32.05
N
ATOM 3247 CA ASN B 177 12.551 13.372 -42.192 1.00 37.49
C
ATOM 3248 C ASN B 177 11.058 13.384 -41.853 1.00 32.07
C
ATOM 3249 O ASN B 177 10.227 13.073 -42.704 1.00 32.22
O
ATOM 3250 CB ASN B 177 12.853 12.200 -43.134 1.00 43.25
C
ATOM 3251 CG ASN B 177 14.279 12.223 -43.656 1.00 42.46
C
ATOM 3252 OD1 ASN B 177 14.599 12.972 -44.579 1.00 48.73

N1+
ATOM 9519 H LYS E 113 16.072 44.253 -34.623 1.00 19.69 H
ATOM 9520 HA LYS E 113 15.069 44.035 -37.002 1.00 18.78
H
ATOM 9521 HB2 LYS E 113 17.112 45.127 -36.544 1.00 24.65
H
ATOM 9522 HB3 LYS E 113 17.787 43.710 -36.317 1.00 24.65
H
ATOM 9523 HG2 LYS E 113 17.486 43.197 -38.557 1.00 24.56
H
ATOM 9524 HG3 LYS E 113 16.789 44.611 -38.789 1.00 24.56
H
ATOM 9525 HD2 LYS E 113 18.809 45.672 -38.228 1.00 27.28
H
ATOM 9526 HD3 LYS E 113 19.497 44.246 -38.071 1.00 27.28
H
ATOM 9527 HE2 LYS E 113 19.125 43.844 -40.352 1.00 29.38
H
ATOM 9528 HE3 LYS E 113 18.511 45.305 -40.492 1.00 29.38
H
ATOM 9529 HZ1 LYS E 113 20.565 46.139 -39.988 1.00 31.27
H
ATOM 9530 HZ2 LYS E 113 21.124 44.808 -39.861 1.00 31.27
H
ATOM 9531 HZ3 LYS E 113 20.682 45.288 -41.155 1.00 31.27
H
ATOM 9532 N ASN E 114 16.360 41.307 -35.924 1.00 14.24
N
ATOM 9533 CA ASN E 114 16.389 39.862 -36.127 1.00 15.14
C
ATOM 9534 C ASN E 114 15.036 39.200 -35.892 1.00 13.48
C
ATOM 9535 O ASN E 114 14.623 38.335 -36.663 1.00 14.71
O
ATOM 9536 CB ASN E 114 17.440 39.224 -35.217 1.00 20.17
C
ATOM 9537 CG ASN E 114 18.851 39.385 -35.758 1.00 27.46
C
ATOM 9538 OD1 ASN E 114 19.069 39.370 -36.971 1.00 22.82
O
ATOM 9539 ND2 ASN E 114 19.815 39.537 -34.858 1.00 24.63
N
ATOM 9540 H ASN E 114 16.790 41.576 -35.230 1.00 17.09
H
ATOM 9541 HA ASN E 114 16.648 39.684 -37.045 1.00 18.17
H
ATOM 9542 HB2 ASN E 114 17.402 39.647 -34.345 1.00 24.21
H
ATOM 9543 HB3 ASN E 114 17.255 38.276 -35.136 1.00 24.21
H
ATOM 9544 HD21 ASN E 114 20.631 39.631 -35.114 1.00 29.56
H
ATOM 9545 HD22 ASN E 114 19.624 39.540 -34.019 1.00 29.56
H
ATOM 9546 N MET E 115 14.350 39.596 -34.827 1.00 14.19
N
ATOM 9547 CA MET E 115 13.049 39.018 -34.518 1.00 15.83
C
ATOM 9548 C MET E 115 12.046 39.333 -35.625 1.00 15.36
C
ATOM 9549 O MET E 115 11.231 38.490 -36.006 1.00 14.90
O
ATOM 9550 CB MET E 115 12.536 39.543 -33.179 1.00 17.26
C
ATOM 9551 CG MET E 115 11.267 38.858 -32.708 1.00 23.77
C
ATOM 9552 SD MET E 115 10.596 39.578 -31.197 1.00 35.74

O
ATOM 3253 ND2 ASN B 177 15.140 11.398 -43.072 1.00 42.22
N
ATOM 3254 H ASN B 177 13.967 13.970 -40.959 1.00 38.46
H
ATOM 3255 HA ASN B 177 12.746 14.191 -42.674 1.00 44.99
H
ATOM 3256 HB2 ASN B 177 12.722 11.367 -42.655 1.00 51.90
H
ATOM 3257 HB3 ASN B 177 12.253 12.243 -43.895 1.00 51.90
H
ATOM 3258 HD21 ASN B 177 15.959 11.376 -43.334 1.00 50.66
H
ATOM 3259 HD22 ASN B 177 14.879 10.886 -42.432 1.00 50.66
H
ATOM 3260 N LEU B 178 10.722 13.744 -40.615 1.00 29.94
N
ATOM 3261 CA LEU B 178 9.326 13.905 -40.208 1.00 27.52
C
ATOM 3262 C LEU B 178 8.926 15.373 -40.174 1.00 28.55
C
ATOM 3263 O LEU B 178 7.933 15.769 -40.785 1.00 28.18
O
ATOM 3264 CB LEU B 178 9.082 13.284 -38.831 1.00 25.65
C
ATOM 3265 CG LEU B 178 8.632 11.822 -38.770 1.00 29.25
C
ATOM 3266 CD1 LEU B 178 8.419 11.427 -37.326 1.00 30.04
C
ATOM 3267 CD2 LEU B 178 7.356 11.576 -39.570 1.00 30.40
C
ATOM 3268 H LEU B 178 11.289 13.902 -39.987 1.00 35.93
H
ATOM 3269 HA LEU B 178 8.755 13.452 -40.848 1.00 33.02
H
ATOM 3270 HB2 LEU B 178 9.907 13.346 -38.326 1.00 30.78
H
ATOM 3271 HB3 LEU B 178 8.398 13.808 -38.385 1.00 30.78
H
ATOM 3272 HG LEU B 178 9.331 11.259 -39.137 1.00 35.10
H
ATOM 3273 HD11 LEU B 178 8.134 10.500 -37.292 1.00 36.05
H
ATOM 3274 HD12 LEU B 178 9.253 11.535 -36.844 1.00 36.05
H
ATOM 3275 HD13 LEU B 178 7.736 11.998 -36.940 1.00 36.05
H
ATOM 3276 HD21 LEU B 178 7.115 10.640 -39.499 1.00 36.49
H
ATOM 3277 HD22 LEU B 178 6.646 12.129 -39.209 1.00 36.49
H
ATOM 3278 HD23 LEU B 178 7.517 11.808 -40.498 1.00 36.49
H
ATOM 3279 N LEU B 179 9.706 16.171 -39.449 1.00 24.55
N
ATOM 3280 CA LEU B 179 9.420 17.591 -39.277 1.00 21.87
C
ATOM 3281 C LEU B 179 10.570 18.473 -39.737 1.00 24.32
C
ATOM 3282 O LEU B 179 11.735 18.189 -39.457 1.00 23.82
O
ATOM 3283 CB LEU B 179 9.114 17.896 -37.810 1.00 23.91
C
ATOM 3284 CG LEU B 179 7.814 17.348 -37.224 1.00 22.72
C
ATOM 3285 CD1 LEU B 179 7.760 17.633 -35.726 1.00 20.68
C
ATOM 3286 CD2 LEU B 179 6.602 17.946 -37.927 1.00 23.32
S
ATOM 9553 CE MET E 115 11.976 39.355 -30.071 1.00 45.72
C
ATOM 9554 H MET E 115 14.614 40.195 -34.270 1.00 17.03
H
ATOM 9555 HA MET E 115 13.142 38.056 -34.444 1.00 19.00
H
ATOM 9556 HB2 MET E 115 13.218 39.402 -32.505 1.00 20.71
H
ATOM 9557 HB3 MET E 115 12.348 40.491 -33.265 1.00 20.71
H
ATOM 9558 HG2 MET E 115 10.592 38.933 -33.400 1.00 28.52
H
ATOM 9559 HG3 MET E 115 11.460 37.923 -32.533 1.00 28.52
H
ATOM 9560 HE1 MET E 115 11.735 39.711 -29.202 1.00 54.87
H
ATOM 9561 HE2 MET E 115 12.173 38.408 -29.998 1.00 54.87
H
ATOM 9562 HE3 MET E 115 12.748 39.828 -30.420 1.00 54.87
H
ATOM 9563 N TRP E 116 12.109 40.558 -36.130 1.00 12.48
N
ATOM 9564 CA TRP E 116 11.240 40.990 -37.216 1.00 15.47
C
ATOM 9565 C TRP E 116 11.452 40.113 -38.447 1.00 14.04
C
ATOM 9566 O TRP E 116 10.498 39.712 -39.112 1.00 11.48
O
ATOM 9567 CB TRP E 116 11.515 42.458 -37.544 1.00 12.64
C
ATOM 9568 CG TRP E 116 10.633 43.043 -38.607 1.00 12.35
C
ATOM 9569 CD1 TRP E 116 10.933 43.189 -39.929 1.00 12.04
C
ATOM 9570 CD2 TRP E 116 9.312 43.572 -38.435 1.00 14.43
C
ATOM 9571 NE1 TRP E 116 9.883 43.779 -40.593 1.00 14.64
N
ATOM 9572 CE2 TRP E 116 8.874 44.021 -39.699 1.00 13.81
C
ATOM 9573 CE3 TRP E 116 8.459 43.711 -37.336 1.00 11.41
C
ATOM 9574 CZ2 TRP E 116 7.624 44.603 -39.892 1.00 14.26
C
ATOM 9575 CZ3 TRP E 116 7.216 44.288 -37.531 1.00 15.87
C
ATOM 9576 CH2 TRP E 116 6.811 44.726 -38.799 1.00 14.11
C
ATOM 9577 H TRP E 116 12.653 41.165 -35.857 1.00 14.98
H
ATOM 9578 HA TRP E 116 10.314 40.907 -36.938 1.00 18.56
H
ATOM 9579 HB2 TRP E 116 11.390 42.983 -36.738 1.00 15.17
H
ATOM 9580 HB3 TRP E 116 12.432 42.540 -37.847 1.00 15.17
H
ATOM 9581 HD1 TRP E 116 11.734 42.930 -40.324 1.00 14.44
H
ATOM 9582 HE1 TRP E 116 9.862 43.961 -41.433 1.00 17.57
H
ATOM 9583 HE3 TRP E 116 8.723 43.427 -36.491 1.00 13.69
H
ATOM 9584 HZ2 TRP E 116 7.351 44.891 -40.733 1.00 17.11
H
ATOM 9585 HZ3 TRP E 116 6.639 44.385 -36.808 1.00 19.05
H
ATOM 9586 HH2 TRP E 116 5.967 45.105 -38.901 1.00 16.94

C
ATOM 3287 H LEU B 179 10.416 15.909 -39.041 1.00 29.47
H
ATOM 3288 HA LEU B 179 8.637 17.821 -39.802 1.00 26.24
H
ATOM 3289 HB2 LEU B 179 9.839 17.539 -37.273 1.00 28.70
H
ATOM 3290 HB3 LEU B 179 9.088 18.860 -37.705 1.00 28.70
H
ATOM 3291 HG LEU B 179 7.791 16.387 -37.349 1.00 27.27
H
ATOM 3292 HD11 LEU B 179 6.931 17.280 -35.368 1.00 24.81
H
ATOM 3293 HD12 LEU B 179 8.516 17.203 -35.296 1.00 24.81
H
ATOM 3294 HD13 LEU B 179 7.800 18.592 -35.586 1.00 24.81
H
ATOM 3295 HD21 LEU B 179 5.795 17.579 -37.533 1.00 27.98
H
ATOM 3296 HD22 LEU B 179 6.616 18.910 -37.816 1.00 27.98
H
ATOM 3297 HD23 LEU B 179 6.642 17.721 -38.870 1.00 27.98
H
ATOM 3298 N THR B 180 10.228 19.547 -40.441 1.00 21.44
N
ATOM 3299 CA THR B 180 11.169 20.621 -40.726 1.00 24.48
C
ATOM 3300 C THR B 180 11.150 21.596 -39.556 1.00 24.18
C
ATOM 3301 O THR B 180 10.148 22.277 -39.330 1.00 20.49
O
ATOM 3302 CB THR B 180 10.814 21.367 -42.029 1.00 26.75
C
ATOM 3303 OG1 THR B 180 10.749 20.439 -43.119 1.00 26.99
O
ATOM 3304 CG2 THR B 180 11.848 22.444 -42.342 1.00 29.06
C
ATOM 3305 H THR B 180 9.444 19.678 -40.769 1.00 25.72
H
ATOM 3306 HA THR B 180 12.063 20.256 -40.812 1.00 29.38
H
ATOM 3307 HB THR B 180 9.951 21.798 -41.926 1.00 32.10
H
ATOM 3308 HG1 THR B 180 10.161 19.858 -42.966 1.00 32.39
H
ATOM 3309 HG21 THR B 180 11.611 22.903 -43.163 1.00 34.88
H
ATOM 3310 HG22 THR B 180 11.883 23.090 -41.619 1.00 34.88
H
ATOM 3311 HG23 THR B 180 12.724 22.041 -42.448 1.00 34.88
H
ATOM 3312 N ILE B 181 12.246 21.645 -38.804 1.00 23.05
N
ATOM 3313 CA ILE B 181 12.353 22.540 -37.656 1.00 22.09
C
ATOM 3314 C ILE B 181 12.910 23.895 -38.081 1.00 26.12
C
ATOM 3315 O ILE B 181 13.964 23.972 -38.711 1.00 23.50
O
ATOM 3316 CB ILE B 181 13.251 21.948 -36.557 1.00 23.97
C
ATOM 3317 CG1 ILE B 181 12.745 20.565 -36.131 1.00 23.66
C
ATOM 3318 CG2 ILE B 181 13.312 22.885 -35.356 1.00 22.95
C
ATOM 3319 CD1 ILE B 181 11.326 20.552 -35.592 1.00 28.66
C
ATOM 3320 H ILE B 181 12.947 21.167 -38.940 1.00 27.67
H
ATOM 9587 N LEU E 117 12.714 39.810 -38.725 1.00 13.03
N
ATOM 9588 CA LEU E 117 13.093 39.003 -39.878 1.00 13.36
C
ATOM 9589 C LEU E 117 12.619 37.564 -39.748 1.00 15.88
C
ATOM 9590 O LEU E 117 12.149 36.968 -40.719 1.00 15.15
O
ATOM 9591 CB LEU E 117 14.618 39.027 -40.063 1.00 13.94
C
ATOM 9592 CG LEU E 117 15.204 38.145 -41.175 1.00 15.98
C
ATOM 9593 CD1 LEU E 117 14.745 38.606 -42.552 1.00 16.70
C
ATOM 9594 CD2 LEU E 117 16.725 38.130 -41.103 1.00 24.05
C
ATOM 9595 H LEU E 117 13.384 40.067 -38.251 1.00 15.63
H
ATOM 9596 HA LEU E 117 12.688 39.381 -40.674 1.00 16.03
H
ATOM 9597 HB2 LEU E 117 14.884 39.940 -40.254 1.00 16.73
H
ATOM 9598 HB3 LEU E 117 15.027 38.744 -39.230 1.00 16.73
H
ATOM 9599 HG LEU E 117 14.892 37.235 -41.048 1.00 19.17
H
ATOM 9600 HD11 LEU E 117 15.135 38.026 -43.225 1.00 20.03
H
ATOM 9601 HD12 LEU E 117 13.777 38.559 -42.594 1.00 20.03
H
ATOM 9602 HD13 LEU E 117 15.039 39.520 -42.693 1.00 20.03
H
ATOM 9603 HD21 LEU E 117 17.069 37.567 -41.814 1.00 28.86
H
ATOM 9604 HD22 LEU E 117 17.055 39.036 -41.209 1.00 28.86
H
ATOM 9605 HD23 LEU E 117 16.997 37.777 -40.241 1.00 28.86
H
ATOM 9606 N THR E 118 12.748 37.002 -38.552 1.00 11.16
N
ATOM 9607 CA THR E 118 12.450 35.592 -38.362 1.00 15.63
C
ATOM 9608 C THR E 118 10.994 35.308 -37.997 1.00 15.23
C
ATOM 9609 O THR E 118 10.612 34.141 -37.919 1.00 16.44
O
ATOM 9610 CB THR E 118 13.340 34.974 -37.268 1.00 17.43
C
ATOM 9611 OG1 THR E 118 13.079 35.606 -36.008 1.00 19.94
O
ATOM 9612 CG2 THR E 118 14.807 35.139 -37.623 1.00 21.12
C
ATOM 9613 H THR E 118 13.004 37.412 -37.840 1.00 13.39
H
ATOM 9614 HA THR E 118 12.639 35.124 -39.190 1.00 18.76
H
ATOM 9615 HB THR E 118 13.149 34.026 -37.197 1.00 20.92
H
ATOM 9616 HG1 THR E 118 12.273 35.500 -35.795 1.00 23.93
H
ATOM 9617 HG21 THR E 118 15.362 34.748 -36.930 1.00 25.34
H
ATOM 9618 HG22 THR E 118 14.996 34.697 -38.465 1.00 25.34
H
ATOM 9619 HG23 THR E 118 15.024 36.081 -37.707 1.00 25.34
H
ATOM 9620 N THR E 119 10.183 36.346 -37.781 1.00 13.58

H
ATOM 3321 HA ILE B 181 11.470 22.681 -37.281 1.00 26.51
H
ATOM 3322 HB ILE B 181 14.147 21.849 -36.914 1.00 28.77
H
ATOM 3323 HG12 ILE B 181 12.773 19.974 -36.899 1.00 28.39
H
ATOM 3324 HG13 ILE B 181 13.327 20.223 -35.434 1.00 28.39
H
ATOM 3325 HG21 ILE B 181 13.883 22.492 -34.677 1.00 27.55
H
ATOM 3326 HG22 ILE B 181 13.676 23.738 -35.640 1.00 27.55
H
ATOM 3327 HG23 ILE B 181 12.416 23.008 -35.005 1.00 27.55
H
ATOM 3328 HD11 ILE B 181 11.089 19.643 -35.348 1.00 34.39
H
ATOM 3329 HD12 ILE B 181 11.279 21.126 -34.812 1.00 34.39
H
ATOM 3330 HD13 ILE B 181 10.724 20.877 -36.279 1.00 34.39
H
ATOM 3331 N ILE B 182 12.203 24.958 -37.706 1.00 23.73
N
ATOM 3332 CA ILE B 182 12.514 26.304 -38.171 1.00 20.26
C
ATOM 3333 C ILE B 182 12.680 27.254 -36.992 1.00 23.35
C
ATOM 3334 O ILE B 182 11.782 27.378 -36.163 1.00 18.77
O
ATOM 3335 CB ILE B 182 11.400 26.838 -39.101 1.00 21.54
C
ATOM 3336 CG1 ILE B 182 11.154 25.858 -40.255 1.00 22.95
C
ATOM 3337 CG2 ILE B 182 11.751 28.230 -39.631 1.00 20.67
C
ATOM 3338 CD1 ILE B 182 9.889 26.137 -41.035 1.00 27.62
C
ATOM 3339 H ILE B 182 11.528 24.923 -37.174 1.00 28.48
H
ATOM 3340 HA ILE B 182 13.346 26.287 -38.669 1.00 24.31
H
ATOM 3341 HB ILE B 182 10.582 26.908 -38.585 1.00 25.85
H
ATOM 3342 HG12 ILE B 182 11.900 25.909 -40.873 1.00 27.54
H
ATOM 3343 HG13 ILE B 182 11.087 24.960 -39.894 1.00 27.54
H
ATOM 3344 HG21 ILE B 182 11.036 28.537 -40.210 1.00 24.80
H
ATOM 3345 HG22 ILE B 182 11.854 28.836 -38.881 1.00 24.80
H
ATOM 3346 HG23 ILE B 182 12.581 28.177 -40.130 1.00 24.80
H
ATOM 3347 HD11 ILE B 182 9.803 25.480 -41.743 1.00 33.14
H
ATOM 3348 HD12 ILE B 182 9.129 26.078 -40.435 1.00 33.14
H
ATOM 3349 HD13 ILE B 182 9.942 27.028 -41.415 1.00 33.14
H
ATOM 3350 N GLU B 183 13.821 27.934 -36.916 1.00 24.54
N
ATOM 3351 CA GLU B 183 14.022 28.911 -35.854 1.00 27.28
C
ATOM 3352 C GLU B 183 13.140 30.122 -36.128 1.00 29.16
C
ATOM 3353 O GLU B 183 13.045 30.599 -37.260 1.00 34.53
O
ATOM 3354 CB GLU B 183 15.494 29.314 -35.730 1.00 36.17
N
ATOM 9621 CA THR E 119 8.800 36.131 -37.326 1.00 12.81
C
ATOM 9622 C THR E 119 7.709 36.798 -38.158 1.00 15.49 C
ATOM 9623 O THR E 119 6.530 36.502 -37.968 1.00 14.16 O
ATOM 9624 CB THR E 119 8.595 36.627 -35.875 1.00 12.82
C
ATOM 9625 OG1 THR E 119 8.665 38.059 -35.835 1.00 12.89
O
ATOM 9626 CG2 THR E 119 9.626 36.020 -34.943 1.00 17.46
C
ATOM 9627 H THR E 119 10.401 37.171 -37.886 1.00 16.30
H
ATOM 9628 HA THR E 119 8.624 35.177 -37.333 1.00 15.37
H
ATOM 9629 HB THR E 119 7.717 36.348 -35.570 1.00 15.38
H
ATOM 9630 HG1 THR E 119 9.416 38.318 -36.110 1.00 15.47
H
ATOM 9631 HG21 THR E 119 9.484 36.341 -34.038 1.00 20.95
H
ATOM 9632 HG22 THR E 119 9.551 35.053 -34.950 1.00 20.95
H
ATOM 9633 HG23 THR E 119 10.518 36.270 -35.229 1.00 20.95
H
ATOM 9634 N SER E 120 8.075 37.705 -39.056 1.00 11.68 N
ATOM 9635 CA SER E 120 7.067 38.444 -39.814 1.00 15.43
C
ATOM 9636 C SER E 120 6.196 37.531 -40.684 1.00 12.04 C
ATOM 9637 O SER E 120 4.966 37.593 -40.619 1.00 10.68 O
ATOM 9638 CB SER E 120 7.737 39.510 -40.682 1.00 14.31
C
ATOM 9639 OG SER E 120 8.074 40.644 -39.901 1.00 13.97
O
ATOM 9640 H SER E 120 8.888 37.911 -39.244 1.00 14.01 H
ATOM 9641 HA SER E 120 6.482 38.899 -39.189 1.00 18.51
H
ATOM 9642 HB2 SER E 120 8.546 39.140 -41.070 1.00 17.18
H
ATOM 9643 HB3 SER E 120 7.124 39.778 -41.384 1.00 17.18
H
ATOM 9644 HG SER E 120 8.604 40.424 -39.288 1.00 16.76
H
ATOM 9645 N GLU E 121 6.827 36.691 -41.502 1.00 13.53 N
ATOM 9646 CA GLU E 121 6.080 35.770 -42.357 1.00 16.10
C
ATOM 9647 C GLU E 121 5.202 34.861 -41.501 1.00 14.09 C
ATOM 9648 O GLU E 121 4.025 34.658 -41.788 1.00 14.66 O
ATOM 9649 CB GLU E 121 7.030 34.933 -43.222 1.00 18.39
C
ATOM 9650 CG GLU E 121 6.315 34.029 -44.220 1.00 17.83
C
ATOM 9651 CD GLU E 121 7.270 33.236 -45.097 1.00 26.57
C
ATOM 9652 OE1 GLU E 121 8.499 33.395 -44.946 1.00 29.79
O
ATOM 9653 OE2 GLU E 121 6.786 32.450 -45.940 1.00 28.08
O1-
ATOM 9654 H GLU E 121 7.681 36.635 -41.580 1.00 16.24 H

C
ATOM 3355 CG GLU B 183 16.063 30.065 -36.915 1.00 45.13
C
ATOM 3356 CD GLU B 183 17.553 30.328 -36.767 1.00 52.61
C
ATOM 3357 OE1 GLU B 183 18.036 30.396 -35.616 1.00 55.37
O
ATOM 3358 OE2 GLU B 183 18.243 30.456 -37.800 1.00 57.38
O1-
ATOM 3359 H GLU B 183 14.482 27.851 -37.459 1.00 29.44
H
ATOM 3360 HA GLU B 183 13.745 28.522 -35.010 1.00 32.74
H
ATOM 3361 HB2 GLU B 183 15.592 29.882 -34.950 1.00 43.40
H
ATOM 3362 HB3 GLU B 183 16.024 28.510 -35.613 1.00 43.40
H
ATOM 3363 HG2 GLU B 183 15.927 29.540 -37.719 1.00 54.15
H
ATOM 3364 HG3 GLU B 183 15.612 30.920 -36.995 1.00 54.15
H
ATOM 3365 N MET B 184 12.478 30.594 -35.080 1.00 29.01
N
ATOM 3366 CA MET B 184 11.478 31.648 -35.192 1.00 25.24
C
ATOM 3367 C MET B 184 11.643 32.571 -33.986 1.00 34.39
C
ATOM 3368 O MET B 184 11.916 33.764 -34.133 1.00 34.16
O
ATOM 3369 CB MET B 184 10.075 31.032 -35.263 1.00 25.23
C
ATOM 3370 CG MET B 184 8.947 31.974 -35.675 1.00 22.62
C
ATOM 3371 SD MET B 184 8.098 32.757 -34.293 1.00 34.48
S
ATOM 3372 CE MET B 184 7.450 31.341 -33.400 1.00 28.01
C
ATOM 3373 H MET B 184 12.592 30.314 -34.275 1.00 34.81
H
ATOM 3374 HA MET B 184 11.631 32.152 -36.006 1.00 30.28
H
ATOM 3375 HB2 MET B 184 10.093 30.305 -35.905 1.00 30.28
H
ATOM 3376 HB3 MET B 184 9.852 30.681 -34.386 1.00 30.28
H
ATOM 3377 HG2 MET B 184 9.317 32.677 -36.231 1.00 27.15
H
ATOM 3378 HG3 MET B 184 8.289 31.470 -36.179 1.00 27.15
H
ATOM 3379 HE1 MET B 184 6.964 31.655 -32.621 1.00 33.61
H
ATOM 3380 HE2 MET B 184 6.855 30.845 -33.984 1.00 33.61
H
ATOM 3381 HE3 MET B 184 8.189 30.777 -33.124 1.00 33.61
H
ATOM 3382 N GLN B 185 11.505 31.998 -32.794 1.00 32.90
N
ATOM 3383 CA GLN B 185 11.808 32.696 -31.549 1.00 32.39
C
ATOM 3384 C GLN B 185 12.769 31.850 -30.723 1.00 34.72
C
ATOM 3385 O GLN B 185 12.721 30.619 -30.769 1.00 28.22
O
ATOM 3386 CB GLN B 185 10.531 32.976 -30.754 1.00 29.62
C
ATOM 3387 CG GLN B 185 9.601 34.000 -31.390 1.00 33.22
C
ATOM 3388 CD GLN B 185 9.964 35.435 -31.046 1.00 40.19

ATOM 9655 HA GLU E 121 5.503 36.279 -42.947 1.00 19.32
H
ATOM 9656 HB2 GLU E 121 7.606 35.532 -43.723 1.00 22.07
H
ATOM 9657 HB3 GLU E 121 7.566 34.370 -42.642 1.00 22.07
H
ATOM 9658 HG2 GLU E 121 5.761 33.399 -43.734 1.00 21.40
H
ATOM 9659 HG3 GLU E 121 5.762 34.576 -44.800 1.00 21.40
H

ATOM 9660 N PHE E 122 5.798 34.331 -40.439 1.00 13.77 N
ATOM 9661 CA PHE E 122 5.101 33.510 -39.458 1.00 14.62
C

ATOM 9662 C PHE E 122 3.851 34.212 -38.924 1.00 14.41 C

ATOM 9663 O PHE E 122 2.760 33.641 -38.928 1.00 13.91 O
ATOM 9664 CB PHE E 122 6.072 33.171 -38.319 1.00 16.68
C
ATOM 9665 CG PHE E 122 5.445 32.476 -37.144 1.00 16.24
C
ATOM 9666 CD1 PHE E 122 5.386 31.093 -37.091 1.00 19.07
C
ATOM 9667 CD2 PHE E 122 4.959 33.204 -36.070 1.00 17.52
C
ATOM 9668 CE1 PHE E 122 4.830 30.451 -36.003 1.00 20.81
C
ATOM 9669 CE2 PHE E 122 4.398 32.568 -34.980 1.00 21.23
C
ATOM 9670 CZ PHE E 122 4.337 31.189 -34.944 1.00 22.10
C

ATOM 9671 H PHE E 122 6.633 34.438 -40.261 1.00 16.53 H
ATOM 9672 HA PHE E 122 4.825 32.680 -39.877 1.00 17.54
H
ATOM 9673 HB2 PHE E 122 6.766 32.589 -38.667 1.00 20.02
H
ATOM 9674 HB3 PHE E 122 6.469 33.994 -37.995 1.00 20.02
H
ATOM 9675 HD1 PHE E 122 5.717 30.591 -37.801 1.00 22.89
H
ATOM 9676 HD2 PHE E 122 4.998 34.133 -36.089 1.00 21.02
H
ATOM 9677 HE1 PHE E 122 4.787 29.522 -35.983 1.00 24.98
H
ATOM 9678 HE2 PHE E 122 4.067 33.068 -34.268 1.00 25.48
H
ATOM 9679 HZ PHE E 122 3.959 30.758 -34.211 1.00 26.52
H

ATOM 9680 N ARG E 123 4.008 35.459 -38.491 1.00 9.96 N
ATOM 9681 CA ARG E 123 2.915 36.190 -37.862 1.00 12.21
C

ATOM 9682 C ARG E 123 1.821 36.555 -38.871 1.00 13.20 C
ATOM 9683 O ARG E 123 0.660 36.720 -38.501 1.00 16.26
O
ATOM 9684 CB ARG E 123 3.461 37.442 -37.164 1.00 13.63
C
ATOM 9685 CG ARG E 123 4.080 37.153 -35.797 1.00 14.82
C
ATOM 9686 CD ARG E 123 5.182 38.138 -35.440 1.00 19.31
C
ATOM 9687 NE ARG E 123 4.809 39.485 -35.833 1.00 25.00
N
ATOM 9688 CZ ARG E 123 5.551 40.304 -36.569 1.00 13.96

C
ATOM 3389 OE1 GLN B 185 11.094 35.730 -30.652 1.00 41.44
O
ATOM 3390 NE2 GLN B 185 8.997 36.337 -31.188 1.00 34.22
N
ATOM 3391 H GLN B 185 11.232 31.190 -32.679 1.00 39.48
H
ATOM 3392 HA GLN B 185 12.237 33.542 -31.749 1.00 38.87
H
ATOM 3393 HB2 GLN B 185 10.036 32.148 -30.659 1.00 35.55
H
ATOM 3394 HB3 GLN B 185 10.779 33.310 -29.877 1.00 35.55
H
ATOM 3395 HG2 GLN B 185 9.641 33.905 -32.355 1.00 39.87
H
ATOM 3396 HG3 GLN B 185 8.696 33.839 -31.080 1.00 39.87
H
ATOM 3397 HE21 GLN B 185 9.150 37.164 -31.007 1.00 41.06
H
ATOM 3398 HE22 GLN B 185 8.218 36.094 -31.461 1.00 41.06
H
ATOM 3399 N LYS B 186 13.654 32.506 -29.980 1.00 34.85
N
ATOM 3400 CA LYS B 186 14.542 31.796 -29.071 1.00 34.85
C
ATOM 3401 C LYS B 186 13.694 31.086 -28.016 1.00 28.04
C
ATOM 3402 O LYS B 186 12.924 31.726 -27.301 1.00 27.27
O
ATOM 3403 CB LYS B 186 15.533 32.763 -28.418 1.00 43.85
C
ATOM 3404 CG LYS B 186 16.859 32.136 -28.014 1.00 64.98
C
ATOM 3405 CD LYS B 186 17.666 31.694 -29.229 1.00 85.87
C
ATOM 3406 CE LYS B 186 19.083 31.299 -28.845 1.00104.79
C
ATOM 3407 NZ LYS B 186 19.756 30.516 -29.918 1.00110.38
N1+
ATOM 3408 H LYS B 186 13.758 33.359 -29.984 1.00 41.82
H
ATOM 3409 HA LYS B 186 15.043 31.127 -29.563 1.00 41.82
H
ATOM 3410 HB2 LYS B 186 15.725 33.478 -29.044 1.00 52.62
H
ATOM 3411 HB3 LYS B 186 15.125 33.130 -27.618 1.00 52.62
H
ATOM 3412 HG2 LYS B 186 17.383 32.788 -27.523 1.00 77.98
H
ATOM 3413 HG3 LYS B 186 16.690 31.357 -27.462 1.00 77.98
H
ATOM 3414 HD2 LYS B 186 17.236 30.925 -29.635 1.00103.05
H
ATOM 3415 HD3 LYS B 186 17.716 32.425 -29.864 1.00103.05
H
ATOM 3416 HE2 LYS B 186 19.604 32.101 -28.684 1.00125.75
H
ATOM 3417 HE3 LYS B 186 19.055 30.753 -28.044 1.00125.75
H
ATOM 3418 HZ1 LYS B 186 19.799 30.999 -30.664 1.00132.46
H
ATOM 3419 HZ2 LYS B 186 20.581 30.301 -29.664 1.00132.46
H
ATOM 3420 HZ3 LYS B 186 19.300 29.770 -30.081 1.00132.46
H
ATOM 3421 N GLY B 187 13.816 29.765 -27.932 1.00 25.29
N
ATOM 3422 CA GLY B 187 13.002 28.997 -27.007 1.00 25.76
C
ATOM 9689 NH1 ARG E 123 6.763 39.963 -36.994 1.00 17.77
N1+
ATOM 9690 NH2 ARG E 123 5.076 41.500 -36.857 1.00 20.81
N

ATOM 9691 H ARG E 123 4.741 35.905 -38.551 1.00 11.95 H
ATOM 9692 HA ARG E 123 2.513 35.625 -37.183 1.00 14.65
H
ATOM 9693 HB2 ARG E 123 4.147 37.839 -37.724 1.00 16.36
H
ATOM 9694 HB3 ARG E 123 2.735 38.072 -37.035 1.00 16.36
H
ATOM 9695 HG2 ARG E 123 3.391 37.212 -35.117 1.00 17.78
H
ATOM 9696 HG3 ARG E 123 4.464 36.262 -35.805 1.00 17.78
H
ATOM 9697 HD2 ARG E 123 5.326 38.127 -34.481 1.00 23.17
H
ATOM 9698 HD3 ARG E 123 5.996 37.896 -35.908 1.00 23.17
H
ATOM 9699 HE ARG E 123 4.045 39.776 -35.567 1.00 30.00
H
ATOM 9700 HH11 ARG E 123 7.080 39.185 -36.811 1.00 21.33
H
ATOM 9701 HH12 ARG E 123 7.225 40.516 -37.464 1.00 21.33
H
ATOM 9702 HH21 ARG E 123 4.296 41.732 -36.579 1.00 24.98
H
ATOM 9703 HH22 ARG E 123 5.547 42.049 -37.323 1.00 24.98
H

ATOM 9704 N LEU E 124 2.184 36.657 -40.146 1.00 11.77 N
ATOM 9705 CA LEU E 124 1.207 36.917 -41.200 1.00 12.92
C

ATOM 9706 C LEU E 124 0.445 35.654 -41.598 1.00 14.87 C

ATOM 9707 O LEU E 124 -0.771 35.691 -41.805 1.00 14.46 O
ATOM 9708 CB LEU E 124 1.890 37.508 -42.437 1.00 14.80
C
ATOM 9709 CG LEU E 124 1.021 37.592 -43.700 1.00 11.83
C
ATOM 9710 CD1 LEU E 124 -0.216 38.439 -43.460 1.00 15.58
C
ATOM 9711 CD2 LEU E 124 1.822 38.135 -44.871 1.00 14.19
C

ATOM 9712 H LEU E 124 2.993 36.579 -40.429 1.00 14.12 H
ATOM 9713 HA LEU E 124 0.561 37.565 -40.877 1.00 15.50
H
ATOM 9714 HB2 LEU E 124 2.182 38.408 -42.225 1.00 17.76
H
ATOM 9715 HB3 LEU E 124 2.661 36.961 -42.652 1.00 17.76
H
ATOM 9716 HG LEU E 124 0.725 36.698 -43.934 1.00 14.19
H
ATOM 9717 HD11 LEU E 124 -0.740 38.470 -44.276 1.00 18.69
H
ATOM 9718 HD12 LEU E 124 -0.738 38.040 -42.746 1.00 18.69
H
ATOM 9719 HD13 LEU E 124 0.059 39.335 -43.209 1.00 18.69
H
ATOM 9720 HD21 LEU E 124 1.250 38.177 -45.652 1.00 17.03
H
ATOM 9721 HD22 LEU E 124 2.144 39.022 -44.648 1.00 17.03
H
ATOM 9722 HD23 LEU E 124 2.572 37.544 -45.041 1.00 17.03

```
C
ATOM   3423  C   GLY B 187      13.264  27.506 -27.086  1.00 23.48
C
ATOM   3424  O   GLY B 187      14.020  27.050 -27.944  1.00 19.67
O
ATOM   3425  H   GLY B 187      14.362  29.294 -28.400  1.00 30.35
H
ATOM   3426  HA2 GLY B 187      13.181  29.291 -26.101  1.00 30.91
H
ATOM   3427  HA3 GLY B 187      12.064  29.152 -27.200  1.00 30.91
H
ATOM   3428  N   ASP B 188      12.629  26.752 -26.190  1.00 17.61
N
ATOM   3429  CA  ASP B 188      12.873  25.316 -26.064  1.00 20.10
C
ATOM   3430  C   ASP B 188      11.623  24.472 -26.317  1.00 17.87
C
ATOM   3431  O   ASP B 188      11.587  23.291 -25.973  1.00 18.91
O
ATOM   3432  CB  ASP B 188      13.420  25.000 -24.673  1.00 22.84
C
ATOM   3433  CG  ASP B 188      14.737  25.686 -24.393  1.00 27.00
C
ATOM   3434  OD1 ASP B 188      15.629  25.638 -25.265  1.00 28.51
O
ATOM   3435  OD2 ASP B 188      14.877  26.274 -23.300  1.00 29.60
O1-
ATOM   3436  H   ASP B 188      12.044  27.053 -25.637  1.00 21.13
H
ATOM   3437  HA  ASP B 188      13.544  25.055 -26.714  1.00 24.12
H
ATOM   3438  HB2 ASP B 188      12.780  25.296 -24.007  1.00 27.41
H
ATOM   3439  HB3 ASP B 188      13.559  24.043 -24.598  1.00 27.41
H
ATOM   3440  N   CYS B 189      10.597  25.079 -26.901  1.00 15.55
N
ATOM   3441  CA  CYS B 189       9.399  24.344 -27.293  1.00 18.29
C
ATOM   3442  C   CYS B 189       9.129  24.575 -28.777  1.00 18.34
C
ATOM   3443  O   CYS B 189       9.771  25.421 -29.403  1.00 16.24
O
ATOM   3444  CB  CYS B 189       8.202  24.763 -26.437  1.00 21.42
C
ATOM   3445  SG  CYS B 189       8.369  24.310 -24.685  1.00 19.88
S
ATOM   3446  H   CYS B 189      10.568  25.919 -27.083  1.00 18.66
H
ATOM   3447  HA  CYS B 189       9.549  23.395 -27.158  1.00 21.95
H
ATOM   3448  HB2 CYS B 189       8.103  25.726 -26.487  1.00 25.71
H
ATOM   3449  HB3 CYS B 189       7.404  24.331 -26.781  1.00 25.71
H
ATOM   3450  N   ALA B 190       8.195  23.813 -29.337  1.00 17.84
N
ATOM   3451  CA  ALA B 190       7.935  23.856 -30.773  1.00 16.98
C
ATOM   3452  C   ALA B 190       6.443  23.850 -31.098  1.00 13.84
C
ATOM   3453  O   ALA B 190       5.680  23.040 -30.566  1.00 13.74
O
ATOM   3454  CB  ALA B 190       8.622  22.686 -31.461  1.00 18.20
C
ATOM   3455  H   ALA B 190       7.697  23.260 -28.907  1.00 21.40
H
ATOM   3456  HA  ALA B 190       8.312  24.674 -31.133  1.00 20.37
H

ATOM   9723  N   LYS E 125       1.158  34.538 -41.705  1.00 13.01      N
ATOM   9724  CA  LYS E 125       0.593  33.347 -42.336  1.00 15.82
C

ATOM   9725  C   LYS E 125      -0.148  32.421 -41.379  1.00 17.64      C

ATOM   9726  O   LYS E 125      -0.543  31.320 -41.758  1.00 13.71      O
ATOM   9727  CB  LYS E 125       1.698  32.572 -43.050  1.00 13.96
C
ATOM   9728  CG  LYS E 125       2.202  33.285 -44.298  1.00 20.01
C
ATOM   9729  CD  LYS E 125       3.130  32.408 -45.114  1.00 23.78
C
ATOM   9730  CE  LYS E 125       3.436  33.035 -46.467  1.00 22.29
C
ATOM   9731  NZ  LYS E 125       4.222  32.110 -47.321  1.00 26.85
N1+

ATOM   9732  H   LYS E 125       1.965  34.443 -41.424  1.00 15.61      H
ATOM   9733  HA  LYS E 125      -0.043  33.633 -43.010  1.00 18.98
H
ATOM   9734  HB2 LYS E 125       2.448  32.461 -42.444  1.00 16.76
H
ATOM   9735  HB3 LYS E 125       1.355  31.705 -43.317  1.00 16.76
H
ATOM   9736  HG2 LYS E 125       1.446  33.526 -44.855  1.00 24.01
H
ATOM   9737  HG3 LYS E 125       2.691  34.080 -44.035  1.00 24.01
H
ATOM   9738  HD2 LYS E 125       3.965  32.292 -44.635  1.00 28.53
H
ATOM   9739  HD3 LYS E 125       2.707  31.548 -45.265  1.00 28.53
H
ATOM   9740  HE2 LYS E 125       2.604  33.238 -46.922  1.00 26.74
H
ATOM   9741  HE3 LYS E 125       3.955  33.844 -46.335  1.00 26.74
H
ATOM   9742  HZ1 LYS E 125       4.392  32.492 -48.106  1.00 32.22
H
ATOM   9743  HZ2 LYS E 125       4.993  31.910 -46.923  1.00 32.22
H
ATOM   9744  HZ3 LYS E 125       3.764  31.359 -47.457  1.00 32.22
H

ATOM   9745  N   LYS E 126      -0.352  32.867 -40.145  1.00 15.49      N
ATOM   9746  CA  LYS E 126      -1.062  32.056 -39.168  1.00 14.17
C

ATOM   9747  C   LYS E 126      -2.423  31.628 -39.718  1.00 14.30      C

ATOM   9748  O   LYS E 126      -2.765  30.447 -39.682  1.00 14.19      O
ATOM   9749  CB  LYS E 126      -1.230  32.826 -37.862  1.00 13.34
C
ATOM   9750  CG  LYS E 126      -1.750  31.990 -36.705  1.00 16.84
C
ATOM   9751  CD  LYS E 126      -1.636  32.761 -35.400  1.00 20.30
C
ATOM   9752  CE  LYS E 126      -2.149  31.960 -34.218  1.00 23.97
C
ATOM   9753  NZ  LYS E 126      -1.883  32.674 -32.933  1.00 26.21
N1+

ATOM   9754  H   LYS E 126      -0.091  33.632 -39.851  1.00 18.59      H
ATOM   9755  HA  LYS E 126      -0.546  31.257 -38.983  1.00 17.00
H
ATOM   9756  HB2 LYS E 126      -0.368  33.187 -37.601  1.00 16.00
```

H
ATOM 3457 HB1 ALA B 190 8.440 22.729 -32.413 1.00 21.84
H
ATOM 3458 HB2 ALA B 190 9.577 22.744 -31.303 1.00 21.84
H
ATOM 3459 HB3 ALA B 190 8.275 21.858 -31.094 1.00 21.84
H
ATOM 3460 N LEU B 191 6.047 24.763 -31.982 1.00 11.45
N
ATOM 3461 CA LEU B 191 4.680 24.829 -32.492 1.00 14.13
C
ATOM 3462 C LEU B 191 4.554 23.994 -33.749 1.00 16.78
C
ATOM 3463 O LEU B 191 5.395 24.100 -34.642 1.00 15.41
O
ATOM 3464 CB LEU B 191 4.288 26.269 -32.817 1.00 12.09
C
ATOM 3465 CG LEU B 191 4.165 27.255 -31.659 1.00 14.17
C
ATOM 3466 CD1 LEU B 191 4.052 28.666 -32.203 1.00 14.01
C
ATOM 3467 CD2 LEU B 191 2.958 26.915 -30.798 1.00 16.56
C
ATOM 3468 H LEU B 191 6.564 25.368 -32.309 1.00 13.74
H
ATOM 3469 HA LEU B 191 4.066 24.482 -31.825 1.00 16.96
H
ATOM 3470 HB2 LEU B 191 4.953 26.629 -33.424 1.00 14.51
H
ATOM 3471 HB3 LEU B 191 3.428 26.250 -33.264 1.00 14.51
H
ATOM 3472 HG LEU B 191 4.959 27.203 -31.105 1.00 17.01
H
ATOM 3473 HD11 LEU B 191 3.974 29.285 -31.461 1.00 16.81
H
ATOM 3474 HD12 LEU B 191 4.847 28.868 -32.721 1.00 16.81
H
ATOM 3475 HD13 LEU B 191 3.265 28.724 -32.768 1.00 16.81
H
ATOM 3476 HD21 LEU B 191 2.900 27.553 -30.070 1.00 19.87
H
ATOM 3477 HD22 LEU B 191 2.158 26.962 -31.345 1.00 19.87
H
ATOM 3478 HD23 LEU B 191 3.065 26.018 -30.445 1.00 19.87
H
ATOM 3479 N TYR B 192 3.513 23.172 -33.834 1.00 16.15
N
ATOM 3480 CA TYR B 192 3.244 22.485 -35.084 1.00 12.87
C
ATOM 3481 C TYR B 192 2.607 23.440 -36.076 1.00 18.63
C
ATOM 3482 O TYR B 192 1.704 24.209 -35.732 1.00 14.22
O
ATOM 3483 CB TYR B 192 2.322 21.279 -34.921 1.00 17.45
C
ATOM 3484 CG TYR B 192 2.041 20.673 -36.280 1.00 18.09
C
ATOM 3485 CD1 TYR B 192 2.958 19.818 -36.876 1.00 18.30
C
ATOM 3486 CD2 TYR B 192 0.901 21.013 -36.997 1.00 15.77
C
ATOM 3487 CE1 TYR B 192 2.731 19.287 -38.131 1.00 17.41
C
ATOM 3488 CE2 TYR B 192 0.666 20.487 -38.257 1.00 19.17
C
ATOM 3489 CZ TYR B 192 1.586 19.625 -38.819 1.00 19.87
C
ATOM 3490 OH TYR B 192 1.361 19.098 -40.072 1.00 20.58
H
ATOM 9757 HB3 LYS E 126 -1.858 33.551 -38.007 1.00 16.00
H
ATOM 9758 HG2 LYS E 126 -2.684 31.775 -36.855 1.00 20.21
H
ATOM 9759 HG3 LYS E 126 -1.223 31.179 -36.630 1.00 20.21
H
ATOM 9760 HD2 LYS E 126 -0.704 32.977 -35.238 1.00 24.36
H
ATOM 9761 HD3 LYS E 126 -2.161 33.575 -35.464 1.00 24.36
H
ATOM 9762 HE2 LYS E 126 -3.106 31.835 -34.305 1.00 28.76
H
ATOM 9763 HE3 LYS E 126 -1.697 31.103 -34.190 1.00 28.76
H
ATOM 9764 HZ1 LYS E 126 -1.008 32.800 -32.830 1.00 31.45
H
ATOM 9765 HZ2 LYS E 126 -2.290 33.466 -32.935 1.00 31.45
H
ATOM 9766 HZ3 LYS E 126 -2.188 32.193 -32.249 1.00 31.45
H

ATOM 9767 N TRP E 127 -3.177 32.587 -40.254 1.00 13.47 N
ATOM 9768 CA TRP E 127 -4.497 32.314 -40.828 1.00 13.36
C

ATOM 9769 C TRP E 127 -4.575 32.682 -42.311 1.00 14.64 C

ATOM 9770 O TRP E 127 -5.632 32.557 -42.929 1.00 13.48 O
ATOM 9771 CB TRP E 127 -5.573 33.078 -40.053 1.00 13.26
C
ATOM 9772 CG TRP E 127 -5.758 32.580 -38.653 1.00 16.00
C
ATOM 9773 CD1 TRP E 127 -5.306 33.163 -37.508 1.00 16.46
C
ATOM 9774 CD2 TRP E 127 -6.437 31.386 -38.256 1.00 14.01
C
ATOM 9775 NE1 TRP E 127 -5.666 32.408 -36.419 1.00 20.27
N
ATOM 9776 CE2 TRP E 127 -6.365 31.312 -36.851 1.00 19.93
C
ATOM 9777 CE3 TRP E 127 -7.108 30.374 -38.951 1.00 20.52
C
ATOM 9778 CZ2 TRP E 127 -6.931 30.266 -36.129 1.00 17.91
C
ATOM 9779 CZ3 TRP E 127 -7.672 29.339 -38.232 1.00 22.57
C
ATOM 9780 CH2 TRP E 127 -7.579 29.291 -36.835 1.00 25.03
C

ATOM 9781 H TRP E 127 -2.944 33.413 -40.298 1.00 16.16 H
ATOM 9782 HA TRP E 127 -4.686 31.367 -40.745 1.00 16.03
H
ATOM 9783 HB2 TRP E 127 -5.322 34.014 -40.006 1.00 15.92
H
ATOM 9784 HB3 TRP E 127 -6.420 32.986 -40.517 1.00 15.92
H
ATOM 9785 HD1 TRP E 127 -4.823 33.957 -37.470 1.00 19.75
H
ATOM 9786 HE1 TRP E 127 -5.484 32.594 -35.599 1.00 24.32
H
ATOM 9787 HE3 TRP E 127 -7.174 30.400 -39.878 1.00 24.62
H
ATOM 9788 HZ2 TRP E 127 -6.873 30.232 -35.201 1.00 21.50
H
ATOM 9789 HZ3 TRP E 127 -8.119 28.660 -38.684 1.00 27.09
H
ATOM 9790 HH2 TRP E 127 -7.969 28.581 -36.378 1.00 30.03

O
ATOM 3491 H TYR B 192 2.962 22.999 -33.197 1.00 19.37
H
ATOM 3492 HA TYR B 192 4.082 22.174 -35.461 1.00 15.44
H
ATOM 3493 HB2 TYR B 192 2.753 20.611 -34.366 1.00 20.94
H
ATOM 3494 HB3 TYR B 192 1.482 21.561 -34.527 1.00 20.94
H
ATOM 3495 HD1 TYR B 192 3.734 19.589 -36.417 1.00 21.96
H
ATOM 3496 HD2 TYR B 192 0.281 21.595 -36.621 1.00 18.92
H
ATOM 3497 HE1 TYR B 192 3.351 18.706 -38.512 1.00 20.89
H
ATOM 3498 HE2 TYR B 192 -0.107 20.714 -38.722 1.00 23.00
H
ATOM 3499 HH TYR B 192 0.633 19.384 -40.377 1.00 24.69
H
ATOM 3500 N ALA B 193 3.077 23.360 -37.315 1.00 12.79
N
ATOM 3501 CA ALA B 193 2.483 24.079 -38.431 1.00 15.94
C
ATOM 3502 C ALA B 193 2.550 23.173 -39.650 1.00 18.77
C
ATOM 3503 O ALA B 193 3.498 22.402 -39.801 1.00 16.34
O
ATOM 3504 CB ALA B 193 3.211 25.385 -38.685 1.00 17.09
C
ATOM 3505 H ALA B 193 3.756 22.883 -37.538 1.00 15.35
H
ATOM 3506 HA ALA B 193 1.553 24.274 -38.238 1.00 19.13
H
ATOM 3507 HB1 ALA B 193 2.792 25.839 -39.433 1.00 20.50
H
ATOM 3508 HB2 ALA B 193 3.156 25.937 -37.890 1.00 20.50
H
ATOM 3509 HB3 ALA B 193 4.139 25.194 -38.892 1.00 20.50
H
ATOM 3510 N SER B 194 1.543 23.243 -40.509 1.00 15.79
N
ATOM 3511 CA SER B 194 1.535 22.414 -41.708 1.00 21.22
C
ATOM 3512 C SER B 194 2.354 23.092 -42.803 1.00 20.82
C
ATOM 3513 O SER B 194 2.449 24.317 -42.813 1.00 23.78
O
ATOM 3514 CB SER B 194 0.109 22.172 -42.191 1.00 20.14
C
ATOM 3515 OG SER B 194 -0.410 23.338 -42.795 1.00 26.86
O
ATOM 3516 H SER B 194 0.859 23.757 -40.424 1.00 18.95
H
ATOM 3517 HA SER B 194 1.941 21.555 -41.509 1.00 25.47
H
ATOM 3518 HB2 SER B 194 0.113 21.453 -42.842 1.00 24.17
H
ATOM 3519 HB3 SER B 194 -0.446 21.933 -41.433 1.00 24.17
H
ATOM 3520 HG SER B 194 -0.416 23.970 -42.241 1.00 32.23
H
ATOM 3521 N SER B 195 2.948 22.328 -43.720 1.00 22.26
N
ATOM 3522 CA SER B 195 2.901 20.869 -43.738 1.00 19.41
C
ATOM 3523 C SER B 195 4.097 20.267 -42.993 1.00 26.14
C
ATOM 3524 O SER B 195 5.234 20.349 -43.461 1.00 25.77
H
ATOM 9791 N PHE E 128 -3.452 33.118 -42.876 1.00 13.43 N
ATOM 9792 CA PHE E 128 -3.425 33.694 -44.221 1.00 12.84
C
ATOM 9793 C PHE E 128 -2.168 33.275 -44.986 1.00 14.69 C
ATOM 9794 O PHE E 128 -1.174 33.999 -44.999 1.00 14.50
O
ATOM 9795 CB PHE E 128 -3.509 35.223 -44.122 1.00 15.03
C
ATOM 9796 CG PHE E 128 -3.640 35.922 -45.446 1.00 15.62
C
ATOM 9797 CD1 PHE E 128 -4.757 35.729 -46.242 1.00 14.48
C
ATOM 9798 CD2 PHE E 128 -2.660 36.800 -45.879 1.00 17.09
C
ATOM 9799 CE1 PHE E 128 -4.884 36.381 -47.456 1.00 14.50
C
ATOM 9800 CE2 PHE E 128 -2.780 37.454 -47.092 1.00 18.86
C
ATOM 9801 CZ PHE E 128 -3.895 37.245 -47.881 1.00 19.29
C
ATOM 9802 H PHE E 128 -2.680 33.091 -42.497 1.00 16.11 H
ATOM 9803 HA PHE E 128 -4.198 33.381 -44.717 1.00 15.40
H
ATOM 9804 HB2 PHE E 128 -4.283 35.457 -43.587 1.00 18.04
H
ATOM 9805 HB3 PHE E 128 -2.703 35.551 -43.694 1.00 18.04
H
ATOM 9806 HD1 PHE E 128 -5.426 35.147 -45.961 1.00 17.38
H
ATOM 9807 HD2 PHE E 128 -1.906 36.942 -45.353 1.00 20.50
H
ATOM 9808 HE1 PHE E 128 -5.636 36.239 -47.985 1.00 17.40
H
ATOM 9809 HE2 PHE E 128 -2.112 38.036 -47.376 1.00 22.63
H
ATOM 9810 HZ PHE E 128 -3.979 37.684 -48.696 1.00 23.15
H
ATOM 9811 N ASP E 129 -2.214 32.108 -45.627 1.00 14.98 N
ATOM 9812 CA ASP E 129 -1.055 31.599 -46.357 1.00 14.76
C
ATOM 9813 C ASP E 129 -1.064 32.076 -47.809 1.00 17.71 C
ATOM 9814 O ASP E 129 -1.931 32.851 -48.215 1.00 15.50 O
ATOM 9815 CB ASP E 129 -0.998 30.064 -46.290 1.00 14.79
C
ATOM 9816 CG ASP E 129 -2.224 29.383 -46.902 1.00 19.45
C
ATOM 9817 OD1 ASP E 129 -2.824 29.921 -47.858 1.00 14.89
O
ATOM 9818 OD2 ASP E 129 -2.571 28.277 -46.430 1.00 17.87
O1-
ATOM 9819 H ASP E 129 -2.903 31.593 -45.653 1.00 17.98 H
ATOM 9820 HA ASP E 129 -0.250 31.942 -45.939 1.00 17.72
H
ATOM 9821 HB2 ASP E 129 -0.215 29.757 -46.773 1.00 17.74
H
ATOM 9822 HB3 ASP E 129 -0.940 29.792 -45.361 1.00 17.74
H
ATOM 9823 N GLY E 130 -0.093 31.611 -48.587 1.00 15.51 N
ATOM 9824 CA GLY E 130 0.049 32.047 -49.964 1.00 15.30

O
ATOM 3525 CB SER B 195 2.879 20.368 -45.182 1.00 28.07
C
ATOM 3526 OG SER B 195 2.594 18.984 -45.234 1.00 34.28
O
ATOM 3527 H SER B 195 3.406 22.652 -44.372 1.00 26.71
H
ATOM 3528 HA SER B 195 2.089 20.571 -43.300 1.00 23.30
H
ATOM 3529 HB2 SER B 195 2.194 20.849 -45.672 1.00 33.69
H
ATOM 3530 HB3 SER B 195 3.747 20.527 -45.584 1.00 33.69
H
ATOM 3531 HG SER B 195 3.180 18.555 -44.813 1.00 41.13
H
ATOM 3532 N PHE B 196 3.832 19.674 -41.832 1.00 24.04
N
ATOM 3533 CA PHE B 196 4.858 19.000 -41.029 1.00 22.02
C
ATOM 3534 C PHE B 196 6.070 19.879 -40.731 1.00 23.97
C
ATOM 3535 O PHE B 196 7.214 19.502 -40.988 1.00 20.66
O
ATOM 3536 CB PHE B 196 5.297 17.709 -41.724 1.00 24.00
C
ATOM 3537 CG PHE B 196 4.251 16.638 -41.695 1.00 22.78
C
ATOM 3538 CD1 PHE B 196 4.128 15.806 -40.596 1.00 23.64
C
ATOM 3539 CD2 PHE B 196 3.373 16.477 -42.751 1.00 28.16
C
ATOM 3540 CE1 PHE B 196 3.156 14.827 -40.556 1.00 24.03
C
ATOM 3541 CE2 PHE B 196 2.399 15.500 -42.716 1.00 29.08
C
ATOM 3542 CZ PHE B 196 2.288 14.675 -41.617 1.00 25.46
C
ATOM 3543 H PHE B 196 3.048 19.646 -41.479 1.00 28.84
H
ATOM 3544 HA PHE B 196 4.465 18.752 -40.178 1.00 26.42
H
ATOM 3545 HB2 PHE B 196 5.499 17.904 -42.652 1.00 28.80
H
ATOM 3546 HB3 PHE B 196 6.088 17.366 -41.279 1.00 28.80
H
ATOM 3547 HD1 PHE B 196 4.709 15.907 -39.877 1.00 28.37
H
ATOM 3548 HD2 PHE B 196 3.440 17.033 -43.493 1.00 33.80
H
ATOM 3549 HE1 PHE B 196 3.086 14.271 -39.814 1.00 28.83
H
ATOM 3550 HE2 PHE B 196 1.817 15.398 -43.434 1.00 34.90
H
ATOM 3551 HZ PHE B 196 1.635 14.013 -41.594 1.00 30.55
H
ATOM 3552 N LYS B 197 5.795 21.056 -40.182 1.00 23.08
N
ATOM 3553 CA LYS B 197 6.829 21.970 -39.726 1.00 20.49
C
ATOM 3554 C LYS B 197 6.749 22.119 -38.220 1.00 18.79
C
ATOM 3555 O LYS B 197 5.683 21.951 -37.624 1.00 16.31
O
ATOM 3556 CB LYS B 197 6.681 23.346 -40.376 1.00 23.24
C
ATOM 3557 CG LYS B 197 6.695 23.349 -41.889 1.00 26.94
C
ATOM 3558 CD LYS B 197 6.409 24.749 -42.412 1.00 35.07
C
ATOM 9825 C GLY E 130 -1.162 31.724 -50.821 1.00 17.27 C
ATOM 9826 O GLY E 130 -1.603 32.546 -51.628 1.00 13.78 O
ATOM 9827 H GLY E 130 0.499 31.040 -48.337 1.00 18.61 H
ATOM 9828 HA2 GLY E 130 0.188 33.007 -49.984 1.00 18.37
H
ATOM 9829 HA3 GLY E 130 0.824 31.618 -50.358 1.00 18.37
H
ATOM 9830 N GLU E 131 -1.702 30.522 -50.651 1.00 11.94 N
ATOM 9831 CA GLU E 131 -2.873 30.109 -51.409 1.00 16.34
C
ATOM 9832 C GLU E 131 -4.066 31.011 -51.092 1.00 17.14 C
ATOM 9833 O GLU E 131 -4.838 31.359 -51.984 1.00 15.64
O
ATOM 9834 CB GLU E 131 -3.210 28.648 -51.121 1.00 18.79
C
ATOM 9835 CG GLU E 131 -4.237 28.065 -52.074 1.00 25.42
C
ATOM 9836 CD GLU E 131 -4.437 26.574 -51.886 1.00 25.71
C
ATOM 9837 OE1 GLU E 131 -3.919 26.017 -50.892 1.00 23.82
O
ATOM 9838 OE2 GLU E 131 -5.110 25.960 -52.743 1.00 28.51
O1-
ATOM 9839 H GLU E 131 -1.409 29.929 -50.101 1.00 14.32 H
ATOM 9840 HA GLU E 131 -2.680 30.190 -52.357 1.00 19.61
H
ATOM 9841 HB2 GLU E 131 -2.401 28.118 -51.195 1.00 22.54
H
ATOM 9842 HB3 GLU E 131 -3.567 28.580 -50.221 1.00 22.54
H
ATOM 9843 HG2 GLU E 131 -5.090 28.503 -51.925 1.00 30.51
H
ATOM 9844 HG3 GLU E 131 -3.942 28.215 -52.986 1.00 30.51
H
ATOM 9845 N ASP E 132 -4.207 31.390 -49.824 1.00 14.43 N
ATOM 9846 CA ASP E 132 -5.244 32.334 -49.421 1.00 16.97
C
ATOM 9847 C ASP E 132 -5.081 33.673 -50.140 1.00 15.70 C
ATOM 9848 O ASP E 132 -6.053 34.244 -50.630 1.00 13.91 O
ATOM 9849 CB ASP E 132 -5.220 32.562 -47.904 1.00 15.21
C
ATOM 9850 CG ASP E 132 -5.483 31.294 -47.113 1.00 17.73
C
ATOM 9851 OD1 ASP E 132 -6.201 30.405 -47.621 1.00 16.20
O
ATOM 9852 OD2 ASP E 132 -4.974 31.192 -45.972 1.00 15.44
O1-
ATOM 9853 H ASP E 132 -3.713 31.114 -49.176 1.00 17.31 H
ATOM 9854 HA ASP E 132 -6.112 31.971 -49.656 1.00 20.37
H
ATOM 9855 HB2 ASP E 132 -4.346 32.898 -47.649 1.00 18.25
H
ATOM 9856 HB3 ASP E 132 -5.905 33.208 -47.671 1.00 18.25
H
ATOM 9857 N CYS E 133 -3.849 34.168 -50.198 1.00 12.86 N
ATOM 9858 CA CYS E 133 -3.571 35.454 -50.826 1.00 12.73

C
ATOM 3559 CE LYS B 197 6.323 24.784 -43.924 1.00 45.32
C
ATOM 3560 NZ LYS B 197 6.012 26.155 -44.422 1.00 56.39
N1+
ATOM 3561 H LYS B 197 4.998 21.354 -40.061 1.00 27.70
H
ATOM 3562 HA LYS B 197 7.702 21.613 -39.955 1.00 24.58
H
ATOM 3563 HB2 LYS B 197 5.838 23.731 -40.092 1.00 27.89
H
ATOM 3564 HB3 LYS B 197 7.412 23.908 -40.077 1.00 27.89
H
ATOM 3565 HG2 LYS B 197 7.570 23.074 -42.205 1.00 32.33
H
ATOM 3566 HG3 LYS B 197 6.009 22.749 -42.221 1.00 32.33
H
ATOM 3567 HD2 LYS B 197 5.561 25.056 -42.054 1.00 42.09
H
ATOM 3568 HD3 LYS B 197 7.123 25.345 -42.135 1.00 42.09
H
ATOM 3569 HE2 LYS B 197 7.175 24.510 -44.299 1.00 54.39
H
ATOM 3570 HE3 LYS B 197 5.619 24.186 -44.218 1.00 54.39
H
ATOM 3571 HZ1 LYS B 197 5.967 26.152 -45.311 1.00 67.66
H
ATOM 3572 HZ2 LYS B 197 5.231 26.428 -44.094 1.00 67.66
H
ATOM 3573 HZ3 LYS B 197 6.648 26.723 -44.167 1.00 67.66
H
ATOM 3574 N GLY B 198 7.886 22.439 -37.617 1.00 17.88
N
ATOM 3575 CA GLY B 198 7.954 22.804 -36.219 1.00 15.29
C
ATOM 3576 C GLY B 198 8.632 24.154 -36.088 1.00 16.13
C
ATOM 3577 O GLY B 198 9.783 24.311 -36.488 1.00 18.89
O
ATOM 3578 H GLY B 198 8.650 22.452 -38.012 1.00 21.46
H
ATOM 3579 HA2 GLY B 198 7.061 22.860 -35.845 1.00 18.34
H
ATOM 3580 HA3 GLY B 198 8.465 22.143 -35.726 1.00 18.34
H
ATOM 3581 N TYR B 199 7.914 25.136 -35.554 1.00 16.00
N
ATOM 3582 CA TYR B 199 8.489 26.452 -35.299 1.00 17.75
C
ATOM 3583 C TYR B 199 8.943 26.544 -33.849 1.00 19.24
C
ATOM 3584 O TYR B 199 8.155 26.330 -32.932 1.00 16.43
O
ATOM 3585 CB TYR B 199 7.481 27.562 -35.600 1.00 15.65
C
ATOM 3586 CG TYR B 199 7.254 27.819 -37.072 1.00 15.66
C
ATOM 3587 CD1 TYR B 199 8.128 28.612 -37.801 1.00 17.35
C
ATOM 3588 CD2 TYR B 199 6.151 27.285 -37.728 1.00 22.19
C
ATOM 3589 CE1 TYR B 199 7.918 28.856 -39.150 1.00 24.18
C
ATOM 3590 CE2 TYR B 199 5.931 27.523 -39.074 1.00 19.74
C
ATOM 3591 CZ TYR B 199 6.817 28.308 -39.780 1.00 27.19
C
ATOM 3592 OH TYR B 199 6.600 28.545 -41.117 1.00 25.40
C

ATOM 9859 C CYS E 133 -3.981 35.443 -52.295 1.00 14.86 C
ATOM 9860 O CYS E 133 -4.539 36.417 -52.798 1.00 15.23
O
ATOM 9861 CB CYS E 133 -2.086 35.805 -50.691 1.00 21.39
C
ATOM 9862 SG CYS E 133 -1.610 37.374 -51.458 1.00 23.37
S

ATOM 9863 H CYS E 133 -3.153 33.776 -49.880 1.00 15.43 H
ATOM 9864 HA CYS E 133 -4.084 36.143 -50.376 1.00 15.28
H
ATOM 9865 HB2 CYS E 133 -1.864 35.860 -49.749 1.00 25.67
H
ATOM 9866 HB3 CYS E 133 -1.562 35.103 -51.109 1.00 25.67
H

ATOM 9867 N ILE E 134 -3.718 34.331 -52.974 1.00 13.95 N

ATOM 9868 CA ILE E 134 -4.075 34.191 -54.382 1.00 13.37 C

ATOM 9869 C ILE E 134 -5.593 34.152 -54.551 1.00 14.47 C

ATOM 9870 O ILE E 134 -6.141 34.750 -55.476 1.00 12.81 O

ATOM 9871 CB ILE E 134 -3.457 32.910 -54.996 1.00 18.31 C
ATOM 9872 CG1 ILE E 134 -1.924 32.990 -54.988 1.00 13.13
C
ATOM 9873 CG2 ILE E 134 -3.982 32.670 -56.416 1.00 19.91
C
ATOM 9874 CD1 ILE E 134 -1.336 34.002 -55.955 1.00 13.23
C

ATOM 9875 H ILE E 134 -3.332 33.639 -52.641 1.00 16.74 H

ATOM 9876 HA ILE E 134 -3.735 34.955 -54.873 1.00 16.04 H

ATOM 9877 HB ILE E 134 -3.721 32.156 -54.447 1.00 21.97 H
ATOM 9878 HG12 ILE E 134 -1.632 33.232 -54.096 1.00 15.76
H
ATOM 9879 HG13 ILE E 134 -1.568 32.118 -55.222 1.00 15.76
H
ATOM 9880 HG21 ILE E 134 -3.576 31.863 -56.770 1.00 23.89
H
ATOM 9881 HG22 ILE E 134 -4.946 32.569 -56.382 1.00 23.89
H
ATOM 9882 HG23 ILE E 134 -3.748 33.430 -56.971 1.00 23.89
H
ATOM 9883 HD11 ILE E 134 -0.369 33.983 -55.881 1.00 15.87
H
ATOM 9884 HD12 ILE E 134 -1.604 33.769 -56.858 1.00 15.87
H
ATOM 9885 HD13 ILE E 134 -1.668 34.885 -55.728 1.00 15.87
H

ATOM 9886 N MET E 135 -6.274 33.436 -53.663 1.00 14.36 N
ATOM 9887 CA MET E 135 -7.724 33.324 -53.753 1.00 16.92
C

ATOM 9888 C MET E 135 -8.391 34.654 -53.402 1.00 16.18 C
ATOM 9889 O MET E 135 -9.399 35.025 -54.011 1.00 14.50
O
ATOM 9890 CB MET E 135 -8.230 32.199 -52.849 1.00 17.85
C
ATOM 9891 CG MET E 135 -7.779 30.819 -53.309 1.00 16.72
C
ATOM 9892 SD MET E 135 -8.442 30.370 -54.924 1.00 24.82

O
ATOM 3593 H TYR B 199 7.087 25.065 -35.329 1.00 19.20
H
ATOM 3594 HA TYR B 199 9.262 26.580 -35.869 1.00 21.30
H
ATOM 3595 HB2 TYR B 199 6.628 27.321 -35.208 1.00 18.77
H
ATOM 3596 HB3 TYR B 199 7.801 28.387 -35.204 1.00 18.77
H
ATOM 3597 HD1 TYR B 199 8.871 28.981 -37.380 1.00 20.82
H
ATOM 3598 HD2 TYR B 199 5.552 26.754 -37.255 1.00 26.63
H
ATOM 3599 HE1 TYR B 199 8.515 29.386 -39.628 1.00 29.02
H
ATOM 3600 HE2 TYR B 199 5.191 27.155 -39.499 1.00 23.69
H
ATOM 3601 HH TYR B 199 7.209 29.034 -41.425 1.00 30.48
H
ATOM 3602 N ILE B 200 10.218 26.861 -33.648 1.00 18.78
N
ATOM 3603 CA ILE B 200 10.764 27.005 -32.305 1.00 20.57
C
ATOM 3604 C ILE B 200 10.151 28.240 -31.654 1.00 22.09
C
ATOM 3605 O ILE B 200 10.139 29.323 -32.242 1.00 21.41
O
ATOM 3606 CB ILE B 200 12.305 27.118 -32.322 1.00 22.56
C
ATOM 3607 CG1 ILE B 200 12.914 25.902 -33.023 1.00 23.09
C
ATOM 3608 CG2 ILE B 200 12.850 27.236 -30.901 1.00 23.03
C
ATOM 3609 CD1 ILE B 200 14.406 26.001 -33.258 1.00 28.91
C
ATOM 3610 H ILE B 200 10.789 26.998 -34.276 1.00 22.53
H
ATOM 3611 HA ILE B 200 10.522 26.229 -31.775 1.00 24.68
H
ATOM 3612 HB ILE B 200 12.551 27.916 -32.816 1.00 27.07
H
ATOM 3613 HG12 ILE B 200 12.753 25.116 -32.478 1.00 27.71
H
ATOM 3614 HG13 ILE B 200 12.486 25.794 -33.887 1.00 27.71
H
ATOM 3615 HG21 ILE B 200 13.816 27.306 -30.939 1.00 27.64
H
ATOM 3616 HG22 ILE B 200 12.476 28.029 -30.485 1.00 27.64
H
ATOM 3617 HG23 ILE B 200 12.594 26.447 -30.399 1.00 27.64
H
ATOM 3618 HD11 ILE B 200 14.709 25.194 -33.704 1.00 34.69
H
ATOM 3619 HD12 ILE B 200 14.587 26.775 -33.814 1.00 34.69
H
ATOM 3620 HD13 ILE B 200 14.854 26.095 -32.403 1.00 34.69
H
ATOM 3621 N GLU B 201 9.629 28.066 -30.445 1.00 18.17
N
ATOM 3622 CA GLU B 201 8.939 29.143 -29.751 1.00 18.13
C
ATOM 3623 C GLU B 201 9.234 29.096 -28.260 1.00 19.85
C
ATOM 3624 O GLU B 201 9.528 28.034 -27.703 1.00 17.15
O
ATOM 3625 CB GLU B 201 7.428 29.050 -30.006 1.00 16.42
C
ATOM 3626 CG GLU B 201 6.564 30.052 -29.239 1.00 24.81
S
ATOM 9893 CE MET E 135 -10.125 29.954 -54.479 1.00 72.84
C
ATOM 9894 H MET E 135 -5.923 33.010 -53.003 1.00 17.23 H
ATOM 9895 HA MET E 135 -7.959 33.093 -54.666 1.00 20.30
H
ATOM 9896 HB2 MET E 135 -7.892 32.341 -51.951 1.00 21.42
H
ATOM 9897 HB3 MET E 135 -9.200 32.211 -52.844 1.00 21.42
H
ATOM 9898 HG2 MET E 135 -6.811 30.806 -53.368 1.00 20.06
H
ATOM 9899 HG3 MET E 135 -8.080 30.158 -52.666 1.00 20.06
H
ATOM 9900 HE1 MET E 135 -10.606 29.688 -55.278 1.00 87.41
H
ATOM 9901 HE2 MET E 135 -10.111 29.222 -53.842 1.00 87.41
H
ATOM 9902 HE3 MET E 135 -10.548 30.731 -54.081 1.00 87.41
H
ATOM 9903 N HIS E 136 -7.832 35.373 -52.432 1.00 11.58 N
ATOM 9904 CA HIS E 136 -8.310 36.721 -52.129 1.00 14.06 C
ATOM 9905 C HIS E 136 -8.086 37.640 -53.325 1.00 14.28 C
ATOM 9906 O HIS E 136 -8.963 38.424 -53.693 1.00 17.87 O
ATOM 9907 CB HIS E 136 -7.610 37.302 -50.899 1.00 12.00 C
ATOM 9908 CG HIS E 136 -8.065 36.709 -49.603 1.00 16.23
C
ATOM 9909 ND1 HIS E 136 -8.066 37.421 -48.422 1.00 14.57
N
ATOM 9910 CD2 HIS E 136 -8.528 35.474 -49.298 1.00 14.11
C
ATOM 9911 CE1 HIS E 136 -8.511 36.650 -47.447 1.00 19.48
C
ATOM 9912 NE2 HIS E 136 -8.798 35.463 -47.952 1.00 16.55
N
ATOM 9913 H HIS E 136 -7.180 35.107 -51.939 1.00 13.89 H
ATOM 9914 HA HIS E 136 -9.262 36.688 -51.948 1.00 16.87 H
ATOM 9915 HB2 HIS E 136 -6.656 37.142 -50.979 1.00 14.40
H
ATOM 9916 HB3 HIS E 136 -7.780 38.256 -50.865 1.00 14.40
H
ATOM 9917 HD1 HIS E 136 -7.815 38.239 -48.334 1.00 17.48
H
ATOM 9918 HD2 HIS E 136 -8.642 34.765 -49.890 1.00 16.93
H
ATOM 9919 HE1 HIS E 136 -8.606 36.900 -46.556 1.00 23.37
H
ATOM 9920 HE2 HIS E 136 -9.106 34.793 -47.509 1.00 19.86
H
ATOM 9921 N LEU E 137 -6.903 37.539 -53.922 1.00 13.80 N
ATOM 9922 CA LEU E 137 -6.548 38.344 -55.086 1.00 14.11
C
ATOM 9923 C LEU E 137 -7.567 38.163 -56.209 1.00 14.94 C
ATOM 9924 O LEU E 137 -8.077 39.134 -56.758 1.00 16.40 O
ATOM 9925 CB LEU E 137 -5.142 37.980 -55.573 1.00 13.09
C
ATOM 9926 CG LEU E 137 -4.711 38.506 -56.945 1.00 15.68

C
ATOM 3627 CD GLU B 201 6.879 31.502 -29.577 1.00 29.39
C
ATOM 3628 OE1 GLU B 201 7.969 31.986 -29.202 1.00 28.55
O
ATOM 3629 OE2 GLU B 201 6.028 32.161 -30.213 1.00 33.83
O1-
ATOM 3630 H GLU B 201 9.663 27.329 -30.003 1.00 21.80
H
ATOM 3631 HA GLU B 201 9.251 29.994 -30.094 1.00 21.75
H
ATOM 3632 HB2 GLU B 201 7.268 29.193 -30.952 1.00 19.70
H
ATOM 3633 HB3 GLU B 201 7.130 28.161 -29.759 1.00 19.70
H
ATOM 3634 HG2 GLU B 201 5.632 29.892 -29.453 1.00 29.77
H
ATOM 3635 HG3 GLU B 201 6.710 29.929 -28.288 1.00 29.77
H
ATOM 3636 N ASN B 202 9.168 30.260 -27.625 1.00 21.76
N
ATOM 3637 CA ASN B 202 9.292 30.361 -26.179 1.00 22.40
C
ATOM 3638 C ASN B 202 8.163 29.592 -25.495 1.00 18.61
C
ATOM 3639 O ASN B 202 6.984 29.863 -25.726 1.00 17.60
O
ATOM 3640 CB ASN B 202 9.284 31.831 -25.750 1.00 25.89
C
ATOM 3641 CG ASN B 202 9.627 32.019 -24.284 1.00 30.35
C
ATOM 3642 OD1 ASN B 202 9.134 31.298 -23.417 1.00 28.07
O
ATOM 3643 ND2 ASN B 202 10.484 32.995 -24.002 1.00 32.66
N
ATOM 3644 H ASN B 202 9.049 31.017 -28.017 1.00 26.11
H
ATOM 3645 HA ASN B 202 10.135 29.969 -25.904 1.00 26.88
H
ATOM 3646 HB2 ASN B 202 9.938 32.317 -26.276 1.00 31.07
H
ATOM 3647 HB3 ASN B 202 8.399 32.199 -25.900 1.00 31.07
H
ATOM 3648 HD21 ASN B 202 10.713 33.144 -23.187 1.00 39.19
H
ATOM 3649 HD22 ASN B 202 10.810 33.477 -24.635 1.00 39.19
H
ATOM 3650 N CYS B 203 8.541 28.633 -24.654 1.00 15.24
N
ATOM 3651 CA CYS B 203 7.584 27.779 -23.962 1.00 18.87
C
ATOM 3652 C CYS B 203 6.517 28.573 -23.207 1.00 18.33
C
ATOM 3653 O CYS B 203 5.426 28.065 -22.954 1.00 20.66
O
ATOM 3654 CB CYS B 203 8.322 26.852 -22.989 1.00 18.37
C
ATOM 3655 SG CYS B 203 9.514 25.728 -23.774 1.00 24.48
S
ATOM 3656 H CYS B 203 9.361 28.456 -24.465 1.00 18.29
H
ATOM 3657 HA CYS B 203 7.132 27.223 -24.615 1.00 22.64
H
ATOM 3658 HB2 CYS B 203 8.809 27.397 -22.351 1.00 22.04
H
ATOM 3659 HB3 CYS B 203 7.668 26.309 -22.522 1.00 22.04
H
ATOM 3660 N SER B 204 6.830 29.819 -22.859 1.00 17.86
C
ATOM 9927 CD1 LEU E 137 -4.834 40.023 -57.025 1.00 19.57
C
ATOM 9928 CD2 LEU E 137 -3.285 38.070 -57.252 1.00 16.15
C
ATOM 9929 H LEU E 137 -6.280 37.003 -53.668 1.00 16.56 H
ATOM 9930 HA LEU E 137 -6.545 39.281 -54.833 1.00 16.93
H
ATOM 9931 HB2 LEU E 137 -4.504 38.317 -54.925 1.00 15.71
H
ATOM 9932 HB3 LEU E 137 -5.079 37.012 -55.607 1.00 15.71
H
ATOM 9933 HG LEU E 137 -5.290 38.125 -57.623 1.00 18.82
H
ATOM 9934 HD11 LEU E 137 -4.553 40.316 -57.906 1.00 23.48
H
ATOM 9935 HD12 LEU E 137 -5.759 40.272 -56.873 1.00 23.48
H
ATOM 9936 HD13 LEU E 137 -4.267 40.422 -56.346 1.00 23.48
H
ATOM 9937 HD21 LEU E 137 -3.031 38.412 -58.123 1.00 19.37
H
ATOM 9938 HD22 LEU E 137 -2.693 38.425 -56.570 1.00 19.37
H
ATOM 9939 HD23 LEU E 137 -3.245 37.100 -57.252 1.00 19.37
H
ATOM 9940 N ARG E 138 -7.872 36.915 -56.536 1.00 15.03
N
ATOM 9941 CA ARG E 138 -8.821 36.624 -57.599 1.00 17.21
C
ATOM 9942 C ARG E 138 -10.223 37.129 -57.242 1.00 18.67
C
ATOM 9943 O ARG E 138 -10.941 37.654 -58.093 1.00 17.07
O
ATOM 9944 CB ARG E 138 -8.835 35.121 -57.883 1.00 17.26
C
ATOM 9945 CG ARG E 138 -7.536 34.621 -58.502 1.00 18.09
C
ATOM 9946 CD ARG E 138 -7.529 33.110 -58.664 1.00 22.76
C
ATOM 9947 NE ARG E 138 -8.525 32.659 -59.628 1.00 25.06
N
ATOM 9948 CZ ARG E 138 -8.955 31.407 -59.728 1.00 30.07
C
ATOM 9949 NH1 ARG E 138 -8.479 30.470 -58.918 1.00 28.66
N1+
ATOM 9950 NH2 ARG E 138 -9.870 31.092 -60.635 1.00 31.23
N
ATOM 9951 H ARG E 138 -7.542 36.217 -56.156 1.00 18.04
H
ATOM 9952 HA ARG E 138 -8.537 37.078 -58.408 1.00 20.66
H
ATOM 9953 HB2 ARG E 138 -8.973 34.644 -57.050 1.00 20.72
H
ATOM 9954 HB3 ARG E 138 -9.556 34.924 -58.501 1.00 20.72
H
ATOM 9955 HG2 ARG E 138 -7.426 35.020 -59.380 1.00 21.70
H
ATOM 9956 HG3 ARG E 138 -6.794 34.867 -57.928 1.00 21.70
H
ATOM 9957 HD2 ARG E 138 -6.655 32.828 -58.978 1.00 27.31
H
ATOM 9958 HD3 ARG E 138 -7.727 32.698 -57.809 1.00 27.31
H
ATOM 9959 HE ARG E 138 -8.856 33.242 -60.167 1.00 30.07
H
ATOM 9960 HH11 ARG E 138 -7.888 30.673 -58.328 1.00 34.40

N
ATOM 3661 CA SER B 204 5.916 30.656 -22.087 1.00 22.50
C
ATOM 3662 C SER B 204 4.864 31.354 -22.948 1.00 20.68
C
ATOM 3663 O SER B 204 3.937 31.963 -22.420 1.00 22.63
O
ATOM 3664 CB SER B 204 6.703 31.710 -21.302 1.00 20.13
C
ATOM 3665 OG SER B 204 7.470 31.104 -20.279 1.00 22.97
O
ATOM 3666 H SER B 204 7.571 30.206 -23.061 1.00 21.43
H
ATOM 3667 HA SER B 204 5.449 30.098 -21.446 1.00 27.00
H
ATOM 3668 HB2 SER B 204 7.298 32.177 -21.909 1.00 24.15
H
ATOM 3669 HB3 SER B 204 6.080 32.335 -20.901 1.00 24.15
H
ATOM 3670 HG SER B 204 7.898 31.690 -19.855 1.00 27.57
H
ATOM 3671 N THR B 205 5.005 31.270 -24.267 1.00 18.95
N
ATOM 3672 CA THR B 205 4.096 31.964 -25.178 1.00 19.15
C
ATOM 3673 C THR B 205 2.756 31.236 -25.307 1.00 18.16
C
ATOM 3674 O THR B 205 2.722 30.073 -25.709 1.00 16.01
O
ATOM 3675 CB THR B 205 4.704 32.103 -26.585 1.00 25.38
C
ATOM 3676 OG1 THR B 205 6.060 32.554 -26.487 1.00 28.77
O
ATOM 3677 CG2 THR B 205 3.896 33.092 -27.420 1.00 24.93
C
ATOM 3678 H THR B 205 5.621 30.817 -24.661 1.00 22.74
H
ATOM 3679 HA THR B 205 3.924 32.855 -24.835 1.00 22.99
H
ATOM 3680 HB THR B 205 4.684 31.241 -27.030 1.00 30.45
H
ATOM 3681 HG1 THR B 205 6.087 33.300 -26.103 1.00 34.52
H
ATOM 3682 HG21 THR B 205 4.286 33.174 -28.305 1.00 29.92
H
ATOM 3683 HG22 THR B 205 2.981 32.784 -27.506 1.00 29.92
H
ATOM 3684 HG23 THR B 205 3.897 33.964 -26.994 1.00 29.92
H
ATOM 3685 N PRO B 206 1.645 31.917 -24.977 1.00 18.00
N
ATOM 3686 CA PRO B 206 0.350 31.248 -25.140 1.00 17.87
C
ATOM 3687 C PRO B 206 0.050 30.892 -26.593 1.00 20.20
C
ATOM 3688 O PRO B 206 0.187 31.737 -27.477 1.00 14.53
O
ATOM 3689 CB PRO B 206 -0.655 32.286 -24.621 1.00 22.87
C
ATOM 3690 CG PRO B 206 0.134 33.198 -23.763 1.00 22.22
C
ATOM 3691 CD PRO B 206 1.494 33.257 -24.382 1.00 21.86
C
ATOM 3692 HA PRO B 206 0.306 30.450 -24.591 1.00 21.45
H
ATOM 3693 HB2 PRO B 206 -1.042 32.767 -25.369 1.00 27.45
H
ATOM 3694 HB3 PRO B 206 -1.345 31.841 -24.104 1.00 27.45
H
ATOM 9961 HH12 ARG E 138 -8.761 29.661 -58.985 1.00 34.40
H
ATOM 9962 HH21 ARG E 138 -10.180 31.697 -61.161 1.00 37.48
H
ATOM 9963 HH22 ARG E 138 -10.149 30.281 -60.700 1.00 37.48
H
ATOM 9964 N SER E 139 -10.603 36.994 -55.978 1.00 16.32
N
ATOM 9965 CA SER E 139 -11.907 37.474 -55.534 1.00 16.34
C
ATOM 9966 C SER E 139 -11.968 39.002 -55.579 1.00 17.91
C
ATOM 9967 O SER E 139 -13.011 39.582 -55.889 1.00 16.73
O
ATOM 9968 CB SER E 139 -12.210 36.973 -54.121 1.00 15.40
C
ATOM 9969 OG SER E 139 -12.117 35.559 -54.052 1.00 15.94
O
ATOM 9970 H SER E 139 -10.129 36.630 -55.359 1.00 19.59
H
ATOM 9971 HA SER E 139 -12.590 37.128 -56.129 1.00 19.61
H
ATOM 9972 HB2 SER E 139 -11.569 37.361 -53.504 1.00 18.47
H
ATOM 9973 HB3 SER E 139 -13.109 37.242 -53.877 1.00 18.47
H
ATOM 9974 HG SER E 139 -12.668 35.209 -54.582 1.00 19.13
H
ATOM 9975 N LEU E 140 -10.851 39.657 -55.274 1.00 16.92
N
ATOM 9976 CA LEU E 140 -10.813 41.119 -55.262 1.00 16.54
C
ATOM 9977 C LEU E 140 -10.772 41.679 -56.680 1.00 16.09
C
ATOM 9978 O LEU E 140 -11.345 42.734 -56.953 1.00 20.02
O
ATOM 9979 CB LEU E 140 -9.612 41.620 -54.459 1.00 14.74
C
ATOM 9980 CG LEU E 140 -9.696 41.416 -52.944 1.00 13.44
C
ATOM 9981 CD1 LEU E 140 -8.341 41.666 -52.303 1.00 16.07
C
ATOM 9982 CD2 LEU E 140 -10.762 42.310 -52.316 1.00 17.46
C
ATOM 9983 H LEU E 140 -10.105 39.281 -55.070 1.00 20.30
H
ATOM 9984 HA LEU E 140 -11.617 41.450 -54.834 1.00 19.85
H
ATOM 9985 HB2 LEU E 140 -8.820 41.157 -54.771 1.00 17.68
H
ATOM 9986 HB3 LEU E 140 -9.514 42.572 -54.618 1.00 17.68
H
ATOM 9987 HG LEU E 140 -9.941 40.494 -52.766 1.00 16.13
H
ATOM 9988 HD11 LEU E 140 -8.415 41.532 -51.346 1.00 19.28
H
ATOM 9989 HD12 LEU E 140 -7.696 41.045 -52.676 1.00 19.28
H
ATOM 9990 HD13 LEU E 140 -8.068 42.578 -52.490 1.00 19.28
H
ATOM 9991 HD21 LEU E 140 -10.784 42.151 -51.359 1.00 20.95
H
ATOM 9992 HD22 LEU E 140 -10.540 43.238 -52.493 1.00 20.95
H
ATOM 9993 HD23 LEU E 140 -11.624 42.096 -52.707 1.00 20.95
H
ATOM 9994 N VAL E 141 -10.099 40.975 -57.583 1.00 19.49

H
ATOM 3695 HG2 PRO B 206 -0.277 34.077 -23.758 1.00 26.66
H
ATOM 3696 HG3 PRO B 206 0.183 32.839 -22.864 1.00 26.66
H
ATOM 3697 HD2 PRO B 206 1.525 33.939 -25.071 1.00 26.23
H
ATOM 3698 HD3 PRO B 206 2.171 33.404 -23.703 1.00 26.23
H
ATOM 3699 N ASN B 207 -0.342 29.644 -26.829 1.00 19.17
N
ATOM 3700 CA ASN B 207 -0.792 29.207 -28.146 1.00 16.49
C
ATOM 3701 C ASN B 207 -1.897 28.165 -28.010 1.00 19.54
C
ATOM 3702 O ASN B 207 -2.061 27.557 -26.950 1.00 15.66
O
ATOM 3703 CB ASN B 207 0.371 28.628 -28.961 1.00 19.53
C
ATOM 3704 CG ASN B 207 1.225 29.702 -29.620 1.00 16.92
C
ATOM 3705 OD1 ASN B 207 0.877 30.221 -30.681 1.00 16.98
O
ATOM 3706 ND2 ASN B 207 2.356 30.023 -29.002 1.00 17.66
N
ATOM 3707 H ASN B 207 -0.356 29.022 -26.235 1.00 23.00
H
ATOM 3708 HA ASN B 207 -1.151 29.968 -28.629 1.00 19.79
H
ATOM 3709 HB2 ASN B 207 0.943 28.111 -28.372 1.00 23.43
H
ATOM 3710 HB3 ASN B 207 0.014 28.058 -29.660 1.00 23.43
H
ATOM 3711 HD21 ASN B 207 2.872 30.625 -29.336 1.00 21.19
H
ATOM 3712 HD22 ASN B 207 2.572 29.630 -28.268 1.00 21.19
H
ATOM 3713 N THR B 208 -2.662 27.961 -29.077 1.00 16.41
N
ATOM 3714 CA THR B 208 -3.612 26.859 -29.105 1.00 14.55
C
ATOM 3715 C THR B 208 -2.801 25.564 -29.139 1.00 16.01
C
ATOM 3716 O THR B 208 -1.589 25.596 -29.359 1.00 12.88
O
ATOM 3717 CB THR B 208 -4.568 26.951 -30.307 1.00 14.56
C
ATOM 3718 OG1 THR B 208 -3.821 27.017 -31.528 1.00 15.04
O
ATOM 3719 CG2 THR B 208 -5.450 28.186 -30.187 1.00 15.59
C
ATOM 3720 H THR B 208 -2.650 28.442 -29.790 1.00 19.70
H
ATOM 3721 HA THR B 208 -4.140 26.868 -28.292 1.00 17.46
H
ATOM 3722 HB THR B 208 -5.141 26.168 -30.322 1.00 17.48
H
ATOM 3723 HG1 THR B 208 -4.345 27.067 -32.183 1.00 18.05
H
ATOM 3724 HG21 THR B 208 -6.051 28.239 -30.947 1.00 18.71
H
ATOM 3725 HG22 THR B 208 -5.975 28.140 -29.372 1.00 18.71
H
ATOM 3726 HG23 THR B 208 -4.900 28.984 -30.164 1.00 18.71
H
ATOM 3727 N TYR B 209 -3.446 24.429 -28.895 1.00 13.50
N
ATOM 3728 CA TYR B 209 -2.703 23.175 -28.800 1.00 13.00
N
ATOM 9995 CA VAL E 141 -10.106 41.360 -58.987 1.00 19.08
C
ATOM 9996 C VAL E 141 -11.545 41.319 -59.499 1.00 21.59
C
ATOM 9997 O VAL E 141 -11.956 42.169 -60.284 1.00 25.99
O
ATOM 9998 CB VAL E 141 -9.200 40.441 -59.836 1.00 19.66
C
ATOM 9999 CG1 VAL E 141 -9.450 40.649 -61.326 1.00 22.61
C
ATOM 10000 CG2 VAL E 141 -7.733 40.702 -59.517 1.00 18.87
C
ATOM 10001 H VAL E 141 -9.633 40.274 -57.409 1.00 23.39
H
ATOM 10002 HA VAL E 141 -9.779 42.270 -59.071 1.00 22.90
H
ATOM 10003 HB VAL E 141 -9.396 39.515 -59.623 1.00 23.59
H
ATOM 10004 HG11 VAL E 141 -8.868 40.059 -61.829 1.00 27.13
H
ATOM 10005 HG12 VAL E 141 -10.378 40.445 -61.522 1.00 27.13
H
ATOM 10006 HG13 VAL E 141 -9.260 41.573 -61.551 1.00 27.13
H
ATOM 10007 HG21 VAL E 141 -7.183 40.116 -60.059 1.00 22.64
H
ATOM 10008 HG22 VAL E 141 -7.528 41.629 -59.717 1.00 22.64
H
ATOM 10009 HG23 VAL E 141 -7.579 40.525 -58.576 1.00 22.64
H
ATOM 10010 N ARG E 142 -12.307 40.335 -59.033 1.00 19.07
N
ATOM 10011 CA ARG E 142 -13.704 40.192 -59.429 1.00 24.24
C
ATOM 10012 C ARG E 142 -14.533 41.405 -59.009 1.00 26.35
C
ATOM 10013 O ARG E 142 -15.269 41.966 -59.821 1.00 28.20
O
ATOM 10014 CB ARG E 142 -14.294 38.913 -58.832 1.00 25.76
C
ATOM 10015 CG ARG E 142 -15.783 38.721 -59.070 1.00 36.68
C
ATOM 10016 CD ARG E 142 -16.117 38.625 -60.548 1.00 44.40
C
ATOM 10017 NE ARG E 142 -17.545 38.399 -60.761 1.00 54.59
N
ATOM 10018 CZ ARG E 142 -18.135 37.208 -60.717 1.00 59.95
C
ATOM 10019 NH1 ARG E 142 -17.425 36.115 -60.469 1.00 56.87
N1+
ATOM 10020 NH2 ARG E 142 -19.440 37.109 -60.921 1.00 68.51
N
ATOM 10021 H ARG E 142 -12.037 39.733 -58.483 1.00 22.89
H
ATOM 10022 HA ARG E 142 -13.751 40.119 -60.395 1.00 29.09
H
ATOM 10023 HB2 ARG E 142 -13.835 38.151 -59.219 1.00 30.91
H
ATOM 10024 HB3 ARG E 142 -14.150 38.925 -57.872 1.00 30.91
H
ATOM 10025 HG2 ARG E 142 -16.071 37.900 -58.641 1.00 44.02
H
ATOM 10026 HG3 ARG E 142 -16.265 39.478 -58.700 1.00 44.02
H
ATOM 10027 HD2 ARG E 142 -15.872 39.455 -60.986 1.00 53.28
H
ATOM 10028 HD3 ARG E 142 -15.631 37.882 -60.939 1.00 53.28

C
ATOM 3729 C TYR B 209 -3.513 21.958 -29.226 1.00 14.49
C
ATOM 3730 O TYR B 209 -4.744 21.996 -29.295 1.00 11.51
O
ATOM 3731 CB TYR B 209 -2.187 22.983 -27.371 1.00 14.00
C
ATOM 3732 CG TYR B 209 -3.260 22.967 -26.303 1.00 13.42
C
ATOM 3733 CD1 TYR B 209 -3.864 24.146 -25.876 1.00 15.48
C
ATOM 3734 CD2 TYR B 209 -3.650 21.777 -25.703 1.00 14.21
C
ATOM 3735 CE1 TYR B 209 -4.840 24.134 -24.894 1.00 19.28
C
ATOM 3736 CE2 TYR B 209 -4.619 21.755 -24.720 1.00 19.66
C
ATOM 3737 CZ TYR B 209 -5.211 22.935 -24.319 1.00 20.66
C
ATOM 3738 OH TYR B 209 -6.178 22.907 -23.343 1.00 19.94
O
ATOM 3739 H TYR B 209 -4.295 24.355 -28.783 1.00 16.20
H
ATOM 3740 HA TYR B 209 -1.931 23.231 -29.385 1.00 15.60
H
ATOM 3741 HB2 TYR B 209 -1.714 22.137 -27.325 1.00 16.80
H
ATOM 3742 HB3 TYR B 209 -1.577 23.708 -27.163 1.00 16.80
H
ATOM 3743 HD1 TYR B 209 -3.615 24.954 -26.263 1.00 18.58
H
ATOM 3744 HD2 TYR B 209 -3.253 20.979 -25.971 1.00 17.06
H
ATOM 3745 HE1 TYR B 209 -5.240 24.928 -24.621 1.00 23.13
H
ATOM 3746 HE2 TYR B 209 -4.874 20.949 -24.333 1.00 23.60
H
ATOM 3747 HH TYR B 209 -6.458 23.684 -23.193 1.00 23.92
H
ATOM 3748 N ILE B 210 -2.782 20.885 -29.516 1.00 14.80
N
ATOM 3749 CA ILE B 210 -3.348 19.627 -29.975 1.00 18.21
C
ATOM 3750 C ILE B 210 -3.006 18.514 -28.994 1.00 15.01
C
ATOM 3751 O ILE B 210 -1.834 18.276 -28.705 1.00 15.25
O
ATOM 3752 CB ILE B 210 -2.818 19.246 -31.373 1.00 15.54
C
ATOM 3753 CG1 ILE B 210 -3.110 20.366 -32.375 1.00 15.83
C
ATOM 3754 CG2 ILE B 210 -3.438 17.936 -31.837 1.00 14.28
C
ATOM 3755 CD1 ILE B 210 -2.421 20.193 -33.707 1.00 18.37
C
ATOM 3756 H ILE B 210 -1.924 20.865 -29.452 1.00 17.76
H
ATOM 3757 HA ILE B 210 -4.314 19.706 -30.024 1.00 21.85
H
ATOM 3758 HB ILE B 210 -1.857 19.127 -31.315 1.00 18.65
H
ATOM 3759 HG12 ILE B 210 -4.066 20.397 -32.538 1.00 18.99
H
ATOM 3760 HG13 ILE B 210 -2.814 21.208 -31.996 1.00 18.99
H
ATOM 3761 HG21 ILE B 210 -3.090 17.718 -32.716 1.00 17.13
H
ATOM 3762 HG22 ILE B 210 -3.207 17.237 -31.207 1.00 17.13
H
ATOM 10029 HE ARG E 142 -18.038 39.084 -60.927 1.00 65.51
H
ATOM 10030 HH11 ARG E 142 -16.578 36.173 -60.334 1.00 68.25
H
ATOM 10031 HH12 ARG E 142 -17.813 35.347 -60.442 1.00 68.25
H
ATOM 10032 HH21 ARG E 142 -19.905 37.814 -61.084 1.00 82.22
H
ATOM 10033 HH22 ARG E 142 -19.822 36.339 -60.894 1.00 82.22
H
ATOM 10034 N LYS E 143 -14.416 41.805 -57.745 1.00 23.88
N
ATOM 10035 CA LYS E 143 -15.118 42.986 -57.251 1.00 28.82
C
ATOM 10036 C LYS E 143 -14.736 44.212 -58.065 1.00 28.57
C
ATOM 10037 O LYS E 143 -15.592 44.986 -58.488 1.00 31.07
O
ATOM 10038 CB LYS E 143 -14.800 43.246 -55.778 1.00 23.54
C
ATOM 10039 CG LYS E 143 -15.219 42.147 -54.829 1.00 28.69
C
ATOM 10040 CD LYS E 143 -15.096 42.597 -53.378 1.00 28.36
C
ATOM 10041 CE LYS E 143 -16.233 43.528 -52.982 1.00 35.13
C
ATOM 10042 NZ LYS E 143 -16.120 43.988 -51.571 1.00 39.13
N1+
ATOM 10043 H LYS E 143 -13.935 41.408 -57.152 1.00 28.66
H
ATOM 10044 HA LYS E 143 -16.074 42.849 -57.337 1.00 34.59
H
ATOM 10045 HB2 LYS E 143 -13.842 43.363 -55.685 1.00 28.25
H
ATOM 10046 HB3 LYS E 143 -15.255 44.057 -55.503 1.00 28.25
H
ATOM 10047 HG2 LYS E 143 -16.144 41.911 -54.998 1.00 34.42
H
ATOM 10048 HG3 LYS E 143 -14.645 41.375 -54.959 1.00 34.42
H
ATOM 10049 HD2 LYS E 143 -15.124 41.819 -52.799 1.00 34.03
H
ATOM 10050 HD3 LYS E 143 -14.259 43.072 -53.261 1.00 34.03
H
ATOM 10051 HE2 LYS E 143 -16.218 44.309 -53.557 1.00 42.15
H
ATOM 10052 HE3 LYS E 143 -17.076 43.059 -53.080 1.00 42.15
H
ATOM 10053 HZ1 LYS E 143 -16.137 43.289 -51.021 1.00 46.95
H
ATOM 10054 HZ2 LYS E 143 -15.355 44.429 -51.455 1.00 46.95
H
ATOM 10055 HZ3 LYS E 143 -16.798 44.529 -51.372 1.00 46.95
H
ATOM 10056 N MET E 144 -13.436 44.376 -58.272 1.00 25.28
N
ATOM 10057 CA MET E 144 -12.900 45.547 -58.948 1.00 27.97
C
ATOM 10058 C MET E 144 -13.406 45.645 -60.384 1.00 35.15
C
ATOM 10059 O MET E 144 -13.712 46.735 -60.871 1.00 34.51
O
ATOM 10060 CB MET E 144 -11.370 45.506 -58.919 1.00 25.24
C
ATOM 10061 CG MET E 144 -10.688 46.653 -59.650 1.00 29.40
C
ATOM 10062 SD MET E 144 -10.298 46.242 -61.360 1.00 42.62

H
ATOM 3763 HG23 ILE B 210 -4.401 18.041 -31.879 1.00 17.13
H
ATOM 3764 HD11 ILE B 210 -2.655 20.938 -34.282 1.00 22.04
H
ATOM 3765 HD12 ILE B 210 -1.461 20.172 -33.565 1.00 22.04
H
ATOM 3766 HD13 ILE B 210 -2.714 19.360 -34.108 1.00 22.04
H
ATOM 3767 N CYS B 211 -4.031 17.845 -28.478 1.00 13.03
N
ATOM 3768 CA CYS B 211 -3.838 16.677 -27.628 1.00 16.24
C
ATOM 3769 C CYS B 211 -3.968 15.420 -28.469 1.00 20.33
C
ATOM 3770 O CYS B 211 -4.712 15.394 -29.452 1.00 17.44
O
ATOM 3771 CB CYS B 211 -4.848 16.651 -26.479 1.00 22.87
C
ATOM 3772 SG CYS B 211 -4.586 17.937 -25.240 1.00 32.56
S
ATOM 3773 H CYS B 211 -4.856 18.049 -28.607 1.00 15.64
H
ATOM 3774 HA CYS B 211 -2.945 16.699 -27.249 1.00 19.49
H
ATOM 3775 HB2 CYS B 211 -5.739 16.770 -26.844 1.00 27.44
H
ATOM 3776 HB3 CYS B 211 -4.789 15.793 -26.031 1.00 27.44
H
ATOM 3777 N MET B 212 -3.236 14.385 -28.075 1.00 20.62
N
ATOM 3778 CA MET B 212 -3.224 13.123 -28.796 1.00 19.04
C
ATOM 3779 C MET B 212 -3.266 11.958 -27.822 1.00 24.41
C
ATOM 3780 O MET B 212 -2.621 11.994 -26.773 1.00 20.80
O
ATOM 3781 CB MET B 212 -1.982 13.025 -29.676 1.00 22.84
C
ATOM 3782 CG MET B 212 -1.792 11.672 -30.333 1.00 22.92
C
ATOM 3783 SD MET B 212 -0.403 11.689 -31.475 1.00 24.54
S
ATOM 3784 CE MET B 212 -0.348 9.970 -31.974 1.00 31.53
C
ATOM 3785 H MET B 212 -2.729 14.391 -27.380 1.00 24.74
H
ATOM 3786 HA MET B 212 -4.003 13.081 -29.372 1.00 22.85
H
ATOM 3787 HB2 MET B 212 -2.047 13.688 -30.381 1.00 27.41
H
ATOM 3788 HB3 MET B 212 -1.199 13.201 -29.131 1.00 27.41
H
ATOM 3789 HG2 MET B 212 -1.616 11.006 -29.650 1.00 27.50
H
ATOM 3790 HG3 MET B 212 -2.592 11.441 -30.830 1.00 27.50
H
ATOM 3791 HE1 MET B 212 0.378 9.849 -32.605 1.00 37.83
H
ATOM 3792 HE2 MET B 212 -0.200 9.419 -31.189 1.00 37.83
H
ATOM 3793 HE3 MET B 212 -1.192 9.735 -32.390 1.00 37.83
H
ATOM 3794 N GLN B 213 -4.031 10.931 -28.178 1.00 22.35
N
ATOM 3795 CA GLN B 213 -4.116 9.713 -27.386 1.00 24.56
C
ATOM 3796 C GLN B 213 -4.148 8.501 -28.309 1.00 31.59
S
ATOM 10063 CE MET E 144 -9.018 45.007 -61.143 1.00 35.57
C
ATOM 10064 H MET E 144 -12.835 43.813 -58.026 1.00 30.34
H
ATOM 10065 HA MET E 144 -13.182 46.340 -58.465 1.00 33.56
H
ATOM 10066 HB2 MET E 144 -11.078 45.533 -57.994 1.00 30.28
H
ATOM 10067 HB3 MET E 144 -11.076 44.679 -59.330 1.00 30.28
H
ATOM 10068 HG2 MET E 144 -11.278 47.423 -59.653 1.00 35.29
H
ATOM 10069 HG3 MET E 144 -9.859 46.870 -59.196 1.00 35.29
H
ATOM 10070 HE1 MET E 144 -8.721 44.703 -62.015 1.00 42.68
H
ATOM 10071 HE2 MET E 144 -8.276 45.403 -60.660 1.00 42.68
H
ATOM 10072 HE3 MET E 144 -9.381 44.262 -60.639 1.00 42.68
H
ATOM 10073 N GLU E 145 -13.501 44.505 -61.059 1.00 31.93
N
ATOM 10074 CA GLU E 145 -13.949 44.488 -62.446 1.00 31.71
C
ATOM 10075 C GLU E 145 -15.462 44.676 -62.551 1.00 30.25
C
ATOM 10076 O GLU E 145 -15.959 45.154 -63.568 1.00 33.30
O
ATOM 10077 CB GLU E 145 -13.522 43.186 -63.125 1.00 33.36
C
ATOM 10078 CG GLU E 145 -12.021 43.118 -63.401 1.00 35.77
C
ATOM 10079 CD GLU E 145 -11.606 41.844 -64.115 1.00 37.01
C
ATOM 10080 OE1 GLU E 145 -12.430 40.908 -64.196 1.00 36.72
O
ATOM 10081 OE2 GLU E 145 -10.454 41.782 -64.598 1.00 37.94
O1-
ATOM 10082 H GLU E 145 -13.313 43.729 -60.738 1.00 38.32
H
ATOM 10083 HA GLU E 145 -13.526 45.222 -62.919 1.00 38.05
H
ATOM 10084 HB2 GLU E 145 -13.754 42.440 -62.550 1.00 40.04
H
ATOM 10085 HB3 GLU E 145 -13.986 43.107 -63.973 1.00 40.04
H
ATOM 10086 HG2 GLU E 145 -11.769 43.869 -63.960 1.00 42.93
H
ATOM 10087 HG3 GLU E 145 -11.544 43.157 -62.558 1.00 42.93
H
ATOM 10088 N ASP E 146 -16.188 44.314 -61.498 1.00 33.13
N
ATOM 10089 CA ASP E 146 -17.638 44.488 -61.473 1.00 33.34
C
ATOM 10090 C ASP E 146 -18.047 45.808 -60.815 1.00 39.24
C
ATOM 10091 O ASP E 146 -19.225 46.021 -60.525 1.00 45.17
O
ATOM 10092 CB ASP E 146 -18.306 43.323 -60.738 1.00 33.65
C
ATOM 10093 CG ASP E 146 -18.110 41.998 -61.444 1.00 38.71
C
ATOM 10094 OD1 ASP E 146 -17.633 42.000 -62.600 1.00 44.37
O
ATOM 10095 OD2 ASP E 146 -18.444 40.953 -60.846 1.00 37.49
O1-
ATOM 10096 H ASP E 146 -15.864 43.964 -60.782 1.00 39.75

C
ATOM 3797 O GLN B 213 -5.071 8.346 -29.111 1.00 28.14
O
ATOM 3798 CB GLN B 213 -5.357 9.735 -26.493 1.00 27.78
C
ATOM 3799 CG GLN B 213 -5.480 8.534 -25.565 1.00 30.43
C
ATOM 3800 CD GLN B 213 -6.836 8.462 -24.893 1.00 33.92
C
ATOM 3801 OE1 GLN B 213 -7.736 7.766 -25.363 1.00 34.06
O
ATOM 3802 NE2 GLN B 213 -6.991 9.185 -23.788 1.00 30.76
N
ATOM 3803 H GLN B 213 -4.519 10.917 -28.886 1.00 26.82
H
ATOM 3804 HA GLN B 213 -3.333 9.644 -26.818 1.00 29.47
H
ATOM 3805 HB2 GLN B 213 -5.329 10.533 -25.941 1.00 33.34
H
ATOM 3806 HB3 GLN B 213 -6.145 9.755 -27.057 1.00 33.34
H
ATOM 3807 HG2 GLN B 213 -5.356 7.722 -26.080 1.00 36.51
H
ATOM 3808 HG3 GLN B 213 -4.803 8.597 -24.873 1.00 36.51
H
ATOM 3809 HE21 GLN B 213 -7.742 9.177 -23.371 1.00 36.91
H
ATOM 3810 HE22 GLN B 213 -6.339 9.661 -23.491 1.00 36.91
H
ATOM 3811 N ARG B 214 -3.137 7.645 -28.192 1.00 26.52
N
ATOM 3812 CA ARG B 214 -3.047 6.450 -29.023 1.00 33.12
C
ATOM 3813 C ARG B 214 -4.103 5.415 -28.633 1.00 37.91
C
ATOM 3814 O ARG B 214 -4.624 5.431 -27.514 1.00 34.52
O
ATOM 3815 CB ARG B 214 -1.646 5.838 -28.929 1.00 42.25
C
ATOM 3816 CG ARG B 214 -0.556 6.668 -29.617 1.00 42.31
C
ATOM 3817 CD ARG B 214 0.652 5.824 -30.026 1.00 42.80
C
ATOM 3818 NE ARG B 214 0.268 4.633 -30.787 1.00 51.67
N
ATOM 3819 CZ ARG B 214 0.147 4.575 -32.112 1.00 45.75
C
ATOM 3820 NH1 ARG B 214 0.385 5.640 -32.865 1.00 40.29
N
ATOM 3821 NH2 ARG B 214 -0.212 3.438 -32.692 1.00 44.70
N
ATOM 3822 H ARG B 214 -2.488 7.735 -27.635 1.00 31.82
H
ATOM 3823 HA ARG B 214 -3.201 6.699 -29.947 1.00 39.74
H
ATOM 3824 HB2 ARG B 214 -1.405 5.751 -27.993 1.00 50.70
H
ATOM 3825 HB3 ARG B 214 -1.659 4.963 -29.347 1.00 50.70
H
ATOM 3826 HG2 ARG B 214 -0.924 7.074 -30.417 1.00 50.77
H
ATOM 3827 HG3 ARG B 214 -0.248 7.356 -29.006 1.00 50.77
H
ATOM 3828 HD2 ARG B 214 1.240 6.360 -30.582 1.00 51.36
H
ATOM 3829 HD3 ARG B 214 1.122 5.534 -29.228 1.00 51.36
H
ATOM 3830 HE ARG B 214 0.108 3.914 -30.343 1.00 62.00
H
ATOM 10097 HA ASP E 146 -17.969 44.495 -62.385 1.00 40.00
H
ATOM 10098 HB2 ASP E 146 -17.924 43.249 -59.850 1.00 40.39
H
ATOM 10099 HB3 ASP E 146 -19.259 43.492 -60.677 1.00 40.39
H
ATOM 10100 N SER E 147 -17.081 46.693 -60.585 1.00 36.27
N
ATOM 10101 CA SER E 147 -17.357 47.964 -59.919 1.00 39.56
C
ATOM 10102 C SER E 147 -18.193 48.896 -60.799 1.00 40.84
C
ATOM 10103 O SER E 147 -17.812 49.204 -61.926 1.00 41.91
O
ATOM 10104 CB SER E 147 -16.049 48.657 -59.528 1.00 40.67
C
ATOM 10105 OG SER E 147 -16.299 49.901 -58.895 1.00 39.95
O
ATOM 10106 H SER E 147 -16.257 46.582 -60.805 1.00 43.52
H
ATOM 10107 HA SER E 147 -17.859 47.792 -59.107 1.00 47.47
H
ATOM 10108 HB2 SER E 147 -15.561 48.084 -58.916 1.00 48.80
H
ATOM 10109 HB3 SER E 147 -15.523 48.811 -60.329 1.00 48.80
H
ATOM 10110 HG SER E 147 -15.573 50.269 -58.687 1.00 47.94
H
ATOM 10111 N LYS E 148 -19.326 49.349 -60.270 1.00 44.08
N
ATOM 10112 CA LYS E 148 -20.219 50.241 -61.006 1.00 49.92
C
ATOM 10113 C LYS E 148 -19.658 51.658 -61.121 1.00 48.76
C
ATOM 10114 O LYS E 148 -20.209 52.494 -61.838 1.00 51.47
O
ATOM 10115 CB LYS E 148 -21.595 50.281 -60.339 1.00 47.47
C
ATOM 10116 CG LYS E 148 -22.494 49.113 -60.710 1.00 50.15
C
ATOM 10117 CD LYS E 148 -23.784 49.125 -59.908 1.00 47.36
C
ATOM 10118 CE LYS E 148 -24.808 48.165 -60.488 1.00 50.24
C
ATOM 10119 NZ LYS E 148 -24.266 46.787 -60.642 1.00 51.53
N1+
ATOM 10120 H LYS E 148 -19.603 49.153 -59.479 1.00 52.90
H
ATOM 10121 HA LYS E 148 -20.335 49.894 -61.905 1.00 59.91
H
ATOM 10122 HB2 LYS E 148 -21.476 50.269 -59.376 1.00 56.96
H
ATOM 10123 HB3 LYS E 148 -22.047 51.098 -60.604 1.00 56.96
H
ATOM 10124 HG2 LYS E 148 -22.721 49.170 -61.651 1.00 60.18
H
ATOM 10125 HG3 LYS E 148 -22.029 48.282 -60.526 1.00 60.18
H
ATOM 10126 HD2 LYS E 148 -23.596 48.855 -58.995 1.00 56.83
H
ATOM 10127 HD3 LYS E 148 -24.162 50.018 -59.922 1.00 56.83
H
ATOM 10128 HE2 LYS E 148 -25.575 48.123 -59.896 1.00 60.29
H
ATOM 10129 HE3 LYS E 148 -25.079 48.481 -61.364 1.00 60.29
H
ATOM 10130 HZ1 LYS E 148 -24.890 46.252 -60.983 1.00 61.84

H
ATOM 3831 HH11 ARG B 214 0.617 6.382 -32.498 1.00 48.35
H
ATOM 3832 HH12 ARG B 214 0.304 5.589 -33.719 1.00 48.35
H
ATOM 3833 HH21 ARG B 214 -0.367 2.741 -32.213 1.00 53.64
H
ATOM 3834 HH22 ARG B 214 -0.289 3.397 -33.548 1.00 53.64
H
ATOM 3835 N THR B 215 -4.411 4.526 -29.575 1.00 42.55
N
ATOM 3836 CA THR B 215 -5.441 3.504 -29.396 1.00 47.95
C
ATOM 3837 C THR B 215 -6.789 4.141 -29.072 1.00 47.59
C
ATOM 3838 O THR B 215 -7.690 4.169 -29.914 1.00 48.20
O
ATOM 3839 CB THR B 215 -5.061 2.502 -28.283 1.00 45.58
C
ATOM 3840 OG1 THR B 215 -3.858 1.816 -28.651 1.00 50.86
O
ATOM 3841 CG2 THR B 215 -6.166 1.475 -28.071 1.00 55.86
C
ATOM 3842 H THR B 215 -4.028 4.494 -30.344 1.00 51.06
H
ATOM 3843 HA THR B 215 -5.537 3.008 -30.223 1.00 57.54
H
ATOM 3844 HB THR B 215 -4.920 2.980 -27.451 1.00 54.70
H
ATOM 3845 HG1 THR B 215 -3.645 1.269 -28.050 1.00 61.03
H
ATOM 3846 HG21 THR B 215 -5.911 0.855 -27.370 1.00 67.03
H
ATOM 3847 HG22 THR B 215 -6.988 1.922 -27.814 1.00 67.03
H
ATOM 3848 HG23 THR B 215 -6.320 0.980 -28.891 1.00 67.03
H

TER 3849 THR B 215
ATOM 3850 N GLU C 93 -21.096 71.394 -8.126 1.00 57.72
N
ATOM 3851 CA GLU C 93 -19.991 72.179 -7.586 1.00 64.40
C
ATOM 3852 C GLU C 93 -18.719 71.951 -8.396 1.00 60.46
C
ATOM 3853 O GLU C 93 -18.309 72.806 -9.183 1.00 62.51
O
ATOM 3854 CB GLU C 93 -19.747 71.824 -6.115 1.00 58.36
C
ATOM 3855 CG GLU C 93 -18.795 72.760 -5.383 1.00 58.10
C
ATOM 3856 CD GLU C 93 -19.458 74.063 -4.971 1.00 61.87
C
ATOM 3857 OE1 GLU C 93 -20.558 74.362 -5.481 1.00 60.81
O
ATOM 3858 OE2 GLU C 93 -18.885 74.786 -4.129 1.00 60.23
O1-
ATOM 3859 HA GLU C 93 -20.216 73.122 -7.636 1.00 77.28
H
ATOM 3860 HB2 GLU C 93 -20.596 71.844 -5.647 1.00 70.03
H
ATOM 3861 HB3 GLU C 93 -19.371 70.930 -6.071 1.00 70.03
H
ATOM 3862 HG2 GLU C 93 -18.474 72.320 -4.580 1.00 69.72
H
ATOM 3863 HG3 GLU C 93 -18.050 72.973 -5.966 1.00 69.72
H
ATOM 3864 N SER C 94 -18.107 70.787 -8.197 1.00 55.28
H
ATOM 10131 HZ2 LYS E 148 -23.562 46.796 -61.187 1.00 61.84
H
ATOM 10132 HZ3 LYS E 148 -24.014 46.470 -59.850 1.00 61.84
H
ATOM 10133 N ARG E 149 -18.566 51.925 -60.411 1.00 53.83
N
ATOM 10134 CA ARG E 149 -17.911 53.229 -60.464 1.00 58.71
C
ATOM 10135 C ARG E 149 -17.092 53.366 -61.747 1.00 57.83
C
ATOM 10136 O ARG E 149 -17.518 54.015 -62.704 1.00 57.91
O
ATOM 10137 CB ARG E 149 -17.015 53.422 -59.237 1.00 55.33
C
ATOM 10138 CG ARG E 149 -16.391 54.807 -59.099 1.00 52.08
C
ATOM 10139 CD ARG E 149 -17.379 55.834 -58.558 1.00 50.40
C
ATOM 10140 NE ARG E 149 -16.679 56.984 -57.985 1.00 49.43
N
ATOM 10141 CZ ARG E 149 -16.619 57.279 -56.687 1.00 45.97
C
ATOM 10142 NH1 ARG E 149 -17.237 56.531 -55.780 1.00 36.16
N1+
ATOM 10143 NH2 ARG E 149 -15.943 58.348 -56.292 1.00 50.80
N
ATOM 10144 H ARG E 149 -18.180 51.363 -59.887 1.00 64.60
H
ATOM 10145 HA ARG E 149 -18.586 53.925 -60.460 1.00 70.45
H
ATOM 10146 HB2 ARG E 149 -17.545 53.260 -58.441 1.00 66.39
H
ATOM 10147 HB3 ARG E 149 -16.291 52.779 -59.281 1.00 66.39
H
ATOM 10148 HG2 ARG E 149 -15.641 54.757 -58.486 1.00 62.50
H
ATOM 10149 HG3 ARG E 149 -16.091 55.108 -59.971 1.00 62.50
H
ATOM 10150 HD2 ARG E 149 -17.944 56.150 -59.280 1.00 60.48
H
ATOM 10151 HD3 ARG E 149 -17.917 55.427 -57.861 1.00 60.48
H
ATOM 10152 HE ARG E 149 -16.273 57.511 -58.530 1.00 59.32
H
ATOM 10153 HH11 ARG E 149 -17.678 55.834 -56.025 1.00 43.39
H
ATOM 10154 HH12 ARG E 149 -17.191 56.739 -54.947 1.00 43.39
H
ATOM 10155 HH21 ARG E 149 -15.543 58.842 -56.871 1.00 60.96
H
ATOM 10156 HH22 ARG E 149 -15.906 58.549 -55.457 1.00 60.96
H

TER 10157 ARG E 149

ATOM 10158 N GLY F 0 -3.228 29.760 20.619 1.00 29.41 N

ATOM 10159 CA GLY F 0 -3.768 30.515 19.453 1.00 26.44 C

ATOM 10160 C GLY F 0 -4.157 29.577 18.329 1.00 26.73 C

ATOM 10161 O GLY F 0 -4.379 28.388 18.561 1.00 25.80 O

ATOM 10162 H1 GLY F 0 -3.701 29.959 21.346 1.00 35.29 H

ATOM 10163 H2 GLY F 0 -3.283 28.886 20.459 1.00 35.29 H
ATOM 10164 H3 GLY F 0 -2.376 29.984 20.750 1.00 35.29 H

N
ATOM 3865 CA SER C 94 -16.857 70.437 -8.856 1.00 48.47
C
ATOM 3866 C SER C 94 -16.938 69.038 -9.447 1.00 42.81
C
ATOM 3867 O SER C 94 -17.428 68.105 -8.805 1.00 35.00
O
ATOM 3868 CB SER C 94 -15.690 70.525 -7.872 1.00 51.57
C
ATOM 3869 OG SER C 94 -15.518 71.852 -7.409 1.00 59.31
O
ATOM 3870 H SER C 94 -18.404 70.172 -7.673 1.00 66.34
H
ATOM 3871 HA SER C 94 -16.691 71.062 -9.579 1.00 58.16
H
ATOM 3872 HB2 SER C 94 -15.872 69.947 -7.115 1.00 61.88
H
ATOM 3873 HB3 SER C 94 -14.878 70.239 -8.320 1.00 61.88
H
ATOM 3874 HG SER C 94 -14.875 71.887 -6.870 1.00 71.18
H
ATOM 3875 N TYR C 95 -16.457 68.908 -10.678 1.00 41.19
N
ATOM 3876 CA TYR C 95 -16.444 67.634 -11.379 1.00 38.72
C
ATOM 3877 C TYR C 95 -15.019 67.168 -11.629 1.00 38.41
C
ATOM 3878 O TYR C 95 -14.099 67.975 -11.764 1.00 32.89
O
ATOM 3879 CB TYR C 95 -17.190 67.743 -12.708 1.00 37.08
C
ATOM 3880 CG TYR C 95 -18.693 67.809 -12.573 1.00 37.60
C
ATOM 3881 CD1 TYR C 95 -19.338 69.017 -12.344 1.00 41.89
C
ATOM 3882 CD2 TYR C 95 -19.469 66.663 -12.685 1.00 34.68
C
ATOM 3883 CE1 TYR C 95 -20.712 69.080 -12.226 1.00 39.87
C
ATOM 3884 CE2 TYR C 95 -20.842 66.716 -12.569 1.00 36.52
C
ATOM 3885 CZ TYR C 95 -21.459 67.926 -12.340 1.00 40.73
C
ATOM 3886 OH TYR C 95 -22.829 67.980 -12.225 1.00 41.72
O
ATOM 3887 H TYR C 95 -16.127 69.557 -11.136 1.00 49.43
H
ATOM 3888 HA TYR C 95 -16.890 66.966 -10.835 1.00 46.47
H
ATOM 3889 HB2 TYR C 95 -16.899 68.549 -13.162 1.00 44.49
H
ATOM 3890 HB3 TYR C 95 -16.976 66.967 -13.249 1.00 44.49
H
ATOM 3891 HD1 TYR C 95 -18.837 69.797 -12.267 1.00 50.27
H
ATOM 3892 HD2 TYR C 95 -19.055 65.845 -12.840 1.00 41.62
H
ATOM 3893 HE1 TYR C 95 -21.132 69.895 -12.072 1.00 47.85
H
ATOM 3894 HE2 TYR C 95 -21.348 65.940 -12.645 1.00 43.82
H
ATOM 3895 HH TYR C 95 -23.074 68.771 -12.087 1.00 50.06
H
ATOM 3896 N CYS C 96 -14.853 65.853 -11.684 1.00 35.27
N
ATOM 3897 CA CYS C 96 -13.590 65.246 -12.064 1.00 33.31
C
ATOM 3898 C CYS C 96 -13.632 64.911 -13.550 1.00 27.94

ATOM 10165 HA2 GLY F 0 -4.551 31.019 19.723 1.00 31.73
H
ATOM 10166 HA3 GLY F 0 -3.097 31.133 19.124 1.00 31.73
H

ATOM 10167 N HIS F 1 -4.237 30.106 17.110 1.00 21.94 N

ATOM 10168 CA HIS F 1 -4.640 29.302 15.960 1.00 20.81 C

ATOM 10169 C HIS F 1 -3.752 29.565 14.754 1.00 20.41 C

ATOM 10170 O HIS F 1 -3.175 30.643 14.618 1.00 18.02 O

ATOM 10171 CB HIS F 1 -6.099 29.577 15.600 1.00 19.93 C

ATOM 10172 CG HIS F 1 -7.065 29.227 16.687 1.00 24.76 C

ATOM 10173 ND1 HIS F 1 -7.406 27.926 16.989 1.00 25.09 N

ATOM 10174 CD2 HIS F 1 -7.762 30.008 17.546 1.00 26.11 C

ATOM 10175 CE1 HIS F 1 -8.273 27.921 17.986 1.00 27.35 C

ATOM 10176 NE2 HIS F 1 -8.505 29.171 18.343 1.00 27.19 N

ATOM 10177 H HIS F 1 -4.063 30.927 16.923 1.00 26.33 H

ATOM 10178 HA HIS F 1 -4.561 28.363 16.190 1.00 24.97 H

ATOM 10179 HB2 HIS F 1 -6.200 30.522 15.405 1.00 23.91 H

ATOM 10180 HB3 HIS F 1 -6.331 29.053 14.817 1.00 23.91 H

ATOM 10181 HD1 HIS F 1 -7.103 27.227 16.590 1.00 30.10 H

ATOM 10182 HD2 HIS F 1 -7.742 30.937 17.589 1.00 31.34 H

ATOM 10183 HE1 HIS F 1 -8.654 27.166 18.372 1.00 32.82 H

ATOM 10184 HE2 HIS F 1 -9.036 29.421 18.972 1.00 32.63 H

ATOM 10185 N LYS F 2 -3.635 28.568 13.884 1.00 17.59 N

ATOM 10186 CA LYS F 2 -2.874 28.734 12.658 1.00 18.28 C

ATOM 10187 C LYS F 2 -3.516 27.985 11.498 1.00 19.46 C

ATOM 10188 O LYS F 2 -4.114 26.920 11.668 1.00 15.97 O

ATOM 10189 CB LYS F 2 -1.424 28.284 12.858 1.00 21.88 C

ATOM 10190 CG LYS F 2 -1.243 26.852 13.311 1.00 29.22 C

ATOM 10191 CD LYS F 2 0.205 26.606 13.713 1.00 30.79 C

ATOM 10192 CE LYS F 2 0.429 25.175 14.167 1.00 40.64 C
ATOM 10193 NZ LYS F 2 1.839 24.947 14.592 1.00 46.99
N1+

ATOM 10194 H LYS F 2 -3.985 27.788 13.982 1.00 21.11 H

ATOM 10195 HA LYS F 2 -2.861 29.676 12.428 1.00 21.93 H
ATOM 10196 HB2 LYS F 2 -0.953 28.385 12.017 1.00 26.26
H
ATOM 10197 HB3 LYS F 2 -1.015 28.855 13.528 1.00 26.26
H
ATOM 10198 HG2 LYS F 2 -1.810 26.681 14.079 1.00 35.07

C
ATOM 3899 O CYS C 96 -14.616 64.360 -14.036 1.00 24.96
O
ATOM 3900 CB CYS C 96 -13.329 63.990 -11.232 1.00 32.47
C
ATOM 3901 SG CYS C 96 -11.682 63.299 -11.433 1.00 36.22
S
ATOM 3902 H CYS C 96 -15.470 65.283 -11.503 1.00 42.33
H
ATOM 3903 HA CYS C 96 -12.867 65.874 -11.909 1.00 39.98
H
ATOM 3904 HB2 CYS C 96 -13.445 64.208 -10.294 1.00 38.96
H
ATOM 3905 HB3 CYS C 96 -13.969 63.307 -11.490 1.00 38.96
H
ATOM 3906 N GLY C 97 -12.573 65.259 -14.272 1.00 28.67
N
ATOM 3907 CA GLY C 97 -12.490 64.946 -15.687 1.00 31.01
C
ATOM 3908 C GLY C 97 -12.065 66.130 -16.535 1.00 33.85
C
ATOM 3909 O GLY C 97 -11.450 67.067 -16.028 1.00 35.84
O
ATOM 3910 H GLY C 97 -11.888 65.677 -13.962 1.00 34.40
H
ATOM 3911 HA2 GLY C 97 -11.849 64.230 -15.820 1.00 37.22
H
ATOM 3912 HA3 GLY C 97 -13.357 64.643 -16.000 1.00 37.22
H
ATOM 3913 N PRO C 98 -12.391 66.097 -17.837 1.00 33.61
N
ATOM 3914 CA PRO C 98 -13.165 65.036 -18.492 1.00 34.25
C
ATOM 3915 C PRO C 98 -12.428 63.695 -18.552 1.00 32.91
C
ATOM 3916 O PRO C 98 -11.200 63.661 -18.522 1.00 33.58
O
ATOM 3917 CB PRO C 98 -13.400 65.596 -19.897 1.00 43.48
C
ATOM 3918 CG PRO C 98 -12.285 66.542 -20.119 1.00 44.16
C
ATOM 3919 CD PRO C 98 -11.991 67.149 -18.785 1.00 39.32
C
ATOM 3920 HA PRO C 98 -14.019 64.916 -18.046 1.00 41.10
H
ATOM 3921 HB2 PRO C 98 -13.374 64.875 -20.546 1.00 52.18
H
ATOM 3922 HB3 PRO C 98 -14.253 66.056 -19.928 1.00 52.18
H
ATOM 3923 HG2 PRO C 98 -11.512 66.060 -20.452 1.00 52.99
H
ATOM 3924 HG3 PRO C 98 -12.560 67.225 -20.751 1.00 52.99
H
ATOM 3925 HD2 PRO C 98 -11.043 67.337 -18.701 1.00 47.19
H
ATOM 3926 HD3 PRO C 98 -12.526 67.946 -18.651 1.00 47.19
H
ATOM 3927 N CYS C 99 -13.195 62.610 -18.619 1.00 29.92
N
ATOM 3928 CA CYS C 99 -12.656 61.259 -18.747 1.00 30.84
C
ATOM 3929 C CYS C 99 -13.492 60.459 -19.732 1.00 33.78
C
ATOM 3930 O CYS C 99 -14.602 60.863 -20.076 1.00 29.20
O
ATOM 3931 CB CYS C 99 -12.646 60.535 -17.400 1.00 24.67
C
ATOM 3932 SG CYS C 99 -11.422 61.121 -16.229 1.00 27.04
H
ATOM 10199 HG3 LYS F 2 -1.467 26.252 12.583 1.00 35.07
H
ATOM 10200 HD2 LYS F 2 0.781 26.775 12.951 1.00 36.94
H
ATOM 10201 HD3 LYS F 2 0.438 27.196 14.446 1.00 36.94
H
ATOM 10202 HE2 LYS F 2 -0.150 24.985 14.921 1.00 48.77
H
ATOM 10203 HE3 LYS F 2 0.233 24.573 13.433 1.00 48.77 H
ATOM 10204 HZ1 LYS F 2 2.043 25.487 15.270 1.00 56.39 H
ATOM 10205 HZ2 LYS F 2 1.944 24.103 14.854 1.00 56.39 H
ATOM 10206 HZ3 LYS F 2 2.391 25.111 13.914 1.00 56.39 H
ATOM 10207 N LEU F 3 -3.404 28.589 10.321 1.00 18.68 N
ATOM 10208 CA LEU F 3 -3.925 28.030 9.086 1.00 17.42 C
ATOM 10209 C LEU F 3 -2.752 27.857 8.134 1.00 16.58 C
ATOM 10210 O LEU F 3 -2.066 28.828 7.807 1.00 15.05 O
ATOM 10211 CB LEU F 3 -4.995 28.945 8.485 1.00 15.28 C
ATOM 10212 CG LEU F 3 -5.747 28.440 7.256 1.00 18.11 C
ATOM 10213 CD1 LEU F 3 -6.670 27.286 7.622 1.00 17.93 C
ATOM 10214 CD2 LEU F 3 -6.527 29.581 6.615 1.00 15.66 C
ATOM 10215 H LEU F 3 -3.016 29.349 10.212 1.00 22.41 H
ATOM 10216 HA LEU F 3 -4.319 27.160 9.258 1.00 20.90 H
ATOM 10217 HB2 LEU F 3 -5.657 29.121 9.171 1.00 18.34 H
ATOM 10218 HB3 LEU F 3 -4.568 29.779 8.234 1.00 18.34 H
ATOM 10219 HG LEU F 3 -5.105 28.115 6.606 1.00 21.73 H
ATOM 10220 HD11 LEU F 3 -7.134 26.987 6.824 1.00 21.52
H
ATOM 10221 HD12 LEU F 3 -6.139 26.561 7.987 1.00 21.52
H
ATOM 10222 HD13 LEU F 3 -7.312 27.592 8.282 1.00 21.52
H
ATOM 10223 HD21 LEU F 3 -6.998 29.243 5.837 1.00 18.80
H
ATOM 10224 HD22 LEU F 3 -7.162 29.931 7.260 1.00 18.80
H
ATOM 10225 HD23 LEU F 3 -5.906 30.278 6.349 1.00 18.80
H
ATOM 10226 N ALA F 4 -2.520 26.620 7.706 1.00 17.17 N
ATOM 10227 CA ALA F 4 -1.347 26.278 6.911 1.00 13.80 C
ATOM 10228 C ALA F 4 -1.737 25.668 5.570 1.00 18.72 C
ATOM 10229 O ALA F 4 -2.616 24.807 5.492 1.00 15.41 O
ATOM 10230 CB ALA F 4 -0.455 25.321 7.681 1.00 16.99 C
ATOM 10231 H ALA F 4 -3.037 25.951 7.865 1.00 20.60 H
ATOM 10232 HA ALA F 4 -0.839 27.085 6.736 1.00 16.56 H

S
ATOM 3933 H CYS C 99 -14.054 62.632 -18.593 1.00 35.90
H
ATOM 3934 HA CYS C 99 -11.746 61.303 -19.079 1.00 37.01
H
ATOM 3935 HB2 CYS C 99 -13.518 60.639 -16.987 1.00 29.60
H
ATOM 3936 HB3 CYS C 99 -12.473 59.593 -17.557 1.00 29.60
H
ATOM 3937 N PRO C 100 -12.963 59.314 -20.190 1.00 30.07
N
ATOM 3938 CA PRO C 100 -13.800 58.399 -20.968 1.00 29.87
C
ATOM 3939 C PRO C 100 -14.997 57.928 -20.148 1.00 33.56
C
ATOM 3940 O PRO C 100 -14.919 57.895 -18.917 1.00 26.53
O
ATOM 3941 CB PRO C 100 -12.852 57.239 -21.291 1.00 30.74
C
ATOM 3942 CG PRO C 100 -11.483 57.830 -21.199 1.00 29.98
C
ATOM 3943 CD PRO C 100 -11.566 58.853 -20.110 1.00 28.76
C
ATOM 3944 HA PRO C 100 -14.102 58.818 -21.789 1.00 35.84
H
ATOM 3945 HB2 PRO C 100 -12.965 56.531 -20.638 1.00 36.89
H
ATOM 3946 HB3 PRO C 100 -13.026 56.912 -22.188 1.00 36.89
H
ATOM 3947 HG2 PRO C 100 -10.843 57.138 -20.971 1.00 35.98
H
ATOM 3948 HG3 PRO C 100 -11.251 58.248 -22.043 1.00 35.98
H
ATOM 3949 HD2 PRO C 100 -11.393 58.444 -19.247 1.00 34.51
H
ATOM 3950 HD3 PRO C 100 -10.956 59.586 -20.286 1.00 34.51
H
ATOM 3951 N LYS C 101 -16.086 57.579 -20.825 1.00 31.45
N
ATOM 3952 CA LYS C 101 -17.315 57.171 -20.154 1.00 38.12
C
ATOM 3953 C LYS C 101 -17.066 56.015 -19.182 1.00 30.89
C
ATOM 3954 O LYS C 101 -16.410 55.034 -19.529 1.00 28.71
O
ATOM 3955 CB LYS C 101 -18.373 56.768 -21.188 1.00 43.70
C
ATOM 3956 CG LYS C 101 -19.776 56.557 -20.620 1.00 55.10
C
ATOM 3957 CD LYS C 101 -20.514 57.877 -20.423 1.00 71.07
C
ATOM 3958 CE LYS C 101 -21.918 57.662 -19.866 1.00 83.53
C
ATOM 3959 NZ LYS C 101 -22.935 57.438 -20.932 1.00 96.55
N1+
ATOM 3960 H LYS C 101 -16.139 57.570 -21.684 1.00 37.74
H
ATOM 3961 HA LYS C 101 -17.662 57.921 -19.645 1.00 45.75
H
ATOM 3962 HB2 LYS C 101 -18.431 57.465 -21.860 1.00 52.44
H
ATOM 3963 HB3 LYS C 101 -18.098 55.936 -21.605 1.00 52.44
H
ATOM 3964 HG2 LYS C 101 -20.291 56.011 -21.235 1.00 66.13
H
ATOM 3965 HG3 LYS C 101 -19.708 56.117 -19.758 1.00 66.13
H
ATOM 3966 HD2 LYS C 101 -20.020 58.428 -19.797 1.00 85.28

ATOM 10233 HB1 ALA F 4 0.319 25.105 7.138 1.00 20.38 H
ATOM 10234 HB2 ALA F 4 -0.172 25.747 8.506 1.00 20.38 H
ATOM 10235 HB3 ALA F 4 -0.955 24.514 7.880 1.00 20.38 H
ATOM 10236 N PHE F 5 -1.065 26.132 4.522 1.00 14.07 N
ATOM 10237 CA PHE F 5 -1.247 25.619 3.171 1.00 15.88 C
ATOM 10238 C PHE F 5 0.038 24.967 2.696 1.00 17.08 C
ATOM 10239 O PHE F 5 1.085 25.610 2.658 1.00 19.17 O
ATOM 10240 CB PHE F 5 -1.642 26.742 2.213 1.00 11.34 C
ATOM 10241 CG PHE F 5 -2.919 27.422 2.580 1.00 10.85 C
ATOM 10242 CD1 PHE F 5 -2.940 28.405 3.554 1.00 13.28 C
ATOM 10243 CD2 PHE F 5 -4.100 27.084 1.953 1.00 12.14 C
ATOM 10244 CE1 PHE F 5 -4.120 29.036 3.893 1.00 13.84 C
ATOM 10245 CE2 PHE F 5 -5.280 27.712 2.288 1.00 11.37 C
ATOM 10246 CZ PHE F 5 -5.291 28.686 3.258 1.00 14.78 C
ATOM 10247 H PHE F 5 -0.481 26.761 4.571 1.00 16.89 H
ATOM 10248 HA PHE F 5 -1.951 24.952 3.169 1.00 19.06 H
ATOM 10249 HB2 PHE F 5 -0.940 27.411 2.209 1.00 13.61 H
ATOM 10250 HB3 PHE F 5 -1.749 26.371 1.323 1.00 13.61 H
ATOM 10251 HD1 PHE F 5 -2.151 28.643 3.984 1.00 15.93 H
ATOM 10252 HD2 PHE F 5 -4.100 26.425 1.296 1.00 14.56 H
ATOM 10253 HE1 PHE F 5 -4.124 29.695 4.549 1.00 16.61 H
ATOM 10254 HE2 PHE F 5 -6.070 27.475 1.859 1.00 13.65 H
ATOM 10255 HZ PHE F 5 -6.087 29.109 3.484 1.00 17.73 H
ATOM 10256 N ASN F 6 -0.047 23.691 2.336 1.00 16.88 N
ATOM 10257 CA ASN F 6 1.106 22.963 1.838 1.00 14.07 C
ATOM 10258 C ASN F 6 0.919 22.591 0.376 1.00 16.67 C
ATOM 10259 O ASN F 6 0.153 21.682 0.056 1.00 16.36 O
ATOM 10260 CB ASN F 6 1.348 21.713 2.679 1.00 20.64 C
ATOM 10261 CG ASN F 6 2.626 21.000 2.300 1.00 26.49 C
ATOM 10262 OD1 ASN F 6 2.607 20.029 1.548 1.00 33.61
O
ATOM 10263 ND2 ASN F 6 3.748 21.486 2.814 1.00 26.66 N
ATOM 10264 H ASN F 6 -0.768 23.223 2.373 1.00 20.26 H
ATOM 10265 HA ASN F 6 1.892 23.528 1.906 1.00 16.89 H
ATOM 10266 HB2 ASN F 6 1.411 21.966 3.613 1.00 24.77 H

H
ATOM 3967 HD3 LYS C 101 -20.593 58.329 -21.278 1.00 85.28
H
ATOM 3968 HE2 LYS C 101 -21.912 56.882 -19.288 1.00100.24
H
ATOM 3969 HE3 LYS C 101 -22.180 58.447 -19.360 1.00100.24
H
ATOM 3970 HZ1 LYS C 101 -23.738 57.318 -20.567 1.00115.86
H
ATOM 3971 HZ2 LYS C 101 -22.967 58.143 -21.474 1.00115.86
H
ATOM 3972 HZ3 LYS C 101 -22.723 56.717 -21.409 1.00115.86
H
ATOM 3973 N ASN C 102 -17.578 56.160 -17.962 1.00 29.40
N
ATOM 3974 CA ASN C 102 -17.566 55.095 -16.957 1.00 21.26
C
ATOM 3975 C ASN C 102 -16.171 54.670 -16.501 1.00 23.13
C
ATOM 3976 O ASN C 102 -15.980 53.538 -16.052 1.00 23.84
O
ATOM 3977 CB ASN C 102 -18.317 53.871 -17.484 1.00 26.84
C
ATOM 3978 CG ASN C 102 -19.758 54.178 -17.827 1.00 37.50
C
ATOM 3979 OD1 ASN C 102 -20.390 55.027 -17.198 1.00 35.99
O
ATOM 3980 ND2 ASN C 102 -20.288 53.491 -18.833 1.00 39.34
N
ATOM 3981 H ASN C 102 -17.948 56.885 -17.684 1.00 35.28
H
ATOM 3982 HA ASN C 102 -18.042 55.411 -16.173 1.00 25.51
H
ATOM 3983 HB2 ASN C 102 -17.878 53.551 -18.287 1.00 32.21
H
ATOM 3984 HB3 ASN C 102 -18.311 53.179 -16.804 1.00 32.21
H
ATOM 3985 HD21 ASN C 102 -21.104 53.630 -19.066 1.00 47.21
H
ATOM 3986 HD22 ASN C 102 -19.814 52.907 -19.251 1.00 47.21
H
ATOM 3987 N TRP C 103 -15.202 55.573 -16.611 1.00 20.50
N
ATOM 3988 CA TRP C 103 -13.880 55.343 -16.034 1.00 23.43
C
ATOM 3989 C TRP C 103 -13.826 55.907 -14.620 1.00 21.27
C
ATOM 3990 O TRP C 103 -14.659 56.727 -14.239 1.00 23.07
O
ATOM 3991 CB TRP C 103 -12.785 55.984 -16.889 1.00 21.36
C
ATOM 3992 CG TRP C 103 -12.438 55.213 -18.124 1.00 22.71
C
ATOM 3993 CD1 TRP C 103 -13.270 54.420 -18.857 1.00 24.15
C
ATOM 3994 CD2 TRP C 103 -11.158 55.158 -18.771 1.00 19.27
C
ATOM 3995 NE1 TRP C 103 -12.591 53.880 -19.923 1.00 20.72
N
ATOM 3996 CE2 TRP C 103 -11.293 54.317 -19.891 1.00 20.30
C
ATOM 3997 CE3 TRP C 103 -9.914 55.737 -18.508 1.00 20.40
C
ATOM 3998 CZ2 TRP C 103 -10.230 54.042 -20.751 1.00 24.78
C
ATOM 3999 CZ3 TRP C 103 -8.862 55.465 -19.360 1.00 20.79
C
ATOM 4000 CH2 TRP C 103 -9.026 54.624 -20.468 1.00 22.99
ATOM 10267 HB3 ASN F 6 0.611 21.096 2.550 1.00 24.77 H
ATOM 10268 HD21 ASN F 6 4.502 21.116 2.629 1.00 32.00
H
ATOM 10269 HD22 ASN F 6 3.722 22.171 3.333 1.00 32.00
H
ATOM 10270 N PHE F 7 1.618 23.318 -0.497 1.00 14.97 N
ATOM 10271 CA PHE F 7 1.580 23.101 -1.939 1.00 12.47 C
ATOM 10272 C PHE F 7 2.716 22.190 -2.376 1.00 15.61 C
ATOM 10273 O PHE F 7 3.871 22.427 -2.029 1.00 16.76 O
ATOM 10274 CB PHE F 7 1.695 24.426 -2.696 1.00 12.90 C
ATOM 10275 CG PHE F 7 0.586 25.391 -2.415 1.00 12.41 C
ATOM 10276 CD1 PHE F 7 0.627 26.208 -1.299 1.00 15.02 C
ATOM 10277 CD2 PHE F 7 -0.491 25.494 -3.277 1.00 13.17
C
ATOM 10278 CE1 PHE F 7 -0.392 27.108 -1.041 1.00 14.33 C
ATOM 10279 CE2 PHE F 7 -1.516 26.392 -3.023 1.00 15.79 C
ATOM 10280 CZ PHE F 7 -1.463 27.200 -1.902 1.00 14.48 C
ATOM 10281 H PHE F 7 2.138 23.963 -0.267 1.00 17.96 H
ATOM 10282 HA PHE F 7 0.739 22.681 -2.180 1.00 14.96 H
ATOM 10283 HB2 PHE F 7 2.529 24.855 -2.448 1.00 15.48 H
ATOM 10284 HB3 PHE F 7 1.692 24.242 -3.649 1.00 15.48 H
ATOM 10285 HD1 PHE F 7 1.348 26.150 -0.714 1.00 18.02 H
ATOM 10286 HD2 PHE F 7 -0.530 24.953 -4.032 1.00 15.81
H
ATOM 10287 HE1 PHE F 7 -0.355 27.649 -0.285 1.00 17.19 H
ATOM 10288 HE2 PHE F 7 -2.238 26.452 -3.607 1.00 18.95 H
ATOM 10289 HZ PHE F 7 -2.150 27.803 -1.729 1.00 17.38 H
ATOM 10290 N ASN F 8 2.390 21.165 -3.153 1.00 17.16 N
ATOM 10291 CA ASN F 8 3.399 20.249 -3.662 1.00 18.00 C
ATOM 10292 C ASN F 8 3.214 19.985 -5.147 1.00 19.06 C
ATOM 10293 O ASN F 8 2.111 19.667 -5.601 1.00 19.50 O
ATOM 10294 CB ASN F 8 3.363 18.931 -2.891 1.00 21.59 C
ATOM 10295 CG ASN F 8 4.399 17.940 -3.386 1.00 25.54 C
ATOM 10296 OD1 ASN F 8 4.066 16.957 -4.047 1.00 28.38
O
ATOM 10297 ND2 ASN F 8 5.664 18.203 -3.080 1.00 27.01 N
ATOM 10298 H ASN F 8 1.588 20.978 -3.400 1.00 20.60 H
ATOM 10299 HA ASN F 8 4.275 20.645 -3.536 1.00 21.60 H
ATOM 10300 HB2 ASN F 8 3.540 19.108 -1.953 1.00 25.91 H

C
ATOM 4001 H TRP C 103 -15.284 56.328 -17.014 1.00 24.60
H
ATOM 4002 HA TRP C 103 -13.712 54.389 -15.989 1.00 28.12
H
ATOM 4003 HB2 TRP C 103 -13.082 56.865 -17.165 1.00 25.64
H
ATOM 4004 HB3 TRP C 103 -11.979 56.063 -16.355 1.00 25.64
H
ATOM 4005 HD1 TRP C 103 -14.169 54.273 -18.669 1.00 28.98
H
ATOM 4006 HE1 TRP C 103 -12.926 53.352 -20.514 1.00 24.87
H
ATOM 4007 HE3 TRP C 103 -9.797 56.298 -17.776 1.00 24.47
H
ATOM 4008 HZ2 TRP C 103 -10.336 53.482 -21.486 1.00 29.74
H
ATOM 4009 HZ3 TRP C 103 -8.030 55.848 -19.196 1.00 24.95
H
ATOM 4010 HH2 TRP C 103 -8.299 54.458 -21.025 1.00 27.58
H
ATOM 4011 N ILE C 104 -12.852 55.455 -13.838 1.00 21.47
N
ATOM 4012 CA ILE C 104 -12.562 56.076 -12.552 1.00 22.27
C
ATOM 4013 C ILE C 104 -11.920 57.428 -12.799 1.00 20.16
C
ATOM 4014 O ILE C 104 -11.097 57.559 -13.694 1.00 20.40
O
ATOM 4015 CB ILE C 104 -11.618 55.218 -11.691 1.00 20.98
C
ATOM 4016 CG1 ILE C 104 -12.318 53.922 -11.276 1.00 23.82
C
ATOM 4017 CG2 ILE C 104 -11.151 56.005 -10.452 1.00 22.89
C
ATOM 4018 CD1 ILE C 104 -11.469 53.000 -10.418 1.00 32.17
C
ATOM 4019 H ILE C 104 -12.343 54.789 -14.030 1.00 25.76
H
ATOM 4020 HA ILE C 104 -13.389 56.212 -12.062 1.00 26.72
H
ATOM 4021 HB ILE C 104 -10.839 54.991 -12.222 1.00 25.18
H
ATOM 4022 HG12 ILE C 104 -13.114 54.147 -10.769 1.00 28.58
H
ATOM 4023 HG13 ILE C 104 -12.567 53.433 -12.076 1.00 28.58
H
ATOM 4024 HG21 ILE C 104 -10.559 55.444 -9.927 1.00 27.46
H
ATOM 4025 HG22 ILE C 104 -10.681 56.802 -10.744 1.00 27.46
H
ATOM 4026 HG23 ILE C 104 -11.927 56.252 -9.925 1.00 27.46
H
ATOM 4027 HD11 ILE C 104 -11.984 52.208 -10.201 1.00 38.61
H
ATOM 4028 HD12 ILE C 104 -10.673 52.752 -10.915 1.00 38.61
H
ATOM 4029 HD13 ILE C 104 -11.220 53.467 -9.605 1.00 38.61
H
ATOM 4030 N CYS C 105 -12.291 58.426 -12.005 1.00 18.50
N
ATOM 4031 CA CYS C 105 -11.642 59.730 -12.068 1.00 21.47
C
ATOM 4032 C CYS C 105 -11.168 60.124 -10.673 1.00 24.11
C
ATOM 4033 O CYS C 105 -11.949 60.137 -9.720 1.00 22.75
O
ATOM 4034 CB CYS C 105 -12.592 60.783 -12.641 1.00 24.61

ATOM 10301 HB3 ASN F 8 2.487 18.527 -2.993 1.00 25.91 H
ATOM 10302 HD21 ASN F 8 6.288 17.671 -3.338 1.00 32.41
H
ATOM 10303 HD22 ASN F 8 5.859 18.906 -2.624 1.00 32.41
H

ATOM 10304 N LEU F 9 4.302 20.141 -5.894 1.00 17.68 N

ATOM 10305 CA LEU F 9 4.342 19.779 -7.306 1.00 18.16 C

ATOM 10306 C LEU F 9 5.423 18.732 -7.510 1.00 19.22 C

ATOM 10307 O LEU F 9 6.607 19.007 -7.327 1.00 16.70 O

ATOM 10308 CB LEU F 9 4.610 21.001 -8.190 1.00 12.54 C

ATOM 10309 CG LEU F 9 4.756 20.712 -9.690 1.00 15.42 C
ATOM 10310 CD1 LEU F 9 3.456 20.192 -10.273 1.00 21.54
C
ATOM 10311 CD2 LEU F 9 5.212 21.955 -10.437 1.00 17.32
C

ATOM 10312 H LEU F 9 5.044 20.461 -5.600 1.00 21.21 H

ATOM 10313 HA LEU F 9 3.490 19.395 -7.564 1.00 21.79 H

ATOM 10314 HB2 LEU F 9 3.874 21.624 -8.084 1.00 15.05 H

ATOM 10315 HB3 LEU F 9 5.434 21.419 -7.893 1.00 15.05 H

ATOM 10316 HG LEU F 9 5.431 20.027 -9.813 1.00 18.50 H
ATOM 10317 HD11 LEU F 9 3.581 20.020 -11.219 1.00 25.85
H
ATOM 10318 HD12 LEU F 9 3.211 19.372 -9.816 1.00 25.85
H
ATOM 10319 HD13 LEU F 9 2.764 20.860 -10.146 1.00 25.85
H
ATOM 10320 HD21 LEU F 9 5.295 21.744 -11.380 1.00 20.79
H
ATOM 10321 HD22 LEU F 9 4.554 22.657 -10.312 1.00 20.79
H
ATOM 10322 HD23 LEU F 9 6.070 22.238 -10.084 1.00 20.79
H

ATOM 10323 N GLU F 10 4.995 17.529 -7.874 1.00 21.49 N

ATOM 10324 CA GLU F 10 5.898 16.421 -8.146 1.00 23.67 C

ATOM 10325 C GLU F 10 6.031 16.251 -9.654 1.00 24.38 C

ATOM 10326 O GLU F 10 5.045 15.994 -10.343 1.00 21.67 O

ATOM 10327 CB GLU F 10 5.380 15.135 -7.494 1.00 28.50 C
ATOM 10328 CG GLU F 10 6.252 13.911 -7.718 1.00 39.90
C

ATOM 10329 CD GLU F 10 5.703 12.675 -7.023 1.00 46.88 C
ATOM 10330 OE1 GLU F 10 5.964 11.553 -7.505 1.00 53.49
O
ATOM 10331 OE2 GLU F 10 5.010 12.825 -5.994 1.00 53.38
O1-

ATOM 10332 H GLU F 10 4.165 17.326 -7.973 1.00 25.79 H

ATOM 10333 HA GLU F 10 6.775 16.620 -7.780 1.00 28.41 H
ATOM 10334 HB2 GLU F 10 5.316 15.279 -6.537 1.00 34.20

C
ATOM 4035 SG CYS C 105 -11.757 62.290 -13.195 1.00 30.83
S
ATOM 4036 H CYS C 105 -12.918 58.373 -11.418 1.00 22.20
H
ATOM 4037 HA CYS C 105 -10.867 59.673 -12.648 1.00 25.76
H
ATOM 4038 HB2 CYS C 105 -13.056 60.403 -13.404 1.00 29.53
H
ATOM 4039 HB3 CYS C 105 -13.232 61.032 -11.957 1.00 29.53
H
ATOM 4040 N TYR C 106 -9.880 60.430 -10.556 1.00 20.57
N
ATOM 4041 CA TYR C 106 -9.279 60.704 -9.259 1.00 19.53
C
ATOM 4042 C TYR C 106 -8.063 61.607 -9.395 1.00 24.23
C
ATOM 4043 O TYR C 106 -7.074 61.243 -10.036 1.00 18.60
O
ATOM 4044 CB TYR C 106 -8.885 59.394 -8.580 1.00 18.96
C
ATOM 4045 CG TYR C 106 -8.336 59.537 -7.183 1.00 17.51
C
ATOM 4046 CD1 TYR C 106 -9.161 59.887 -6.128 1.00 20.97
C
ATOM 4047 CD2 TYR C 106 -6.995 59.293 -6.912 1.00 20.26
C
ATOM 4048 CE1 TYR C 106 -8.669 60.006 -4.846 1.00 22.20
C
ATOM 4049 CE2 TYR C 106 -6.494 59.405 -5.629 1.00 20.01
C
ATOM 4050 CZ TYR C 106 -7.339 59.764 -4.599 1.00 22.79
C
ATOM 4051 OH TYR C 106 -6.864 59.881 -3.313 1.00 24.09
O
ATOM 4052 H TYR C 106 -9.332 60.486 -11.217 1.00 24.68
H
ATOM 4053 HA TYR C 106 -9.928 61.153 -8.696 1.00 23.44
H
ATOM 4054 HB2 TYR C 106 -9.670 58.826 -8.529 1.00 22.75
H
ATOM 4055 HB3 TYR C 106 -8.205 58.960 -9.119 1.00 22.75
H
ATOM 4056 HD1 TYR C 106 -10.062 60.051 -6.288 1.00 25.17
H
ATOM 4057 HD2 TYR C 106 -6.425 59.049 -7.606 1.00 24.31
H
ATOM 4058 HE1 TYR C 106 -9.237 60.246 -4.149 1.00 26.64
H
ATOM 4059 HE2 TYR C 106 -5.594 59.243 -5.461 1.00 24.02
H
ATOM 4060 HH TYR C 106 -6.042 59.709 -3.293 1.00 28.90
H
ATOM 4061 N LYS C 107 -8.157 62.784 -8.783 1.00 23.77
N
ATOM 4062 CA LYS C 107 -7.070 63.754 -8.756 1.00 22.66
C
ATOM 4063 C LYS C 107 -6.482 63.992 -10.144 1.00 26.25
C
ATOM 4064 O LYS C 107 -5.304 63.722 -10.384 1.00 25.69
O
ATOM 4065 CB LYS C 107 -5.982 63.288 -7.786 1.00 23.70
C
ATOM 4066 CG LYS C 107 -6.453 63.225 -6.341 1.00 25.76
C
ATOM 4067 CD LYS C 107 -5.337 62.830 -5.392 1.00 24.07
C
ATOM 4068 CE LYS C 107 -5.787 62.932 -3.946 1.00 25.09
H
ATOM 10335 HB3 GLU F 10 4.501 14.939 -7.854 1.00 34.20
H
ATOM 10336 HG2 GLU F 10 6.301 13.726 -8.668 1.00 47.88
H
ATOM 10337 HG3 GLU F 10 7.139 14.085 -7.366 1.00 47.88
H

ATOM 10338 N ILE F 11 7.251 16.419 -10.156 1.00 23.21 N

ATOM 10339 CA ILE F 11 7.533 16.310 -11.584 1.00 25.02 C

ATOM 10340 C ILE F 11 8.327 15.040 -11.859 1.00 29.40 C

ATOM 10341 O ILE F 11 9.479 14.924 -11.444 1.00 28.51 O

ATOM 10342 CB ILE F 11 8.328 17.527 -12.103 1.00 22.20 C
ATOM 10343 CG1 ILE F 11 7.615 18.831 -11.736 1.00 24.16
C
ATOM 10344 CG2 ILE F 11 8.526 17.429 -13.613 1.00 24.02
C

ATOM 10345 CD1 ILE F 11 8.442 20.071 -11.975 1.00 25.01 C

ATOM 10346 H ILE F 11 7.945 16.600 -9.681 1.00 27.85 H

ATOM 10347 HA ILE F 11 6.697 16.260 -12.073 1.00 30.03 H

ATOM 10348 HB ILE F 11 9.200 17.526 -11.679 1.00 26.63 H
ATOM 10349 HG12 ILE F 11 6.808 18.906 -12.270 1.00 28.99
H
ATOM 10350 HG13 ILE F 11 7.384 18.806 -10.794 1.00 28.99
H
ATOM 10351 HG21 ILE F 11 9.027 18.203 -13.916 1.00 28.83
H
ATOM 10352 HG22 ILE F 11 9.016 16.617 -13.815 1.00 28.83
H
ATOM 10353 HG23 ILE F 11 7.657 17.408 -14.044 1.00 28.83
H
ATOM 10354 HD11 ILE F 11 7.923 20.850 -11.720 1.00 30.01
H
ATOM 10355 HD12 ILE F 11 9.248 20.020 -11.438 1.00 30.01
H
ATOM 10356 HD13 ILE F 11 8.672 20.120 -12.916 1.00 30.01
H

ATOM 10357 N ASN F 12 7.703 14.090 -12.549 1.00 32.32 N
ATOM 10358 CA ASN F 12 8.372 12.856 -12.939 1.00 39.08
C

ATOM 10359 C ASN F 12 8.394 12.742 -14.461 1.00 41.01 C

ATOM 10360 O ASN F 12 7.444 12.261 -15.081 1.00 32.24 O
ATOM 10361 CB ASN F 12 7.683 11.646 -12.306 1.00 42.36
C
ATOM 10362 CG ASN F 12 8.618 10.462 -12.149 1.00 49.52
C
ATOM 10363 OD1 ASN F 12 9.445 10.190 -13.019 1.00 51.85
O
ATOM 10364 ND2 ASN F 12 8.501 9.760 -11.027 1.00 49.58
N

ATOM 10365 H ASN F 12 6.884 14.138 -12.805 1.00 38.78 H
ATOM 10366 HA ASN F 12 9.289 12.879 -12.625 1.00 46.89
H
ATOM 10367 HB2 ASN F 12 7.358 11.891 -11.426 1.00 50.83
H
ATOM 10368 HB3 ASN F 12 6.943 11.372 -12.870 1.00 50.83

C
ATOM 4069 NZ LYS C 107 -4.764 62.412 -3.002 1.00 28.21
N1+
ATOM 4070 H LYS C 107 -8.860 63.049 -8.365 1.00 28.53
H
ATOM 4071 HA LYS C 107 -7.415 64.600 -8.431 1.00 27.19
H
ATOM 4072 HB2 LYS C 107 -5.690 62.399 -8.043 1.00 28.45
H
ATOM 4073 HB3 LYS C 107 -5.236 63.906 -7.830 1.00 28.45
H
ATOM 4074 HG2 LYS C 107 -6.780 64.099 -6.076 1.00 30.91
H
ATOM 4075 HG3 LYS C 107 -7.161 62.567 -6.266 1.00 30.91
H
ATOM 4076 HD2 LYS C 107 -5.077 61.911 -5.566 1.00 28.88
H
ATOM 4077 HD3 LYS C 107 -4.581 63.424 -5.519 1.00 28.88
H
ATOM 4078 HE2 LYS C 107 -5.952 63.863 -3.729 1.00 30.11
H
ATOM 4079 HE3 LYS C 107 -6.599 62.414 -3.828 1.00 30.11
H
ATOM 4080 HZ1 LYS C 107 -4.009 62.875 -3.086 1.00 33.85
H
ATOM 4081 HZ2 LYS C 107 -5.058 62.486 -2.165 1.00 33.85
H
ATOM 4082 HZ3 LYS C 107 -4.598 61.555 -3.175 1.00 33.85
H
ATOM 4083 N ASN C 108 -7.324 64.477 -11.052 1.00 24.30
N
ATOM 4084 CA ASN C 108 -6.908 64.862 -12.399 1.00 29.43
C
ATOM 4085 C ASN C 108 -6.390 63.700 -13.248 1.00 29.94
C
ATOM 4086 O ASN C 108 -5.692 63.920 -14.238 1.00 30.74
O
ATOM 4087 CB ASN C 108 -5.834 65.950 -12.322 1.00 37.42
C
ATOM 4088 CG ASN C 108 -6.243 67.111 -11.434 1.00 39.33
C
ATOM 4089 OD1 ASN C 108 -7.357 67.623 -11.536 1.00 36.77
O
ATOM 4090 ND2 ASN C 108 -5.341 67.526 -10.549 1.00 38.25
N
ATOM 4091 H ASN C 108 -8.163 64.595 -10.908 1.00 29.16
H
ATOM 4092 HA ASN C 108 -7.674 65.239 -12.859 1.00 35.31
H
ATOM 4093 HB2 ASN C 108 -5.020 65.566 -11.959 1.00 44.91
H
ATOM 4094 HB3 ASN C 108 -5.670 66.296 -13.213 1.00 44.91
H
ATOM 4095 HD21 ASN C 108 -5.525 68.181 -10.023 1.00 45.91
H
ATOM 4096 HD22 ASN C 108 -4.574 67.140 -10.503 1.00 45.91
H
ATOM 4097 N ASN C 109 -6.729 62.472 -12.863 1.00 22.35
N
ATOM 4098 CA ASN C 109 -6.364 61.294 -13.650 1.00 21.33
C
ATOM 4099 C ASN C 109 -7.542 60.352 -13.846 1.00 21.79
C
ATOM 4100 O ASN C 109 -8.331 60.125 -12.924 1.00 20.85
O
ATOM 4101 CB ASN C 109 -5.211 60.538 -12.986 1.00 24.32
C
ATOM 4102 CG ASN C 109 -3.921 61.337 -12.968 1.00 22.95
H
ATOM 10369 HD21 ASN F 12 9.008 9.079 -10.891 1.00 59.50
H
ATOM 10370 HD22 ASN F 12 7.918 9.986 -10.437 1.00 59.50
H

ATOM 10371 N GLY F 13 9.490 13.206 -15.057 1.00 43.87 N
ATOM 10372 CA GLY F 13 9.594 13.288 -16.500 1.00 37.61
C

ATOM 10373 C GLY F 13 8.548 14.247 -17.031 1.00 34.27 C

ATOM 10374 O GLY F 13 8.500 15.409 -16.628 1.00 38.41 O
ATOM 10375 H GLY F 13 10.190 13.479 -14.639 1.00 52.65
H
ATOM 10376 HA2 GLY F 13 10.474 13.609 -16.752 1.00 45.13
H
ATOM 10377 HA3 GLY F 13 9.451 12.414 -16.895 1.00 45.13
H

ATOM 10378 N SER F 14 7.700 13.754 -17.927 1.00 32.43 N
ATOM 10379 CA SER F 14 6.603 14.550 -18.467 1.00 38.16
C

ATOM 10380 C SER F 14 5.368 14.442 -17.574 1.00 38.46 C

ATOM 10381 O SER F 14 4.368 15.130 -17.790 1.00 34.82 O
ATOM 10382 CB SER F 14 6.270 14.101 -19.894 1.00 40.70
C
ATOM 10383 OG SER F 14 5.954 12.720 -19.938 1.00 40.46
O

ATOM 10384 H SER F 14 7.739 12.955 -18.242 1.00 38.92 H
ATOM 10385 HA SER F 14 6.872 15.481 -18.499 1.00 45.79
H
ATOM 10386 HB2 SER F 14 5.508 14.609 -20.213 1.00 48.84
H
ATOM 10387 HB3 SER F 14 7.038 14.266 -20.462 1.00 48.84
H
ATOM 10388 HG SER F 14 5.288 12.562 -19.450 1.00 48.55
H

ATOM 10389 N ASP F 15 5.451 13.578 -16.567 1.00 36.67 N
ATOM 10390 CA ASP F 15 4.350 13.349 -15.640 1.00 37.21
C

ATOM 10391 C ASP F 15 4.410 14.336 -14.473 1.00 36.51 C

ATOM 10392 O ASP F 15 5.475 14.545 -13.888 1.00 27.52 O
ATOM 10393 CB ASP F 15 4.402 11.911 -15.119 1.00 43.65
C
ATOM 10394 CG ASP F 15 3.030 11.302 -14.934 1.00 50.64
C
ATOM 10395 OD1 ASP F 15 2.191 11.418 -15.853 1.00 56.62
O
ATOM 10396 OD2 ASP F 15 2.794 10.697 -13.868 1.00 55.33
O1-

ATOM 10397 H ASP F 15 6.148 13.103 -16.398 1.00 44.00 H
ATOM 10398 HA ASP F 15 3.508 13.476 -16.105 1.00 44.65
H
ATOM 10399 HB2 ASP F 15 4.890 11.363 -15.754 1.00 52.39
H
ATOM 10400 HB3 ASP F 15 4.852 11.903 -14.260 1.00 52.39
H

ATOM 10401 N THR F 16 3.269 14.937 -14.138 1.00 29.26 N
ATOM 10402 CA THR F 16 3.188 15.852 -13.000 1.00 30.25

C
ATOM 4103 OD1 ASN C 109 -3.364 61.656 -14.015 1.00 30.85
O
ATOM 4104 ND2 ASN C 109 -3.434 61.653 -11.775 1.00 23.23
N
ATOM 4105 H ASN C 109 -7.173 62.292 -12.148 1.00 26.82
H
ATOM 4106 HA ASN C 109 -6.065 61.583 -14.526 1.00 25.60
H
ATOM 4107 HB2 ASN C 109 -5.452 60.336 -12.068 1.00 29.18
H
ATOM 4108 HB3 ASN C 109 -5.049 59.716 -13.475 1.00 29.18
H
ATOM 4109 HD21 ASN C 109 -2.705 62.105 -11.713 1.00 27.87
H
ATOM 4110 HD22 ASN C 109 -3.848 61.405 -11.062 1.00 27.87
H
ATOM 4111 N CYS C 110 -7.646 59.804 -15.053 1.00 16.78
N
ATOM 4112 CA CYS C 110 -8.675 58.825 -15.382 1.00 19.50
C
ATOM 4113 C CYS C 110 -8.083 57.420 -15.392 1.00 18.25
C
ATOM 4114 O CYS C 110 -6.991 57.210 -15.923 1.00 16.64
O
ATOM 4115 CB CYS C 110 -9.296 59.131 -16.745 1.00 22.08
C
ATOM 4116 SG CYS C 110 -9.588 60.882 -17.059 1.00 25.44
S
ATOM 4117 H CYS C 110 -7.122 59.987 -15.710 1.00 20.14
H
ATOM 4118 HA CYS C 110 -9.376 58.857 -14.712 1.00 23.40
H
ATOM 4119 HB2 CYS C 110 -8.700 58.804 -17.438 1.00 26.50
H
ATOM 4120 HB3 CYS C 110 -10.150 58.675 -16.807 1.00 26.50
H
ATOM 4121 N TYR C 111 -8.806 56.462 -14.823 1.00 16.40
N
ATOM 4122 CA TYR C 111 -8.350 55.074 -14.793 1.00 16.58
C
ATOM 4123 C TYR C 111 -9.442 54.103 -15.219 1.00 18.92
C
ATOM 4124 O TYR C 111 -10.626 54.362 -15.018 1.00 17.47
O
ATOM 4125 CB TYR C 111 -7.872 54.690 -13.391 1.00 15.45
C
ATOM 4126 CG TYR C 111 -6.797 55.583 -12.823 1.00 14.27
C
ATOM 4127 CD1 TYR C 111 -5.456 55.321 -13.059 1.00 17.54
C
ATOM 4128 CD2 TYR C 111 -7.124 56.680 -12.039 1.00 17.77
C
ATOM 4129 CE1 TYR C 111 -4.470 56.131 -12.535 1.00 19.61
C
ATOM 4130 CE2 TYR C 111 -6.148 57.495 -11.509 1.00 15.51
C
ATOM 4131 CZ TYR C 111 -4.822 57.216 -11.760 1.00 17.01
C
ATOM 4132 OH TYR C 111 -3.845 58.025 -11.239 1.00 17.34
O
ATOM 4133 H TYR C 111 -9.569 56.589 -14.446 1.00 19.67
H
ATOM 4134 HA TYR C 111 -7.603 54.973 -15.404 1.00 19.90
H
ATOM 4135 HB2 TYR C 111 -8.630 54.723 -12.786 1.00 18.53
H
ATOM 4136 HB3 TYR C 111 -7.518 53.788 -13.421 1.00 18.53
C
ATOM 10403 C THR F 16 1.993 15.543 -12.102 1.00 31.07 C
ATOM 10404 O THR F 16 0.939 15.126 -12.576 1.00 34.24 O
ATOM 10405 CB THR F 16 3.080 17.323 -13.451 1.00 27.23
C
ATOM 10406 OG1 THR F 16 1.821 17.538 -14.099 1.00 33.36
O
ATOM 10407 CG2 THR F 16 4.217 17.692 -14.394 1.00 29.69
C
ATOM 10408 H THR F 16 2.525 14.831 -14.556 1.00 35.11 H
ATOM 10409 HA THR F 16 3.993 15.762 -12.467 1.00 36.30
H
ATOM 10410 HB THR F 16 3.137 17.898 -12.672 1.00 32.67
H
ATOM 10411 HG1 THR F 16 1.758 18.338 -14.346 1.00 40.03
H
ATOM 10412 HG21 THR F 16 4.134 18.619 -14.667 1.00 35.62
H
ATOM 10413 HG22 THR F 16 5.070 17.570 -13.948 1.00 35.62
H
ATOM 10414 HG23 THR F 16 4.190 17.128 -15.183 1.00 35.62
H
ATOM 10415 N HIS F 17 2.176 15.746 -10.799 1.00 27.94 N
ATOM 10416 CA HIS F 17 1.086 15.654 -9.832 1.00 28.47 C
ATOM 10417 C HIS F 17 1.094 16.890 -8.941 1.00 23.00 C
ATOM 10418 O HIS F 17 2.112 17.220 -8.337 1.00 21.84 O
ATOM 10419 CB HIS F 17 1.207 14.388 -8.985 1.00 30.82 C
ATOM 10420 CG HIS F 17 1.084 13.122 -9.773 1.00 44.45 C
ATOM 10421 ND1 HIS F 17 2.129 12.592 -10.499 1.00 46.02
N
ATOM 10422 CD2 HIS F 17 0.037 12.283 -9.954 1.00 47.05 C
ATOM 10423 CE1 HIS F 17 1.733 11.479 -11.089 1.00 48.47
C
ATOM 10424 NE2 HIS F 17 0.467 11.269 -10.775 1.00 52.45
N
ATOM 10425 H HIS F 17 2.935 15.943 -10.446 1.00 33.53 H
ATOM 10426 HA HIS F 17 0.239 15.625 -10.304 1.00 34.16 H
ATOM 10427 HB2 HIS F 17 2.075 14.385 -8.551 1.00 36.99 H
ATOM 10428 HB3 HIS F 17 0.505 14.391 -8.316 1.00 36.99 H
ATOM 10429 HD1 HIS F 17 2.917 12.931 -10.557 1.00 55.22
H
ATOM 10430 HD2 HIS F 17 -0.813 12.374 -9.589 1.00 56.46 H
ATOM 10431 HE1 HIS F 17 2.255 10.936 -11.635 1.00 58.17
H
ATOM 10432 HE2 HIS F 17 -0.011 10.605 -11.042 1.00 62.94
H
ATOM 10433 N SER F 18 -0.044 17.573 -8.879 1.00 17.98 N
ATOM 10434 CA SER F 18 -0.177 18.794 -8.094 1.00 20.45 C
ATOM 10435 C SER F 18 -1.131 18.561 -6.932 1.00 21.00 C
ATOM 10436 O SER F 18 -2.266 18.124 -7.135 1.00 23.24 O

H
ATOM 4137 HD1 TYR C 111 -5.218 54.589 -13.580 1.00 21.04
H
ATOM 4138 HD2 TYR C 111 -8.019 56.868 -11.868 1.00 21.32
H
ATOM 4139 HE1 TYR C 111 -3.574 55.945 -12.703 1.00 23.53
H
ATOM 4140 HE2 TYR C 111 -6.382 58.229 -10.987 1.00 18.62
H
ATOM 4141 HH TYR C 111 -4.194 58.643 -10.790 1.00 20.81
H
ATOM 4142 N GLN C 112 -9.035 52.978 -15.797 1.00 18.21
N
ATOM 4143 CA GLN C 112 -9.954 51.869 -16.025 1.00 19.09
C
ATOM 4144 C GLN C 112 -9.246 50.536 -15.845 1.00 17.43
C
ATOM 4145 O GLN C 112 -8.135 50.330 -16.337 1.00 15.67
O
ATOM 4146 CB GLN C 112 -10.578 51.946 -17.416 1.00 21.52
C
ATOM 4147 CG GLN C 112 -11.604 50.841 -17.706 1.00 22.47
C
ATOM 4148 CD GLN C 112 -12.794 50.862 -16.753 1.00 23.56
C
ATOM 4149 OE1 GLN C 112 -12.685 50.483 -15.585 1.00 22.27
O
ATOM 4150 NE2 GLN C 112 -13.941 51.302 -17.256 1.00 30.82
N
ATOM 4151 H GLN C 112 -8.231 52.831 -16.067 1.00 21.85
H
ATOM 4152 HA GLN C 112 -10.671 51.917 -15.373 1.00 22.91
H
ATOM 4153 HB2 GLN C 112 -11.030 52.799 -17.509 1.00 25.83
H
ATOM 4154 HB3 GLN C 112 -9.873 51.875 -18.079 1.00 25.83
H
ATOM 4155 HG2 GLN C 112 -11.942 50.954 -18.608 1.00 26.97
H
ATOM 4156 HG3 GLN C 112 -11.170 49.978 -17.621 1.00 26.97
H
ATOM 4157 HE21 GLN C 112 -14.643 51.335 -16.760 1.00 36.99
H
ATOM 4158 HE22 GLN C 112 -13.982 51.555 -18.077 1.00 36.99
H
ATOM 4159 N PHE C 113 -9.911 49.643 -15.122 1.00 16.74
N
ATOM 4160 CA PHE C 113 -9.411 48.302 -14.867 1.00 19.52
C
ATOM 4161 C PHE C 113 -10.086 47.323 -15.811 1.00 21.23
C
ATOM 4162 O PHE C 113 -11.263 47.011 -15.651 1.00 24.99
O
ATOM 4163 CB PHE C 113 -9.663 47.898 -13.415 1.00 17.97
C
ATOM 4164 CG PHE C 113 -8.873 48.695 -12.419 1.00 25.87
C
ATOM 4165 CD1 PHE C 113 -9.189 50.019 -12.163 1.00 23.02
C
ATOM 4166 CD2 PHE C 113 -7.817 48.119 -11.734 1.00 25.71
C
ATOM 4167 CE1 PHE C 113 -8.466 50.751 -11.248 1.00 25.64
C
ATOM 4168 CE2 PHE C 113 -7.091 48.849 -10.815 1.00 27.12
C
ATOM 4169 CZ PHE C 113 -7.416 50.166 -10.572 1.00 26.16
C
ATOM 4170 H PHE C 113 -10.675 49.797 -14.759 1.00 20.08

ATOM 10437 CB SER F 18 -0.679 19.942 -8.971 1.00 22.54 C
ATOM 10438 OG SER F 18 0.180 20.143 -10.082 1.00 30.00
O
ATOM 10439 H SER F 18 -0.765 17.345 -9.289 1.00 21.57 H
ATOM 10440 HA SER F 18 0.689 19.041 -7.734 1.00 24.54 H
ATOM 10441 HB2 SER F 18 -1.568 19.727 -9.294 1.00 27.05
H
ATOM 10442 HB3 SER F 18 -0.706 20.754 -8.442 1.00 27.05
H
ATOM 10443 HG SER F 18 -0.107 20.775 -10.555 1.00 36.00
H
ATOM 10444 N THR F 19 -0.665 18.867 -5.722 1.00 17.83 N
ATOM 10445 CA THR F 19 -1.425 18.615 -4.501 1.00 18.00 C
ATOM 10446 C THR F 19 -1.416 19.828 -3.570 1.00 16.45 C
ATOM 10447 O THR F 19 -0.451 20.592 -3.537 1.00 14.39 O
ATOM 10448 CB THR F 19 -0.853 17.389 -3.744 1.00 22.55 C
ATOM 10449 OG1 THR F 19 -0.964 16.223 -4.568 1.00 32.42
O
ATOM 10450 CG2 THR F 19 -1.601 17.142 -2.441 1.00 34.29
C
ATOM 10451 H THR F 19 0.103 19.228 -5.581 1.00 21.39 H
ATOM 10452 HA THR F 19 -2.346 18.421 -4.735 1.00 21.60 H
ATOM 10453 HB THR F 19 0.081 17.548 -3.535 1.00 27.06 H
ATOM 10454 HG1 THR F 19 -0.656 15.555 -4.164 1.00 38.90
H
ATOM 10455 HG21 THR F 19 -1.226 16.372 -1.985 1.00 41.15
H
ATOM 10456 HG22 THR F 19 -1.526 17.917 -1.863 1.00 41.15
H
ATOM 10457 HG23 THR F 19 -2.539 16.975 -2.624 1.00 41.15
H
ATOM 10458 N VAL F 20 -2.497 20.001 -2.817 1.00 15.56 N
ATOM 10459 CA VAL F 20 -2.525 20.990 -1.749 1.00 13.89 C
ATOM 10460 C VAL F 20 -3.255 20.430 -0.534 1.00 18.50 C
ATOM 10461 O VAL F 20 -4.337 19.854 -0.660 1.00 18.47 O
ATOM 10462 CB VAL F 20 -3.205 22.307 -2.177 1.00 12.52 C
ATOM 10463 CG1 VAL F 20 -2.985 23.371 -1.111 1.00 15.06
C
ATOM 10464 CG2 VAL F 20 -2.673 22.791 -3.519 1.00 17.29
C
ATOM 10465 H VAL F 20 -3.228 19.557 -2.906 1.00 18.67 H
ATOM 10466 HA VAL F 20 -1.615 21.194 -1.484 1.00 16.67 H
ATOM 10467 HB VAL F 20 -4.160 22.159 -2.265 1.00 15.03 H
ATOM 10468 HG11 VAL F 20 -3.417 24.193 -1.393 1.00 18.07
H
ATOM 10469 HG12 VAL F 20 -3.369 23.065 -0.275 1.00 18.07
H
ATOM 10470 HG13 VAL F 20 -2.032 23.518 -1.005 1.00 18.07

H
ATOM 4171 HA PHE C 113 -8.455 48.277 -15.031 1.00 23.43
H
ATOM 4172 HB2 PHE C 113 -10.604 48.022 -13.215 1.00 21.57
H
ATOM 4173 HB3 PHE C 113 -9.423 46.964 -13.305 1.00 21.57
H
ATOM 4174 HD1 PHE C 113 -9.896 50.418 -12.615 1.00 27.62
H
ATOM 4175 HD2 PHE C 113 -7.594 47.231 -11.895 1.00 30.85
H
ATOM 4176 HE1 PHE C 113 -8.687 51.639 -11.085 1.00 30.77
H
ATOM 4177 HE2 PHE C 113 -6.382 48.452 -10.361 1.00 32.55
H
ATOM 4178 HZ PHE C 113 -6.927 50.660 -9.953 1.00 31.39
H
ATOM 4179 N PHE C 114 -9.339 46.858 -16.805 1.00 16.23
N
ATOM 4180 CA PHE C 114 -9.855 45.885 -17.757 1.00 21.01
C
ATOM 4181 C PHE C 114 -9.597 44.462 -17.277 1.00 23.07
C
ATOM 4182 O PHE C 114 -8.447 44.064 -17.067 1.00 19.02
O
ATOM 4183 CB PHE C 114 -9.229 46.114 -19.132 1.00 22.60
C
ATOM 4184 CG PHE C 114 -9.646 47.407 -19.764 1.00 22.75
C
ATOM 4185 CD1 PHE C 114 -10.804 47.479 -20.517 1.00 26.86
C
ATOM 4186 CD2 PHE C 114 -8.895 48.556 -19.584 1.00 23.18
C
ATOM 4187 CE1 PHE C 114 -11.197 48.673 -21.094 1.00 30.06
C
ATOM 4188 CE2 PHE C 114 -9.283 49.751 -20.162 1.00 23.89
C
ATOM 4189 CZ PHE C 114 -10.435 49.809 -20.914 1.00 22.95
C
ATOM 4190 H PHE C 114 -8.525 47.092 -16.950 1.00 19.48
H
ATOM 4191 HA PHE C 114 -10.815 46.003 -17.841 1.00 25.21
H
ATOM 4192 HB2 PHE C 114 -8.264 46.125 -19.039 1.00 27.12
H
ATOM 4193 HB3 PHE C 114 -9.496 45.393 -19.723 1.00 27.12
H
ATOM 4194 HD1 PHE C 114 -11.320 46.716 -20.642 1.00 32.23
H
ATOM 4195 HD2 PHE C 114 -8.116 48.521 -19.078 1.00 27.81
H
ATOM 4196 HE1 PHE C 114 -11.974 48.710 -21.603 1.00 36.07
H
ATOM 4197 HE2 PHE C 114 -8.769 50.517 -20.039 1.00 28.67
H
ATOM 4198 HZ PHE C 114 -10.698 50.612 -21.303 1.00 27.54
H
ATOM 4199 N ASP C 115 -10.676 43.702 -17.113 1.00 17.95
N
ATOM 4200 CA ASP C 115 -10.596 42.336 -16.605 1.00 23.68
C
ATOM 4201 C ASP C 115 -10.397 41.329 -17.734 1.00 26.50
C
ATOM 4202 O ASP C 115 -10.405 40.120 -17.503 1.00 28.70
O
ATOM 4203 CB ASP C 115 -11.856 41.988 -15.810 1.00 32.14
C
ATOM 4204 CG ASP C 115 -13.112 42.022 -16.662 1.00 34.91
H
ATOM 10471 HG21 VAL F 20 -3.121 23.618 -3.757 1.00 20.75
H
ATOM 10472 HG22 VAL F 20 -1.718 22.941 -3.444 1.00 20.75
H
ATOM 10473 HG23 VAL F 20 -2.850 22.114 -4.191 1.00 20.75
H

ATOM 10474 N ASP F 21 -2.642 20.603 0.634 1.00 16.80 N

ATOM 10475 CA ASP F 21 -3.255 20.265 1.914 1.00 17.58 C

ATOM 10476 C ASP F 21 -3.462 21.536 2.730 1.00 17.01 C

ATOM 10477 O ASP F 21 -2.575 22.388 2.787 1.00 15.14 O

ATOM 10478 CB ASP F 21 -2.381 19.285 2.699 1.00 20.49 C

ATOM 10479 CG ASP F 21 -2.160 17.976 1.967 1.00 26.72 C
ATOM 10480 OD1 ASP F 21 -3.111 17.480 1.325 1.00 29.73
O
ATOM 10481 OD2 ASP F 21 -1.031 17.446 2.035 1.00 37.52
O1-

ATOM 10482 H ASP F 21 -1.848 20.923 0.712 1.00 20.16 H

ATOM 10483 HA ASP F 21 -4.120 19.853 1.760 1.00 21.09 H
ATOM 10484 HB2 ASP F 21 -1.514 19.690 2.856 1.00 24.59
H
ATOM 10485 HB3 ASP F 21 -2.812 19.086 3.545 1.00 24.59
H

ATOM 10486 N VAL F 22 -4.628 21.667 3.355 1.00 14.74 N

ATOM 10487 CA VAL F 22 -4.883 22.786 4.259 1.00 14.88 C

ATOM 10488 C VAL F 22 -5.074 22.258 5.674 1.00 15.42 C

ATOM 10489 O VAL F 22 -5.919 21.397 5.914 1.00 16.90 O

ATOM 10490 CB VAL F 22 -6.116 23.601 3.839 1.00 16.70 C
ATOM 10491 CG1 VAL F 22 -6.207 24.883 4.654 1.00 16.95
C
ATOM 10492 CG2 VAL F 22 -6.058 23.927 2.351 1.00 15.61
C

ATOM 10493 H VAL F 22 -5.288 21.121 3.274 1.00 17.68 H

ATOM 10494 HA VAL F 22 -4.114 23.378 4.257 1.00 17.85 H

ATOM 10495 HB VAL F 22 -6.916 23.078 4.004 1.00 20.04 H
ATOM 10496 HG11 VAL F 22 -6.991 25.380 4.373 1.00 20.34
H
ATOM 10497 HG12 VAL F 22 -6.280 24.654 5.594 1.00 20.34
H
ATOM 10498 HG13 VAL F 22 -5.408 25.411 4.503 1.00 20.34
H
ATOM 10499 HG21 VAL F 22 -6.845 24.441 2.110 1.00 18.74
H
ATOM 10500 HG22 VAL F 22 -5.257 24.445 2.172 1.00 18.74
H
ATOM 10501 HG23 VAL F 22 -6.036 23.099 1.847 1.00 18.74
H

ATOM 10502 N ASP F 23 -4.271 22.776 6.598 1.00 19.93 N

ATOM 10503 CA ASP F 23 -4.308 22.361 7.994 1.00 18.92 C
ATOM 10504 C ASP F 23 -4.743 23.509 8.899 1.00 20.49 C

C
ATOM 4205 OD1 ASP C 115 -13.093 42.679 -17.724 1.00 35.65
O
ATOM 4206 OD2 ASP C 115 -14.118 41.395 -16.269 1.00 44.70
O1-
ATOM 4207 H ASP C 115 -11.477 43.958 -17.291 1.00 21.53
H
ATOM 4208 HA ASP C 115 -9.836 42.267 -16.006 1.00 28.42
H
ATOM 4209 HB2 ASP C 115 -11.764 41.093 -15.446 1.00 38.57
H
ATOM 4210 HB3 ASP C 115 -11.964 42.629 -15.090 1.00 38.57
H
ATOM 4211 N GLU C 116 -10.227 41.832 -18.952 1.00 22.96
N
ATOM 4212 CA GLU C 116 -9.886 40.989 -20.091 1.00 27.29
C
ATOM 4213 C GLU C 116 -8.406 40.646 -20.029 1.00 28.42
C
ATOM 4214 O GLU C 116 -7.556 41.538 -20.019 1.00 29.30
O
ATOM 4215 CB GLU C 116 -10.212 41.689 -21.415 1.00 32.71
C
ATOM 4216 CG GLU C 116 -11.703 41.836 -21.705 1.00 41.30
C
ATOM 4217 CD GLU C 116 -12.404 42.802 -20.764 1.00 43.24
C
ATOM 4218 OE1 GLU C 116 -11.789 43.823 -20.383 1.00 32.76
O
ATOM 4219 OE2 GLU C 116 -13.572 42.536 -20.403 1.00 49.42
O1-
ATOM 4220 H GLU C 116 -10.304 42.667 -19.146 1.00 27.55
H
ATOM 4221 HA GLU C 116 -10.395 40.165 -20.046 1.00 32.74
H
ATOM 4222 HB2 GLU C 116 -9.827 42.579 -21.397 1.00 39.25
H
ATOM 4223 HB3 GLU C 116 -9.820 41.178 -22.140 1.00 39.25
H
ATOM 4224 HG2 GLU C 116 -11.816 42.166 -22.610 1.00 49.56
H
ATOM 4225 HG3 GLU C 116 -12.128 40.969 -21.614 1.00 49.56
H
ATOM 4226 N SER C 117 -8.096 39.357 -19.979 1.00 18.99
N
ATOM 4227 CA SER C 117 -6.709 38.922 -19.893 1.00 24.06
C
ATOM 4228 C SER C 117 -6.009 39.087 -21.240 1.00 23.72
C
ATOM 4229 O SER C 117 -6.420 38.498 -22.238 1.00 23.97
O
ATOM 4230 CB SER C 117 -6.636 37.470 -19.425 1.00 24.23
C
ATOM 4231 OG SER C 117 -5.313 37.131 -19.059 1.00 33.70
O
ATOM 4232 H SER C 117 -8.669 38.716 -19.994 1.00 22.79
H
ATOM 4233 HA SER C 117 -6.245 39.472 -19.243 1.00 28.88
H
ATOM 4234 HB2 SER C 117 -7.216 37.356 -18.656 1.00 29.08
H
ATOM 4235 HB3 SER C 117 -6.923 36.890 -20.147 1.00 29.08
H
ATOM 4236 HG SER C 117 -5.052 37.628 -18.434 1.00 40.44
H
ATOM 4237 N LYS C 118 -4.950 39.895 -21.255 1.00 19.67
N
ATOM 4238 CA LYS C 118 -4.202 40.183 -22.476 1.00 18.97
ATOM 10505 O ASP F 23 -4.200 24.612 8.815 1.00 16.14 O
ATOM 10506 CB ASP F 23 -2.935 21.862 8.448 1.00 23.31 C
ATOM 10507 CG ASP F 23 -2.429 20.687 7.628 1.00 32.67 C
ATOM 10508 OD1 ASP F 23 -3.251 19.964 7.023 1.00 26.04
O
ATOM 10509 OD2 ASP F 23 -1.196 20.485 7.601 1.00 34.54
O1-
ATOM 10510 H ASP F 23 -3.684 23.383 6.436 1.00 23.92 H
ATOM 10511 HA ASP F 23 -4.945 21.636 8.096 1.00 22.70 H
ATOM 10512 HB2 ASP F 23 -2.293 22.584 8.363 1.00 27.97
H
ATOM 10513 HB3 ASP F 23 -2.993 21.577 9.373 1.00 27.97
H
ATOM 10514 N LEU F 24 -5.720 23.238 9.758 1.00 17.08 N
ATOM 10515 CA LEU F 24 -6.114 24.167 10.813 1.00 21.44
C
ATOM 10516 C LEU F 24 -5.627 23.618 12.149 1.00 25.10 C
ATOM 10517 O LEU F 24 -6.105 22.581 12.603 1.00 24.75 O
ATOM 10518 CB LEU F 24 -7.631 24.360 10.835 1.00 23.19
C
ATOM 10519 CG LEU F 24 -8.183 25.284 11.926 1.00 26.52
C
ATOM 10520 CD1 LEU F 24 -7.713 26.717 11.715 1.00 25.95
C
ATOM 10521 CD2 LEU F 24 -9.702 25.220 11.967 1.00 24.61
C
ATOM 10522 H LEU F 24 -6.177 22.510 9.751 1.00 20.50 H
ATOM 10523 HA LEU F 24 -5.695 25.028 10.662 1.00 25.72
H
ATOM 10524 HB2 LEU F 24 -7.903 24.729 9.980 1.00 27.83
H
ATOM 10525 HB3 LEU F 24 -8.046 23.492 10.956 1.00 27.83
H
ATOM 10526 HG LEU F 24 -7.850 24.986 12.787 1.00 31.82
H
ATOM 10527 HD11 LEU F 24 -8.078 27.275 12.419 1.00 31.14
H
ATOM 10528 HD12 LEU F 24 -6.743 26.738 11.745 1.00 31.14
H
ATOM 10529 HD13 LEU F 24 -8.025 27.027 10.851 1.00 31.14
H
ATOM 10530 HD21 LEU F 24 -10.024 25.813 12.664 1.00 29.53
H
ATOM 10531 HD22 LEU F 24 -10.052 25.499 11.107 1.00 29.53
H
ATOM 10532 HD23 LEU F 24 -9.974 24.308 12.156 1.00 29.53
H
ATOM 10533 N ASP F 25 -4.675 24.310 12.767 1.00 21.21 N
ATOM 10534 CA ASP F 25 -4.059 23.837 14.002 1.00 25.53
C
ATOM 10535 C ASP F 25 -3.507 22.423 13.815 1.00 28.79 C
ATOM 10536 O ASP F 25 -3.845 21.506 14.564 1.00 30.42 O
ATOM 10537 CB ASP F 25 -5.064 23.874 15.157 1.00 22.66
C
ATOM 10538 CG ASP F 25 -5.581 25.275 15.433 1.00 25.89

C
ATOM 4239 C LYS C 118 -2.705 40.264 -22.190 1.00 19.32
C
ATOM 4240 O LYS C 118 -2.304 40.608 -21.081 1.00 17.06
O
ATOM 4241 CB LYS C 118 -4.674 41.499 -23.096 1.00 20.06
C
ATOM 4242 CG LYS C 118 -6.039 41.439 -23.756 1.00 24.89
C
ATOM 4243 CD LYS C 118 -6.415 42.794 -24.345 1.00 27.05
C
ATOM 4244 CE LYS C 118 -7.689 42.712 -25.171 1.00 30.29
C
ATOM 4245 NZ LYS C 118 -8.838 42.217 -24.367 1.00 41.79
N1+
ATOM 4246 H LYS C 118 -4.642 40.295 -20.559 1.00 23.60
H
ATOM 4247 HA LYS C 118 -4.351 39.472 -23.119 1.00 22.76
H
ATOM 4248 HB2 LYS C 118 -4.715 42.172 -22.399 1.00 24.07
H
ATOM 4249 HB3 LYS C 118 -4.034 41.769 -23.773 1.00 24.07
H
ATOM 4250 HG2 LYS C 118 -6.022 40.787 -24.474 1.00 29.87
H
ATOM 4251 HG3 LYS C 118 -6.706 41.196 -23.095 1.00 29.87
H
ATOM 4252 HD2 LYS C 118 -6.561 43.426 -23.624 1.00 32.46
H
ATOM 4253 HD3 LYS C 118 -5.699 43.102 -24.921 1.00 32.46
H
ATOM 4254 HE2 LYS C 118 -7.910 43.596 -25.504 1.00 36.35
H
ATOM 4255 HE3 LYS C 118 -7.550 42.100 -25.910 1.00 36.35
H
ATOM 4256 HZ1 LYS C 118 -8.661 41.403 -24.053 1.00 50.14
H
ATOM 4257 HZ2 LYS C 118 -8.988 42.765 -23.682 1.00 50.14
H
ATOM 4258 HZ3 LYS C 118 -9.569 42.179 -24.873 1.00 50.14
H
ATOM 4259 N ASN C 119 -1.876 39.965 -23.186 1.00 16.38
N
ATOM 4260 CA ASN C 119 -0.438 40.141 -23.016 1.00 19.02
C
ATOM 4261 C ASN C 119 -0.135 41.640 -23.019 1.00 17.17
C
ATOM 4262 O ASN C 119 -1.030 42.453 -23.271 1.00 15.21
O
ATOM 4263 CB ASN C 119 0.354 39.374 -24.095 1.00 16.08
C
ATOM 4264 CG ASN C 119 0.249 39.985 -25.491 1.00 21.42
C
ATOM 4265 OD1 ASN C 119 0.176 41.202 -25.669 1.00 20.88
O
ATOM 4266 ND2 ASN C 119 0.267 39.119 -26.500 1.00 28.85
N
ATOM 4267 H ASN C 119 -2.115 39.664 -23.956 1.00 19.65
H
ATOM 4268 HA ASN C 119 -0.179 39.788 -22.151 1.00 22.82
H
ATOM 4269 HB2 ASN C 119 1.291 39.363 -23.846 1.00 19.30
H
ATOM 4270 HB3 ASN C 119 0.016 38.466 -24.144 1.00 19.30
H
ATOM 4271 HD21 ASN C 119 0.211 39.402 -27.311 1.00 34.62
H
ATOM 4272 HD22 ASN C 119 0.334 38.276 -26.343 1.00 34.62

C
ATOM 10539 OD1 ASP F 25 -4.835 26.240 15.169 1.00 27.08
O
ATOM 10540 OD2 ASP F 25 -6.731 25.415 15.905 1.00 28.60
O1-

ATOM 10541 H ASP F 25 -4.366 25.063 12.489 1.00 25.45 H
ATOM 10542 HA ASP F 25 -3.318 24.420 14.230 1.00 30.64
H
ATOM 10543 HB2 ASP F 25 -5.823 23.312 14.935 1.00 27.20
H
ATOM 10544 HB3 ASP F 25 -4.634 23.548 15.963 1.00 27.20
H

ATOM 10545 N ASP F 26 -2.662 22.266 12.799 1.00 27.45 N
ATOM 10546 CA ASP F 26 -2.002 20.994 12.492 1.00 36.24
C

ATOM 10547 C ASP F 26 -2.989 19.837 12.303 1.00 34.78 C

ATOM 10548 O ASP F 26 -2.632 18.668 12.463 1.00 43.46 O
ATOM 10549 CB ASP F 26 -0.987 20.646 13.588 1.00 40.63
C
ATOM 10550 CG ASP F 26 0.210 21.582 13.591 1.00 47.72
C
ATOM 10551 OD1 ASP F 26 1.038 21.493 12.657 1.00 56.36
O
ATOM 10552 OD2 ASP F 26 0.328 22.403 14.526 1.00 47.17
O1-

ATOM 10553 H ASP F 26 -2.448 22.899 12.256 1.00 32.93 H
ATOM 10554 HA ASP F 26 -1.511 21.095 11.662 1.00 43.49
H
ATOM 10555 HB2 ASP F 26 -1.421 20.710 14.453 1.00 48.76
H
ATOM 10556 HB3 ASP F 26 -0.663 19.743 13.445 1.00 48.76
H

ATOM 10557 N SER F 27 -4.227 20.173 11.955 1.00 32.09 N
ATOM 10558 CA SER F 27 -5.231 19.180 11.597 1.00 34.04
C

ATOM 10559 C SER F 27 -5.743 19.470 10.195 1.00 27.53 C

ATOM 10560 O SER F 27 -6.229 20.565 9.922 1.00 25.46 O
ATOM 10561 CB SER F 27 -6.386 19.183 12.596 1.00 35.84
C
ATOM 10562 OG SER F 27 -7.408 18.294 12.181 1.00 39.50
O

ATOM 10563 H SER F 27 -4.513 20.984 11.919 1.00 38.51 H
ATOM 10564 HA SER F 27 -4.827 18.298 11.600 1.00 40.85
H
ATOM 10565 HB2 SER F 27 -6.055 18.903 13.463 1.00 43.01
H
ATOM 10566 HB3 SER F 27 -6.752 20.080 12.654 1.00 43.01
H
ATOM 10567 HG SER F 27 -8.039 18.302 12.736 1.00 47.40
H

ATOM 10568 N GLN F 28 -5.626 18.486 9.309 1.00 27.54 N

ATOM 10569 CA GLN F 28 -6.030 18.651 7.918 1.00 23.96 C

ATOM 10570 C GLN F 28 -7.541 18.819 7.811 1.00 23.35 C

ATOM 10571 O GLN F 28 -8.295 18.020 8.367 1.00 23.17 O
ATOM 10572 CB GLN F 28 -5.567 17.450 7.091 1.00 27.17 C

H
ATOM 4273 N TRP C 120 1.108 42.013 -22.734 1.00 17.45
N
ATOM 4274 CA TRP C 120 1.443 43.427 -22.571 1.00 16.39
C
ATOM 4275 C TRP C 120 1.229 44.216 -23.861 1.00 19.16
C
ATOM 4276 O TRP C 120 0.768 45.360 -23.822 1.00 20.05
O
ATOM 4277 CB TRP C 120 2.888 43.592 -22.098 1.00 15.72
C
ATOM 4278 CG TRP C 120 3.216 45.005 -21.718 1.00 18.60
C
ATOM 4279 CD1 TRP C 120 3.152 45.554 -20.470 1.00 18.56
C
ATOM 4280 CD2 TRP C 120 3.652 46.053 -22.593 1.00 18.79
C
ATOM 4281 NE1 TRP C 120 3.518 46.876 -20.514 1.00 17.94
N
ATOM 4282 CE2 TRP C 120 3.830 47.208 -21.805 1.00 20.55
C
ATOM 4283 CE3 TRP C 120 3.903 46.128 -23.966 1.00 23.33
C
ATOM 4284 CZ2 TRP C 120 4.251 48.420 -22.342 1.00 21.40
C
ATOM 4285 CZ3 TRP C 120 4.321 47.334 -24.497 1.00 19.62
C
ATOM 4286 CH2 TRP C 120 4.492 48.463 -23.687 1.00 24.59
C
ATOM 4287 H TRP C 120 1.771 41.475 -22.631 1.00 20.94
H
ATOM 4288 HA TRP C 120 0.864 43.807 -21.892 1.00 19.67
H
ATOM 4289 HB2 TRP C 120 3.032 43.032 -21.319 1.00 18.86
H
ATOM 4290 HB3 TRP C 120 3.487 43.327 -22.813 1.00 18.86
H
ATOM 4291 HD1 TRP C 120 2.895 45.098 -19.701 1.00 22.28
H
ATOM 4292 HE1 TRP C 120 3.550 47.408 -19.839 1.00 21.53
H
ATOM 4293 HE3 TRP C 120 3.791 45.383 -24.511 1.00 28.00
H
ATOM 4294 HZ2 TRP C 120 4.366 49.172 -21.806 1.00 25.69
H
ATOM 4295 HZ3 TRP C 120 4.493 47.396 -25.409 1.00 23.55
H
ATOM 4296 HH2 TRP C 120 4.776 49.260 -24.072 1.00 29.50
H
ATOM 4297 N TYR C 121 1.555 43.605 -24.998 1.00 17.25
N
ATOM 4298 CA TYR C 121 1.432 44.280 -26.289 1.00 19.29
C
ATOM 4299 C TYR C 121 -0.035 44.502 -26.645 1.00 19.51
C
ATOM 4300 O TYR C 121 -0.406 45.554 -27.164 1.00 22.89
O
ATOM 4301 CB TYR C 121 2.124 43.472 -27.392 1.00 22.07
C
ATOM 4302 CG TYR C 121 3.470 42.922 -26.983 1.00 18.97
C
ATOM 4303 CD1 TYR C 121 4.582 43.748 -26.897 1.00 21.63
C
ATOM 4304 CD2 TYR C 121 3.627 41.577 -26.675 1.00 18.97
C
ATOM 4305 CE1 TYR C 121 5.812 43.250 -26.517 1.00 22.33
C
ATOM 4306 CE2 TYR C 121 4.853 41.070 -26.296 1.00 21.40
C
ATOM 10573 CG GLN F 28 -5.639 17.658 5.595 1.00 25.49
C
ATOM 10574 CD GLN F 28 -5.293 16.399 4.820 1.00 29.69 C
ATOM 10575 OE1 GLN F 28 -4.307 16.362 4.086 1.00 31.67
O
ATOM 10576 NE2 GLN F 28 -6.104 15.361 4.984 1.00 33.72
N
ATOM 10577 H GLN F 28 -5.312 17.706 9.491 1.00 33.05 H
ATOM 10578 HA GLN F 28 -5.610 19.447 7.556 1.00 28.76 H
ATOM 10579 HB2 GLN F 28 -4.644 17.254 7.317 1.00 32.60
H
ATOM 10580 HB3 GLN F 28 -6.126 16.688 7.310 1.00 32.60
H
ATOM 10581 HG2 GLN F 28 -6.540 17.922 5.355 1.00 30.58
H
ATOM 10582 HG3 GLN F 28 -5.009 18.351 5.341 1.00 30.58
H
ATOM 10583 HE21 GLN F 28 -5.950 14.625 4.566 1.00 40.46
H
ATOM 10584 HE22 GLN F 28 -6.783 15.424 5.508 1.00 40.46
H
ATOM 10585 N ILE F 29 -7.974 19.862 7.102 1.00 18.13 N
ATOM 10586 CA ILE F 29 -9.397 20.159 6.940 1.00 18.44 C
ATOM 10587 C ILE F 29 -9.830 20.136 5.472 1.00 17.32 C
ATOM 10588 O ILE F 29 -11.008 19.952 5.170 1.00 15.77 O
ATOM 10589 CB ILE F 29 -9.757 21.539 7.544 1.00 16.85 C
ATOM 10590 CG1 ILE F 29 -8.943 22.655 6.879 1.00 18.54 C
ATOM 10591 CG2 ILE F 29 -9.505 21.533 9.044 1.00 21.09 C
ATOM 10592 CD1 ILE F 29 -9.442 24.060 7.198 1.00 16.42 C
ATOM 10593 H ILE F 29 -7.456 20.418 6.700 1.00 21.76 H
ATOM 10594 HA ILE F 29 -9.912 19.486 7.411 1.00 22.13 H
ATOM 10595 HB ILE F 29 -10.699 21.708 7.389 1.00 20.22 H
ATOM 10596 HG12 ILE F 29 -8.024 22.592 7.181 1.00 22.25
H
ATOM 10597 HG13 ILE F 29 -8.982 22.538 5.917 1.00 22.25
H
ATOM 10598 HG21 ILE F 29 -9.735 22.404 9.405 1.00 25.31
H
ATOM 10599 HG22 ILE F 29 -10.056 20.848 9.454 1.00 25.31
H
ATOM 10600 HG23 ILE F 29 -8.568 21.345 9.206 1.00 25.31
H
ATOM 10601 HD11 ILE F 29 -8.879 24.705 6.742 1.00 19.71 H
ATOM 10602 HD12 ILE F 29 -10.358 24.147 6.891 1.00 19.71
H
ATOM 10603 HD13 ILE F 29 -9.399 24.201 8.156 1.00 19.71 H
ATOM 10604 N ILE F 30 -8.874 20.338 4.571 1.00 18.05 N
ATOM 10605 CA ILE F 30 -9.146 20.395 3.137 1.00 16.43 C
ATOM 10606 C ILE F 30 -7.997 19.753 2.372 1.00 17.64 C

C
ATOM 4307 CZ TYR C 121 5.939 41.910 -26.216 1.00 21.86
C
ATOM 4308 OH TYR C 121 7.161 41.408 -25.840 1.00 22.74
O
ATOM 4309 H TYR C 121 1.850 42.799 -25.049 1.00 20.71
H
ATOM 4310 HA TYR C 121 1.863 45.148 -26.236 1.00 23.15
H
ATOM 4311 HB2 TYR C 121 1.558 42.722 -27.633 1.00 26.49
H
ATOM 4312 HB3 TYR C 121 2.259 44.044 -28.163 1.00 26.49
H
ATOM 4313 HD1 TYR C 121 4.496 44.652 -27.097 1.00 25.95
H
ATOM 4314 HD2 TYR C 121 2.893 41.008 -26.726 1.00 22.76
H
ATOM 4315 HE1 TYR C 121 6.550 43.815 -26.464 1.00 26.80
H
ATOM 4316 HE2 TYR C 121 4.944 40.167 -26.092 1.00 25.68
H
ATOM 4317 HH TYR C 121 7.734 42.021 -25.835 1.00 27.29
H
ATOM 4318 N GLU C 122 -0.864 43.503 -26.363 1.00 19.03
N
ATOM 4319 CA GLU C 122 -2.296 43.606 -26.607 1.00 20.24
C
ATOM 4320 C GLU C 122 -2.911 44.657 -25.688 1.00 22.15
C
ATOM 4321 O GLU C 122 -3.781 45.424 -26.098 1.00 21.67
O
ATOM 4322 CB GLU C 122 -2.969 42.249 -26.399 1.00 23.32
C
ATOM 4323 CG GLU C 122 -2.577 41.198 -27.442 1.00 28.93
C
ATOM 4324 CD GLU C 122 -3.051 39.794 -27.089 1.00 31.55
C
ATOM 4325 OE1 GLU C 122 -3.184 39.484 -25.884 1.00 26.49
O
ATOM 4326 OE2 GLU C 122 -3.289 38.996 -28.023 1.00 36.30
O1-
ATOM 4327 H GLU C 122 -0.619 42.750 -26.028 1.00 22.84
H
ATOM 4328 HA GLU C 122 -2.445 43.881 -27.525 1.00 24.29
H
ATOM 4329 HB2 GLU C 122 -2.720 41.907 -25.526 1.00 27.98
H
ATOM 4330 HB3 GLU C 122 -3.931 42.366 -26.444 1.00 27.98
H
ATOM 4331 HG2 GLU C 122 -2.970 41.440 -28.295 1.00 34.71
H
ATOM 4332 HG3 GLU C 122 -1.610 41.176 -27.517 1.00 34.71
H
ATOM 4333 N SER C 123 -2.442 44.696 -24.446 1.00 20.16
N
ATOM 4334 CA SER C 123 -2.934 45.664 -23.473 1.00 21.59
C
ATOM 4335 C SER C 123 -2.539 47.085 -23.865 1.00 20.70
C
ATOM 4336 O SER C 123 -3.328 48.019 -23.717 1.00 19.90
O
ATOM 4337 CB SER C 123 -2.405 45.335 -22.080 1.00 19.87
C
ATOM 4338 OG SER C 123 -2.871 44.070 -21.655 1.00 17.57
O
ATOM 4339 H SER C 123 -1.836 44.169 -24.140 1.00 24.19
H
ATOM 4340 HA SER C 123 -3.903 45.619 -23.445 1.00 25.91

ATOM 10607 O ILE F 30 -6.847 19.815 2.805 1.00 16.22 O

ATOM 10608 CB ILE F 30 -9.324 21.855 2.635 1.00 16.66 C
ATOM 10609 CG1 ILE F 30 -10.499 22.548 3.327 1.00 19.53
C

ATOM 10610 CG2 ILE F 30 -9.533 21.893 1.120 1.00 17.34 C

ATOM 10611 CD1 ILE F 30 -10.513 24.061 3.112 1.00 22.20 C

ATOM 10612 H ILE F 30 -8.044 20.446 4.768 1.00 21.66 H

ATOM 10613 HA ILE F 30 -9.959 19.902 2.943 1.00 19.72 H

ATOM 10614 HB ILE F 30 -8.515 22.348 2.842 1.00 20.00 H
ATOM 10615 HG12 ILE F 30 -11.329 22.189 2.974 1.00 23.44
H
ATOM 10616 HG13 ILE F 30 -10.445 22.382 4.281 1.00 23.44
H
ATOM 10617 HG21 ILE F 30 -9.641 22.816 0.840 1.00 20.81
H
ATOM 10618 HG22 ILE F 30 -8.759 21.503 0.685 1.00 20.81
H
ATOM 10619 HG23 ILE F 30 -10.329 21.385 0.899 1.00 20.81
H
ATOM 10620 HD11 ILE F 30 -11.278 24.438 3.574 1.00 26.64
H

ATOM 10621 HD12 ILE F 30 -9.692 24.437 3.468 1.00 26.64 H
ATOM 10622 HD13 ILE F 30 -10.576 24.244 2.161 1.00 26.64
H

ATOM 10623 N THR F 31 -8.312 19.148 1.231 1.00 18.54 N

ATOM 10624 CA THR F 31 -7.291 18.625 0.330 1.00 18.58 C

ATOM 10625 C THR F 31 -7.672 18.886 -1.126 1.00 20.44 C

ATOM 10626 O THR F 31 -8.849 19.000 -1.466 1.00 19.16 O

ATOM 10627 CB THR F 31 -7.064 17.111 0.539 1.00 20.21 C
ATOM 10628 OG1 THR F 31 -5.973 16.673 -0.278 1.00 30.33
O
ATOM 10629 CG2 THR F 31 -8.309 16.315 0.191 1.00 26.70
C

ATOM 10630 H THR F 31 -9.117 19.028 0.954 1.00 22.25 H

ATOM 10631 HA THR F 31 -6.453 19.080 0.507 1.00 22.30 H

ATOM 10632 HB THR F 31 -6.850 16.947 1.471 1.00 24.26 H
ATOM 10633 HG1 THR F 31 -5.273 17.088 -0.070 1.00 36.39
H
ATOM 10634 HG21 THR F 31 -8.147 15.369 0.328 1.00 32.04
H
ATOM 10635 HG22 THR F 31 -9.048 16.594 0.753 1.00 32.04
H
ATOM 10636 HG23 THR F 31 -8.547 16.463 -0.738 1.00 32.04
H

ATOM 10637 N PHE F 32 -6.655 18.973 -1.976 1.00 19.67 N

ATOM 10638 CA PHE F 32 -6.820 19.291 -3.391 1.00 18.78 C

ATOM 10639 C PHE F 32 -5.886 18.375 -4.181 1.00 19.20 C
ATOM 10640 O PHE F 32 -4.713 18.254 -3.833 1.00 16.31 O

H
ATOM 4341 HB2 SER C 123 -1.436 45.323 -22.105 1.00 23.85
H
ATOM 4342 HB3 SER C 123 -2.713 46.011 -21.457 1.00 23.85
H
ATOM 4343 HG SER C 123 -2.612 43.475 -22.188 1.00 21.09
H
ATOM 4344 N GLN C 124 -1.318 47.244 -24.366 1.00 24.47
N
ATOM 4345 CA GLN C 124 -0.843 48.550 -24.805 1.00 22.72
C
ATOM 4346 C GLN C 124 -1.706 49.080 -25.946 1.00 24.57
C
ATOM 4347 O GLN C 124 -2.072 50.256 -25.962 1.00 20.57
O
ATOM 4348 CB GLN C 124 0.619 48.478 -25.256 1.00 26.56
C
ATOM 4349 CG GLN C 124 1.218 49.843 -25.591 1.00 36.95
C
ATOM 4350 CD GLN C 124 2.420 49.764 -26.513 1.00 46.63
C
ATOM 4351 OE1 GLN C 124 2.512 48.882 -27.367 1.00 51.66
O
ATOM 4352 NE2 GLN C 124 3.351 50.695 -26.344 1.00 54.16
N
ATOM 4353 H GLN C 124 -0.745 46.610 -24.462 1.00 29.36
H
ATOM 4354 HA GLN C 124 -0.901 49.176 -24.066 1.00 27.27
H
ATOM 4355 HB2 GLN C 124 1.148 48.087 -24.543 1.00 31.87
H
ATOM 4356 HB3 GLN C 124 0.675 47.925 -26.050 1.00 31.87
H
ATOM 4357 HG2 GLN C 124 0.542 50.384 -26.029 1.00 44.35
H
ATOM 4358 HG3 GLN C 124 1.501 50.272 -24.769 1.00 44.35
H
ATOM 4359 HE21 GLN C 124 4.053 50.696 -26.840 1.00 64.99
H
ATOM 4360 HE22 GLN C 124 3.253 51.297 -25.737 1.00 64.99
H
ATOM 4361 N ALA C 125 -2.013 48.209 -26.905 1.00 22.47
N
ATOM 4362 CA ALA C 125 -2.833 48.589 -28.053 1.00 26.65
C
ATOM 4363 C ALA C 125 -4.243 48.953 -27.612 1.00 27.08
C
ATOM 4364 O ALA C 125 -4.863 49.867 -28.162 1.00 28.57
O
ATOM 4365 CB ALA C 125 -2.877 47.464 -29.074 1.00 20.86
C
ATOM 4366 H ALA C 125 -1.758 47.388 -26.914 1.00 26.96
H
ATOM 4367 HA ALA C 125 -2.440 49.368 -28.479 1.00 31.98
H
ATOM 4368 HB1 ALA C 125 -3.426 47.741 -29.825 1.00 25.03
H
ATOM 4369 HB2 ALA C 125 -1.974 47.276 -29.375 1.00 25.03
H
ATOM 4370 HB3 ALA C 125 -3.258 46.676 -28.658 1.00 25.03
H
ATOM 4371 N SER C 126 -4.747 48.225 -26.622 1.00 19.59
N
ATOM 4372 CA SER C 126 -6.082 48.473 -26.088 1.00 26.30
C
ATOM 4373 C SER C 126 -6.193 49.891 -25.531 1.00 26.98
C
ATOM 4374 O SER C 126 -7.138 50.616 -25.844 1.00 26.20

ATOM 10641 CB PHE F 32 -6.511 20.772 -3.633 1.00 15.72 C
ATOM 10642 CG PHE F 32 -6.536 21.186 -5.076 1.00 18.98
C
ATOM 10643 CD1 PHE F 32 -7.727 21.534 -5.696 1.00 19.61
C
ATOM 10644 CD2 PHE F 32 -5.362 21.262 -5.804 1.00 16.15
C
ATOM 10645 CE1 PHE F 32 -7.745 21.928 -7.026 1.00 20.12
C
ATOM 10646 CE2 PHE F 32 -5.374 21.660 -7.130 1.00 17.52
C

ATOM 10647 CZ PHE F 32 -6.568 21.992 -7.741 1.00 20.04 C

ATOM 10648 H PHE F 32 -5.835 18.848 -1.750 1.00 23.60 H

ATOM 10649 HA PHE F 32 -7.734 19.114 -3.663 1.00 22.53 H
ATOM 10650 HB2 PHE F 32 -7.168 21.307 -3.162 1.00 18.87
H
ATOM 10651 HB3 PHE F 32 -5.625 20.964 -3.288 1.00 18.87
H
ATOM 10652 HD1 PHE F 32 -8.523 21.492 -5.217 1.00 23.54
H
ATOM 10653 HD2 PHE F 32 -4.555 21.039 -5.399 1.00 19.38
H
ATOM 10654 HE1 PHE F 32 -8.550 22.153 -7.433 1.00 24.14
H
ATOM 10655 HE2 PHE F 32 -4.579 21.699 -7.611 1.00 21.02
H

ATOM 10656 HZ PHE F 32 -6.578 22.257 -8.632 1.00 24.04 H

ATOM 10657 N ASP F 33 -6.405 17.714 -5.216 1.00 19.97 N

ATOM 10658 CA ASP F 33 -5.646 16.676 -5.927 1.00 21.68 C

ATOM 10659 C ASP F 33 -5.216 17.090 -7.332 1.00 27.22 C

ATOM 10660 O ASP F 33 -4.852 16.243 -8.152 1.00 29.98 O

ATOM 10661 CB ASP F 33 -6.465 15.379 -6.003 1.00 24.51 C
ATOM 10662 CG ASP F 33 -7.686 15.488 -6.923 1.00 28.43
C
ATOM 10663 OD1 ASP F 33 -7.945 16.569 -7.497 1.00 23.84
O
ATOM 10664 OD2 ASP F 33 -8.402 14.475 -7.060 1.00 25.95
O1-

ATOM 10665 H ASP F 33 -7.196 17.846 -5.528 1.00 23.96 H

ATOM 10666 HA ASP F 33 -4.841 16.483 -5.421 1.00 26.01 H
ATOM 10667 HB2 ASP F 33 -5.899 14.669 -6.343 1.00 29.41
H
ATOM 10668 HB3 ASP F 33 -6.781 15.154 -5.114 1.00 29.41
H

ATOM 10669 N GLY F 34 -5.262 18.390 -7.604 1.00 24.60 N

ATOM 10670 CA GLY F 34 -4.859 18.922 -8.894 1.00 23.43 C

ATOM 10671 C GLY F 34 -6.046 19.347 -9.735 1.00 23.46 C

ATOM 10672 O GLY F 34 -5.911 20.193 -10.618 1.00 27.08 O

ATOM 10673 H GLY F 34 -5.527 18.991 -7.048 1.00 29.52 H
ATOM 10674 HA2 GLY F 34 -4.284 19.692 -8.762 1.00 28.12

O
ATOM 4375 CB SER C 126 -6.419 47.449 -25.003 1.00 24.52
C
ATOM 4376 OG SER C 126 -7.657 47.745 -24.384 1.00 25.71
O
ATOM 4377 H SER C 126 -4.333 47.575 -26.239 1.00 23.51
H
ATOM 4378 HA SER C 126 -6.731 48.379 -26.802 1.00 31.56
H
ATOM 4379 HB2 SER C 126 -6.472 46.569 -25.407 1.00 29.43
H
ATOM 4380 HB3 SER C 126 -5.720 47.462 -24.330 1.00 29.43
H
ATOM 4381 HG SER C 126 -7.826 47.174 -23.792 1.00 30.85
H
ATOM 4382 N CYS C 127 -5.218 50.285 -24.717 1.00 24.31
N
ATOM 4383 CA CYS C 127 -5.209 51.616 -24.121 1.00 23.85
C
ATOM 4384 C CYS C 127 -5.053 52.705 -25.182 1.00 28.40
C
ATOM 4385 O CYS C 127 -5.731 53.734 -25.127 1.00 25.10
O
ATOM 4386 CB CYS C 127 -4.088 51.731 -23.086 1.00 21.86
C
ATOM 4387 SG CYS C 127 -4.254 50.602 -21.682 1.00 18.33
S
ATOM 4388 H CYS C 127 -4.546 49.796 -24.493 1.00 29.17
H
ATOM 4389 HA CYS C 127 -6.053 51.762 -23.665 1.00 28.62
H
ATOM 4390 HB2 CYS C 127 -3.243 51.539 -23.521 1.00 26.23
H
ATOM 4391 HB3 CYS C 127 -4.079 52.636 -22.737 1.00 26.23
H
ATOM 4392 N MET C 128 -4.159 52.476 -26.142 1.00 24.31
N
ATOM 4393 CA MET C 128 -3.917 53.445 -27.210 1.00 28.72
C
ATOM 4394 C MET C 128 -5.173 53.665 -28.049 1.00 28.90
C
ATOM 4395 O MET C 128 -5.436 54.776 -28.504 1.00 34.94
O
ATOM 4396 CB MET C 128 -2.770 52.985 -28.114 1.00 29.76
C
ATOM 4397 CG MET C 128 -1.377 53.258 -27.565 1.00 41.22
C
ATOM 4398 SD MET C 128 -0.084 53.092 -28.823 1.00 57.79
S
ATOM 4399 CE MET C 128 -0.259 51.366 -29.269 1.00 79.41
C
ATOM 4400 H MET C 128 -3.679 51.765 -26.199 1.00 29.18
H
ATOM 4401 HA MET C 128 -3.658 54.289 -26.810 1.00 34.46
H
ATOM 4402 HB2 MET C 128 -2.848 52.028 -28.251 1.00 35.71
H
ATOM 4403 HB3 MET C 128 -2.844 53.443 -28.966 1.00 35.71
H
ATOM 4404 HG2 MET C 128 -1.345 54.165 -27.220 1.00 49.47
H
ATOM 4405 HG3 MET C 128 -1.187 52.626 -26.854 1.00 49.47
H
ATOM 4406 HE1 MET C 128 0.395 51.149 -29.952 1.00 95.30
H
ATOM 4407 HE2 MET C 128 -0.109 50.820 -28.481 1.00 95.30
H
ATOM 4408 HE3 MET C 128 -1.155 51.218 -29.609 1.00 95.30
H
ATOM 10675 HA3 GLY F 34 -4.362 18.246 -9.382 1.00 28.12
H

ATOM 10676 N LYS F 35 -7.206 18.754 -9.457 1.00 24.09 N
ATOM 10677 CA LYS F 35 -8.438 19.056 -10.187 1.00 31.50
C

ATOM 10678 C LYS F 35 -9.588 19.327 -9.223 1.00 23.95 C

ATOM 10679 O LYS F 35 -10.257 20.354 -9.316 1.00 24.63 O
ATOM 10680 CB LYS F 35 -8.813 17.902 -11.122 1.00 36.85
C
ATOM 10681 CG LYS F 35 -9.995 18.210 -12.039 1.00 53.02
C
ATOM 10682 CD LYS F 35 -10.999 17.062 -12.114 1.00 67.53
C
ATOM 10683 CE LYS F 35 -10.483 15.894 -12.943 1.00 93.83
C
ATOM 10684 NZ LYS F 35 -9.481 15.062 -12.222 1.00102.55
N1+

ATOM 10685 H LYS F 35 -7.308 18.164 -8.840 1.00 28.91 H
ATOM 10686 HA LYS F 35 -8.302 19.851 -10.726 1.00 37.80
H
ATOM 10687 HB2 LYS F 35 -8.049 17.693 -11.683 1.00 44.22
H
ATOM 10688 HB3 LYS F 35 -9.048 17.128 -10.586 1.00 44.22
H
ATOM 10689 HG2 LYS F 35 -10.459 18.993 -11.704 1.00 63.63
H
ATOM 10690 HG3 LYS F 35 -9.664 18.378 -12.935 1.00 63.63
H
ATOM 10691 HD2 LYS F 35 -11.179 16.739 -11.218 1.00 81.03
H
ATOM 10692 HD3 LYS F 35 -11.818 17.383 -12.523 1.00 81.03
H
ATOM 10693 HE2 LYS F 35 -11.230 15.323 -13.181 1.00112.59
H
ATOM 10694 HE3 LYS F 35 -10.062 16.239 -13.746 1.00112.59
H
ATOM 10695 HZ1 LYS F 35 -9.843 14.724 -11.482 1.00123.06
H
ATOM 10696 HZ2 LYS F 35 -9.209 14.394 -12.743 1.00123.06
H
ATOM 10697 HZ3 LYS F 35 -8.778 15.559 -11.998 1.00123.06
H

ATOM 10698 N ASP F 36 -9.807 18.396 -8.299 1.00 24.43 N
ATOM 10699 CA ASP F 36 -10.926 18.476 -7.367 1.00 25.36
C

ATOM 10700 C ASP F 36 -10.472 18.842 -5.959 1.00 23.53 C

ATOM 10701 O ASP F 36 -9.384 18.462 -5.523 1.00 20.70 O
ATOM 10702 CB ASP F 36 -11.679 17.146 -7.340 1.00 30.39
C
ATOM 10703 CG ASP F 36 -12.330 16.821 -8.671 1.00 38.61
C
ATOM 10704 OD1 ASP F 36 -12.966 17.723 -9.258 1.00 37.40
O
ATOM 10705 OD2 ASP F 36 -12.199 15.669 -9.134 1.00 42.12
O1-

ATOM 10706 H ASP F 36 -9.314 17.699 -8.191 1.00 29.32 H
ATOM 10707 HA ASP F 36 -11.541 19.162 -7.671 1.00 30.43
H
ATOM 10708 HB2 ASP F 36 -11.056 16.433 -7.128 1.00 36.46

H
ATOM 4409 N SER C 129 -5.945 52.601 -28.246 1.00 29.07
N
ATOM 4410 CA SER C 129 -7.157 52.672 -29.055 1.00 32.00
C
ATOM 4411 C SER C 129 -8.256 53.469 -28.358 1.00 36.56
C
ATOM 4412 O SER C 129 -9.307 53.735 -28.945 1.00 32.22
O
ATOM 4413 CB SER C 129 -7.669 51.267 -29.377 1.00 33.16
C
ATOM 4414 OG SER C 129 -8.267 50.670 -28.237 1.00 33.58
O
ATOM 4415 H SER C 129 -5.788 51.821 -27.920 1.00 34.88
H
ATOM 4416 HA SER C 129 -6.952 53.115 -29.893 1.00 38.40
H
ATOM 4417 HB2 SER C 129 -8.329 51.325 -30.085 1.00 39.79
H
ATOM 4418 HB3 SER C 129 -6.922 50.718 -29.664 1.00 39.79
H
ATOM 4419 HG SER C 129 -7.706 50.613 -27.615 1.00 40.30
H
ATOM 4420 N GLN C 130 -8.010 53.834 -27.102 1.00 33.51
N
ATOM 4421 CA GLN C 130 -8.946 54.642 -26.331 1.00 30.27
C
ATOM 4422 C GLN C 130 -8.314 55.976 -25.955 1.00 26.64
C
ATOM 4423 O GLN C 130 -8.730 56.622 -24.995 1.00 31.87
O
ATOM 4424 CB GLN C 130 -9.393 53.881 -25.082 1.00 30.65
C
ATOM 4425 CG GLN C 130 -10.037 52.545 -25.414 1.00 34.01
C
ATOM 4426 CD GLN C 130 -10.477 51.776 -24.191 1.00 33.95
C
ATOM 4427 OE1 GLN C 130 -11.212 52.290 -23.347 1.00 40.96
O
ATOM 4428 NE2 GLN C 130 -10.033 50.529 -24.089 1.00 34.20
N
ATOM 4429 H GLN C 130 -7.297 53.622 -26.670 1.00 40.22
H
ATOM 4430 HA GLN C 130 -9.731 54.822 -26.872 1.00 36.32
H
ATOM 4431 HB2 GLN C 130 -8.620 53.711 -24.521 1.00 36.78
H
ATOM 4432 HB3 GLN C 130 -10.043 54.416 -24.601 1.00 36.78
H
ATOM 4433 HG2 GLN C 130 -10.819 52.701 -25.966 1.00 40.81
H
ATOM 4434 HG3 GLN C 130 -9.396 51.998 -25.896 1.00 40.81
H
ATOM 4435 HE21 GLN C 130 -10.254 50.047 -23.411 1.00 41.04
H
ATOM 4436 HE22 GLN C 130 -9.523 50.203 -24.700 1.00 41.04
H
ATOM 4437 N ASN C 131 -7.312 56.382 -26.730 1.00 25.72
N
ATOM 4438 CA ASN C 131 -6.593 57.631 -26.495 1.00 31.52
C
ATOM 4439 C ASN C 131 -6.008 57.676 -25.091 1.00 30.51
C
ATOM 4440 O ASN C 131 -5.996 58.719 -24.433 1.00 30.75
O
ATOM 4441 CB ASN C 131 -7.512 58.833 -26.721 1.00 40.00
C
ATOM 4442 CG ASN C 131 -6.739 60.121 -26.931 1.00 45.49
H
ATOM 10709 HB3 ASP F 36 -12.376 17.189 -6.667 1.00 36.46
H
ATOM 10710 N ILE F 37 -11.317 19.592 -5.262 1.00 22.26 N
ATOM 10711 CA ILE F 37 -11.081 19.940 -3.868 1.00 19.23 C
ATOM 10712 C ILE F 37 -12.106 19.217 -3.019 1.00 20.45 C
ATOM 10713 O ILE F 37 -13.226 18.982 -3.467 1.00 15.18 O
ATOM 10714 CB ILE F 37 -11.176 21.460 -3.636 1.00 19.93 C
ATOM 10715 CG1 ILE F 37 -10.676 21.821 -2.235 1.00 23.69
C
ATOM 10716 CG2 ILE F 37 -12.600 21.958 -3.851 1.00 19.45
C
ATOM 10717 CD1 ILE F 37 -10.392 23.301 -2.070 1.00 21.55
C
ATOM 10718 H ILE F 37 -12.046 19.918 -5.581 1.00 26.71 H
ATOM 10719 HA ILE F 37 -10.197 19.642 -3.604 1.00 23.08 H
ATOM 10720 HB ILE F 37 -10.602 21.899 -4.283 1.00 23.92 H
ATOM 10721 HG12 ILE F 37 -11.351 21.572 -1.585 1.00 28.43
H
ATOM 10722 HG13 ILE F 37 -9.854 21.337 -2.060 1.00 28.43
H
ATOM 10723 HG21 ILE F 37 -12.625 22.916 -3.698 1.00 23.34
H
ATOM 10724 HG22 ILE F 37 -12.868 21.762 -4.762 1.00 23.34
H
ATOM 10725 HG23 ILE F 37 -13.190 21.507 -3.227 1.00 23.34
H
ATOM 10726 HD11 ILE F 37 -10.080 23.463 -1.166 1.00 25.86
H
ATOM 10727 HD12 ILE F 37 -9.710 23.564 -2.708 1.00 25.86
H
ATOM 10728 HD13 ILE F 37 -11.208 23.799 -2.233 1.00 25.86
H
ATOM 10729 N ARG F 38 -11.738 18.858 -1.797 1.00 17.84 N
ATOM 10730 CA ARG F 38 -12.697 18.217 -0.916 1.00 20.68
C
ATOM 10731 C ARG F 38 -12.396 18.455 0.558 1.00 19.35 C
ATOM 10732 O ARG F 38 -11.235 18.589 0.953 1.00 18.38
O
ATOM 10733 CB ARG F 38 -12.754 16.714 -1.198 1.00 22.95
C
ATOM 10734 CG ARG F 38 -11.423 16.000 -1.117 1.00 28.32
C
ATOM 10735 CD ARG F 38 -11.562 14.534 -1.510 1.00 33.42
C
ATOM 10736 NE ARG F 38 -10.260 13.892 -1.685 1.00 43.09
N
ATOM 10737 CZ ARG F 38 -9.592 13.252 -0.728 1.00 44.56
C
ATOM 10738 NH1 ARG F 38 -10.092 13.147 0.498 1.00 41.53
N1+
ATOM 10739 NH2 ARG F 38 -8.414 12.710 -1.002 1.00 57.47
N
ATOM 10740 H ARG F 38 -10.954 18.971 -1.461 1.00 21.40 H
ATOM 10741 HA ARG F 38 -13.576 18.584 -1.098 1.00 24.81
H
ATOM 10742 HB2 ARG F 38 -13.348 16.301 -0.551 1.00 27.54

C
ATOM 4443 OD1 ASN C 131 -6.120 60.320 -27.975 1.00 53.22
O
ATOM 4444 ND2 ASN C 131 -6.769 61.001 -25.937 1.00 44.21
N
ATOM 4445 H ASN C 131 -7.025 55.944 -27.412 1.00 30.86
H
ATOM 4446 HA ASN C 131 -5.859 57.695 -27.126 1.00 37.83
H
ATOM 4447 HB2 ASN C 131 -8.053 58.675 -27.511 1.00 48.00
H
ATOM 4448 HB3 ASN C 131 -8.082 58.947 -25.945 1.00 48.00
H
ATOM 4449 HD21 ASN C 131 -6.346 61.746 -26.009 1.00 53.05
H
ATOM 4450 HD22 ASN C 131 -7.211 60.826 -25.220 1.00 53.05
H
ATOM 4451 N ALA C 132 -5.522 56.526 -24.641 1.00 27.31
N
ATOM 4452 CA ALA C 132 -4.952 56.397 -23.311 1.00 24.35
C
ATOM 4453 C ALA C 132 -3.654 55.604 -23.376 1.00 22.93
C
ATOM 4454 O ALA C 132 -3.175 55.264 -24.456 1.00 22.28
O
ATOM 4455 CB ALA C 132 -5.946 55.724 -22.377 1.00 24.10
C
ATOM 4456 H ALA C 132 -5.512 55.796 -25.096 1.00 32.77
H
ATOM 4457 HA ALA C 132 -4.753 57.279 -22.960 1.00 29.22
H
ATOM 4458 HB1 ALA C 132 -5.548 55.647 -21.496 1.00 28.92
H
ATOM 4459 HB2 ALA C 132 -6.750 56.264 -22.331 1.00 28.92
H
ATOM 4460 HB3 ALA C 132 -6.157 54.843 -22.724 1.00 28.92
H
ATOM 4461 N SER C 133 -3.086 55.317 -22.211 1.00 23.85
N
ATOM 4462 CA SER C 133 -1.908 54.470 -22.123 1.00 19.49
C
ATOM 4463 C SER C 133 -2.035 53.561 -20.913 1.00 19.76
C
ATOM 4464 O SER C 133 -2.954 53.714 -20.106 1.00 21.65
O
ATOM 4465 CB SER C 133 -0.637 55.315 -22.035 1.00 28.62
C
ATOM 4466 OG SER C 133 -0.593 56.041 -20.822 1.00 30.86
O
ATOM 4467 H SER C 133 -3.368 55.604 -21.451 1.00 28.62
H
ATOM 4468 HA SER C 133 -1.851 53.916 -22.917 1.00 23.39
H
ATOM 4469 HB2 SER C 133 0.135 54.730 -22.081 1.00 34.34
H
ATOM 4470 HB3 SER C 133 -0.622 55.940 -22.777 1.00 34.34
H
ATOM 4471 HG SER C 133 -1.256 56.554 -20.769 1.00 37.04
H
ATOM 4472 N LEU C 134 -1.131 52.597 -20.799 1.00 15.30
N
ATOM 4473 CA LEU C 134 -1.085 51.753 -19.618 1.00 16.31
C
ATOM 4474 C LEU C 134 -0.722 52.605 -18.413 1.00 18.61
C
ATOM 4475 O LEU C 134 -0.102 53.660 -18.558 1.00 17.38
O
ATOM 4476 CB LEU C 134 -0.082 50.615 -19.800 1.00 18.05
H
ATOM 10743 HB3 ARG F 38 -13.104 16.580 -2.092 1.00 27.54
H
ATOM 10744 HG2 ARG F 38 -10.795 16.421 -1.725 1.00 33.98
H
ATOM 10745 HG3 ARG F 38 -11.091 16.041 -0.207 1.00 33.98
H
ATOM 10746 HD2 ARG F 38 -12.041 14.060 -0.812 1.00 40.11
H
ATOM 10747 HD3 ARG F 38 -12.045 14.473 -2.349 1.00 40.11
H
ATOM 10748 HE ARG F 38 -9.899 13.931 -2.465 1.00 51.71
H
ATOM 10749 HH11 ARG F 38 -10.856 13.497 0.682 1.00 49.84
H
ATOM 10750 HH12 ARG F 38 -9.651 12.730 1.107 1.00 49.84
H
ATOM 10751 HH21 ARG F 38 -8.085 12.773 -1.794 1.00 68.96
H
ATOM 10752 HH22 ARG F 38 -7.979 12.293 -0.388 1.00 68.96
H

ATOM 10753 N PRO F 39 -13.454 18.510 1.378 1.00 18.43 N
ATOM 10754 CA PRO F 39 -13.287 18.624 2.828 1.00 18.67
C

ATOM 10755 C PRO F 39 -12.741 17.328 3.420 1.00 21.97 C
ATOM 10756 O PRO F 39 -13.015 16.261 2.874 1.00 21.02
O
ATOM 10757 CB PRO F 39 -14.706 18.905 3.320 1.00 22.75
C
ATOM 10758 CG PRO F 39 -15.585 18.250 2.306 1.00 22.23
C
ATOM 10759 CD PRO F 39 -14.875 18.401 0.993 1.00 22.99
C
ATOM 10760 HA PRO F 39 -12.704 19.365 3.054 1.00 22.40
H
ATOM 10761 HB2 PRO F 39 -14.835 18.509 4.196 1.00 27.30
H
ATOM 10762 HB3 PRO F 39 -14.861 19.862 3.346 1.00 27.30
H
ATOM 10763 HG2 PRO F 39 -15.696 17.312 2.528 1.00 26.68
H
ATOM 10764 HG3 PRO F 39 -16.445 18.699 2.282 1.00 26.68
H
ATOM 10765 HD2 PRO F 39 -15.016 17.616 0.441 1.00 27.59
H
ATOM 10766 HD3 PRO F 39 -15.166 19.209 0.543 1.00 27.59
H

ATOM 10767 N THR F 40 -11.976 17.424 4.505 1.00 17.56 N
ATOM 10768 CA THR F 40 -11.433 16.245 5.182 1.00 19.85
C

ATOM 10769 C THR F 40 -11.726 16.306 6.680 1.00 21.64 C

ATOM 10770 O THR F 40 -11.068 15.646 7.482 1.00 25.05 O

ATOM 10771 CB THR F 40 -9.914 16.121 4.970 1.00 22.38 C
ATOM 10772 OG1 THR F 40 -9.253 17.246 5.562 1.00 22.26
O
ATOM 10773 CG2 THR F 40 -9.581 16.061 3.486 1.00 26.29
C

ATOM 10774 H THR F 40 -11.755 18.169 4.874 1.00 21.07 H
ATOM 10775 HA THR F 40 -11.855 15.449 4.823 1.00 23.82
H
ATOM 10776 HB THR F 40 -9.596 15.305 5.387 1.00 26.85 H

C
ATOM 4477 CG LEU C 134 -0.545 49.502 -20.739 1.00 18.46
C
ATOM 4478 CD1 LEU C 134 0.622 48.613 -21.151 1.00 18.54
C
ATOM 4479 CD2 LEU C 134 -1.633 48.677 -20.070 1.00 13.57
C
ATOM 4480 H LEU C 134 -0.535 52.413 -21.391 1.00 18.36
H
ATOM 4481 HA LEU C 134 -1.961 51.366 -19.465 1.00 19.57
H
ATOM 4482 HB2 LEU C 134 0.740 50.982 -20.162 1.00 21.66
H
ATOM 4483 HB3 LEU C 134 0.094 50.215 -18.934 1.00 21.66
H
ATOM 4484 HG LEU C 134 -0.919 49.899 -21.541 1.00 22.15
H
ATOM 4485 HD11 LEU C 134 0.296 47.919 -21.745 1.00 22.25
H
ATOM 4486 HD12 LEU C 134 1.285 49.154 -21.608 1.00 22.25
H
ATOM 4487 HD13 LEU C 134 1.011 48.214 -20.357 1.00 22.25
H
ATOM 4488 HD21 LEU C 134 -1.916 47.976 -20.678 1.00 16.29
H
ATOM 4489 HD22 LEU C 134 -1.278 48.287 -19.256 1.00 16.29
H
ATOM 4490 HD23 LEU C 134 -2.383 49.256 -19.859 1.00 16.29
H
ATOM 4491 N LEU C 135 -1.122 52.145 -17.232 1.00 17.61
N
ATOM 4492 CA LEU C 135 -0.861 52.863 -15.990 1.00 16.82
C
ATOM 4493 C LEU C 135 0.574 53.365 -15.907 1.00 17.04
C
ATOM 4494 O LEU C 135 1.521 52.614 -16.145 1.00 17.43
O
ATOM 4495 CB LEU C 135 -1.160 51.962 -14.792 1.00 13.74
C
ATOM 4496 CG LEU C 135 -0.816 52.517 -13.409 1.00 13.56
C
ATOM 4497 CD1 LEU C 135 -1.668 53.736 -13.089 1.00 14.51
C
ATOM 4498 CD2 LEU C 135 -0.994 51.438 -12.348 1.00 14.41
C
ATOM 4499 H LEU C 135 -1.553 51.409 -17.123 1.00 21.14
H
ATOM 4500 HA LEU C 135 -1.450 53.632 -15.941 1.00 20.18
H
ATOM 4501 HB2 LEU C 135 -2.109 51.762 -14.793 1.00 16.49
H
ATOM 4502 HB3 LEU C 135 -0.660 51.138 -14.901 1.00 16.49
H
ATOM 4503 HG LEU C 135 0.114 52.793 -13.402 1.00 16.27
H
ATOM 4504 HD11 LEU C 135 -1.429 54.066 -12.209 1.00 17.41
H
ATOM 4505 HD12 LEU C 135 -1.502 54.421 -13.756 1.00 17.41
H
ATOM 4506 HD13 LEU C 135 -2.604 53.480 -13.104 1.00 17.41
H
ATOM 4507 HD21 LEU C 135 -0.772 51.810 -11.480 1.00 17.29
H
ATOM 4508 HD22 LEU C 135 -1.917 51.139 -12.354 1.00 17.29
H
ATOM 4509 HD23 LEU C 135 -0.404 50.695 -12.551 1.00 17.29
H
ATOM 4510 N LYS C 136 0.716 54.650 -15.601 1.00 17.22

ATOM 10777 HG1 THR F 40 -8.423 17.183 5.449 1.00 26.71
H
ATOM 10778 HG21 THR F 40 -8.622 15.983 3.364 1.00 31.55
H
ATOM 10779 HG22 THR F 40 -10.014 15.294 3.080 1.00 31.55
H
ATOM 10780 HG23 THR F 40 -9.890 16.868 3.044 1.00 31.55
H

ATOM 10781 N ILE F 41 -12.714 17.115 7.042 1.00 20.01 N

ATOM 10782 CA ILE F 41 -13.138 17.273 8.426 1.00 20.07 C

ATOM 10783 C ILE F 41 -14.638 17.573 8.393 1.00 21.37 C

ATOM 10784 O ILE F 41 -15.103 18.248 7.473 1.00 19.23 O

ATOM 10785 CB ILE F 41 -12.348 18.400 9.131 1.00 20.97 C
ATOM 10786 CG1 ILE F 41 -12.551 18.369 10.647 1.00 25.82
C
ATOM 10787 CG2 ILE F 41 -12.723 19.766 8.564 1.00 19.25
C
ATOM 10788 CD1 ILE F 41 -11.871 17.205 11.329 1.00 28.28
C

ATOM 10789 H ILE F 41 -13.164 17.595 6.490 1.00 24.01 H

ATOM 10790 HA ILE F 41 -12.997 16.444 8.909 1.00 24.09 H

ATOM 10791 HB ILE F 41 -11.405 18.256 8.956 1.00 25.16 H
ATOM 10792 HG12 ILE F 41 -12.191 19.186 11.027 1.00 30.99
H
ATOM 10793 HG13 ILE F 41 -13.500 18.310 10.834 1.00 30.99
H
ATOM 10794 HG21 ILE F 41 -12.213 20.450 9.024 1.00 23.10
H
ATOM 10795 HG22 ILE F 41 -12.517 19.780 7.616 1.00 23.10
H
ATOM 10796 HG23 ILE F 41 -13.673 19.913 8.698 1.00 23.10
H
ATOM 10797 HD11 ILE F 41 -12.044 17.254 12.282 1.00 33.93
H
ATOM 10798 HD12 ILE F 41 -12.227 16.378 10.969 1.00 33.93
H
ATOM 10799 HD13 ILE F 41 -10.917 17.255 11.162 1.00 33.93
H

ATOM 10800 N PRO F 42 -15.407 17.061 9.370 1.00 22.08 N
ATOM 10801 CA PRO F 42 -16.864 17.242 9.291 1.00 25.38
C

ATOM 10802 C PRO F 42 -17.359 18.688 9.171 1.00 23.43 C
ATOM 10803 O PRO F 42 -18.349 18.910 8.474 1.00 22.02
O
ATOM 10804 CB PRO F 42 -17.353 16.627 10.603 1.00 29.94
C
ATOM 10805 CG PRO F 42 -16.363 15.564 10.893 1.00 28.27
C
ATOM 10806 CD PRO F 42 -15.038 16.104 10.431 1.00 25.21
C
ATOM 10807 HA PRO F 42 -17.220 16.726 8.551 1.00 30.46
H
ATOM 10808 HB2 PRO F 42 -17.354 17.299 11.302 1.00 35.92
H
ATOM 10809 HB3 PRO F 42 -18.239 16.251 10.481 1.00 35.92
H
ATOM 10810 HG2 PRO F 42 -16.346 15.387 11.846 1.00 33.93

N
ATOM 4511 CA LYS C 136 2.000 55.223 -15.224 1.00 18.54
C
ATOM 4512 C LYS C 136 1.937 55.661 -13.766 1.00 20.47
C
ATOM 4513 O LYS C 136 1.050 56.424 -13.383 1.00 19.64
O
ATOM 4514 CB LYS C 136 2.365 56.409 -16.117 1.00 20.46
C
ATOM 4515 CG LYS C 136 3.646 57.121 -15.689 1.00 23.01
C
ATOM 4516 CD LYS C 136 3.990 58.278 -16.612 1.00 23.30
C
ATOM 4517 CE LYS C 136 5.219 59.029 -16.123 1.00 27.96
C
ATOM 4518 NZ LYS C 136 5.543 60.212 -16.968 1.00 28.81
N1+
ATOM 4519 H LYS C 136 0.072 55.219 -15.605 1.00 20.67
H
ATOM 4520 HA LYS C 136 2.692 54.549 -15.312 1.00 22.25
H
ATOM 4521 HB2 LYS C 136 2.490 56.091 -17.025 1.00 24.55
H
ATOM 4522 HB3 LYS C 136 1.642 57.055 -16.090 1.00 24.55
H
ATOM 4523 HG2 LYS C 136 3.530 57.473 -14.792 1.00 27.61
H
ATOM 4524 HG3 LYS C 136 4.382 56.490 -15.708 1.00 27.61
H
ATOM 4525 HD2 LYS C 136 4.175 57.936 -17.500 1.00 27.96
H
ATOM 4526 HD3 LYS C 136 3.245 58.899 -16.639 1.00 27.96
H
ATOM 4527 HE2 LYS C 136 5.061 59.341 -15.218 1.00 33.55
H
ATOM 4528 HE3 LYS C 136 5.983 58.431 -16.140 1.00 33.55
H
ATOM 4529 HZ1 LYS C 136 5.701 59.954 -17.805 1.00 34.57
H
ATOM 4530 HZ2 LYS C 136 4.860 60.783 -16.965 1.00 34.57
H
ATOM 4531 HZ3 LYS C 136 6.265 60.623 -16.650 1.00 34.57
H
ATOM 4532 N VAL C 137 2.879 55.174 -12.962 1.00 17.55
N
ATOM 4533 CA VAL C 137 2.946 55.507 -11.540 1.00 20.81
C
ATOM 4534 C VAL C 137 3.952 56.623 -11.309 1.00 21.28
C
ATOM 4535 O VAL C 137 5.166 56.402 -11.400 1.00 21.39
O
ATOM 4536 CB VAL C 137 3.340 54.286 -10.685 1.00 17.34
C
ATOM 4537 CG1 VAL C 137 3.489 54.674 -9.218 1.00 17.08
C
ATOM 4538 CG2 VAL C 137 2.308 53.180 -10.832 1.00 19.83
C
ATOM 4539 H VAL C 137 3.501 54.639 -13.221 1.00 21.06
H
ATOM 4540 HA VAL C 137 2.075 55.816 -11.243 1.00 24.98
H
ATOM 4541 HB VAL C 137 4.194 53.945 -10.994 1.00 20.81
H
ATOM 4542 HG11 VAL C 137 3.737 53.887 -8.708 1.00 20.50
H
ATOM 4543 HG12 VAL C 137 4.179 55.351 -9.140 1.00 20.50
H
ATOM 4544 HG13 VAL C 137 2.643 55.024 -8.897 1.00 20.50
H
ATOM 10811 HG3 PRO F 42 -16.594 14.761 10.400 1.00 33.93
H
ATOM 10812 HD2 PRO F 42 -14.588 16.563 11.158 1.00 30.25
H
ATOM 10813 HD3 PRO F 42 -14.490 15.391 10.067 1.00 30.25
H

ATOM 10814 N PHE F 43 -16.709 19.651 9.818 1.00 23.12 N
ATOM 10815 CA PHE F 43 -17.256 21.005 9.831 1.00 24.79
C

ATOM 10816 C PHE F 43 -17.066 21.713 8.486 1.00 23.64 C

ATOM 10817 O PHE F 43 -17.626 22.787 8.262 1.00 21.80 O
ATOM 10818 CB PHE F 43 -16.650 21.828 10.981 1.00 27.53
C
ATOM 10819 CG PHE F 43 -15.249 22.323 10.736 1.00 22.90
C
ATOM 10820 CD1 PHE F 43 -15.021 23.465 9.986 1.00 24.94
C
ATOM 10821 CD2 PHE F 43 -14.165 21.676 11.301 1.00 25.76
C
ATOM 10822 CE1 PHE F 43 -13.736 23.932 9.777 1.00 25.31
C
ATOM 10823 CE2 PHE F 43 -12.876 22.141 11.097 1.00 25.44
C
ATOM 10824 CZ PHE F 43 -12.663 23.270 10.336 1.00 23.75
C
ATOM 10825 H PHE F 43 -15.970 19.552 10.246 1.00 27.75
H
ATOM 10826 HA PHE F 43 -18.211 20.945 9.992 1.00 29.75
H
ATOM 10827 HB2 PHE F 43 -17.212 22.604 11.136 1.00 33.04
H
ATOM 10828 HB3 PHE F 43 -16.630 21.277 11.779 1.00 33.04
H
ATOM 10829 HD1 PHE F 43 -15.740 23.916 9.606 1.00 29.93
H
ATOM 10830 HD2 PHE F 43 -14.302 20.913 11.816 1.00 30.91
H
ATOM 10831 HE1 PHE F 43 -13.595 24.694 9.263 1.00 30.37
H
ATOM 10832 HE2 PHE F 43 -12.154 21.691 11.473 1.00 30.53
H
ATOM 10833 HZ PHE F 43 -11.798 23.582 10.195 1.00 28.50
H

ATOM 10834 N MET F 44 -16.306 21.100 7.584 1.00 22.56 N
ATOM 10835 CA MET F 44 -16.106 21.657 6.248 1.00 22.07
C

ATOM 10836 C MET F 44 -17.100 21.090 5.233 1.00 25.90 C

ATOM 10837 O MET F 44 -17.186 21.573 4.099 1.00 24.02 O
ATOM 10838 CB MET F 44 -14.672 21.401 5.776 1.00 23.53
C
ATOM 10839 CG MET F 44 -13.629 22.258 6.480 1.00 17.23
C
ATOM 10840 SD MET F 44 -13.962 24.032 6.367 1.00 24.19
S
ATOM 10841 CE MET F 44 -14.044 24.258 4.597 1.00 16.78
C

ATOM 10842 H MET F 44 -15.893 20.357 7.720 1.00 27.07 H
ATOM 10843 HA MET F 44 -16.230 22.618 6.295 1.00 26.49
H
ATOM 10844 HB2 MET F 44 -14.451 20.471 5.940 1.00 28.24

H
ATOM 4545 HG21 VAL C 137 2.576 52.424 -10.287 1.00 23.80
H
ATOM 4546 HG22 VAL C 137 1.446 53.512 -10.537 1.00 23.80
H
ATOM 4547 HG23 VAL C 137 2.260 52.915 -11.764 1.00 23.80
H
ATOM 4548 N TYR C 138 3.447 57.812 -10.992 1.00 20.38
N
ATOM 4549 CA TYR C 138 4.298 58.989 -10.848 1.00 21.11
C
ATOM 4550 C TYR C 138 4.204 59.608 -9.457 1.00 24.17
C
ATOM 4551 O TYR C 138 5.071 60.393 -9.071 1.00 24.32
O
ATOM 4552 CB TYR C 138 3.940 60.037 -11.906 1.00 22.43
C
ATOM 4553 CG TYR C 138 2.622 60.739 -11.663 1.00 20.09
C
ATOM 4554 CD1 TYR C 138 1.442 60.245 -12.197 1.00 21.54
C
ATOM 4555 CD2 TYR C 138 2.560 61.899 -10.899 1.00 24.15
C
ATOM 4556 CE1 TYR C 138 0.238 60.882 -11.978 1.00 23.42
C
ATOM 4557 CE2 TYR C 138 1.361 62.542 -10.673 1.00 24.55
C
ATOM 4558 CZ TYR C 138 0.204 62.029 -11.214 1.00 24.76
C
ATOM 4559 OH TYR C 138 -0.991 62.663 -10.994 1.00 25.68
O
ATOM 4560 H TYR C 138 2.612 57.965 -10.855 1.00 24.46
H
ATOM 4561 HA TYR C 138 5.221 58.726 -10.992 1.00 25.34
H
ATOM 4562 HB2 TYR C 138 4.636 60.712 -11.923 1.00 26.92
H
ATOM 4563 HB3 TYR C 138 3.887 59.600 -12.770 1.00 26.92
H
ATOM 4564 HD1 TYR C 138 1.462 59.471 -12.712 1.00 25.85
H
ATOM 4565 HD2 TYR C 138 3.341 62.246 -10.531 1.00 28.98
H
ATOM 4566 HE1 TYR C 138 -0.546 60.538 -12.342 1.00 28.11
H
ATOM 4567 HE2 TYR C 138 1.334 63.316 -10.159 1.00 29.46
H
ATOM 4568 HH TYR C 138 -0.872 63.344 -10.517 1.00 30.82
H
ATOM 4569 N SER C 139 3.160 59.265 -8.704 1.00 20.17
N
ATOM 4570 CA SER C 139 2.980 59.837 -7.369 1.00 25.07
C
ATOM 4571 C SER C 139 2.203 58.946 -6.407 1.00 22.13
C
ATOM 4572 O SER C 139 1.051 58.586 -6.664 1.00 19.25
O
ATOM 4573 CB SER C 139 2.267 61.184 -7.468 1.00 26.51
C
ATOM 4574 OG SER C 139 1.936 61.668 -6.178 1.00 27.30
O
ATOM 4575 H SER C 139 2.547 58.709 -8.939 1.00 24.21
H
ATOM 4576 HA SER C 139 3.854 59.995 -6.980 1.00 30.08
H
ATOM 4577 HB2 SER C 139 2.854 61.821 -7.905 1.00 31.82
H
ATOM 4578 HB3 SER C 139 1.453 61.074 -7.984 1.00 31.82
H
ATOM 10845 HB3 MET F 44 -14.618 21.589 4.826 1.00 28.24
H
ATOM 10846 HG2 MET F 44 -13.609 22.019 7.420 1.00 20.67
H
ATOM 10847 HG3 MET F 44 -12.763 22.092 6.078 1.00 20.67
H
ATOM 10848 HE1 MET F 44 -14.222 25.193 4.407 1.00 20.13
H
ATOM 10849 HE2 MET F 44 -13.196 23.996 4.206 1.00 20.13
H
ATOM 10850 HE3 MET F 44 -14.758 23.706 4.242 1.00 20.13
H

ATOM 10851 N ILE F 45 -17.856 20.074 5.637 1.00 23.53 N

ATOM 10852 CA ILE F 45 -18.861 19.487 4.759 1.00 23.76 C

ATOM 10853 C ILE F 45 -19.891 20.542 4.379 1.00 24.02 C

ATOM 10854 O ILE F 45 -20.445 21.213 5.246 1.00 22.40 O

ATOM 10855 CB ILE F 45 -19.570 18.284 5.427 1.00 24.34 C
ATOM 10856 CG1 ILE F 45 -18.585 17.130 5.642 1.00 26.48
C
ATOM 10857 CG2 ILE F 45 -20.768 17.817 4.596 1.00 27.47
C

ATOM 10858 CD1 ILE F 45 -18.072 16.491 4.363 1.00 31.71 C

ATOM 10859 H ILE F 45 -17.806 19.707 6.413 1.00 28.23 H

ATOM 10860 HA ILE F 45 -18.433 19.174 3.947 1.00 28.52 H

ATOM 10861 HB ILE F 45 -19.896 18.569 6.295 1.00 29.20 H
ATOM 10862 HG12 ILE F 45 -17.818 17.464 6.132 1.00 31.78
H
ATOM 10863 HG13 ILE F 45 -19.027 16.438 6.159 1.00 31.78
H
ATOM 10864 HG21 ILE F 45 -21.188 17.065 5.043 1.00 32.97
H
ATOM 10865 HG22 ILE F 45 -21.400 18.549 4.516 1.00 32.97
H
ATOM 10866 HG23 ILE F 45 -20.458 17.550 3.717 1.00 32.97
H
ATOM 10867 HD11 ILE F 45 -17.459 15.775 4.593 1.00 38.05
H
ATOM 10868 HD12 ILE F 45 -18.824 16.136 3.864 1.00 38.05
H
ATOM 10869 HD13 ILE F 45 -17.613 17.164 3.837 1.00 38.05
H

ATOM 10870 N GLY F 46 -20.129 20.692 3.080 1.00 23.90 N
ATOM 10871 CA GLY F 46 -21.162 21.585 2.590 1.00 29.90
C

ATOM 10872 C GLY F 46 -20.766 23.050 2.590 1.00 30.07 C

ATOM 10873 O GLY F 46 -21.596 23.918 2.325 1.00 26.85 O

ATOM 10874 H GLY F 46 -19.699 20.281 2.459 1.00 28.68 H
ATOM 10875 HA2 GLY F 46 -21.392 21.336 1.681 1.00 35.88
H
ATOM 10876 HA3 GLY F 46 -21.954 21.487 3.141 1.00 35.88
H

ATOM 10877 N ASP F 47 -19.503 23.332 2.889 1.00 25.37 N
ATOM 10878 CA ASP F 47 -19.003 24.700 2.842 1.00 22.15

H
ATOM 4579 HG SER C 139 1.545 62.408 -6.240 1.00 32.76
H
ATOM 4580 N LYS C 140 2.828 58.620 -5.280 1.00 15.89
N
ATOM 4581 CA LYS C 140 2.167 57.822 -4.254 1.00 23.70
C
ATOM 4582 C LYS C 140 0.968 58.551 -3.655 1.00 24.90
C
ATOM 4583 O LYS C 140 -0.012 57.922 -3.258 1.00 26.09
O
ATOM 4584 CB LYS C 140 3.150 57.456 -3.142 1.00 28.92
C
ATOM 4585 CG LYS C 140 4.057 56.282 -3.470 1.00 29.54
C
ATOM 4586 CD LYS C 140 4.867 55.875 -2.252 1.00 37.47
C
ATOM 4587 CE LYS C 140 5.648 54.596 -2.489 1.00 37.64
C
ATOM 4588 NZ LYS C 140 6.295 54.118 -1.233 1.00 49.87
N1+
ATOM 4589 H LYS C 140 3.634 58.848 -5.085 1.00 19.07
H
ATOM 4590 HA LYS C 140 1.847 56.998 -4.653 1.00 28.44
H
ATOM 4591 HB2 LYS C 140 3.715 58.224 -2.962 1.00 34.70
H
ATOM 4592 HB3 LYS C 140 2.646 57.226 -2.346 1.00 34.70
H
ATOM 4593 HG2 LYS C 140 3.517 55.525 -3.746 1.00 35.45
H
ATOM 4594 HG3 LYS C 140 4.671 56.536 -4.177 1.00 35.45
H
ATOM 4595 HD2 LYS C 140 5.499 56.581 -2.040 1.00 44.96
H
ATOM 4596 HD3 LYS C 140 4.267 55.729 -1.504 1.00 44.96
H
ATOM 4597 HE2 LYS C 140 5.045 53.905 -2.803 1.00 45.16
H
ATOM 4598 HE3 LYS C 140 6.343 54.762 -3.145 1.00 45.16
H
ATOM 4599 HZ1 LYS C 140 6.748 53.368 -1.391 1.00 59.85
H
ATOM 4600 HZ2 LYS C 140 6.857 54.736 -0.926 1.00 59.85
H
ATOM 4601 HZ3 LYS C 140 5.676 53.957 -0.614 1.00 59.85
H
ATOM 4602 N GLU C 141 1.046 59.876 -3.593 1.00 24.55
N
ATOM 4603 CA GLU C 141 -0.002 60.674 -2.963 1.00 26.23
C
ATOM 4604 C GLU C 141 -1.169 60.917 -3.914 1.00 24.95
C
ATOM 4605 O GLU C 141 -2.327 60.758 -3.534 1.00 21.89
O
ATOM 4606 CB GLU C 141 0.559 62.010 -2.474 1.00 26.15
C
ATOM 4607 CG GLU C 141 1.543 61.885 -1.314 1.00 34.78
C
ATOM 4608 CD GLU C 141 2.855 61.219 -1.707 1.00 37.55
C
ATOM 4609 OE1 GLU C 141 3.227 61.278 -2.899 1.00 33.99
O
ATOM 4610 OE2 GLU C 141 3.514 60.634 -0.820 1.00 45.19
O1-
ATOM 4611 H GLU C 141 1.698 60.339 -3.910 1.00 29.46
H
ATOM 4612 HA GLU C 141 -0.342 60.193 -2.192 1.00 31.47
C
ATOM 10879 C ASP F 47 -19.092 25.225 1.417 1.00 19.48 C
ATOM 10880 O ASP F 47 -18.683 24.548 0.479 1.00 23.63 O
ATOM 10881 CB ASP F 47 -17.561 24.767 3.347 1.00 24.63
C
ATOM 10882 CG ASP F 47 -16.915 26.115 3.090 1.00 24.37
C
ATOM 10883 OD1 ASP F 47 -17.287 27.091 3.769 1.00 27.78
O
ATOM 10884 OD2 ASP F 47 -16.032 26.196 2.212 1.00 27.63
O1-
ATOM 10885 H ASP F 47 -18.915 22.749 3.122 1.00 30.44 H
ATOM 10886 HA ASP F 47 -19.552 25.262 3.410 1.00 26.58
H
ATOM 10887 HB2 ASP F 47 -17.553 24.607 4.304 1.00 29.56
H
ATOM 10888 HB3 ASP F 47 -17.034 24.090 2.893 1.00 29.56
H
ATOM 10889 N GLU F 48 -19.637 26.426 1.256 1.00 18.86 N
ATOM 10890 CA GLU F 48 -19.825 27.004 -0.074 1.00 23.59
C
ATOM 10891 C GLU F 48 -19.089 28.332 -0.224 1.00 18.84 C
ATOM 10892 O GLU F 48 -19.333 29.078 -1.173 1.00 23.99 O
ATOM 10893 CB GLU F 48 -21.321 27.185 -0.365 1.00 24.87
C
ATOM 10894 CG GLU F 48 -22.059 28.030 0.656 1.00 25.98
C
ATOM 10895 CD GLU F 48 -23.557 28.110 0.393 1.00 27.03
C
ATOM 10896 OE1 GLU F 48 -23.975 28.028 -0.781 1.00 27.18
O
ATOM 10897 OE2 GLU F 48 -24.316 28.257 1.368 1.00 24.72
O1-
ATOM 10898 H GLU F 48 -19.907 26.928 1.900 1.00 22.64 H
ATOM 10899 HA GLU F 48 -19.467 26.390 -0.734 1.00 28.31
H
ATOM 10900 HB2 GLU F 48 -21.420 27.614 -1.229 1.00 29.84
H
ATOM 10901 HB3 GLU F 48 -21.742 26.311 -0.384 1.00 29.84
H
ATOM 10902 HG2 GLU F 48 -21.930 27.643 1.536 1.00 31.18
H
ATOM 10903 HG3 GLU F 48 -21.702 28.932 0.635 1.00 31.18
H
ATOM 10904 N ILE F 49 -18.176 28.615 0.701 1.00 21.84 N
ATOM 10905 CA ILE F 49 -17.393 29.848 0.657 1.00 19.58 C
ATOM 10906 C ILE F 49 -15.911 29.570 0.422 1.00 21.99 C
ATOM 10907 O ILE F 49 -15.314 30.091 -0.521 1.00 18.32 O
ATOM 10908 CB ILE F 49 -17.560 30.650 1.958 1.00 22.04 C
ATOM 10909 CG1 ILE F 49 -19.021 31.077 2.119 1.00 19.68
C
ATOM 10910 CG2 ILE F 49 -16.648 31.883 1.960 1.00 22.59
C
ATOM 10911 CD1 ILE F 49 -19.377 31.490 3.521 1.00 29.80 C
ATOM 10912 H ILE F 49 -17.990 28.106 1.369 1.00 26.21 H

H
ATOM 4613 HB2 GLU C 141 1.022 62.442 -3.209 1.00 31.39
H
ATOM 4614 HB3 GLU C 141 -0.178 62.568 -2.178 1.00 31.39
H
ATOM 4615 HG2 GLU C 141 1.747 62.772 -0.978 1.00 41.74
H
ATOM 4616 HG3 GLU C 141 1.136 61.352 -0.613 1.00 41.74
H
ATOM 4617 N ASP C 142 -0.867 61.296 -5.152 1.00 22.41
N
ATOM 4618 CA ASP C 142 -1.915 61.567 -6.129 1.00 21.49
C
ATOM 4619 C ASP C 142 -2.560 60.282 -6.633 1.00 21.91
C
ATOM 4620 O ASP C 142 -3.686 60.300 -7.128 1.00 24.05
O
ATOM 4621 CB ASP C 142 -1.357 62.369 -7.307 1.00 24.21
C
ATOM 4622 CG ASP C 142 -0.908 63.760 -6.901 1.00 29.23
C
ATOM 4623 OD1 ASP C 142 -1.248 64.193 -5.776 1.00 30.52
O
ATOM 4624 OD2 ASP C 142 -0.223 64.424 -7.707 1.00 33.69
O1-
ATOM 4625 H ASP C 142 -0.067 61.403 -5.450 1.00 26.89
H
ATOM 4626 HA ASP C 142 -2.606 62.101 -5.707 1.00 25.79
H
ATOM 4627 HB2 ASP C 142 -0.590 61.901 -7.674 1.00 29.05
H
ATOM 4628 HB3 ASP C 142 -2.046 62.460 -7.983 1.00 29.05
H
ATOM 4629 N GLN C 143 -1.849 59.167 -6.501 1.00 17.21
N
ATOM 4630 CA GLN C 143 -2.357 57.882 -6.969 1.00 20.06
C
ATOM 4631 C GLN C 143 -2.424 56.890 -5.819 1.00 19.18
C
ATOM 4632 O GLN C 143 -2.183 55.696 -5.994 1.00 17.46
O
ATOM 4633 CB GLN C 143 -1.479 57.342 -8.097 1.00 18.97
C
ATOM 4634 CG GLN C 143 -1.248 58.349 -9.217 1.00 17.93
C
ATOM 4635 CD GLN C 143 -0.285 57.837 -10.270 1.00 21.93
C
ATOM 4636 OE1 GLN C 143 0.917 57.724 -10.024 1.00 19.88
O
ATOM 4637 NE2 GLN C 143 -0.808 57.520 -11.450 1.00 17.07
N
ATOM 4638 H GLN C 143 -1.069 59.128 -6.143 1.00 20.65
H
ATOM 4639 HA GLN C 143 -3.255 58.002 -7.317 1.00 24.08
H
ATOM 4640 HB2 GLN C 143 -0.614 57.098 -7.732 1.00 22.76
H
ATOM 4641 HB3 GLN C 143 -1.906 56.561 -8.482 1.00 22.76
H
ATOM 4642 HG2 GLN C 143 -2.094 58.540 -9.651 1.00 21.52
H
ATOM 4643 HG3 GLN C 143 -0.877 59.162 -8.840 1.00 21.52
H
ATOM 4644 HE21 GLN C 143 -0.302 57.225 -12.079 1.00 20.49
H
ATOM 4645 HE22 GLN C 143 -1.653 57.609 -11.584 1.00 20.49
H
ATOM 4646 N ASP C 144 -2.770 57.395 -4.639 1.00 22.78

ATOM 10913 HA ILE F 49 -17.714 30.397 -0.075 1.00 23.50 H

ATOM 10914 HB ILE F 49 -17.317 30.082 2.707 1.00 26.45 H
ATOM 10915 HG12 ILE F 49 -19.192 31.832 1.534 1.00 23.61
H
ATOM 10916 HG13 ILE F 49 -19.594 30.334 1.874 1.00 23.61
H
ATOM 10917 HG21 ILE F 49 -16.775 32.368 2.791 1.00 27.11
H
ATOM 10918 HG22 ILE F 49 -15.726 31.594 1.883 1.00 27.11
H
ATOM 10919 HG23 ILE F 49 -16.882 32.449 1.208 1.00 27.11
H
ATOM 10920 HD11 ILE F 49 -20.312 31.747 3.546 1.00 35.76
H
ATOM 10921 HD12 ILE F 49 -19.222 30.743 4.119 1.00 35.76
H
ATOM 10922 HD13 ILE F 49 -18.820 32.242 3.779 1.00 35.76
H

ATOM 10923 N PHE F 50 -15.317 28.749 1.279 1.00 14.92 N
ATOM 10924 CA PHE F 50 -13.876 28.544 1.238 1.00 18.72
C

ATOM 10925 C PHE F 50 -13.449 27.474 0.235 1.00 15.47 C

ATOM 10926 O PHE F 50 -12.438 27.643 -0.442 1.00 15.17 O
ATOM 10927 CB PHE F 50 -13.374 28.203 2.637 1.00 14.79
C
ATOM 10928 CG PHE F 50 -13.688 29.267 3.644 1.00 20.85
C
ATOM 10929 CD1 PHE F 50 -12.912 30.413 3.720 1.00 23.04
C
ATOM 10930 CD2 PHE F 50 -14.778 29.144 4.488 1.00 21.71
C
ATOM 10931 CE1 PHE F 50 -13.206 31.407 4.633 1.00 21.89
C
ATOM 10932 CE2 PHE F 50 -15.074 30.134 5.408 1.00 21.18
C
ATOM 10933 CZ PHE F 50 -14.288 31.268 5.475 1.00 19.57
C

ATOM 10934 H PHE F 50 -15.724 28.301 1.890 1.00 17.90 H
ATOM 10935 HA PHE F 50 -13.454 29.376 0.972 1.00 22.46
H
ATOM 10936 HB2 PHE F 50 -13.794 27.379 2.930 1.00 17.74
H
ATOM 10937 HB3 PHE F 50 -12.411 28.092 2.608 1.00 17.74
H
ATOM 10938 HD1 PHE F 50 -12.181 30.512 3.153 1.00 27.65
H
ATOM 10939 HD2 PHE F 50 -15.310 28.383 4.445 1.00 26.06
H
ATOM 10940 HE1 PHE F 50 -12.674 32.169 4.681 1.00 26.27
H
ATOM 10941 HE2 PHE F 50 -15.805 30.039 5.975 1.00 25.42
H
ATOM 10942 HZ PHE F 50 -14.486 31.934 6.094 1.00 23.49
H

ATOM 10943 N LEU F 51 -14.215 26.389 0.130 1.00 15.59 N
ATOM 10944 CA LEU F 51 -13.877 25.314 -0.803 1.00 16.84
C

ATOM 10945 C LEU F 51 -13.816 25.809 -2.251 1.00 14.18 C
ATOM 10946 O LEU F 51 -12.842 25.549 -2.949 1.00 17.50 O

N
ATOM 4647 CA ASP C 144 -2.791 56.572 -3.438 1.00 23.80
C
ATOM 4648 C ASP C 144 -3.893 55.512 -3.492 1.00 19.24
C
ATOM 4649 O ASP C 144 -3.854 54.538 -2.740 1.00 21.24
O
ATOM 4650 CB ASP C 144 -2.949 57.449 -2.188 1.00 24.80
C
ATOM 4651 CG ASP C 144 -4.205 58.296 -2.215 1.00 24.61
C
ATOM 4652 OD1 ASP C 144 -4.881 58.345 -3.264 1.00 31.09
O
ATOM 4653 OD2 ASP C 144 -4.511 58.927 -1.183 1.00 34.04
O1-
ATOM 4654 H ASP C 144 -2.998 58.214 -4.509 1.00 27.33
H
ATOM 4655 HA ASP C 144 -1.942 56.108 -3.366 1.00 28.56
H
ATOM 4656 HB2 ASP C 144 -2.991 56.878 -1.405 1.00 29.76
H
ATOM 4657 HB3 ASP C 144 -2.188 58.046 -2.123 1.00 29.76
H
ATOM 4658 N LEU C 145 -4.864 55.678 -4.386 1.00 18.41
N
ATOM 4659 CA LEU C 145 -5.892 54.652 -4.544 1.00 19.62
C
ATOM 4660 C LEU C 145 -5.274 53.321 -4.976 1.00 20.78
C
ATOM 4661 O LEU C 145 -5.893 52.270 -4.826 1.00 14.96
O
ATOM 4662 CB LEU C 145 -6.968 55.078 -5.553 1.00 19.66
C
ATOM 4663 CG LEU C 145 -6.615 55.709 -6.908 1.00 27.10
C
ATOM 4664 CD1 LEU C 145 -5.336 55.184 -7.518 1.00 25.70
C
ATOM 4665 CD2 LEU C 145 -7.776 55.498 -7.879 1.00 21.56
C
ATOM 4666 H LEU C 145 -4.950 56.360 -4.903 1.00 22.09
H
ATOM 4667 HA LEU C 145 -6.328 54.513 -3.689 1.00 23.55
H
ATOM 4668 HB2 LEU C 145 -7.493 54.288 -5.756 1.00 23.59
H
ATOM 4669 HB3 LEU C 145 -7.540 55.718 -5.102 1.00 23.59
H
ATOM 4670 HG LEU C 145 -6.508 56.665 -6.784 1.00 32.52
H
ATOM 4671 HD11 LEU C 145 -5.185 55.630 -8.366 1.00 30.83
H
ATOM 4672 HD12 LEU C 145 -4.600 55.366 -6.913 1.00 30.83
H
ATOM 4673 HD13 LEU C 145 -5.422 54.228 -7.657 1.00 30.83
H
ATOM 4674 HD21 LEU C 145 -7.550 55.898 -8.734 1.00 25.87
H
ATOM 4675 HD22 LEU C 145 -7.927 54.547 -7.989 1.00 25.87
H
ATOM 4676 HD23 LEU C 145 -8.571 55.920 -7.517 1.00 25.87
H
ATOM 4677 N LEU C 146 -4.048 53.365 -5.494 1.00 16.14
N
ATOM 4678 CA LEU C 146 -3.384 52.158 -5.983 1.00 16.03
C
ATOM 4679 C LEU C 146 -2.981 51.231 -4.840 1.00 17.57
C
ATOM 4680 O LEU C 146 -2.655 50.065 -5.067 1.00 16.74

ATOM 10947 CB LEU F 51 -14.878 24.157 -0.695 1.00 16.15
C
ATOM 10948 CG LEU F 51 -14.747 23.235 0.521 1.00 23.56
C
ATOM 10949 CD1 LEU F 51 -15.930 22.279 0.591 1.00 25.39
C
ATOM 10950 CD2 LEU F 51 -13.442 22.452 0.490 1.00 18.07
C

ATOM 10951 H LEU F 51 -14.931 26.251 0.585 1.00 18.71 H
ATOM 10952 HA LEU F 51 -13.000 24.967 -0.573 1.00 20.21
H
ATOM 10953 HB2 LEU F 51 -15.772 24.533 -0.673 1.00 19.38
H
ATOM 10954 HB3 LEU F 51 -14.785 23.603 -1.485 1.00 19.38
H
ATOM 10955 HG LEU F 51 -14.751 23.775 1.327 1.00 28.27
H
ATOM 10956 HD11 LEU F 51 -15.826 21.705 1.367 1.00 30.46
H
ATOM 10957 HD12 LEU F 51 -16.748 22.794 0.667 1.00 30.46
H
ATOM 10958 HD13 LEU F 51 -15.950 21.742 -0.217 1.00 30.46
H
ATOM 10959 HD21 LEU F 51 -13.398 21.882 1.274 1.00 21.69
H
ATOM 10960 HD22 LEU F 51 -13.418 21.911 -0.314 1.00 21.69
H
ATOM 10961 HD23 LEU F 51 -12.700 23.076 0.492 1.00 21.69
H

ATOM 10962 N PRO F 52 -14.858 26.512 -2.718 1.00 15.74 N
ATOM 10963 CA PRO F 52 -14.770 27.012 -4.094 1.00 16.28
C

ATOM 10964 C PRO F 52 -13.685 28.072 -4.276 1.00 16.85 C
ATOM 10965 O PRO F 52 -13.036 28.106 -5.322 1.00 15.38
O
ATOM 10966 CB PRO F 52 -16.167 27.601 -4.350 1.00 19.09
C
ATOM 10967 CG PRO F 52 -16.760 27.811 -3.003 1.00 20.50
C
ATOM 10968 CD PRO F 52 -16.194 26.736 -2.139 1.00 20.80
C
ATOM 10969 HA PRO F 52 -14.611 26.279 -4.710 1.00 19.54
H
ATOM 10970 HB2 PRO F 52 -16.084 28.443 -4.822 1.00 22.91
H
ATOM 10971 HB3 PRO F 52 -16.697 26.971 -4.862 1.00 22.91
H
ATOM 10972 HG2 PRO F 52 -16.507 28.686 -2.669 1.00 24.59
H
ATOM 10973 HG3 PRO F 52 -17.725 27.732 -3.057 1.00 24.59
H
ATOM 10974 HD2 PRO F 52 -16.119 27.042 -1.222 1.00 24.96
H
ATOM 10975 HD3 PRO F 52 -16.731 25.930 -2.204 1.00 24.96
H

ATOM 10976 N PHE F 53 -13.485 28.921 -3.273 1.00 15.61 N
ATOM 10977 CA PHE F 53 -12.478 29.970 -3.374 1.00 15.34
C

ATOM 10978 C PHE F 53 -11.083 29.361 -3.477 1.00 14.81 C

ATOM 10979 O PHE F 53 -10.293 29.756 -4.334 1.00 15.50 O
ATOM 10980 CB PHE F 53 -12.555 30.922 -2.180 1.00 15.16

O
ATOM 4681 CB LEU C 146 -2.154 52.524 -6.821 1.00 17.95
C
ATOM 4682 CG LEU C 146 -2.410 53.275 -8.132 1.00 15.53
C
ATOM 4683 CD1 LEU C 146 -1.089 53.618 -8.817 1.00 16.96
C
ATOM 4684 CD2 LEU C 146 -3.292 52.460 -9.064 1.00 19.12
C
ATOM 4685 H LEU C 146 -3.579 54.081 -5.574 1.00 19.36
H
ATOM 4686 HA LEU C 146 -3.999 51.673 -6.555 1.00 19.23
H
ATOM 4687 HB2 LEU C 146 -1.575 53.083 -6.280 1.00 21.54
H
ATOM 4688 HB3 LEU C 146 -1.688 51.704 -7.048 1.00 21.54
H
ATOM 4689 HG LEU C 146 -2.870 54.106 -7.935 1.00 18.63
H
ATOM 4690 HD11 LEU C 146 -1.276 54.092 -9.642 1.00 20.36
H
ATOM 4691 HD12 LEU C 146 -0.564 54.179 -8.225 1.00 20.36
H
ATOM 4692 HD13 LEU C 146 -0.610 52.797 -9.007 1.00 20.36
H
ATOM 4693 HD21 LEU C 146 -3.435 52.962 -9.882 1.00 22.95
H
ATOM 4694 HD22 LEU C 146 -2.850 51.621 -9.264 1.00 22.95
H
ATOM 4695 HD23 LEU C 146 -4.142 52.291 -8.627 1.00 22.95
H
ATOM 4696 N LYS C 147 -3.014 51.744 -3.613 1.00 19.33
N
ATOM 4697 CA LYS C 147 -2.750 50.925 -2.433 1.00 19.87
C
ATOM 4698 C LYS C 147 -3.839 49.877 -2.192 1.00 17.73
C
ATOM 4699 O LYS C 147 -3.603 48.867 -1.526 1.00 19.26
O
ATOM 4700 CB LYS C 147 -2.628 51.807 -1.188 1.00 23.96
C
ATOM 4701 CG LYS C 147 -1.400 52.698 -1.163 1.00 34.05
C
ATOM 4702 CD LYS C 147 -1.286 53.467 0.152 1.00 43.75
C
ATOM 4703 CE LYS C 147 -2.464 54.413 0.354 1.00 52.91
C
ATOM 4704 NZ LYS C 147 -2.213 55.423 1.423 1.00 63.31
N1+
ATOM 4705 H LYS C 147 -3.187 52.568 -3.436 1.00 23.19
H
ATOM 4706 HA LYS C 147 -1.908 50.459 -2.555 1.00 23.84
H
ATOM 4707 HB2 LYS C 147 -3.409 52.380 -1.136 1.00 28.75
H
ATOM 4708 HB3 LYS C 147 -2.592 51.234 -0.405 1.00 28.75
H
ATOM 4709 HG2 LYS C 147 -0.606 52.150 -1.263 1.00 40.86
H
ATOM 4710 HG3 LYS C 147 -1.458 53.341 -1.886 1.00 40.86
H
ATOM 4711 HD2 LYS C 147 -1.272 52.838 0.890 1.00 52.50
H
ATOM 4712 HD3 LYS C 147 -0.472 53.994 0.145 1.00 52.50
H
ATOM 4713 HE2 LYS C 147 -2.634 54.888 -0.474 1.00 63.49
H
ATOM 4714 HE3 LYS C 147 -3.245 53.896 0.607 1.00 63.49
C
ATOM 10981 CG PHE F 53 -11.510 32.002 -2.204 1.00 15.82
C
ATOM 10982 CD1 PHE F 53 -11.679 33.131 -2.989 1.00 15.97
C
ATOM 10983 CD2 PHE F 53 -10.356 31.885 -1.448 1.00 15.98
C
ATOM 10984 CE1 PHE F 53 -10.719 34.123 -3.016 1.00 18.86
C
ATOM 10985 CE2 PHE F 53 -9.392 32.879 -1.470 1.00 13.90
C
ATOM 10986 CZ PHE F 53 -9.574 33.995 -2.256 1.00 13.75 C
ATOM 10987 H PHE F 53 -13.916 28.910 -2.528 1.00 18.73 H
ATOM 10988 HA PHE F 53 -12.640 30.486 -4.179 1.00 18.41
H
ATOM 10989 HB2 PHE F 53 -13.425 31.350 -2.176 1.00 18.19
H
ATOM 10990 HB3 PHE F 53 -12.436 30.411 -1.364 1.00 18.19
H
ATOM 10991 HD1 PHE F 53 -12.448 33.222 -3.504 1.00 19.16
H
ATOM 10992 HD2 PHE F 53 -10.229 31.133 -0.916 1.00 19.17
H
ATOM 10993 HE1 PHE F 53 -10.844 34.877 -3.546 1.00 22.64
H
ATOM 10994 HE2 PHE F 53 -8.620 32.791 -0.958 1.00 16.68
H
ATOM 10995 HZ PHE F 53 -8.927 34.664 -2.272 1.00 16.50 H
ATOM 10996 N TYR F 54 -10.790 28.389 -2.616 1.00 13.52 N
ATOM 10997 CA TYR F 54 -9.500 27.707 -2.649 1.00 13.81 C
ATOM 10998 C TYR F 54 -9.324 26.904 -3.935 1.00 13.72 C
ATOM 10999 O TYR F 54 -8.222 26.831 -4.473 1.00 12.92 O
ATOM 11000 CB TYR F 54 -9.338 26.783 -1.436 1.00 12.43 C
ATOM 11001 CG TYR F 54 -9.215 27.502 -0.107 1.00 13.97
C
ATOM 11002 CD1 TYR F 54 -8.682 28.785 -0.029 1.00 15.04
C
ATOM 11003 CD2 TYR F 54 -9.637 26.899 1.070 1.00 14.73
C
ATOM 11004 CE1 TYR F 54 -8.575 29.442 1.182 1.00 13.01
C
ATOM 11005 CE2 TYR F 54 -9.531 27.545 2.282 1.00 13.82
C
ATOM 11006 CZ TYR F 54 -9.002 28.814 2.333 1.00 14.13 C
ATOM 11007 OH TYR F 54 -8.901 29.461 3.537 1.00 13.26
O
ATOM 11008 H TYR F 54 -11.322 28.106 -2.003 1.00 16.22 H
ATOM 11009 HA TYR F 54 -8.793 28.371 -2.614 1.00 16.57 H
ATOM 11010 HB2 TYR F 54 -10.112 26.201 -1.384 1.00 14.92
H
ATOM 11011 HB3 TYR F 54 -8.536 26.250 -1.557 1.00 14.92
H
ATOM 11012 HD1 TYR F 54 -8.395 29.208 -0.805 1.00 18.05
H
ATOM 11013 HD2 TYR F 54 -9.996 26.041 1.039 1.00 17.67
H
ATOM 11014 HE1 TYR F 54 -8.217 30.299 1.221 1.00 15.61

H
ATOM 4715 HZ1 LYS C 147 -2.921 55.955 1.511 1.00 75.97
H
ATOM 4716 HZ2 LYS C 147 -2.060 55.014 2.198 1.00 75.97
H
ATOM 4717 HZ3 LYS C 147 -1.504 55.918 1.213 1.00 75.97
H
ATOM 4718 N LEU C 148 -5.028 50.122 -2.732 1.00 15.82
N
ATOM 4719 CA LEU C 148 -6.210 49.333 -2.387 1.00 18.04
C
ATOM 4720 C LEU C 148 -6.593 48.304 -3.450 1.00 18.60
C
ATOM 4721 O LEU C 148 -7.686 47.744 -3.405 1.00 15.31
O
ATOM 4722 CB LEU C 148 -7.395 50.269 -2.151 1.00 23.06
C
ATOM 4723 CG LEU C 148 -7.130 51.452 -1.217 1.00 32.15
C
ATOM 4724 CD1 LEU C 148 -8.009 52.619 -1.612 1.00 32.37
C
ATOM 4725 CD2 LEU C 148 -7.363 51.056 0.236 1.00 30.03
C
ATOM 4726 H LEU C 148 -5.179 50.745 -3.306 1.00 18.98
H
ATOM 4727 HA LEU C 148 -6.038 48.856 -1.560 1.00 21.65
H
ATOM 4728 HB2 LEU C 148 -7.674 50.632 -3.007 1.00 27.68
H
ATOM 4729 HB3 LEU C 148 -8.122 49.753 -1.768 1.00 27.68
H
ATOM 4730 HG LEU C 148 -6.204 51.727 -1.308 1.00 38.58
H
ATOM 4731 HD11 LEU C 148 -7.833 53.363 -1.015 1.00 38.84
H
ATOM 4732 HD12 LEU C 148 -7.804 52.873 -2.526 1.00 38.84
H
ATOM 4733 HD13 LEU C 148 -8.939 52.351 -1.544 1.00 38.84
H
ATOM 4734 HD21 LEU C 148 -7.188 51.822 0.804 1.00 36.04
H
ATOM 4735 HD22 LEU C 148 -8.284 50.770 0.341 1.00 36.04
H
ATOM 4736 HD23 LEU C 148 -6.763 50.329 0.466 1.00 36.04
H
ATOM 4737 N VAL C 149 -5.697 48.054 -4.398 1.00 16.71
N
ATOM 4738 CA VAL C 149 -6.011 47.210 -5.548 1.00 14.87
C
ATOM 4739 C VAL C 149 -5.503 45.783 -5.380 1.00 14.53
C
ATOM 4740 O VAL C 149 -4.311 45.568 -5.166 1.00 16.23
O
ATOM 4741 CB VAL C 149 -5.409 47.803 -6.833 1.00 18.92
C
ATOM 4742 CG1 VAL C 149 -5.723 46.926 -8.036 1.00 20.42
C
ATOM 4743 CG2 VAL C 149 -5.930 49.222 -7.054 1.00 20.99
C
ATOM 4744 H VAL C 149 -4.894 48.363 -4.399 1.00 20.06
H
ATOM 4745 HA VAL C 149 -6.975 47.174 -5.658 1.00 17.84
H
ATOM 4746 HB VAL C 149 -4.445 47.849 -6.738 1.00 22.71
H
ATOM 4747 HG11 VAL C 149 -5.330 47.326 -8.828 1.00 24.51
H
ATOM 4748 HG12 VAL C 149 -5.347 46.044 -7.890 1.00 24.51
H
ATOM 11015 HE2 TYR F 54 -9.820 27.127 3.061 1.00 16.58
H
ATOM 11016 HH TYR F 54 -9.194 28.970 4.152 1.00 15.91 H
ATOM 11017 N LYS F 55 -10.403 26.303 -4.429 1.00 13.00 N
ATOM 11018 CA LYS F 55 -10.321 25.526 -5.661 1.00 15.12
C
ATOM 11019 C LYS F 55 -9.743 26.382 -6.786 1.00 14.25 C
ATOM 11020 O LYS F 55 -8.873 25.934 -7.535 1.00 15.64 O
ATOM 11021 CB LYS F 55 -11.695 24.982 -6.060 1.00 17.19
C
ATOM 11022 CG LYS F 55 -11.638 23.938 -7.159 1.00 18.78
C
ATOM 11023 CD LYS F 55 -13.025 23.546 -7.643 1.00 22.88
C
ATOM 11024 CE LYS F 55 -12.935 22.564 -8.795 1.00 27.95
C
ATOM 11025 NZ LYS F 55 -14.263 22.302 -9.406 1.00 35.34
N1+
ATOM 11026 H LYS F 55 -11.186 26.330 -4.075 1.00 15.60 H
ATOM 11027 HA LYS F 55 -9.727 24.772 -5.522 1.00 18.15 H
ATOM 11028 HB2 LYS F 55 -12.108 24.574 -5.283 1.00 20.62
H
ATOM 11029 HB3 LYS F 55 -12.243 25.717 -6.376 1.00 20.62
H
ATOM 11030 HG2 LYS F 55 -11.145 24.296 -7.913 1.00 22.53
H
ATOM 11031 HG3 LYS F 55 -11.200 23.142 -6.820 1.00 22.53
H
ATOM 11032 HD2 LYS F 55 -13.512 23.124 -6.918 1.00 27.45
H
ATOM 11033 HD3 LYS F 55 -13.495 24.337 -7.950 1.00 27.45
H
ATOM 11034 HE2 LYS F 55 -12.354 22.929 -9.480 1.00 33.53
H
ATOM 11035 HE3 LYS F 55 -12.581 21.722 -8.469 1.00 33.53
H
ATOM 11036 HZ1 LYS F 55 -14.180 21.724 -10.078 1.00 42.41
H
ATOM 11037 HZ2 LYS F 55 -14.816 21.961 -8.798 1.00 42.41
H
ATOM 11038 HZ3 LYS F 55 -14.609 23.060 -9.719 1.00 42.41
H
ATOM 11039 N ASN F 56 -10.210 27.622 -6.886 1.00 12.64 N
ATOM 11040 CA ASN F 56 -9.713 28.541 -7.906 1.00 15.26 C
ATOM 11041 C ASN F 56 -8.293 29.017 -7.618 1.00 16.59 C
ATOM 11042 O ASN F 56 -7.447 29.059 -8.511 1.00 15.03 O
ATOM 11043 CB ASN F 56 -10.640 29.751 -8.028 1.00 18.33
C
ATOM 11044 CG ASN F 56 -11.983 29.397 -8.634 1.00 28.04
C
ATOM 11045 OD1 ASN F 56 -12.091 28.463 -9.428 1.00 30.73
O
ATOM 11046 ND2 ASN F 56 -13.016 30.147 -8.264 1.00 32.03
N
ATOM 11047 H ASN F 56 -10.815 27.957 -6.376 1.00 15.17 H
ATOM 11048 HA ASN F 56 -9.706 28.085 -8.762 1.00 18.31 H

H
ATOM 4749 HG13 VAL C 149 -6.685 46.864 -8.139 1.00 24.51
H
ATOM 4750 HG21 VAL C 149 -5.539 49.577 -7.868 1.00 25.18
H
ATOM 4751 HG22 VAL C 149 -6.896 49.194 -7.136 1.00 25.18
H
ATOM 4752 HG23 VAL C 149 -5.677 49.772 -6.297 1.00 25.18
H
ATOM 4753 N LYS C 150 -6.408 44.816 -5.500 1.00 13.93
N
ATOM 4754 CA LYS C 150 -6.044 43.402 -5.450 1.00 18.06
C
ATOM 4755 C LYS C 150 -5.531 42.912 -6.797 1.00 15.46
C
ATOM 4756 O LYS C 150 -5.715 43.570 -7.819 1.00 15.34
O
ATOM 4757 CB LYS C 150 -7.238 42.538 -5.030 1.00 16.72
C
ATOM 4758 CG LYS C 150 -7.584 42.607 -3.553 1.00 17.69
C
ATOM 4759 CD LYS C 150 -8.705 41.641 -3.194 1.00 15.55
C
ATOM 4760 CE LYS C 150 -8.218 40.202 -3.082 1.00 17.69
C
ATOM 4761 NZ LYS C 150 -7.374 39.972 -1.871 1.00 15.20
N1+
ATOM 4762 H LYS C 150 -7.249 44.953 -5.613 1.00 16.72
H
ATOM 4763 HA LYS C 150 -5.338 43.279 -4.796 1.00 21.68
H
ATOM 4764 HB2 LYS C 150 -8.019 42.826 -5.528 1.00 20.06
H
ATOM 4765 HB3 LYS C 150 -7.040 41.612 -5.241 1.00 20.06
H
ATOM 4766 HG2 LYS C 150 -6.802 42.373 -3.030 1.00 21.22
H
ATOM 4767 HG3 LYS C 150 -7.877 43.506 -3.335 1.00 21.22
H
ATOM 4768 HD2 LYS C 150 -9.084 41.898 -2.339 1.00 18.65
H
ATOM 4769 HD3 LYS C 150 -9.386 41.675 -3.884 1.00 18.65
H
ATOM 4770 HE2 LYS C 150 -8.986 39.612 -3.029 1.00 21.23
H
ATOM 4771 HE3 LYS C 150 -7.686 39.987 -3.864 1.00 21.23
H
ATOM 4772 HZ1 LYS C 150 -6.656 40.498 -1.896 1.00 18.24
H
ATOM 4773 HZ2 LYS C 150 -7.841 40.156 -1.136 1.00 18.24
H
ATOM 4774 HZ3 LYS C 150 -7.110 39.123 -1.841 1.00 18.24
H
ATOM 4775 N SER C 151 -4.903 41.742 -6.777 1.00 16.11
N
ATOM 4776 CA SER C 151 -4.426 41.078 -7.985 1.00 17.40
C
ATOM 4777 C SER C 151 -3.319 41.859 -8.690 1.00 14.09
C
ATOM 4778 O SER C 151 -2.799 42.846 -8.168 1.00 16.03
O
ATOM 4779 CB SER C 151 -5.585 40.834 -8.952 1.00 14.05
C
ATOM 4780 OG SER C 151 -5.188 39.954 -9.988 1.00 14.91
O
ATOM 4781 H SER C 151 -4.736 41.302 -6.057 1.00 19.33
H
ATOM 4782 HA SER C 151 -4.063 40.213 -7.739 1.00 20.89

ATOM 11049 HB2 ASN F 56 -10.797 30.119 -7.144 1.00 22.00
H
ATOM 11050 HB3 ASN F 56 -10.220 30.416 -8.595 1.00 22.00
H
ATOM 11051 HD21 ASN F 56 -13.799 29.986 -8.581 1.00 38.43
H
ATOM 11052 HD22 ASN F 56 -12.901 30.792 -7.708 1.00 38.43
H

ATOM 11053 N VAL F 57 -8.039 29.391 -6.370 1.00 12.10 N

ATOM 11054 CA VAL F 57 -6.714 29.855 -5.972 1.00 12.15 C

ATOM 11055 C VAL F 57 -5.674 28.762 -6.181 1.00 12.63 C

ATOM 11056 O VAL F 57 -4.603 29.015 -6.738 1.00 16.24 O

ATOM 11057 CB VAL F 57 -6.708 30.312 -4.500 1.00 12.42 C
ATOM 11058 CG1 VAL F 57 -5.284 30.566 -4.000 1.00 13.82
C
ATOM 11059 CG2 VAL F 57 -7.555 31.571 -4.342 1.00 13.89
C

ATOM 11060 H VAL F 57 -8.617 29.386 -5.733 1.00 14.52 H

ATOM 11061 HA VAL F 57 -6.467 30.615 -6.522 1.00 14.57 H

ATOM 11062 HB VAL F 57 -7.100 29.615 -3.951 1.00 14.90 H
ATOM 11063 HG11 VAL F 57 -5.321 30.851 -3.074 1.00 16.59
H
ATOM 11064 HG12 VAL F 57 -4.772 29.745 -4.074 1.00 16.59
H
ATOM 11065 HG13 VAL F 57 -4.878 31.260 -4.544 1.00 16.59
H
ATOM 11066 HG21 VAL F 57 -7.541 31.845 -3.412 1.00 16.67
H
ATOM 11067 HG22 VAL F 57 -7.184 32.272 -4.900 1.00 16.67
H
ATOM 11068 HG23 VAL F 57 -8.464 31.375 -4.617 1.00 16.67
H

ATOM 11069 N PHE F 58 -5.994 27.548 -5.740 1.00 12.82 N

ATOM 11070 CA PHE F 58 -5.062 26.430 -5.830 1.00 13.09 C

ATOM 11071 C PHE F 58 -4.801 26.058 -7.285 1.00 14.82 C

ATOM 11072 O PHE F 58 -3.660 25.848 -7.676 1.00 12.06 O

ATOM 11073 CB PHE F 58 -5.588 25.207 -5.070 1.00 12.73 C
ATOM 11074 CG PHE F 58 -5.695 25.402 -3.578 1.00 12.49
C
ATOM 11075 CD1 PHE F 58 -5.281 26.581 -2.974 1.00 12.83
C
ATOM 11076 CD2 PHE F 58 -6.213 24.396 -2.777 1.00 13.83
C
ATOM 11077 CE1 PHE F 58 -5.388 26.751 -1.603 1.00 13.49
C
ATOM 11078 CE2 PHE F 58 -6.322 24.566 -1.405 1.00 16.44
C

ATOM 11079 CZ PHE F 58 -5.906 25.747 -0.821 1.00 11.02 C

ATOM 11080 H PHE F 58 -6.749 27.346 -5.381 1.00 15.38 H

ATOM 11081 HA PHE F 58 -4.217 26.690 -5.431 1.00 15.71 H
ATOM 11082 HB2 PHE F 58 -6.473 24.991 -5.403 1.00 15.28

H
ATOM 4783 HB2 SER C 151 -6.325 40.438 -8.467 1.00 16.86
H
ATOM 4784 HB3 SER C 151 -5.856 41.679 -9.342 1.00 16.86
H
ATOM 4785 HG SER C 151 -5.828 39.824 -10.515 1.00 17.89
H
ATOM 4786 N TYR C 152 -2.961 41.385 -9.877 1.00 12.60
N
ATOM 4787 CA TYR C 152 -1.828 41.905 -10.624 1.00 11.73
C
ATOM 4788 C TYR C 152 -2.312 42.429 -11.968 1.00 17.09
C
ATOM 4789 O TYR C 152 -3.220 41.852 -12.575 1.00 15.23
O
ATOM 4790 CB TYR C 152 -0.770 40.814 -10.824 1.00 14.94
C
ATOM 4791 CG TYR C 152 -0.394 40.065 -9.562 1.00 13.45
C
ATOM 4792 CD1 TYR C 152 -0.119 40.743 -8.383 1.00 17.53
C
ATOM 4793 CD2 TYR C 152 -0.317 38.678 -9.552 1.00 13.04
C
ATOM 4794 CE1 TYR C 152 0.229 40.064 -7.232 1.00 15.99
C
ATOM 4795 CE2 TYR C 152 0.031 37.989 -8.407 1.00 17.54
C
ATOM 4796 CZ TYR C 152 0.303 38.688 -7.246 1.00 17.26
C
ATOM 4797 OH TYR C 152 0.650 38.009 -6.097 1.00 14.46
O
ATOM 4798 H TYR C 152 -3.371 40.745 -10.280 1.00 15.12
H
ATOM 4799 HA TYR C 152 -1.425 42.639 -10.134 1.00 14.07
H
ATOM 4800 HB2 TYR C 152 -1.110 40.166 -11.461 1.00 17.93
H
ATOM 4801 HB3 TYR C 152 0.036 41.224 -11.174 1.00 17.93
H
ATOM 4802 HD1 TYR C 152 -0.165 41.672 -8.369 1.00 21.04
H
ATOM 4803 HD2 TYR C 152 -0.496 38.205 -10.333 1.00 15.65
H
ATOM 4804 HE1 TYR C 152 0.412 40.533 -6.450 1.00 19.18
H
ATOM 4805 HE2 TYR C 152 0.080 37.060 -8.416 1.00 21.05
H
ATOM 4806 HH TYR C 152 0.657 37.182 -6.243 1.00 17.36
H
ATOM 4807 N HIS C 153 -1.711 43.521 -12.428 1.00 11.85
N
ATOM 4808 CA HIS C 153 -2.185 44.203 -13.628 1.00 13.69
C
ATOM 4809 C HIS C 153 -1.038 44.802 -14.415 1.00 13.10
C
ATOM 4810 O HIS C 153 -0.106 45.358 -13.836 1.00 13.18
O
ATOM 4811 CB HIS C 153 -3.182 45.302 -13.254 1.00 12.79
C
ATOM 4812 CG HIS C 153 -4.220 44.860 -12.274 1.00 15.44
C
ATOM 4813 ND1 HIS C 153 -5.444 44.357 -12.661 1.00 13.49
N
ATOM 4814 CD2 HIS C 153 -4.210 44.830 -10.920 1.00 15.97
C
ATOM 4815 CE1 HIS C 153 -6.146 44.043 -11.587 1.00 16.56
C
ATOM 4816 NE2 HIS C 153 -5.419 44.317 -10.518 1.00 16.62
H
ATOM 11083 HB3 PHE F 58 -4.988 24.461 -5.227 1.00 15.28
H
ATOM 11084 HD1 PHE F 58 -4.931 27.267 -3.496 1.00 15.39
H
ATOM 11085 HD2 PHE F 58 -6.497 23.600 -3.166 1.00 16.60
H
ATOM 11086 HE1 PHE F 58 -5.107 27.546 -1.211 1.00 16.19
H
ATOM 11087 HE2 PHE F 58 -6.672 23.884 -0.878 1.00 19.73
H

ATOM 11088 HZ PHE F 58 -5.975 25.862 0.099 1.00 13.22 H

ATOM 11089 N SER F 59 -5.853 25.970 -8.089 1.00 12.82 N

ATOM 11090 CA SER F 59 -5.685 25.598 -9.486 1.00 16.28 C

ATOM 11091 C SER F 59 -4.855 26.649 -10.229 1.00 18.53 C

ATOM 11092 O SER F 59 -4.011 26.307 -11.056 1.00 15.62 O
ATOM 11093 CB SER F 59 -7.046 25.406 -10.159 1.00 19.61
C
ATOM 11094 OG SER F 59 -7.896 26.504 -9.896 1.00 29.67
O

ATOM 11095 H SER F 59 -6.667 26.119 -7.853 1.00 15.39 H

ATOM 11096 HA SER F 59 -5.208 24.754 -9.532 1.00 19.54 H
ATOM 11097 HB2 SER F 59 -6.917 25.329 -11.118 1.00 23.54
H
ATOM 11098 HB3 SER F 59 -7.458 24.598 -9.815 1.00 23.54
H
ATOM 11099 HG SER F 59 -7.551 27.212 -10.189 1.00 35.60
H

ATOM 11100 N GLU F 60 -5.070 27.925 -9.914 1.00 17.84 N
ATOM 11101 CA GLU F 60 -4.311 29.000 -10.554 1.00 15.88
C

ATOM 11102 C GLU F 60 -2.856 29.027 -10.090 1.00 14.19 C

ATOM 11103 O GLU F 60 -1.958 29.374 -10.859 1.00 16.59 O
ATOM 11104 CB GLU F 60 -4.966 30.356 -10.286 1.00 19.52
C
ATOM 11105 CG GLU F 60 -6.207 30.607 -11.124 1.00 26.68
C
ATOM 11106 CD GLU F 60 -5.906 30.696 -12.609 1.00 34.90
C
ATOM 11107 OE1 GLU F 60 -5.129 31.593 -13.010 1.00 37.82
O
ATOM 11108 OE2 GLU F 60 -6.442 29.866 -13.377 1.00 35.67
O1-

ATOM 11109 H GLU F 60 -5.646 28.194 -9.335 1.00 21.40 H
ATOM 11110 HA GLU F 60 -4.313 28.855 -11.513 1.00 19.05
H
ATOM 11111 HB2 GLU F 60 -5.223 30.400 -9.352 1.00 23.42
H
ATOM 11112 HB3 GLU F 60 -4.326 31.058 -10.485 1.00 23.42
H
ATOM 11113 HG2 GLU F 60 -6.833 29.877 -10.988 1.00 32.02
H
ATOM 11114 HG3 GLU F 60 -6.610 31.445 -10.849 1.00 32.02
H

ATOM 11115 N PHE F 61 -2.630 28.671 -8.829 1.00 16.80 N
ATOM 11116 CA PHE F 61 -1.278 28.576 -8.290 1.00 13.01 C

N
ATOM 4817 H HIS C 153 -1.025 43.888 -12.063 1.00 14.22
H
ATOM 4818 HA HIS C 153 -2.641 43.563 -14.198 1.00 16.43
H
ATOM 4819 HB2 HIS C 153 -2.697 46.043 -12.859 1.00 15.35
H
ATOM 4820 HB3 HIS C 153 -3.638 45.598 -14.057 1.00 15.35
H
ATOM 4821 HD1 HIS C 153 -5.710 44.265 -13.474 1.00 16.19
H
ATOM 4822 HD2 HIS C 153 -3.515 45.104 -10.366 1.00 19.16
H
ATOM 4823 HE1 HIS C 153 -7.005 43.687 -11.584 1.00 19.87
H
ATOM 4824 HE2 HIS C 153 -5.665 44.199 -9.702 1.00 19.95
H
ATOM 4825 N TRP C 154 -1.104 44.682 -15.738 1.00 15.58
N
ATOM 4826 CA TRP C 154 -0.104 45.295 -16.598 1.00 15.13
C
ATOM 4827 C TRP C 154 -0.118 46.805 -16.411 1.00 15.13
C
ATOM 4828 O TRP C 154 -1.175 47.430 -16.468 1.00 13.30
O
ATOM 4829 CB TRP C 154 -0.353 44.977 -18.078 1.00 15.45
C
ATOM 4830 CG TRP C 154 0.036 43.598 -18.543 1.00 17.21
C
ATOM 4831 CD1 TRP C 154 -0.751 42.717 -19.229 1.00 18.69
C
ATOM 4832 CD2 TRP C 154 1.310 42.957 -18.385 1.00 17.34
C
ATOM 4833 NE1 TRP C 154 -0.049 41.567 -19.506 1.00 16.22
N
ATOM 4834 CE2 TRP C 154 1.217 41.687 -18.995 1.00 17.13
C
ATOM 4835 CE3 TRP C 154 2.518 43.329 -17.783 1.00 15.92
C
ATOM 4836 CZ2 TRP C 154 2.283 40.790 -19.019 1.00 16.67
C
ATOM 4837 CZ3 TRP C 154 3.576 42.435 -17.809 1.00 13.50
C
ATOM 4838 CH2 TRP C 154 3.451 41.182 -18.422 1.00 14.99
C
ATOM 4839 H TRP C 154 -1.718 44.251 -16.159 1.00 18.70
H
ATOM 4840 HA TRP C 154 0.775 44.964 -16.357 1.00 18.16
H
ATOM 4841 HB2 TRP C 154 -1.301 45.083 -18.256 1.00 18.54
H
ATOM 4842 HB3 TRP C 154 0.147 45.612 -18.613 1.00 18.54
H
ATOM 4843 HD1 TRP C 154 -1.633 42.875 -19.480 1.00 22.43
H
ATOM 4844 HE1 TRP C 154 -0.357 40.881 -19.924 1.00 19.46
H
ATOM 4845 HE3 TRP C 154 2.608 44.160 -17.375 1.00 19.10
H
ATOM 4846 HZ2 TRP C 154 2.203 39.957 -19.424 1.00 20.01
H
ATOM 4847 HZ3 TRP C 154 4.383 42.671 -17.413 1.00 16.20
H
ATOM 4848 HH2 TRP C 154 4.179 40.603 -18.422 1.00 17.99
H
ATOM 4849 N MET C 155 1.060 47.377 -16.184 1.00 13.13
N
ATOM 4850 CA MET C 155 1.247 48.820 -16.244 1.00 15.17

ATOM 11117 C PHE F 61 -0.415 27.700 -9.188 1.00 15.28 C

ATOM 11118 O PHE F 61 0.721 28.048 -9.504 1.00 14.04 O

ATOM 11119 CB PHE F 61 -1.302 28.013 -6.866 1.00 12.89 C
ATOM 11120 CG PHE F 61 0.067 27.780 -6.272 1.00 11.72
C
ATOM 11121 CD1 PHE F 61 0.710 26.560 -6.430 1.00 12.06
C
ATOM 11122 CD2 PHE F 61 0.698 28.775 -5.538 1.00 12.10
C
ATOM 11123 CE1 PHE F 61 1.968 26.342 -5.878 1.00 14.29
C
ATOM 11124 CE2 PHE F 61 1.954 28.563 -4.982 1.00 12.57
C

ATOM 11125 CZ PHE F 61 2.589 27.347 -5.152 1.00 11.10 C

ATOM 11126 H PHE F 61 -3.247 28.479 -8.262 1.00 20.16 H

ATOM 11127 HA PHE F 61 -0.883 29.462 -8.260 1.00 15.61 H
ATOM 11128 HB2 PHE F 61 -1.771 28.638 -6.292 1.00 15.46
H
ATOM 11129 HB3 PHE F 61 -1.768 27.162 -6.876 1.00 15.46
H
ATOM 11130 HD1 PHE F 61 0.299 25.884 -6.917 1.00 14.47
H
ATOM 11131 HD2 PHE F 61 0.277 29.596 -5.421 1.00 14.52
H
ATOM 11132 HE1 PHE F 61 2.391 25.522 -5.994 1.00 17.15
H
ATOM 11133 HE2 PHE F 61 2.368 29.240 -4.496 1.00 15.08
H

ATOM 11134 HZ PHE F 61 3.429 27.203 -4.781 1.00 13.32 H

ATOM 11135 N PHE F 62 -0.962 26.564 -9.605 1.00 15.38 N
ATOM 11136 CA PHE F 62 -0.203 25.622 -10.419 1.00 14.52
C

ATOM 11137 C PHE F 62 -0.191 26.018 -11.891 1.00 14.12 C

ATOM 11138 O PHE F 62 0.847 25.938 -12.546 1.00 17.38 O
ATOM 11139 CB PHE F 62 -0.762 24.209 -10.254 1.00 17.80
C
ATOM 11140 CG PHE F 62 -0.503 23.620 -8.899 1.00 18.12
C
ATOM 11141 CD1 PHE F 62 0.767 23.192 -8.550 1.00 17.73
C
ATOM 11142 CD2 PHE F 62 -1.521 23.503 -7.972 1.00 13.87
C
ATOM 11143 CE1 PHE F 62 1.015 22.657 -7.305 1.00 14.74
C
ATOM 11144 CE2 PHE F 62 -1.279 22.972 -6.723 1.00 16.22
C

ATOM 11145 CZ PHE F 62 -0.008 22.548 -6.389 1.00 16.45 C

ATOM 11146 H PHE F 62 -1.767 26.316 -9.432 1.00 18.46 H
ATOM 11147 HA PHE F 62 0.715 25.614 -10.108 1.00 17.42
H
ATOM 11148 HB2 PHE F 62 -1.722 24.233 -10.389 1.00 21.36
H
ATOM 11149 HB3 PHE F 62 -0.350 23.630 -10.914 1.00 21.36
H
ATOM 11150 HD1 PHE F 62 1.461 23.267 -9.165 1.00 21.28

C
ATOM 4851 C MET C 155 2.264 49.134 -17.341 1.00 17.69
C
ATOM 4852 O MET C 155 2.792 48.226 -17.983 1.00 15.06
O
ATOM 4853 CB MET C 155 1.705 49.374 -14.895 1.00 13.10
C
ATOM 4854 CG MET C 155 2.991 48.776 -14.369 1.00 12.38
C
ATOM 4855 SD MET C 155 3.439 49.474 -12.769 1.00 15.66
S
ATOM 4856 CE MET C 155 4.634 48.273 -12.207 1.00 16.77
C
ATOM 4857 H MET C 155 1.776 46.943 -15.989 1.00 15.75
H
ATOM 4858 HA MET C 155 0.402 49.239 -16.468 1.00 18.20
H
ATOM 4859 HB2 MET C 155 1.841 50.330 -14.983 1.00 15.72
H
ATOM 4860 HB3 MET C 155 1.012 49.202 -14.238 1.00 15.72
H
ATOM 4861 HG2 MET C 155 2.879 47.818 -14.262 1.00 14.86
H
ATOM 4862 HG3 MET C 155 3.710 48.962 -14.994 1.00 14.86
H
ATOM 4863 HE1 MET C 155 4.961 48.538 -11.333 1.00 20.13
H
ATOM 4864 HE2 MET C 155 4.205 47.404 -12.150 1.00 20.13
H
ATOM 4865 HE3 MET C 155 5.369 48.239 -12.839 1.00 20.13
H
ATOM 4866 N GLY C 156 2.542 50.415 -17.549 1.00 15.94
N
ATOM 4867 CA GLY C 156 3.297 50.843 -18.714 1.00 17.37
C
ATOM 4868 C GLY C 156 4.802 50.829 -18.544 1.00 19.77
C
ATOM 4869 O GLY C 156 5.513 51.512 -19.281 1.00 21.61
O
ATOM 4870 H GLY C 156 2.304 51.057 -17.029 1.00 19.13
H
ATOM 4871 HA2 GLY C 156 3.076 50.264 -19.461 1.00 20.84
H
ATOM 4872 HA3 GLY C 156 3.031 51.746 -18.947 1.00 20.84
H
ATOM 4873 N LEU C 157 5.289 50.047 -17.585 1.00 18.34
N
ATOM 4874 CA LEU C 157 6.714 50.015 -17.271 1.00 17.73
C
ATOM 4875 C LEU C 157 7.415 48.890 -18.029 1.00 18.37
C
ATOM 4876 O LEU C 157 7.014 47.726 -17.935 1.00 16.44
O
ATOM 4877 CB LEU C 157 6.922 49.845 -15.762 1.00 19.33
C
ATOM 4878 CG LEU C 157 8.315 50.182 -15.225 1.00 17.68
C
ATOM 4879 CD1 LEU C 157 8.587 51.676 -15.326 1.00 18.67
C
ATOM 4880 CD2 LEU C 157 8.458 49.706 -13.788 1.00 20.64
C
ATOM 4881 H LEU C 157 4.812 49.522 -17.099 1.00 22.01
H
ATOM 4882 HA LEU C 157 7.117 50.856 -17.538 1.00 21.28
H
ATOM 4883 HB2 LEU C 157 6.290 50.418 -15.302 1.00 23.19
H
ATOM 4884 HB3 LEU C 157 6.742 48.919 -15.534 1.00 23.19
H
ATOM 11151 HD2 PHE F 62 -2.378 23.790 -8.191 1.00 16.64
H
ATOM 11152 HE1 PHE F 62 1.872 22.372 -7.082 1.00 17.69
H
ATOM 11153 HE2 PHE F 62 -1.972 22.897 -6.108 1.00 19.47
H

ATOM 11154 HZ PHE F 62 0.155 22.185 -5.548 1.00 19.74 H

ATOM 11155 N SER F 63 -1.332 26.448 -12.416 1.00 15.98 N
ATOM 11156 CA SER F 63 -1.421 26.766 -13.841 1.00 18.60
C

ATOM 11157 C SER F 63 -0.623 28.019 -14.201 1.00 16.33 C

ATOM 11158 O SER F 63 -0.291 28.231 -15.362 1.00 19.99 O
ATOM 11159 CB SER F 63 -2.885 26.932 -14.267 1.00 22.18
C
ATOM 11160 OG SER F 63 -3.490 28.031 -13.617 1.00 24.58
O

ATOM 11161 H SER F 63 -2.062 26.565 -11.977 1.00 19.18 H
ATOM 11162 HA SER F 63 -1.050 26.026 -14.347 1.00 22.32
H
ATOM 11163 HB2 SER F 63 -2.918 27.076 -15.225 1.00 26.61
H
ATOM 11164 HB3 SER F 63 -3.372 26.125 -14.037 1.00 26.61
H
ATOM 11165 HG SER F 63 -4.290 28.105 -13.863 1.00 29.50
H

ATOM 11166 N LEU F 64 -0.302 28.840 -13.206 1.00 15.47 N
ATOM 11167 CA LEU F 64 0.496 30.041 -13.437 1.00 15.54
C

ATOM 11168 C LEU F 64 1.991 29.730 -13.469 1.00 18.63 C

ATOM 11169 O LEU F 64 2.785 30.540 -13.943 1.00 13.90 O
ATOM 11170 CB LEU F 64 0.224 31.088 -12.353 1.00 15.69
C
ATOM 11171 CG LEU F 64 -1.059 31.911 -12.474 1.00 16.40
C
ATOM 11172 CD1 LEU F 64 -1.282 32.718 -11.207 1.00 17.92
C
ATOM 11173 CD2 LEU F 64 -0.993 32.831 -13.679 1.00 21.55
C

ATOM 11174 H LEU F 64 -0.534 28.724 -12.386 1.00 18.57 H
ATOM 11175 HA LEU F 64 0.250 30.424 -14.293 1.00 18.64
H
ATOM 11176 HB2 LEU F 64 0.190 30.632 -11.498 1.00 18.83
H
ATOM 11177 HB3 LEU F 64 0.964 31.715 -12.350 1.00 18.83
H
ATOM 11178 HG LEU F 64 -1.813 31.312 -12.590 1.00 19.68
H
ATOM 11179 HD11 LEU F 64 -2.099 33.233 -11.301 1.00 21.51
H
ATOM 11180 HD12 LEU F 64 -1.359 32.110 -10.456 1.00 21.51
H
ATOM 11181 HD13 LEU F 64 -0.528 33.314 -11.076 1.00 21.51
H
ATOM 11182 HD21 LEU F 64 -1.817 33.340 -13.732 1.00 25.87
H
ATOM 11183 HD22 LEU F 64 -0.238 33.432 -13.576 1.00 25.87
H
ATOM 11184 HD23 LEU F 64 -0.882 32.295 -14.479 1.00 25.87

H
ATOM 4885 HG LEU C 157 8.979 49.720 -15.760 1.00 21.22
H
ATOM 4886 HD11 LEU C 157 9.474 51.859 -14.979 1.00 22.41
H
ATOM 4887 HD12 LEU C 157 8.533 51.944 -16.257 1.00 22.41
H
ATOM 4888 HD13 LEU C 157 7.922 52.153 -14.805 1.00 22.41
H
ATOM 4889 HD21 LEU C 157 9.346 49.930 -13.469 1.00 24.77
H
ATOM 4890 HD22 LEU C 157 7.788 50.147 -13.242 1.00 24.77
H
ATOM 4891 HD23 LEU C 157 8.327 48.745 -13.759 1.00 24.77
H
ATOM 4892 N VAL C 158 8.462 49.247 -18.774 1.00 19.08
N
ATOM 4893 CA VAL C 158 9.199 48.292 -19.595 1.00 18.04
C
ATOM 4894 C VAL C 158 10.704 48.381 -19.349 1.00 20.45
C
ATOM 4895 O VAL C 158 11.209 49.396 -18.873 1.00 18.61
O
ATOM 4896 CB VAL C 158 8.931 48.512 -21.093 1.00 17.89
C
ATOM 4897 CG1 VAL C 158 7.446 48.311 -21.402 1.00 18.67
C
ATOM 4898 CG2 VAL C 158 9.398 49.897 -21.522 1.00 16.63
C
ATOM 4899 H VAL C 158 8.768 50.049 -18.819 1.00 22.89
H
ATOM 4900 HA VAL C 158 8.911 47.394 -19.369 1.00 21.65
H
ATOM 4901 HB VAL C 158 9.433 47.857 -21.602 1.00 21.47
H
ATOM 4902 HG11 VAL C 158 7.299 48.454 -22.350 1.00 22.40
H
ATOM 4903 HG12 VAL C 158 7.194 47.405 -21.161 1.00 22.40
H
ATOM 4904 HG13 VAL C 158 6.927 48.947 -20.887 1.00 22.40
H
ATOM 4905 HG21 VAL C 158 9.218 50.011 -22.469 1.00 19.96
H
ATOM 4906 HG22 VAL C 158 8.916 50.565 -21.010 1.00 19.96
H
ATOM 4907 HG23 VAL C 158 10.350 49.975 -21.354 1.00 19.96
H
ATOM 4908 N HIS C 159 11.405 47.314 -19.716 1.00 16.25
N
ATOM 4909 CA HIS C 159 12.812 47.135 -19.375 1.00 21.00
C
ATOM 4910 C HIS C 159 13.698 47.078 -20.616 1.00 21.62
C
ATOM 4911 O HIS C 159 13.470 46.273 -21.516 1.00 19.38
O
ATOM 4912 CB HIS C 159 12.968 45.855 -18.552 1.00 25.11
C
ATOM 4913 CG HIS C 159 14.385 45.484 -18.249 1.00 23.93
C
ATOM 4914 ND1 HIS C 159 15.041 44.462 -18.901 1.00 30.14
N
ATOM 4915 CD2 HIS C 159 15.265 45.983 -17.348 1.00 28.59
C
ATOM 4916 CE1 HIS C 159 16.269 44.354 -18.423 1.00 30.59
C
ATOM 4917 NE2 HIS C 159 16.430 45.265 -17.479 1.00 31.14
N
ATOM 4918 H HIS C 159 11.079 46.663 -20.174 1.00 19.50
H
ATOM 11185 N PHE F 65 2.371 28.568 -12.946 1.00 14.47 N
ATOM 11186 CA PHE F 65 3.784 28.206 -12.848 1.00 14.00
C
ATOM 11187 C PHE F 65 4.326 27.740 -14.195 1.00 19.33 C
ATOM 11188 O PHE F 65 3.872 26.736 -14.741 1.00 18.05 O
ATOM 11189 CB PHE F 65 3.987 27.113 -11.797 1.00 12.53
C
ATOM 11190 CG PHE F 65 5.433 26.750 -11.565 1.00 13.60
C
ATOM 11191 CD1 PHE F 65 6.370 27.728 -11.278 1.00 13.02
C
ATOM 11192 CD2 PHE F 65 5.845 25.432 -11.616 1.00 13.09
C
ATOM 11193 CE1 PHE F 65 7.694 27.395 -11.059 1.00 15.49
C
ATOM 11194 CE2 PHE F 65 7.169 25.093 -11.392 1.00 15.62
C
ATOM 11195 CZ PHE F 65 8.092 26.076 -11.117 1.00 16.41
C
ATOM 11196 H PHE F 65 1.833 27.972 -12.641 1.00 17.36 H
ATOM 11197 HA PHE F 65 4.292 28.985 -12.573 1.00 16.80
H
ATOM 11198 HB2 PHE F 65 3.619 27.419 -10.954 1.00 15.03
H
ATOM 11199 HB3 PHE F 65 3.523 26.312 -12.087 1.00 15.03
H
ATOM 11200 HD1 PHE F 65 6.108 28.619 -11.239 1.00 15.62
H
ATOM 11201 HD2 PHE F 65 5.225 24.764 -11.803 1.00 15.71
H
ATOM 11202 HE1 PHE F 65 8.316 28.061 -10.870 1.00 18.58
H
ATOM 11203 HE2 PHE F 65 7.436 24.202 -11.434 1.00 18.74
H
ATOM 11204 HZ PHE F 65 8.982 25.851 -10.969 1.00 19.69
H
ATOM 11205 N ARG F 66 5.282 28.493 -14.731 1.00 15.25 N
ATOM 11206 CA ARG F 66 5.986 28.096 -15.943 1.00 17.61
C
ATOM 11207 C ARG F 66 7.345 27.528 -15.594 1.00 25.02 C
ATOM 11208 O ARG F 66 8.085 28.103 -14.797 1.00 25.04
O
ATOM 11209 CB ARG F 66 6.142 29.273 -16.894 1.00 18.04
C
ATOM 11210 CG ARG F 66 4.896 29.554 -17.694 1.00 22.17
C
ATOM 11211 CD ARG F 66 4.516 30.995 -17.574 1.00 24.66
C
ATOM 11212 NE ARG F 66 5.588 31.875 -18.023 1.00 26.85
N
ATOM 11213 CZ ARG F 66 5.720 33.140 -17.643 1.00 26.45
C
ATOM 11214 NH1 ARG F 66 4.850 33.681 -16.797 1.00 25.82
N1+
ATOM 11215 NH2 ARG F 66 6.724 33.865 -18.107 1.00 29.31
N
ATOM 11216 H ARG F 66 5.544 29.245 -14.407 1.00 18.30 H
ATOM 11217 HA ARG F 66 5.476 27.406 -16.396 1.00 21.13
H
ATOM 11218 HB2 ARG F 66 6.352 30.068 -16.379 1.00 21.65

H
ATOM 4919 HA HIS C 159 13.104 47.882 -18.830 1.00 25.20
H
ATOM 4920 HB2 HIS C 159 12.507 45.971 -17.706 1.00 30.13
H
ATOM 4921 HB3 HIS C 159 12.570 45.119 -19.043 1.00 30.13
H
ATOM 4922 HD1 HIS C 159 14.706 43.974 -19.525 1.00 36.16
H
ATOM 4923 HD2 HIS C 159 15.112 46.683 -16.756 1.00 34.31
H
ATOM 4924 HE1 HIS C 159 16.910 43.742 -18.703 1.00 36.71
H
ATOM 4925 HE2 HIS C 159 17.147 45.390 -17.022 1.00 37.37
H
ATOM 4926 N ILE C 160 14.703 47.947 -20.656 1.00 25.17
N
ATOM 4927 CA ILE C 160 15.714 47.923 -21.708 1.00 25.24
C
ATOM 4928 C ILE C 160 16.835 46.958 -21.317 1.00 32.27
C
ATOM 4929 O ILE C 160 17.581 47.241 -20.379 1.00 31.75
O
ATOM 4930 CB ILE C 160 16.310 49.328 -21.947 1.00 29.66
C
ATOM 4931 CG1 ILE C 160 15.219 50.296 -22.407 1.00 26.24
C
ATOM 4932 CG2 ILE C 160 17.433 49.264 -22.976 1.00 33.94
C
ATOM 4933 CD1 ILE C 160 15.673 51.741 -22.507 1.00 35.20
C
ATOM 4934 H ILE C 160 14.822 48.571 -20.076 1.00 30.21
H
ATOM 4935 HA ILE C 160 15.314 47.613 -22.535 1.00 30.29
H
ATOM 4936 HB ILE C 160 16.677 49.653 -21.110 1.00 35.59
H
ATOM 4937 HG12 ILE C 160 14.910 50.022 -23.284 1.00 31.49
H
ATOM 4938 HG13 ILE C 160 14.485 50.260 -21.774 1.00 31.49
H
ATOM 4939 HG21 ILE C 160 17.790 50.156 -23.108 1.00 40.72
H
ATOM 4940 HG22 ILE C 160 18.129 48.674 -22.646 1.00 40.72
H
ATOM 4941 HG23 ILE C 160 17.077 48.923 -23.811 1.00 40.72
H
ATOM 4942 HD11 ILE C 160 14.926 52.285 -22.803 1.00 42.25
H
ATOM 4943 HD12 ILE C 160 15.974 52.038 -21.635 1.00 42.25
H
ATOM 4944 HD13 ILE C 160 16.400 51.799 -23.147 1.00 42.25
H
ATOM 4945 N PRO C 161 16.965 45.817 -22.025 1.00 32.29
N
ATOM 4946 CA PRO C 161 18.018 44.864 -21.642 1.00 33.49
C
ATOM 4947 C PRO C 161 19.426 45.439 -21.793 1.00 38.43
C
ATOM 4948 O PRO C 161 20.344 45.006 -21.093 1.00 39.19
O
ATOM 4949 CB PRO C 161 17.810 43.692 -22.612 1.00 34.26
C
ATOM 4950 CG PRO C 161 16.429 43.848 -23.134 1.00 31.11
C
ATOM 4951 CD PRO C 161 16.174 45.321 -23.164 1.00 27.41
C
ATOM 4952 HA PRO C 161 17.887 44.559 -20.731 1.00 40.18
H
ATOM 11219 HB3 ARG F 66 6.860 29.082 -17.517 1.00 21.65
H
ATOM 11220 HG2 ARG F 66 5.060 29.356 -18.629 1.00 26.60
H
ATOM 11221 HG3 ARG F 66 4.165 29.014 -17.356 1.00 26.60
H
ATOM 11222 HD2 ARG F 66 3.734 31.165 -18.123 1.00 29.59
H
ATOM 11223 HD3 ARG F 66 4.325 31.199 -16.646 1.00 29.59
H
ATOM 11224 HE ARG F 66 6.139 31.571 -18.609 1.00 32.21
H
ATOM 11225 HH11 ARG F 66 4.195 33.211 -16.495 1.00 30.99
H
ATOM 11226 HH12 ARG F 66 4.940 34.500 -16.552 1.00 30.99
H
ATOM 11227 HH21 ARG F 66 7.289 33.516 -18.654 1.00 35.18
H
ATOM 11228 HH22 ARG F 66 6.814 34.684 -17.861 1.00 35.18
H
ATOM 11229 N ARG F 67 7.660 26.395 -16.206 1.00 21.33 N
ATOM 11230 CA ARG F 67 8.865 25.653 -15.896 1.00 25.35
C
ATOM 11231 C ARG F 67 9.889 25.840 -17.006 1.00 30.18 C
ATOM 11232 O ARG F 67 9.701 26.664 -17.904 1.00 29.69
O
ATOM 11233 CB ARG F 67 8.526 24.172 -15.705 1.00 22.56
C
ATOM 11234 CG ARG F 67 7.327 23.950 -14.797 1.00 21.84
C
ATOM 11235 CD ARG F 67 7.287 22.543 -14.225 1.00 23.91
C
ATOM 11236 NE ARG F 67 7.381 21.509 -15.253 1.00 27.20
N
ATOM 11237 CZ ARG F 67 6.343 20.966 -15.883 1.00 31.04
C
ATOM 11238 NH1 ARG F 67 5.103 21.355 -15.613 1.00 27.45
N1+
ATOM 11239 NH2 ARG F 67 6.548 20.027 -16.798 1.00 29.30
N
ATOM 11240 H ARG F 67 7.178 26.030 -16.818 1.00 25.59 H
ATOM 11241 HA ARG F 67 9.246 25.989 -15.069 1.00 30.42
H
ATOM 11242 HB2 ARG F 67 8.324 23.781 -16.570 1.00 27.07
H
ATOM 11243 HB3 ARG F 67 9.289 23.723 -15.309 1.00 27.07
H
ATOM 11244 HG2 ARG F 67 7.370 24.575 -14.056 1.00 26.21
H
ATOM 11245 HG3 ARG F 67 6.513 24.092 -15.306 1.00 26.21
H
ATOM 11246 HD2 ARG F 67 8.034 22.429 -13.617 1.00 28.69
H
ATOM 11247 HD3 ARG F 67 6.451 22.419 -13.751 1.00 28.69
H
ATOM 11248 HE ARG F 67 8.166 21.230 -15.466 1.00 32.65
H
ATOM 11249 HH11 ARG F 67 4.962 21.962 -15.021 1.00 32.94
H
ATOM 11250 HH12 ARG F 67 4.440 20.998 -16.028 1.00 32.94
H
ATOM 11251 HH21 ARG F 67 7.349 19.771 -16.980 1.00 35.16
H
ATOM 11252 HH22 ARG F 67 5.880 19.676 -17.211 1.00 35.16

H
ATOM 4953 HB2 PRO C 161 18.456 43.747 -23.333 1.00 41.12
H
ATOM 4954 HB3 PRO C 161 17.902 42.853 -22.134 1.00 41.12
H
ATOM 4955 HG2 PRO C 161 16.374 43.474 -24.028 1.00 37.33
H
ATOM 4956 HG3 PRO C 161 15.804 43.405 -22.539 1.00 37.33
H
ATOM 4957 HD2 PRO C 161 16.497 45.705 -23.994 1.00 32.89
H
ATOM 4958 HD3 PRO C 161 15.231 45.505 -23.028 1.00 32.89
H
ATOM 4959 N THR C 162 19.577 46.399 -22.701 1.00 41.08
N
ATOM 4960 CA THR C 162 20.863 47.035 -22.974 1.00 43.65
C
ATOM 4961 C THR C 162 21.495 47.605 -21.709 1.00 48.57
C
ATOM 4962 O THR C 162 22.589 47.196 -21.318 1.00 52.38
O
ATOM 4963 CB THR C 162 20.704 48.164 -24.030 1.00 41.19
C
ATOM 4964 OG1 THR C 162 20.643 47.588 -25.339 1.00 51.79
O
ATOM 4965 CG2 THR C 162 21.861 49.168 -23.983 1.00 50.32
C
ATOM 4966 H THR C 162 18.934 46.707 -23.182 1.00 49.29
H
ATOM 4967 HA THR C 162 21.470 46.371 -23.337 1.00 52.38
H
ATOM 4968 HB THR C 162 19.880 48.646 -23.857 1.00 49.42
H
ATOM 4969 HG1 THR C 162 19.988 47.065 -25.393 1.00 62.14
H
ATOM 4970 HG21 THR C 162 21.730 49.857 -24.653 1.00 60.38
H
ATOM 4971 HG22 THR C 162 21.904 49.584 -23.107 1.00 60.38
H
ATOM 4972 HG23 THR C 162 22.701 48.714 -24.157 1.00 60.38
H
ATOM 4973 N ASN C 163 20.799 48.544 -21.075 1.00 46.77
N
ATOM 4974 CA ASN C 163 21.340 49.264 -19.928 1.00 44.73
C
ATOM 4975 C ASN C 163 20.590 48.965 -18.630 1.00 46.38
C
ATOM 4976 O ASN C 163 20.716 49.698 -17.648 1.00 47.39
O
ATOM 4977 CB ASN C 163 21.324 50.768 -20.213 1.00 48.30
C
ATOM 4978 CG ASN C 163 19.972 51.258 -20.685 1.00 47.25
C
ATOM 4979 OD1 ASN C 163 18.934 50.711 -20.313 1.00 46.02
O
ATOM 4980 ND2 ASN C 163 19.978 52.292 -21.520 1.00 46.65
N
ATOM 4981 H ASN C 163 20.003 48.784 -21.292 1.00 56.13
H
ATOM 4982 HA ASN C 163 22.264 48.998 -19.802 1.00 53.68
H
ATOM 4983 HB2 ASN C 163 21.550 51.246 -19.399 1.00 57.96
H
ATOM 4984 HB3 ASN C 163 21.974 50.965 -20.905 1.00 57.96
H
ATOM 4985 HD21 ASN C 163 19.236 52.608 -21.817 1.00 55.98
H
ATOM 4986 HD22 ASN C 163 20.724 52.645 -21.762 1.00 55.98
H
ATOM 11253 N VAL F 68 10.975 25.085 -16.925 1.00 32.53 N
ATOM 11254 CA VAL F 68 11.988 25.069 -17.970 1.00 34.51
C
ATOM 11255 C VAL F 68 12.281 23.609 -18.307 1.00 38.41 C
ATOM 11256 O VAL F 68 12.207 22.750 -17.429 1.00 36.57
O
ATOM 11257 CB VAL F 68 13.276 25.800 -17.529 1.00 41.03
C
ATOM 11258 CG1 VAL F 68 13.813 25.221 -16.223 1.00 39.01
C
ATOM 11259 CG2 VAL F 68 14.334 25.746 -18.624 1.00 43.43
C
ATOM 11260 H VAL F 68 11.152 24.564 -16.264 1.00 39.04 H
ATOM 11261 HA VAL F 68 11.642 25.505 -18.763 1.00 41.42
H
ATOM 11262 HB VAL F 68 13.063 26.733 -17.371 1.00 49.24
H
ATOM 11263 HG11 VAL F 68 14.619 25.699 -15.974 1.00 46.81
H
ATOM 11264 HG12 VAL F 68 13.140 25.323 -15.532 1.00 46.81
H
ATOM 11265 HG13 VAL F 68 14.014 24.280 -16.354 1.00 46.81
H
ATOM 11266 HG21 VAL F 68 15.128 26.213 -18.318 1.00 52.11
H
ATOM 11267 HG22 VAL F 68 14.547 24.819 -18.811 1.00 52.11
H
ATOM 11268 HG23 VAL F 68 13.985 26.174 -19.421 1.00 52.11
H
ATOM 11269 N PRO F 69 12.585 23.312 -19.583 1.00 40.10
N
ATOM 11270 CA PRO F 69 12.933 21.923 -19.904 1.00 43.70
C
ATOM 11271 C PRO F 69 14.276 21.526 -19.307 1.00 46.21
C
ATOM 11272 O PRO F 69 15.248 22.268 -19.453 1.00 49.34
O
ATOM 11273 CB PRO F 69 12.994 21.915 -21.437 1.00 42.03
C
ATOM 11274 CG PRO F 69 12.269 23.147 -21.865 1.00 44.28
C
ATOM 11275 CD PRO F 69 12.538 24.147 -20.794 1.00 37.27
C
ATOM 11276 HA PRO F 69 12.243 21.314 -19.599 1.00 52.45
H
ATOM 11277 HB2 PRO F 69 13.919 21.944 -21.728 1.00 50.44
H
ATOM 11278 HB3 PRO F 69 12.552 21.122 -21.777 1.00 50.44
H
ATOM 11279 HG2 PRO F 69 12.619 23.453 -22.716 1.00 53.14
H
ATOM 11280 HG3 PRO F 69 11.319 22.961 -21.930 1.00 53.14
H
ATOM 11281 HD2 PRO F 69 13.392 24.582 -20.941 1.00 44.72
H
ATOM 11282 HD3 PRO F 69 11.813 24.789 -20.737 1.00 44.72
H
ATOM 11283 N THR F 70 14.325 20.373 -18.647 1.00 48.67
N
ATOM 11284 CA THR F 70 15.550 19.908 -18.009 1.00 60.44
C
ATOM 11285 C THR F 70 15.727 18.407 -18.178 1.00 59.62
C
ATOM 11286 O THR F 70 14.758 17.671 -18.367 1.00 55.15

H
ATOM 4987 N GLY C 164 19.813 47.885 -18.633 1.00 43.17
N
ATOM 4988 CA GLY C 164 19.118 47.429 -17.441 1.00 38.67
C
ATOM 4989 C GLY C 164 18.202 48.466 -16.815 1.00 39.65
C
ATOM 4990 O GLY C 164 17.958 48.435 -15.609 1.00 42.49
O
ATOM 4991 H GLY C 164 19.673 47.394 -19.326 1.00 51.80
H
ATOM 4992 HA2 GLY C 164 18.584 46.651 -17.664 1.00 46.40
H
ATOM 4993 HA3 GLY C 164 19.772 47.165 -16.775 1.00 46.40
H
ATOM 4994 N SER C 165 17.686 49.376 -17.636 1.00 34.82
N
ATOM 4995 CA SER C 165 16.856 50.474 -17.153 1.00 32.20
C
ATOM 4996 C SER C 165 15.364 50.169 -17.287 1.00 27.87
C
ATOM 4997 O SER C 165 14.943 49.486 -18.223 1.00 25.68
O
ATOM 4998 CB SER C 165 17.193 51.756 -17.917 1.00 38.18
C
ATOM 4999 OG SER C 165 16.391 52.837 -17.475 1.00 43.62
O
ATOM 5000 H SER C 165 17.803 49.378 -18.488 1.00 41.79
H
ATOM 5001 HA SER C 165 17.048 50.625 -16.214 1.00 38.64
H
ATOM 5002 HB2 SER C 165 18.126 51.976 -17.769 1.00 45.81
H
ATOM 5003 HB3 SER C 165 17.032 51.611 -18.863 1.00 45.81
H
ATOM 5004 HG SER C 165 16.586 53.533 -17.903 1.00 52.34
H
ATOM 5005 N TRP C 166 14.579 50.679 -16.340 1.00 31.94
N
ATOM 5006 CA TRP C 166 13.119 50.583 -16.387 1.00 23.07
C
ATOM 5007 C TRP C 166 12.515 51.944 -16.699 1.00 27.85
C
ATOM 5008 O TRP C 166 12.805 52.927 -16.018 1.00 29.97
O
ATOM 5009 CB TRP C 166 12.561 50.059 -15.063 1.00 22.45
C
ATOM 5010 CG TRP C 166 12.817 48.608 -14.846 1.00 20.87
C
ATOM 5011 CD1 TRP C 166 13.887 48.054 -14.214 1.00 28.32
C
ATOM 5012 CD2 TRP C 166 11.989 47.519 -15.267 1.00 20.19
C
ATOM 5013 NE1 TRP C 166 13.779 46.685 -14.212 1.00 29.81
N
ATOM 5014 CE2 TRP C 166 12.622 46.331 -14.853 1.00 21.03
C
ATOM 5015 CE3 TRP C 166 10.773 47.434 -15.951 1.00 18.26
C
ATOM 5016 CZ2 TRP C 166 12.082 45.074 -15.100 1.00 20.42
C
ATOM 5017 CZ3 TRP C 166 10.238 46.186 -16.198 1.00 19.14
C
ATOM 5018 CH2 TRP C 166 10.890 45.020 -15.772 1.00 22.75
C
ATOM 5019 H TRP C 166 14.873 51.093 -15.646 1.00 38.33
H
ATOM 5020 HA TRP C 166 12.861 49.968 -17.091 1.00 27.68
O
ATOM 11287 CB THR F 70 15.565 20.240 -16.507 1.00 59.77
C
ATOM 11288 OG1 THR F 70 14.479 19.568 -15.855 1.00 58.31
O
ATOM 11289 CG2 THR F 70 15.441 21.742 -16.286 1.00 62.29
C
ATOM 11290 H THR F 70 13.657 19.840 -18.554 1.00 58.41
H
ATOM 11291 HA THR F 70 16.309 20.349 -18.422 1.00 72.53
H
ATOM 11292 HB THR F 70 16.404 19.943 -16.121 1.00 71.73
H
ATOM 11293 HG1 THR F 70 14.482 19.746 -15.034 1.00 69.97
H
ATOM 11294 HG21 THR F 70 15.451 21.939 -15.336 1.00 74.75
H
ATOM 11295 HG22 THR F 70 16.182 22.201 -16.711 1.00 74.75
H
ATOM 11296 HG23 THR F 70 14.609 22.065 -16.666 1.00 74.75
H
ATOM 11297 N SER F 71 16.978 17.966 -18.107 1.00 61.53
N
ATOM 11298 CA SER F 71 17.303 16.549 -18.178 1.00 66.52
C
ATOM 11299 C SER F 71 16.917 15.841 -16.883 1.00 61.49
C
ATOM 11300 O SER F 71 16.835 14.613 -16.840 1.00 59.94
O
ATOM 11301 CB SER F 71 18.795 16.361 -18.457 1.00 70.57
C
ATOM 11302 OG SER F 71 19.580 17.021 -17.479 1.00 74.17
O
ATOM 11303 H SER F 71 17.665 18.476 -18.016 1.00 73.84
H
ATOM 11304 HA SER F 71 16.805 16.144 -18.905 1.00 79.82
H
ATOM 11305 HB2 SER F 71 19.002 15.414 -18.441 1.00 84.68
H
ATOM 11306 HB3 SER F 71 19.002 16.731 -19.330 1.00 84.68
H
ATOM 11307 HG SER F 71 20.396 16.911 -17.642 1.00 89.01
H
ATOM 11308 N THR F 72 16.682 16.626 -15.833 1.00 62.01
N
ATOM 11309 CA THR F 72 16.339 16.091 -14.517 1.00 54.74
C
ATOM 11310 C THR F 72 15.134 15.150 -14.598 1.00 49.84
C
ATOM 11311 O THR F 72 14.027 15.588 -14.906 1.00 53.35
O
ATOM 11312 CB THR F 72 16.026 17.225 -13.522 1.00 57.21
C
ATOM 11313 OG1 THR F 72 17.057 18.220 -13.583 1.00 59.71
O
ATOM 11314 CG2 THR F 72 15.929 16.683 -12.103 1.00 49.20
C
ATOM 11315 H THR F 72 16.715 17.485 -15.859 1.00 74.41
H
ATOM 11316 HA THR F 72 17.093 15.587 -14.173 1.00 65.69
H
ATOM 11317 HB THR F 72 15.176 17.629 -13.753 1.00 68.66
H
ATOM 11318 HG1 THR F 72 16.890 18.840 -13.042 1.00 71.65
H
ATOM 11319 HG21 THR F 72 15.732 17.405 -11.485 1.00 59.04
H
ATOM 11320 HG22 THR F 72 15.223 16.021 -12.049 1.00 59.04

H
ATOM 5021 HB2 TRP C 166 12.974 50.547 -14.334 1.00 26.94
H
ATOM 5022 HB3 TRP C 166 11.601 50.197 -15.051 1.00 26.94
H
ATOM 5023 HD1 TRP C 166 14.591 48.532 -13.838 1.00 33.98
H
ATOM 5024 HE1 TRP C 166 14.345 46.139 -13.865 1.00 35.77
H
ATOM 5025 HE3 TRP C 166 10.335 48.203 -16.237 1.00 21.91
H
ATOM 5026 HZ2 TRP C 166 12.513 44.299 -14.818 1.00 24.50
H
ATOM 5027 HZ3 TRP C 166 9.429 46.117 -16.653 1.00 22.96
H
ATOM 5028 HH2 TRP C 166 10.506 44.192 -15.952 1.00 27.30
H
ATOM 5029 N GLN C 167 11.676 52.003 -17.727 1.00 22.33
N
ATOM 5030 CA GLN C 167 11.066 53.265 -18.126 1.00 24.92
C
ATOM 5031 C GLN C 167 9.614 53.084 -18.554 1.00 20.54
C
ATOM 5032 O GLN C 167 9.185 51.984 -18.912 1.00 18.82
O
ATOM 5033 CB GLN C 167 11.872 53.904 -19.257 1.00 26.21
C
ATOM 5034 CG GLN C 167 11.910 53.089 -20.540 1.00 31.52
C
ATOM 5035 CD GLN C 167 12.781 53.730 -21.610 1.00 33.46
C
ATOM 5036 OE1 GLN C 167 13.768 54.399 -21.306 1.00 35.78
O
ATOM 5037 NE2 GLN C 167 12.412 53.532 -22.870 1.00 34.85
N
ATOM 5038 H GLN C 167 11.444 51.330 -18.209 1.00 26.80
H
ATOM 5039 HA GLN C 167 11.080 53.873 -17.370 1.00 29.90
H
ATOM 5040 HB2 GLN C 167 11.482 54.767 -19.467 1.00 31.45
H
ATOM 5041 HB3 GLN C 167 12.787 54.024 -18.958 1.00 31.45
H
ATOM 5042 HG2 GLN C 167 12.269 52.209 -20.347 1.00 37.82
H
ATOM 5043 HG3 GLN C 167 11.009 53.011 -20.892 1.00 37.82
H
ATOM 5044 HE21 GLN C 167 12.872 53.873 -23.511 1.00 41.82
H
ATOM 5045 HE22 GLN C 167 11.713 53.062 -23.044 1.00 41.82
H
ATOM 5046 N TRP C 168 8.865 54.180 -18.504 1.00 19.48
N
ATOM 5047 CA TRP C 168 7.471 54.186 -18.926 1.00 24.91
C
ATOM 5048 C TRP C 168 7.401 54.322 -20.439 1.00 28.19
C
ATOM 5049 O TRP C 168 8.390 54.684 -21.077 1.00 29.68
O
ATOM 5050 CB TRP C 168 6.715 55.320 -18.236 1.00 22.90
C
ATOM 5051 CG TRP C 168 6.806 55.241 -16.746 1.00 18.59
C
ATOM 5052 CD1 TRP C 168 7.589 56.003 -15.932 1.00 20.28
C
ATOM 5053 CD2 TRP C 168 6.101 54.331 -15.890 1.00 18.57
C
ATOM 5054 NE1 TRP C 168 7.410 55.631 -14.620 1.00 19.79
H
ATOM 11321 HG23 THR F 72 16.769 16.270 -11.848 1.00 59.04
H
ATOM 11322 N PRO F 73 15.345 13.851 -14.327 1.00 47.67
N
ATOM 11323 CA PRO F 73 14.252 12.884 -14.470 1.00 42.23
C
ATOM 11324 C PRO F 73 13.246 12.910 -13.323 1.00 44.81
C
ATOM 11325 O PRO F 73 12.230 12.217 -13.393 1.00 43.07
O
ATOM 11326 CB PRO F 73 14.984 11.543 -14.503 1.00 43.10
C
ATOM 11327 CG PRO F 73 16.189 11.769 -13.668 1.00 42.60
C
ATOM 11328 CD PRO F 73 16.597 13.199 -13.901 1.00 44.19
C
ATOM 11329 HA PRO F 73 13.788 13.019 -15.311 1.00 50.67
H
ATOM 11330 HB2 PRO F 73 14.422 10.851 -14.121 1.00 51.72
H
ATOM 11331 HB3 PRO F 73 15.231 11.325 -15.416 1.00 51.72
H
ATOM 11332 HG2 PRO F 73 15.967 11.627 -12.734 1.00 51.12
H
ATOM 11333 HG3 PRO F 73 16.894 11.164 -13.946 1.00 51.12
H
ATOM 11334 HD2 PRO F 73 16.923 13.596 -13.078 1.00 53.02
H
ATOM 11335 HD3 PRO F 73 17.261 13.249 -14.607 1.00 53.02
H
ATOM 11336 N TYR F 74 13.524 13.683 -12.280 1.00 43.68
N
ATOM 11337 CA TYR F 74 12.612 13.764 -11.146 1.00 36.00
C
ATOM 11338 C TYR F 74 12.852 15.007 -10.302 1.00 34.98
C
ATOM 11339 O TYR F 74 13.985 15.312 -9.931 1.00 37.75 O
ATOM 11340 CB TYR F 74 12.740 12.518 -10.271 1.00 34.00
C
ATOM 11341 CG TYR F 74 11.779 12.501 -9.107 1.00 33.28
C
ATOM 11342 CD1 TYR F 74 10.522 11.926 -9.231 1.00 37.86
C
ATOM 11343 CD2 TYR F 74 12.124 13.064 -7.884 1.00 31.82
C
ATOM 11344 CE1 TYR F 74 9.637 11.908 -8.173 1.00 40.32
C
ATOM 11345 CE2 TYR F 74 11.245 13.051 -6.819 1.00 28.53
C
ATOM 11346 CZ TYR F 74 10.003 12.472 -6.969 1.00 35.36
C
ATOM 11347 OH TYR F 74 9.120 12.456 -5.915 1.00 37.99
O
ATOM 11348 H TYR F 74 14.230 14.169 -12.204 1.00 52.42
H
ATOM 11349 HA TYR F 74 11.702 13.801 -11.479 1.00 43.20
H
ATOM 11350 HB2 TYR F 74 12.565 11.734 -10.814 1.00 40.80
H
ATOM 11351 HB3 TYR F 74 13.641 12.477 -9.913 1.00 40.80
H
ATOM 11352 HD1 TYR F 74 10.273 11.545 -10.042 1.00 45.43
H
ATOM 11353 HD2 TYR F 74 12.961 13.455 -7.781 1.00 38.18
H
ATOM 11354 HE1 TYR F 74 8.799 11.519 -8.272 1.00 48.39

N
ATOM 5055 CE2 TRP C 168 6.501 54.607 -14.568 1.00 18.17
C
ATOM 5056 CE3 TRP C 168 5.168 53.313 -16.114 1.00 19.34
C
ATOM 5057 CZ2 TRP C 168 6.000 53.903 -13.474 1.00 19.51
C
ATOM 5058 CZ3 TRP C 168 4.672 52.614 -15.028 1.00 18.19
C
ATOM 5059 CH2 TRP C 168 5.090 52.912 -13.724 1.00 17.53
C
ATOM 5060 H TRP C 168 9.146 54.943 -18.225 1.00 23.37
H
ATOM 5061 HA TRP C 168 7.056 53.346 -18.676 1.00 29.89
H
ATOM 5062 HB2 TRP C 168 7.091 56.169 -18.516 1.00 27.48
H
ATOM 5063 HB3 TRP C 168 5.778 55.272 -18.483 1.00 27.48
H
ATOM 5064 HD1 TRP C 168 8.158 56.679 -16.222 1.00 24.34
H
ATOM 5065 HE1 TRP C 168 7.804 55.985 -13.942 1.00 23.74
H
ATOM 5066 HE3 TRP C 168 4.886 53.110 -16.977 1.00 23.20
H
ATOM 5067 HZ2 TRP C 168 6.276 54.098 -12.607 1.00 23.42
H
ATOM 5068 HZ3 TRP C 168 4.051 51.936 -15.166 1.00 21.83
H
ATOM 5069 HH2 TRP C 168 4.739 52.427 -13.013 1.00 21.04
H
ATOM 5070 N GLU C 169 6.242 54.030 -21.020 1.00 30.70
N
ATOM 5071 CA GLU C 169 6.122 54.022 -22.474 1.00 35.60
C
ATOM 5072 C GLU C 169 6.155 55.434 -23.049 1.00 36.18
C
ATOM 5073 O GLU C 169 6.337 55.608 -24.254 1.00 37.85
O
ATOM 5074 CB GLU C 169 4.844 53.301 -22.910 1.00 39.61
C
ATOM 5075 CG GLU C 169 3.559 53.974 -22.490 1.00 33.74
C
ATOM 5076 CD GLU C 169 2.372 53.021 -22.532 1.00 38.01
C
ATOM 5077 OE1 GLU C 169 2.228 52.285 -23.532 1.00 37.73
O
ATOM 5078 OE2 GLU C 169 1.587 53.002 -21.562 1.00 35.40
O1-
ATOM 5079 H GLU C 169 5.517 53.835 -20.600 1.00 36.84
H
ATOM 5080 HA GLU C 169 6.876 53.536 -22.844 1.00 42.72
H
ATOM 5081 HB2 GLU C 169 4.840 53.240 -23.878 1.00 47.53
H
ATOM 5082 HB3 GLU C 169 4.847 52.410 -22.528 1.00 47.53
H
ATOM 5083 HG2 GLU C 169 3.653 54.299 -21.581 1.00 40.49
H
ATOM 5084 HG3 GLU C 169 3.375 54.712 -23.092 1.00 40.49
H
ATOM 5085 N ASP C 170 5.994 56.440 -22.192 1.00 34.47
N
ATOM 5086 CA ASP C 170 6.132 57.827 -22.629 1.00 33.57
C
ATOM 5087 C ASP C 170 7.609 58.221 -22.703 1.00 33.88
C
ATOM 5088 O ASP C 170 7.943 59.327 -23.127 1.00 37.21
H
ATOM 11355 HE2 TYR F 74 11.489 13.431 -6.006 1.00 34.24
H
ATOM 11356 HH TYR F 74 9.464 12.829 -5.246 1.00 45.59 H
ATOM 11357 N GLU F 75 11.767 15.712 -9.998 1.00 32.78 N
ATOM 11358 CA GLU F 75 11.816 16.888 -9.141 1.00 25.81
C
ATOM 11359 C GLU F 75 10.590 16.935 -8.235 1.00 29.12 C
ATOM 11360 O GLU F 75 9.484 16.581 -8.649 1.00 30.51 O
ATOM 11361 CB GLU F 75 11.892 18.167 -9.974 1.00 35.92
C
ATOM 11362 CG GLU F 75 13.193 18.358 -10.729 1.00 38.70
C
ATOM 11363 CD GLU F 75 13.265 19.711 -11.411 1.00 41.84
C
ATOM 11364 OE1 GLU F 75 12.460 19.955 -12.333 1.00 39.49
O
ATOM 11365 OE2 GLU F 75 14.120 20.535 -11.018 1.00 43.44
O1-
ATOM 11366 H GLU F 75 10.977 15.524 -10.282 1.00 39.33
H
ATOM 11367 HA GLU F 75 12.607 16.843 -8.581 1.00 30.97
H
ATOM 11368 HB2 GLU F 75 11.174 18.154 -10.626 1.00 43.10
H
ATOM 11369 HB3 GLU F 75 11.781 18.928 -9.383 1.00 43.10
H
ATOM 11370 HG2 GLU F 75 13.934 18.294 -10.107 1.00 46.44
H
ATOM 11371 HG3 GLU F 75 13.269 17.672 -11.411 1.00 46.44
H
ATOM 11372 N ASP F 76 10.798 17.370 -6.998 1.00 27.11 N
ATOM 11373 CA ASP F 76 9.716 17.527 -6.037 1.00 25.30 C
ATOM 11374 C ASP F 76 9.802 18.922 -5.426 1.00 18.73 C
ATOM 11375 O ASP F 76 10.778 19.253 -4.754 1.00 19.05 O
ATOM 11376 CB ASP F 76 9.793 16.447 -4.956 1.00 25.98 C
ATOM 11377 CG ASP F 76 8.511 16.323 -4.158 1.00 33.41 C
ATOM 11378 OD1 ASP F 76 7.419 16.365 -4.766 1.00 28.50
O
ATOM 11379 OD2 ASP F 76 8.596 16.176 -2.919 1.00 44.45
O1-
ATOM 11380 H ASP F 76 11.571 17.585 -6.687 1.00 32.53 H
ATOM 11381 HA ASP F 76 8.864 17.444 -6.493 1.00 30.36 H
ATOM 11382 HB2 ASP F 76 9.969 15.591 -5.377 1.00 31.18
H
ATOM 11383 HB3 ASP F 76 10.509 16.667 -4.340 1.00 31.18
H
ATOM 11384 N LEU F 77 8.786 19.738 -5.689 1.00 15.80 N
ATOM 11385 CA LEU F 77 8.767 21.135 -5.256 1.00 15.34 C
ATOM 11386 C LEU F 77 7.693 21.357 -4.206 1.00 19.57 C
ATOM 11387 O LEU F 77 6.536 20.990 -4.414 1.00 16.25 O
ATOM 11388 CB LEU F 77 8.520 22.055 -6.447 1.00 13.25 C

O
ATOM 5089 CB ASP C 170 5.363 58.777 -21.699 1.00 36.54
C
ATOM 5090 CG ASP C 170 6.038 58.968 -20.348 1.00 37.03
C
ATOM 5091 OD1 ASP C 170 6.943 58.181 -19.995 1.00 34.20
O
ATOM 5092 OD2 ASP C 170 5.647 59.913 -19.628 1.00 37.14
O1-
ATOM 5093 H ASP C 170 5.805 56.348 -21.358 1.00 41.36
H
ATOM 5094 HA ASP C 170 5.756 57.914 -23.519 1.00 40.28
H
ATOM 5095 HB2 ASP C 170 5.293 59.646 -22.124 1.00 43.84
H
ATOM 5096 HB3 ASP C 170 4.477 58.414 -21.541 1.00 43.84
H
ATOM 5097 N GLY C 171 8.484 57.311 -22.277 1.00 32.03
N
ATOM 5098 CA GLY C 171 9.920 57.506 -22.382 1.00 35.58
C
ATOM 5099 C GLY C 171 10.576 57.946 -21.087 1.00 32.10
C
ATOM 5100 O GLY C 171 11.790 57.817 -20.924 1.00 32.64
O
ATOM 5101 H GLY C 171 8.262 56.562 -21.919 1.00 38.44
H
ATOM 5102 HA2 GLY C 171 10.334 56.676 -22.664 1.00 42.69
H
ATOM 5103 HA3 GLY C 171 10.101 58.180 -23.056 1.00 42.69
H
ATOM 5104 N SER C 172 9.777 58.463 -20.159 1.00 32.52
N
ATOM 5105 CA SER C 172 10.301 58.957 -18.891 1.00 30.32
C
ATOM 5106 C SER C 172 10.860 57.828 -18.032 1.00 29.58
C
ATOM 5107 O SER C 172 10.442 56.675 -18.146 1.00 27.69
O
ATOM 5108 CB SER C 172 9.213 59.703 -18.117 1.00 33.73
C
ATOM 5109 OG SER C 172 8.138 58.839 -17.786 1.00 33.64
O
ATOM 5110 H SER C 172 8.924 58.538 -20.240 1.00 39.02
H
ATOM 5111 HA SER C 172 11.022 59.582 -19.070 1.00 36.38
H
ATOM 5112 HB2 SER C 172 9.595 60.058 -17.299 1.00 40.48
H
ATOM 5113 HB3 SER C 172 8.876 60.428 -18.666 1.00 40.48
H
ATOM 5114 HG SER C 172 7.797 58.524 -18.486 1.00 40.37
H
ATOM 5115 N ILE C 173 11.811 58.174 -17.170 1.00 28.71
N
ATOM 5116 CA ILE C 173 12.416 57.214 -16.256 1.00 33.40
C
ATOM 5117 C ILE C 173 11.462 56.904 -15.106 1.00 29.48
C
ATOM 5118 O ILE C 173 10.612 57.725 -14.757 1.00 29.36
O
ATOM 5119 CB ILE C 173 13.759 57.752 -15.691 1.00 31.94
C
ATOM 5120 CG1 ILE C 173 14.496 56.691 -14.868 1.00 40.78
C
ATOM 5121 CG2 ILE C 173 13.529 59.000 -14.843 1.00 39.11
C
ATOM 5122 CD1 ILE C 173 14.933 55.482 -15.661 1.00 47.43

ATOM 11389 CG LEU F 77 9.510 21.914 -7.604 1.00 18.29 C
ATOM 11390 CD1 LEU F 77 8.906 22.436 -8.889 1.00 24.51
C
ATOM 11391 CD2 LEU F 77 10.790 22.653 -7.281 1.00 21.55
C

ATOM 11392 H LEU F 77 8.083 19.504 -6.125 1.00 18.96 H

ATOM 11393 HA LEU F 77 9.626 21.362 -4.868 1.00 18.41 H
ATOM 11394 HB2 LEU F 77 7.635 21.872 -6.798 1.00 15.90
H
ATOM 11395 HB3 LEU F 77 8.562 22.974 -6.138 1.00 15.90
H

ATOM 11396 HG LEU F 77 9.724 20.976 -7.728 1.00 21.95 H
ATOM 11397 HD11 LEU F 77 9.553 22.336 -9.605 1.00 29.41
H
ATOM 11398 HD12 LEU F 77 8.106 21.927 -9.092 1.00 29.41
H
ATOM 11399 HD13 LEU F 77 8.682 23.373 -8.775 1.00 29.41
H
ATOM 11400 HD21 LEU F 77 11.407 22.554 -8.024 1.00 25.86
H
ATOM 11401 HD22 LEU F 77 10.587 23.591 -7.143 1.00 25.86
H
ATOM 11402 HD23 LEU F 77 11.178 22.276 -6.476 1.00 25.86
H

ATOM 11403 N THR F 78 8.072 21.965 -3.086 1.00 13.26 N

ATOM 11404 CA THR F 78 7.124 22.221 -2.009 1.00 15.50 C

ATOM 11405 C THR F 78 7.129 23.689 -1.608 1.00 15.27 C

ATOM 11406 O THR F 78 8.182 24.310 -1.481 1.00 15.66 O

ATOM 11407 CB THR F 78 7.432 21.361 -0.771 1.00 15.80 C
ATOM 11408 OG1 THR F 78 7.512 19.982 -1.150 1.00 21.65
O
ATOM 11409 CG2 THR F 78 6.354 21.526 0.287 1.00 19.77
C

ATOM 11410 H THR F 78 8.872 22.239 -2.925 1.00 15.91 H

ATOM 11411 HA THR F 78 6.231 21.997 -2.315 1.00 18.60 H

ATOM 11412 HB THR F 78 8.280 21.639 -0.389 1.00 18.96 H
ATOM 11413 HG1 THR F 78 8.122 19.875 -1.718 1.00 25.98
H
ATOM 11414 HG21 THR F 78 6.562 20.978 1.060 1.00 23.73
H
ATOM 11415 HG22 THR F 78 6.299 22.454 0.563 1.00 23.73
H
ATOM 11416 HG23 THR F 78 5.494 21.252 -0.071 1.00 23.73
H

ATOM 11417 N TYR F 79 5.934 24.232 -1.417 1.00 14.59 N

ATOM 11418 CA TYR F 79 5.771 25.580 -0.895 1.00 14.36 C

ATOM 11419 C TYR F 79 4.795 25.527 0.268 1.00 13.77 C

ATOM 11420 O TYR F 79 3.654 25.085 0.126 1.00 11.30 O

ATOM 11421 CB TYR F 79 5.286 26.537 -1.984 1.00 15.36 C
ATOM 11422 CG TYR F 79 4.973 27.937 -1.494 1.00 12.43 C

C
ATOM 5123 H ILE C 173 12.126 58.971 -17.095 1.00 34.45
H
ATOM 5124 HA ILE C 173 12.596 56.388 -16.732 1.00 40.08
H
ATOM 5125 HB ILE C 173 14.324 57.997 -16.440 1.00 38.33
H
ATOM 5126 HG12 ILE C 173 15.290 57.093 -14.482 1.00 48.94
H
ATOM 5127 HG13 ILE C 173 13.908 56.383 -14.160 1.00 48.94
H
ATOM 5128 HG21 ILE C 173 14.382 59.313 -14.504 1.00 46.93
H
ATOM 5129 HG22 ILE C 173 13.120 59.685 -15.395 1.00 46.93
H
ATOM 5130 HG23 ILE C 173 12.941 58.776 -14.105 1.00 46.93
H
ATOM 5131 HD11 ILE C 173 14.151 55.057 -16.044 1.00 56.92
H
ATOM 5132 HD12 ILE C 173 15.534 55.768 -16.366 1.00 56.92
H
ATOM 5133 HD13 ILE C 173 15.389 54.864 -15.068 1.00 56.92
H
ATOM 5134 N LEU C 174 11.589 55.712 -14.534 1.00 25.61
N
ATOM 5135 CA LEU C 174 10.914 55.404 -13.281 1.00 23.61
C
ATOM 5136 C LEU C 174 11.490 56.287 -12.185 1.00 26.93
C
ATOM 5137 O LEU C 174 12.652 56.136 -11.819 1.00 26.37
O
ATOM 5138 CB LEU C 174 11.087 53.932 -12.917 1.00 21.37
C
ATOM 5139 CG LEU C 174 10.642 53.521 -11.513 1.00 18.27
C
ATOM 5140 CD1 LEU C 174 9.132 53.664 -11.367 1.00 19.70
C
ATOM 5141 CD2 LEU C 174 11.086 52.100 -11.213 1.00 21.64
C
ATOM 5142 H LEU C 174 12.059 55.066 -14.851 1.00 30.74
H
ATOM 5143 HA LEU C 174 9.967 55.593 -13.366 1.00 28.33
H
ATOM 5144 HB2 LEU C 174 10.575 53.402 -13.548 1.00 25.65
H
ATOM 5145 HB3 LEU C 174 12.027 53.708 -12.998 1.00 25.65
H
ATOM 5146 HG LEU C 174 11.061 54.109 -10.865 1.00 21.92
H
ATOM 5147 HD11 LEU C 174 8.875 53.398 -10.470 1.00 23.64
H
ATOM 5148 HD12 LEU C 174 8.886 54.590 -11.521 1.00 23.64
H
ATOM 5149 HD13 LEU C 174 8.697 53.093 -12.019 1.00 23.64
H
ATOM 5150 HD21 LEU C 174 10.794 51.860 -10.320 1.00 25.97
H
ATOM 5151 HD22 LEU C 174 10.687 51.501 -11.864 1.00 25.97
H
ATOM 5152 HD23 LEU C 174 12.053 52.054 -11.269 1.00 25.97
H
ATOM 5153 N SER C 175 10.689 57.209 -11.661 1.00 26.24
N
ATOM 5154 CA SER C 175 11.166 58.084 -10.595 1.00 23.83
C
ATOM 5155 C SER C 175 11.378 57.288 -9.308 1.00 25.15
C
ATOM 5156 O SER C 175 10.734 56.258 -9.099 1.00 21.90
O
ATOM 11423 CD1 TYR F 79 5.935 28.706 -0.856 1.00 14.93
C
ATOM 11424 CD2 TYR F 79 3.715 28.493 -1.685 1.00 15.01
C
ATOM 11425 CE1 TYR F 79 5.651 29.988 -0.417 1.00 16.52
C
ATOM 11426 CE2 TYR F 79 3.424 29.768 -1.249 1.00 12.69
C
ATOM 11427 CZ TYR F 79 4.392 30.510 -0.614 1.00 14.82 C
ATOM 11428 OH TYR F 79 4.099 31.784 -0.184 1.00 18.09
O
ATOM 11429 H TYR F 79 5.191 23.833 -1.585 1.00 17.51 H
ATOM 11430 HA TYR F 79 6.624 25.901 -0.564 1.00 17.24 H
ATOM 11431 HB2 TYR F 79 5.975 26.611 -2.663 1.00 18.43
H
ATOM 11432 HB3 TYR F 79 4.477 26.175 -2.378 1.00 18.43
H
ATOM 11433 HD1 TYR F 79 6.785 28.354 -0.721 1.00 17.91
H
ATOM 11434 HD2 TYR F 79 3.056 27.995 -2.112 1.00 18.01
H
ATOM 11435 HE1 TYR F 79 6.305 30.491 0.012 1.00 19.83
H
ATOM 11436 HE2 TYR F 79 2.575 30.124 -1.383 1.00 15.23
H
ATOM 11437 HH TYR F 79 4.774 32.127 0.179 1.00 21.71 H
ATOM 11438 N PHE F 80 5.280 25.957 1.426 1.00 14.96 N
ATOM 11439 CA PHE F 80 4.514 25.945 2.660 1.00 15.84 C
ATOM 11440 C PHE F 80 4.224 27.377 3.071 1.00 15.28 C
ATOM 11441 O PHE F 80 5.138 28.191 3.150 1.00 15.47 O
ATOM 11442 CB PHE F 80 5.287 25.213 3.754 1.00 20.98 C
ATOM 11443 CG PHE F 80 4.626 25.256 5.097 1.00 22.06 C
ATOM 11444 CD1 PHE F 80 3.607 24.372 5.411 1.00 22.52
C
ATOM 11445 CD2 PHE F 80 5.030 26.173 6.052 1.00 19.44
C
ATOM 11446 CE1 PHE F 80 3.000 24.406 6.653 1.00 24.51
C
ATOM 11447 CE2 PHE F 80 4.426 26.211 7.295 1.00 20.54
C
ATOM 11448 CZ PHE F 80 3.412 25.328 7.596 1.00 20.28 C
ATOM 11449 H PHE F 80 6.075 26.269 1.522 1.00 17.96 H
ATOM 11450 HA PHE F 80 3.671 25.487 2.516 1.00 19.00 H
ATOM 11451 HB2 PHE F 80 5.381 24.282 3.500 1.00 25.17
H
ATOM 11452 HB3 PHE F 80 6.163 25.619 3.842 1.00 25.17
H
ATOM 11453 HD1 PHE F 80 3.327 23.749 4.780 1.00 27.02
H
ATOM 11454 HD2 PHE F 80 5.714 26.771 5.855 1.00 23.33
H
ATOM 11455 HE1 PHE F 80 2.316 23.809 6.854 1.00 29.42
H
ATOM 11456 HE2 PHE F 80 4.704 26.833 7.929 1.00 24.65

O
ATOM 5157 CB SER C 175 10.187 59.234 -10.365 1.00 27.90
C
ATOM 5158 OG SER C 175 10.203 60.135 -11.461 1.00 34.12
O
ATOM 5159 H SER C 175 9.875 57.348 -11.901 1.00 31.49
H
ATOM 5160 HA SER C 175 12.019 58.464 -10.856 1.00 28.60
H
ATOM 5161 HB2 SER C 175 9.293 58.873 -10.266 1.00 33.49
H
ATOM 5162 HB3 SER C 175 10.444 59.711 -9.560 1.00 33.49
H
ATOM 5163 HG SER C 175 9.662 60.763 -11.324 1.00 40.94
H
ATOM 5164 N PRO C 176 12.289 57.760 -8.440 1.00 23.75
N
ATOM 5165 CA PRO C 176 12.646 57.005 -7.232 1.00 23.82
C
ATOM 5166 C PRO C 176 11.560 57.003 -6.157 1.00 26.93
C
ATOM 5167 O PRO C 176 10.702 57.885 -6.138 1.00 25.00
O
ATOM 5168 CB PRO C 176 13.901 57.729 -6.726 1.00 30.63
C
ATOM 5169 CG PRO C 176 13.790 59.110 -7.259 1.00 34.23
C
ATOM 5170 CD PRO C 176 13.094 58.987 -8.584 1.00 32.51
C
ATOM 5171 HA PRO C 176 12.873 56.091 -7.461 1.00 28.59
H
ATOM 5172 HB2 PRO C 176 13.907 57.735 -5.756 1.00 36.75
H
ATOM 5173 HB3 PRO C 176 14.694 57.290 -7.073 1.00 36.75
H
ATOM 5174 HG2 PRO C 176 13.266 59.652 -6.648 1.00 41.08
H
ATOM 5175 HG3 PRO C 176 14.676 59.486 -7.374 1.00 41.08
H
ATOM 5176 HD2 PRO C 176 12.518 59.753 -8.734 1.00 39.01
H
ATOM 5177 HD3 PRO C 176 13.742 58.884 -9.298 1.00 39.01
H
ATOM 5178 N ASN C 177 11.611 56.003 -5.280 1.00 20.91
N
ATOM 5179 CA ASN C 177 10.723 55.914 -4.124 1.00 26.58
C
ATOM 5180 C ASN C 177 9.249 55.841 -4.507 1.00 27.22
C
ATOM 5181 O ASN C 177 8.392 56.360 -3.795 1.00 27.05
O
ATOM 5182 CB ASN C 177 10.957 57.102 -3.188 1.00 28.67
C
ATOM 5183 CG ASN C 177 12.372 57.143 -2.644 1.00 32.73
C
ATOM 5184 OD1 ASN C 177 12.886 56.139 -2.152 1.00 39.20
O
ATOM 5185 ND2 ASN C 177 13.013 58.302 -2.739 1.00 33.01
N
ATOM 5186 H ASN C 177 12.166 55.348 -5.335 1.00 25.10
H
ATOM 5187 HA ASN C 177 10.937 55.106 -3.632 1.00 31.90
H
ATOM 5188 HB2 ASN C 177 10.799 57.926 -3.676 1.00 34.41
H
ATOM 5189 HB3 ASN C 177 10.348 57.039 -2.436 1.00 34.41
H
ATOM 5190 HD21 ASN C 177 13.818 58.374 -2.444 1.00 39.62
H

ATOM 11457 HZ PHE F 80 3.005 25.353 8.432 1.00 24.33 H

ATOM 11458 N TYR F 81 2.952 27.686 3.295 1.00 13.47 N

ATOM 11459 CA TYR F 81 2.553 29.014 3.746 1.00 15.11 C

ATOM 11460 C TYR F 81 1.595 28.918 4.926 1.00 17.28 C

ATOM 11461 O TYR F 81 0.586 28.208 4.869 1.00 14.65 O

ATOM 11462 CB TYR F 81 1.905 29.803 2.614 1.00 12.73 C

ATOM 11463 CG TYR F 81 1.506 31.189 3.044 1.00 17.49 C
ATOM 11464 CD1 TYR F 81 2.430 32.225 3.046 1.00 16.62
C
ATOM 11465 CD2 TYR F 81 0.213 31.459 3.469 1.00 14.65
C
ATOM 11466 CE1 TYR F 81 2.073 33.496 3.451 1.00 19.10
C
ATOM 11467 CE2 TYR F 81 -0.152 32.725 3.879 1.00 18.37
C

ATOM 11468 CZ TYR F 81 0.781 33.739 3.866 1.00 19.41 C

ATOM 11469 OH TYR F 81 0.420 35.004 4.267 1.00 20.36 O

ATOM 11470 H TYR F 81 2.295 27.140 3.193 1.00 16.17 H

ATOM 11471 HA TYR F 81 3.341 29.499 4.038 1.00 18.13 H
ATOM 11472 HB2 TYR F 81 2.535 29.884 1.881 1.00 15.28
H
ATOM 11473 HB3 TYR F 81 1.107 29.337 2.318 1.00 15.28
H
ATOM 11474 HD1 TYR F 81 3.302 32.061 2.768 1.00 19.95
H
ATOM 11475 HD2 TYR F 81 -0.418 30.776 3.480 1.00 17.58
H
ATOM 11476 HE1 TYR F 81 2.700 34.182 3.444 1.00 22.92
H
ATOM 11477 HE2 TYR F 81 -1.023 32.894 4.157 1.00 22.05
H

ATOM 11478 HH TYR F 81 -0.389 35.014 4.493 1.00 24.43 H

ATOM 11479 N GLU F 82 1.910 29.648 5.991 1.00 15.52 N

ATOM 11480 CA GLU F 82 1.145 29.563 7.224 1.00 15.50 C

ATOM 11481 C GLU F 82 0.925 30.935 7.832 1.00 19.21 C

ATOM 11482 O GLU F 82 1.858 31.731 7.929 1.00 16.31 O

ATOM 11483 CB GLU F 82 1.865 28.661 8.228 1.00 18.78 C

ATOM 11484 CG GLU F 82 1.115 28.456 9.537 1.00 21.18 C
ATOM 11485 CD GLU F 82 1.954 27.739 10.577 1.00 28.40
C
ATOM 11486 OE1 GLU F 82 2.678 28.425 11.330 1.00 28.83
O
ATOM 11487 OE2 GLU F 82 1.893 26.492 10.637 1.00 29.39
O1-

ATOM 11488 H GLU F 82 2.567 30.202 6.022 1.00 18.63 H

ATOM 11489 HA GLU F 82 0.278 29.173 7.034 1.00 18.59 H
ATOM 11490 HB2 GLU F 82 1.996 27.789 7.824 1.00 22.54

H
ATOM 5191 HD22 ASN C 177 12.623 58.981 -3.095 1.00 39.62
H
ATOM 5192 N LEU C 178 8.961 55.193 -5.631 1.00 22.55
N
ATOM 5193 CA LEU C 178 7.586 55.018 -6.087 1.00 22.76
C
ATOM 5194 C LEU C 178 7.205 53.547 -6.144 1.00 24.97
C
ATOM 5195 O LEU C 178 6.143 53.162 -5.657 1.00 27.82
O
ATOM 5196 CB LEU C 178 7.390 55.657 -7.461 1.00 21.51
C
ATOM 5197 CG LEU C 178 7.366 57.186 -7.511 1.00 24.49
C
ATOM 5198 CD1 LEU C 178 7.248 57.640 -8.953 1.00 24.38
C
ATOM 5199 CD2 LEU C 178 6.224 57.756 -6.679 1.00 22.93
C
ATOM 5200 H LEU C 178 9.549 54.842 -6.152 1.00 27.06
H
ATOM 5201 HA LEU C 178 6.989 55.459 -5.463 1.00 27.31
H
ATOM 5202 HB2 LEU C 178 8.113 55.363 -8.037 1.00 25.81
H
ATOM 5203 HB3 LEU C 178 6.546 55.345 -7.822 1.00 25.81
H
ATOM 5204 HG LEU C 178 8.200 57.528 -7.154 1.00 29.39
H
ATOM 5205 HD11 LEU C 178 7.233 58.609 -8.978 1.00 29.25
H
ATOM 5206 HD12 LEU C 178 8.011 57.307 -9.451 1.00 29.25
H
ATOM 5207 HD13 LEU C 178 6.427 57.286 -9.329 1.00 29.25
H
ATOM 5208 HD21 LEU C 178 6.245 58.724 -6.738 1.00 27.52
H
ATOM 5209 HD22 LEU C 178 5.383 57.421 -7.027 1.00 27.52
H
ATOM 5210 HD23 LEU C 178 6.336 57.478 -5.757 1.00 27.52
H
ATOM 5211 N LEU C 179 8.075 52.732 -6.735 1.00 19.58
N
ATOM 5212 CA LEU C 179 7.821 51.303 -6.896 1.00 17.86
C
ATOM 5213 C LEU C 179 8.977 50.444 -6.402 1.00 21.63
C
ATOM 5214 O LEU C 179 10.147 50.751 -6.648 1.00 22.35
O
ATOM 5215 CB LEU C 179 7.558 50.971 -8.367 1.00 21.35
C
ATOM 5216 CG LEU C 179 6.290 51.513 -9.021 1.00 19.98
C
ATOM 5217 CD1 LEU C 179 6.291 51.174 -10.502 1.00 19.74
C
ATOM 5218 CD2 LEU C 179 5.044 50.954 -8.349 1.00 21.35
C
ATOM 5219 H LEU C 179 8.831 52.987 -7.057 1.00 23.50
H
ATOM 5220 HA LEU C 179 7.030 51.064 -6.388 1.00 21.44
H
ATOM 5221 HB2 LEU C 179 8.306 51.307 -8.885 1.00 25.62
H
ATOM 5222 HB3 LEU C 179 7.526 50.005 -8.451 1.00 25.62
H
ATOM 5223 HG LEU C 179 6.274 52.479 -8.932 1.00 23.97
H
ATOM 5224 HD11 LEU C 179 5.482 51.524 -10.906 1.00 23.68
H
ATOM 11491 HB3 GLU F 82 2.725 29.056 8.440 1.00 22.54
H
ATOM 11492 HG2 GLU F 82 0.864 29.321 9.897 1.00 25.42
H
ATOM 11493 HG3 GLU F 82 0.323 27.922 9.369 1.00 25.42
H

ATOM 11494 N CYS F 83 -0.314 31.205 8.236 1.00 16.05 N

ATOM 11495 CA CYS F 83 -0.618 32.408 8.996 1.00 14.60 C

ATOM 11496 C CYS F 83 -1.077 31.989 10.386 1.00 17.53 C

ATOM 11497 O CYS F 83 -1.688 30.932 10.562 1.00 19.01 O

ATOM 11498 CB CYS F 83 -1.672 33.270 8.287 1.00 21.05 C

ATOM 11499 SG CYS F 83 -3.338 32.591 8.159 1.00 20.77 S

ATOM 11500 H CYS F 83 -0.996 30.705 8.082 1.00 19.26 H

ATOM 11501 HA CYS F 83 0.189 32.937 9.092 1.00 17.52 H
ATOM 11502 HB2 CYS F 83 -1.742 34.112 8.763 1.00 25.26
H
ATOM 11503 HB3 CYS F 83 -1.363 33.440 7.383 1.00 25.26
H

ATOM 11504 N ASP F 84 -0.746 32.815 11.370 1.00 13.89 N
ATOM 11505 CA ASP F 84 -1.007 32.510 12.768 1.00 17.39
C

ATOM 11506 C ASP F 84 -1.702 33.696 13.425 1.00 21.87 C

ATOM 11507 O ASP F 84 -1.286 34.844 13.257 1.00 19.44 O
ATOM 11508 CB ASP F 84 0.302 32.175 13.492 1.00 19.88
C
ATOM 11509 CG ASP F 84 0.095 31.813 14.952 1.00 29.70
C
ATOM 11510 OD1 ASP F 84 -0.328 32.693 15.737 1.00 23.11
O
ATOM 11511 OD2 ASP F 84 0.378 30.651 15.318 1.00 31.40
O1-

ATOM 11512 H ASP F 84 -0.361 33.574 11.250 1.00 16.67 H
ATOM 11513 HA ASP F 84 -1.595 31.740 12.826 1.00 20.87
H
ATOM 11514 HB2 ASP F 84 0.721 31.418 13.053 1.00 23.86
H
ATOM 11515 HB3 ASP F 84 0.889 32.946 13.456 1.00 23.86
H

ATOM 11516 N TYR F 85 -2.766 33.406 14.165 1.00 17.83 N
ATOM 11517 CA TYR F 85 -3.500 34.426 14.897 1.00 20.90
C

ATOM 11518 C TYR F 85 -3.523 34.050 16.370 1.00 21.48 C

ATOM 11519 O TYR F 85 -4.217 33.118 16.776 1.00 22.77 O
ATOM 11520 CB TYR F 85 -4.918 34.575 14.344 1.00 20.94
C
ATOM 11521 CG TYR F 85 -5.590 35.873 14.726 1.00 19.46
C
ATOM 11522 CD1 TYR F 85 -5.044 37.093 14.351 1.00 23.95
C
ATOM 11523 CD2 TYR F 85 -6.781 35.880 15.443 1.00 24.58
C
ATOM 11524 CE1 TYR F 85 -5.652 38.284 14.690 1.00 21.09

H
ATOM 5225 HD12 LEU C 179 7.070 51.578 -10.917 1.00 23.68
H
ATOM 5226 HD13 LEU C 179 6.324 50.210 -10.605 1.00 23.68
H
ATOM 5227 HD21 LEU C 179 4.259 51.318 -8.788 1.00 25.62
H
ATOM 5228 HD22 LEU C 179 5.050 49.987 -8.429 1.00 25.62
H
ATOM 5229 HD23 LEU C 179 5.049 51.209 -7.414 1.00 25.62
H
ATOM 5230 N THR C 180 8.639 49.362 -5.708 1.00 18.15
N
ATOM 5231 CA THR C 180 9.600 48.313 -5.406 1.00 22.56
C
ATOM 5232 C THR C 180 9.556 47.299 -6.548 1.00 20.55
C
ATOM 5233 O THR C 180 8.552 46.607 -6.729 1.00 17.30
O
ATOM 5234 CB THR C 180 9.293 47.614 -4.066 1.00 21.01
C
ATOM 5235 OG1 THR C 180 9.224 48.585 -3.015 1.00 25.27
O
ATOM 5236 CG2 THR C 180 10.368 46.594 -3.730 1.00 28.16
C
ATOM 5237 H THR C 180 7.851 49.213 -5.399 1.00 21.78
H
ATOM 5238 HA THR C 180 10.492 48.691 -5.362 1.00 27.08
H
ATOM 5239 HB THR C 180 8.443 47.151 -4.132 1.00 25.22
H
ATOM 5240 HG1 THR C 180 8.616 49.142 -3.178 1.00 30.32
H
ATOM 5241 HG21 THR C 180 10.163 46.163 -2.886 1.00 33.79
H
ATOM 5242 HG22 THR C 180 10.413 45.920 -4.426 1.00 33.79
H
ATOM 5243 HG23 THR C 180 11.230 47.033 -3.659 1.00 33.79
H
ATOM 5244 N ILE C 181 10.633 47.229 -7.325 1.00 19.65
N
ATOM 5245 CA ILE C 181 10.726 46.266 -8.420 1.00 19.28
C
ATOM 5246 C ILE C 181 11.226 44.924 -7.902 1.00 16.96
C
ATOM 5247 O ILE C 181 12.275 44.842 -7.261 1.00 13.49
O
ATOM 5248 CB ILE C 181 11.659 46.760 -9.540 1.00 21.11
C
ATOM 5249 CG1 ILE C 181 11.236 48.150 -10.022 1.00 18.12
C
ATOM 5250 CG2 ILE C 181 11.664 45.776 -10.704 1.00 19.77
C
ATOM 5251 CD1 ILE C 181 9.805 48.234 -10.525 1.00 25.78
C
ATOM 5252 H ILE C 181 11.327 47.730 -7.240 1.00 23.58
H
ATOM 5253 HA ILE C 181 9.843 46.133 -8.800 1.00 23.13
H
ATOM 5254 HB ILE C 181 12.560 46.819 -9.185 1.00 25.33
H
ATOM 5255 HG12 ILE C 181 11.326 48.775 -9.285 1.00 21.74
H
ATOM 5256 HG13 ILE C 181 11.820 48.417 -10.749 1.00 21.74
H
ATOM 5257 HG21 ILE C 181 12.258 46.107 -11.395 1.00 23.73
H
ATOM 5258 HG22 ILE C 181 11.974 44.913 -10.386 1.00 23.73
C
ATOM 11525 CE2 TYR F 85 -7.401 37.068 15.784 1.00 25.21
C
ATOM 11526 CZ TYR F 85 -6.831 38.266 15.402 1.00 24.37
C
ATOM 11527 OH TYR F 85 -7.436 39.454 15.734 1.00 24.90
O
ATOM 11528 H TYR F 85 -3.086 32.614 14.260 1.00 21.40 H
ATOM 11529 HA TYR F 85 -3.045 35.278 14.806 1.00 25.08
H
ATOM 11530 HB2 TYR F 85 -4.881 34.535 13.375 1.00 25.13
H
ATOM 11531 HB3 TYR F 85 -5.463 33.848 14.683 1.00 25.13
H
ATOM 11532 HD1 TYR F 85 -4.248 37.108 13.870 1.00 28.73
H
ATOM 11533 HD2 TYR F 85 -7.165 35.073 15.699 1.00 29.50
H
ATOM 11534 HE1 TYR F 85 -5.272 39.093 14.434 1.00 25.31
H
ATOM 11535 HE2 TYR F 85 -8.196 37.059 16.266 1.00 30.25
H
ATOM 11536 HH TYR F 85 -8.142 39.306 16.164 1.00 29.88
H
ATOM 11537 N THR F 86 -2.739 34.777 17.158 1.00 20.16 N
ATOM 11538 CA THR F 86 -2.580 34.497 18.577 1.00 23.51
C
ATOM 11539 C THR F 86 -2.558 35.808 19.355 1.00 22.77 C
ATOM 11540 O THR F 86 -1.775 36.704 19.040 1.00 22.32 O
ATOM 11541 CB THR F 86 -1.280 33.708 18.847 1.00 27.41
C
ATOM 11542 OG1 THR F 86 -1.277 32.503 18.069 1.00 22.82
O
ATOM 11543 CG2 THR F 86 -1.153 33.353 20.320 1.00 24.65
C
ATOM 11544 H THR F 86 -2.280 35.452 16.887 1.00 24.20 H
ATOM 11545 HA THR F 86 -3.331 33.967 18.889 1.00 28.22
H
ATOM 11546 HB THR F 86 -0.517 34.252 18.598 1.00 32.89
H
ATOM 11547 HG1 THR F 86 -1.322 32.690 17.251 1.00 27.38
H
ATOM 11548 HG21 THR F 86 -0.333 32.858 20.472 1.00 29.58
H
ATOM 11549 HG22 THR F 86 -1.138 34.161 20.856 1.00 29.58
H
ATOM 11550 HG23 THR F 86 -1.906 32.806 20.596 1.00 29.58
H
ATOM 11551 N ASP F 87 -3.415 35.920 20.367 1.00 21.80 N
ATOM 11552 CA ASP F 87 -3.493 37.140 21.166 1.00 21.76
C
ATOM 11553 C ASP F 87 -3.709 38.351 20.255 1.00 25.94 C
ATOM 11554 O ASP F 87 -3.058 39.382 20.404 1.00 24.45 O
ATOM 11555 CB ASP F 87 -2.221 37.313 22.002 1.00 24.06
C
ATOM 11556 CG ASP F 87 -2.336 38.433 23.021 1.00 25.87
C
ATOM 11557 OD1 ASP F 87 -3.451 38.663 23.533 1.00 26.46
O
ATOM 11558 OD2 ASP F 87 -1.309 39.082 23.305 1.00 27.96

H
ATOM 5259 HG23 ILE C 181 10.762 45.695 -11.053 1.00 23.73
H
ATOM 5260 HD11 ILE C 181 9.623 49.144 -10.808 1.00 30.93
H
ATOM 5261 HD12 ILE C 181 9.698 47.627 -11.274 1.00 30.93
H
ATOM 5262 HD13 ILE C 181 9.203 47.984 -9.807 1.00 30.93
H
ATOM 5263 N ILE C 182 10.471 43.873 -8.193 1.00 15.47
N
ATOM 5264 CA ILE C 182 10.754 42.552 -7.654 1.00 15.31
C
ATOM 5265 C ILE C 182 10.921 41.530 -8.770 1.00 20.29
C
ATOM 5266 O ILE C 182 10.081 41.426 -9.662 1.00 15.60
O
ATOM 5267 CB ILE C 182 9.631 42.095 -6.703 1.00 19.87
C
ATOM 5268 CG1 ILE C 182 9.419 43.135 -5.596 1.00 18.35
C
ATOM 5269 CG2 ILE C 182 9.959 40.735 -6.096 1.00 17.54
C
ATOM 5270 CD1 ILE C 182 8.174 42.899 -4.758 1.00 19.47
C
ATOM 5271 H ILE C 182 9.782 43.900 -8.707 1.00 18.56
H
ATOM 5272 HA ILE C 182 11.582 42.586 -7.149 1.00 18.37
H
ATOM 5273 HB ILE C 182 8.810 42.015 -7.212 1.00 23.85
H
ATOM 5274 HG12 ILE C 182 10.185 43.117 -5.001 1.00 22.02
H
ATOM 5275 HG13 ILE C 182 9.340 44.012 -6.003 1.00 22.02
H
ATOM 5276 HG21 ILE C 182 9.237 40.472 -5.504 1.00 21.04
H
ATOM 5277 HG22 ILE C 182 10.054 40.085 -6.811 1.00 21.04
H
ATOM 5278 HG23 ILE C 182 10.788 40.803 -5.598 1.00 21.04
H
ATOM 5279 HD11 ILE C 182 8.111 43.594 -4.084 1.00 23.36
H
ATOM 5280 HD12 ILE C 182 7.395 42.926 -5.335 1.00 23.36
H
ATOM 5281 HD13 ILE C 182 8.241 42.030 -4.331 1.00 23.36
H
ATOM 5282 N GLU C 183 12.013 40.776 -8.717 1.00 17.61
N
ATOM 5283 CA GLU C 183 12.211 39.676 -9.648 1.00 20.35
C
ATOM 5284 C GLU C 183 11.144 38.620 -9.401 1.00 20.70
C
ATOM 5285 O GLU C 183 10.829 38.289 -8.258 1.00 21.07
O
ATOM 5286 CB GLU C 183 13.610 39.075 -9.500 1.00 26.30
C
ATOM 5287 CG GLU C 183 14.730 40.031 -9.891 1.00 27.61
C
ATOM 5288 CD GLU C 183 16.108 39.407 -9.763 1.00 38.86
C
ATOM 5289 OE1 GLU C 183 16.214 38.165 -9.858 1.00 36.41
O
ATOM 5290 OE2 GLU C 183 17.086 40.160 -9.564 1.00 42.70
O1-
ATOM 5291 H GLU C 183 12.653 40.881 -8.152 1.00 21.14
H
ATOM 5292 HA GLU C 183 12.114 40.002 -10.556 1.00 24.42
H
ATOM 11559 H ASP F 87 -3.962 35.304 20.612 1.00 26.15
H
ATOM 11560 HA ASP F 87 -4.248 37.077 21.772 1.00 26.11
H
ATOM 11561 HB2 ASP F 87 -2.043 36.489 22.480 1.00 28.88
H
ATOM 11562 HB3 ASP F 87 -1.480 37.521 21.411 1.00 28.88
H
ATOM 11563 N ASN F 88 -4.611 38.192 19.291 1.00 22.91
N
ATOM 11564 CA ASN F 88 -4.971 39.255 18.351 1.00 24.97
C
ATOM 11565 C ASN F 88 -3.803 39.741 17.489 1.00 23.23
C
ATOM 11566 O ASN F 88 -3.880 40.805 16.877 1.00 24.47
O
ATOM 11567 CB ASN F 88 -5.580 40.433 19.112 1.00 25.84
C
ATOM 11568 CG ASN F 88 -6.788 40.027 19.930 1.00 36.58
C
ATOM 11569 OD1 ASN F 88 -6.720 39.928 21.155 1.00 44.27
O
ATOM 11570 ND2 ASN F 88 -7.905 39.783 19.253 1.00 40.67
N
ATOM 11571 H ASN F 88 -5.040 37.459 19.157 1.00 27.49
H
ATOM 11572 HA ASN F 88 -5.651 38.913 17.750 1.00 29.96
H
ATOM 11573 HB2 ASN F 88 -4.916 40.798 19.717 1.00 31.01
H
ATOM 11574 HB3 ASN F 88 -5.861 41.110 18.477 1.00 31.01
H
ATOM 11575 HD21 ASN F 88 -8.619 39.549 19.671 1.00 48.81
H
ATOM 11576 HD22 ASN F 88 -7.914 39.859 18.396 1.00 48.81
H
ATOM 11577 N LYS F 89 -2.736 38.952 17.429 1.00 19.11
N
ATOM 11578 CA LYS F 89 -1.563 39.305 16.639 1.00 23.78
C
ATOM 11579 C LYS F 89 -1.421 38.394 15.422 1.00 22.87
C
ATOM 11580 O LYS F 89 -1.475 37.167 15.537 1.00 22.29
O
ATOM 11581 CB LYS F 89 -0.303 39.240 17.503 1.00 26.55
C
ATOM 11582 CG LYS F 89 -0.226 40.350 18.549 1.00 32.53
C
ATOM 11583 CD LYS F 89 0.900 40.113 19.546 1.00 46.00
C
ATOM 11584 CE LYS F 89 1.075 41.298 20.484 1.00 56.99
C
ATOM 11585 NZ LYS F 89 -0.193 41.656 21.180 1.00 56.00
N1+
ATOM 11586 H LYS F 89 -2.667 38.200 17.840 1.00 22.93
H
ATOM 11587 HA LYS F 89 -1.661 40.216 16.321 1.00 28.53
H
ATOM 11588 HB2 LYS F 89 -0.286 38.390 17.970 1.00 31.86
H
ATOM 11589 HB3 LYS F 89 0.475 39.318 16.930 1.00 31.86
H
ATOM 11590 HG2 LYS F 89 -0.064 41.197 18.104 1.00 39.04
H
ATOM 11591 HG3 LYS F 89 -1.062 40.384 19.040 1.00 39.04
H
ATOM 11592 HD2 LYS F 89 0.695 39.330 20.080 1.00 55.20

H
ATOM 5293 HB2 GLU C 183 13.746 38.821 -8.574 1.00 31.56
H
ATOM 5294 HB3 GLU C 183 13.676 38.292 -10.069 1.00 31.56
H
ATOM 5295 HG2 GLU C 183 14.607 40.300 -10.815 1.00 33.13
H
ATOM 5296 HG3 GLU C 183 14.697 40.809 -9.312 1.00 33.13
H
ATOM 5297 N MET C 184 10.573 38.109 -10.482 1.00 22.39
N
ATOM 5298 CA MET C 184 9.533 37.098 -10.391 1.00 21.60
C
ATOM 5299 C MET C 184 9.735 36.135 -11.546 1.00 22.55
C
ATOM 5300 O MET C 184 10.063 34.965 -11.347 1.00 23.79
O
ATOM 5301 CB MET C 184 8.144 37.747 -10.426 1.00 20.97
C
ATOM 5302 CG MET C 184 6.990 36.814 -10.069 1.00 19.42
C
ATOM 5303 SD MET C 184 6.346 35.883 -11.472 1.00 22.46
S
ATOM 5304 CE MET C 184 5.613 37.205 -12.438 1.00 23.45
C
ATOM 5305 H MET C 184 10.773 38.334 -11.287 1.00 26.87
H
ATOM 5306 HA MET C 184 9.624 36.618 -9.553 1.00 25.92
H
ATOM 5307 HB2 MET C 184 8.131 38.484 -9.796 1.00 25.17
H
ATOM 5308 HB3 MET C 184 7.983 38.082 -11.322 1.00 25.17
H
ATOM 5309 HG2 MET C 184 7.298 36.177 -9.405 1.00 23.30
H
ATOM 5310 HG3 MET C 184 6.263 37.343 -9.704 1.00 23.30
H
ATOM 5311 HE1 MET C 184 5.221 36.829 -13.241 1.00 28.15
H
ATOM 5312 HE2 MET C 184 4.927 37.640 -11.907 1.00 28.15
H
ATOM 5313 HE3 MET C 184 6.304 37.843 -12.674 1.00 28.15
H
ATOM 5314 N GLN C 185 9.571 36.648 -12.758 1.00 18.88
N
ATOM 5315 CA GLN C 185 9.795 35.862 -13.960 1.00 24.05
C
ATOM 5316 C GLN C 185 10.736 36.628 -14.880 1.00 25.86
C
ATOM 5317 O GLN C 185 10.834 37.853 -14.793 1.00 24.87
O
ATOM 5318 CB GLN C 185 8.463 35.568 -14.648 1.00 25.95
C
ATOM 5319 CG GLN C 185 8.465 34.367 -15.561 1.00 37.07
C
ATOM 5320 CD GLN C 185 8.668 33.057 -14.826 1.00 34.64
C
ATOM 5321 OE1 GLN C 185 9.787 32.701 -14.462 1.00 43.56
O
ATOM 5322 NE2 GLN C 185 7.578 32.330 -14.609 1.00 35.60
N
ATOM 5323 H GLN C 185 9.327 37.459 -12.911 1.00 22.66
H
ATOM 5324 HA GLN C 185 10.213 35.019 -13.723 1.00 28.86
H
ATOM 5325 HB2 GLN C 185 7.791 35.416 -13.966 1.00 31.14
H
ATOM 5326 HB3 GLN C 185 8.215 36.340 -15.182 1.00 31.14
H
ATOM 11593 HD3 LYS F 89 1.732 39.982 19.064 1.00 55.20
H
ATOM 11594 HE2 LYS F 89 1.737 41.076 21.158 1.00 68.38
H
ATOM 11595 HE3 LYS F 89 1.366 42.069 19.972 1.00 68.38
H
ATOM 11596 HZ1 LYS F 89 -0.817 41.870 20.583 1.00 67.20
H
ATOM 11597 HZ2 LYS F 89 -0.479 40.965 21.663 1.00 67.20
H
ATOM 11598 HZ3 LYS F 89 -0.058 42.350 21.720 1.00 67.20
H

ATOM 11599 N SER F 90 -1.243 39.015 14.259 1.00 20.20 N
ATOM 11600 CA SER F 90 -1.063 38.297 13.002 1.00 20.82
C

ATOM 11601 C SER F 90 0.418 38.076 12.691 1.00 21.90 C

ATOM 11602 O SER F 90 1.195 39.028 12.641 1.00 19.40 O
ATOM 11603 CB SER F 90 -1.719 39.065 11.852 1.00 22.35
C
ATOM 11604 OG SER F 90 -3.108 39.241 12.070 1.00 20.82
O

ATOM 11605 H SER F 90 -1.223 39.870 14.171 1.00 24.24 H
ATOM 11606 HA SER F 90 -1.490 37.428 13.068 1.00 24.98
H
ATOM 11607 HB2 SER F 90 -1.300 39.937 11.779 1.00 26.83
H
ATOM 11608 HB3 SER F 90 -1.591 38.568 11.029 1.00 26.83
H
ATOM 11609 HG SER F 90 -3.486 38.493 12.133 1.00 24.99
H

ATOM 11610 N THR F 91 0.805 36.820 12.486 1.00 14.45 N
ATOM 11611 CA THR F 91 2.164 36.504 12.056 1.00 22.20
C

ATOM 11612 C THR F 91 2.125 35.449 10.960 1.00 21.21 C

ATOM 11613 O THR F 91 1.136 34.728 10.808 1.00 20.13 O
ATOM 11614 CB THR F 91 3.048 36.012 13.223 1.00 22.36
C
ATOM 11615 OG1 THR F 91 2.488 34.825 13.793 1.00 21.83
O
ATOM 11616 CG2 THR F 91 3.171 37.091 14.297 1.00 25.53
C

ATOM 11617 H THR F 91 0.299 36.132 12.589 1.00 17.34 H
ATOM 11618 HA THR F 91 2.571 37.304 11.688 1.00 26.63
H
ATOM 11619 HB THR F 91 3.937 35.816 12.888 1.00 26.83
H
ATOM 11620 HG1 THR F 91 2.443 34.221 13.212 1.00 26.19
H
ATOM 11621 HG21 THR F 91 3.727 36.772 15.025 1.00 30.64
H
ATOM 11622 HG22 THR F 91 3.571 37.890 13.920 1.00 30.64
H
ATOM 11623 HG23 THR F 91 2.293 37.312 14.646 1.00 30.64
H

ATOM 11624 N PHE F 92 3.210 35.371 10.198 1.00 18.86 N

ATOM 11625 CA PHE F 92 3.250 34.542 9.005 1.00 17.69 C
ATOM 11626 C PHE F 92 4.564 33.793 8.890 1.00 21.66 C

H
ATOM 5327 HG2 GLN C 185 7.612 34.322 -16.022 1.00 44.49
H
ATOM 5328 HG3 GLN C 185 9.184 34.463 -16.205 1.00 44.49
H
ATOM 5329 HE21 GLN C 185 7.639 31.578 -14.196 1.00 42.72
H
ATOM 5330 HE22 GLN C 185 6.812 32.611 -14.881 1.00 42.72
H
ATOM 5331 N LYS C 186 11.446 35.921 -15.749 1.00 25.22
N
ATOM 5332 CA LYS C 186 12.328 36.599 -16.689 1.00 33.47
C
ATOM 5333 C LYS C 186 11.493 37.254 -17.785 1.00 26.33
C
ATOM 5334 O LYS C 186 10.665 36.607 -18.428 1.00 24.54
O
ATOM 5335 CB LYS C 186 13.351 35.630 -17.283 1.00 44.39
C
ATOM 5336 CG LYS C 186 14.454 35.205 -16.308 1.00 62.35
C
ATOM 5337 CD LYS C 186 15.252 36.385 -15.736 1.00 70.73
C
ATOM 5338 CE LYS C 186 15.913 37.222 -16.825 1.00 85.50
C
ATOM 5339 NZ LYS C 186 16.696 38.358 -16.263 1.00 92.86
N1+
ATOM 5340 H LYS C 186 11.437 35.063 -15.816 1.00 30.26
H
ATOM 5341 HA LYS C 186 12.812 37.298 -16.222 1.00 40.16
H
ATOM 5342 HB2 LYS C 186 12.889 34.829 -17.573 1.00 53.27
H
ATOM 5343 HB3 LYS C 186 13.778 36.056 -18.044 1.00 53.27
H
ATOM 5344 HG2 LYS C 186 14.050 34.732 -15.564 1.00 74.83
H
ATOM 5345 HG3 LYS C 186 15.075 34.622 -16.771 1.00 74.83
H
ATOM 5346 HD2 LYS C 186 14.653 36.961 -15.237 1.00 84.87
H
ATOM 5347 HD3 LYS C 186 15.949 36.044 -15.154 1.00 84.87
H
ATOM 5348 HE2 LYS C 186 16.519 36.660 -17.334 1.00102.60
H
ATOM 5349 HE3 LYS C 186 15.228 37.586 -17.407 1.00102.60
H
ATOM 5350 HZ1 LYS C 186 17.069 38.826 -16.922 1.00111.43
H
ATOM 5351 HZ2 LYS C 186 16.161 38.893 -15.795 1.00111.43
H
ATOM 5352 HZ3 LYS C 186 17.337 38.050 -15.729 1.00111.43
H
ATOM 5353 N GLY C 187 11.707 38.550 -17.977 1.00 22.70
N
ATOM 5354 CA GLY C 187 10.938 39.312 -18.943 1.00 24.36
C
ATOM 5355 C GLY C 187 11.284 40.784 -18.913 1.00 21.56
C
ATOM 5356 O GLY C 187 12.096 41.226 -18.094 1.00 17.20
O
ATOM 5357 H GLY C 187 12.298 39.013 -17.555 1.00 27.25
H
ATOM 5358 HA2 GLY C 187 11.111 38.972 -19.835 1.00 29.23
H
ATOM 5359 HA3 GLY C 187 9.991 39.213 -18.754 1.00 29.23
H
ATOM 5360 N ASP C 188 10.659 41.544 -19.808 1.00 18.15

ATOM 11627 O PHE F 92 5.582 34.199 9.449 1.00 17.52 O

ATOM 11628 CB PHE F 92 3.034 35.404 7.762 1.00 16.77 C

ATOM 11629 CG PHE F 92 1.834 36.297 7.852 1.00 17.86 C
ATOM 11630 CD1 PHE F 92 0.583 35.834 7.480 1.00 20.94
C
ATOM 11631 CD2 PHE F 92 1.955 37.598 8.316 1.00 19.25
C
ATOM 11632 CE1 PHE F 92 -0.527 36.654 7.567 1.00 20.21
C
ATOM 11633 CE2 PHE F 92 0.852 38.419 8.407 1.00 21.07
C

ATOM 11634 CZ PHE F 92 -0.390 37.951 8.033 1.00 18.70 C

ATOM 11635 H PHE F 92 3.942 35.793 10.354 1.00 22.63 H

ATOM 11636 HA PHE F 92 2.533 33.890 9.047 1.00 21.23 H
ATOM 11637 HB2 PHE F 92 3.814 35.967 7.632 1.00 20.13
H
ATOM 11638 HB3 PHE F 92 2.915 34.823 6.994 1.00 20.13
H
ATOM 11639 HD1 PHE F 92 0.489 34.963 7.168 1.00 25.13
H
ATOM 11640 HD2 PHE F 92 2.790 37.919 8.571 1.00 23.10
H
ATOM 11641 HE1 PHE F 92 -1.363 36.335 7.314 1.00 24.25
H
ATOM 11642 HE2 PHE F 92 0.946 39.290 8.719 1.00 25.28
H

ATOM 11643 HZ PHE F 92 -1.134 38.506 8.092 1.00 22.43 H

ATOM 11644 N ASP F 93 4.528 32.693 8.151 1.00 18.85 N

ATOM 11645 CA ASP F 93 5.714 31.893 7.904 1.00 19.59 C

ATOM 11646 C ASP F 93 5.583 31.237 6.539 1.00 21.25 C

ATOM 11647 O ASP F 93 4.484 30.852 6.130 1.00 15.85 O

ATOM 11648 CB ASP F 93 5.887 30.841 9.000 1.00 23.31 C

ATOM 11649 CG ASP F 93 7.131 29.997 8.810 1.00 31.07 C
ATOM 11650 OD1 ASP F 93 8.143 30.533 8.309 1.00 32.52
O1-
ATOM 11651 OD2 ASP F 93 7.093 28.797 9.164 1.00 33.33
O

ATOM 11652 H ASP F 93 3.817 32.386 7.778 1.00 22.62 H

ATOM 11653 HA ASP F 93 6.497 32.466 7.898 1.00 23.51 H
ATOM 11654 HB2 ASP F 93 5.955 31.288 9.859 1.00 27.98
H
ATOM 11655 HB3 ASP F 93 5.119 30.249 8.994 1.00 27.98
H

ATOM 11656 N GLN F 94 6.695 31.128 5.825 1.00 16.48 N

ATOM 11657 CA GLN F 94 6.698 30.390 4.575 1.00 21.95 C

ATOM 11658 C GLN F 94 8.029 29.686 4.368 1.00 20.37 C

ATOM 11659 O GLN F 94 9.078 30.195 4.754 1.00 17.80 O
ATOM 11660 CB GLN F 94 6.378 31.314 3.394 1.00 16.26 C

N
ATOM 5361 CA ASP C 188 10.960 42.961 -19.960 1.00 17.36
C
ATOM 5362 C ASP C 188 9.738 43.846 -19.697 1.00 19.06
C
ATOM 5363 O ASP C 188 9.709 45.001 -20.117 1.00 15.87
O
ATOM 5364 CB ASP C 188 11.509 43.226 -21.365 1.00 19.74
C
ATOM 5365 CG ASP C 188 12.824 42.513 -21.618 1.00 23.22
C
ATOM 5366 OD1 ASP C 188 13.720 42.596 -20.754 1.00 19.57
O
ATOM 5367 OD2 ASP C 188 12.958 41.864 -22.675 1.00 26.62
O1-
ATOM 5368 H ASP C 188 10.050 41.258 -20.344 1.00 21.78
H
ATOM 5369 HA ASP C 188 11.648 43.206 -19.321 1.00 20.83
H
ATOM 5370 HB2 ASP C 188 10.866 42.914 -22.020 1.00 23.69
H
ATOM 5371 HB3 ASP C 188 11.657 44.179 -21.472 1.00 23.69
H
ATOM 5372 N CYS C 189 8.739 43.299 -19.006 1.00 16.64
N
ATOM 5373 CA CYS C 189 7.539 44.052 -18.630 1.00 17.86
C
ATOM 5374 C CYS C 189 7.259 43.887 -17.138 1.00 16.95
C
ATOM 5375 O CYS C 189 7.791 42.980 -16.504 1.00 15.25
O
ATOM 5376 CB CYS C 189 6.326 43.596 -19.447 1.00 16.46
C
ATOM 5377 SG CYS C 189 6.412 43.997 -21.213 1.00 19.92
S
ATOM 5378 H CYS C 189 8.730 42.481 -18.739 1.00 19.97
H
ATOM 5379 HA CYS C 189 7.686 44.995 -18.808 1.00 21.43
H
ATOM 5380 HB2 CYS C 189 6.245 42.632 -19.368 1.00 19.75
H
ATOM 5381 HB3 CYS C 189 5.532 44.021 -19.088 1.00 19.75
H
ATOM 5382 N ALA C 190 6.424 44.763 -16.584 1.00 14.88
N
ATOM 5383 CA ALA C 190 6.146 44.757 -15.149 1.00 15.16
C
ATOM 5384 C ALA C 190 4.655 44.804 -14.854 1.00 12.33
C
ATOM 5385 O ALA C 190 3.901 45.546 -15.487 1.00 12.28
O
ATOM 5386 CB ALA C 190 6.845 45.927 -14.478 1.00 18.64
C
ATOM 5387 H ALA C 190 6.003 45.373 -17.020 1.00 17.85
H
ATOM 5388 HA ALA C 190 6.500 43.940 -14.766 1.00 18.19
H
ATOM 5389 HB1 ALA C 190 6.651 45.907 -13.528 1.00 22.37
H
ATOM 5390 HB2 ALA C 190 7.801 45.847 -14.622 1.00 22.37
H
ATOM 5391 HB3 ALA C 190 6.520 46.754 -14.866 1.00 22.37
H
ATOM 5392 N LEU C 191 4.249 43.993 -13.882 1.00 10.76
N
ATOM 5393 CA LEU C 191 2.888 43.985 -13.375 1.00 12.20
C
ATOM 5394 C LEU C 191 2.805 44.849 -12.132 1.00 13.93

ATOM 11661 CG GLN F 94 7.372 32.427 3.149 1.00 21.74 C

ATOM 11662 CD GLN F 94 7.010 33.272 1.933 1.00 28.61 C
ATOM 11663 OE1 GLN F 94 5.878 33.231 1.442 1.00 23.71
O
ATOM 11664 NE2 GLN F 94 7.976 34.041 1.440 1.00 34.71
N

ATOM 11665 H GLN F 94 7.454 31.469 6.042 1.00 19.77 H

ATOM 11666 HA GLN F 94 6.007 29.709 4.613 1.00 26.34 H
ATOM 11667 HB2 GLN F 94 6.337 30.777 2.587 1.00 19.52
H
ATOM 11668 HB3 GLN F 94 5.513 31.725 3.553 1.00 19.52
H
ATOM 11669 HG2 GLN F 94 7.393 33.009 3.925 1.00 26.09
H
ATOM 11670 HG3 GLN F 94 8.249 32.042 2.998 1.00 26.09
H
ATOM 11671 HE21 GLN F 94 7.823 34.537 0.754 1.00 41.66
H
ATOM 11672 HE22 GLN F 94 8.754 34.042 1.806 1.00 41.66
H

ATOM 11673 N ASP F 95 7.961 28.494 3.780 1.00 19.52 N

ATOM 11674 CA ASP F 95 9.139 27.680 3.502 1.00 19.57 C

ATOM 11675 C ASP F 95 9.090 27.193 2.064 1.00 21.52 C

ATOM 11676 O ASP F 95 8.010 27.017 1.496 1.00 17.71 O

ATOM 11677 CB ASP F 95 9.219 26.471 4.443 1.00 24.75 C

ATOM 11678 CG ASP F 95 9.408 26.861 5.898 1.00 36.23 C
ATOM 11679 OD1 ASP F 95 10.173 27.809 6.181 1.00 35.86
O
ATOM 11680 OD2 ASP F 95 8.792 26.202 6.762 1.00 36.50
O1-

ATOM 11681 H ASP F 95 7.225 28.128 3.527 1.00 23.42 H

ATOM 11682 HA ASP F 95 9.939 28.216 3.619 1.00 23.48 H
ATOM 11683 HB2 ASP F 95 8.395 25.964 4.375 1.00 29.70
H
ATOM 11684 HB3 ASP F 95 9.971 25.918 4.182 1.00 29.70
H

ATOM 11685 N TYR F 96 10.266 26.978 1.488 1.00 17.67 N
ATOM 11686 CA TYR F 96 10.397 26.363 0.173 1.00 17.08
C

ATOM 11687 C TYR F 96 11.265 25.123 0.294 1.00 20.00 C

ATOM 11688 O TYR F 96 12.344 25.188 0.880 1.00 20.02 O
ATOM 11689 CB TYR F 96 11.028 27.329 -0.828 1.00 18.79
C
ATOM 11690 CG TYR F 96 10.392 28.694 -0.885 1.00 16.85
C
ATOM 11691 CD1 TYR F 96 10.737 29.681 0.029 1.00 18.78
C
ATOM 11692 CD2 TYR F 96 9.463 29.005 -1.866 1.00 17.98
C
ATOM 11693 CE1 TYR F 96 10.164 30.932 -0.025 1.00 20.39
C
ATOM 11694 CE2 TYR F 96 8.886 30.254 -1.929 1.00 16.11

C
ATOM 5395 O LEU C 191 3.653 44.741 -11.246 1.00 12.07
O
ATOM 5396 CB LEU C 191 2.440 42.565 -13.034 1.00 11.91
C
ATOM 5397 CG LEU C 191 2.300 41.584 -14.194 1.00 12.77
C
ATOM 5398 CD1 LEU C 191 2.254 40.162 -13.660 1.00 15.07
C
ATOM 5399 CD2 LEU C 191 1.046 41.904 -14.990 1.00 15.63
C
ATOM 5400 H LEU C 191 4.761 43.423 -13.491 1.00 12.91
H
ATOM 5401 HA LEU C 191 2.288 44.347 -14.046 1.00 14.65
H
ATOM 5402 HB2 LEU C 191 3.085 42.186 -12.416 1.00 14.29
H
ATOM 5403 HB3 LEU C 191 1.575 42.619 -12.599 1.00 14.29
H
ATOM 5404 HG LEU C 191 3.066 41.667 -14.782 1.00 15.32
H
ATOM 5405 HD11 LEU C 191 2.165 39.548 -14.406 1.00 18.08
H
ATOM 5406 HD12 LEU C 191 3.076 39.980 -13.178 1.00 18.08
H
ATOM 5407 HD13 LEU C 191 1.494 40.073 -13.065 1.00 18.08 H
ATOM 5408 HD21 LEU C 191 0.969 41.274 -15.723 1.00 18.76 H
ATOM 5409 HD22 LEU C 191 0.275 41.829 -14.406 1.00 18.76 H
ATOM 5410 HD23 LEU C 191 1.114 42.808 -15.335 1.00 18.76 H
ATOM 5411 N TYR C 192 1.786 45.698 -12.056 1.00 12.40 N
ATOM 5412 CA TYR C 192 1.539 46.417 -10.818 1.00 15.75 C
ATOM 5413 C TYR C 192 0.917 45.485 -9.793 1.00 13.37 C
ATOM 5414 O TYR C 192 0.058 44.669 -10.119 1.00 12.80 O
ATOM 5415 CB TYR C 192 0.619 47.621 -11.010 1.00 12.40 C
ATOM 5416 CG TYR C 192 0.350 48.273 -9.679 1.00 17.77 C
ATOM 5417 CD1 TYR C 192 1.268 49.153 -9.128 1.00 19.33 C
ATOM 5418 CD2 TYR C 192 -0.786 47.958 -8.939 1.00 18.28 C
ATOM 5419 CE1 TYR C 192 1.051 49.729 -7.899 1.00 17.95 C
ATOM 5420 CE2 TYR C 192 -1.010 48.531 -7.701 1.00 20.59 C
ATOM 5421 CZ TYR C 192 -0.085 49.416 -7.187 1.00 20.36 C
ATOM 5422 OH TYR C 192 -0.287 49.996 -5.957 1.00 19.55 O
ATOM 5423 H TYR C 192 1.236 45.873 -12.693 1.00 14.88 H
ATOM 5424 HA TYR C 192 2.383 46.736 -10.463 1.00 18.89 H
ATOM 5425 HB2 TYR C 192 1.047 48.268 -11.591 1.00 14.88 H
ATOM 5426 HB3 TYR C 192 -0.226 47.329 -11.388 1.00 14.88 H
ATOM 5427 HD1 TYR C 192 2.038 49.366 -9.603 1.00 23.20 H
ATOM 5428 HD2 TYR C 192 -1.407 47.360 -9.286 1.00 21.93 H
ATOM 5429 HE1 TYR C 192 1.673 50.325 -7.548 1.00 21.53 H
ATOM 5430 HE2 TYR C 192 -1.777 48.322 -7.219 1.00 24.70 H
ATOM 5431 HH TYR C 192 -1.011 49.725 -5.627 1.00 23.47 H
ATOM 5432 N ALA C 193 1.363 45.625 -8.552 1.00 14.31 N
ATOM 5433 CA ALA C 193 0.773 44.931 -7.416 1.00 14.94 C
ATOM 5434 C ALA C 193 0.867 45.856 -6.211 1.00 17.89 C
ATOM 5435 O ALA C 193 1.874 46.539 -6.034 1.00 18.07 O
ATOM 5436 CB ALA C 193 1.488 43.614 -7.146 1.00 13.51 C
ATOM 5437 H ALA C 193 2.025 46.130 -8.337 1.00 17.18 H
ATOM 5438 HA ALA C 193 -0.162 44.747 -7.595 1.00 17.93 H
ATOM 5439 HB1 ALA C 193 1.071 43.179 -6.386 1.00 16.22 H
ATOM 5440 HB2 ALA C 193 1.416 43.050 -7.932 1.00 16.22 H
ATOM 5441 HB3 ALA C 193 2.421 43.796 -6.954 1.00 16.22 H
ATOM 5442 N SER C 194 -0.171 45.893 -5.385 1.00 15.21 N
ATOM 5443 CA SER C 194 -0.150 46.773 -4.220 1.00 19.46 C
ATOM 5444 C SER C 194 0.589 46.101 -3.063 1.00 18.48 C
ATOM 5445 O SER C 194 0.561 44.878 -2.952 1.00 20.00 O
ATOM 5446 CB SER C 194 -1.569 47.149 -3.798 1.00 18.63 C
ATOM 5447 OG SER C 194 -2.308 45.998 -3.450 1.00 27.89 O
ATOM 5448 H SER C 194 -0.889 45.428 -5.472 1.00 18.26 H
ATOM 5449 HA SER C 194 0.323 47.589 -4.447 1.00 23.36 H
C
ATOM 11695 CZ TYR F 96 9.239 31.214 -1.006 1.00 20.26 C
ATOM 11696 OH TYR F 96 8.666 32.462 -1.069 1.00 22.81
O
ATOM 11697 H TYR F 96 11.020 27.185 1.848 1.00 21.20 H
ATOM 11698 HA TYR F 96 9.523 26.101 -0.155 1.00 20.50 H
ATOM 11699 HB2 TYR F 96 11.962 27.451 -0.593 1.00 22.55
H
ATOM 11700 HB3 TYR F 96 10.965 26.940 -1.715 1.00 22.55
H
ATOM 11701 HD1 TYR F 96 11.361 29.492 0.692 1.00 22.54
H
ATOM 11702 HD2 TYR F 96 9.223 28.358 -2.489 1.00 21.57
H
ATOM 11703 HE1 TYR F 96 10.401 31.583 0.595 1.00 24.47
H
ATOM 11704 HE2 TYR F 96 8.261 30.447 -2.590 1.00 19.33
H
ATOM 11705 HH TYR F 96 8.124 32.497 -1.710 1.00 27.37 H
ATOM 11706 N LEU F 97 10.806 24.001 -0.258 1.00 19.54 N
ATOM 11707 CA LEU F 97 11.617 22.782 -0.290 1.00 21.34 C
ATOM 11708 C LEU F 97 11.827 22.285 -1.721 1.00 21.46 C
ATOM 11709 O LEU F 97 10.891 22.245 -2.520 1.00 15.94 O
ATOM 11710 CB LEU F 97 10.973 21.670 0.540 1.00 21.85 C
ATOM 11711 CG LEU F 97 10.355 22.043 1.891 1.00 24.09 C
ATOM 11712 CD1 LEU F 97 9.634 20.841 2.480 1.00 34.93 C
ATOM 11713 CD2 LEU F 97 11.413 22.551 2.856 1.00 31.03 C
ATOM 11714 H LEU F 97 10.031 23.918 -0.621 1.00 23.45 H
ATOM 11715 HA LEU F 97 12.488 22.973 0.091 1.00 25.61 H
ATOM 11716 HB2 LEU F 97 10.267 21.272 0.008 1.00 26.22 H
ATOM 11717 HB3 LEU F 97 11.652 21.000 0.717 1.00 26.22 H
ATOM 11718 HG LEU F 97 9.704 22.749 1.758 1.00 28.91 H
ATOM 11719 HD11 LEU F 979.248 21.092 3.334 1.00 41.92 H
ATOM 11720 HD12 LEU F 97 8.934 20.563 1.869 1.00 41.92 H
ATOM 11721 HD13 LEU F 97 10.271 20.120 2.603 1.00 41.92 H
ATOM 11722 HD21 LEU F 97 10.989 22.777 3.699 1.00 37.24 H
ATOM 11723 HD22 LEU F 97 12.074 21.855 2.995 1.00 37.24 H
ATOM 11724 HD23 LEU F 97 11.835 23.338 2.476 1.00 37.24 H
ATOM 11725 N TYR F 98 13.066 21.914 -2.030 1.00 21.23 N
ATOM 11726 CA TYR F 98 13.397 21.259 -3.293 1.00 18.28 C
ATOM 11727 C TYR F 98 13.879 19.850 -2.981 1.00 22.72 C
ATOM 11728 O TYR F 98 14.924 19.675 -2.353 1.00 20.74 O
ATOM 11729 CB TYR F 98 14.465 22.044 -4.058 1.00 18.19 C
ATOM 11730 CG TYR F 98 14.779 21.475 -5.426 1.00 21.19 C
ATOM 11731 CD1 TYR F 98 13.950 21.729 -6.511 1.00 23.23 C
ATOM 11732 CD2 TYR F 98 15.905 20.689 -5.632 1.00 23.20 C
ATOM 11733 CE1 TYR F 98 14.233 21.213 -7.764 1.00 29.19 C
ATOM 11734 CE2 TYR F 98 16.196 20.170 -6.879 1.00 24.25 C
ATOM 11735 CZ TYR F 98 15.357 20.434 -7.941 1.00 27.82 C
ATOM 11736 OH TYR F 98 15.644 19.918 -9.183 1.00 33.31 O
ATOM 11737 H TYR F 98 13.744 22.032 -1.515 1.00 25.47 H
ATOM 11738 HA TYR F 98 12.603 21.199 -3.846 1.00 21.94 H
ATOM 11739 HB2 TYR F 98 14.157 22.955 -4.179 1.00 21.83 H
ATOM 11740 HB3 TYR F 98 15.286 22.041 -3.541 1.00 21.83 H
ATOM 11741 HD1 TYR F 98 13.192 22.254 -6.393 1.00 27.87 H
ATOM 11742 HD2 TYR F 98 16.473 20.508 -4.918 1.00 27.84 H
ATOM 11743 HE1 TYR F 98 13.668 21.391 -8.482 1.00 35.03 H
ATOM 11744 HE2 TYR F 98 16.953 19.644 -7.001 1.00 29.10 H
ATOM 11745 HH TYR F 98 15.057 20.155 -9.736 1.00 39.98 H
ATOM 11746 N ASN F 99 13.103 18.855 -3.405 1.00 20.11 N
ATOM 11747 CA ASN F 99 13.368 17.458 -3.066 1.00 23.25 C
ATOM 11748 C ASN F 99 13.517 17.267 -1.558 1.00 25.58 C
ATOM 11749 O ASN F 99 14.394 16.536 -1.090 1.00 21.44 O

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ATOM   5450  HB2 SER C 194     -1.525  47.740  -3.030  1.00 22.35           H
ATOM   5451  HB3 SER C 194     -2.011  47.596  -4.537  1.00 22.35           H
ATOM   5452  HG  SER C 194     -1.935  45.600  -2.811  1.00 33.47           H
ATOM   5453  N   SER C 195      1.243  46.877  -2.197  1.00 20.90           N
ATOM   5454  CA  SER C 195      1.276  48.334  -2.265  1.00 24.71           C
ATOM   5455  C   SER C 195      2.483  48.832  -3.053  1.00 20.24           C
ATOM   5456  O   SER C 195      3.625  48.682  -2.618  1.00 19.16           O
ATOM   5457  CB  SER C 195      1.300  48.929  -0.858  1.00 22.44           C
ATOM   5458  OG  SER C 195      1.256  50.341  -0.920  1.00 28.76           O
ATOM   5459  H   SER C 195      1.694  46.564  -1.535  1.00 25.08           H
ATOM   5460  HA  SER C 195      0.474  48.648  -2.712  1.00 29.65           H
ATOM   5461  HB2 SER C 195      0.528  48.609  -0.365  1.00 26.93           H
ATOM   5462  HB3 SER C 195      2.117  48.656  -0.412  1.00 26.93           H
ATOM   5463  HG  SER C 195      1.270  50.663  -0.144  1.00 34.51           H
ATOM   5464  N   PHE C 196      2.215  49.423  -4.213  1.00 20.32           N
ATOM   5465  CA  PHE C 196      3.249  50.046  -5.035  1.00 19.27           C
ATOM   5466  C   PHE C 196      4.443  49.138  -5.290  1.00 23.51           C
ATOM   5467  O   PHE C 196      5.581  49.456  -4.933  1.00 18.74           O
ATOM   5468  CB  PHE C 196      3.708  51.345  -4.384  1.00 20.31           C
ATOM   5469  CG  PHE C 196      2.685  52.432  -4.451  1.00 21.15           C
ATOM   5470  CD1 PHE C 196      2.543  53.189  -5.599  1.00 21.62           C
ATOM   5471  CD2 PHE C 196      1.849  52.685  -3.378  1.00 27.55           C
ATOM   5472  CE1 PHE C 196      1.592  54.182  -5.673  1.00 19.96           C
ATOM   5473  CE2 PHE C 196      0.899  53.680  -3.447  1.00 23.40           C
ATOM   5474  CZ  PHE C 196      0.772  54.430  -4.595  1.00 21.78           C
ATOM   5475  H   PHE C 196      1.427  49.477  -4.553  1.00 24.38
H
ATOM   5476  HA  PHE C 196      2.864  50.271  -5.896  1.00 23.12
H
ATOM   5477  HB2 PHE C 196      3.902  51.176  -3.448  1.00 24.38
H
ATOM   5478  HB3 PHE C 196      4.507  51.658  -4.836  1.00 24.38
H
ATOM   5479  HD1 PHE C 196      3.095  53.025  -6.329  1.00 25.94
H
ATOM   5480  HD2 PHE C 196      1.932  52.181  -2.601  1.00 33.05
H
ATOM   5481  HE1 PHE C 196      1.508  54.688  -6.448  1.00 23.95
H
ATOM   5482  HE2 PHE C 196      0.345  53.846  -2.719  1.00 28.08
H
ATOM   5483  HZ  PHE C 196      0.131  55.102  -4.643  1.00 26.14
H
ATOM   5484  N   LYS C 197      4.165  48.003  -5.919  1.00 18.00
N
ATOM   5485  CA  LYS C 197      5.197  47.054  -6.288  1.00 21.33
C
ATOM   5486  C   LYS C 197      5.092  46.769  -7.776  1.00 18.93
C
ATOM   5487  O   LYS C 197      4.018  46.905  -8.367  1.00 15.60
O
ATOM   5488  CB  LYS C 197      5.064  45.765  -5.474  1.00 21.85
C
ATOM   5489  CG  LYS C 197      4.958  46.002  -3.977  1.00 27.27
C
ATOM   5490  CD  LYS C 197      5.109  44.719  -3.183  1.00 29.38
C
ATOM   5491  CE  LYS C 197      3.988  43.739  -3.459  1.00 32.12
C
ATOM   5492  NZ  LYS C 197      4.083  42.540  -2.575  1.00 44.07
N1+
ATOM   5493  H   LYS C 197      3.372  47.759  -6.146  1.00 21.60
H
ATOM   5494  HA  LYS C 197      6.069  47.440  -6.110  1.00 25.60
H
ATOM   5495  HB2 LYS C 197      4.264  45.296  -5.759  1.00 26.23
H
ATOM   5496  HB3 LYS C 197      5.844  45.212  -5.634  1.00 26.23

ATOM  11750  CB  ASN F  99     14.621  16.955  -3.789  1.00 22.66           C
ATOM  11751  CG  ASN F  99     14.430  16.862  -5.291  1.00 24.21           C
ATOM  11752  OD1 ASN F  99     13.320  16.636  -5.779  1.00 25.43           O
ATOM  11753  ND2 ASN F  99     15.517  17.028  -6.034  1.00 21.89           N
ATOM  11754  H   ASN F  99     12.407  18.965  -3.899  1.00 24.13           H
ATOM  11755  HA  ASN F  99     12.619  16.918  -3.360  1.00 27.90           H
ATOM  11756  HB2 ASN F  99     15.353  17.567  -3.617  1.00 27.19           H
ATOM  11757  HB3 ASN F  99     14.842  16.070  -3.459  1.00 27.19           H
ATOM  11758 HD21 ASN F  99     15.462  16.985  -6.891  1.00 26.27           H
ATOM  11759 HD22 ASN F  99     16.275  17.180  -5.658  1.00 26.27           H
ATOM  11760  N   GLY F 100     12.658  17.940  -0.799  1.00 20.75           N
ATOM  11761  CA  GLY F 100     12.618  17.775   0.642  1.00 27.43           C
ATOM  11762  C   GLY F 100     13.626  18.633   1.379  1.00 25.00           C
ATOM  11763  O   GLY F 100     13.587  18.729   2.607  1.00 23.15           O
ATOM  11764  H   GLY F 100     12.084  18.504  -1.103  1.00 24.90           H
ATOM  11765  HA2 GLY F 100     11.732  18.004   0.965  1.00 32.92           H
ATOM  11766  HA3 GLY F 100     12.792  16.847   0.862  1.00 32.92           H
ATOM  11767  N   GLU F 101     14.529  19.255   0.628  1.00 27.20           N
ATOM  11768  CA  GLU F 101     15.572  20.100   1.201  1.00 28.99           C
ATOM  11769  C   GLU F 101     15.137  21.559   1.206  1.00 26.31           C
ATOM  11770  O   GLU F 101     14.827  22.123   0.158  1.00 22.95           O
ATOM  11771  CB  GLU F 101     16.874  19.947   0.413  1.00 28.96           C
ATOM  11772  CG  GLU F 101     18.114  20.440   1.148  1.00 43.62           C
ATOM  11773  CD  GLU F 101     18.632  19.442   2.169  1.00 55.65           C
ATOM  11774  OE1 GLU F 101     18.669  18.230   1.862  1.00 48.87           O
ATOM  11775  OE2 GLU F 101     19.007  19.872   3.280  1.00 57.62
O1-
ATOM  11776  H   GLU F 101     14.560  19.203  -0.230  1.00 32.65
H
ATOM  11777  HA  GLU F 101     15.737  19.828   2.117  1.00 34.79
H
ATOM  11778  HB2 GLU F 101     17.006  19.008   0.209  1.00 34.75
H
ATOM  11779  HB3 GLU F 101     16.799  20.453  -0.411  1.00 34.75
H
ATOM  11780  HG2 GLU F 101     18.819  20.603   0.503  1.00 52.34
H
ATOM  11781  HG3 GLU F 101     17.897  21.262   1.616  1.00 52.34
H
ATOM  11782  N   GLU F 102     15.126  22.176   2.383  1.00 28.54
N
ATOM  11783  CA  GLU F 102     14.689  23.561   2.500  1.00 25.54
C
ATOM  11784  C   GLU F 102     15.733  24.512   1.927  1.00 24.67
C
ATOM  11785  O   GLU F 102     16.936  24.287   2.062  1.00 21.93
O
ATOM  11786  CB  GLU F 102     14.396  23.912   3.962  1.00 33.49
C
ATOM  11787  CG  GLU F 102     13.833  25.312   4.156  1.00 37.89
C
ATOM  11788  CD  GLU F 102     13.340  25.561   5.574  1.00 47.13
C
ATOM  11789  OE1 GLU F 102     13.153  26.742   5.939  1.00 46.84
O
ATOM  11790  OE2 GLU F 102     13.134  24.578   6.319  1.00 51.60
O1-
ATOM  11791  H   GLU F 102     15.366  21.816   3.126  1.00 34.25
H
ATOM  11792  HA  GLU F 102     13.869  23.677   1.995  1.00 30.65
H
ATOM  11793  HB2 GLU F 102     13.749  23.281   4.312  1.00 40.19
H
ATOM  11794  HB3 GLU F 102     15.221  23.852   4.469  1.00 40.19
H
ATOM  11795  HG2 GLU F 102     14.527  25.961   3.962  1.00 45.47
H
ATOM  11796  HG3 GLU F 102     13.084  25.437   3.553  1.00 45.47
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H
ATOM 5497 HG2 LYS C 197 5.660 46.612 -3.702 1.00 32.72
H
ATOM 5498 HG3 LYS C 197 4.089 46.381 -3.776 1.00 32.72
H
ATOM 5499 HD2 LYS C 197 5.948 44.294 -3.422 1.00 35.26
H
ATOM 5500 HD3 LYS C 197 5.100 44.929 -2.236 1.00 35.26
H
ATOM 5501 HE2 LYS C 197 3.135 44.172 -3.295 1.00 38.55
H
ATOM 5502 HE3 LYS C 197 4.042 43.442 -4.381 1.00 38.55
H
ATOM 5503 HZ1 LYS C 197 3.416 41.977 -2.752 1.00 52.89
H
ATOM 5504 HZ2 LYS C 197 4.857 42.123 -2.710 1.00 52.89
H
ATOM 5505 HZ3 LYS C 197 4.033 42.787 -1.721 1.00 52.89
H
ATOM 5506 N GLY C 198 6.222 46.404 -8.372 1.00 13.97
N
ATOM 5507 CA GLY C 198 6.273 45.977 -9.754 1.00 12.15
C
ATOM 5508 C GLY C 198 6.935 44.618 -9.848 1.00 15.82
C
ATOM 5509 O GLY C 198 8.119 44.484 -9.540 1.00 16.91
O
ATOM 5510 H GLY C 198 6.988 46.398 -7.982 1.00 16.76
H
ATOM 5511 HA2 GLY C 198 5.375 45.916 -10.116 1.00 14.58
H
ATOM 5512 HA3 GLY C 198 6.783 46.613 -10.280 1.00 14.58
H
ATOM 5513 N TYR C 199 6.172 43.605 -10.251 1.00 14.27
N
ATOM 5514 CA TYR C 199 6.716 42.267 -10.466 1.00 14.60
C
ATOM 5515 C TYR C 199 7.146 42.099 -11.920 1.00 15.48
C
ATOM 5516 O TYR C 199 6.360 42.327 -12.829 1.00 12.77
O
ATOM 5517 CB TYR C 199 5.689 41.192 -10.101 1.00 14.93
C
ATOM 5518 CG TYR C 199 5.489 41.006 -8.615 1.00 20.52
C
ATOM 5519 CD1 TYR C 199 6.359 40.220 -7.870 1.00 15.96
C
ATOM 5520 CD2 TYR C 199 4.425 41.609 -7.956 1.00 18.27
C
ATOM 5521 CE1 TYR C 199 6.179 40.044 -6.509 1.00 18.35
C
ATOM 5522 CE2 TYR C 199 4.236 41.438 -6.596 1.00 20.42
C
ATOM 5523 CZ TYR C 199 5.116 40.654 -5.877 1.00 22.28
C
ATOM 5524 OH TYR C 199 4.931 40.486 -4.522 1.00 27.53
O
ATOM 5525 H TYR C 199 5.329 43.667 -10.408 1.00 17.12
H
ATOM 5526 HA TYR C 199 7.496 42.145 -9.903 1.00 17.52
H
ATOM 5527 HB2 TYR C 199 4.833 41.436 -10.486 1.00 17.92
H
ATOM 5528 HB3 TYR C 199 5.983 40.344 -10.468 1.00 17.92
H
ATOM 5529 HD1 TYR C 199 7.077 39.807 -8.293 1.00 19.15
H
ATOM 5530 HD2 TYR C 199 3.830 42.137 -8.438 1.00 21.93
H
ATOM 11797 N TYR F 103 15.269 25.577 1.284 1.00 19.00 N
ATOM 11798 CA TYR F 103 16.175 26.558 0.700 1.00 23.12
C
ATOM 11799 C TYR F 103 15.507 27.925 0.622 1.00 24.60 C
ATOM 11800 O TYR F 103 14.283 28.026 0.729 1.00 18.78
O
ATOM 11801 CB TYR F 103 16.632 26.099 -0.686 1.00 18.11
C
ATOM 11802 CG TYR F 103 15.564 26.151 -1.759 1.00 20.57
C
ATOM 11803 CD1 TYR F 103 14.489 25.272 -1.743 1.00 19.73
C
ATOM 11804 CD2 TYR F 103 15.647 27.066 -2.802 1.00 19.76
C
ATOM 11805 CE1 TYR F 103 13.516 25.314 -2.731 1.00 17.89
C
ATOM 11806 CE2 TYR F 103 14.681 27.117 -3.790 1.00 15.45
C
ATOM 11807 CZ TYR F 103 13.618 26.236 -3.751 1.00 18.31
C
ATOM 11808 OH TYR F 103 12.652 26.280 -4.734 1.00 17.87
O
ATOM 11809 H TYR F 103 14.435 25.755 1.172 1.00 22.80 H
ATOM 11810 HA TYR F 103 16.960 26.639 1.265 1.00 27.75
H
ATOM 11811 HB2 TYR F 103 17.364 26.667 -0.974 1.00 21.74
H
ATOM 11812 HB3 TYR F 103 16.939 25.181 -0.622 1.00 21.74
H
ATOM 11813 HD1 TYR F 103 14.417 24.650 -1.056 1.00 23.67
H
ATOM 11814 HD2 TYR F 103 16.362 27.660 -2.831 1.00 23.72
H
ATOM 11815 HE1 TYR F 103 12.798 24.722 -2.705 1.00 21.47
H
ATOM 11816 HE2 TYR F 103 14.749 27.738 -4.479 1.00 18.54
H
ATOM 11817 HH TYR F 103 12.834 26.883 -5.290 1.00 21.44
H
ATOM 11818 N THR F 104 16.319 28.969 0.452 1.00 20.25
N
ATOM 11819 CA THR F 104 15.819 30.341 0.376 1.00 19.66
C
ATOM 11820 C THR F 104 16.621 31.227 -0.581 1.00 24.00
C
ATOM 11821 O THR F 104 16.243 32.373 -0.830 1.00 25.47
O
ATOM 11822 CB THR F 104 15.834 31.022 1.762 1.00 23.07
C
ATOM 11823 OG1 THR F 104 17.182 31.117 2.235 1.00 27.80
O
ATOM 11824 CG2 THR F 104 14.996 30.247 2.763 1.00 27.54
C
ATOM 11825 H THR F 104 17.174 28.907 0.378 1.00 24.30
H
ATOM 11826 HA THR F 104 14.901 30.322 0.064 1.00 23.59
H
ATOM 11827 HB THR F 104 15.461 31.914 1.682 1.00 27.69
H
ATOM 11828 HG1 THR F 104 17.196 31.487 2.989 1.00 33.36
H
ATOM 11829 HG21 THR F 104 15.017 30.689 3.626 1.00 33.05
H
ATOM 11830 HG22 THR F 104 14.077 30.196 2.457 1.00 33.05

H
ATOM 5531 HE1 TYR C 199 6.771 39.517 -6.024 1.00 22.01
H
ATOM 5532 HE2 TYR C 199 3.520 41.849 -6.168 1.00 24.50
H
ATOM 5533 HH TYR C 199 4.251 40.909 -4.270 1.00 33.04
H
ATOM 5534 N ILE C 200 8.396 41.698 -12.128 1.00 16.81
N
ATOM 5535 CA ILE C 200 8.926 41.482 -13.471 1.00 15.74
C
ATOM 5536 C ILE C 200 8.280 40.245 -14.100 1.00 16.52
C
ATOM 5537 O ILE C 200 8.284 39.168 -13.505 1.00 15.20
O
ATOM 5538 CB ILE C 200 10.460 41.318 -13.442 1.00 16.14
C
ATOM 5539 CG1 ILE C 200 11.100 42.522 -12.738 1.00 15.26
C
ATOM 5540 CG2 ILE C 200 11.010 41.152 -14.861 1.00 16.45
C
ATOM 5541 CD1 ILE C 200 12.613 42.437 -12.586 1.00 18.39
C
ATOM 5542 H ILE C 200 8.964 41.543 -11.501 1.00 20.17
H
ATOM 5543 HA ILE C 200 8.713 42.249 -14.025 1.00 18.88
H
ATOM 5544 HB ILE C 200 10.673 40.519 -12.936 1.00 19.37
H
ATOM 5545 HG12 ILE C 200 10.900 43.322 -13.249 1.00 18.31
H
ATOM 5546 HG13 ILE C 200 10.719 42.600 -11.849 1.00 18.31
H
ATOM 5547 HG21 ILE C 200 11.974 41.051 -14.816 1.00 19.74
H
ATOM 5548 HG22 ILE C 200 10.613 40.363 -15.263 1.00 19.74
H
ATOM 5549 HG23 ILE C 200 10.784 41.939 -15.381 1.00 19.74
H
ATOM 5550 HD11 ILE C 200 12.930 43.234 -12.133 1.00 22.06
H
ATOM 5551 HD12 ILE C 200 12.834 41.650 -12.064 1.00 22.06
H
ATOM 5552 HD13 ILE C 200 13.016 42.374 -13.466 1.00 22.06
H
ATOM 5553 N GLU C 201 7.728 40.405 -15.302 1.00 15.15
N
ATOM 5554 CA GLU C 201 6.998 39.327 -15.966 1.00 17.24
C
ATOM 5555 C GLU C 201 7.281 39.288 -17.467 1.00 21.31
C
ATOM 5556 O GLU C 201 7.635 40.302 -18.076 1.00 15.67
O
ATOM 5557 CB GLU C 201 5.491 39.485 -15.712 1.00 17.25
C
ATOM 5558 CG GLU C 201 4.600 38.460 -16.405 1.00 20.61
C
ATOM 5559 CD GLU C 201 4.918 37.025 -16.012 1.00 24.32
C
ATOM 5560 OE1 GLU C 201 5.957 36.492 -16.457 1.00 24.36
O
ATOM 5561 OE2 GLU C 201 4.120 36.426 -15.262 1.00 26.94
O1-
ATOM 5562 H GLU C 201 7.763 41.134 -15.757 1.00 18.18
H
ATOM 5563 HA GLU C 201 7.277 38.479 -15.587 1.00 20.69
H
ATOM 5564 HB2 GLU C 201 5.330 39.412 -14.758 1.00 20.70
H
ATOM 11831 HG23 THR F 104 15.345 29.347 2.861 1.00 33.05
H

ATOM 11832 N VAL F 105 17.720 30.704 -1.118 1.00 21.71 N
ATOM 11833 CA VAL F 105 18.623 31.506 -1.936 1.00 19.03
C

ATOM 11834 C VAL F 105 18.462 31.235 -3.432 1.00 21.46 C
ATOM 11835 O VAL F 105 18.561 30.094 -3.889 1.00 20.83
O
ATOM 11836 CB VAL F 105 20.087 31.255 -1.536 1.00 26.65
C
ATOM 11837 CG1 VAL F 105 21.028 32.107 -2.377 1.00 28.48
C
ATOM 11838 CG2 VAL F 105 20.282 31.546 -0.051 1.00 23.67
C

ATOM 11839 H VAL F 105 17.965 29.885 -1.023 1.00 26.06 H
ATOM 11840 HA VAL F 105 18.430 32.445 -1.784 1.00 22.83
H
ATOM 11841 HB VAL F 105 20.304 30.322 -1.692 1.00 31.98
H
ATOM 11842 HG11 VAL F 105 21.942 31.930 -2.105 1.00 34.18
H
ATOM 11843 HG12 VAL F 105 20.910 31.879 -3.312 1.00 34.18
H
ATOM 11844 HG13 VAL F 105 20.816 33.043 -2.236 1.00 34.18
H
ATOM 11845 HG21 VAL F 105 21.209 31.382 0.183 1.00 28.41
H
ATOM 11846 HG22 VAL F 105 20.056 32.474 0.121 1.00 28.41
H
ATOM 11847 HG23 VAL F 105 19.703 30.963 0.464 1.00 28.41
H

ATOM 11848 N LYS F 106 18.229 32.302 -4.187 1.00 19.36 N
ATOM 11849 CA LYS F 106 18.092 32.220 -5.634 1.00 29.10
C

ATOM 11850 C LYS F 106 19.465 32.283 -6.295 1.00 29.24 C
ATOM 11851 O LYS F 106 20.302 33.093 -5.904 1.00 32.55
O
ATOM 11852 CB LYS F 106 17.203 33.358 -6.144 1.00 29.53
C
ATOM 11853 CG LYS F 106 17.008 33.392 -7.652 1.00 35.32
C
ATOM 11854 CD LYS F 106 16.478 34.740 -8.106 1.00 37.47
C
ATOM 11855 CE LYS F 106 16.168 34.747 -9.600 1.00 50.78
C
ATOM 11856 NZ LYS F 106 17.386 34.542 -10.437 1.00 52.11
N1+

ATOM 11857 H LYS F 106 18.145 33.100 -3.877 1.00 23.23 H
ATOM 11858 HA LYS F 106 17.676 31.377 -5.871 1.00 34.92
H
ATOM 11859 HB2 LYS F 106 16.327 33.272 -5.738 1.00 35.44
H
ATOM 11860 HB3 LYS F 106 17.602 34.203 -5.882 1.00 35.44
H
ATOM 11861 HG2 LYS F 106 17.859 33.236 -8.090 1.00 42.38
H
ATOM 11862 HG3 LYS F 106 16.367 32.710 -7.909 1.00 42.38
H
ATOM 11863 HD2 LYS F 106 15.660 34.941 -7.626 1.00 44.96
H
ATOM 11864 HD3 LYS F 106 17.145 35.422 -7.932 1.00 44.96

H
ATOM 5565 HB3 GLU C 201 5.218 40.364 -16.020 1.00 20.70
H
ATOM 5566 HG2 GLU C 201 3.676 38.637 -16.170 1.00 24.73
H
ATOM 5567 HG3 GLU C 201 4.718 38.540 -17.365 1.00 24.73
H
ATOM 5568 N ASN C 202 7.143 38.099 -18.050 1.00 18.71
N
ATOM 5569 CA ASN C 202 7.219 37.925 -19.497 1.00 20.17
C
ATOM 5570 C ASN C 202 6.078 38.663 -20.179 1.00 18.49
C
ATOM 5571 O ASN C 202 4.912 38.461 -19.844 1.00 16.77
O
ATOM 5572 CB ASN C 202 7.176 36.435 -19.857 1.00 23.56
C
ATOM 5573 CG ASN C 202 7.406 36.177 -21.341 1.00 23.40
C
ATOM 5574 OD1 ASN C 202 6.838 36.850 -22.202 1.00 21.30
O
ATOM 5575 ND2 ASN C 202 8.248 35.191 -21.643 1.00 23.28
N
ATOM 5576 H ASN C 202 7.002 37.368 -17.621 1.00 22.45
H
ATOM 5577 HA ASN C 202 8.056 38.292 -19.821 1.00 24.21
H
ATOM 5578 HB2 ASN C 202 7.869 35.971 -19.362 1.00 28.27
H
ATOM 5579 HB3 ASN C 202 6.305 36.079 -19.623 1.00 28.27
H
ATOM 5580 HD21 ASN C 202 8.413 35.004 -22.466 1.00 27.94
H
ATOM 5581 HD22 ASN C 202 8.626 34.741 -21.015 1.00 27.94
H
ATOM 5582 N CYS C 203 6.418 39.501 -21.153 1.00 15.62
N
ATOM 5583 CA CYS C 203 5.443 40.379 -21.787 1.00 17.19
C
ATOM 5584 C CYS C 203 4.362 39.611 -22.551 1.00 21.25
C
ATOM 5585 O CYS C 203 3.338 40.187 -22.922 1.00 19.77
O
ATOM 5586 CB CYS C 203 6.159 41.353 -22.727 1.00 20.68
C
ATOM 5587 SG CYS C 203 7.423 42.375 -21.911 1.00 23.41
S
ATOM 5588 H CYS C 203 7.215 39.580 -21.467 1.00 18.74
H
ATOM 5589 HA CYS C 203 5.003 40.902 -21.099 1.00 20.63
H
ATOM 5590 HB2 CYS C 203 6.596 40.846 -23.428 1.00 24.82
H
ATOM 5591 HB3 CYS C 203 5.501 41.951 -23.115 1.00 24.82
H
ATOM 5592 N SER C 204 4.585 38.317 -22.774 1.00 16.75
N
ATOM 5593 CA SER C 204 3.614 37.469 -23.470 1.00 19.18
C
ATOM 5594 C SER C 204 2.544 36.908 -22.539 1.00 19.81
C
ATOM 5595 O SER C 204 1.558 36.328 -22.991 1.00 19.37
O
ATOM 5596 CB SER C 204 4.327 36.306 -24.161 1.00 22.12
C
ATOM 5597 OG SER C 204 5.221 36.785 -25.144 1.00 22.09
O
ATOM 5598 H SER C 204 5.297 37.901 -22.530 1.00 20.11
H
ATOM 11865 HE2 LYS F 106 15.544 34.031 -9.797 1.00 60.93
H
ATOM 11866 HE3 LYS F 106 15.779 35.603 -9.839 1.00 60.93
H
ATOM 11867 HZ1 LYS F 106 17.166 34.552 -11.300 1.00 62.53
H
ATOM 11868 HZ2 LYS F 106 17.975 35.191 -10.281 1.00 62.53
H
ATOM 11869 HZ3 LYS F 106 17.760 33.758 -10.243 1.00 62.53
H
ATOM 11870 N THR F 107 19.691 31.424 -7.287 1.00 31.35
N
ATOM 11871 CA THR F 107 20.912 31.469 -8.090 1.00 36.12
C
ATOM 11872 C THR F 107 20.608 32.090 -9.449 1.00 43.02
C
ATOM 11873 O THR F 107 19.463 32.429 -9.740 1.00 33.93
O
ATOM 11874 CB THR F 107 21.524 30.071 -8.287 1.00 39.11
C
ATOM 11875 OG1 THR F 107 20.604 29.231 -8.994 1.00 41.98
O
ATOM 11876 CG2 THR F 107 21.855 29.442 -6.942 1.00 37.13
C
ATOM 11877 H THR F 107 19.147 30.798 -7.517 1.00 37.62
H
ATOM 11878 HA THR F 107 21.567 32.026 -7.642 1.00 43.34
H
ATOM 11879 HB THR F 107 22.345 30.149 -8.797 1.00 46.93
H
ATOM 11880 HG1 THR F 107 20.936 28.468 -9.103 1.00 50.37
H
ATOM 11881 HG21 THR F 107 22.240 28.562 -7.073 1.00 44.55
H
ATOM 11882 HG22 THR F 107 22.491 29.997 -6.464 1.00 44.55
H
ATOM 11883 HG23 THR F 107 21.048 29.357 -6.409 1.00 44.55
H
ATOM 11884 N GLN F 108 21.632 32.231 -10.284 1.00 47.01
N
ATOM 11885 CA GLN F 108 21.497 32.983 -11.527 1.00 54.07
C
ATOM 11886 C GLN F 108 20.864 32.173 -12.657 1.00 53.72
C
ATOM 11887 O GLN F 108 20.083 32.708 -13.446 1.00 54.72
O
ATOM 11888 CB GLN F 108 22.867 33.498 -11.976 1.00 67.40
C
ATOM 11889 CG GLN F 108 23.526 34.461 -10.992 1.00 74.36
C
ATOM 11890 CD GLN F 108 22.732 35.740 -10.791 1.00 78.47
C
ATOM 11891 OE1 GLN F 108 21.891 36.101 -11.615 1.00 79.85
O
ATOM 11892 NE2 GLN F 108 22.997 36.433 -9.688 1.00 78.07
N
ATOM 11893 H GLN F 108 22.415 31.902 -10.154 1.00 56.42
H
ATOM 11894 HA GLN F 108 20.930 33.753 -11.364 1.00 64.88
H
ATOM 11895 HB2 GLN F 108 23.462 32.741 -12.091 1.00 80.88
H
ATOM 11896 HB3 GLN F 108 22.763 33.965 -12.820 1.00 80.88
H
ATOM 11897 HG2 GLN F 108 23.610 34.022 -10.130 1.00 89.23
H
ATOM 11898 HG3 GLN F 108 24.403 34.703 -11.327 1.00 89.23

H
ATOM 5599 HA SER C 204 3.169 37.996 -24.152 1.00 23.02
H
ATOM 5600 HB2 SER C 204 4.825 35.802 -23.499 1.00 26.54
H
ATOM 5601 HB3 SER C 204 3.666 35.737 -24.585 1.00 26.54
H
ATOM 5602 HG SER C 204 5.799 37.281 -24.789 1.00 26.51
H
ATOM 5603 N THR C 205 2.747 37.067 -21.237 1.00 15.82
N
ATOM 5604 CA THR C 205 1.848 36.478 -20.254 1.00 17.27
C
ATOM 5605 C THR C 205 0.512 37.224 -20.200 1.00 23.16
C
ATOM 5606 O THR C 205 0.486 38.427 -19.927 1.00 18.56
O
ATOM 5607 CB THR C 205 2.486 36.480 -18.855 1.00 20.49
C
ATOM 5608 OG1 THR C 205 3.798 35.907 -18.927 1.00 19.75
O
ATOM 5609 CG2 THR C 205 1.643 35.677 -17.877 1.00 22.93
C
ATOM 5610 H THR C 205 3.399 37.513 -20.897 1.00 18.99
H
ATOM 5611 HA THR C 205 1.669 35.557 -20.501 1.00 20.72
H
ATOM 5612 HB THR C 205 2.549 37.392 -18.530 1.00 24.58
H
ATOM 5613 HG1 THR C 205 3.751 35.117 -19.208 1.00 23.70
H
ATOM 5614 HG21 THR C 205 2.055 35.686 -16.999 1.00 27.51
H
ATOM 5615 HG22 THR C 205 0.754 36.061 -17.812 1.00 27.51
H
ATOM 5616 HG23 THR C 205 1.568 34.759 -18.181 1.00 27.51
H
ATOM 5617 N PRO C 206 -0.604 36.517 -20.459 1.00 17.76
N
ATOM 5618 CA PRO C 206 -1.898 37.193 -20.323 1.00 19.80
C
ATOM 5619 C PRO C 206 -2.147 37.676 -18.898 1.00 20.72
C
ATOM 5620 O PRO C 206 -1.969 36.923 -17.940 1.00 18.27
O
ATOM 5621 CB PRO C 206 -2.913 36.112 -20.718 1.00 22.87
C
ATOM 5622 CG PRO C 206 -2.139 35.122 -21.513 1.00 28.25
C
ATOM 5623 CD PRO C 206 -0.760 35.128 -20.926 1.00 20.21
C
ATOM 5624 HA PRO C 206 -1.960 37.941 -20.939 1.00 23.76
H
ATOM 5625 HB2 PRO C 206 -3.278 35.700 -19.919 1.00 27.44
H
ATOM 5626 HB3 PRO C 206 -3.618 36.506 -21.255 1.00 27.44
H
ATOM 5627 HG2 PRO C 206 -2.544 34.245 -21.425 1.00 33.91
H
ATOM 5628 HG3 PRO C 206 -2.116 35.397 -22.443 1.00 33.91
H
ATOM 5629 HD2 PRO C 206 -0.707 34.511 -20.180 1.00 24.25
H
ATOM 5630 HD3 PRO C 206 -0.101 34.923 -21.608 1.00 24.25
H
ATOM 5631 N ASN C 207 -2.542 38.936 -18.774 1.00 19.76
N
ATOM 5632 CA ASN C 207 -2.912 39.512 -17.490 1.00 19.32
H
ATOM 11899 HE21 GLN F 108 22.575 37.165 -9.529 1.00 93.69
H
ATOM 11900 HE22 GLN F 108 23.591 36.149 -9.135 1.00 93.69
H
ATOM 11901 N GLU F 109 21.200 30.890 -12.737 1.00 54.38
N
ATOM 11902 CA GLU F 109 20.771 30.063 -13.861 1.00 55.52
C
ATOM 11903 C GLU F 109 19.268 29.776 -13.827 1.00 49.42
C
ATOM 11904 O GLU F 109 18.635 29.804 -12.770 1.00 41.41
O
ATOM 11905 CB GLU F 109 21.559 28.746 -13.896 1.00 59.16
C
ATOM 11906 CG GLU F 109 21.309 27.793 -12.727 1.00 62.14
C
ATOM 11907 CD GLU F 109 22.090 28.152 -11.473 1.00 66.16
C
ATOM 11908 OE1 GLU F 109 22.681 29.252 -11.421 1.00 64.71
O
ATOM 11909 OE2 GLU F 109 22.112 27.325 -10.536 1.00 67.28
O1-
ATOM 11910 H GLU F 109 21.676 30.474 -12.154 1.00 65.26
H
ATOM 11911 HA GLU F 109 20.960 30.540 -14.685 1.00 66.62
H
ATOM 11912 HB2 GLU F 109 21.328 28.272 -14.711 1.00 70.99
H
ATOM 11913 HB3 GLU F 109 22.506 28.955 -13.902 1.00 70.99
H
ATOM 11914 HG2 GLU F 109 20.365 27.812 -12.505 1.00 74.57
H
ATOM 11915 HG3 GLU F 109 21.567 26.897 -12.992 1.00 74.57
H
ATOM 11916 N ALA F 110 18.709 29.500 -15.002 1.00 43.62
N
ATOM 11917 CA ALA F 110 17.279 29.251 -15.145 1.00 41.53
C
ATOM 11918 C ALA F 110 16.936 27.807 -14.800 1.00 41.29
C
ATOM 11919 O ALA F 110 17.257 26.886 -15.551 1.00 39.37
O
ATOM 11920 CB ALA F 110 16.829 29.575 -16.559 1.00 42.06
C
ATOM 11921 H ALA F 110 19.144 29.450 -15.742 1.00 52.34
H
ATOM 11922 HA ALA F 110 16.795 29.829 -14.535 1.00 49.84
H
ATOM 11923 HB1 ALA F 110 15.877 29.403 -16.634 1.00 50.48
H
ATOM 11924 HB2 ALA F 110 17.012 30.510 -16.742 1.00 50.48
H
ATOM 11925 HB3 ALA F 110 17.317 29.014 -17.182 1.00 50.48
H
ATOM 11926 N THR F 111 16.278 27.623 -13.659 1.00 31.19
N
ATOM 11927 CA THR F 111 15.901 26.300 -13.185 1.00 28.12
C
ATOM 11928 C THR F 111 14.513 26.335 -12.563 1.00 26.09
C
ATOM 11929 O THR F 111 14.038 27.391 -12.146 1.00 23.00
O
ATOM 11930 CB THR F 111 16.895 25.766 -12.140 1.00 31.61
C
ATOM 11931 OG1 THR F 111 16.881 26.618 -10.986 1.00 23.43
O
ATOM 11932 CG2 THR F 111 18.309 25.704 -12.718 1.00 34.93

C
ATOM 5633 C ASN C 207 -3.985 40.567 -17.689 1.00 19.48
C
ATOM 5634 O ASN C 207 -4.119 41.121 -18.782 1.00 15.57
O
ATOM 5635 CB ASN C 207 -1.701 40.140 -16.796 1.00 18.33
C
ATOM 5636 CG ASN C 207 -0.820 39.120 -16.109 1.00 16.71
C
ATOM 5637 OD1 ASN C 207 -1.106 38.690 -14.991 1.00 18.99
O
ATOM 5638 ND2 ASN C 207 0.266 38.735 -16.768 1.00 18.70
N
ATOM 5639 H ASN C 207 -2.604 39.487 -19.431 1.00 23.72
H
ATOM 5640 HA ASN C 207 -3.268 38.816 -16.915 1.00 23.19
H
ATOM 5641 HB2 ASN C 207 -1.163 40.603 -17.457 1.00 21.99
H
ATOM 5642 HB3 ASN C 207 -2.013 40.767 -16.124 1.00 21.99
H
ATOM 5643 HD21 ASN C 207 0.799 38.157 -16.420 1.00 22.44
H
ATOM 5644 HD22 ASN C 207 0.437 39.064 -17.544 1.00 22.44
H
ATOM 5645 N THR C 208 -4.742 40.847 -16.634 1.00 16.68
N
ATOM 5646 CA THR C 208 -5.613 42.012 -16.630 1.00 15.95
C
ATOM 5647 C THR C 208 -4.721 43.246 -16.681 1.00 17.24
C
ATOM 5648 O THR C 208 -3.514 43.148 -16.471 1.00 15.69
O
ATOM 5649 CB THR C 208 -6.522 42.041 -15.393 1.00 19.27
C
ATOM 5650 OG1 THR C 208 -5.725 42.005 -14.204 1.00 15.59
O
ATOM 5651 CG2 THR C 208 -7.471 40.844 -15.408 1.00 21.85
C
ATOM 5652 H THR C 208 -4.770 40.380 -15.912 1.00 20.02
H
ATOM 5653 HA THR C 208 -6.172 42.003 -17.423 1.00 19.14
H
ATOM 5654 HB THR C 208 -7.053 42.853 -15.402 1.00 23.12
H
ATOM 5655 HG1 THR C 208 -6.220 42.021 -13.525 1.00 18.71
H
ATOM 5656 HG21 THR C 208 -8.044 40.866 -14.625 1.00 26.22
H
ATOM 5657 HG22 THR C 208 -8.025 40.869 -16.204 1.00 26.22
H
ATOM 5658 HG23 THR C 208 -6.963 40.018 -15.403 1.00 26.22
H
ATOM 5659 N TYR C 209 -5.292 44.405 -16.979 1.00 16.72
N
ATOM 5660 CA TYR C 209 -4.470 45.597 -17.141 1.00 13.53
C
ATOM 5661 C TYR C 209 -5.203 46.876 -16.759 1.00 14.40
C
ATOM 5662 O TYR C 209 -6.437 46.914 -16.687 1.00 12.53
O
ATOM 5663 CB TYR C 209 -3.958 45.689 -18.585 1.00 14.96
C
ATOM 5664 CG TYR C 209 -5.040 45.726 -19.649 1.00 18.50
C
ATOM 5665 CD1 TYR C 209 -5.741 44.580 -19.996 1.00 19.53
C
ATOM 5666 CD2 TYR C 209 -5.343 46.907 -20.318 1.00 14.68
C
ATOM 11933 H THR F 111 16.036 28.261 -13.136 1.00 37.43
H
ATOM 11934 HA THR F 111 15.885 25.683 -13.933 1.00 33.75
H
ATOM 11935 HB THR F 111 16.634 24.869 -11.879 1.00 37.94
H
ATOM 11936 HG1 THR F 111 17.422 26.332 -10.411 1.00 28.12
H
ATOM 11937 HG21 THR F 111 18.925 25.366 -12.050 1.00 41.92
H
ATOM 11938 HG22 THR F 111 18.326 25.115 -13.489 1.00 41.92
H
ATOM 11939 HG23 THR F 111 18.594 26.590 -12.992 1.00 41.92
H
ATOM 11940 N ASN F 112 13.867 25.178 -12.499 1.00 21.68
N
ATOM 11941 CA ASN F 112 12.586 25.072 -11.820 1.00 22.81
C
ATOM 11942 C ASN F 112 12.736 25.457 -10.350 1.00 22.60
C
ATOM 11943 O ASN F 112 11.832 26.046 -9.758 1.00 18.34
O
ATOM 11944 CB ASN F 112 12.023 23.655 -11.945 1.00 25.23
C
ATOM 11945 CG ASN F 112 11.577 23.326 -13.359 1.00 30.83
C
ATOM 11946 OD1 ASN F 112 11.337 24.221 -14.171 1.00 29.96
O
ATOM 11947 ND2 ASN F 112 11.458 22.038 -13.658 1.00 31.13
N
ATOM 11948 H ASN F 112 14.149 24.441 -12.841 1.00 26.01
H
ATOM 11949 HA ASN F 112 11.956 25.685 -12.230 1.00 27.37
H
ATOM 11950 HB2 ASN F 112 12.709 23.019 -11.691 1.00 30.28
H
ATOM 11951 HB3 ASN F 112 11.255 23.567 -11.360 1.00 30.28
H
ATOM 11952 HD21 ASN F 112 11.209 21.801 -14.446 1.00 37.36
H
ATOM 11953 HD22 ASN F 112 11.631 21.441 -13.063 1.00 37.36
H

ATOM 11954 N LYS F 113 13.890 25.129 -9.774 1.00 18.06 N
ATOM 11955 CA LYS F 113 14.159 25.425 -8.374 1.00 17.23
C

ATOM 11956 C LYS F 113 14.117 26.924 -8.124 1.00 15.57 C
ATOM 11957 O LYS F 113 13.505 27.381 -7.160 1.00 20.36
O
ATOM 11958 CB LYS F 113 15.518 24.858 -7.957 1.00 22.25
C
ATOM 11959 CG LYS F 113 15.804 24.952 -6.465 1.00 19.36
C
ATOM 11960 CD LYS F 113 17.161 24.356 -6.130 1.00 25.27
C
ATOM 11961 CE LYS F 113 17.450 24.430 -4.645 1.00 23.84
C
ATOM 11962 NZ LYS F 113 18.808 23.913 -4.317 1.00 30.60
N1+
ATOM 11963 H LYS F 113 14.537 24.732 -10.178 1.00 21.67
H
ATOM 11964 HA LYS F 113 13.477 25.009 -7.824 1.00 20.67
H
ATOM 11965 HB2 LYS F 113 15.553 23.921 -8.206 1.00 26.70
H
ATOM 11966 HB3 LYS F 113 16.215 25.346 -8.422 1.00 26.70

C
ATOM 5667 CE1 TYR C 209 -6.723 44.609 -20.970 1.00 19.93
C
ATOM 5668 CE2 TYR C 209 -6.317 46.947 -21.291 1.00 21.82
C
ATOM 5669 CZ TYR C 209 -7.005 45.797 -21.615 1.00 26.03
C
ATOM 5670 OH TYR C 209 -7.976 45.843 -22.585 1.00 20.92
O
ATOM 5671 H TYR C 209 -6.136 44.528 -17.090 1.00 20.07
H
ATOM 5672 HA TYR C 209 -3.696 45.520 -16.561 1.00 16.23
H
ATOM 5673 HB2 TYR C 209 -3.432 46.500 -18.675 1.00 17.95
H
ATOM 5674 HB3 TYR C 209 -3.399 44.917 -18.764 1.00 17.95
H
ATOM 5675 HD1 TYR C 209 -5.551 43.780 -19.562 1.00 23.43
H
ATOM 5676 HD2 TYR C 209 -4.881 47.685 -20.102 1.00 17.62
H
ATOM 5677 HE1 TYR C 209 -7.187 43.834 -21.191 1.00 23.92
H
ATOM 5678 HE2 TYR C 209 -6.511 47.745 -21.727 1.00 26.18
H
ATOM 5679 HH TYR C 209 -8.317 45.082 -22.686 1.00 25.10
H
ATOM 5680 N ILE C 210 -4.411 47.914 -16.502 1.00 12.10
N
ATOM 5681 CA ILE C 210 -4.920 49.213 -16.091 1.00 14.56
C
ATOM 5682 C ILE C 210 -4.546 50.283 -17.113 1.00 16.31
C
ATOM 5683 O ILE C 210 -3.369 50.482 -17.419 1.00 14.03
O
ATOM 5684 CB ILE C 210 -4.370 49.618 -14.707 1.00 15.33
C
ATOM 5685 CG1 ILE C 210 -4.746 48.564 -13.661 1.00 15.55
C
ATOM 5686 CG2 ILE C 210 -4.904 50.989 -14.300 1.00 16.97
C
ATOM 5687 CD1 ILE C 210 -4.066 48.749 -12.314 1.00 17.10
C
ATOM 5688 H ILE C 210 -3.554 47.886 -16.562 1.00 14.52
H
ATOM 5689 HA ILE C 210 -5.887 49.174 -16.033 1.00 17.47
H
ATOM 5690 HB ILE C 210 -3.403 49.667 -14.761 1.00 18.39
H
ATOM 5691 HG12 ILE C 210 -5.704 48.599 -13.515 1.00 18.66
H
ATOM 5692 HG13 ILE C 210 -4.498 47.689 -13.998 1.00 18.66
H
ATOM 5693 HG21 ILE C 210 -4.546 51.222 -13.429 1.00 20.36
H
ATOM 5694 HG22 ILE C 210 -4.625 51.645 -14.958 1.00 20.36
H
ATOM 5695 HG23 ILE C 210 -5.873 50.951 -14.260 1.00 20.36
H
ATOM 5696 HD11 ILE C 210 -4.357 48.045 -11.714 1.00 20.51
H
ATOM 5697 HD12 ILE C 210 -3.105 48.704 -12.437 1.00 20.51
H
ATOM 5698 HD13 ILE C 210 -4.313 49.615 -11.953 1.00 20.51
H
ATOM 5699 N CYS C 211 -5.558 50.963 -17.639 1.00 16.07
N
ATOM 5700 CA CYS C 211 -5.348 52.082 -18.544 1.00 16.50
H
ATOM 11967 HG2 LYS F 113 15.804 25.883 -6.196 1.00 23.23
H
ATOM 11968 HG3 LYS F 113 15.125 24.459 -5.977 1.00 23.23
H
ATOM 11969 HD2 LYS F 113 17.177 23.424 -6.397 1.00 30.32
H
ATOM 11970 HD3 LYS F 113 17.852 24.851 -6.599 1.00 30.32
H
ATOM 11971 HE2 LYS F 113 17.401 25.355 -4.356 1.00 28.61
H
ATOM 11972 HE3 LYS F 113 16.798 23.895 -4.166 1.00 28.61
H
ATOM 11973 HZ1 LYS F 113 18.878 23.062 -4.568 1.00 36.72
H
ATOM 11974 HZ2 LYS F 113 19.427 24.392 -4.741 1.00 36.72
H
ATOM 11975 HZ3 LYS F 113 18.951 23.968 -3.440 1.00 36.72
H
ATOM 11976 N ASN F 114 14.770 27.687 -8.994 1.00 15.69
N
ATOM 11977 CA ASN F 114 14.793 29.140 -8.867 1.00 19.32
C
ATOM 11978 C ASN F 114 13.446 29.792 -9.159 1.00 20.12
C
ATOM 11979 O ASN F 114 13.054 30.750 -8.496 1.00 17.64
O
ATOM 11980 CB ASN F 114 15.845 29.734 -9.800 1.00 23.98
C
ATOM 11981 CG ASN F 114 17.251 29.576 -9.266 1.00 26.05
C
ATOM 11982 OD1 ASN F 114 17.485 29.674 -8.060 1.00 23.54
O
ATOM 11983 ND2 ASN F 114 18.198 29.334 -10.163 1.00 28.63
N
ATOM 11984 H ASN F 114 15.208 27.387 -9.670 1.00 18.83
H
ATOM 11985 HA ASN F 114 15.041 29.369 -7.958 1.00 23.19
H
ATOM 11986 HB2 ASN F 114 15.798 29.283 -10.658 1.00 28.78
H
ATOM 11987 HB3 ASN F 114 15.671 30.681 -9.912 1.00 28.78
H
ATOM 11988 HD21 ASN F 114 19.015 29.237 -9.910 1.00 34.35
H
ATOM 11989 HD22 ASN F 114 17.996 29.275 -10.997 1.00 34.35
H
ATOM 11990 N MET F 115 12.749 29.282 -10.164 1.00 18.73
N
ATOM 11991 CA MET F 115 11.481 29.867 -10.572 1.00 22.34
C
ATOM 11992 C MET F 115 10.409 29.580 -9.524 1.00 17.47
C
ATOM 11993 O MET F 115 9.539 30.411 -9.270 1.00 19.13 O
ATOM 11994 CB MET F 115 11.063 29.327 -11.943 1.00 24.76
C
ATOM 11995 CG MET F 115 12.071 29.623 -13.060 1.00 34.49
C
ATOM 11996 SD MET F 115 11.705 28.781 -14.614 1.00 53.25
S
ATOM 11997 CE MET F 115 10.474 29.881 -15.303 1.00 35.96
C
ATOM 11998 H MET F 115 12.988 28.598 -10.627 1.00 22.48
H
ATOM 11999 HA MET F 115 11.591 30.827 -10.652 1.00 26.81
H
ATOM 12000 HB2 MET F 115 10.962 28.365 -11.883 1.00 29.71

C
ATOM 5701 C CYS C 211 -5.448 53.379 -17.768 1.00 16.84
C
ATOM 5702 O CYS C 211 -6.188 53.471 -16.787 1.00 17.47
O
ATOM 5703 CB CYS C 211 -6.366 52.068 -19.685 1.00 24.73
C
ATOM 5704 SG CYS C 211 -6.116 50.730 -20.874 1.00 30.48
S
ATOM 5705 H CYS C 211 -6.386 50.791 -17.484 1.00 19.28
H
ATOM 5706 HA CYS C 211 -4.459 52.023 -18.927 1.00 19.81
H
ATOM 5707 HB2 CYS C 211 -7.255 51.969 -19.310 1.00 29.68
H
ATOM 5708 HB3 CYS C 211 -6.305 52.908 -20.167 1.00 29.68
H
ATOM 5709 N MET C 212 -4.706 54.380 -18.222 1.00 19.38
N
ATOM 5710 CA MET C 212 -4.653 55.668 -17.551 1.00 17.22
C
ATOM 5711 C MET C 212 -4.669 56.802 -18.563 1.00 21.46
C
ATOM 5712 O MET C 212 -4.066 56.699 -19.634 1.00 19.72
O
ATOM 5713 CB MET C 212 -3.402 55.756 -16.681 1.00 17.06
C
ATOM 5714 CG MET C 212 -3.232 57.075 -15.955 1.00 20.46
C
ATOM 5715 SD MET C 212 -1.732 57.072 -14.950 1.00 22.92
S
ATOM 5716 CE MET C 212 -1.636 58.792 -14.465 1.00 27.66
C
ATOM 5717 H MET C 212 -4.217 54.337 -18.928 1.00 23.26
H
ATOM 5718 HA MET C 212 -5.426 55.752 -16.971 1.00 20.66
H
ATOM 5719 HB2 MET C 212 -3.439 55.054 -16.013 1.00 20.47
H
ATOM 5720 HB3 MET C 212 -2.623 55.628 -17.245 1.00 20.47
H
ATOM 5721 HG2 MET C 212 -3.164 57.793 -16.603 1.00 24.55
H
ATOM 5722 HG3 MET C 212 -3.992 57.220 -15.369 1.00 24.55
H
ATOM 5723 HE1 MET C 212 -1.569 59.341 -15.262 1.00 33.19
H
ATOM 5724 HE2 MET C 212 -2.436 59.025 -13.968 1.00 33.19
H
ATOM 5725 HE3 MET C 212 -0.852 58.919 -13.908 1.00 33.19
H
ATOM 5726 N GLN C 213 -5.370 57.878 -18.219 1.00 17.77
N
ATOM 5727 CA GLN C 213 -5.404 59.079 -19.048 1.00 25.12
C
ATOM 5728 C GLN C 213 -5.400 60.318 -18.160 1.00 26.47
C
ATOM 5729 O GLN C 213 -6.282 60.489 -17.319 1.00 26.02
O
ATOM 5730 CB GLN C 213 -6.639 59.080 -19.953 1.00 26.62
C
ATOM 5731 CG GLN C 213 -6.655 60.187 -20.999 1.00 29.95
C
ATOM 5732 CD GLN C 213 -8.002 60.315 -21.689 1.00 32.31
C
ATOM 5733 OE1 GLN C 213 -8.926 60.930 -21.157 1.00 30.11
O
ATOM 5734 NE2 GLN C 213 -8.121 59.727 -22.874 1.00 31.23
H
ATOM 12001 HB3 MET F 115 10.217 29.732 -12.193 1.00 29.71
H
ATOM 12002 HG2 MET F 115 12.074 30.578 -13.234 1.00 41.38
H
ATOM 12003 HG3 MET F 115 12.952 29.340 -12.769 1.00 41.38
H
ATOM 12004 HE1 MET F 115 10.187 29.534 -16.162 1.00 43.15
H
ATOM 12005 HE2 MET F 115 9.719 29.930 -14.696 1.00 43.15
H
ATOM 12006 HE3 MET F 115 10.866 30.762 -15.416 1.00 43.15
H
ATOM 12007 N TRP F 116 10.477 28.397 -8.921 1.00 15.95
N
ATOM 12008 CA TRP F 116 9.571 28.024 -7.839 1.00 16.43
C
ATOM 12009 C TRP F 116 9.757 28.966 -6.659 1.00 17.46 C
ATOM 12010 O TRP F 116 8.794 29.369 -6.003 1.00 13.97 O
ATOM 12011 CB TRP F 116 9.830 26.579 -7.413 1.00 17.21
C
ATOM 12012 CG TRP F 116 8.910 26.053 -6.352 1.00 14.30
C
ATOM 12013 CD1 TRP F 116 9.177 25.930 -5.020 1.00 16.57
C
ATOM 12014 CD2 TRP F 116 7.579 25.557 -6.541 1.00 14.31
C
ATOM 12015 NE1 TRP F 116 8.094 25.392 -4.366 1.00 15.96
N
ATOM 12016 CE2 TRP F 116 7.098 25.158 -5.277 1.00 14.58
C
ATOM 12017 CE3 TRP F 116 6.746 25.414 -7.655 1.00 14.42
C
ATOM 12018 CZ2 TRP F 116 5.824 24.620 -5.099 1.00 17.85
C
ATOM 12019 CZ3 TRP F 116 5.477 24.887 -7.475 1.00 12.40
C
ATOM 12020 CH2 TRP F 116 5.031 24.492 -6.209 1.00 14.26
C
ATOM 12021 H TRP F 116 11.046 27.785 -9.124 1.00 19.15
H
ATOM 12022 HA TRP F 116 8.654 28.094 -8.146 1.00 19.71
H
ATOM 12023 HB2 TRP F 116 9.735 26.007 -8.191 1.00 20.66
H
ATOM 12024 HB3 TRP F 116 10.736 26.515 -7.071 1.00 20.66
H
ATOM 12025 HD1 TRP F 116 9.977 26.174 -4.613 1.00 19.88
H
ATOM 12026 HE1 TRP F 116 8.047 25.233 -3.522 1.00 19.16
H
ATOM 12027 HE3 TRP F 116 7.037 25.670 -8.501 1.00 17.30
H
ATOM 12028 HZ2 TRP F 116 5.522 24.363 -4.257 1.00 21.42
H
ATOM 12029 HZ3 TRP F 116 4.915 24.787 -8.210 1.00 14.88
H
ATOM 12030 HH2 TRP F 116 4.174 24.144 -6.117 1.00 17.11
H
ATOM 12031 N LEU F 117 11.014 29.315 -6.407 1.00 18.59 N
ATOM 12032 CA LEU F 117 11.380 30.189 -5.300 1.00 17.51
C
ATOM 12033 C LEU F 117 10.905 31.619 -5.506 1.00 16.16 C
ATOM 12034 O LEU F 117 10.428 32.268 -4.571 1.00 15.98

N
ATOM 5735 H GLN C 213 -5.840 57.938 -17.502 1.00 21.33
H
ATOM 5736 HA GLN C 213 -4.614 59.103 -19.610 1.00 30.14
H
ATOM 5737 HB2 GLN C 213 -6.682 58.232 -20.421 1.00 31.94
H
ATOM 5738 HB3 GLN C 213 -7.429 59.188 -19.400 1.00 31.94
H
ATOM 5739 HG2 GLN C 213 -6.456 61.033 -20.568 1.00 35.94
H
ATOM 5740 HG3 GLN C 213 -5.987 59.993 -21.676 1.00 35.94
H
ATOM 5741 HE21 GLN C 213 -7.455 59.302 -23.213 1.00 37.48
H
ATOM 5742 HE22 GLN C 213 -8.865 59.772 -23.304 1.00 37.48
H
ATOM 5743 N ARG C 214 -4.398 61.171 -18.344 1.00 27.50
N
ATOM 5744 CA ARG C 214 -4.329 62.438 -17.626 1.00 31.88
C
ATOM 5745 C ARG C 214 -5.318 63.436 -18.229 1.00 33.93
C
ATOM 5746 O ARG C 214 -5.446 63.533 -19.451 1.00 35.59
O
ATOM 5747 CB ARG C 214 -2.905 62.994 -17.664 1.00 40.82
C
ATOM 5748 CG ARG C 214 -1.878 62.073 -17.022 1.00 40.28
C
ATOM 5749 CD ARG C 214 -0.473 62.643 -17.093 1.00 53.54
C
ATOM 5750 NE ARG C 214 -0.373 63.945 -16.438 1.00 62.54
N
ATOM 5751 CZ ARG C 214 -0.186 64.121 -15.133 1.00 62.56
C
ATOM 5752 NH1 ARG C 214 -0.083 63.078 -14.320 1.00 49.80
N1+
ATOM 5753 NH2 ARG C 214 -0.106 65.349 -14.635 1.00 61.54
N
ATOM 5754 H ARG C 214 -3.741 61.038 -18.883 1.00 33.00
H
ATOM 5755 HA ARG C 214 -4.573 62.293 -16.699 1.00 38.26
H
ATOM 5756 HB2 ARG C 214 -2.647 63.131 -18.588 1.00 48.98
H
ATOM 5757 HB3 ARG C 214 -2.886 63.839 -17.187 1.00 48.98
H
ATOM 5758 HG2 ARG C 214 -2.104 61.945 -16.088 1.00 48.33
H
ATOM 5759 HG3 ARG C 214 -1.881 61.221 -17.487 1.00 48.33
H
ATOM 5760 HD2 ARG C 214 0.140 62.035 -16.651 1.00 64.25
H
ATOM 5761 HD3 ARG C 214 -0.221 62.753 -18.024 1.00 64.25
H
ATOM 5762 HE ARG C 214 -0.440 64.647 -16.931 1.00 75.04
H
ATOM 5763 HH11 ARG C 214 -0.133 62.279 -14.636 1.00 59.76
H
ATOM 5764 HH12 ARG C 214 0.037 63.199 -13.477 1.00 59.76
H
ATOM 5765 HH21 ARG C 214 -0.174 66.030 -15.157 1.00 73.85
H
ATOM 5766 HH22 ARG C 214 0.012 65.465 -13.791 1.00 73.85
H
ATOM 5767 N THR C 215 -6.025 64.167 -17.372 1.00 36.74
N
ATOM 5768 CA THR C 215 -7.027 65.127 -17.832 1.00 41.57
O
ATOM 12035 CB LEU F 117 12.897 30.180 -5.108 1.00 17.18
C
ATOM 12036 CG LEU F 117 13.448 31.119 -4.034 1.00 17.88
C
ATOM 12037 CD1 LEU F 117 12.913 30.744 -2.657 1.00 21.03
C
ATOM 12038 CD2 LEU F 117 14.966 31.092 -4.048 1.00 24.18
C
ATOM 12039 H LEU F 117 11.687 29.052 -6.874 1.00 22.30 H
ATOM 12040 HA LEU F 117 10.973 29.853 -4.486 1.00 21.01
H
ATOM 12041 HB2 LEU F 117 13.169 29.280 -4.870 1.00 20.62
H
ATOM 12042 HB3 LEU F 117 13.311 30.430 -5.948 1.00 20.62
H
ATOM 12043 HG LEU F 117 13.163 32.025 -4.230 1.00 21.45
H
ATOM 12044 HD11 LEU F 117 13.279 31.355 -1.999 1.00 25.23
H
ATOM 12045 HD12 LEU F 117 11.945 30.809 -2.666 1.00 25.23
H
ATOM 12046 HD13 LEU F 117 13.182 29.835 -2.450 1.00 25.23
H
ATOM 12047 HD21 LEU F 117 15.298 31.692 -3.362 1.00 29.02
H
ATOM 12048 HD22 LEU F 117 15.266 30.187 -3.871 1.00 29.02
H
ATOM 12049 HD23 LEU F 117 15.278 31.380 -4.920 1.00 29.02
H
ATOM 12050 N THR F 118 11.042 32.121 -6.726 1.00 13.53
N
ATOM 12051 CA THR F 118 10.730 33.519 -6.985 1.00 18.81
C
ATOM 12052 C THR F 118 9.255 33.762 -7.325 1.00 16.55 C
ATOM 12053 O THR F 118 8.828 34.914 -7.373 1.00 17.08 O
ATOM 12054 CB THR F 118 11.598 34.082 -8.133 1.00 20.28
C
ATOM 12055 OG1 THR F 118 11.412 33.302 -9.320 1.00 22.13
O
ATOM 12056 CG2 THR F 118 13.070 34.063 -7.747 1.00 26.66
C
ATOM 12057 H THR F 118 11.311 31.679 -7.414 1.00 16.23
H
ATOM 12058 HA THR F 118 10.933 34.031 -6.187 1.00 22.57
H
ATOM 12059 HB THR F 118 11.341 35.000 -8.309 1.00 24.34
H
ATOM 12060 HG1 THR F 118 10.606 33.323 -9.554 1.00 26.55
H
ATOM 12061 HG21 THR F 118 13.607 34.417 -8.472 1.00 31.99
H
ATOM 12062 HG22 THR F 118 13.211 34.605 -6.955 1.00 31.99
H
ATOM 12063 HG23 THR F 118 13.352 33.153 -7.561 1.00 31.99
H
ATOM 12064 N THR F 119 8.475 32.701 -7.541 1.00 16.31 N
ATOM 12065 CA THR F 119 7.098 32.874 -8.023 1.00 13.93
C
ATOM 12066 C THR F 119 6.010 32.287 -7.133 1.00 15.23 C
ATOM 12067 O THR F 119 4.835 32.608 -7.309 1.00 15.00 O
ATOM 12068 CB THR F 119 6.908 32.252 -9.429 1.00 15.38

C
ATOM 5769 C THR C 215 -6.376 66.389 -18.393 1.00 37.21
C
ATOM 5770 O THR C 215 -5.421 66.913 -17.819 1.00 43.79
O
ATOM 5771 CB THR C 215 -7.992 65.528 -16.697 1.00 37.58
C
ATOM 5772 OG1 THR C 215 -7.256 66.123 -15.621 1.00 31.78
O
ATOM 5773 CG2 THR C 215 -8.750 64.313 -16.184 1.00 39.25
C
ATOM 5774 H THR C 215 -5.945 64.125 -16.517 1.00 44.09
H
ATOM 5775 HA THR C 215 -7.551 64.721 -18.540 1.00 49.88
H
ATOM 5776 HB THR C 215 -8.637 66.169 -17.036 1.00 45.09
H
ATOM 5777 HG1 THR C 215 -6.693 65.577 -15.322 1.00 38.13
H
ATOM 5778 HG21 THR C 215 -9.354 64.576 -15.471 1.00 47.10
H
ATOM 5779 HG22 THR C 215 -9.266 63.916 -16.903 1.00 47.10
H
ATOM 5780 HG23 THR C 215 -8.126 63.654 -15.841 1.00 47.10
H
TER 5781 THR C 215
ATOM 5782 N GLU D 93 -16.518 60.935 -24.144 1.00 50.72
N
ATOM 5783 CA GLU D 93 -15.948 61.865 -23.176 1.00 55.05
C
ATOM 5784 C GLU D 93 -17.021 62.338 -22.200 1.00 56.26
C
ATOM 5785 O GLU D 93 -18.143 62.642 -22.604 1.00 53.30
O
ATOM 5786 CB GLU D 93 -15.318 63.062 -23.888 1.00 63.84
C
ATOM 5787 CG GLU D 93 -14.372 63.872 -23.016 1.00 63.90
C
ATOM 5788 CD GLU D 93 -13.844 65.113 -23.716 1.00 77.81
C
ATOM 5789 OE1 GLU D 93 -14.545 65.642 -24.605 1.00 77.09
O
ATOM 5790 OE2 GLU D 93 -12.725 65.558 -23.379 1.00 78.31
O1-
ATOM 5791 HA GLU D 93 -15.255 61.413 -22.669 1.00 66.06
H
ATOM 5792 HB2 GLU D 93 -14.813 62.740 -24.651 1.00 76.60
H
ATOM 5793 HB3 GLU D 93 -16.025 63.654 -24.188 1.00 76.60
H
ATOM 5794 HG2 GLU D 93 -14.844 64.157 -22.217 1.00 76.68
H
ATOM 5795 HG3 GLU D 93 -13.613 63.319 -22.773 1.00 76.68
H
ATOM 5796 N SER D 94 -16.675 62.405 -20.918 1.00 45.44
N
ATOM 5797 CA SER D 94 -17.646 62.768 -19.894 1.00 42.83
C
ATOM 5798 C SER D 94 -16.982 63.218 -18.597 1.00 36.20
C
ATOM 5799 O SER D 94 -15.871 62.800 -18.274 1.00 34.62
O
ATOM 5800 CB SER D 94 -18.576 61.582 -19.613 1.00 47.30
C
ATOM 5801 OG SER D 94 -19.526 61.895 -18.609 1.00 57.24
O
ATOM 5802 H SER D 94 -15.886 62.245 -20.616 1.00 54.53
H
C
ATOM 12069 OG1 THR F 119 6.994 30.823 -9.354 1.00 15.55
O
ATOM 12070 CG2 THR F 119 7.938 32.794 -10.407 1.00 22.64
C
ATOM 12071 H THR F 119 8.712 31.883 -7.419 1.00 19.57 H
ATOM 12072 HA THR F 119 6.924 33.825 -8.102 1.00 16.72
H
ATOM 12073 HB THR F 119 6.029 32.495 -9.760 1.00 18.46
H
ATOM 12074 HG1 THR F 119 7.746 30.596 -9.056 1.00 18.65
H
ATOM 12075 HG21 THR F 119 7.806 32.396 -11.281 1.00 27.16
H
ATOM 12076 HG22 THR F 119 7.850 33.757 -10.482 1.00 27.16
H
ATOM 12077 HG23 THR F 119 8.833 32.582 -10.096 1.00 27.16
H
ATOM 12078 N SER F 120 6.372 31.435 -6.184 1.00 14.66 N
ATOM 12079 CA SER F 120 5.353 30.736 -5.405 1.00 13.72
C
ATOM 12080 C SER F 120 4.494 31.689 -4.583 1.00 15.42 C
ATOM 12081 O SER F 120 3.267 31.564 -4.561 1.00 14.45 O
ATOM 12082 CB SER F 120 6.000 29.701 -4.490 1.00 13.00
C
ATOM 12083 OG SER F 120 6.308 28.529 -5.215 1.00 13.36
O
ATOM 12084 H SER F 120 7.183 31.245 -5.972 1.00 17.59 H
ATOM 12085 HA SER F 120 4.766 30.264 -6.016 1.00 16.46
H
ATOM 12086 HB2 SER F 120 6.817 30.070 -4.121 1.00 15.60
H
ATOM 12087 HB3 SER F 120 5.382 29.479 -3.776 1.00 15.60
H
ATOM 12088 HG SER F 120 6.841 28.709 -5.839 1.00 16.03
H
ATOM 12089 N GLU F 121 5.127 32.640 -3.906 1.00 12.33 N
ATOM 12090 CA GLU F 121 4.374 33.607 -3.114 1.00 15.40
C
ATOM 12091 C GLU F 121 3.490 34.461 -4.020 1.00 15.41 C
ATOM 12092 O GLU F 121 2.297 34.645 -3.758 1.00 13.55 O
ATOM 12093 CB GLU F 121 5.317 34.491 -2.307 1.00 17.29
C
ATOM 12094 CG GLU F 121 4.607 35.381 -1.317 1.00 19.47
C
ATOM 12095 CD GLU F 121 5.568 36.252 -0.541 1.00 26.69
C
ATOM 12096 OE1 GLU F 121 6.760 35.884 -0.447 1.00 27.63
O
ATOM 12097 OE2 GLU F 121 5.132 37.303 -0.028 1.00 31.22
O1-
ATOM 12098 H GLU F 121 5.980 32.748 -3.888 1.00 14.80 H
ATOM 12099 HA GLU F 121 3.801 33.131 -2.493 1.00 18.48
H
ATOM 12100 HB2 GLU F 121 5.931 33.926 -1.813 1.00 20.74
H
ATOM 12101 HB3 GLU F 121 5.811 35.061 -2.918 1.00 20.74
H
ATOM 12102 HG2 GLU F 121 3.992 35.960 -1.794 1.00 23.37
H

ATOM 5803 HA SER D 94 -18.189 63.502 -20.221 1.00 51.40
H
ATOM 5804 HB2 SER D 94 -19.046 61.353 -20.430 1.00 56.75
H
ATOM 5805 HB3 SER D 94 -18.042 60.828 -19.317 1.00 56.75
H
ATOM 5806 HG SER D 94 -20.025 61.234 -18.470 1.00 68.69
H
ATOM 5807 N TYR D 95 -17.673 64.086 -17.866 1.00 33.40
N
ATOM 5808 CA TYR D 95 -17.266 64.466 -16.520 1.00 33.91
C
ATOM 5809 C TYR D 95 -17.891 63.519 -15.505 1.00 30.98
C
ATOM 5810 O TYR D 95 -18.999 63.025 -15.711 1.00 31.07
O
ATOM 5811 CB TYR D 95 -17.675 65.905 -16.213 1.00 39.04
C
ATOM 5812 CG TYR D 95 -16.785 66.949 -16.840 1.00 41.85
C
ATOM 5813 CD1 TYR D 95 -15.603 67.336 -16.227 1.00 42.03
C
ATOM 5814 CD2 TYR D 95 -17.130 67.557 -18.040 1.00 50.41
C
ATOM 5815 CE1 TYR D 95 -14.785 68.293 -16.790 1.00 48.64
C
ATOM 5816 CE2 TYR D 95 -16.319 68.517 -18.613 1.00 52.83
C
ATOM 5817 CZ TYR D 95 -15.147 68.881 -17.983 1.00 57.25
C
ATOM 5818 OH TYR D 95 -14.331 69.837 -18.545 1.00 60.24
O
ATOM 5819 H TYR D 95 -18.394 64.473 -18.132 1.00 40.08
H
ATOM 5820 HA TYR D 95 -16.301 64.400 -16.446 1.00 40.69
H
ATOM 5821 HB2 TYR D 95 -18.576 66.050 -16.542 1.00 46.85
H
ATOM 5822 HB3 TYR D 95 -17.653 66.037 -15.252 1.00 46.85
H
ATOM 5823 HD1 TYR D 95 -15.356 66.941 -15.421 1.00 50.44
H
ATOM 5824 HD2 TYR D 95 -17.920 67.312 -18.465 1.00 60.50
H
ATOM 5825 HE1 TYR D 95 -13.994 68.541 -16.368 1.00 58.37
H
ATOM 5826 HE2 TYR D 95 -16.561 68.915 -19.418 1.00 63.40
H
ATOM 5827 HH TYR D 95 -14.664 70.113 -19.265 1.00 72.28
H
ATOM 5828 N CYS D 96 -17.171 63.269 -14.415 1.00 25.95
N
ATOM 5829 CA CYS D 96 -17.651 62.404 -13.343 1.00 25.00
C
ATOM 5830 C CYS D 96 -17.873 63.227 -12.080 1.00 26.60
C
ATOM 5831 O CYS D 96 -17.011 64.017 -11.687 1.00 24.78
O
ATOM 5832 CB CYS D 96 -16.654 61.274 -13.078 1.00 24.34
C
ATOM 5833 SG CYS D 96 -17.220 60.018 -11.906 1.00 25.98
S
ATOM 5834 H CYS D 96 -16.388 63.595 -14.272 1.00 31.14
H
ATOM 5835 HA CYS D 96 -18.498 62.010 -13.603 1.00 30.00
H
ATOM 5836 HB2 CYS D 96 -16.465 60.826 -13.918 1.00 29.21
H

ATOM 12103 HG3 GLU F 121 4.122 34.828 -0.684 1.00 23.37
H

ATOM 12104 N PHE F 122 4.095 34.977 -5.083 1.00 13.83 N
ATOM 12105 CA PHE F 122 3.375 35.708 -6.123 1.00 14.10
C

ATOM 12106 C PHE F 122 2.122 34.964 -6.586 1.00 15.86 C

ATOM 12107 O PHE F 122 1.038 35.545 -6.674 1.00 14.66 O
ATOM 12108 CB PHE F 122 4.314 35.954 -7.308 1.00 15.83
C
ATOM 12109 CG PHE F 122 3.651 36.569 -8.505 1.00 17.67
C
ATOM 12110 CD1 PHE F 122 3.586 37.944 -8.644 1.00 16.84
C
ATOM 12111 CD2 PHE F 122 3.124 35.770 -9.510 1.00 15.73
C
ATOM 12112 CE1 PHE F 122 2.991 38.512 -9.751 1.00 19.00
C
ATOM 12113 CE2 PHE F 122 2.525 36.331 -10.617 1.00 21.26
C
ATOM 12114 CZ PHE F 122 2.461 37.707 -10.740 1.00 21.83
C

ATOM 12115 H PHE F 122 4.940 34.915 -5.230 1.00 16.59 H
ATOM 12116 HA PHE F 122 3.101 36.570 -5.772 1.00 16.92
H
ATOM 12117 HB2 PHE F 122 5.023 36.552 -7.024 1.00 19.00
H
ATOM 12118 HB3 PHE F 122 4.694 35.105 -7.585 1.00 19.00
H
ATOM 12119 HD1 PHE F 122 3.942 38.490 -7.982 1.00 20.21
H
ATOM 12120 HD2 PHE F 122 3.166 34.845 -9.430 1.00 18.87
H
ATOM 12121 HE1 PHE F 122 2.946 39.438 -9.831 1.00 22.80
H
ATOM 12122 HE2 PHE F 122 2.170 35.786 -11.281 1.00 25.51
H
ATOM 12123 HZ PHE F 122 2.057 38.089 -11.485 1.00 26.20
H

ATOM 12124 N ARG F 123 2.271 33.671 -6.857 1.00 14.87 N
ATOM 12125 CA ARG F 123 1.185 32.875 -7.423 1.00 15.14
C

ATOM 12126 C ARG F 123 0.102 32.529 -6.394 1.00 16.12 C
ATOM 12127 O ARG F 123 -1.047 32.276 -6.759 1.00 15.25
O
ATOM 12128 CB ARG F 123 1.752 31.598 -8.055 1.00 17.25
C
ATOM 12129 CG ARG F 123 2.417 31.851 -9.407 1.00 15.66
C
ATOM 12130 CD ARG F 123 2.949 30.582 -10.069 1.00 16.20
C
ATOM 12131 NE ARG F 123 4.170 30.101 -9.428 1.00 17.22
N
ATOM 12132 CZ ARG F 123 4.237 29.081 -8.574 1.00 13.04
C
ATOM 12133 NH1 ARG F 123 3.150 28.391 -8.242 1.00 11.59
N1+
ATOM 12134 NH2 ARG F 123 5.408 28.743 -8.054 1.00 13.48
N

ATOM 12135 H ARG F 123 2.996 33.228 -6.721 1.00 17.85 H
ATOM 12136 HA ARG F 123 0.763 33.388 -8.129 1.00 18.17
H

ATOM 5837 HB3 CYS D 96 -15.838 61.659 -12.724 1.00 29.21
H
ATOM 5838 N GLY D 97 -19.032 63.042 -11.454 1.00 23.68
N
ATOM 5839 CA GLY D 97 -19.358 63.738 -10.223 1.00 26.95
C
ATOM 5840 C GLY D 97 -20.783 64.263 -10.206 1.00 29.72
C
ATOM 5841 O GLY D 97 -21.654 63.711 -10.880 1.00 30.29
O
ATOM 5842 H GLY D 97 -19.651 62.512 -11.730 1.00 28.42
H
ATOM 5843 HA2 GLY D 97 -19.245 63.135 -9.472 1.00 32.33
H
ATOM 5844 HA3 GLY D 97 -18.755 64.489 -10.108 1.00 32.33
H
ATOM 5845 N PRO D 98 -21.033 65.333 -9.432 1.00 27.73
N
ATOM 5846 CA PRO D 98 -20.059 66.060 -8.605 1.00 26.68
C
ATOM 5847 C PRO D 98 -19.526 65.247 -7.425 1.00 25.52
C
ATOM 5848 O PRO D 98 -20.262 64.465 -6.822 1.00 24.79
O
ATOM 5849 CB PRO D 98 -20.855 67.272 -8.110 1.00 31.02
C
ATOM 5850 CG PRO D 98 -22.272 66.852 -8.178 1.00 32.89
C
ATOM 5851 CD PRO D 98 -22.370 65.945 -9.363 1.00 31.01
C
ATOM 5852 HA PRO D 98 -19.315 66.363 -9.148 1.00 32.02
H
ATOM 5853 HB2 PRO D 98 -20.601 67.480 -7.197 1.00 37.23
H
ATOM 5854 HB3 PRO D 98 -20.692 68.030 -8.693 1.00 37.23
H
ATOM 5855 HG2 PRO D 98 -22.510 66.380 -7.366 1.00 39.46
H
ATOM 5856 HG3 PRO D 98 -22.837 67.632 -8.298 1.00 39.46
H
ATOM 5857 HD2 PRO D 98 -23.046 65.266 -9.214 1.00 37.21
H
ATOM 5858 HD3 PRO D 98 -22.550 66.456 -10.167 1.00 37.21
H
ATOM 5859 N CYS D 99 -18.247 65.439 -7.115 1.00 22.53
N
ATOM 5860 CA CYS D 99 -17.605 64.787 -5.978 1.00 24.42
C
ATOM 5861 C CYS D 99 -16.595 65.739 -5.345 1.00 27.19
C
ATOM 5862 O CYS D 99 -16.094 66.638 -6.017 1.00 26.74
O
ATOM 5863 CB CYS D 99 -16.895 63.496 -6.407 1.00 28.73
C
ATOM 5864 SG CYS D 99 -17.971 62.187 -7.066 1.00 27.37
S
ATOM 5865 H CYS D 99 -17.719 65.952 -7.559 1.00 27.03
H
ATOM 5866 HA CYS D 99 -18.275 64.563 -5.313 1.00 29.30
H
ATOM 5867 HB2 CYS D 99 -16.250 63.716 -7.097 1.00 34.48
H
ATOM 5868 HB3 CYS D 99 -16.432 63.131 -5.637 1.00 34.48
H
ATOM 5869 N PRO D 100 -16.293 65.547 -4.051 1.00 23.29
N
ATOM 5870 CA PRO D 100 -15.166 66.276 -3.458 1.00 27.44
C

ATOM 12137 HB2 ARG F 123 2.418 31.220 -7.460 1.00 20.70
H
ATOM 12138 HB3 ARG F 123 1.030 30.965 -8.191 1.00 20.70
H
ATOM 12139 HG2 ARG F 123 1.767 32.250 -10.006 1.00 18.79
H
ATOM 12140 HG3 ARG F 123 3.164 32.456 -9.280 1.00 18.79
H
ATOM 12141 HD2 ARG F 123 2.278 29.884 -10.005 1.00 19.44
H
ATOM 12142 HD3 ARG F 123 3.149 30.769 -11.000 1.00 19.44
H
ATOM 12143 HE ARG F 123 4.904 30.508 -9.617 1.00 20.67
H
ATOM 12144 HH11 ARG F 123 2.387 28.605 -8.575 1.00 13.91
H
ATOM 12145 HH12 ARG F 123 3.210 27.734 -7.691 1.00 13.91
H
ATOM 12146 HH21 ARG F 123 6.116 29.182 -8.266 1.00 16.17
H
ATOM 12147 HH22 ARG F 123 5.460 28.083 -7.505 1.00 16.17
H

ATOM 12148 N LEU F 124 0.455 32.535 -5.113 1.00 15.08 N
ATOM 12149 CA LEU F 124 -0.532 32.315 -4.062 1.00 16.64
C

ATOM 12150 C LEU F 124 -1.329 33.584 -3.789 1.00 17.66 C

ATOM 12151 O LEU F 124 -2.555 33.542 -3.651 1.00 14.64 O
ATOM 12152 CB LEU F 124 0.137 31.848 -2.766 1.00 12.40
C
ATOM 12153 CG LEU F 124 -0.767 31.818 -1.525 1.00 15.66
C
ATOM 12154 CD1 LEU F 124 -1.960 30.901 -1.736 1.00 18.94
C
ATOM 12155 CD2 LEU F 124 0.001 31.410 -0.273 1.00 12.65
C

ATOM 12156 H LEU F 124 1.256 32.662 -4.827 1.00 18.10 H
ATOM 12157 HA LEU F 124 -1.151 31.626 -4.347 1.00 19.97
H
ATOM 12158 HB2 LEU F 124 0.473 30.948 -2.903 1.00 14.88
H
ATOM 12159 HB3 LEU F 124 0.877 32.443 -2.572 1.00 14.88
H
ATOM 12160 HG LEU F 124 -1.112 32.712 -1.376 1.00 18.80
H
ATOM 12161 HD11 LEU F 124 -2.507 30.907 -0.935 1.00 22.72
H
ATOM 12162 HD12 LEU F 124 -2.475 31.223 -2.492 1.00 22.72
H
ATOM 12163 HD13 LEU F 124 -1.639 30.003 -1.912 1.00 22.72
H
ATOM 12164 HD21 LEU F 124 -0.607 31.405 0.482 1.00 15.18
H
ATOM 12165 HD22 LEU F 124 0.373 30.524 -0.406 1.00 15.18
H
ATOM 12166 HD23 LEU F 124 0.715 32.049 -0.120 1.00 15.18
H

ATOM 12167 N LYS F 125 -0.628 34.711 -3.714 1.00 16.52 N
ATOM 12168 CA LYS F 125 -1.208 35.923 -3.146 1.00 13.85
C

ATOM 12169 C LYS F 125 -1.934 36.817 -4.144 1.00 18.09 C

ATOM 12170 O LYS F 125 -2.316 37.935 -3.802 1.00 17.06 O

ATOM 5871 C PRO D 100 -13.882 66.019 -4.245 1.00 28.68
C
ATOM 5872 O PRO D 100 -13.681 64.904 -4.730 1.00 26.75
O
ATOM 5873 CB PRO D 100 -15.073 65.703 -2.043 1.00 29.15
C
ATOM 5874 CG PRO D 100 -16.420 65.125 -1.767 1.00 25.98
C
ATOM 5875 CD PRO D 100 -16.950 64.656 -3.079 1.00 24.13
C
ATOM 5876 HA PRO D 100 -15.349 67.228 -3.420 1.00 32.93
H
ATOM 5877 HB2 PRO D 100 -14.392 65.013 -2.014 1.00 34.98
H
ATOM 5878 HB3 PRO D 100 -14.869 66.414 -1.415 1.00 34.98
H
ATOM 5879 HG2 PRO D 100 -16.333 64.382 -1.150 1.00 31.17
H
ATOM 5880 HG3 PRO D 100 -16.996 65.811 -1.394 1.00 31.17
H
ATOM 5881 HD2 PRO D 100 -16.693 63.734 -3.238 1.00 28.95
H
ATOM 5882 HD3 PRO D 100 -17.913 64.769 -3.115 1.00 28.95
H
ATOM 5883 N LYS D 101 -13.027 67.031 -4.357 1.00 31.41
N
ATOM 5884 CA LYS D 101 -11.915 66.997 -5.306 1.00 34.02
C
ATOM 5885 C LYS D 101 -10.851 65.943 -4.997 1.00 34.04
C
ATOM 5886 O LYS D 101 -10.078 65.570 -5.884 1.00 40.88
O
ATOM 5887 CB LYS D 101 -11.254 68.377 -5.379 1.00 40.64
C
ATOM 5888 CG LYS D 101 -12.150 69.458 -5.975 1.00 44.15
C
ATOM 5889 CD LYS D 101 -11.383 70.749 -6.223 1.00 55.25
C
ATOM 5890 CE LYS D 101 -12.306 71.866 -6.691 1.00 57.18
C
ATOM 5891 NZ LYS D 101 -11.566 73.132 -6.955 1.00 56.55
N1+
ATOM 5892 H LYS D 101 -13.069 67.753 -3.892 1.00 37.69
H
ATOM 5893 HA LYS D 101 -12.271 66.799 -6.186 1.00 40.82
H
ATOM 5894 HB2 LYS D 101 -11.011 68.655 -4.482 1.00 48.77
H
ATOM 5895 HB3 LYS D 101 -10.459 68.314 -5.931 1.00 48.77
H
ATOM 5896 HG2 LYS D 101 -12.505 69.147 -6.823 1.00 52.98
H
ATOM 5897 HG3 LYS D 101 -12.874 69.649 -5.358 1.00 52.98
H
ATOM 5898 HD2 LYS D 101 -10.957 71.032 -5.399 1.00 66.30
H
ATOM 5899 HD3 LYS D 101 -10.716 70.598 -6.911 1.00 66.30
H
ATOM 5900 HE2 LYS D 101 -12.743 71.594 -7.513 1.00 68.62
H
ATOM 5901 HE3 LYS D 101 -12.967 72.040 -6.003 1.00 68.62
H
ATOM 5902 HZ1 LYS D 101 -12.132 73.763 -7.226 1.00 67.86
H
ATOM 5903 HZ2 LYS D 101 -11.160 73.407 -6.213 1.00 67.86
H
ATOM 5904 HZ3 LYS D 101 -10.955 73.000 -7.588 1.00 67.86
H

ATOM 12171 CB LYS F 125 -0.117 36.732 -2.443 1.00 16.06
C
ATOM 12172 CG LYS F 125 0.491 36.018 -1.252 1.00 20.08
C
ATOM 12173 CD LYS F 125 1.351 36.960 -0.420 1.00 22.60
C
ATOM 12174 CE LYS F 125 1.664 36.362 0.940 1.00 23.37 C
ATOM 12175 NZ LYS F 125 2.510 37.267 1.764 1.00 23.92
N1+
ATOM 12176 H LYS F 125 0.183 34.801 -3.985 1.00 19.83 H
ATOM 12177 HA LYS F 125 -1.854 35.662 -2.471 1.00 16.62
H
ATOM 12178 HB2 LYS F 125 0.595 36.915 -3.076 1.00 19.28
H
ATOM 12179 HB3 LYS F 125 -0.499 37.566 -2.127 1.00 19.28
H
ATOM 12180 HG2 LYS F 125 -0.219 35.674 -0.688 1.00 24.10
H
ATOM 12181 HG3 LYS F 125 1.052 35.291 -1.567 1.00 24.10
H
ATOM 12182 HD2 LYS F 125 2.188 37.123 -0.881 1.00 27.13
H
ATOM 12183 HD3 LYS F 125 0.874 37.794 -0.283 1.00 27.13
H
ATOM 12184 HE2 LYS F 125 0.834 36.205 1.417 1.00 28.04
H
ATOM 12185 HE3 LYS F 125 2.142 35.527 0.818 1.00 28.04
H
ATOM 12186 HZ1 LYS F 125 3.282 37.423 1.348 1.00 28.71
H
ATOM 12187 HZ2 LYS F 125 2.090 38.041 1.894 1.00 28.71
H
ATOM 12188 HZ3 LYS F 125 2.678 36.891 2.553 1.00 28.71
H
ATOM 12189 N LYS F 126 -2.143 36.328 -5.363 1.00 14.39 N
ATOM 12190 CA LYS F 126 -2.855 37.102 -6.371 1.00 15.04
C
ATOM 12191 C LYS F 126 -4.200 37.597 -5.829 1.00 15.14 C
ATOM 12192 O LYS F 126 -4.500 38.788 -5.906 1.00 13.71 O
ATOM 12193 CB LYS F 126 -3.057 36.270 -7.637 1.00 15.31
C
ATOM 12194 CG LYS F 126 -3.569 37.060 -8.822 1.00 14.58
C
ATOM 12195 CD LYS F 126 -3.293 36.319 -10.120 1.00 18.23
C
ATOM 12196 CE LYS F 126 -3.981 36.970 -11.302 1.00 24.64
C
ATOM 12197 NZ LYS F 126 -3.627 36.281 -12.575 1.00 24.00
N1+
ATOM 12198 H LYS F 126 -1.883 35.553 -5.630 1.00 17.27 H
ATOM 12199 HA LYS F 126 -2.323 37.879 -6.605 1.00 18.05
H
ATOM 12200 HB2 LYS F 126 -2.207 35.876 -7.889 1.00 18.37
H
ATOM 12201 HB3 LYS F 126 -3.700 35.569 -7.449 1.00 18.37
H
ATOM 12202 HG2 LYS F 126 -4.528 37.183 -8.738 1.00 17.49
H
ATOM 12203 HG3 LYS F 126 -3.119 37.918 -8.857 1.00 17.49
H
ATOM 12204 HD2 LYS F 126 -2.338 36.318 -10.289 1.00 21.87
H

ATOM 5905 N ASN D 102 -10.804 65.470 -3.755 1.00 27.12 N
ATOM 5906 CA ASN D 102 -9.836 64.445 -3.366 1.00 27.98 C
ATOM 5907 C ASN D 102 -10.503 63.098 -3.072 1.00 26.71 C
ATOM 5908 O ASN D 102 -9.946 62.263 -2.360 1.00 25.40 O
ATOM 5909 CB ASN D 102 -9.026 64.914 -2.150 1.00 30.15 C
ATOM 5910 CG ASN D 102 -9.898 65.481 -1.045 1.00 36.72 C
ATOM 5911 OD1 ASN D 102 -11.120 65.332 -1.062 1.00 37.16 O
ATOM 5912 ND2 ASN D 102 -9.271 66.145 -0.078 1.00 41.06 N
ATOM 5913 H ASN D 102 -11.322 65.725 -3.118 1.00 32.55 H
ATOM 5914 HA ASN D 102 -9.215 64.311 -4.099 1.00 33.58 H
ATOM 5915 HB2 ASN D 102 -8.535 64.160 -1.787 1.00 36.19 H
ATOM 5916 HB3 ASN D 102 -8.409 65.608 -2.430 1.00 36.19 H
ATOM 5917 HD21 ASN D 102 -9.720 66.485 0.571 1.00 49.28 H
ATOM 5918 HD22 ASN D 102 -8.416 66.233 -0.102 1.00 49.28 H
ATOM 5919 N TRP D 103 -11.696 62.897 -3.630 1.00 25.27 N
ATOM 5920 CA TRP D 103 -12.400 61.619 -3.534 1.00 19.72 C
ATOM 5921 C TRP D 103 -12.378 60.891 -4.872 1.00 20.07 C
ATOM 5922 O TRP D 103 -12.240 61.516 -5.927 1.00 20.39 O
ATOM 5923 CB TRP D 103 -13.853 61.822 -3.094 1.00 22.50 C
ATOM 5924 CG TRP D 103 -14.018 62.103 -1.636 1.00 21.05 C
ATOM 5925 CD1 TRP D 103 -13.247 62.919 -0.865 1.00 26.32 C
ATOM 5926 CD2 TRP D 103 -15.014 61.552 -0.768 1.00 22.01 C
ATOM 5927 NE1 TRP D 103 -13.708 62.920 0.430 1.00 31.25 N
ATOM 5928 CE2 TRP D 103 -14.792 62.088 0.516 1.00 23.75 C
ATOM 5929 CE3 TRP D 103 -16.075 60.660 -0.952 1.00 21.83 C
ATOM 5930 CZ2 TRP D 103 -15.589 61.759 1.611 1.00 26.02 C
ATOM 5931 CZ3 TRP D 103 -16.868 60.336 0.136 1.00 24.01 C
ATOM 5932 CH2 TRP D 103 -16.620 60.884 1.401 1.00 22.41 C
ATOM 5933 H TRP D 103 -12.124 63.494 -4.077 1.00 30.33 H
ATOM 5934 HA TRP D 103 -11.959 61.060 -2.876 1.00 23.66 H
ATOM 5935 HB2 TRP D 103 -14.225 62.572 -3.583 1.00 27.00 H
ATOM 5936 HB3 TRP D 103 -14.355 61.017 -3.298 1.00 27.00 H
ATOM 5937 HD1 TRP D 103 -12.520 63.412 -1.172 1.00 31.59 H
ATOM 5938 HE1 TRP D 103 -13.369 63.369 1.081 1.00 37.50 H

ATOM 12205 HD3 LYS F 126 -3.620 35.409 -10.043 1.00 21.87 H
ATOM 12206 HE2 LYS F 126 -4.943 36.917 -11.183 1.00 29.56 H
ATOM 12207 HE3 LYS F 126 -3.700 37.896 -11.367 1.00 29.56 H
ATOM 12208 HZ1 LYS F 126 -4.039 36.675 -13.258 1.00 28.80 H
ATOM 12209 HZ2 LYS F 126 -2.748 36.318 -12.706 1.00 28.80 H
ATOM 12210 HZ3 LYS F 126 -3.878 35.427 -12.538 1.00 28.80 H

ATOM 12211 N TRP F 127 -4.983 36.690 -5.245 1.00 15.14 N
ATOM 12212 CA TRP F 127 -6.284 37.040 -4.663 1.00 15.40 C

ATOM 12213 C TRP F 127 -6.357 36.731 -3.163 1.00 15.55 C

ATOM 12214 O TRP F 127 -7.408 36.886 -2.532 1.00 13.20 O
ATOM 12215 CB TRP F 127 -7.397 36.293 -5.400 1.00 11.59 C
ATOM 12216 CG TRP F 127 -7.543 36.706 -6.833 1.00 15.11 C
ATOM 12217 CD1 TRP F 127 -7.053 36.059 -7.931 1.00 17.05 C
ATOM 12218 CD2 TRP F 127 -8.229 37.863 -7.323 1.00 15.18 C
ATOM 12219 NE1 TRP F 127 -7.390 36.744 -9.075 1.00 17.58 N
ATOM 12220 CE2 TRP F 127 -8.114 37.854 -8.729 1.00 18.89 C
ATOM 12221 CE3 TRP F 127 -8.930 38.906 -6.710 1.00 19.66 C
ATOM 12222 CZ2 TRP F 127 -8.675 38.847 -9.531 1.00 19.66 C
ATOM 12223 CZ3 TRP F 127 -9.486 39.891 -7.507 1.00 17.24 C
ATOM 12224 CH2 TRP F 127 -9.353 39.854 -8.904 1.00 23.08 C

ATOM 12225 H TRP F 127 -4.783 35.856 -5.172 1.00 18.17 H
ATOM 12226 HA TRP F 127 -6.434 37.991 -4.779 1.00 18.48 H
ATOM 12227 HB2 TRP F 127 -7.202 35.343 -5.382 1.00 13.91 H
ATOM 12228 HB3 TRP F 127 -8.240 36.466 -4.953 1.00 13.91 H
ATOM 12229 HD1 TRP F 127 -6.560 35.270 -7.908 1.00 20.46 H
ATOM 12230 HE1 TRP F 127 -7.183 36.511 -9.877 1.00 21.10 H
ATOM 12231 HE3 TRP F 127 -9.022 38.937 -5.785 1.00 23.59 H
ATOM 12232 HZ2 TRP F 127 -8.589 38.826 -10.457 1.00 23.59 H
ATOM 12233 HZ3 TRP F 127 -9.954 40.589 -7.111 1.00 20.69 H
ATOM 12234 HH2 TRP F 127 -9.737 40.530 -9.415 1.00 27.70 H

ATOM 12235 N PHE F 128 -5.230 36.311 -2.599 1.00 13.38 N
ATOM 12236 CA PHE F 128 -5.188 35.772 -1.243 1.00 17.23 C

ATOM 12237 C PHE F 128 -3.938 36.245 -0.498 1.00 16.62 C

ATOM 12238 O PHE F 128 -2.925 35.552 -0.476 1.00 14.93 O

ATOM 5939 HE3 TRP D 103 -16.245 60.292 -1.789 1.00 26.20
H
ATOM 5940 HZ2 TRP D 103 -15.427 62.122 2.452 1.00 31.22
H
ATOM 5941 HZ3 TRP D 103 -17.577 59.744 0.025 1.00 28.82
H
ATOM 5942 HH2 TRP D 103 -17.169 60.649 2.114 1.00 26.90
H
ATOM 5943 N ILE D 104 -12.524 59.571 -4.821 1.00 16.86
N
ATOM 5944 CA ILE D 104 -12.597 58.755 -6.027 1.00 17.78
C
ATOM 5945 C ILE D 104 -13.993 58.831 -6.627 1.00 18.20
C
ATOM 5946 O ILE D 104 -14.975 58.549 -5.944 1.00 18.57
O
ATOM 5947 CB ILE D 104 -12.255 57.281 -5.735 1.00 20.02
C
ATOM 5948 CG1 ILE D 104 -10.857 57.168 -5.119 1.00 20.67
C
ATOM 5949 CG2 ILE D 104 -12.338 56.446 -7.015 1.00 19.79
C
ATOM 5950 CD1 ILE D 104 -10.571 55.825 -4.483 1.00 17.10
C
ATOM 5951 H ILE D 104 -12.585 59.120 -4.092 1.00 20.23
H
ATOM 5952 HA ILE D 104 -11.965 59.091 -6.681 1.00 21.34
H
ATOM 5953 HB ILE D 104 -12.901 56.935 -5.099 1.00 24.02
H
ATOM 5954 HG12 ILE D 104 -10.197 57.313 -5.815 1.00 24.80
H
ATOM 5955 HG13 ILE D 104 -10.763 57.847 -4.432 1.00 24.80
H
ATOM 5956 HG21 ILE D 104 -12.120 55.525 -6.805 1.00 23.75
H
ATOM 5957 HG22 ILE D 104 -13.240 56.500 -7.368 1.00 23.75
H
ATOM 5958 HG23 ILE D 104 -11.707 56.798 -7.662 1.00 23.75
H
ATOM 5959 HD11 ILE D 104 -9.673 55.834 -4.118 1.00 20.52
H
ATOM 5960 HD12 ILE D 104 -11.215 55.668 -3.774 1.00 20.52
H
ATOM 5961 HD13 ILE D 104 -10.648 55.134 -5.159 1.00 20.52
H
ATOM 5962 N CYS D 105 -14.076 59.199 -7.902 1.00 17.45
N
ATOM 5963 CA CYS D 105 -15.354 59.239 -8.602 1.00 17.74
C
ATOM 5964 C CYS D 105 -15.465 58.067 -9.573 1.00 21.30
C
ATOM 5965 O CYS D 105 -14.560 57.821 -10.371 1.00 19.85
O
ATOM 5966 CB CYS D 105 -15.524 60.563 -9.345 1.00 20.49
C
ATOM 5967 SG CYS D 105 -17.186 60.797 -10.022 1.00 29.47
S
ATOM 5968 H CYS D 105 -13.404 59.431 -8.385 1.00 20.94
H
ATOM 5969 HA CYS D 105 -16.073 59.163 -7.955 1.00 21.29
H
ATOM 5970 HB2 CYS D 105 -15.347 61.293 -8.731 1.00 24.59
H
ATOM 5971 HB3 CYS D 105 -14.895 60.592 -10.083 1.00 24.59
H
ATOM 5972 N TYR D 106 -16.577 57.343 -9.481 1.00 17.44
N

ATOM 12239 CB PHE F 128 -5.234 34.241 -1.310 1.00 12.61
C
ATOM 12240 CG PHE F 128 -5.412 33.567 0.020 1.00 15.61
C
ATOM 12241 CD1 PHE F 128 -6.504 33.855 0.818 1.00 17.23
C
ATOM 12242 CD2 PHE F 128 -4.503 32.619 0.454 1.00 13.57
C
ATOM 12243 CE1 PHE F 128 -6.674 33.226 2.031 1.00 14.89
C
ATOM 12244 CE2 PHE F 128 -4.668 31.985 1.669 1.00 16.18
C
ATOM 12245 CZ PHE F 128 -5.756 32.288 2.459 1.00 14.81
C

ATOM 12246 H PHE F 128 -4.463 36.329 -2.987 1.00 16.05 H
ATOM 12247 HA PHE F 128 -5.967 36.079 -0.753 1.00 20.67
H
ATOM 12248 HB2 PHE F 128 -5.976 33.977 -1.876 1.00 15.13
H
ATOM 12249 HB3 PHE F 128 -4.402 33.922 -1.693 1.00 15.13
H
ATOM 12250 HD1 PHE F 128 -7.126 34.486 0.536 1.00 20.67
H
ATOM 12251 HD2 PHE F 128 -3.767 32.412 -0.075 1.00 16.29
H
ATOM 12252 HE1 PHE F 128 -7.409 33.432 2.563 1.00 17.87
H
ATOM 12253 HE2 PHE F 128 -4.047 31.355 1.954 1.00 19.41
H
ATOM 12254 HZ PHE F 128 -5.870 31.864 3.278 1.00 17.78
H

ATOM 12255 N ASP F 129 -4.011 37.426 0.108 1.00 16.80 N
ATOM 12256 CA ASP F 129 -2.863 37.972 0.828 1.00 17.78
C

ATOM 12257 C ASP F 129 -2.895 37.537 2.290 1.00 19.18 C

ATOM 12258 O ASP F 129 -3.800 36.814 2.714 1.00 16.91 O
ATOM 12259 CB ASP F 129 -2.819 39.504 0.714 1.00 18.37
C
ATOM 12260 CG ASP F 129 -4.066 40.185 1.263 1.00 16.63
C
ATOM 12261 OD1 ASP F 129 -4.707 39.642 2.181 1.00 16.14
O
ATOM 12262 OD2 ASP F 129 -4.394 41.289 0.779 1.00 16.62
O1-

ATOM 12263 H ASP F 129 -4.708 37.928 0.119 1.00 20.16 H
ATOM 12264 HA ASP F 129 -2.050 37.621 0.432 1.00 21.34
H
ATOM 12265 HB2 ASP F 129 -2.055 39.834 1.212 1.00 22.04
H
ATOM 12266 HB3 ASP F 129 -2.734 39.747 -0.221 1.00 22.04
H

ATOM 12267 N GLY F 130 -1.900 37.976 3.052 1.00 15.15 N
ATOM 12268 CA GLY F 130 -1.783 37.608 4.450 1.00 17.82
C

ATOM 12269 C GLY F 130 -2.997 37.984 5.277 1.00 16.60 C

ATOM 12270 O GLY F 130 -3.425 37.224 6.147 1.00 14.67 O

ATOM 12271 H GLY F 130 -1.273 38.496 2.775 1.00 18.18 H
ATOM 12272 HA2 GLY F 130 -1.654 36.649 4.518 1.00 21.38
H

ATOM 5973 CA TYR D 106 -16.858 56.216 -10.365 1.00 18.50 C
ATOM 5974 C TYR D 106 -18.354 56.134 -10.632 1.00 19.85 C
ATOM 5975 O TYR D 106 -19.139 55.879 -9.718 1.00 18.05 O
ATOM 5976 CB TYR D 106 -16.362 54.902 -9.755 1.00 15.27 C
ATOM 5977 CG TYR D 106 -16.488 53.707 -10.675 1.00 17.55 C
ATOM 5978 CD1 TYR D 106 -15.878 53.702 -11.922 1.00 20.29 C
ATOM 5979 CD2 TYR D 106 -17.202 52.577 -10.293 1.00 20.08 C
ATOM 5980 CE1 TYR D 106 -15.981 52.613 -12.768 1.00 20.50 C
ATOM 5981 CE2 TYR D 106 -17.309 51.476 -11.136 1.00 18.23 C
ATOM 5982 CZ TYR D 106 -16.692 51.502 -12.373 1.00 22.08 C
ATOM 5983 OH TYR D 106 -16.785 50.418 -13.224 1.00 18.81 O
ATOM 5984 H TYR D 106 -17.196 57.488 -8.902 1.00 20.92 H
ATOM 5985 HA TYR D 106 -16.403 56.351 -11.211 1.00 22.20 H
ATOM 5986 HB2 TYR D 106 -15.425 55.000 -9.524 1.00 18.33 H
ATOM 5987 HB3 TYR D 106 -16.879 54.715 -8.956 1.00 18.33 H
ATOM 5988 HD1 TYR D 106 -15.394 54.448 -12.195 1.00 24.35 H
ATOM 5989 HD2 TYR D 106 -17.616 52.557 -9.460 1.00 24.10 H
ATOM 5990 HE1 TYR D 106 -15.565 52.629 -13.600 1.00 24.60 H
ATOM 5991 HE2 TYR D 106 -17.790 50.727 -10.869 1.00 21.87 H
ATOM 5992 HH TYR D 106 -17.243 49.811 -12.867 1.00 22.58 H
ATOM 5993 N LYS D 107 -18.732 56.351 -11.888 1.00 16.29 N
ATOM 5994 CA LYS D 107 -20.132 56.364 -12.294 1.00 20.57 C
ATOM 5995 C LYS D 107 -20.916 57.330 -11.404 1.00 24.05 C
ATOM 5996 O LYS D 107 -21.998 57.015 -10.907 1.00 17.53 O
ATOM 5997 CB LYS D 107 -20.708 54.947 -12.249 1.00 20.83 C
ATOM 5998 CG LYS D 107 -19.963 53.987 -13.184 1.00 20.22 C
ATOM 5999 CD LYS D 107 -20.505 52.566 -13.145 1.00 20.35 C
ATOM 6000 CE LYS D 107 -19.817 51.694 -14.198 1.00 23.07 C
ATOM 6001 NZ LYS D 107 -20.217 50.259 -14.138 1.00 21.00 N1+
ATOM 6002 H LYS D 107 -18.185 56.495 -12.536 1.00 19.55 H
ATOM 6003 HA LYS D 107 -20.193 56.682 -13.208 1.00 24.68 H
ATOM 6004 HB2 LYS D 107 -20.637 54.604 -11.344 1.00 24.99 H
ATOM 6005 HB3 LYS D 107 -21.638 54.974 -12.523 1.00 24.99 H
ATOM 6006 HG2 LYS D 107 -20.041 54.311 -14.094 1.00 24.26 H
ATOM 12273 HA3 GLY F 130 -1.007 38.048 4.832 1.00 21.38 H
ATOM 12274 N GLU F 131 -3.560 39.156 5.010 1.00 13.72 N
ATOM 12275 CA GLU F 131 -4.732 39.598 5.751 1.00 18.76 C
ATOM 12276 C GLU F 131 -5.928 38.710 5.433 1.00 16.47 C
ATOM 12277 O GLU F 131 -6.715 38.380 6.322 1.00 13.63 O
ATOM 12278 CB GLU F 131 -5.052 41.056 5.440 1.00 19.73 C
ATOM 12279 CG GLU F 131 -6.078 41.653 6.382 1.00 26.43 C
ATOM 12280 CD GLU F 131 -6.202 43.154 6.229 1.00 27.13 C
ATOM 12281 OE1 GLU F 131 -5.568 43.715 5.309 1.00 19.31 O
ATOM 12282 OE2 GLU F 131 -6.931 43.773 7.034 1.00 31.50 O1-
ATOM 12283 H GLU F 131 -3.285 39.709 4.412 1.00 16.47 H
ATOM 12284 HA GLU F 131 -4.550 39.527 6.702 1.00 22.52 H
ATOM 12285 HB2 GLU F 131 -4.239 41.579 5.514 1.00 23.68 H
ATOM 12286 HB3 GLU F 131 -5.404 41.115 4.538 1.00 23.68 H
ATOM 12287 HG2 GLU F 131 -6.945 41.260 6.196 1.00 31.71 H
ATOM 12288 HG3 GLU F 131 -5.816 41.465 7.296 1.00 31.71 H
ATOM 12289 N ASP F 132 -6.067 38.318 4.169 1.00 15.33 N
ATOM 12290 CA ASP F 132 -7.115 37.374 3.801 1.00 13.35 C
ATOM 12291 C ASP F 132 -6.949 36.086 4.596 1.00 14.58 C
ATOM 12292 O ASP F 132 -7.918 35.557 5.137 1.00 15.18 O
ATOM 12293 CB ASP F 132 -7.094 37.063 2.305 1.00 15.90 C
ATOM 12294 CG ASP F 132 -7.322 38.286 1.444 1.00 17.33 C
ATOM 12295 OD1 ASP F 132 -8.013 39.232 1.887 1.00 16.63 O
ATOM 12296 OD2 ASP F 132 -6.809 38.292 0.308 1.00 18.06 O1-
ATOM 12297 H ASP F 132 -5.575 38.581 3.515 1.00 18.40 H
ATOM 12298 HA ASP F 132 -7.980 37.756 4.018 1.00 16.02 H
ATOM 12299 HB2 ASP F 132 -6.229 36.690 2.073 1.00 19.08 H
ATOM 12300 HB3 ASP F 132 -7.794 36.422 2.107 1.00 19.08 H
ATOM 12301 N CYS F 133 -5.716 35.591 4.680 1.00 14.32 N
ATOM 12302 CA CYS F 133 -5.449 34.328 5.364 1.00 14.59 C
ATOM 12303 C CYS F 133 -5.892 34.382 6.825 1.00 15.41 C
ATOM 12304 O CYS F 133 -6.499 33.441 7.328 1.00 14.68 O
ATOM 12305 CB CYS F 133 -3.964 33.968 5.286 1.00 18.53 C
ATOM 12306 SG CYS F 133 -3.547 32.418 6.119 1.00 24.44 S

ATOM 6007 HG3 LYS D 107 -19.029 53.957 -12.923 1.00 24.26
H
ATOM 6008 HD2 LYS D 107 -20.338 52.180 -12.271 1.00 24.42
H
ATOM 6009 HD3 LYS D 107 -21.457 52.579 -13.332 1.00 24.42
H
ATOM 6010 HE2 LYS D 107 -20.045 52.029 -15.080 1.00 27.69
H
ATOM 6011 HE3 LYS D 107 -18.857 51.741 -14.065 1.00 27.69
H
ATOM 6012 HZ1 LYS D 107 -21.095 50.182 -14.267 1.00 25.20
H
ATOM 6013 HZ2 LYS D 107 -19.791 49.797 -14.768 1.00 25.20
H
ATOM 6014 HZ3 LYS D 107 -20.011 49.919 -13.341 1.00 25.20
H
ATOM 6015 N ASN D 108 -20.318 58.503 -11.205 1.00 23.09
N
ATOM 6016 CA ASN D 108 -20.912 59.622 -10.473 1.00 24.38
C
ATOM 6017 C ASN D 108 -21.096 59.378 -8.976 1.00 22.29
C
ATOM 6018 O ASN D 108 -21.565 60.261 -8.262 1.00 28.01
O
ATOM 6019 CB ASN D 108 -22.253 60.012 -11.103 1.00 25.10
C
ATOM 6020 CG ASN D 108 -22.084 60.642 -12.471 1.00 28.43
C
ATOM 6021 OD1 ASN D 108 -21.044 61.229 -12.769 1.00 25.66
O
ATOM 6022 ND2 ASN D 108 -23.107 60.529 -13.310 1.00 30.87
N
ATOM 6023 H ASN D 108 -19.530 58.682 -11.500 1.00 27.71
H
ATOM 6024 HA ASN D 108 -20.321 60.386 -10.565 1.00 29.25
H
ATOM 6025 HB2 ASN D 108 -22.800 59.217 -11.203 1.00 30.12
H
ATOM 6026 HB3 ASN D 108 -22.698 60.654 -10.529 1.00 30.12
H
ATOM 6027 HD21 ASN D 108 -23.057 60.871 -14.098 1.00 37.04
H
ATOM 6028 HD22 ASN D 108 -23.820 60.115 -13.066 1.00 37.04
H
ATOM 6029 N ASN D 109 -20.704 58.205 -8.494 1.00 21.22
N
ATOM 6030 CA ASN D 109 -20.646 57.967 -7.056 1.00 19.34
C
ATOM 6031 C ASN D 109 -19.262 58.340 -6.533 1.00 19.61
C
ATOM 6032 O ASN D 109 -18.267 58.162 -7.232 1.00 16.71
O
ATOM 6033 CB ASN D 109 -20.973 56.512 -6.733 1.00 19.32
C
ATOM 6034 CG ASN D 109 -22.421 56.167 -7.013 1.00 25.66
C
ATOM 6035 OD1 ASN D 109 -23.322 56.973 -6.770 1.00 19.34
O
ATOM 6036 ND2 ASN D 109 -22.652 54.969 -7.533 1.00 19.02
N
ATOM 6037 H ASN D 109 -20.467 57.532 -8.974 1.00 25.47
H
ATOM 6038 HA ASN D 109 -21.300 58.530 -6.613 1.00 23.20
H
ATOM 6039 HB2 ASN D 109 -20.415 55.934 -7.278 1.00 23.19
H
ATOM 6040 HB3 ASN D 109 -20.801 56.350 -5.792 1.00 23.19
H

ATOM 12307 H CYS F 133 -5.017 35.968 4.350 1.00 17.18 H
ATOM 12308 HA CYS F 133 -5.951 33.622 4.927 1.00 17.51
H
ATOM 12309 HB2 CYS F 133 -3.712 33.881 4.353 1.00 22.24
H
ATOM 12310 HB3 CYS F 133 -3.448 34.677 5.702 1.00 22.24
H

ATOM 12311 N ILE F 134 -5.593 35.489 7.496 1.00 14.80 N

ATOM 12312 CA ILE F 134 -5.980 35.661 8.890 1.00 12.54 C

ATOM 12313 C ILE F 134 -7.507 35.701 9.031 1.00 14.20 C

ATOM 12314 O ILE F 134 -8.068 35.120 9.957 1.00 14.69 O

ATOM 12315 CB ILE F 134 -5.370 36.952 9.483 1.00 14.54 C
ATOM 12316 CG1 ILE F 134 -3.842 36.854 9.542 1.00 15.52
C
ATOM 12317 CG2 ILE F 134 -5.935 37.240 10.873 1.00 18.23
C
ATOM 12318 CD1 ILE F 134 -3.302 35.789 10.488 1.00 20.56
C

ATOM 12319 H ILE F 134 -5.165 36.157 7.165 1.00 17.76 H

ATOM 12320 HA ILE F 134 -5.650 34.908 9.406 1.00 15.05 H

ATOM 12321 HB ILE F 134 -5.604 37.692 8.902 1.00 17.45 H
ATOM 12322 HG12 ILE F 134 -3.512 36.651 8.653 1.00 18.62
H
ATOM 12323 HG13 ILE F 134 -3.489 37.710 9.832 1.00 18.62
H
ATOM 12324 HG21 ILE F 134 -5.533 38.054 11.214 1.00 21.87
H
ATOM 12325 HG22 ILE F 134 -6.896 37.348 10.806 1.00 21.87
H
ATOM 12326 HG23 ILE F 134 -5.725 36.496 11.459 1.00 21.87
H
ATOM 12327 HD11 ILE F 134 -2.333 35.802 10.457 1.00 24.67
H
ATOM 12328 HD12 ILE F 134 -3.608 35.983 11.388 1.00 24.67
H
ATOM 12329 HD13 ILE F 134 -3.631 34.921 10.206 1.00 24.67
H

ATOM 12330 N MET F 135 -8.184 36.386 8.117 1.00 12.68 N
ATOM 12331 CA MET F 135 -9.635 36.491 8.203 1.00 14.96
C
ATOM 12332 C MET F 135 -10.291 35.143 7.899 1.00 17.64
C
ATOM 12333 O MET F 135 -11.291 34.786 8.528 1.00 18.23
O
ATOM 12334 CB MET F 135 -10.156 37.577 7.261 1.00 15.55
C
ATOM 12335 CG MET F 135 -9.677 38.983 7.625 1.00 18.93
C
ATOM 12336 SD MET F 135 -10.279 39.567 9.225 1.00 25.83
S
ATOM 12337 CE MET F 135 -11.971 39.939 8.804 1.00 23.03
C

ATOM 12338 H MET F 135 -7.833 36.795 7.446 1.00 15.22 H
ATOM 12339 HA MET F 135 -9.872 36.751 9.107 1.00 17.96
H
ATOM 12340 HB2 MET F 135 -9.852 37.384 6.360 1.00 18.66
H

ATOM 6041 HD21 ASN D 109 -23.457 54.725 -7.710 1.00 22.82
H
ATOM 6042 HD22 ASN D 109 -21.996 54.436 -7.693 1.00 22.82
H
ATOM 6043 N CYS D 110 -19.204 58.867 -5.312 1.00 17.46
N
ATOM 6044 CA CYS D 110 -17.941 59.308 -4.726 1.00 16.88
C
ATOM 6045 C CYS D 110 -17.547 58.402 -3.573 1.00 19.16
C
ATOM 6046 O CYS D 110 -18.374 58.079 -2.725 1.00 17.29
O
ATOM 6047 CB CYS D 110 -18.047 60.751 -4.237 1.00 22.60
C
ATOM 6048 SG CYS D 110 -18.972 61.837 -5.338 1.00 23.11
S
ATOM 6049 H CYS D 110 -19.886 58.981 -4.801 1.00 20.95
H
ATOM 6050 HA CYS D 110 -17.244 59.265 -5.399 1.00 20.25
H
ATOM 6051 HB2 CYS D 110 -18.493 60.756 -3.375 1.00 27.12
H
ATOM 6052 HB3 CYS D 110 -17.153 61.116 -4.145 1.00 27.12
H
ATOM 6053 N TYR D 111 -16.280 58.001 -3.545 1.00 18.03
N
ATOM 6054 CA TYR D 111 -15.768 57.132 -2.489 1.00 17.44
C
ATOM 6055 C TYR D 111 -14.471 57.677 -1.920 1.00 15.34
C
ATOM 6056 O TYR D 111 -13.731 58.388 -2.600 1.00 20.20
O
ATOM 6057 CB TYR D 111 -15.515 55.718 -3.016 1.00 18.77
C
ATOM 6058 CG TYR D 111 -16.678 55.089 -3.737 1.00 20.60
C
ATOM 6059 CD1 TYR D 111 -16.879 55.308 -5.090 1.00 15.51
C
ATOM 6060 CD2 TYR D 111 -17.561 54.251 -3.070 1.00 20.76
C
ATOM 6061 CE1 TYR D 111 -17.936 54.723 -5.757 1.00 18.59
C
ATOM 6062 CE2 TYR D 111 -18.625 53.664 -3.728 1.00 17.85
C
ATOM 6063 CZ TYR D 111 -18.806 53.903 -5.071 1.00 18.90
C
ATOM 6064 OH TYR D 111 -19.868 53.323 -5.732 1.00 19.85
O
ATOM 6065 H TYR D 111 -15.691 58.220 -4.132 1.00 21.63
H
ATOM 6066 HA TYR D 111 -16.418 57.080 -1.772 1.00 20.92
H
ATOM 6067 HB2 TYR D 111 -14.769 55.748 -3.635 1.00 22.52
H
ATOM 6068 HB3 TYR D 111 -15.291 55.145 -2.266 1.00 22.52
H
ATOM 6069 HD1 TYR D 111 -16.294 55.862 -5.556 1.00 18.61
H
ATOM 6070 HD2 TYR D 111 -17.440 54.089 -2.162 1.00 24.91
H
ATOM 6071 HE1 TYR D 111 -18.064 54.885 -6.664 1.00 22.30
H
ATOM 6072 HE2 TYR D 111 -19.212 53.110 -3.267 1.00 21.42
H
ATOM 6073 HH TYR D 111 -19.863 53.553 -6.540 1.00 23.82
H
ATOM 6074 N GLN D 112 -14.190 57.329 -0.673 1.00 17.91
N

ATOM 12341 HB3 MET F 135 -11.126 37.577 7.288 1.00 18.66
H
ATOM 12342 HG2 MET F 135 -8.707 38.985 7.655 1.00 22.72
H
ATOM 12343 HG3 MET F 135 -9.986 39.605 6.947 1.00 22.72
H
ATOM 12344 HE1 MET F 135 -12.427 40.272 9.593 1.00 27.63
H
ATOM 12345 HE2 MET F 135 -11.982 40.613 8.107 1.00 27.63
H
ATOM 12346 HE3 MET F 135 -12.403 39.129 8.490 1.00 27.63
H

ATOM 12347 N HIS F 136 -9.727 34.394 6.950 1.00 17.74 N
ATOM 12348 CA HIS F 136 -10.191 33.034 6.677 1.00 14.38
C

ATOM 12349 C HIS F 136 -10.007 32.155 7.908 1.00 15.88 C

ATOM 12350 O HIS F 136 -10.899 31.400 8.284 1.00 15.42 O

ATOM 12351 CB HIS F 136 -9.443 32.412 5.489 1.00 16.15 C

ATOM 12352 CG HIS F 136 -9.875 32.932 4.152 1.00 15.03 C
ATOM 12353 ND1 HIS F 136 -9.959 32.127 3.035 1.00 15.21
N
ATOM 12354 CD2 HIS F 136 -10.236 34.172 3.748 1.00 13.64
C
ATOM 12355 CE1 HIS F 136 -10.355 32.850 2.003 1.00 15.34
C
ATOM 12356 NE2 HIS F 136 -10.530 34.094 2.408 1.00 15.92
N

ATOM 12357 H HIS F 136 -9.074 34.650 6.451 1.00 21.29 H
ATOM 12358 HA HIS F 136 -11.136 33.058 6.461 1.00 17.26
H
ATOM 12359 HB2 HIS F 136 -8.495 32.598 5.586 1.00 19.38
H
ATOM 12360 HB3 HIS F 136 -9.591 31.453 5.495 1.00 19.38
H
ATOM 12361 HD1 HIS F 136 -9.780 31.286 3.013 1.00 18.25
H
ATOM 12362 HD2 HIS F 136 -10.277 34.935 4.279 1.00 16.36
H
ATOM 12363 HE1 HIS F 136 -10.489 32.535 1.138 1.00 18.41
H
ATOM 12364 HE2 HIS F 136 -10.788 34.749 1.914 1.00 19.10
H

ATOM 12365 N LEU F 137 -8.833 32.255 8.523 1.00 14.21 N
ATOM 12366 CA LEU F 137 -8.515 31.483 9.717 1.00 16.46
C

ATOM 12367 C LEU F 137 -9.530 31.739 10.832 1.00 16.07 C
ATOM 12368 O LEU F 137 -10.045 30.804 11.433 1.00 16.54
O
ATOM 12369 CB LEU F 137 -7.101 31.819 10.196 1.00 16.82
C
ATOM 12370 CG LEU F 137 -6.696 31.348 11.597 1.00 17.25
C
ATOM 12371 CD1 LEU F 137 -6.909 29.855 11.775 1.00 21.45
C
ATOM 12372 CD2 LEU F 137 -5.239 31.707 11.858 1.00 16.99
C

ATOM 12373 H LEU F 137 -8.195 32.769 8.263 1.00 17.06 H
ATOM 12374 HA LEU F 137 -8.542 30.538 9.499 1.00 19.75
H

ATOM 6075 CA GLN D 112 -12.866 57.552 -0.119 1.00 20.98
C
ATOM 6076 C GLN D 112 -12.549 56.483 0.914 1.00 18.40
C
ATOM 6077 O GLN D 112 -13.417 56.045 1.668 1.00 17.57
O
ATOM 6078 CB GLN D 112 -12.750 58.949 0.496 1.00 23.03
C
ATOM 6079 CG GLN D 112 -11.326 59.331 0.905 1.00 24.86
C
ATOM 6080 CD GLN D 112 -10.317 59.175 -0.225 1.00 29.43
C
ATOM 6081 OE1 GLN D 112 -9.797 58.083 -0.469 1.00 32.59
O
ATOM 6082 NE2 GLN D 112 -10.033 60.270 -0.920 1.00 35.19
N
ATOM 6083 H GLN D 112 -14.747 56.965 -0.128 1.00 21.49
H
ATOM 6084 HA GLN D 112 -12.211 57.483 -0.831 1.00 25.18
H
ATOM 6085 HB2 GLN D 112 -13.057 59.602 -0.152 1.00 27.63
H
ATOM 6086 HB3 GLN D 112 -13.306 58.987 1.290 1.00 27.63
H
ATOM 6087 HG2 GLN D 112 -11.318 60.259 1.187 1.00 29.83
H
ATOM 6088 HG3 GLN D 112 -11.045 58.760 1.637 1.00 29.83
H
ATOM 6089 HE21 GLN D 112 -9.469 60.234 -1.568 1.00 42.23
H
ATOM 6090 HE22 GLN D 112 -10.414 61.015 -0.721 1.00 42.23
H
ATOM 6091 N PHE D 113 -11.293 56.059 0.921 1.00 15.24
N
ATOM 6092 CA PHE D 113 -10.808 55.082 1.878 1.00 19.47
C
ATOM 6093 C PHE D 113 -10.013 55.796 2.963 1.00 22.57
C
ATOM 6094 O PHE D 113 -9.202 56.678 2.676 1.00 28.44
O
ATOM 6095 CB PHE D 113 -9.955 54.026 1.172 1.00 25.43
C
ATOM 6096 CG PHE D 113 -10.730 53.179 0.198 1.00 22.13
C
ATOM 6097 CD1 PHE D 113 -11.227 53.727 -0.976 1.00 29.41
C
ATOM 6098 CD2 PHE D 113 -10.953 51.836 0.450 1.00 23.89
C
ATOM 6099 CE1 PHE D 113 -11.940 52.951 -1.877 1.00 30.31
C
ATOM 6100 CE2 PHE D 113 -11.666 51.054 -0.447 1.00 21.37
C
ATOM 6101 CZ PHE D 113 -12.160 51.613 -1.610 1.00 23.83
C
ATOM 6102 H PHE D 113 -10.692 56.330 0.369 1.00 18.29
H
ATOM 6103 HA PHE D 113 -11.562 54.637 2.294 1.00 23.37
H
ATOM 6104 HB2 PHE D 113 -9.247 54.472 0.681 1.00 30.51
H
ATOM 6105 HB3 PHE D 113 -9.571 53.436 1.839 1.00 30.51
H
ATOM 6106 HD1 PHE D 113 -11.084 54.627 -1.159 1.00 35.29
H
ATOM 6107 HD2 PHE D 113 -10.625 51.455 1.232 1.00 28.66
H
ATOM 6108 HE1 PHE D 113 -12.270 53.330 -2.659 1.00 36.37
H
ATOM 12375 HB2 LEU F 137 -6.472 31.425 9.572 1.00 20.18
H
ATOM 12376 HB3 LEU F 137 -7.000 32.784 10.182 1.00 20.18
H
ATOM 12377 HG LEU F 137 -7.240 31.808 12.254 1.00 20.69
H
ATOM 12378 HD11 LEU F 137 -6.640 29.603 12.672 1.00 25.74
H
ATOM 12379 HD12 LEU F 137 -7.848 29.653 11.641 1.00 25.74
H
ATOM 12380 HD13 LEU F 137 -6.372 29.380 11.122 1.00 25.74
H
ATOM 12381 HD21 LEU F 137 -4.994 31.404 12.747 1.00 20.39
H
ATOM 12382 HD22 LEU F 137 -4.682 31.271 11.195 1.00 20.39
H
ATOM 12383 HD23 LEU F 137 -5.136 32.670 11.797 1.00 20.39
H
ATOM 12384 N ARG F 138 -9.817 33.006 11.100 1.00 15.78
N
ATOM 12385 CA ARG F 138 -10.767 33.360 12.147 1.00 21.48
C
ATOM 12386 C ARG F 138 -12.162 32.844 11.802 1.00 20.46
C
ATOM 12387 O ARG F 138 -12.903 32.389 12.676 1.00 17.61
O
ATOM 12388 CB ARG F 138 -10.791 34.875 12.353 1.00 20.11
C
ATOM 12389 CG ARG F 138 -9.496 35.437 12.926 1.00 22.32
C
ATOM 12390 CD ARG F 138 -9.536 36.954 13.003 1.00 22.66
C
ATOM 12391 NE ARG F 138 -10.564 37.424 13.925 1.00 25.37
N
ATOM 12392 CZ ARG F 138 -10.969 38.686 14.016 1.00 33.49
C
ATOM 12393 NH1 ARG F 138 -10.435 39.618 13.241 1.00 30.85
N1+
ATOM 12394 NH2 ARG F 138 -11.917 39.018 14.882 1.00 35.00
N
ATOM 12395 H ARG F 138 -9.477 33.681 10.690 1.00 18.94
H
ATOM 12396 HA ARG F 138 -10.490 32.946 12.979 1.00 25.77
H
ATOM 12397 HB2 ARG F 138 -10.948 35.305 11.498 1.00 24.13
H
ATOM 12398 HB3 ARG F 138 -11.507 35.096 12.969 1.00 24.13
H
ATOM 12399 HG2 ARG F 138 -9.364 35.090 13.822 1.00 26.78
H
ATOM 12400 HG3 ARG F 138 -8.755 35.181 12.354 1.00 26.78
H
ATOM 12401 HD2 ARG F 138 -8.678 37.281 13.315 1.00 27.20
H
ATOM 12402 HD3 ARG F 138 -9.731 37.313 12.123 1.00 27.20
H
ATOM 12403 HE ARG F 138 -10.932 36.845 14.443 1.00 30.44
H
ATOM 12404 HH11 ARG F 138 -9.821 39.407 12.676 1.00 37.02
H
ATOM 12405 HH12 ARG F 138 -10.700 40.433 13.303 1.00 37.02
H
ATOM 12406 HH21 ARG F 138 -12.267 38.417 15.388 1.00 42.00
H
ATOM 12407 HH22 ARG F 138 -12.178 39.836 14.942 1.00 42.00
H
ATOM 12408 N SER F 139 -12.505 32.898 10.520 1.00 17.64
N

ATOM 6109 HE2 PHE D 113 -11.812 50.154 -0.265 1.00 25.65
H
ATOM 6110 HZ PHE D 113 -12.637 51.089 -2.213 1.00 28.60
H
ATOM 6111 N PHE D 114 -10.275 55.420 4.209 1.00 21.22
N
ATOM 6112 CA PHE D 114 -9.633 56.027 5.368 1.00 22.84
C
ATOM 6113 C PHE D 114 -8.840 54.967 6.111 1.00 25.57
C
ATOM 6114 O PHE D 114 -9.409 53.987 6.590 1.00 20.97
O
ATOM 6115 CB PHE D 114 -10.682 56.665 6.280 1.00 25.74
C
ATOM 6116 CG PHE D 114 -11.434 57.787 5.629 1.00 22.57
C
ATOM 6117 CD1 PHE D 114 -12.523 57.530 4.817 1.00 23.79
C
ATOM 6118 CD2 PHE D 114 -11.041 59.102 5.819 1.00 30.88
C
ATOM 6119 CE1 PHE D 114 -13.208 58.562 4.209 1.00 26.61
C
ATOM 6120 CE2 PHE D 114 -11.723 60.139 5.214 1.00 23.44
C
ATOM 6121 CZ PHE D 114 -12.809 59.869 4.409 1.00 28.06
C
ATOM 6122 H PHE D 114 -10.835 54.801 4.413 1.00 25.46
H
ATOM 6123 HA PHE D 114 -9.020 56.719 5.073 1.00 27.40
H
ATOM 6124 HB2 PHE D 114 -11.325 55.987 6.540 1.00 30.89
H
ATOM 6125 HB3 PHE D 114 -10.240 57.019 7.067 1.00 30.89
H
ATOM 6126 HD1 PHE D 114 -12.796 56.652 4.678 1.00 28.55
H
ATOM 6127 HD2 PHE D 114 -10.308 59.288 6.361 1.00 37.05
H
ATOM 6128 HE1 PHE D 114 -13.941 58.378 3.667 1.00 31.94
H
ATOM 6129 HE2 PHE D 114 -11.451 61.018 5.351 1.00 28.13
H
ATOM 6130 HZ PHE D 114 -13.271 60.565 4.001 1.00 33.67
H
ATOM 6131 N ASP D 115 -7.526 55.161 6.199 1.00 23.12
N
ATOM 6132 CA ASP D 115 -6.645 54.131 6.737 1.00 26.22
C
ATOM 6133 C ASP D 115 -6.365 54.317 8.228 1.00 30.31
C
ATOM 6134 O ASP D 115 -5.656 53.516 8.831 1.00 25.41
O
ATOM 6135 CB ASP D 115 -5.328 54.096 5.957 1.00 27.72
C
ATOM 6136 CG ASP D 115 -4.615 55.436 5.940 1.00 34.76
C
ATOM 6137 OD1 ASP D 115 -5.100 56.389 6.587 1.00 33.82
O
ATOM 6138 OD2 ASP D 115 -3.558 55.530 5.282 1.00 32.71
O1-
ATOM 6139 H ASP D 115 -7.122 55.879 5.954 1.00 27.74
H
ATOM 6140 HA ASP D 115 -7.075 53.269 6.626 1.00 31.46
H
ATOM 6141 HB2 ASP D 115 -4.735 53.447 6.367 1.00 33.26
H
ATOM 6142 HB3 ASP D 115 -5.512 53.843 5.039 1.00 33.26
H

ATOM 12409 CA SER F 139 -13.798 32.413 10.056 1.00 19.10
C
ATOM 12410 C SER F 139 -13.890 30.893 10.165 1.00 20.53
C
ATOM 12411 O SER F 139 -14.945 30.348 10.492 1.00 20.71
O
ATOM 12412 CB SER F 139 -14.042 32.855 8.613 1.00 21.03
C
ATOM 12413 OG SER F 139 -14.120 34.266 8.526 1.00 16.92
O
ATOM 12414 H SER F 139 -12.003 33.212 9.896 1.00 21.17
H
ATOM 12415 HA SER F 139 -14.496 32.797 10.609 1.00 22.92
H
ATOM 12416 HB2 SER F 139 -13.308 32.545 8.059 1.00 25.24
H
ATOM 12417 HB3 SER F 139 -14.877 32.473 8.302 1.00 25.24
H
ATOM 12418 HG SER F 139 -13.402 34.611 8.793 1.00 20.30
H

ATOM 12419 N LEU F 140 -12.783 30.210 9.897 1.00 17.28 N
ATOM 12420 CA LEU F 140 -12.766 28.753 9.949 1.00 20.30
C
ATOM 12421 C LEU F 140 -12.769 28.260 11.394 1.00 21.22
C
ATOM 12422 O LEU F 140 -13.346 27.216 11.695 1.00 23.85
O
ATOM 12423 CB LEU F 140 -11.554 28.201 9.195 1.00 21.20
C
ATOM 12424 CG LEU F 140 -11.611 28.339 7.669 1.00 20.22
C
ATOM 12425 CD1 LEU F 140 -10.258 28.037 7.052 1.00 19.97
C
ATOM 12426 CD2 LEU F 140 -12.680 27.431 7.075 1.00 21.22
C

ATOM 12427 H LEU F 140 -12.030 30.565 9.682 1.00 20.74 H
ATOM 12428 HA LEU F 140 -13.566 28.415 9.517 1.00 24.37
H
ATOM 12429 HB2 LEU F 140 -10.762 28.671 9.500 1.00 25.44
H
ATOM 12430 HB3 LEU F 140 -11.469 27.257 9.399 1.00 25.44
H
ATOM 12431 HG LEU F 140 -11.841 29.254 7.446 1.00 24.27
H
ATOM 12432 HD11 LEU F 140 -10.323 28.132 6.088 1.00 23.96
H
ATOM 12433 HD12 LEU F 140 -9.605 28.662 7.402 1.00 23.96
H
ATOM 12434 HD13 LEU F 140 -10.003 27.129 7.279 1.00 23.96
H
ATOM 12435 HD21 LEU F 140 -12.689 27.542 6.112 1.00 25.46
H
ATOM 12436 HD22 LEU F 140 -12.473 26.510 7.300 1.00 25.46
H
ATOM 12437 HD23 LEU F 140 -13.543 27.676 7.445 1.00 25.46
H
ATOM 12438 N VAL F 141 -12.132 29.008 12.288 1.00 19.00
N
ATOM 12439 CA VAL F 141 -12.164 28.668 13.704 1.00 23.28
C
ATOM 12440 C VAL F 141 -13.590 28.802 14.237 1.00 25.21
C
ATOM 12441 O VAL F 141 -14.020 28.017 15.081 1.00 24.34
O
ATOM 12442 CB VAL F 141 -11.210 29.556 14.528 1.00 19.95
C

ATOM 6143 N GLU D 116 -6.920 55.373 8.817 1.00 29.51
N
ATOM 6144 CA GLU D 116 -6.821 55.578 10.259 1.00 35.02
C
ATOM 6145 C GLU D 116 -7.960 54.814 10.921 1.00 33.34
C
ATOM 6146 O GLU D 116 -9.096 55.282 10.940 1.00 33.54
O
ATOM 6147 CB GLU D 116 -6.880 57.067 10.624 1.00 38.38
C
ATOM 6148 CG GLU D 116 -5.921 57.960 9.836 1.00 42.91
C
ATOM 6149 CD GLU D 116 -6.444 58.351 8.458 1.00 44.87
C
ATOM 6150 OE1 GLU D 116 -7.627 58.078 8.155 1.00 38.52
O
ATOM 6151 OE2 GLU D 116 -5.664 58.934 7.673 1.00 52.44
O1-
ATOM 6152 H GLU D 116 -7.360 55.986 8.404 1.00 35.41
H
ATOM 6153 HA GLU D 116 -5.980 55.216 10.580 1.00 42.03
H
ATOM 6154 HB2 GLU D 116 -7.781 57.389 10.462 1.00 46.06
H
ATOM 6155 HB3 GLU D 116 -6.665 57.163 11.565 1.00 46.06
H
ATOM 6156 HG2 GLU D 116 -5.768 58.775 10.338 1.00 51.49
H
ATOM 6157 HG3 GLU D 116 -5.083 57.487 9.712 1.00 51.49
H
ATOM 6158 N SER D 117 -7.650 53.636 11.457 1.00 30.25
N
ATOM 6159 CA SER D 117 -8.674 52.697 11.907 1.00 27.86
C
ATOM 6160 C SER D 117 -9.509 53.219 13.077 1.00 33.38
C
ATOM 6161 O SER D 117 -8.988 53.810 14.022 1.00 30.47
O
ATOM 6162 CB SER D 117 -8.028 51.365 12.297 1.00 31.01
C
ATOM 6163 OG SER D 117 -7.150 51.529 13.392 1.00 34.10
O
ATOM 6164 H SER D 117 -6.845 53.355 11.571 1.00 36.30
H
ATOM 6165 HA SER D 117 -9.279 52.525 11.169 1.00 33.44
H
ATOM 6166 HB2 SER D 117 -8.725 50.737 12.543 1.00 37.21
H
ATOM 6167 HB3 SER D 117 -7.527 51.024 11.539 1.00 37.21
H
ATOM 6168 HG SER D 117 -6.803 50.792 13.595 1.00 40.92
H
ATOM 6169 N LYS D 118 -10.814 52.976 12.992 1.00 27.74
N
ATOM 6170 CA LYS D 118 -11.771 53.385 14.015 1.00 27.96
C
ATOM 6171 C LYS D 118 -12.805 52.284 14.202 1.00 31.80
C
ATOM 6172 O LYS D 118 -12.946 51.409 13.343 1.00 27.27
O
ATOM 6173 CB LYS D 118 -12.464 54.689 13.619 1.00 25.67
C
ATOM 6174 CG LYS D 118 -11.533 55.875 13.440 1.00 29.25
C
ATOM 6175 CD LYS D 118 -12.293 57.075 12.904 1.00 36.12
C
ATOM 6176 CE LYS D 118 -11.416 58.312 12.827 1.00 36.20
C
ATOM 12443 CG1 VAL F 141 -11.452 29.377 16.024 1.00 26.02
C
ATOM 12444 CG2 VAL F 141 -9.758 29.225 14.198 1.00 24.20
C
ATOM 12445 H VAL F 141 -11.678 29.714 12.101 1.00 22.80
H
ATOM 12446 HA VAL F 141 -11.886 27.745 13.814 1.00 27.94
H
ATOM 12447 HB VAL F 141 -11.367 30.487 14.305 1.00 23.94
H
ATOM 12448 HG11 VAL F 141 -10.838 29.947 16.514 1.00 31.23
H
ATOM 12449 HG12 VAL F 141 -12.368 29.624 16.227 1.00 31.23
H
ATOM 12450 HG13 VAL F 141 -11.300 28.448 16.259 1.00 31.23
H
ATOM 12451 HG21 VAL F 141 -9.177 29.794 14.727 1.00 29.04
H
ATOM 12452 HG22 VAL F 141 -9.591 28.293 14.410 1.00 29.04
H
ATOM 12453 HG23 VAL F 141 -9.605 29.382 13.253 1.00 29.04
H
ATOM 12454 N ARG F 142 -14.315 29.802 13.745 1.00 21.37
N
ATOM 12455 CA ARG F 142 -15.718 29.978 14.107 1.00 23.25
C
ATOM 12456 C ARG F 142 -16.534 28.742 13.722 1.00 30.62
C
ATOM 12457 O ARG F 142 -17.319 28.235 14.525 1.00 27.61
O
ATOM 12458 CB ARG F 142 -16.286 31.230 13.436 1.00 28.79
C
ATOM 12459 CG ARG F 142 -17.776 31.456 13.656 1.00 34.59
C
ATOM 12460 CD ARG F 142 -18.109 31.669 15.122 1.00 36.74
C
ATOM 12461 NE ARG F 142 -19.526 31.963 15.311 1.00 43.29
N
ATOM 12462 CZ ARG F 142 -20.073 33.164 15.149 1.00 47.11
C
ATOM 12463 NH1 ARG F 142 -19.325 34.201 14.794 1.00 40.67
N1+
ATOM 12464 NH2 ARG F 142 -21.373 33.330 15.342 1.00 53.09
N
ATOM 12465 H ARG F 142 -14.017 30.395 13.197 1.00 25.65
H
ATOM 12466 HA ARG F 142 -15.785 30.095 15.068 1.00 27.90
H
ATOM 12467 HB2 ARG F 142 -15.818 32.006 13.782 1.00 34.55
H
ATOM 12468 HB3 ARG F 142 -16.138 31.161 12.479 1.00 34.55
H
ATOM 12469 HG2 ARG F 142 -18.054 32.244 13.164 1.00 41.50
H
ATOM 12470 HG3 ARG F 142 -18.265 30.678 13.345 1.00 41.50
H
ATOM 12471 HD2 ARG F 142 -17.896 30.864 15.619 1.00 44.08
H
ATOM 12472 HD3 ARG F 142 -17.595 32.419 15.461 1.00 44.08
H
ATOM 12473 HE ARG F 142 -20.043 31.315 15.542 1.00 51.95
H
ATOM 12474 HH11 ARG F 142 -18.480 34.099 14.666 1.00 48.80
H
ATOM 12475 HH12 ARG F 142 -19.684 34.975 14.691 1.00 48.80
H
ATOM 12476 HH21 ARG F 142 -21.862 32.662 15.573 1.00 63.71
H

ATOM 6177 NZ LYS D 118 -10.988 58.767 14.175 1.00 46.64
N1+
ATOM 6178 H LYS D 118 -11.179 52.564 12.332 1.00 33.29
H
ATOM 6179 HA LYS D 118 -11.309 53.523 14.856 1.00 33.55
H
ATOM 6180 HB2 LYS D 118 -12.928 54.550 12.778 1.00 30.81
H
ATOM 6181 HB3 LYS D 118 -13.105 54.921 14.310 1.00 30.81
H
ATOM 6182 HG2 LYS D 118 -11.146 56.114 14.297 1.00 35.10
H
ATOM 6183 HG3 LYS D 118 -10.836 55.645 12.806 1.00 35.10
H
ATOM 6184 HD2 LYS D 118 -12.615 56.876 12.011 1.00 43.34
H
ATOM 6185 HD3 LYS D 118 -13.039 57.269 13.493 1.00 43.34
H
ATOM 6186 HE2 LYS D 118 -10.621 58.108 12.310 1.00 43.44
H
ATOM 6187 HE3 LYS D 118 -11.914 59.031 12.408 1.00 43.44
H
ATOM 6188 HZ1 LYS D 118 -10.477 59.492 14.103 1.00 55.96
H
ATOM 6189 HZ2 LYS D 118 -11.701 58.965 14.670 1.00 55.96
H
ATOM 6190 HZ3 LYS D 118 -10.524 58.125 14.580 1.00 55.96
H
ATOM 6191 N ASN D 119 -13.531 52.314 15.316 1.00 28.46
N
ATOM 6192 CA ASN D 119 -14.632 51.378 15.495 1.00 27.04
C
ATOM 6193 C ASN D 119 -15.773 51.811 14.585 1.00 24.03
C
ATOM 6194 O ASN D 119 -15.713 52.884 13.985 1.00 24.95
O
ATOM 6195 CB ASN D 119 -15.068 51.301 16.964 1.00 27.48
C
ATOM 6196 CG ASN D 119 -15.649 52.600 17.483 1.00 26.83
C
ATOM 6197 OD1 ASN D 119 -16.565 53.173 16.895 1.00 25.34
O
ATOM 6198 ND2 ASN D 119 -15.119 53.069 18.606 1.00 37.21
N
ATOM 6199 H ASN D 119 -13.408 52.858 15.971 1.00 34.15
H
ATOM 6200 HA ASN D 119 -14.345 50.494 15.220 1.00 32.45
H
ATOM 6201 HB2 ASN D 119 -15.747 50.613 17.054 1.00 32.97
H
ATOM 6202 HB3 ASN D 119 -14.298 51.079 17.510 1.00 32.97
H
ATOM 6203 HD21 ASN D 119 -15.411 53.803 18.945 1.00 44.65
H
ATOM 6204 HD22 ASN D 119 -14.484 52.638 18.994 1.00 44.65
H
ATOM 6205 N TRP D 120 -16.807 50.986 14.472 1.00 21.37
N
ATOM 6206 CA TRP D 120 -17.855 51.238 13.492 1.00 24.98
C
ATOM 6207 C TRP D 120 -18.589 52.545 13.770 1.00 24.15
C
ATOM 6208 O TRP D 120 -18.945 53.274 12.844 1.00 19.58
O
ATOM 6209 CB TRP D 120 -18.855 50.083 13.460 1.00 21.60
C
ATOM 6210 CG TRP D 120 -19.879 50.242 12.386 1.00 23.54
C
ATOM 12477 HH22 ARG F 142 -21.727 34.107 15.239 1.00 63.71
H
ATOM 12478 N LYS F 143 -16.343 28.261 12.495 1.00 24.90
N
ATOM 12479 CA LYS F 143 -17.016 27.049 12.034 1.00 28.02
C
ATOM 12480 C LYS F 143 -16.646 25.854 12.897 1.00 28.44
C
ATOM 12481 O LYS F 143 -17.509 25.084 13.314 1.00 28.33
O
ATOM 12482 CB LYS F 143 -16.656 26.740 10.581 1.00 27.89
C
ATOM 12483 CG LYS F 143 -17.165 27.743 9.576 1.00 21.75
C
ATOM 12484 CD LYS F 143 -16.613 27.446 8.190 1.00 24.93
C
ATOM 12485 CE LYS F 143 -17.698 26.971 7.242 1.00 33.41
C
ATOM 12486 NZ LYS F 143 -18.262 25.655 7.631 1.00 38.22
N1+
ATOM 12487 H LYS F 143 -15.826 28.619 11.908 1.00 29.88
H
ATOM 12488 HA LYS F 143 -17.976 27.177 12.089 1.00 33.63
H
ATOM 12489 HB2 LYS F 143 -15.689 26.711 10.502 1.00 33.47
H
ATOM 12490 HB3 LYS F 143 -17.028 25.876 10.347 1.00 33.47
H
ATOM 12491 HG2 LYS F 143 -18.133 27.697 9.536 1.00 26.10
H
ATOM 12492 HG3 LYS F 143 -16.879 28.633 9.835 1.00 26.10
H
ATOM 12493 HD2 LYS F 143 -16.221 28.253 7.822 1.00 29.91
H
ATOM 12494 HD3 LYS F 143 -15.942 26.748 8.256 1.00 29.91
H
ATOM 12495 HE2 LYS F 143 -18.420 27.618 7.239 1.00 40.09
H
ATOM 12496 HE3 LYS F 143 -17.324 26.886 6.351 1.00 40.09
H
ATOM 12497 HZ1 LYS F 143 -17.620 25.038 7.635 1.00 45.86
H
ATOM 12498 HZ2 LYS F 143 -18.619 25.706 8.445 1.00 45.86
H
ATOM 12499 HZ3 LYS F 143 -18.893 25.412 7.052 1.00 45.86
H
ATOM 12500 N MET F 144 -15.350 25.703 13.146 1.00 24.38
N
ATOM 12501 CA MET F 144 -14.836 24.550 13.866 1.00 27.30
C
ATOM 12502 C MET F 144 -15.415 24.490 15.276 1.00 34.88
C
ATOM 12503 O MET F 144 -15.839 23.429 15.735 1.00 35.17
O
ATOM 12504 CB MET F 144 -13.307 24.597 13.910 1.00 31.14
C
ATOM 12505 CG MET F 144 -12.660 23.367 14.523 1.00 31.20
C
ATOM 12506 SD MET F 144 -11.998 23.709 16.160 1.00 44.38
S
ATOM 12507 CE MET F 144 -10.619 24.779 15.748 1.00 36.74
C
ATOM 12508 H MET F 144 -14.743 26.263 12.906 1.00 29.26
H
ATOM 12509 HA MET F 144 -15.093 23.745 13.389 1.00 32.76
H
ATOM 12510 HB2 MET F 144 -12.973 24.685 13.004 1.00 37.36
H

ATOM 6211 CD1 TRP D 120 -19.797 49.787 11.102 1.00 24.11
C
ATOM 6212 CD2 TRP D 120 -21.137 50.917 12.493 1.00 26.63
C
ATOM 6213 NE1 TRP D 120 -20.927 50.135 10.404 1.00 25.43
N
ATOM 6214 CE2 TRP D 120 -21.766 50.828 11.236 1.00 27.74
C
ATOM 6215 CE3 TRP D 120 -21.793 51.587 13.531 1.00 30.26
C
ATOM 6216 CZ2 TRP D 120 -23.020 51.379 10.989 1.00 28.23
C
ATOM 6217 CZ3 TRP D 120 -23.036 52.136 13.283 1.00 28.53
C
ATOM 6218 CH2 TRP D 120 -23.637 52.030 12.022 1.00 29.49
C
ATOM 6219 H TRP D 120 -16.924 50.278 14.947 1.00 25.65
H
ATOM 6220 HA TRP D 120 -17.452 51.305 12.612 1.00 29.98
H
ATOM 6221 HB2 TRP D 120 -18.377 49.255 13.300 1.00 25.92
H
ATOM 6222 HB3 TRP D 120 -19.317 50.041 14.312 1.00 25.92
H
ATOM 6223 HD1 TRP D 120 -19.079 49.312 10.750 1.00 28.93
H
ATOM 6224 HE1 TRP D 120 -21.084 49.945 9.580 1.00 30.52
H
ATOM 6225 HE3 TRP D 120 -21.400 51.661 14.370 1.00 36.31
H
ATOM 6226 HZ2 TRP D 120 -23.421 51.312 10.153 1.00 33.87
H
ATOM 6227 HZ3 TRP D 120 -23.482 52.583 13.965 1.00 34.24
H
ATOM 6228 HH2 TRP D 120 -24.475 52.408 11.885 1.00 35.38
H
ATOM 6229 N TYR D 121 -18.808 52.839 15.047 1.00 27.37
N
ATOM 6230 CA TYR D 121 -19.558 54.028 15.438 1.00 29.38
C
ATOM 6231 C TYR D 121 -18.799 55.295 15.065 1.00 22.01
C
ATOM 6232 O TYR D 121 -19.365 56.214 14.481 1.00 23.03
O
ATOM 6233 CB TYR D 121 -19.857 54.001 16.939 1.00 32.74
C
ATOM 6234 CG TYR D 121 -20.587 52.751 17.378 1.00 29.99
C
ATOM 6235 CD1 TYR D 121 -21.946 52.598 17.144 1.00 35.21
C
ATOM 6236 CD2 TYR D 121 -19.911 51.718 18.016 1.00 32.98
C
ATOM 6237 CE1 TYR D 121 -22.616 51.452 17.538 1.00 36.69
C
ATOM 6238 CE2 TYR D 121 -20.571 50.569 18.414 1.00 36.17
C
ATOM 6239 CZ TYR D 121 -21.922 50.442 18.172 1.00 40.29
C
ATOM 6240 OH TYR D 121 -22.582 49.300 18.566 1.00 49.60
O
ATOM 6241 H TYR D 121 -18.531 52.365 15.709 1.00 32.84
H
ATOM 6242 HA TYR D 121 -20.405 54.036 14.964 1.00 35.25
H
ATOM 6243 HB2 TYR D 121 -19.020 54.046 17.428 1.00 39.29
H
ATOM 6244 HB3 TYR D 121 -20.412 54.765 17.163 1.00 39.29
H
ATOM 12511 HB3 MET F 144 -13.035 25.365 14.435 1.00 37.36
H
ATOM 12512 HG2 MET F 144 -13.323 22.664 14.605 1.00 37.44
H
ATOM 12513 HG3 MET F 144 -11.930 23.074 13.955 1.00 37.44
H
ATOM 12514 HE1 MET F 144 -10.168 25.040 16.566 1.00 44.09
H
ATOM 12515 HE2 MET F 144 -10.007 24.296 15.172 1.00 44.09
H
ATOM 12516 HE3 MET F 144 -10.956 25.565 15.290 1.00 44.09
H
ATOM 12517 N GLU F 145 -15.455 25.636 15.948 1.00 29.62
N
ATOM 12518 CA GLU F 145 -15.954 25.704 17.316 1.00 35.30
C
ATOM 12519 C GLU F 145 -17.462 25.475 17.409 1.00 33.13
C
ATOM 12520 O GLU F 145 -17.954 24.977 18.420 1.00 34.65
O
ATOM 12521 CB GLU F 145 -15.597 27.055 17.934 1.00 31.57
C
ATOM 12522 CG GLU F 145 -14.112 27.209 18.208 1.00 33.34
C
ATOM 12523 CD GLU F 145 -13.765 28.538 18.842 1.00 32.82
C
ATOM 12524 OE1 GLU F 145 -14.628 29.444 18.853 1.00 41.83
O
ATOM 12525 OE2 GLU F 145 -12.625 28.672 19.332 1.00 37.68
O1-
ATOM 12526 H GLU F 145 -15.197 26.392 15.631 1.00 35.54
H
ATOM 12527 HA GLU F 145 -15.518 25.015 17.841 1.00 42.36
H
ATOM 12528 HB2 GLU F 145 -15.864 27.760 17.324 1.00 37.89
H
ATOM 12529 HB3 GLU F 145 -16.069 27.150 18.776 1.00 37.89
H
ATOM 12530 HG2 GLU F 145 -13.828 26.506 18.813 1.00 40.00
H
ATOM 12531 HG3 GLU F 145 -13.628 27.142 17.370 1.00 40.00
H
ATOM 12532 N ASP F 146 -18.190 25.837 16.359 1.00 33.24
N
ATOM 12533 CA ASP F 146 -19.641 25.667 16.339 1.00 37.33
C
ATOM 12534 C ASP F 146 -20.054 24.299 15.791 1.00 42.30
C
ATOM 12535 O ASP F 146 -21.244 24.010 15.660 1.00 50.59
O
ATOM 12536 CB ASP F 146 -20.292 26.776 15.510 1.00 34.15
C
ATOM 12537 CG ASP F 146 -20.188 28.139 16.169 1.00 38.34
C
ATOM 12538 OD1 ASP F 146 -19.944 28.201 17.393 1.00 39.97
O
ATOM 12539 OD2 ASP F 146 -20.362 29.152 15.460 1.00 37.23
O1-
ATOM 12540 H ASP F 146 -17.868 26.186 15.641 1.00 39.88
H
ATOM 12541 HA ASP F 146 -19.976 25.737 17.247 1.00 44.79
H
ATOM 12542 HB2 ASP F 146 -19.853 26.825 14.647 1.00 40.97
H
ATOM 12543 HB3 ASP F 146 -21.233 26.570 15.393 1.00 40.97
H
ATOM 12544 N SER F 147 -19.073 23.459 15.476 1.00 44.15
N

ATOM 6245 HD1 TYR D 121 -22.416 53.277 16.716 1.00 42.26
H
ATOM 6246 HD2 TYR D 121 -19.000 51.801 18.180 1.00 39.57
H
ATOM 6247 HE1 TYR D 121 -23.527 51.364 17.376 1.00 44.02
H
ATOM 6248 HE2 TYR D 121 -20.106 49.887 18.842 1.00 43.40
H
ATOM 6249 HH TYR D 121 -22.045 48.771 18.937 1.00 59.52
H
ATOM 6250 N GLU D 122 -17.513 55.332 15.395 1.00 23.53
N
ATOM 6251 CA GLU D 122 -16.664 56.463 15.044 1.00 26.93
C
ATOM 6252 C GLU D 122 -16.509 56.579 13.530 1.00 25.72
C
ATOM 6253 O GLU D 122 -16.406 57.680 12.991 1.00 23.66
O
ATOM 6254 CB GLU D 122 -15.294 56.318 15.702 1.00 31.25
C
ATOM 6255 CG GLU D 122 -15.338 56.331 17.223 1.00 35.27
C
ATOM 6256 CD GLU D 122 -14.056 55.821 17.855 1.00 43.03
C
ATOM 6257 OE1 GLU D 122 -13.270 55.135 17.162 1.00 42.60
O
ATOM 6258 OE2 GLU D 122 -13.837 56.104 19.051 1.00 53.83
O1-
ATOM 6259 H GLU D 122 -17.105 54.710 15.826 1.00 28.23
H
ATOM 6260 HA GLU D 122 -17.071 57.281 15.370 1.00 32.32
H
ATOM 6261 HB2 GLU D 122 -14.902 55.475 15.424 1.00 37.50
H
ATOM 6262 HB3 GLU D 122 -14.730 57.053 15.415 1.00 37.50
H
ATOM 6263 HG2 GLU D 122 -15.480 57.241 17.526 1.00 42.33
H
ATOM 6264 HG3 GLU D 122 -16.066 55.764 17.522 1.00 42.33
H
ATOM 6265 N SER D 123 -16.486 55.436 12.848 1.00 21.52
N
ATOM 6266 CA SER D 123 -16.412 55.419 11.391 1.00 23.20
C
ATOM 6267 C SER D 123 -17.680 56.030 10.804 1.00 23.42
C
ATOM 6268 O SER D 123 -17.620 56.862 9.898 1.00 20.31
O
ATOM 6269 CB SER D 123 -16.216 53.993 10.871 1.00 21.62
C
ATOM 6270 OG SER D 123 -14.982 53.454 11.306 1.00 19.63
O
ATOM 6271 H SER D 123 -16.512 54.655 13.208 1.00 25.82
H
ATOM 6272 HA SER D 123 -15.656 55.954 11.103 1.00 27.84
H
ATOM 6273 HB2 SER D 123 -16.938 53.435 11.202 1.00 25.94
H
ATOM 6274 HB3 SER D 123 -16.229 54.007 9.901 1.00 25.94
H
ATOM 6275 HG SER D 123 -14.957 53.434 12.146 1.00 23.55
H
ATOM 6276 N GLN D 124 -18.827 55.611 11.331 1.00 20.37
N
ATOM 6277 CA GLN D 124 -20.107 56.170 10.922 1.00 24.01
C
ATOM 6278 C GLN D 124 -20.123 57.683 11.103 1.00 25.04
C
ATOM 12545 CA SER F 147 -19.348 22.137 14.921 1.00 50.25
C
ATOM 12546 C SER F 147 -20.056 21.244 15.935 1.00 51.65
C
ATOM 12547 O SER F 147 -19.657 21.172 17.098 1.00 47.99
O
ATOM 12548 CB SER F 147 -18.052 21.468 14.460 1.00 45.00
C
ATOM 12549 OG SER F 147 -18.303 20.164 13.961 1.00 48.06
O
ATOM 12550 H SER F 147 -18.236 23.631 15.575 1.00 52.98
H
ATOM 12551 HA SER F 147 -19.928 22.233 14.149 1.00 60.30
H
ATOM 12552 HB2 SER F 147 -17.654 22.003 13.756 1.00 54.00
H
ATOM 12553 HB3 SER F 147 -17.444 21.406 15.213 1.00 54.00
H
ATOM 12554 HG SER F 147 -17.584 19.809 13.712 1.00 57.67
H
ATOM 12555 N LYS F 148 -21.095 20.552 15.474 1.00 56.81
N
ATOM 12556 CA LYS F 148 -21.896 19.678 16.328 1.00 60.25
C
ATOM 12557 C LYS F 148 -21.256 18.299 16.469 1.00 62.99
C
ATOM 12558 O LYS F 148 -21.945 17.311 16.731 1.00 62.68
O
ATOM 12559 CB LYS F 148 -23.312 19.528 15.761 1.00 56.25
C
ATOM 12560 CG LYS F 148 -23.992 20.839 15.384 1.00 64.67
C
ATOM 12561 CD LYS F 148 -25.039 21.247 16.406 1.00 71.20
C
ATOM 12562 CE LYS F 148 -25.557 22.651 16.134 1.00 76.82
C
ATOM 12563 NZ LYS F 148 -24.495 23.682 16.310 1.00 75.60
N1+
ATOM 12564 H LYS F 148 -21.360 20.572 14.656 1.00 68.17
H
ATOM 12565 HA LYS F 148 -21.964 20.071 17.211 1.00 72.30
H
ATOM 12566 HB2 LYS F 148 -23.268 18.980 14.962 1.00 67.50
H
ATOM 12567 HB3 LYS F 148 -23.866 19.091 16.426 1.00 67.50
H
ATOM 12568 HG2 LYS F 148 -23.325 21.542 15.336 1.00 77.61
H
ATOM 12569 HG3 LYS F 148 -24.431 20.736 14.525 1.00 77.61
H
ATOM 12570 HD2 LYS F 148 -25.788 20.632 16.361 1.00 85.44
H
ATOM 12571 HD3 LYS F 148 -24.645 21.234 17.292 1.00 85.44
H
ATOM 12572 HE2 LYS F 148 -25.877 22.701 15.219 1.00 92.19
H
ATOM 12573 HE3 LYS F 148 -26.277 22.850 16.752 1.00 92.19
H
ATOM 12574 HZ1 LYS F 148 -23.822 23.524 15.749 1.00 90.72
H
ATOM 12575 HZ2 LYS F 148 -24.826 24.491 16.145 1.00 90.72
H
ATOM 12576 HZ3 LYS F 148 -24.187 23.660 17.145 1.00 90.72
H
ATOM 12577 N ARG F 149 -19.938 18.236 16.295 1.00 62.51
N
ATOM 12578 CA ARG F 149 -19.219 16.968 16.305 1.00 65.70
C

ATOM 6279 O GLN D 124 -20.549 58.420 10.214 1.00 21.92
O
ATOM 6280 CB GLN D 124 -21.238 55.534 11.725 1.00 28.29
C
ATOM 6281 CG GLN D 124 -22.605 56.135 11.471 1.00 32.29
C
ATOM 6282 CD GLN D 124 -23.667 55.497 12.338 1.00 34.18
C
ATOM 6283 OE1 GLN D 124 -23.490 55.356 13.549 1.00 37.41
O
ATOM 6284 NE2 GLN D 124 -24.773 55.089 11.722 1.00 37.93
N
ATOM 6285 H GLN D 124 -18.888 55.000 11.933 1.00 24.45
H
ATOM 6286 HA GLN D 124 -20.255 55.975 9.983 1.00 28.81
H
ATOM 6287 HB2 GLN D 124 -21.284 54.591 11.501 1.00 33.95
H
ATOM 6288 HB3 GLN D 124 -21.042 55.636 12.669 1.00 33.95
H
ATOM 6289 HG2 GLN D 124 -22.579 57.083 11.672 1.00 38.75
H
ATOM 6290 HG3 GLN D 124 -22.848 55.995 10.543 1.00 38.75
H
ATOM 6291 HE21 GLN D 124 -25.405 54.720 12.174 1.00 45.51
H
ATOM 6292 HE22 GLN D 124 -24.855 55.194 10.873 1.00 45.51
H
ATOM 6293 N ALA D 125 -19.652 58.135 12.260 1.00 25.98
N
ATOM 6294 CA ALA D 125 -19.640 59.555 12.584 1.00 27.07
C
ATOM 6295 C ALA D 125 -18.721 60.311 11.636 1.00 24.27
C
ATOM 6296 O ALA D 125 -19.057 61.397 11.168 1.00 27.08
O
ATOM 6297 CB ALA D 125 -19.207 59.766 14.027 1.00 26.32
C
ATOM 6298 H ALA D 125 -19.331 57.633 12.880 1.00 31.18
H
ATOM 6299 HA ALA D 125 -20.537 59.912 12.483 1.00 32.48
H
ATOM 6300 HB1 ALA D 125 -19.206 60.716 14.221 1.00 31.59
H
TER 12601 ARG F 149
HETATM12602 O HOH A 301 -4.239 8.778 -55.547 1.00 45.04
O
HETATM12603 O HOH A 302 -24.027 13.065 -38.411 1.00 31.04
O
HETATM12604 O HOH A 303 -26.938 32.739 -45.146 1.00 27.98
O
HETATM12605 O HOH A 304 -26.382 16.536 -35.436 1.00 35.92
O
HETATM12606 O HOH A 305 -19.043 4.283 -27.862 1.00 40.38
O
HETATM12607 O HOH A 306 -19.017 7.187 -59.366 1.00 28.55
O
HETATM12608 O HOH A 307 -13.369 10.269 -60.520 1.00 31.03
O
HETATM12609 O HOH A 308 -19.209 3.822 -43.074 1.00 38.43
O
HETATM12610 O HOH A 309 -23.006 34.055 -48.572 1.00 21.85
O
HETATM12611 O HOH A 310 -13.086 4.848 -49.321 1.00 25.83
O
HETATM12612 O HOH A 311 -26.139 21.686 -35.299 1.00 30.33
O
HETATM12613 O HOH A 312 -28.024 21.488 -43.474 1.00 27.79
O
ATOM 12579 C ARG F 149 -17.746 17.180 16.640 1.00 70.51
C
ATOM 12580 O ARG F 149 -17.410 17.671 17.718 1.00 79.82
O
ATOM 12581 CB ARG F 149 -19.361 16.277 14.948 1.00 59.09
C
ATOM 12582 CG ARG F 149 -18.637 14.951 14.834 1.00 53.79
C
ATOM 12583 CD ARG F 149 -18.960 14.289 13.514 1.00 43.18
C
ATOM 12584 NE ARG F 149 -18.021 13.226 13.181 1.00 43.60
N
ATOM 12585 CZ ARG F 149 -18.019 12.580 12.021 1.00 40.65
C
ATOM 12586 NH1 ARG F 149 -18.915 12.894 11.095 1.00 30.30
N1+
ATOM 12587 NH2 ARG F 149 -17.125 11.627 11.791 1.00 40.71
N
ATOM 12588 H ARG F 149 -19.434 18.921 16.169 1.00 75.01
H
ATOM 12589 HA ARG F 149 -19.603 16.389 16.982 1.00 78.85
H
ATOM 12590 HB2 ARG F 149 -20.303 16.112 14.782 1.00 70.91
H
ATOM 12591 HB3 ARG F 149 -19.007 16.865 14.263 1.00 70.91
H
ATOM 12592 HG2 ARG F 149 -17.679 15.101 14.877 1.00 64.55
H
ATOM 12593 HG3 ARG F 149 -18.921 14.363 15.551 1.00 64.55
H
ATOM 12594 HD2 ARG F 149 -19.848 13.902 13.562 1.00 51.81
H
ATOM 12595 HD3 ARG F 149 -18.925 14.954 12.808 1.00 51.81
H
ATOM 12596 HE ARG F 149 -17.372 13.078 13.725 1.00 52.32
H
ATOM 12597 HH11 ARG F 149 -19.492 13.514 11.246 1.00 36.36
H
ATOM 12598 HH12 ARG F 149 -18.919 12.478 10.342 1.00 36.36
H
ATOM 12599 HH21 ARG F 149 -16.546 11.425 12.394 1.00 48.86
H
ATOM 12600 HH22 ARG F 149 -17.127 11.207 11.040 1.00 48.86
H
HETATM12933 O HOH D 370 -13.314 41.381 16.992 1.00 38.82
O
HETATM12934 O HOH D 371 -12.620 44.975 19.857 1.00 38.87
O
HETATM12935 O HOH D 372 -34.361 45.041 6.117 1.00 40.66
O
HETATM12936 O HOH D 373 -19.902 30.159 10.064 1.00 39.21
O
HETATM12937 O HOH D 374 -19.665 42.831 -10.863 1.00 37.18
O
HETATM12938 O HOH D 375 -26.348 36.818 9.412 1.00 40.39
O
HETATM12939 O HOH D 376 -4.888 48.505 8.181 1.00 40.81
O
HETATM12940 O HOH D 377 -38.516 50.575 6.009 1.00 40.44
O
HETATM12941 O HOH D 378 -20.538 43.117 -13.094 1.00 39.95
O
HETATM12942 O HOH D 379 -19.702 45.502 -14.659 1.00 39.92
O
HETATM12943 O HOH D 380 -5.678 50.415 4.198 1.00 39.75
O
HETATM12944 O HOH D 381 -30.979 39.861 1.528 1.00 41.67

O
HETATM12614 O HOH A 313 -27.846 27.929 -39.556 1.00 26.71
O
HETATM12615 O HOH A 314 -24.877 25.289 -37.453 1.00 23.03
O
HETATM12616 O HOH A 315 -23.432 2.197 -46.149 1.00 45.83
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CONECT 3932 4116
CONECT 4035 3901
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CONECT 7309 7519
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CONECT 7636 6319
CONECT 9055 9862
CONECT 9862 9055
CONECT1149912306
CONECT1230611499

CLAIMS

What is claimed is:

1. A composition, the composition comprising a cytokine linked to a ligand, wherein the ligand is not a corresponding binding partner to the cytokine.

2. The composition of claim 1, wherein the cytokine is part of the IL2 subfamily.

3. The composition of claim 2, wherein the cytokine is selected from the group consisting of IL2, IL7, IL15, IL21 and a mutant thereof.

4. The composition of claim 1, wherein the cytokine is interleukin-2 (IL2), a mutated IL2, or a variant thereof.

5. The composition of claim 4, wherein the mutated IL2 comprises at least one mutation selected from the group consisting of R38A, F42K and C125S.

6. The composition of claim 4, wherein the IL2 comprises the amino acid sequence set forth in SEQ ID NO:5 or SEQ ID NO:6

7. The composition of claim 1, wherein the cytokine is part of the IL1 family.

8. The composition of claim 7, wherein the cytokine is IL18 or a mutant thereof.

9. The composition of claim1, wherein the cytokine is selected from the group consisting of IL2, IL15, IL18 and mutants thereof.

10. The composition of any of claims 1-9, wherein the ligand is a MHC class-I-related glycoprotein.

11. The composition of any of claims 1-9, wherein the ligand is orthopoxvirus major histocompatibility complex class I-like protein (OMCP) or a variant thereof.

12. The composition of any of claims 1-9, wherein the ligand binds to a receptor expressed on natural killer (NK) cells and CD8+ cytotoxic T lymphocytes (CTLs).

13. The composition of any of claims 1-9, wherein the ligand does not bind to a receptor on vascular endothelial cells or regulatory T cells (T_{regs}).

14. The composition of any of claims 1-9, wherein the ligand binds to NKG2D receptor.

15. The composition of any of claims 1-9, wherein the ligand comprises the amino acid sequence set forth in SEQ ID NO:7, SEQ ID NO:13 or SEQ ID NO:14.

16. The composition of any of claims 1-9, further comprising a linker.

17. The composition of any of claims 1-9, further comprising a linker, wherein the linker is a peptide linker and comprises about 20 to about 30 amino acids.

18. The composition of any of claims 1-9, further comprising a linker, wherein the linker comprises the amino acid sequence selected from the group consisting of $(AAS)_n$, $(AAAL)_n$, $(G_nS)_n$ or $(G_2S)_n$, wherein A is alanine, S is serine, L is leucine, and G is glycine and wherein n is an integer from 1-20, or 1-10, or 3-10.

19. The composition of any of claims 1-9, further comprising a linker, wherein the linker is a peptide linker and comprises at least one tag selected from the group consisting of a FLAG tag and a His tag.

20. The composition of any of claims 1-9, further comprising a linker, wherein the linker comprises the amino acid sequence set forth in SEQ ID NO:8.

21. The composition of claim 1, wherein the cytokine and the ligand form a fusion peptide comprising the amino acid sequence set forth in SEQ ID NO:2.

22. A nucleic acid molecule comprising the nucleic acid sequence set forth in SEQ ID NO:1.

23. A method to deliver a cytokine to a target cell, the method comprising contacting a target cell with a composition comprising a cytokine linked to a ligand, wherein the ligand specifically binds to a receptor on the target cell and the ligand is not a corresponding binding partner to the cytokine.

24. The method of claim 23, wherein the target cell is a NK cell or a CD8+ CTL.

25. A method to activate immune cells, the method comprising contacting an immune cell with a composition comprising a proinflammatory cytokine linked to a ligand, wherein the ligand specifically binds to a receptor on the immune cell thereby activating the cell and the ligand is not a corresponding binding partner to the cytokine.

26. The method of claim 25, wherein the immune cells are NK cells and CD8+ CTLs.

27. The method of claim 26, wherein the activated NK cells lyse tumor cells.

28. The method of claim 25, wherein the proinflammatory cytokine is selected from the group consisting of IL2, IL7, IL15, IL18, IL21 and a mutant thereof.

29. A method to treat a tumor, the method comprising:
    a) identifying a subject with a tumor; and
    b) administering to the subject a therapeutically effective amount of a composition comprising a proinflammatory cytokine linked to a ligand, wherein the ligand specifically binds to a receptor on a target cell and the ligand is not a corresponding binding partner to the cytokine.

30. The method of claim 29, wherein the target cell is an immune cell that is activated to lyse tumor cells.

31. The method of claim 29, wherein the tumor is selected from the group consisting of melanoma, renal cell carcinoma, lung cancer and blood cancer.

32. The method of claim 29, wherein the composition is administered twice daily.

33. The method of claim 29, wherein the proinflammatory cytokine is IL2 or a mutant thereof, and wherein the dose of IL2 or mutant thereof is about 250,000 IU/kg to about 750,000 IU/kg.

34. A method to treat a viral infection, the method comprising administering to the subject a therapeutically effective amount of a composition comprising a proinflammatory cytokine linked to a ligand, wherein the ligand specifically binds to a receptor on a target cell and the ligand is not a corresponding binding partner to the cytokine.

35. The method of claim 34, wherein the target cell is an immune cell that is activated to lyse the infected host cell.

36. The method of claim 34, wherein the viral infection is caused by a flavivirus.

37. The method of claim 36, wherein the flavivirus is West Nile virus (WNV).

38. A chimeric peptide comprising a cytokine peptide and a ligand peptide, wherein the cytokine peptide is not a binding partner of the ligand peptide.

39. The chimeric peptide of claim 38, wherein the cytokine peptide is in the IL2 subfamily.

40. The chimeric peptide of claim 38, wherein the cytokine peptide is in the IL1 family.

41. The chimeric peptide of claim 38, wherein the cytokine peptide is selected from the group consisting of IL2, IL7, IL15, IL18, IL21, and mutants thereof.

42. The chimeric peptide of claim 38, wherein the cytokine peptide is interleukin-2 (IL2) or a mutant thereof.

43. The chimeric peptide of claim 38, wherein the cytokine peptide comprises the amino acid sequence set forth in SEQ ID NO: 5.

44. The chimeric peptide of claim 38, wherein the cytokine peptide is a mutant interleukin-2 (IL2).

45. The chimeric peptide of claim 44, wherein the mutant interleukin-2 comprises at least one mutation selected from the group consisting of R38A, F42K and C125S.

46. The chimeric peptide of claim 38, wherein the cytokine peptide comprises the amino acid sequence set forth in SEQ ID NO: 6.

47. The chimeric peptide of any of claims 38-46, wherein the ligand peptide is a MHC class-I-related glycoprotein.

48. The chimeric peptide of any of claims 38-46, wherein the ligand peptide is orthopoxvirus major histocompatibility complex class I-like protein (OMCP) or a portion thereof, or a mutant OMCP.

49. The chimeric peptide of any of claims 38-46, wherein the ligand peptide binds to a receptor expressed on natural killer (NK) cells and CD8+ cytotoxic T lymphocytes (CTLs).

50. The chimeric peptide of any of claims 38-46, wherein the ligand peptide binds to an NKG2D receptor.

51. The chimeric peptide of any of claims 38-46, wherein the ligand peptide comprises the amino acid sequence set forth in SEQ ID NO:7, SEQ ID NO:13, SEQ ID NO:14 or a portion thereof that is capable of binding to the NKG2D receptor.

52. The chimeric peptide of any of claims 38-46, further comprising a linker peptide.

53. The chimeric peptide of any of claims 38-46, further comprising a linker peptide comprising the amino acid sequence set forth in SEQ ID NO: 8.

54. The chimeric peptide of any of claims 38-46, further comprising a linker peptide comprising the amino acid sequence selected from the group consisting of $(AAS)_n$, $(AAAL)_n$, $(G_nS)_n$ or $(G_2S)_n$, wherein A is alanine, S is serine, L is leucine, and G is glycine and wherein n is an integer from 1-20, or 1-10, or 3-10.

55. The chimeric peptide of any of claims 38-46, further comprising a linker peptide comprising at least one tag selected from the group consisting of a FLAG tag and a His tag.

56. The chimeric peptide of any of claims 38-46, further comprising a linker peptide about 20 to about 30 amino acids.

57. A chimeric peptide comprising a cytokine peptide and a ligand peptide, wherein the ligand peptide binds to an NKG2D receptor.

58. The chimeric peptide of claim 57, wherein the cytokine peptide is in the IL2 subfamily.

59. The chimeric peptide of claim 57, wherein the cytokine peptide is in the IL1 family.

60. The chimeric peptide of claim 57, wherein the cytokine peptide is selected from the group consisting of IL2, IL7, IL15, IL18 and IL21.

61. The chimeric peptide of claim 57, wherein the cytokine peptide is interleukin-2 (IL2).

62. The chimeric peptide of claim 57, wherein the cytokine peptide comprises the amino acid sequence set forth in SEQ ID NO: 5.

63. The chimeric peptide of claim 57, wherein the cytokine peptide is a mutant interleukin-2 (IL2).

64. The chimeric peptide of claim 63, wherein the mutant interleukin-2 comprises at least one mutation selected from the group consisting of R38A, F42K and C125S.

65. The chimeric peptide of claim 57, wherein the cytokine peptide comprises the amino acid sequence set forth in SEQ ID NO: 6.

66. The chimeric peptide of claim 57, further comprising a linker peptide.

67. The chimeric peptide of claim 66, wherein the linker peptide comprises the amino acid sequence set forth in SEQ ID NO: 8.

68. The chimeric peptide of claim 66, wherein the linker peptide comprises the amino acid sequence selected from the group consisting of (AAS)n, (AAAL)n, ((Gu)S)n or (G_2S)n, wherein A is alanine, S is serine, L is leucine, G is glycine and Gu is glutamine and wherein n is an integer from 1-20, or 1-10, or 3-10.

69. The chimeric peptide of claim 66, wherein the linker peptide comprises at least one tag selected from the group consisting of a FLAG tag and a His tag.

70. The chimeric peptide of claim 66, wherein the linker peptide comprises about 20 to about 30 amino acids.

71. The chimeric peptide of any of claims 57-70, wherein the ligand peptide is a MHC class-I-related glycoprotein.

72. The chimeric peptide of any of claims 57-70, wherein the ligand peptide is orthopoxvirus major histocompatibility complex class I-like protein (OMCP) or a portion thereof, or a mutant OMCP.

73. The chimeric peptide of any of claims 57-70, wherein the ligand peptide comprises the amino acid sequence set forth in SEQ ID NO:7, SEQ ID NO:13, SEQ ID NO:14 or a portion thereof.

74. A nucleic acid molecule comprising a sequence encoding the chimeric peptide of any of claims 38-73.

75. A pharmaceutical composition comprising the chimeric peptide of any of claims 38-73.

76. A method of treating a subject diagnosed with cancer comprising administering to the subject the pharmaceutical composition of claim 75.

77. A composition, the composition comprising a cytokine linked to a ligand with a linker, wherein the ligand is not a corresponding binding partner to the cytokine.

78. The composition of claim 77, wherein the linker is a peptide linker and comprises about 20 to about 30 amino acids.

79. The composition of claim 77, wherein the linker comprises the amino acid sequence selected from the group consisting of $(AAS)_n$, $(AAAL)_n$, $(G_nS)_n$ or $(G_2S)_n$, wherein A is alanine, S is serine, L is leucine, and G is glycine and wherein n is an integer from 1-20, or 1-10, or 3-10.

80. The composition of claim 77, wherein the linker is a peptide linker and comprises at least one tag selected from the group consisting of a FLAG tag and a His tag.

81. The composition of claim 77, wherein the linker comprises the amino acid sequence set forth in SEQ ID NO:8.

82. The composition of claim 77, wherein the cytokine is part of the IL2 subfamily.

83. The composition of claim 82, wherein the cytokine is selected from the group consisting of IL2, IL7, IL15, IL21 and a mutant thereof.

84. The composition of claim 77, wherein the cytokine is interleukin-2 (IL2), a mutated IL2, or a variant thereof.

85. The composition of claim 84, wherein the mutated IL2 comprises at least one mutation selected from the group consisting of R38A, F42K and C125S.

86. The composition of claim 84, wherein the IL2 comprises the amino acid sequence set forth in SEQ ID NO:5 or SEQ ID NO:6

87. The composition of claim 77, wherein the cytokine is part of the IL1 family.

88. The composition of claim 87, wherein the cytokine is IL18 or a mutant thereof.

89. The composition of claim 77, wherein the cytokine is selected from the group consisting of IL2, IL15, IL18 and mutants thereof.

90. The composition of any of claims 77-89, wherein the ligand is a MHC class-I-related glycoprotein.

91. The composition of any of claims 77-89, wherein the ligand is orthopoxvirus major histocompatibility complex class I-like protein (OMCP) or a variant thereof.

92. The composition of any of claims 77-89, wherein the ligand binds to a receptor expressed on natural killer (NK) cells and CD8+ cytotoxic T lymphocytes (CTLs).

93. The composition of any of claims 77-89, wherein the ligand does not bind to a receptor on vascular endothelial cells or regulatory T cells (T_{regs}).

94. The composition of any of claims 77-89, wherein the ligand binds to NKG2D receptor.

95. The composition of any of claims 77-89, wherein the ligand comprises the amino acid sequence set forth in SEQ ID NO:7, SEQ ID NO:13 or SEQ ID NO:14.

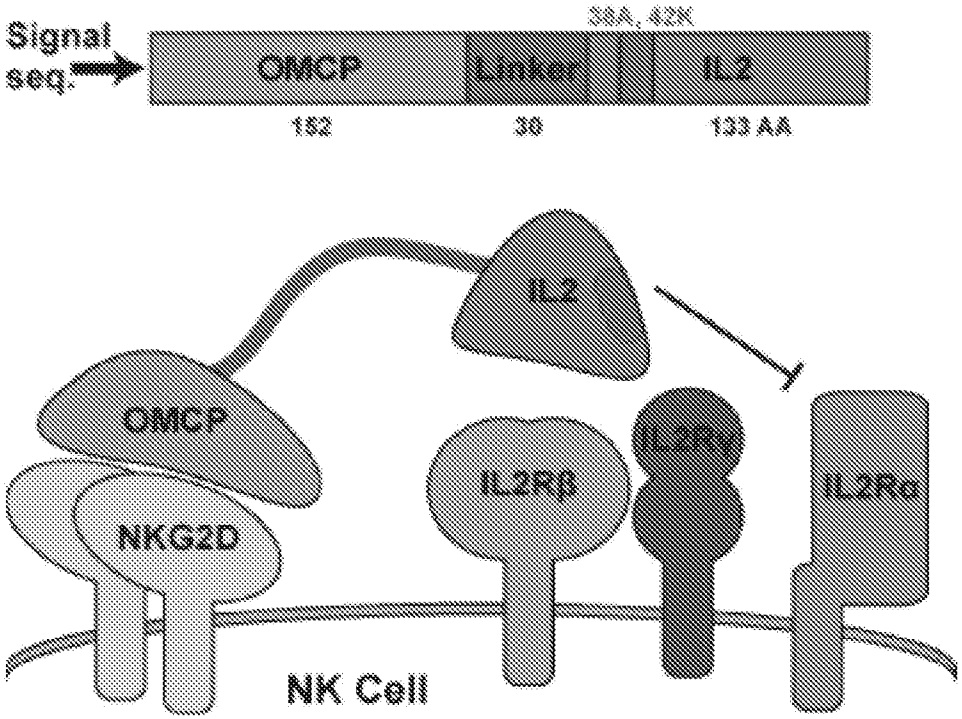

38A, 42K
Signal seq.
OMCP
Linker
IL2
152
30
133 AA
IL2
OMCP
IL2Rγ
IL2Rβ
IL2Rα
NKG2D
NK Cell

FIG. 1A

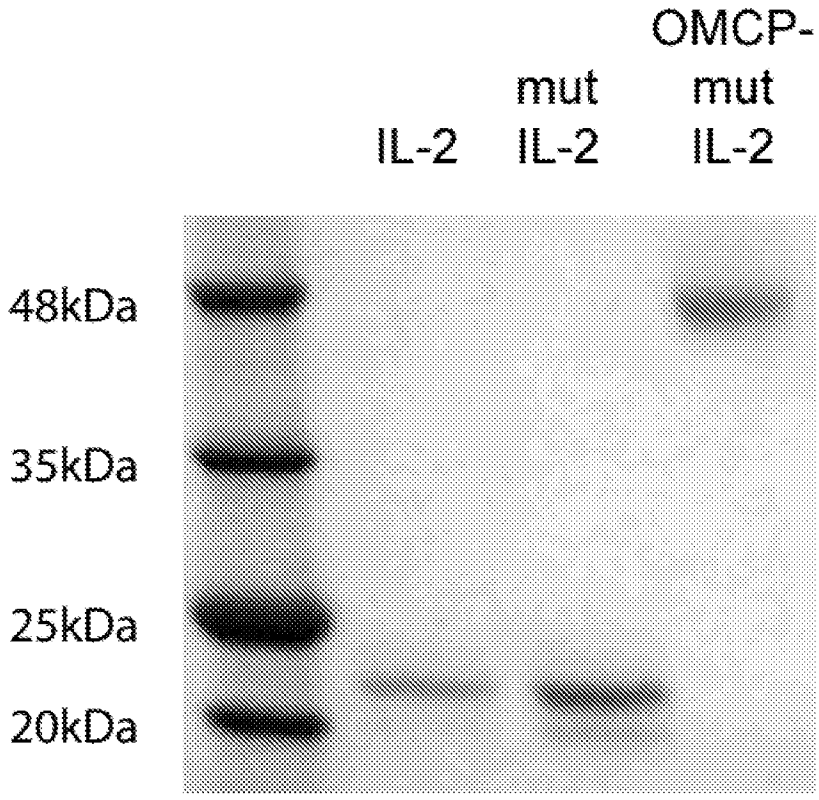

IL-2
mut IL-2
OMCP-mut IL-2
48kDa
35kDa
25kDa
20kDa

FIG. 1B

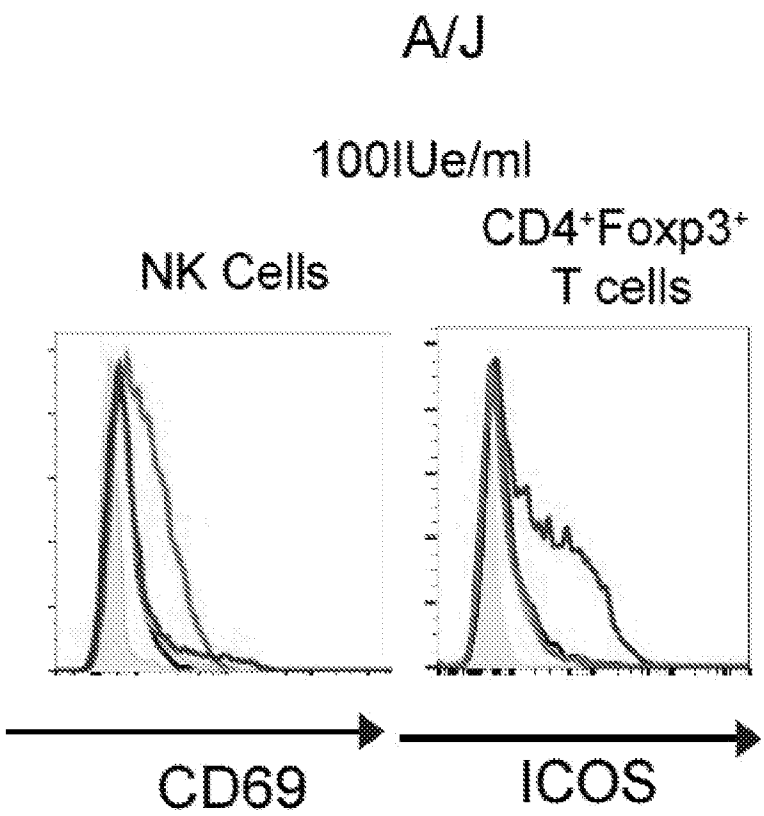


FIG. 1C

OMCP-mutIL-2, wild-type IL-2, mutIL-2, Saline

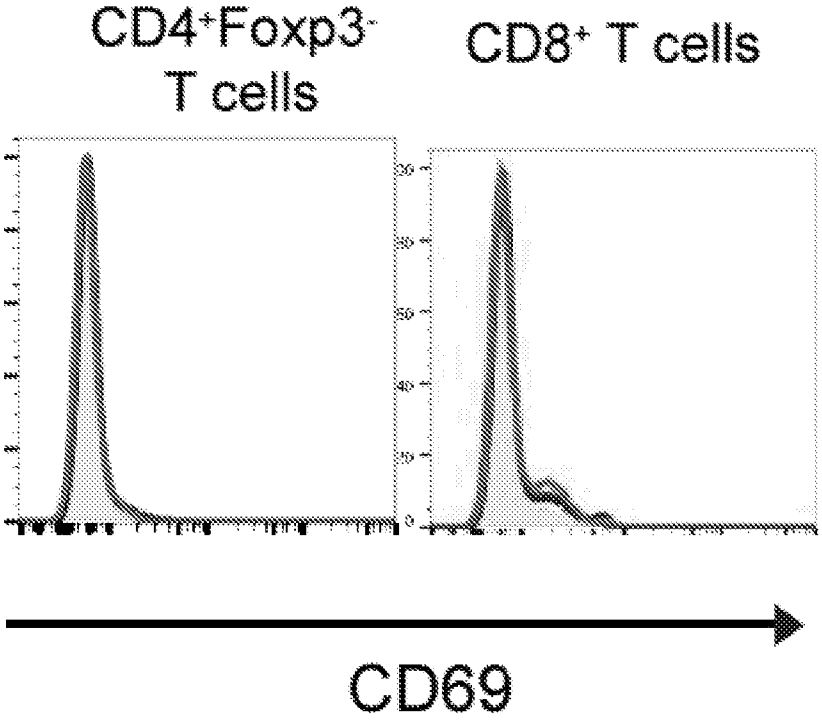


FIG. 1D

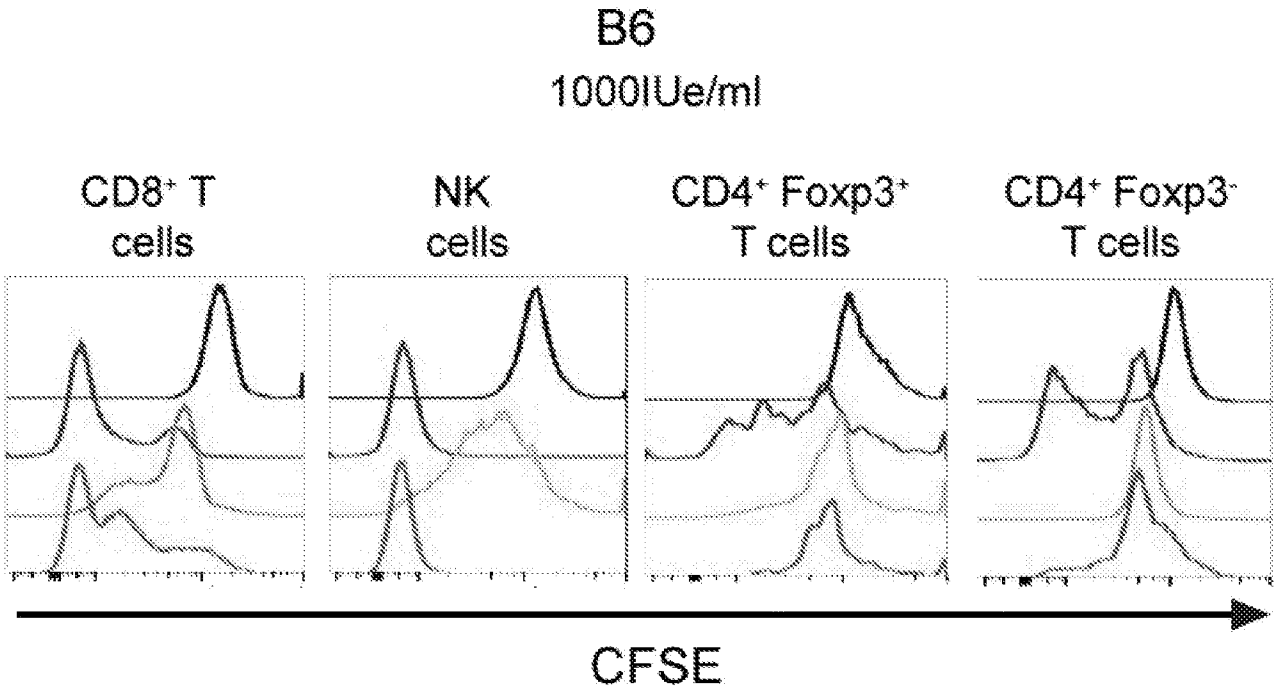


FIG. 1E

OMCP-mutIL-2, wild-type IL-2, mutIL-2, Saline

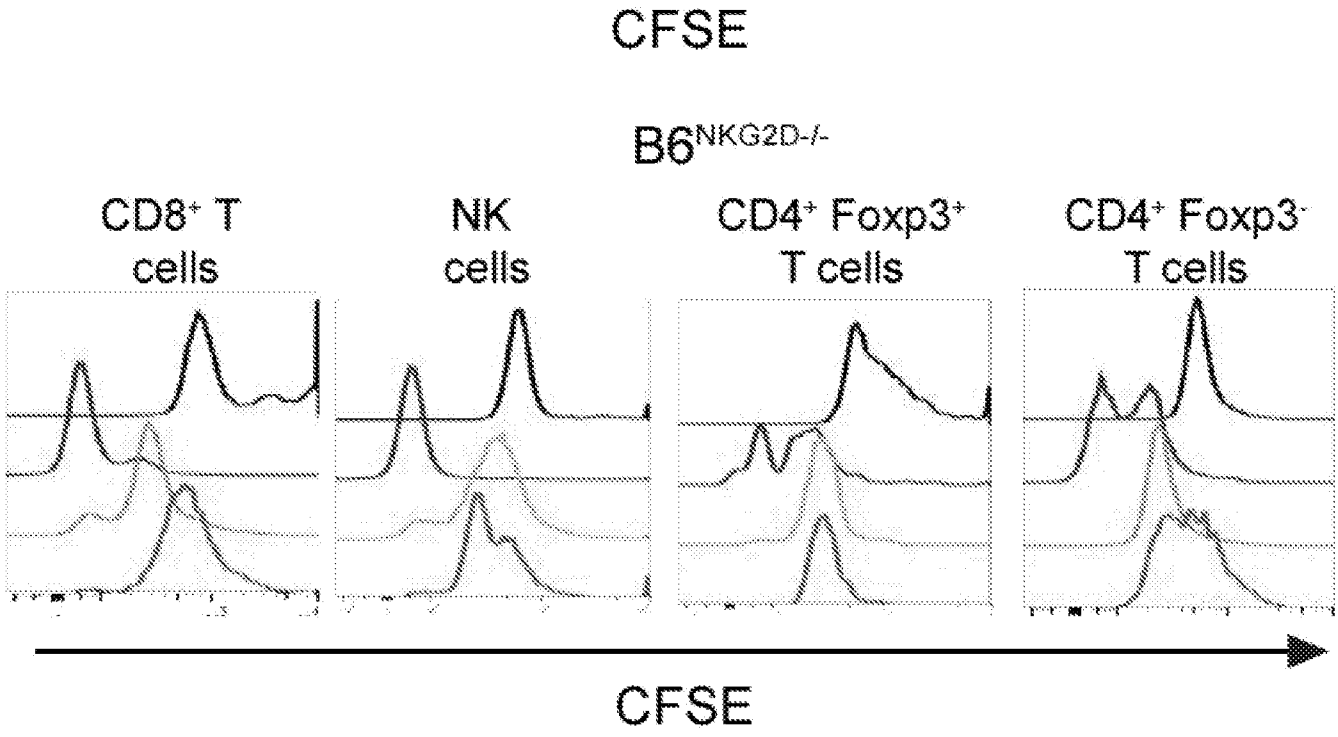


FIG. 1F

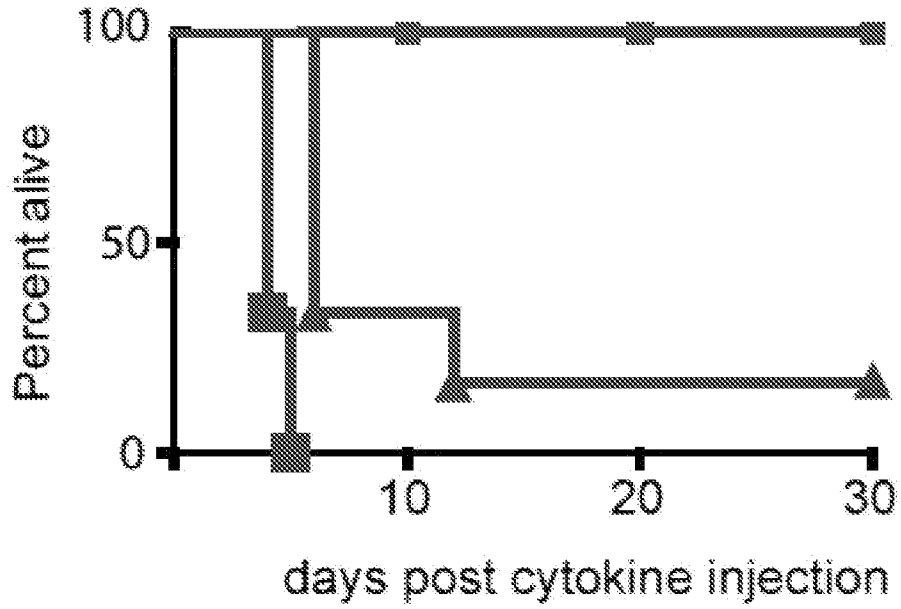

100
50
0
Percent alive
10
20
30
days post cytokine injection

FIG. 2A

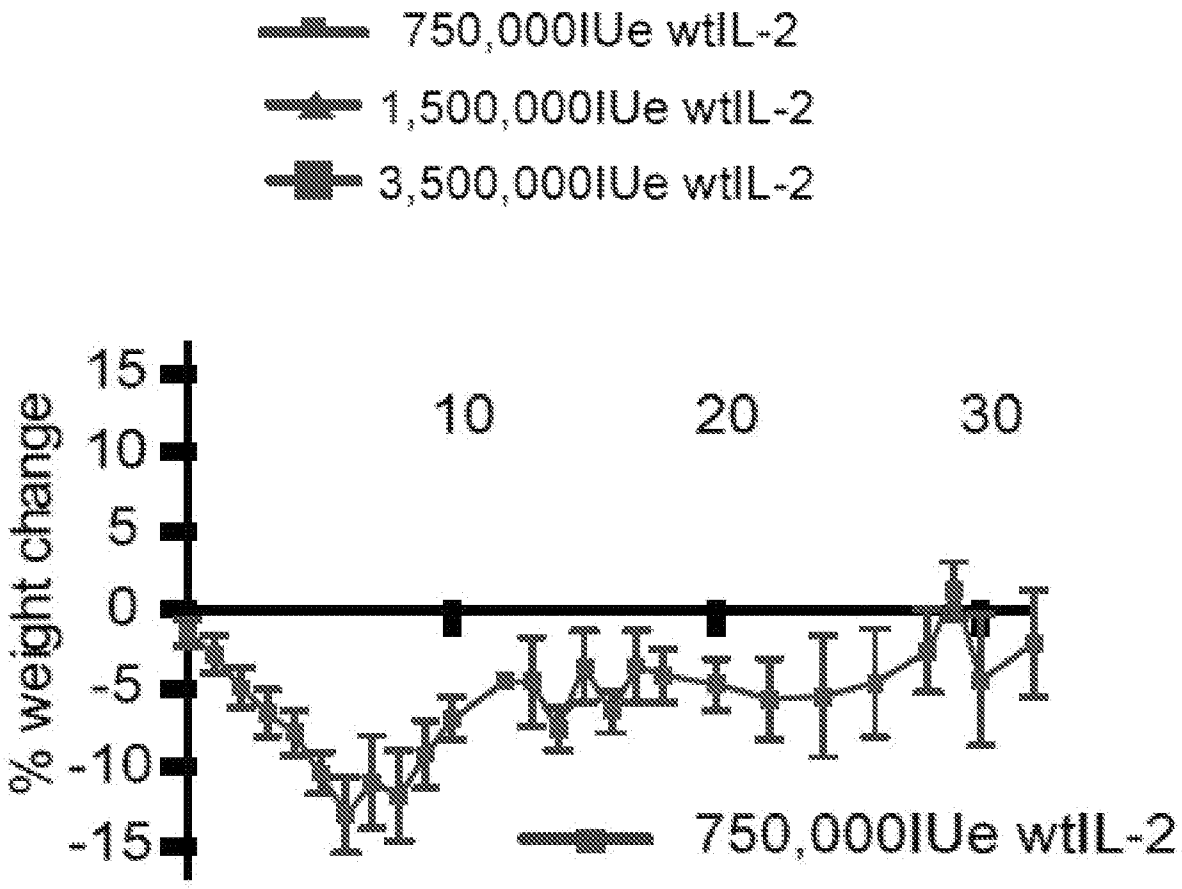

750,000IUe wtIL-2
1,500,000IUe wtIL-2
3,500,000IUe wtIL-2
15
10
5
0
-5
-10
-15
% weight change
10
20
30
750,000IUe wtIL-2

FIG. 2B

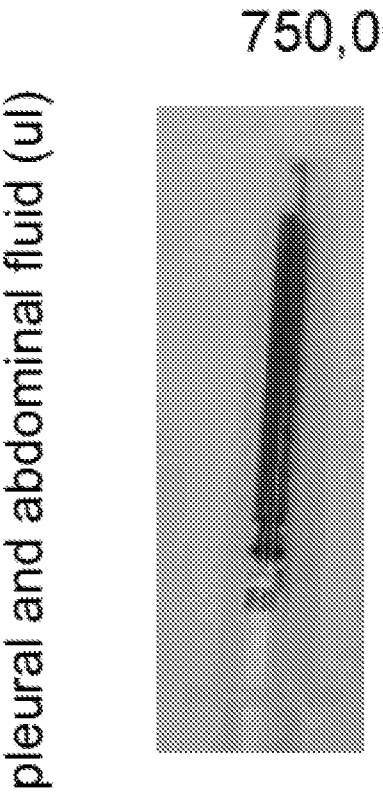

750,000IUe wtIL-2
pleural and abdominal fluid (ul)

FIG. 2C

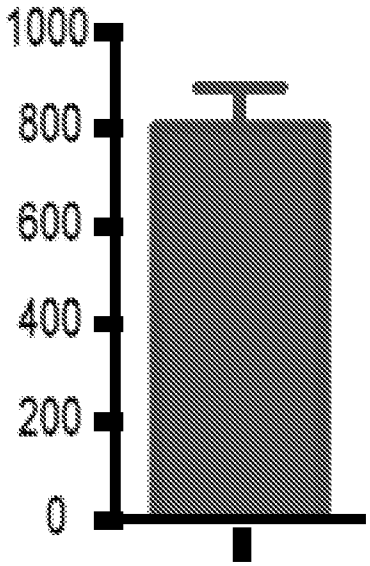

1000
800
600
400
200
0

FIG. 2D

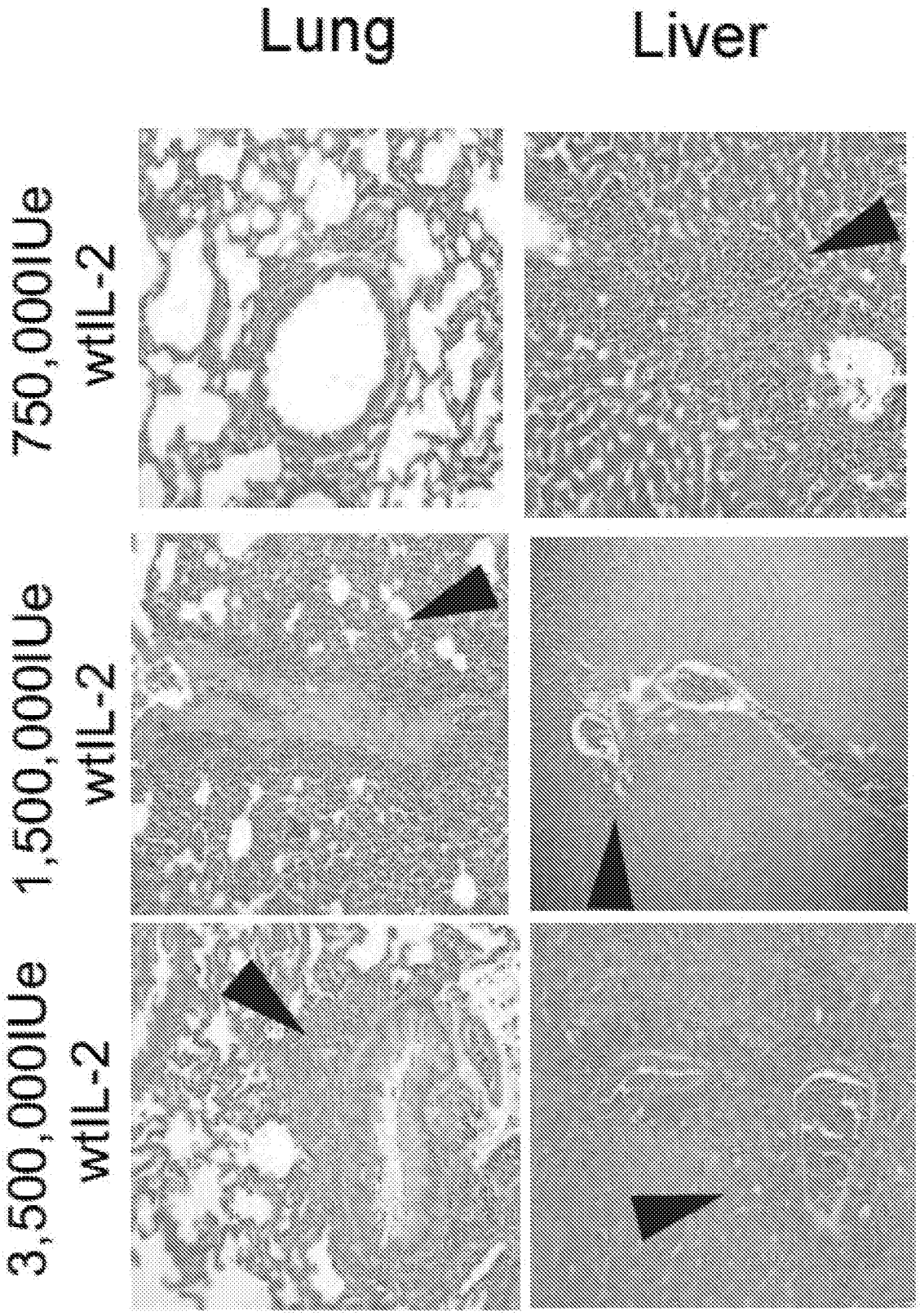

Lung
Liver
750,000IUe wtIL-2
1,500,000IUe wtIL-2
3,500,000IUe wtIL-2

FIG. 2E

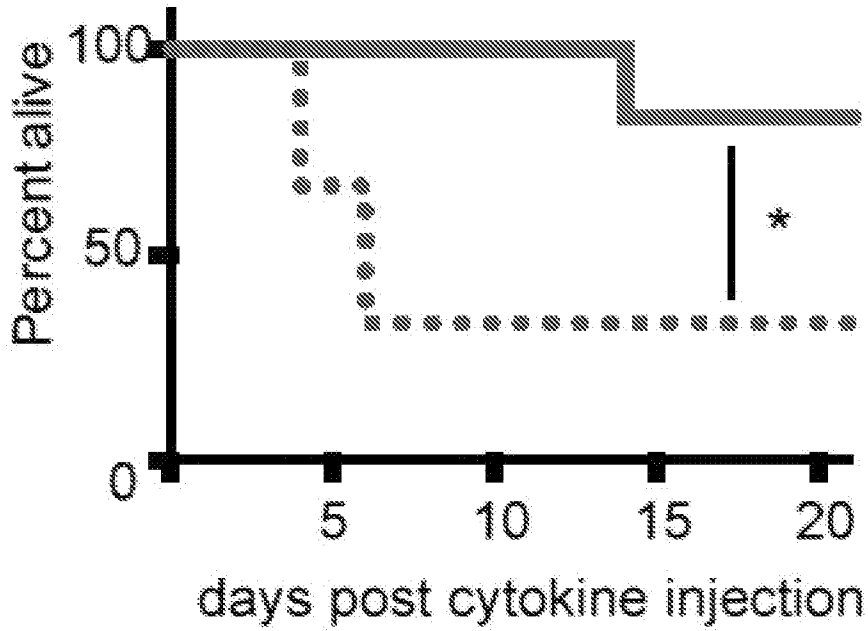
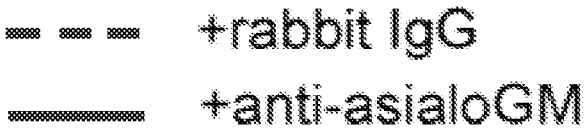

Percent alive
100
50
0
5
10
15
20
days post cytokine injection
*

FIG. 2F


+rabbit IgG
+anti-asialoGM

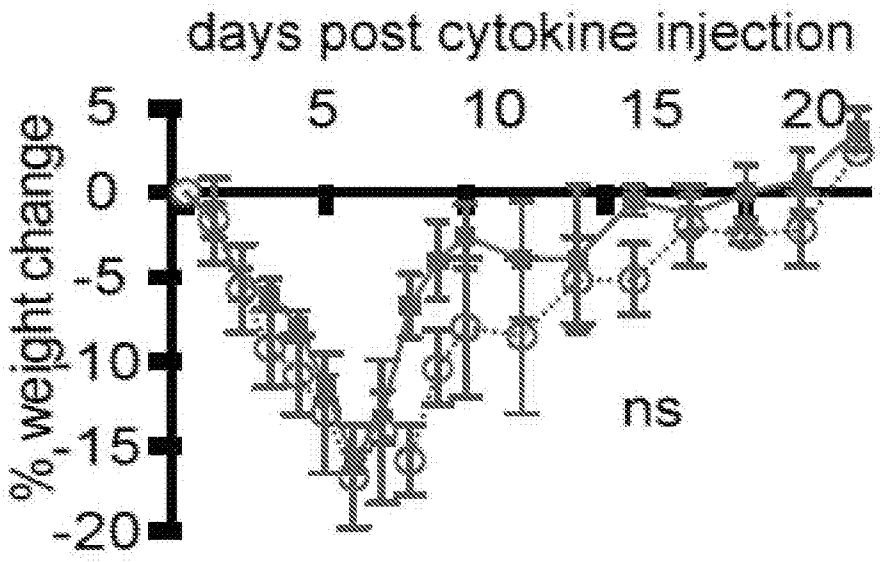

days post cytokine injection
% weight change
5
0
-5
-10
-15
-20
5
10
15
20
ns

FIG. 2G

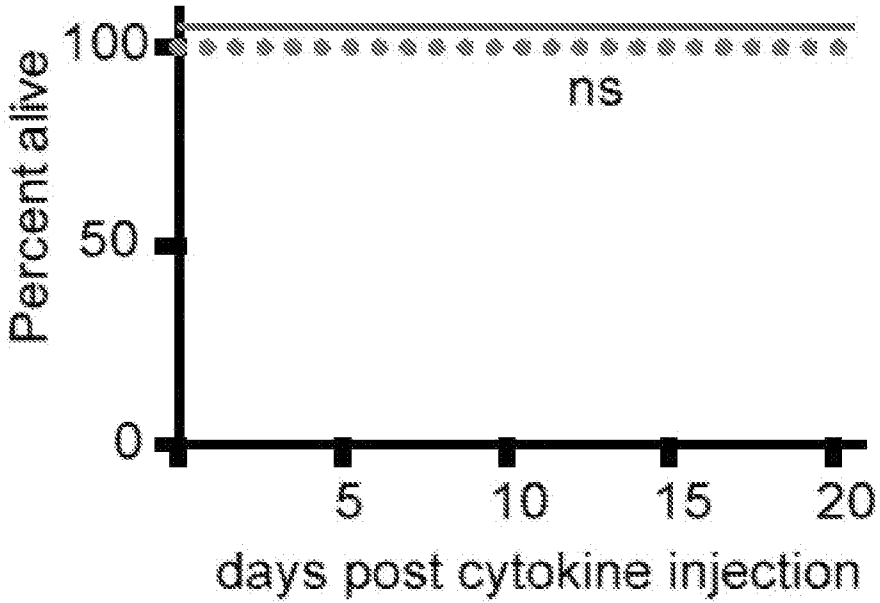
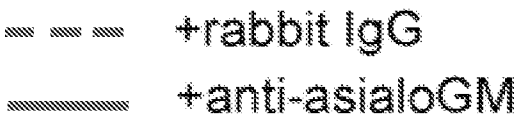

100
50
0
Percent alive
ns
5
10
15
20
days post cytokine injection

FIG. 2H


+rabbit IgG
+anti-asialoGM

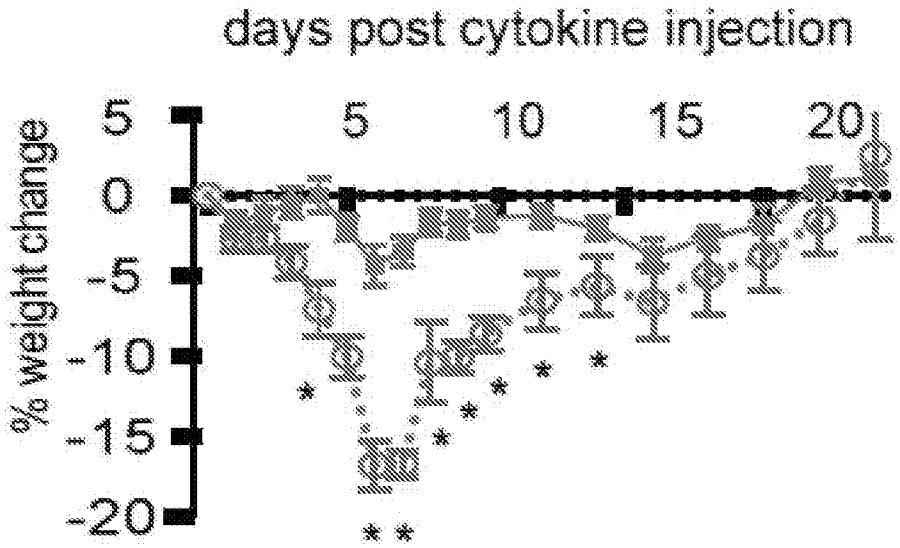

days post cytokine injection
5
0
-5
-10
-15
-20
% weight change
5
10
15
20

FIG. 2I

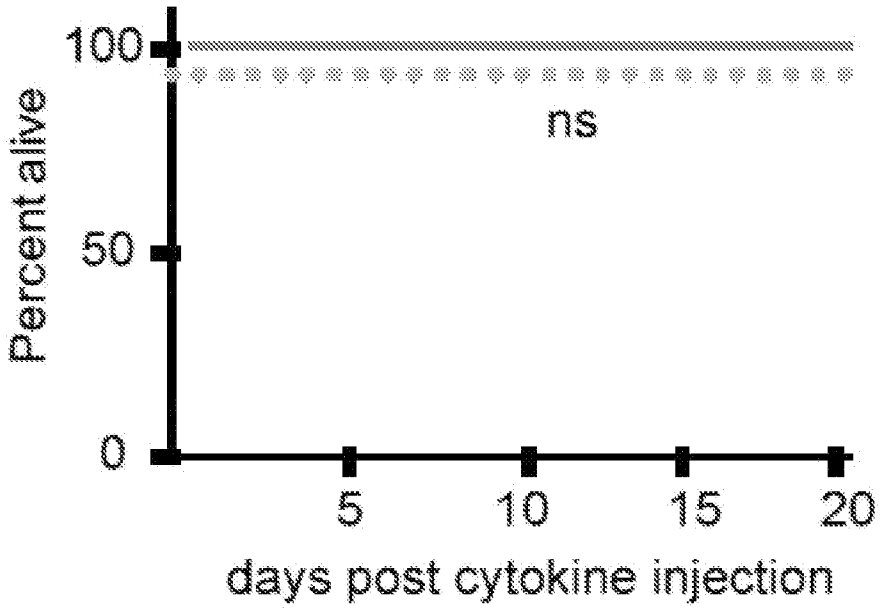
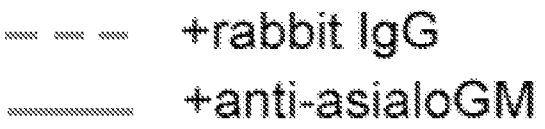

100
50
0
Percent alive
ns
5
10
15
20
days post cytokine injection

FIG. 2J


+rabbit IgG
+anti-asialoGM

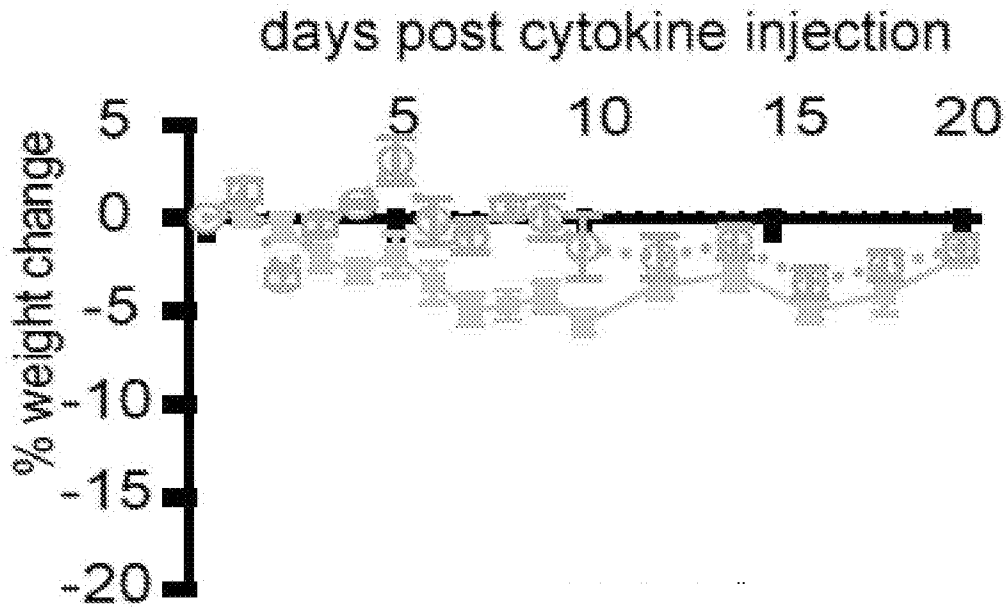

days post cytokine injection
5
0
-5
-10
-15
-20
% weight change
5
10
15
20

FIG. 2K

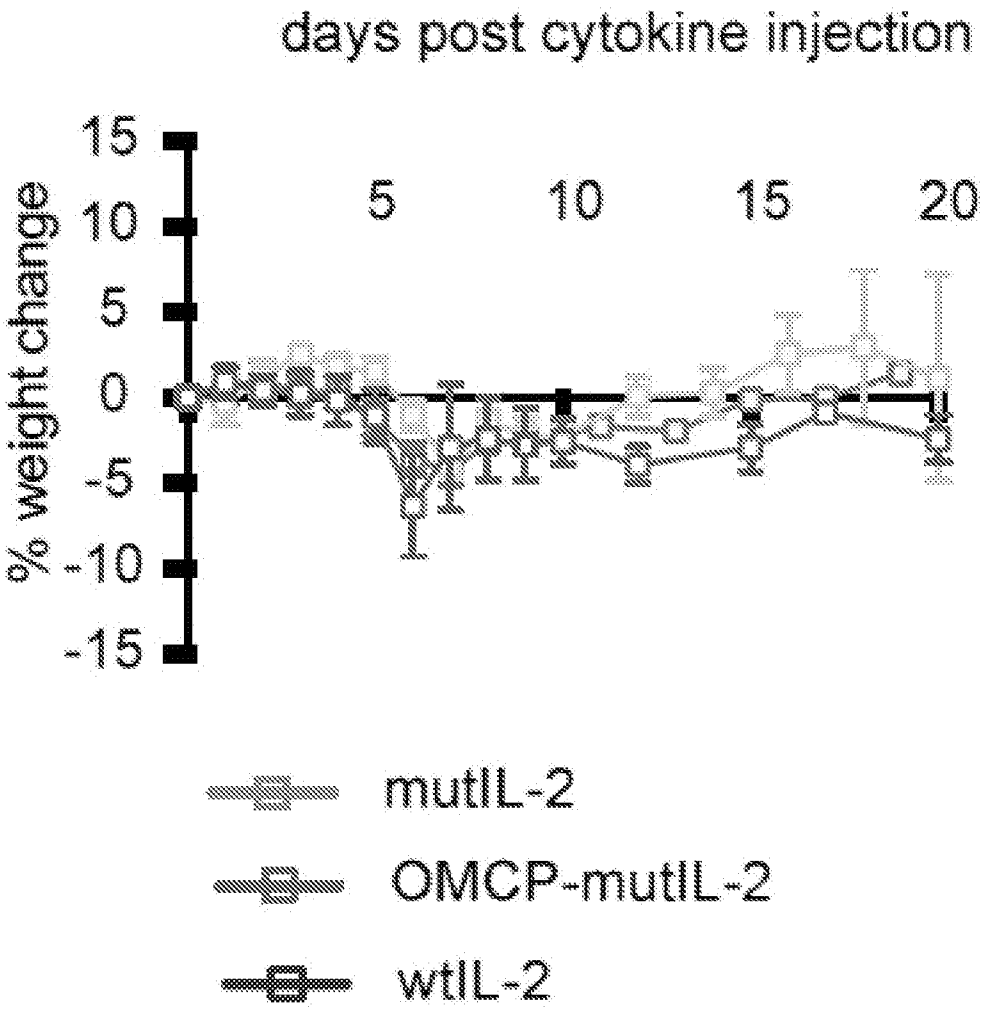

days post cytokine injection
% weight change
15
10
5
0
-5
-10
-15
5
10
15
20
mutIL-2
OMCP-mutIL-2
wtIL-2

FIG. 2L

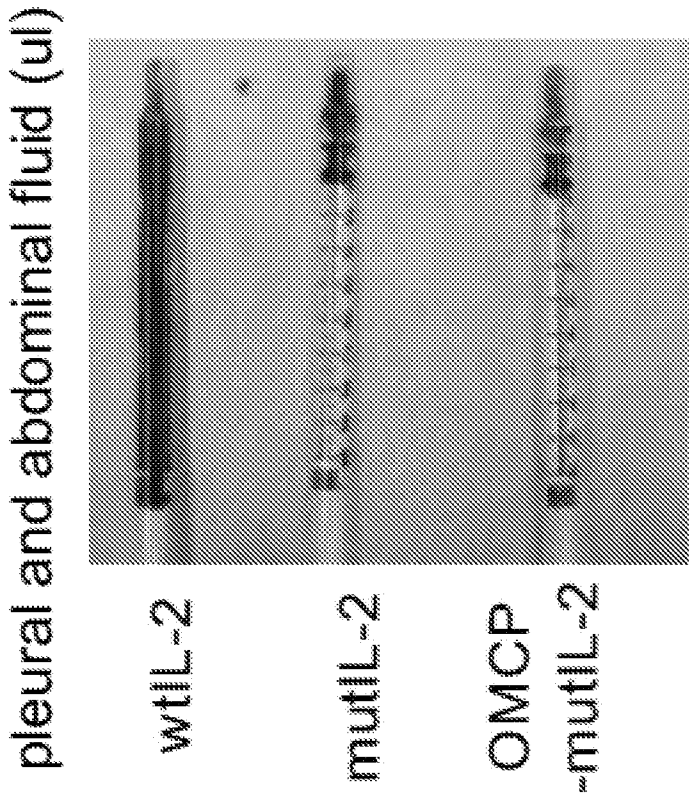

pleural and abdominal fluid (ul)
wtIL-2
mutIL-2
OMCP -mutIL-2

FIG. 2M

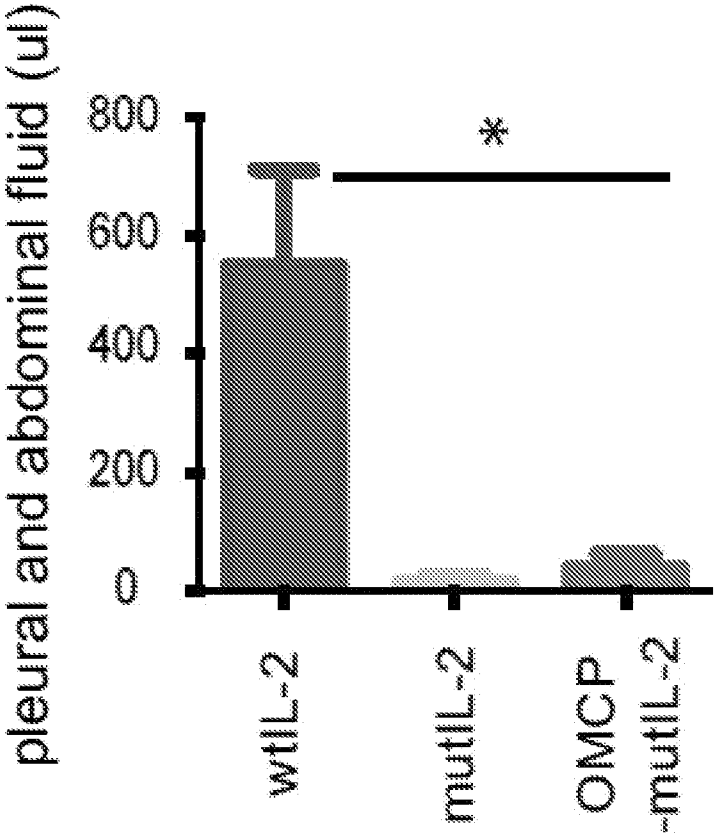

pleural and abdominal fluid (ul)
800
600
400
200
0
*
wtIL-2
mutIL-2
OMCP -mutIL-2

FIG. 2N

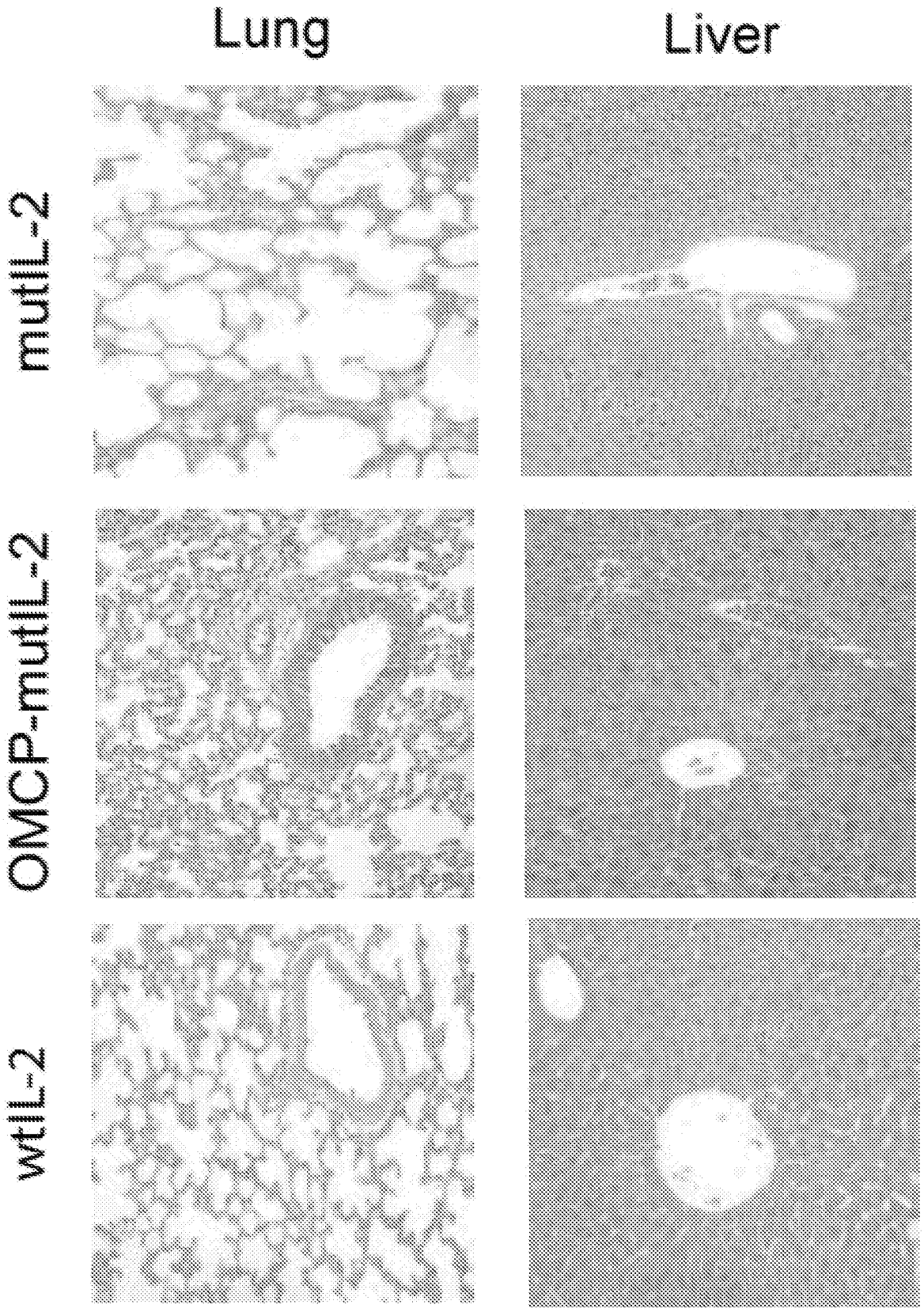


FIG. 20

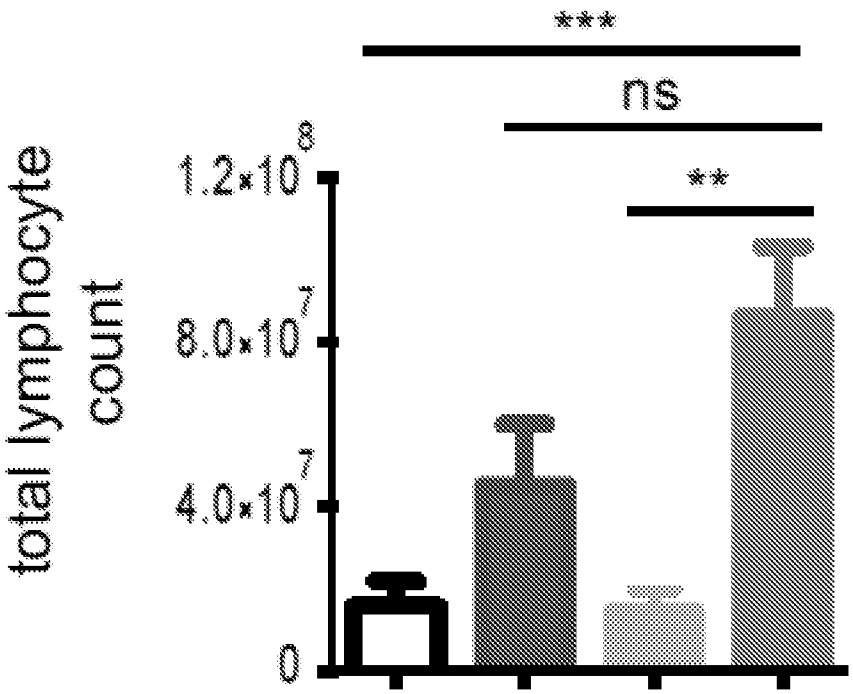

***
ns
**
total lymphocyte count
1.2×10^8
8.0×10^7
4.0×10^7
0

FIG. 3A

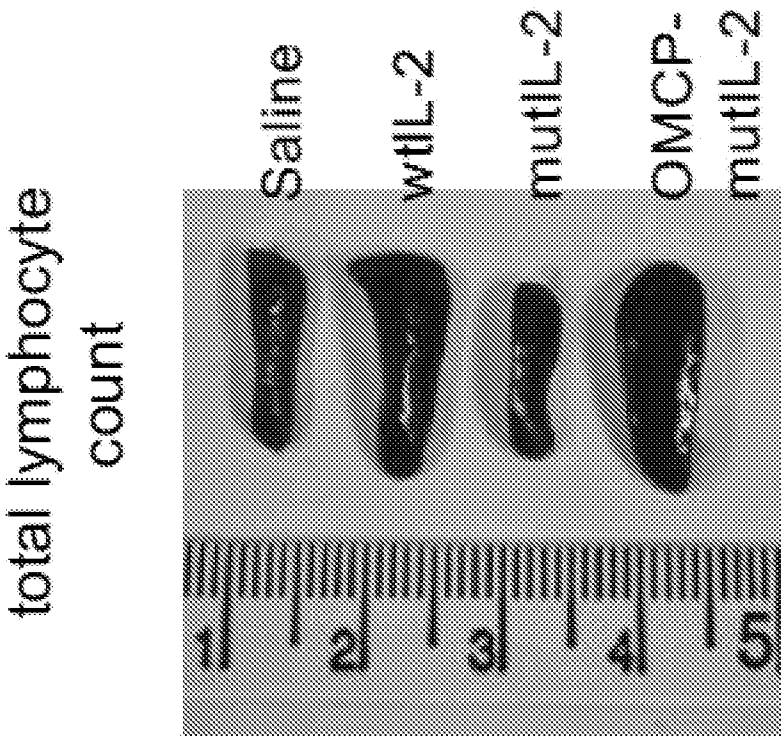
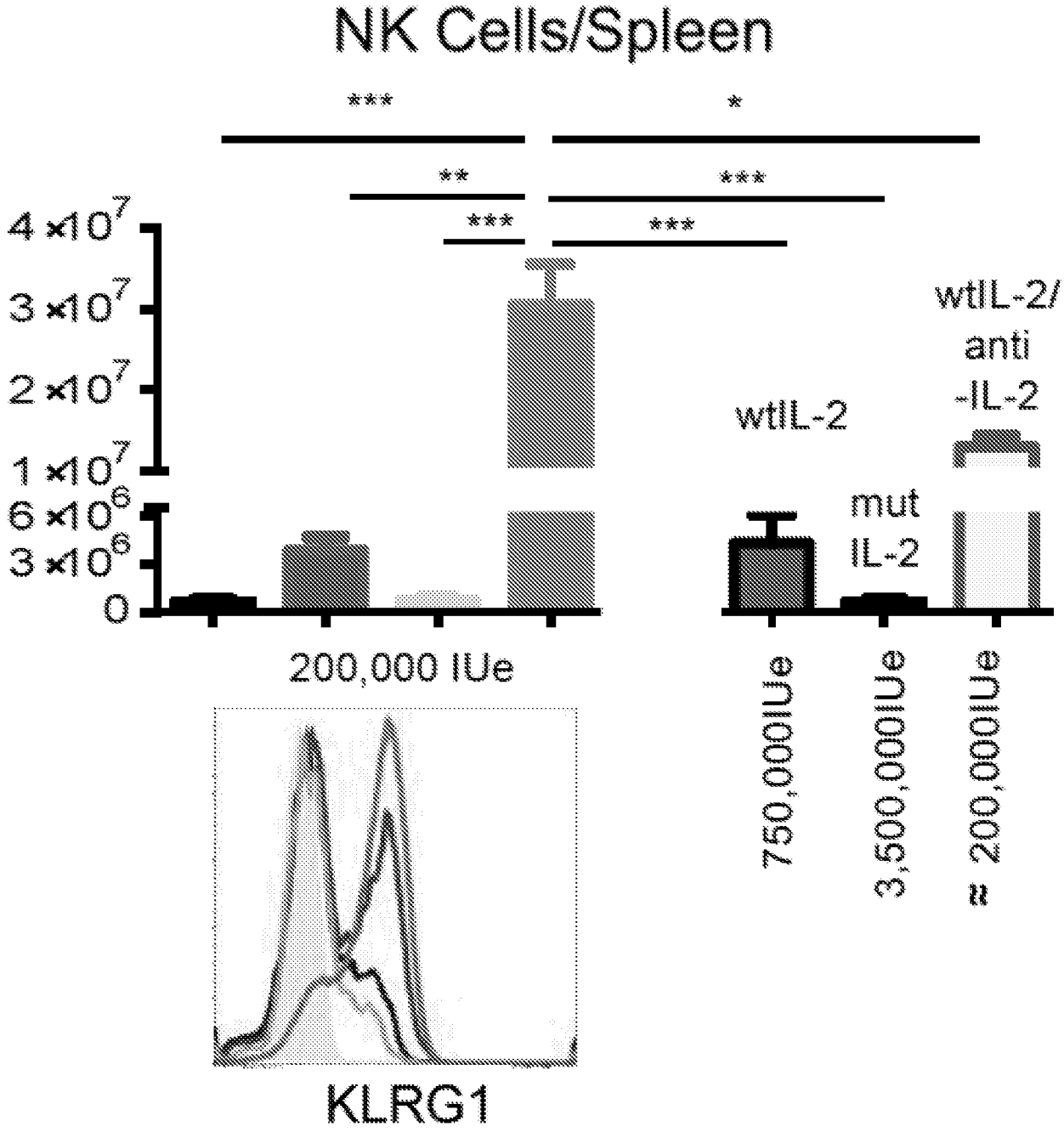

total lymphocyte count
Saline
wtIL-2
mutIL-2
OMCP-mutIL-2
1
2
3
4
5

FIG. 3B



Saline, wtIL-2, mutIL-2, OMCP-mutIL-2

FIG. 3C

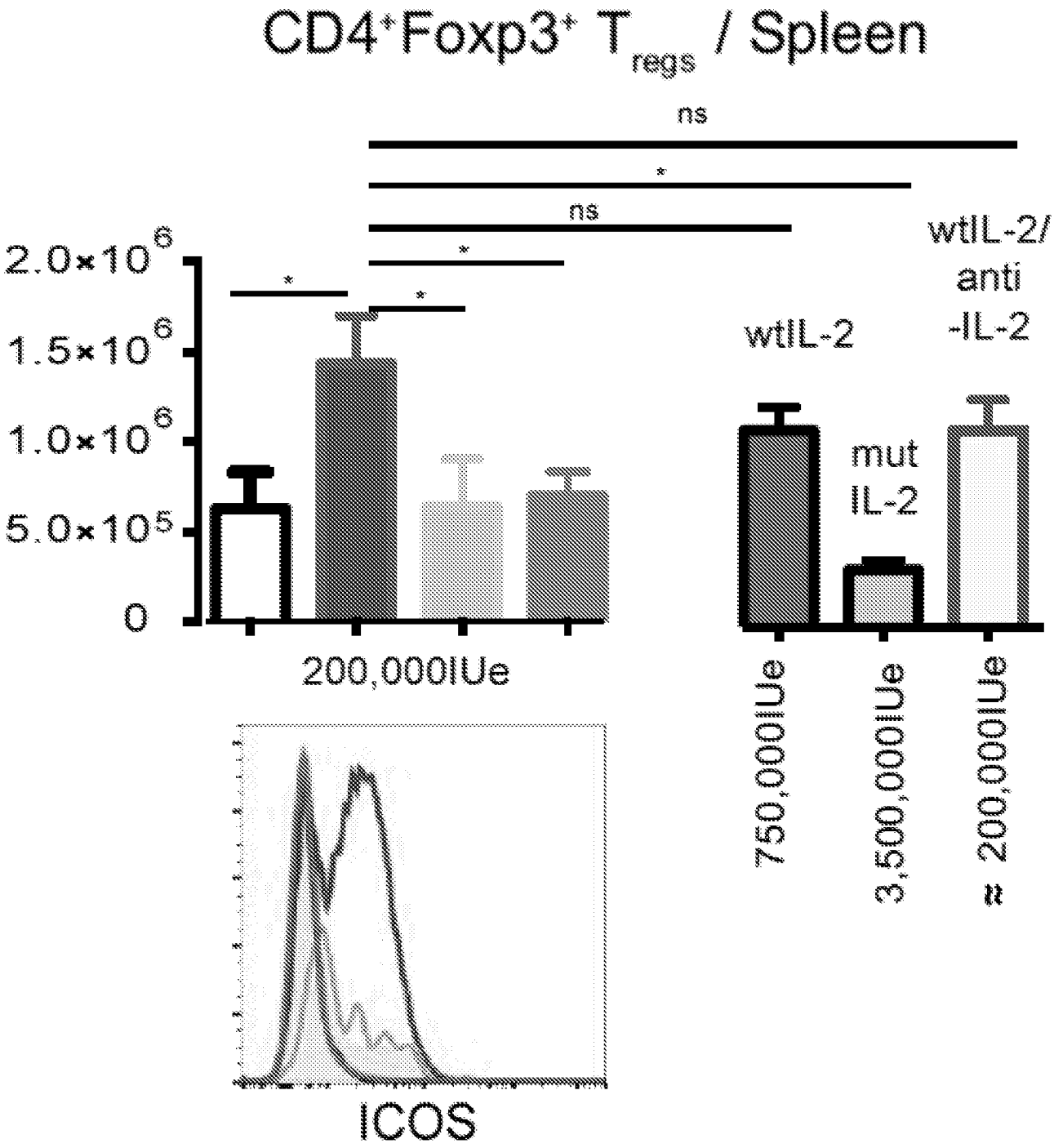
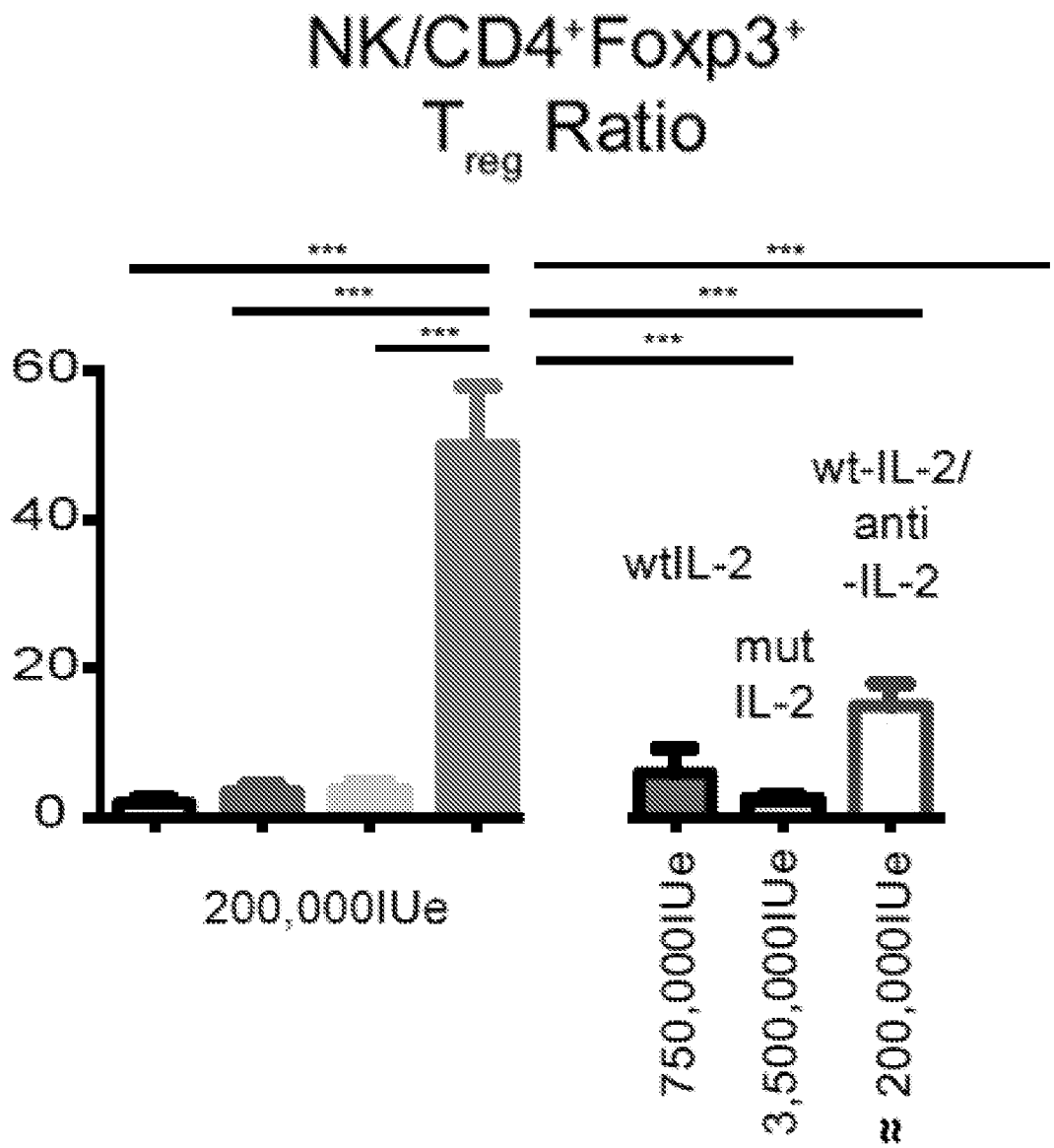

CD4+Foxp3+ Tregs / Spleen
ns
*
ns
*
*
*
2.0×10^6
1.5×10^6
1.0×10^6
5.0×10^5
0
wtIL-2/
anti
-IL-2
wtIL-2
mut
IL-2
200,000IUe
750,000IUe
3,500,000IUe
≈ 200,000IUe
ICOS
Saline, wtIL-2, mutIL-2, OMCP-mutIL-2

FIG. 3D



Saline, wtIL-2, mutIL-2, OMCP-mutIL-2

FIG. 3E

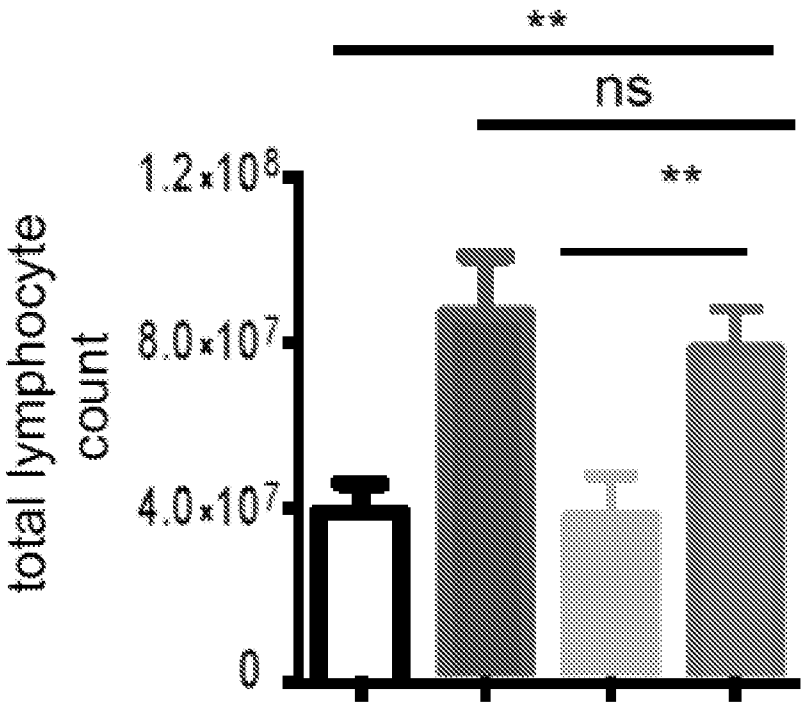

**
ns
**
total lymphocyte count
1.2×10^8
8.0×10^7
4.0×10^7
0

FIG. 3F

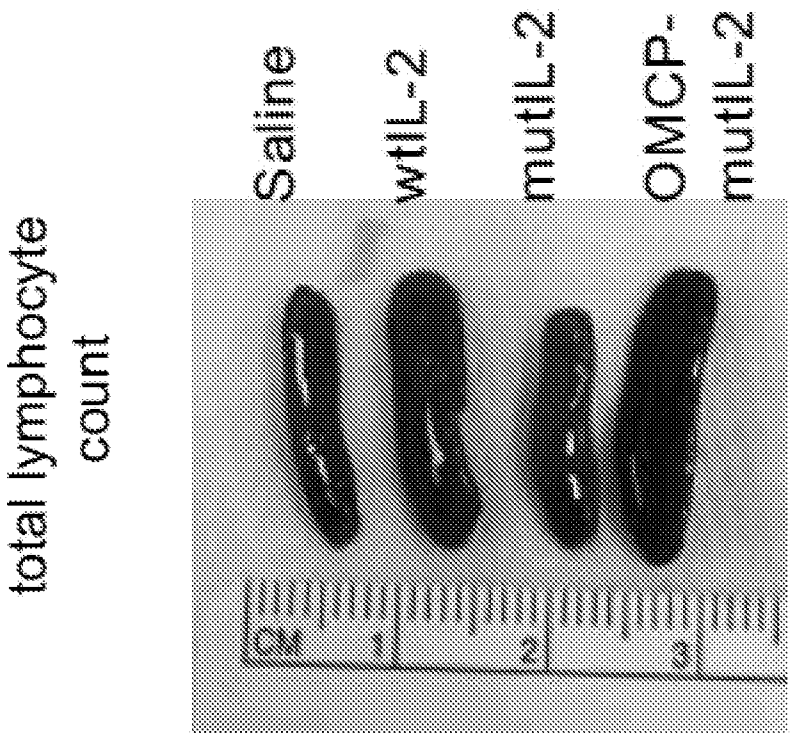

Saline
wtIL-2
mutIL-2
OMCP-mutIL-2
total lymphocyte count

FIG. 3G

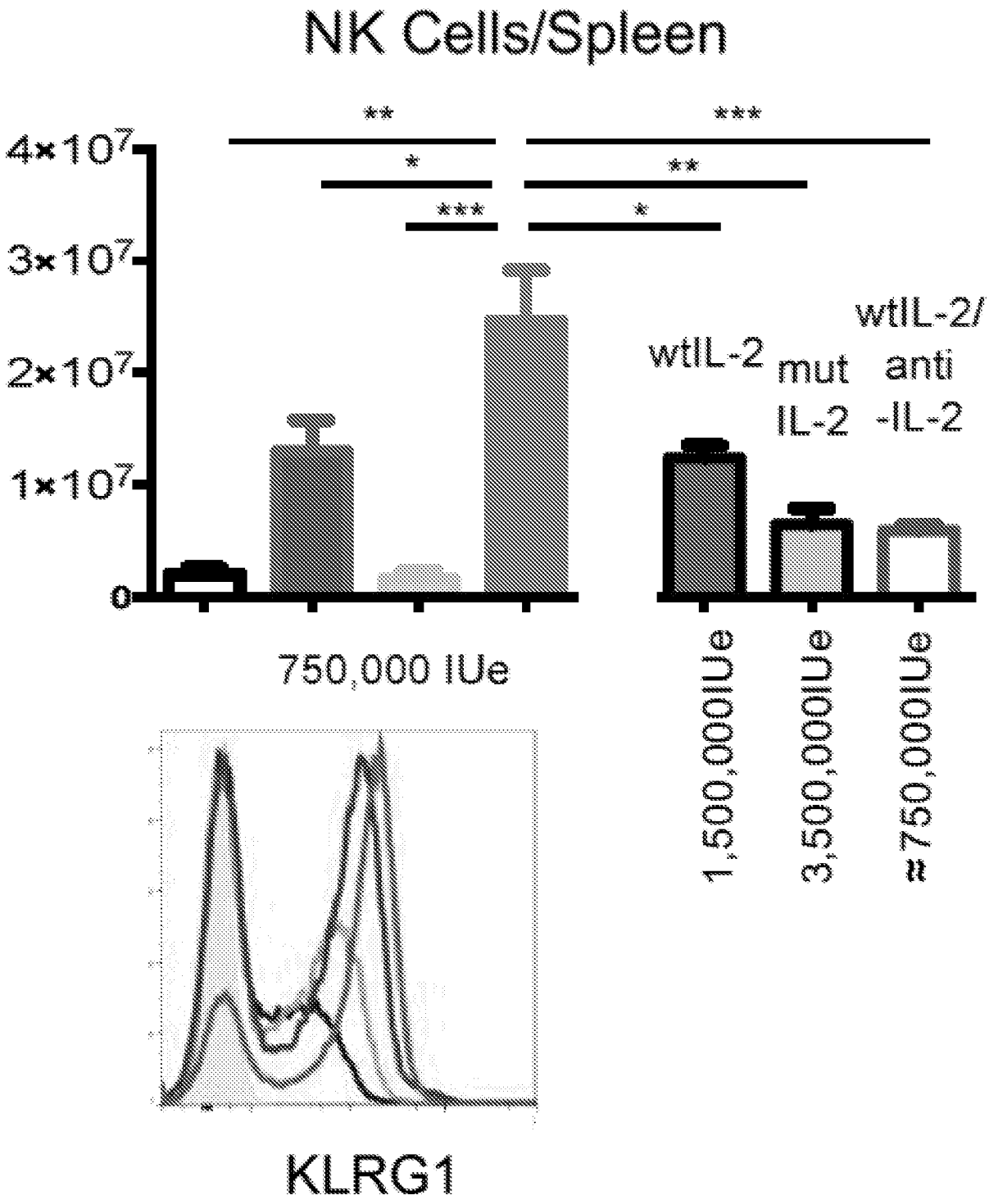
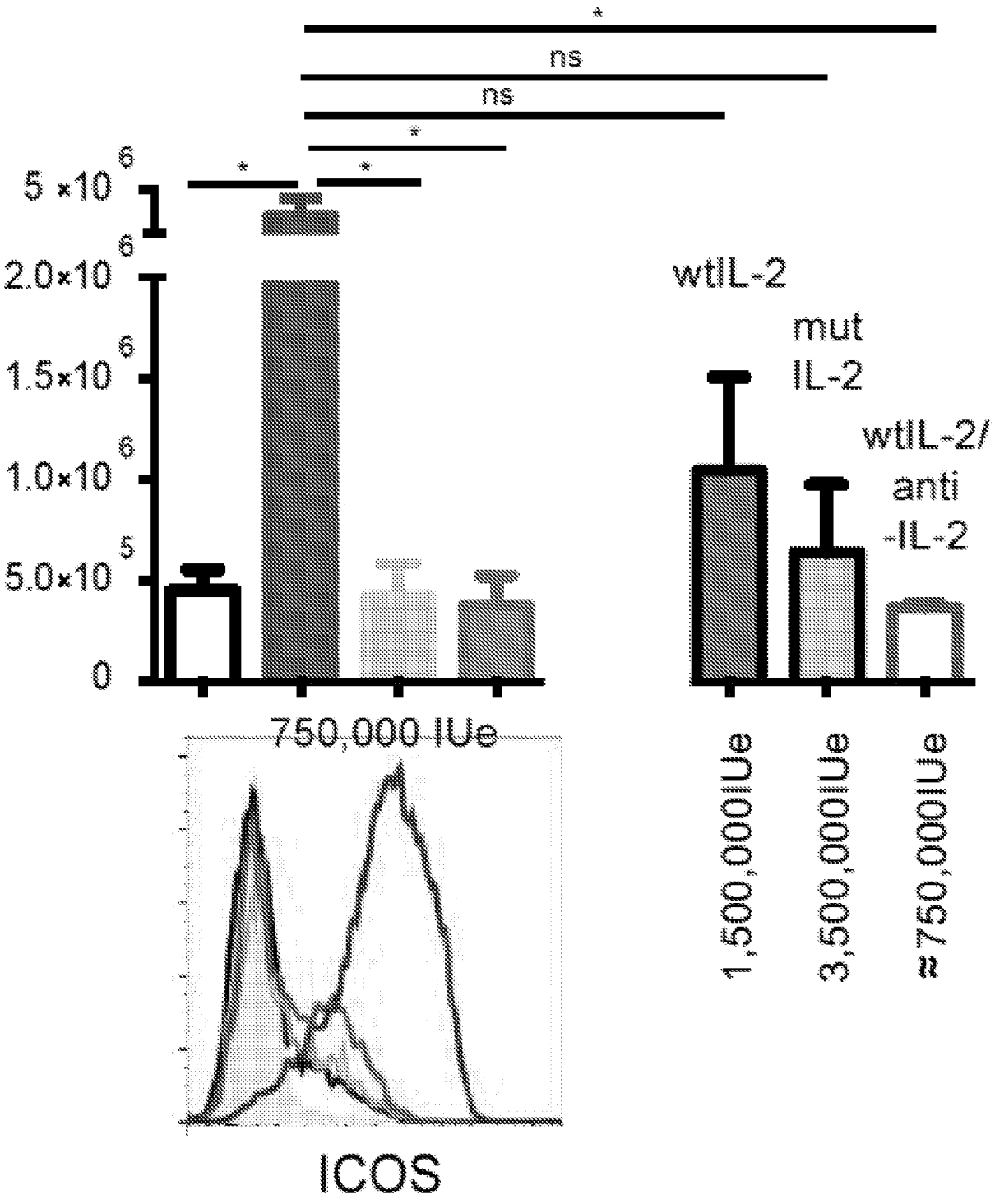
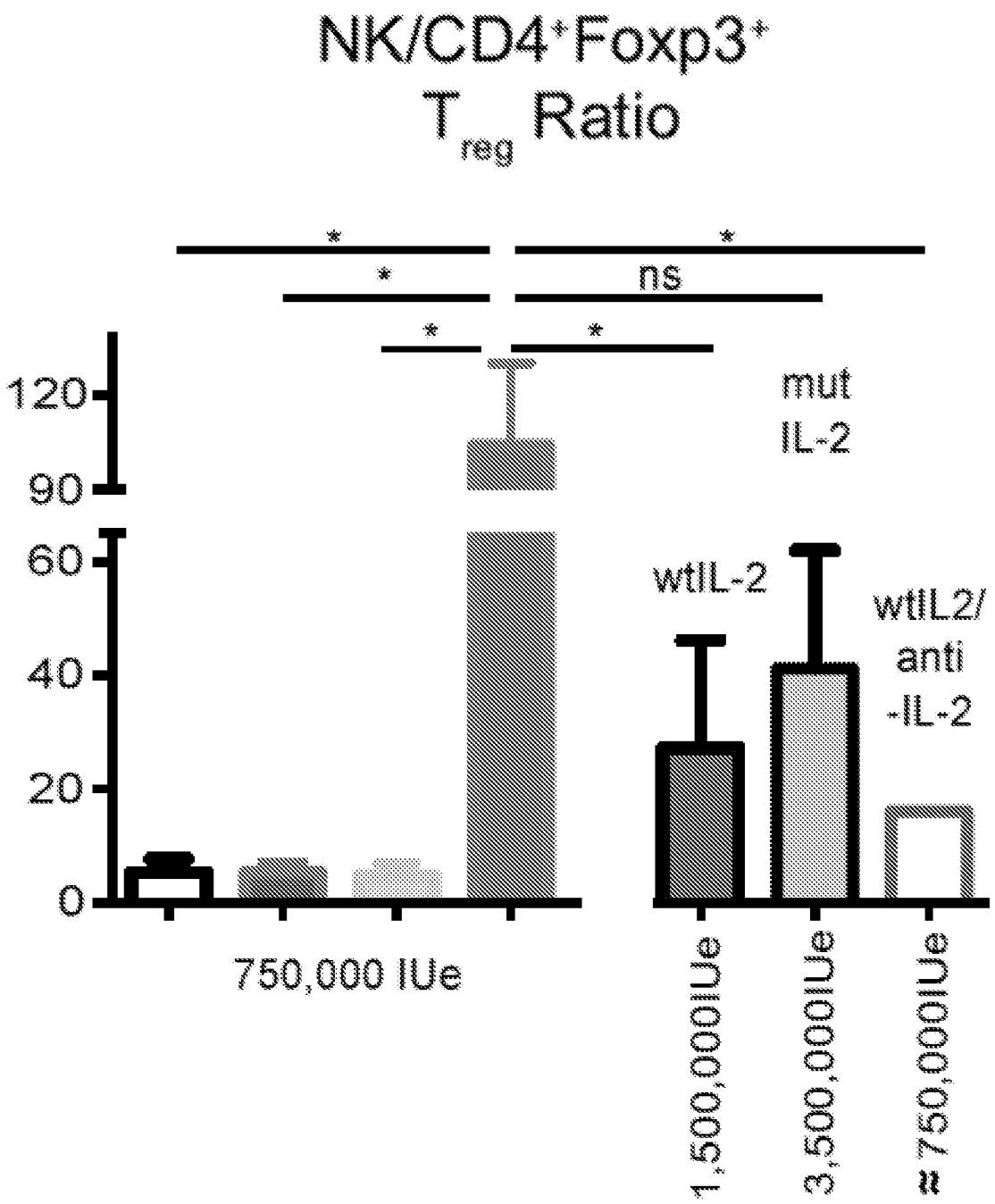

NK Cells/Spleen
**
***
*
**
***
*
4×10^7
3×10^7
2×10^7
1×10^7
0
wtIL-2
wtIL-2/ mut IL-2
wtIL-2/ anti -IL-2
750,000 IUe
1,500,000IUe
3,500,000IUe
7,750,000IUe
KLRG1
Saline, wtIL-2, mutIL-2, OMCP-mutIL-2

FIG. 3H



Saline, wtIL-2, mutIL-2, OMCP-mutIL-2

FIG. 3I



Saline, wtIL-2, mutIL-2, OMCP-mutIL-2

FIG. 3J

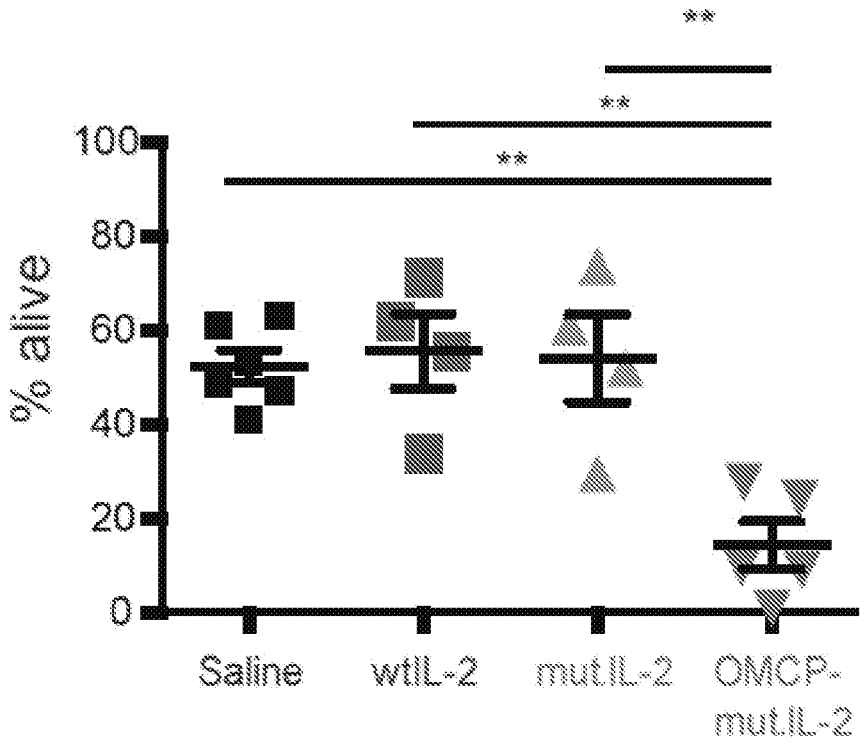

**
**
**
100
80
60
40
20
0
% alive
Saline
wtIL-2
mutIL-2
OMCP-mutIL-2

FIG. 4A

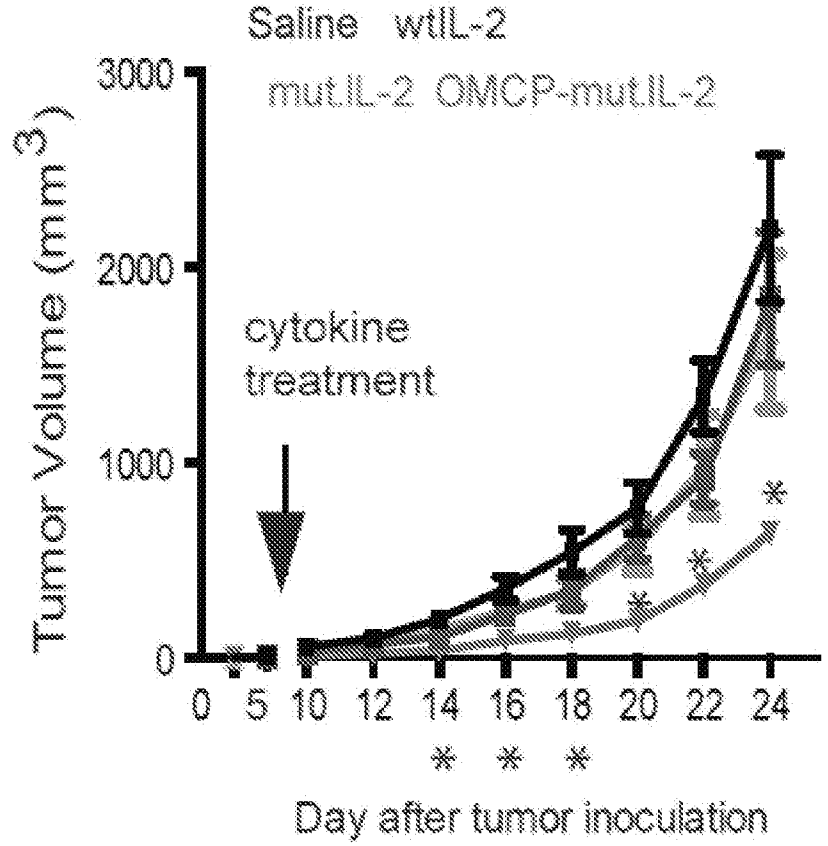

Saline wtIL-2
mutIL-2 OMCP-mutIL-2
3000
2000
1000
0
Tumor Volume (mm3)
cytokine
treatment
0 5 10 12 14 16 18 20 22 24
Day after tumor inoculation

FIG. 4B

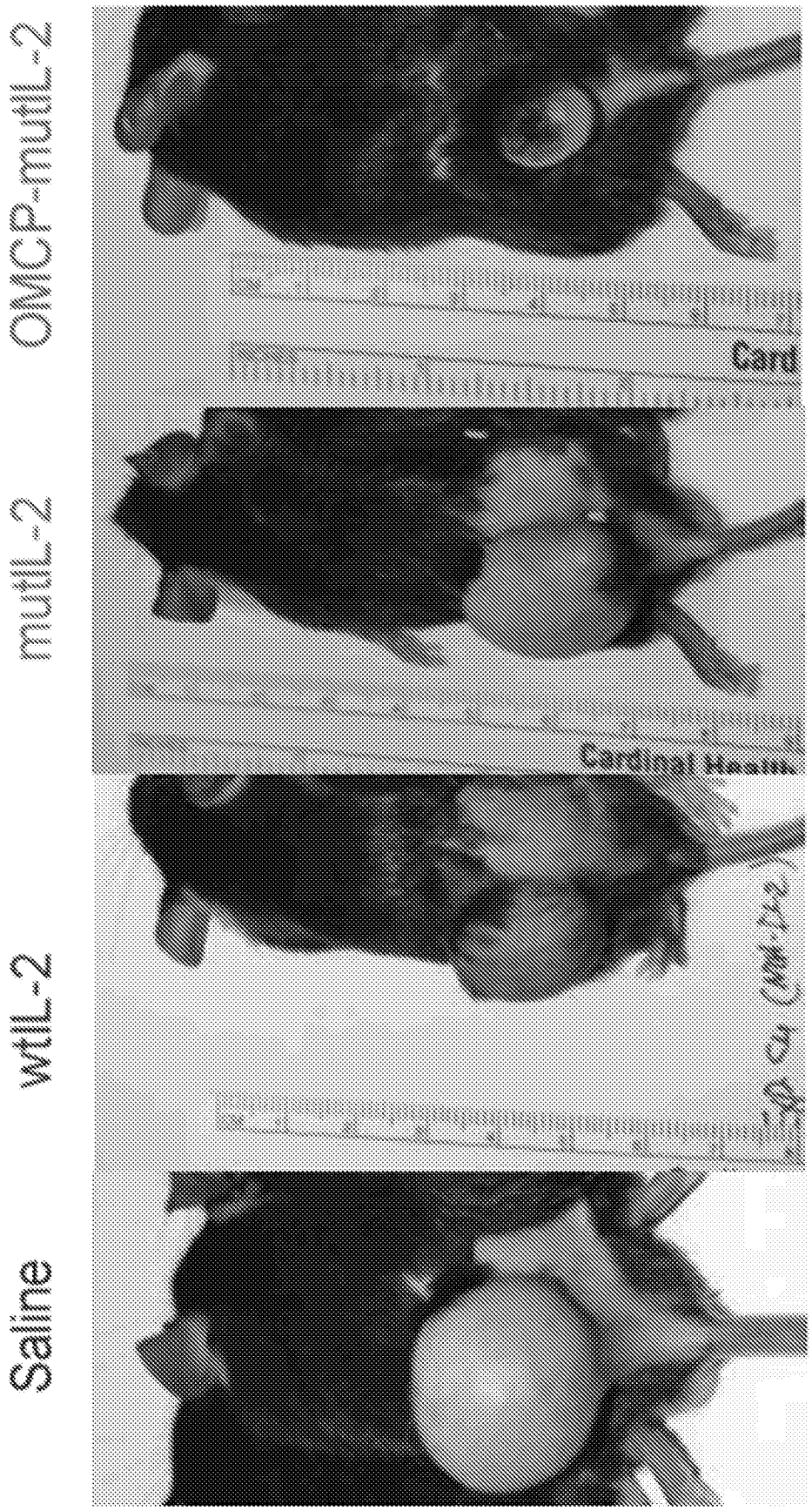


FIG. 4C

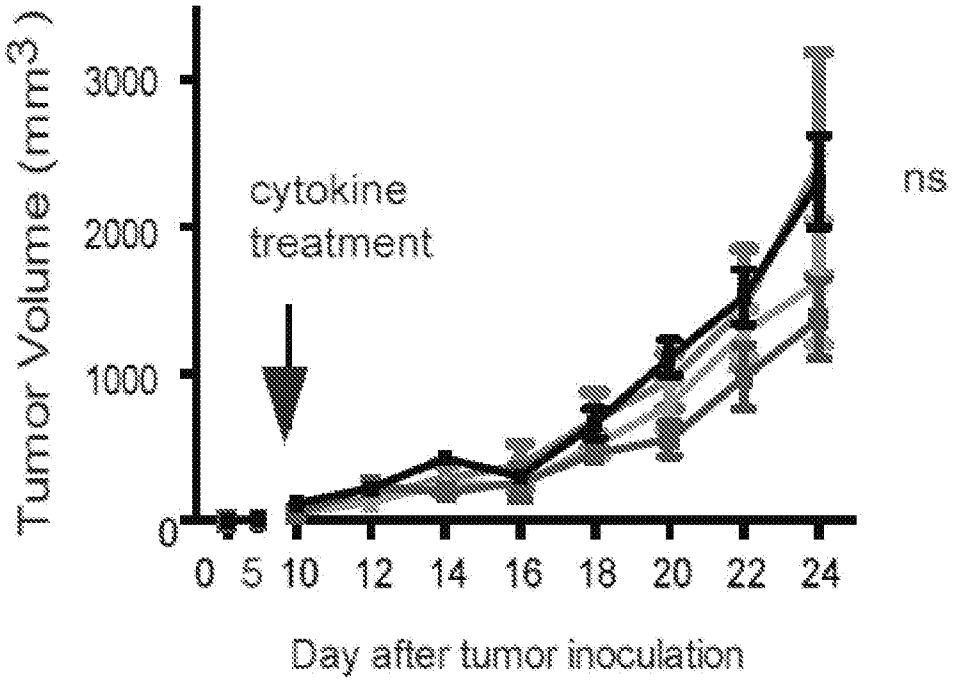

Tumor Volume (mm3)
3000
2000
1000
0
cytokine
treatment
ns
0 5 10 12 14 16 18 20 22 24
Day after tumor inoculation

FIG. 4D

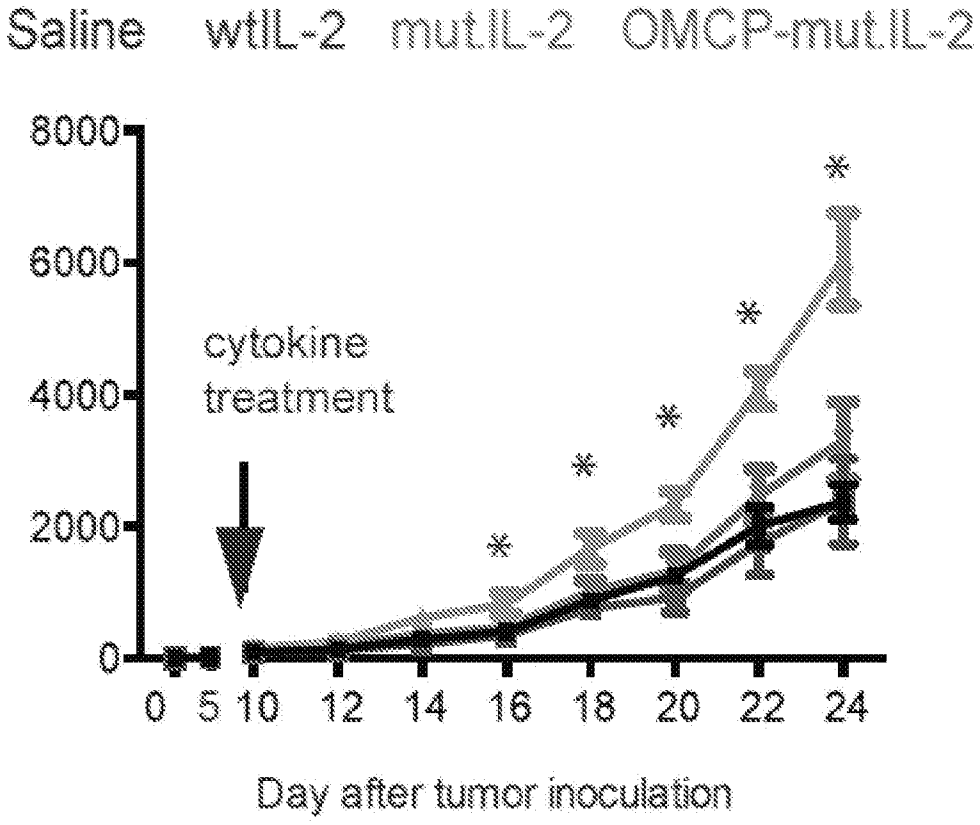

Saline wtIL-2 mutIL-2 OMCP-mutIL-2
8000
6000
4000
2000
0
cytokine
treatment
*
0 5 10 12 14 16 18 20 22 24
Day after tumor inoculation

FIG. 4E

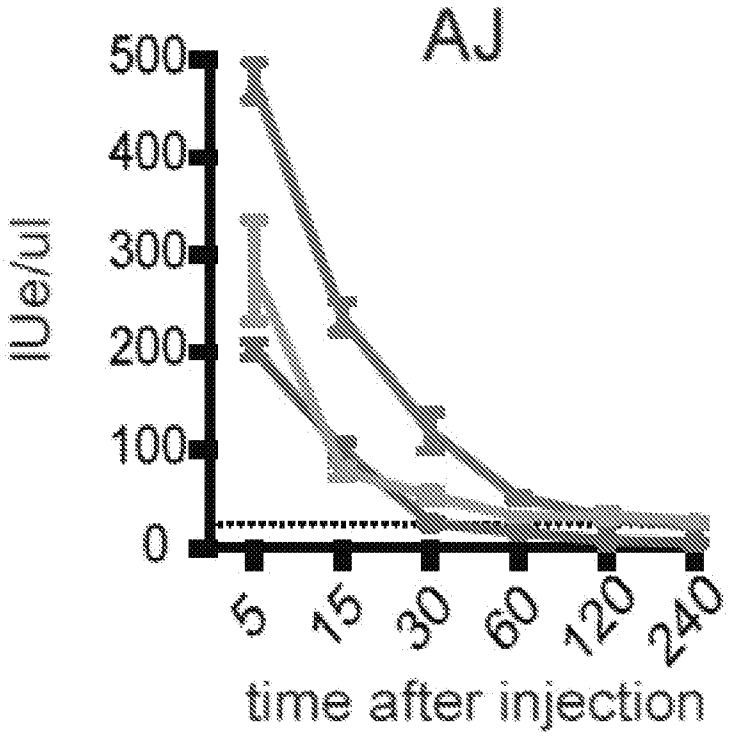


FIG. 5A

OMCP-mutIL-2, wtIL-2, mutIL-2

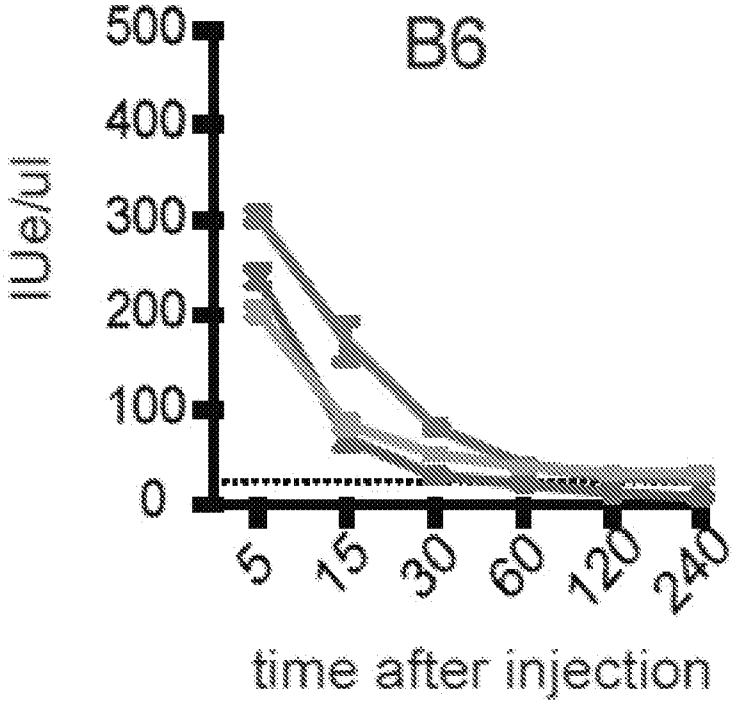


FIG. 5B

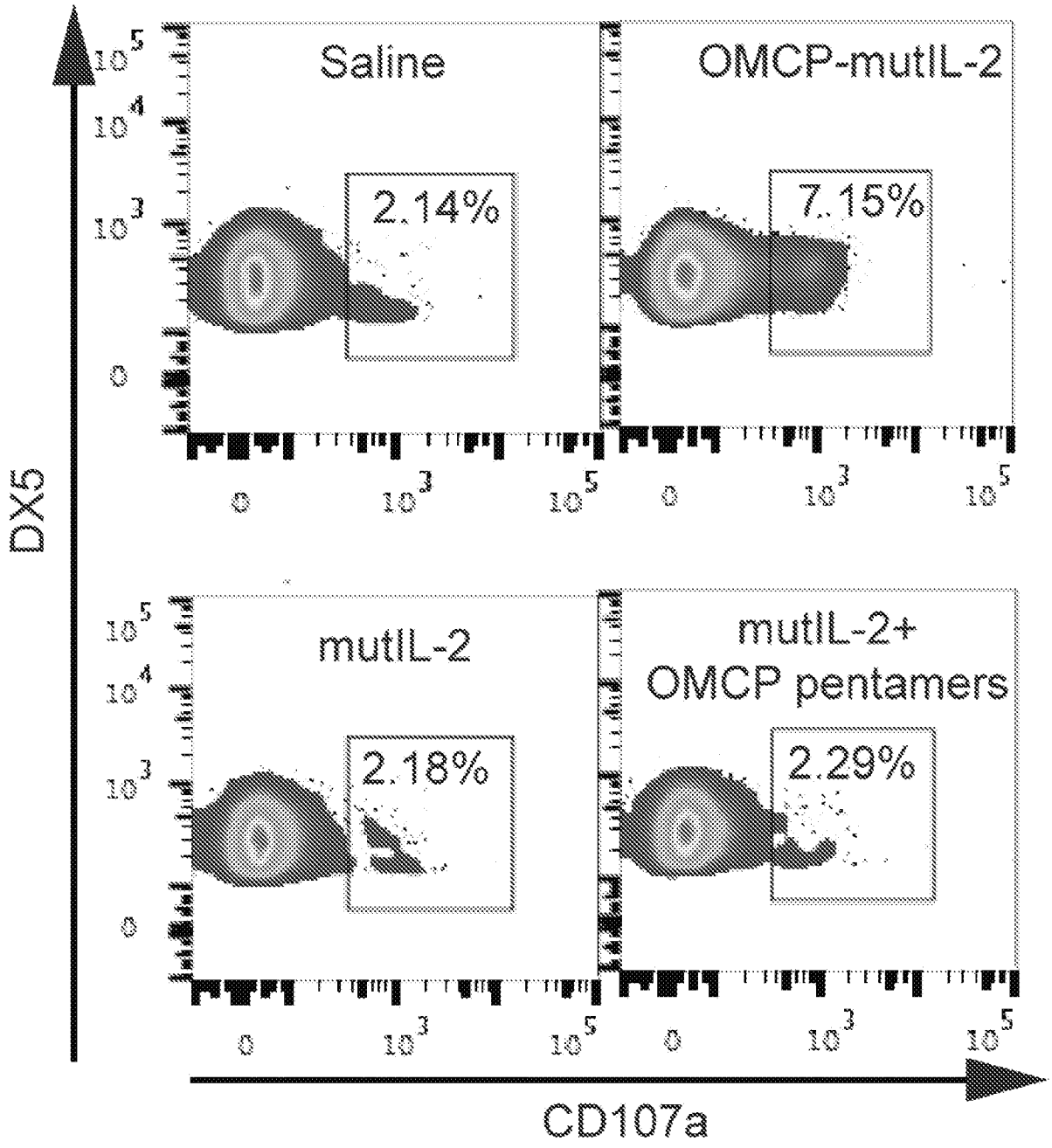

Saline
2.14%
OMCP-mutIL-2
7.15%
mutIL-2
2.18%
mutIL-2+
OMCP pentamers
2.29%
DX5
CD107a
0
10^3
10^4
10^5

FIG. 5C

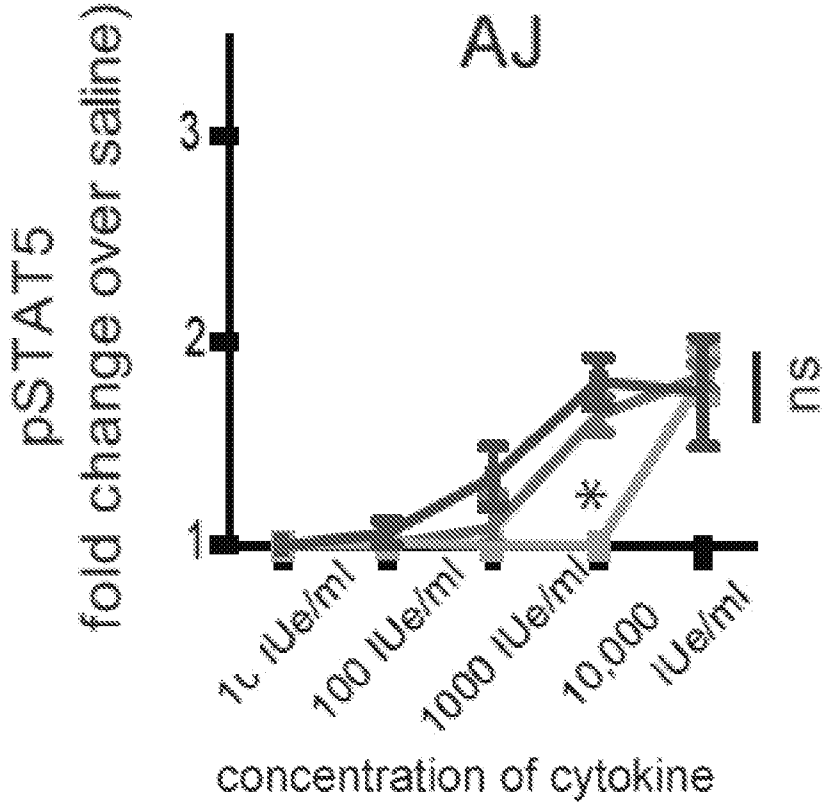

AJ
pSTAT5
fold change over saline)
3
2
1
ns
*
10 IUe/ml
100 IUe/ml
1000 IUe/ml
10,000
IUe/ml
concentration of cytokine

FIG. 5D

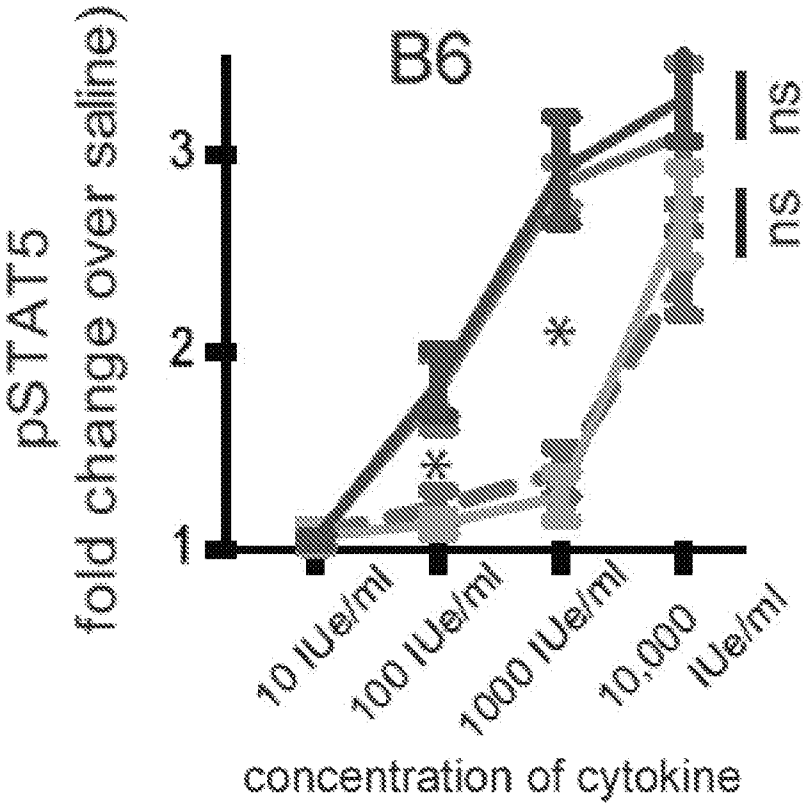

B6
pSTAT5
fold change over saline)
3
2
1
ns
ns
*
*
10 IUe/ml
100 IUe/ml
1000 IUe/ml
10,000
IUe/ml
concentration of cytokine

FIG. 5E

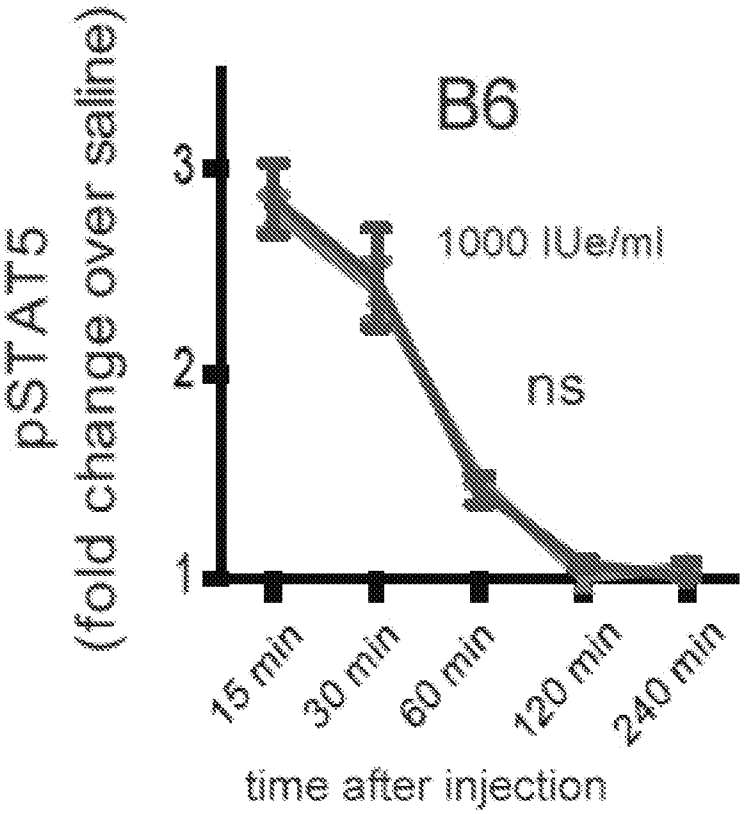

B6
1000 IUe/ml
ns
pSTAT5
(fold change over saline)
3
2
1
15 min
30 min
60 min
120 min
240 min
time after injection

FIG. 5F

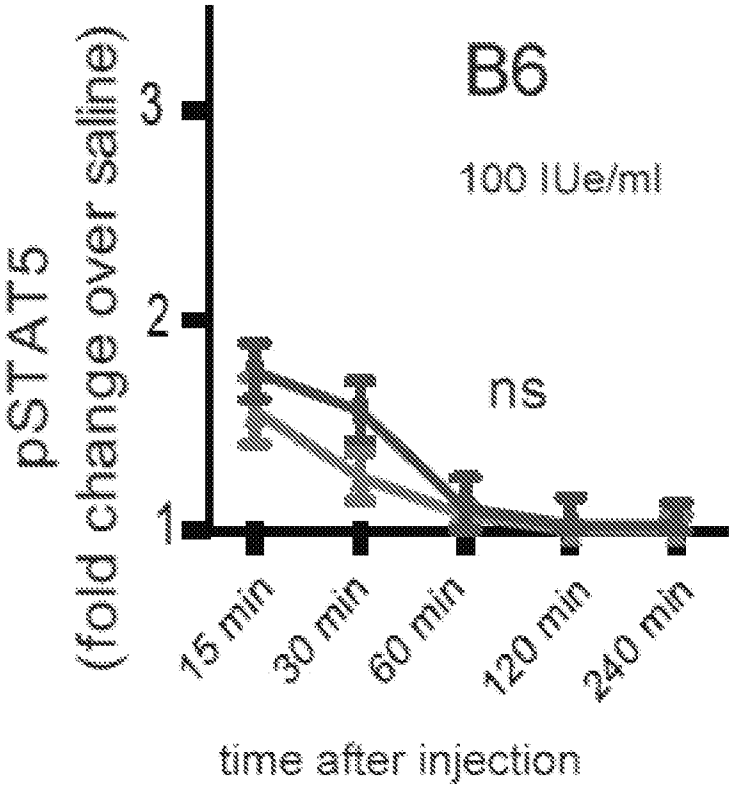

B6
100 IUe/ml
ns
pSTAT5
(fold change over saline)
3
2
1
15 min
30 min
60 min
120 min
240 min
time after injection

FIG. 5G

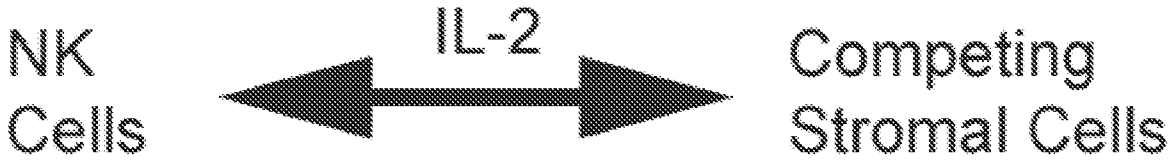

NK
Cells
IL-2
Competing
Stromal Cells

FIG. 5H

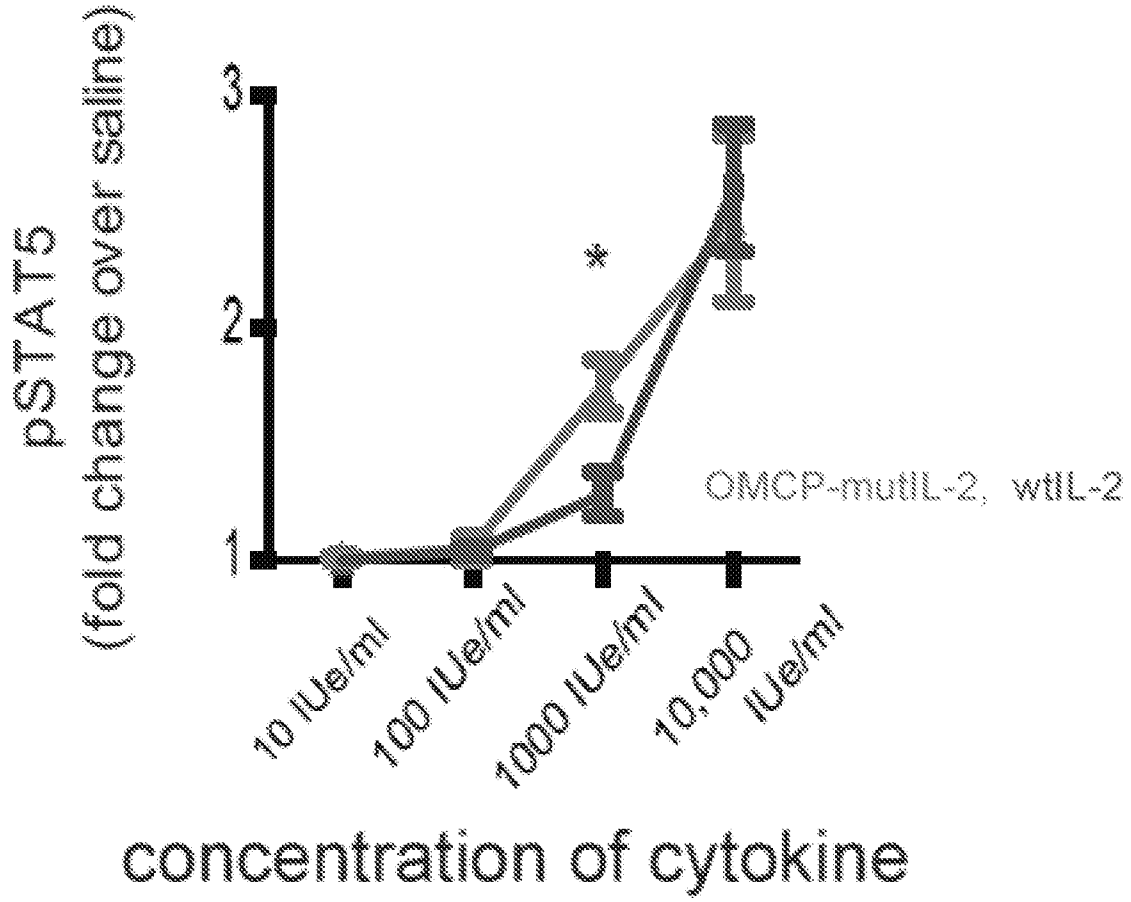

pSTAT5
(fold change over saline)
3
2
1
*
OMCP-mutIL-2, wtIL-2
10 IUe/ml
100 IUe/ml
1000 IUe/ml
10,000 IUe/ml
concentration of cytokine

FIG. 5I

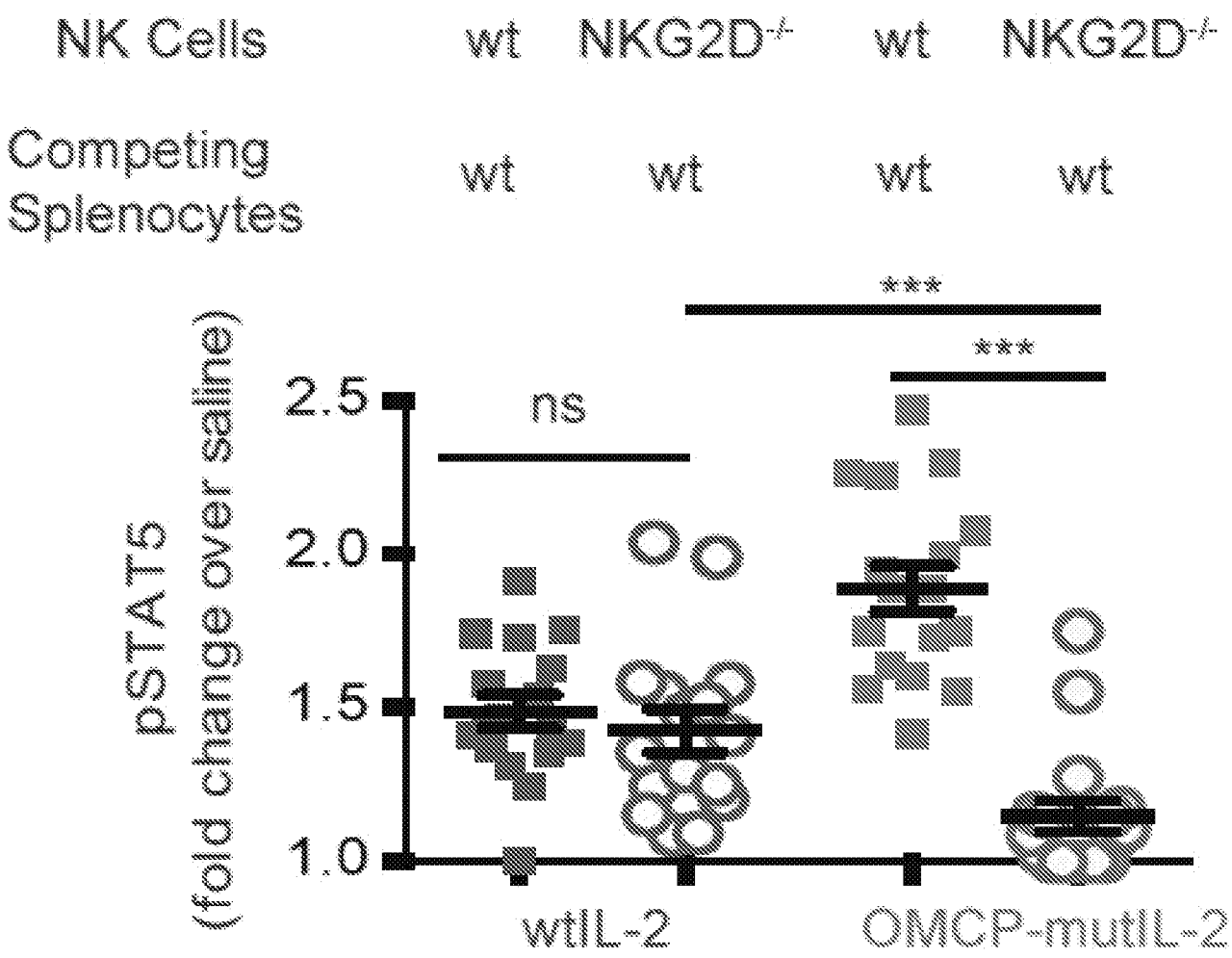

NK Cells
wt
NKG2D-/-
wt
NKG2D-/-
Competing Splenocytes
wt
wt
wt
wt
***
***
ns
pSTAT5 (fold change over saline)
2.5
2.0
1.5
1.0
wtIL-2
OMCP-mutIL-2

FIG. 5J

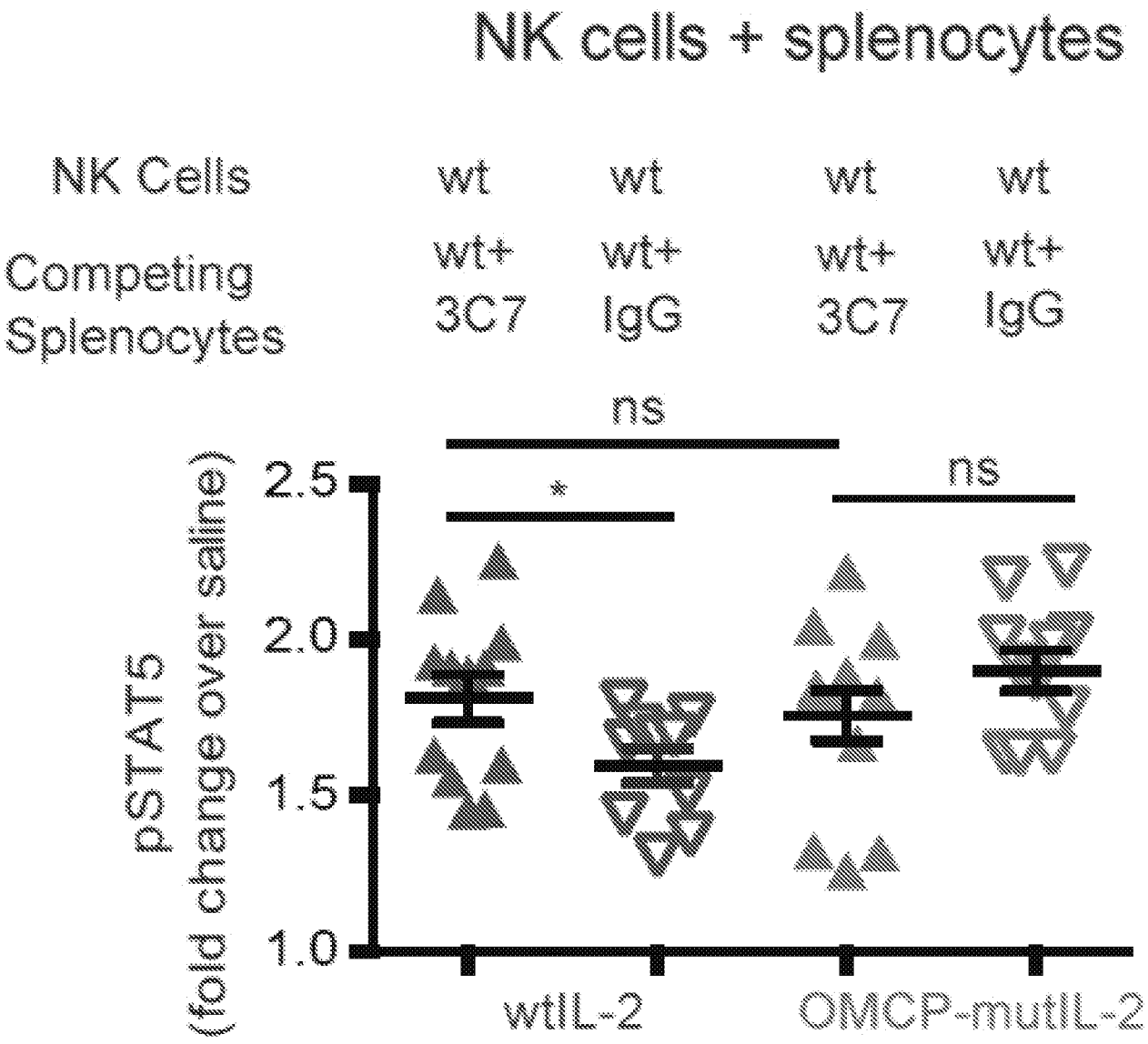

NK cells + splenocytes
NK Cells
wt
wt
wt
wt
Competing Splenocytes
wt+ 3C7
wt+ IgG
wt+ 3C7
wt+ IgG
ns
*
ns
pSTAT5 (fold change over saline)
2.5
2.0
1.5
1.0
wtIL-2
OMCP-mutIL-2

FIG. 5K

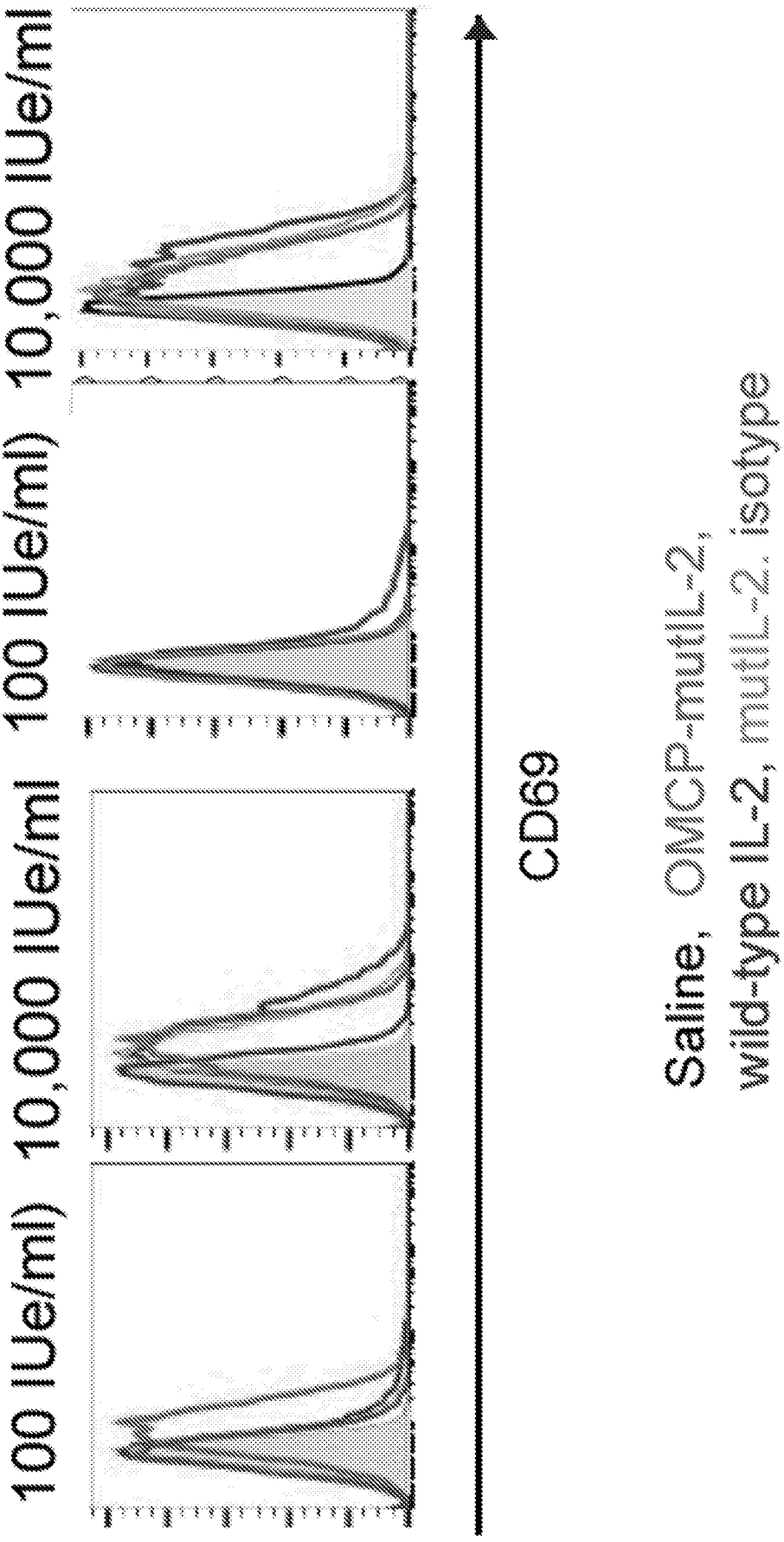

100 IUe/ml)
10,000 IUe/ml
100 IUe/ml)
10,000 IUe/ml
CD69
Saline, OMCP-mutIL-2,
wild-type IL-2, mutIL-2, isotype

FIG. 6

Saline

FIG. 7A

200,000IUe

FIG. 7B

750,000IUe

FIG. 7C

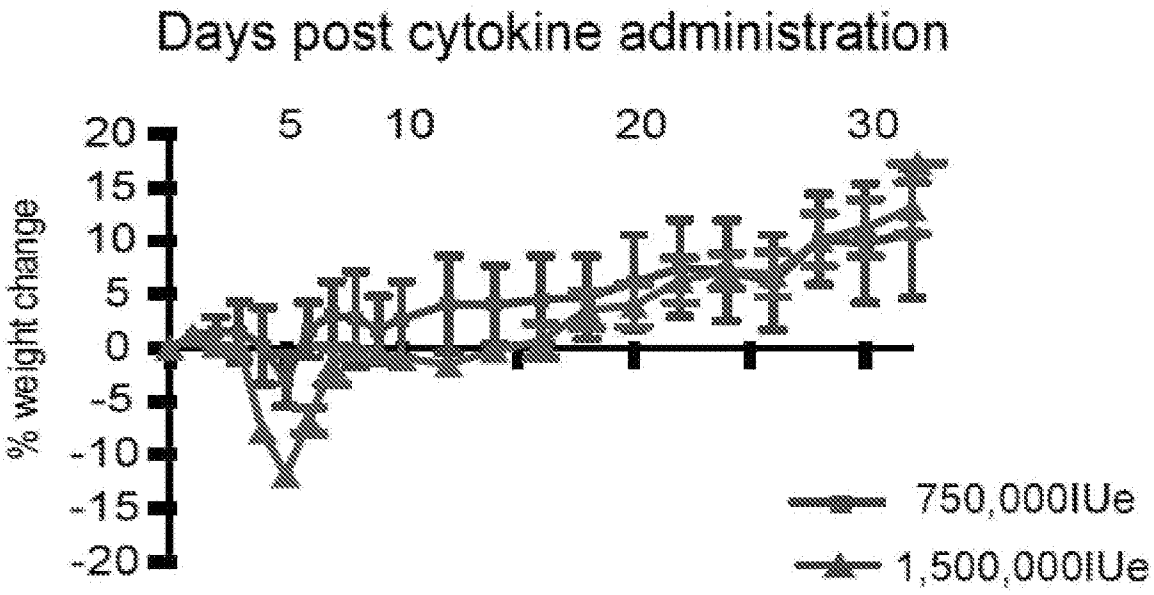


FIG. 7D

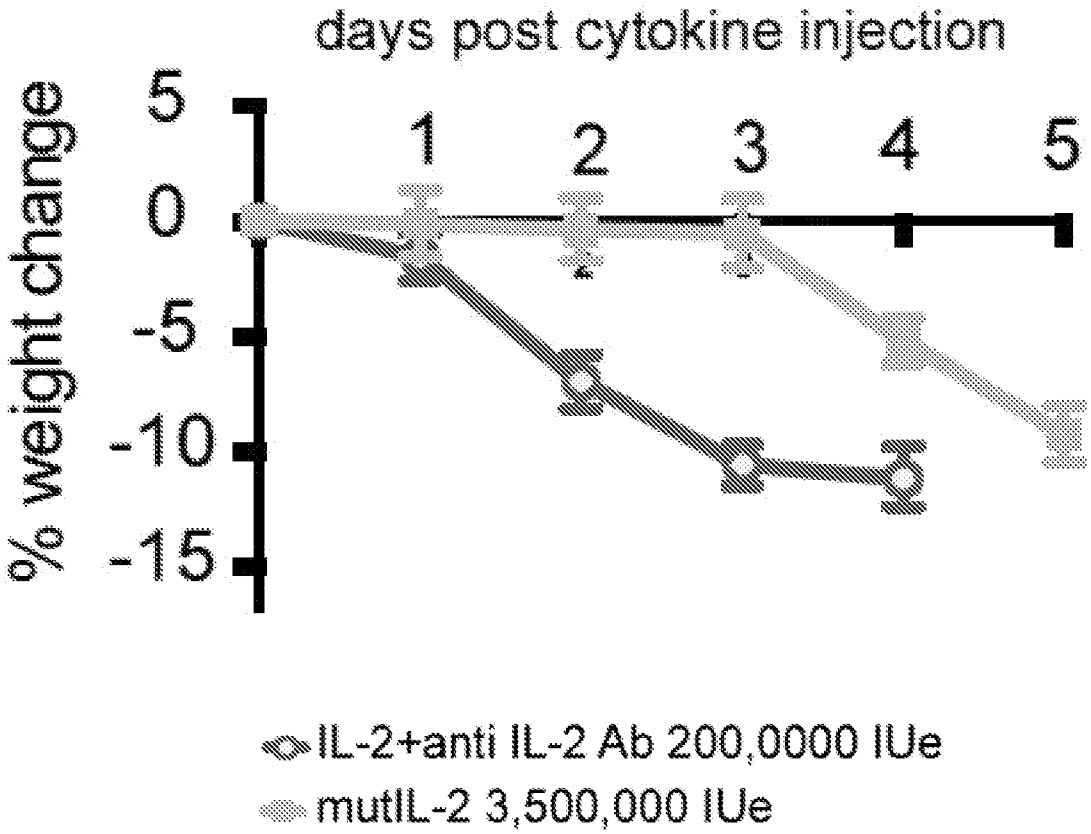

days post cytokine injection
% weight change
5
0
-5
-10
-15
1
2
3
4
5
IL-2+anti IL-2 Ab 200,0000 IUe
mutIL-2 3,500,000 IUe

FIG. 8A

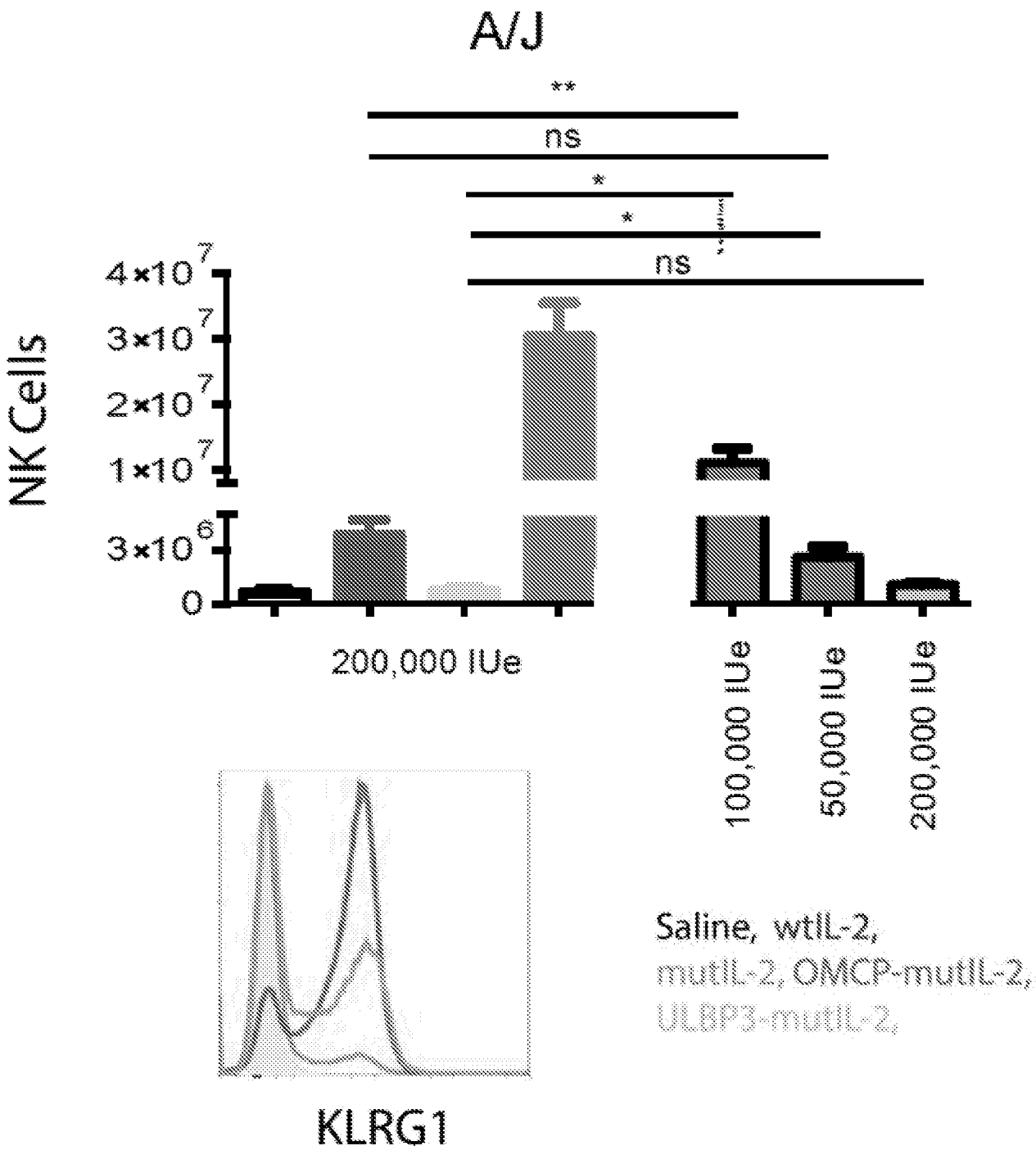

A/J
**
ns
*
*
ns
NK Cells
4×10^7
3×10^7
2×10^7
1×10^7
3×10^6
0
200,000 IUe
100,000 IUe
50,000 IUe
200,000 IUe
Saline, wtIL-2,
mutIL-2, OMCP-mutIL-2,
ULBP3-mutIL-2,
KLRG1

FIG. 8B

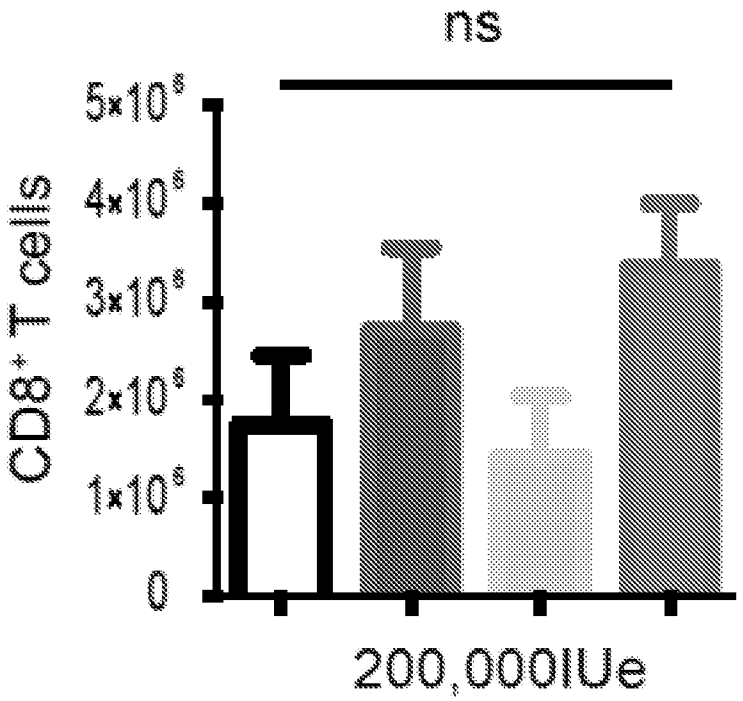


FIG. 8C

Saline, wtIL-2, mutIL-2, OMCP-mutIL-2,

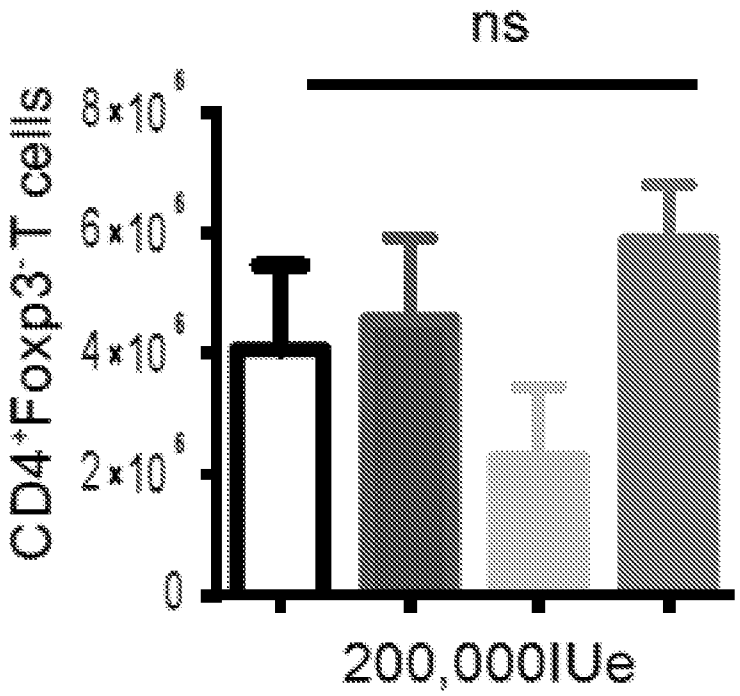


FIG. 8D

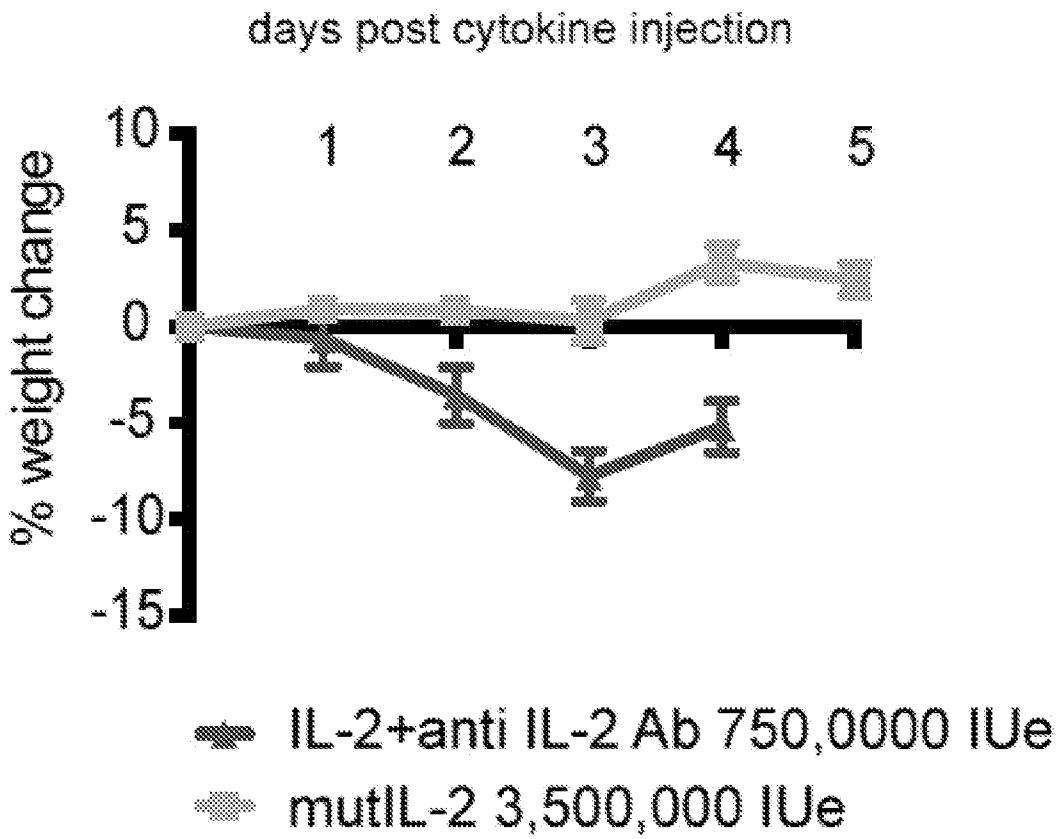

days post cytokine injection
% weight change
10
5
0
-5
-10
-15
1
2
3
4
5
IL-2+anti IL-2 Ab 750,0000 IUe
mutIL-2 3,500,000 IUe

FIG. 8E

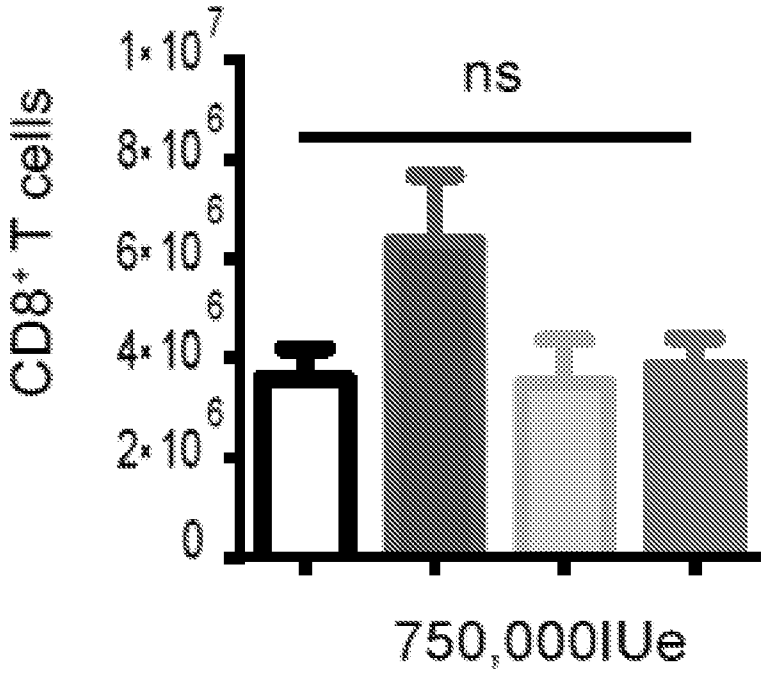


FIG. 8F

Saline, wtIL-2, mutIL-2, OMCP-mutIL-2,

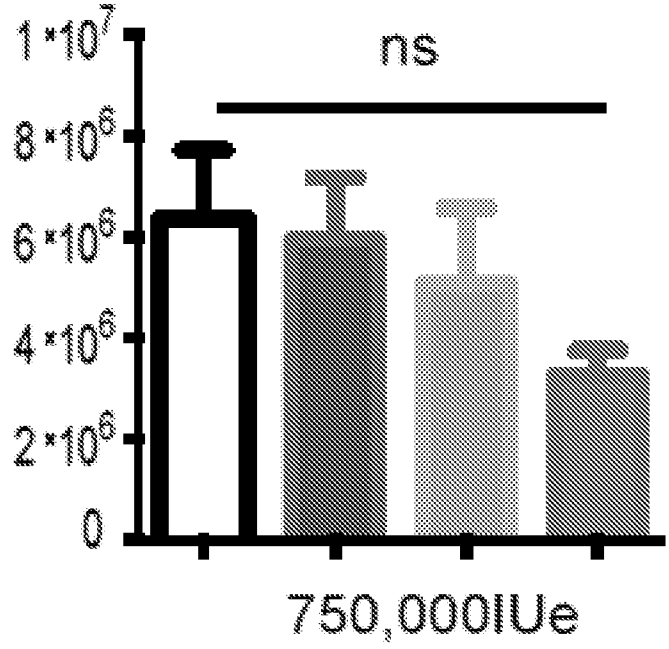


FIG. 8G

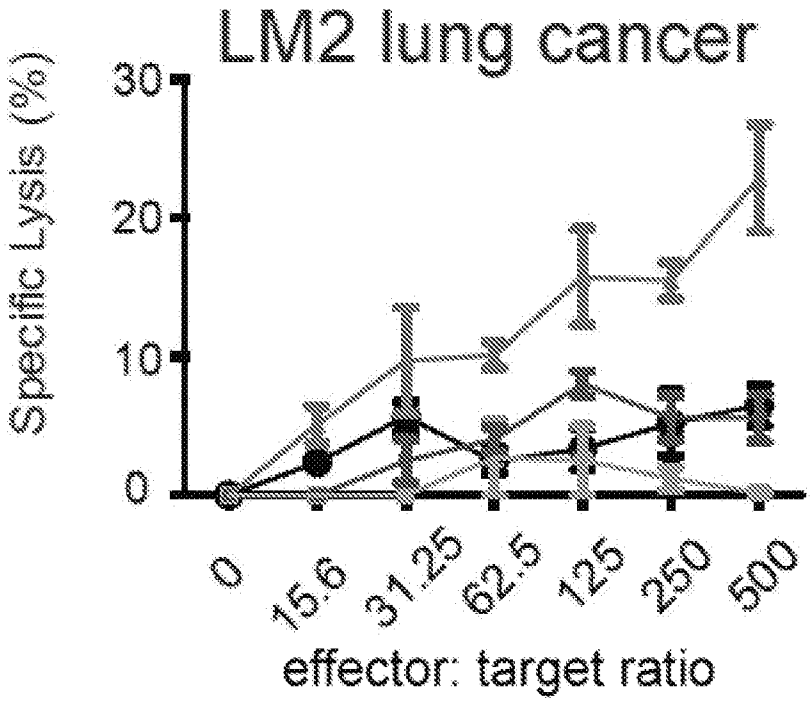


FIG. 9A

saline, wtIL-2, mutIL-2, OMCP-mutIL-2

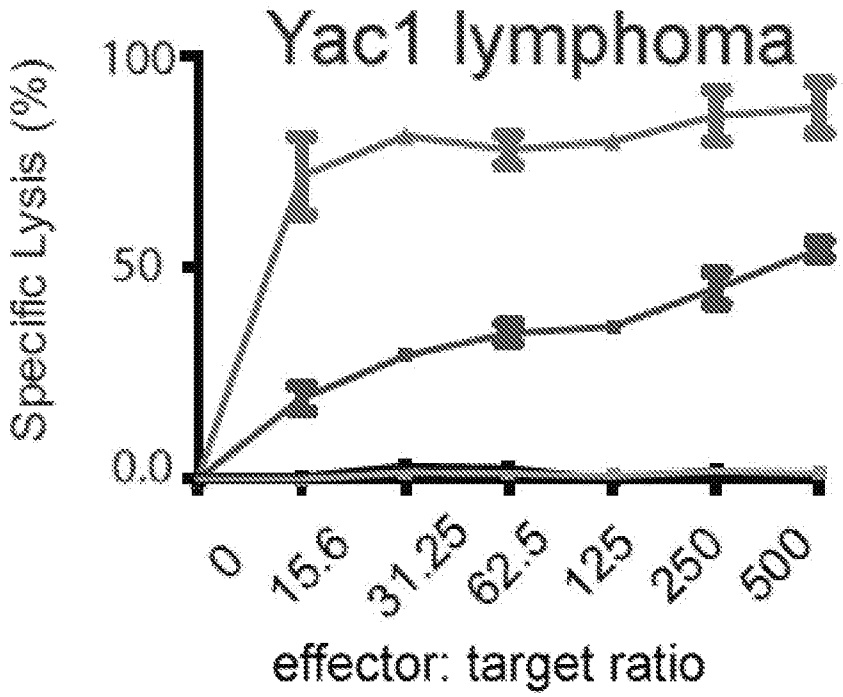
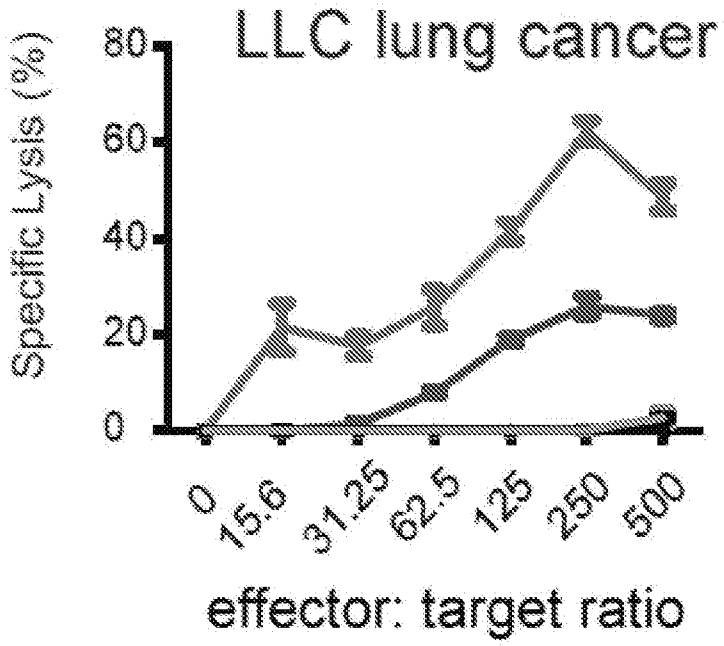


FIG. 9B



saline, wtIL-2, mutIL-2, OMCP-mutIL-2

FIG. 9C

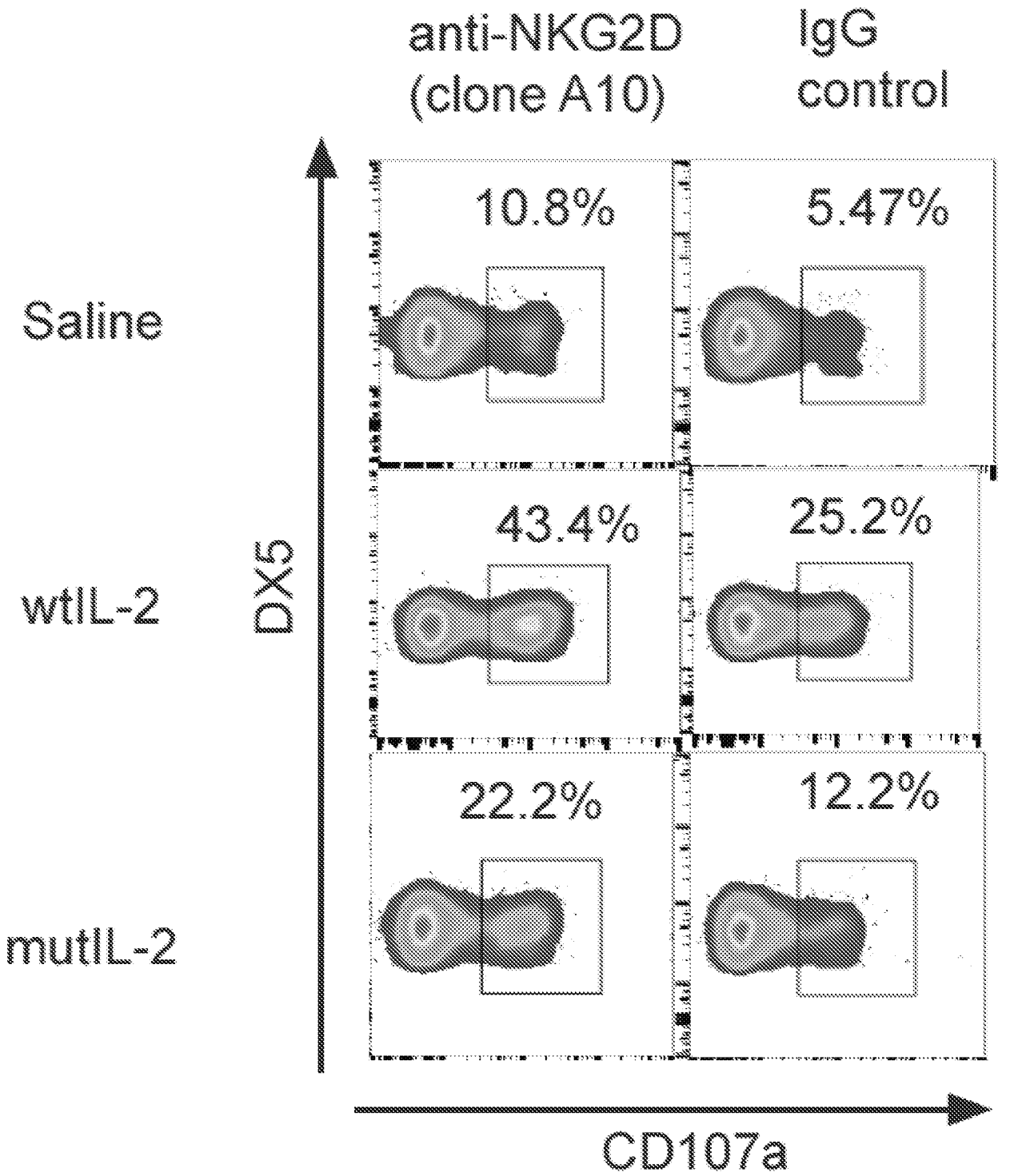

anti-NKG2D
(clone A10)
IgG
control
Saline
wtIL-2
mutIL-2
DX5
CD107a
10.8%
5.47%
43.4%
25.2%
22.2%
12.2%

FIG. 10A

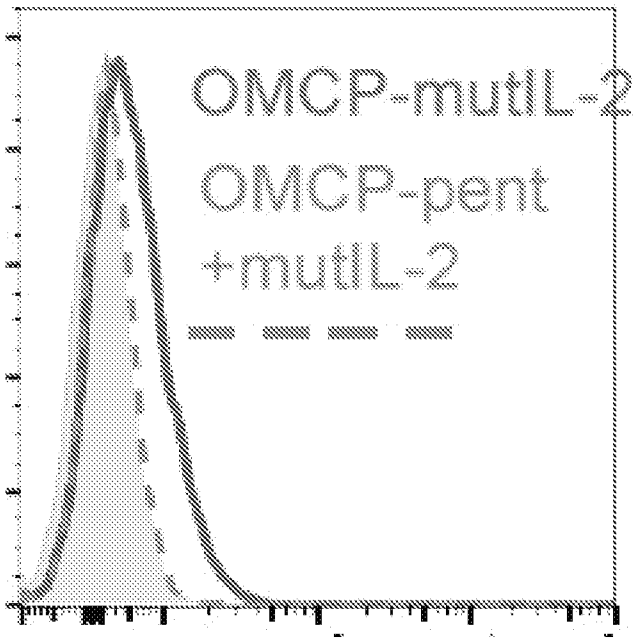


FIG. 10B

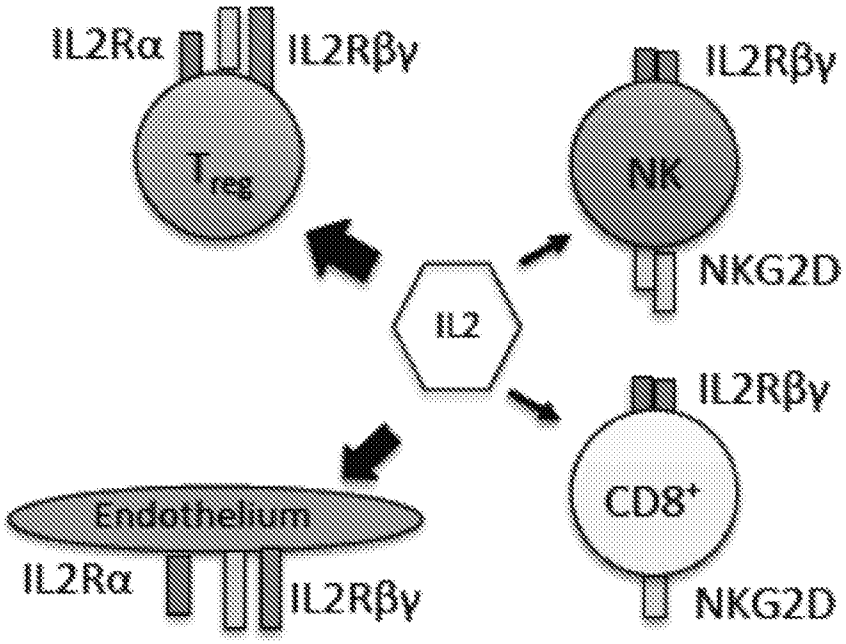


FIG. 11A

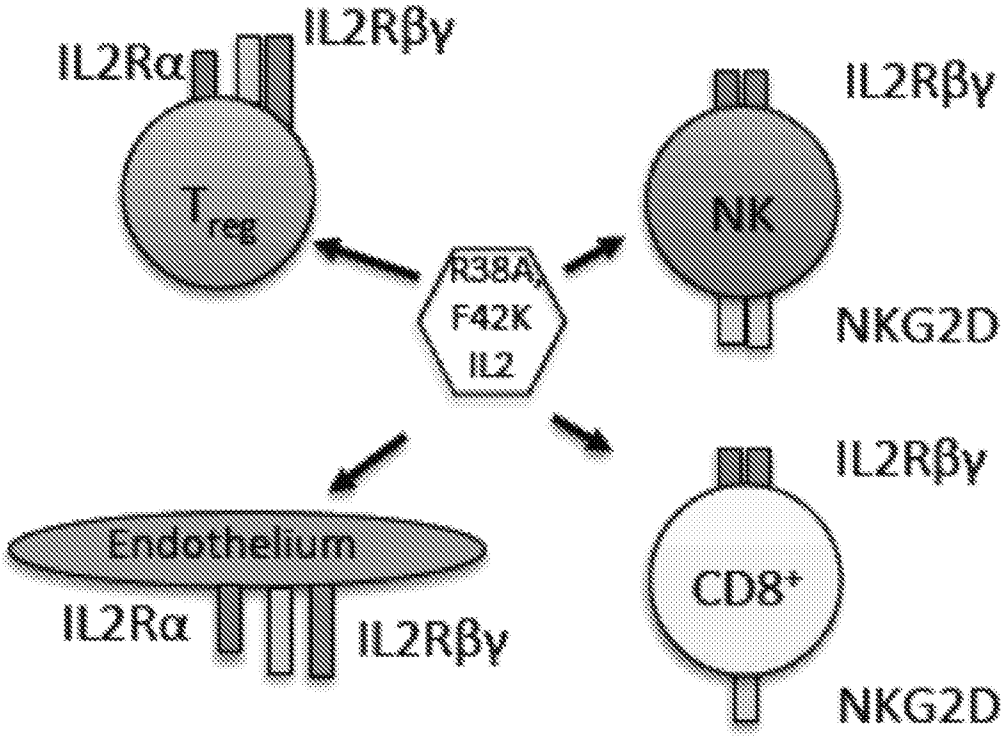


FIG. 11B

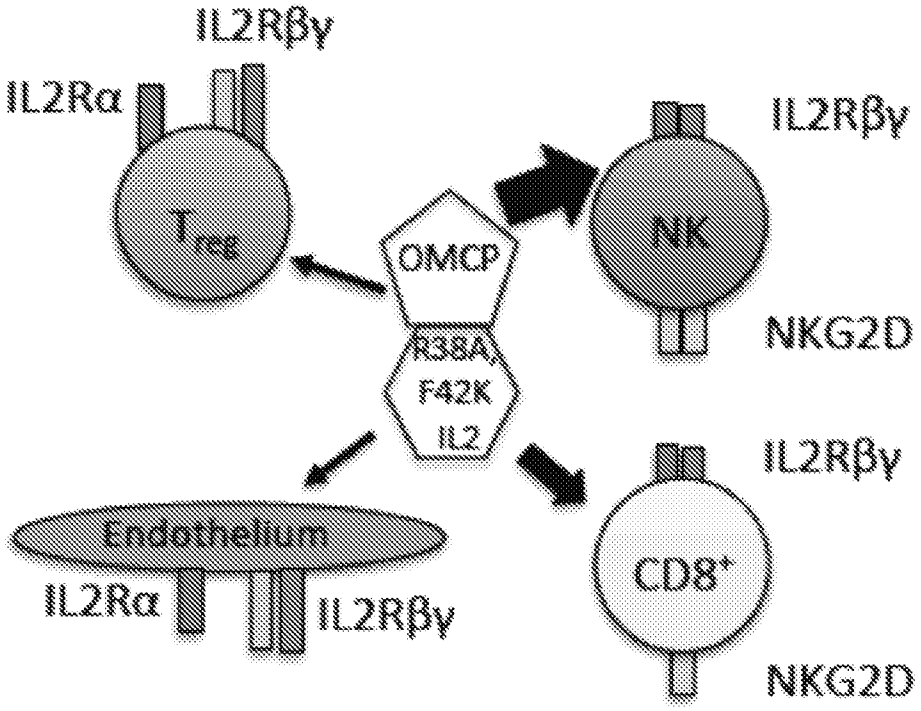

IL2Rβγ
IL2Rα
T reg
OMCP
R38A
F42K
IL2
IL2Rβγ
NK
NKG2D
IL2Rβγ
CD8+
NKG2D
Endothelium
IL2Rα
IL2Rβγ

FIG. 11C

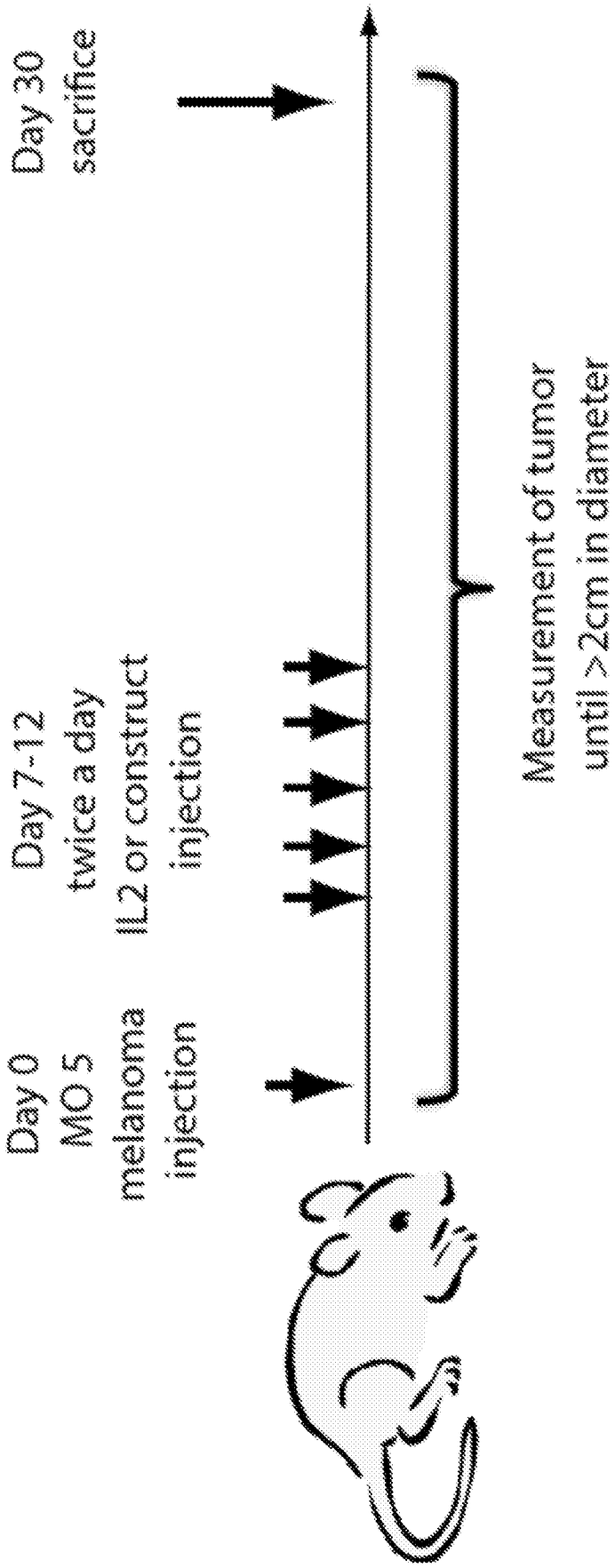

Day 0
MO 5
melanoma
injection
Day 7-12
twice a day
IL2 or construct
injection
Day 30
sacrifice
Measurement of tumor
until >2cm in diameter

FIG. 12

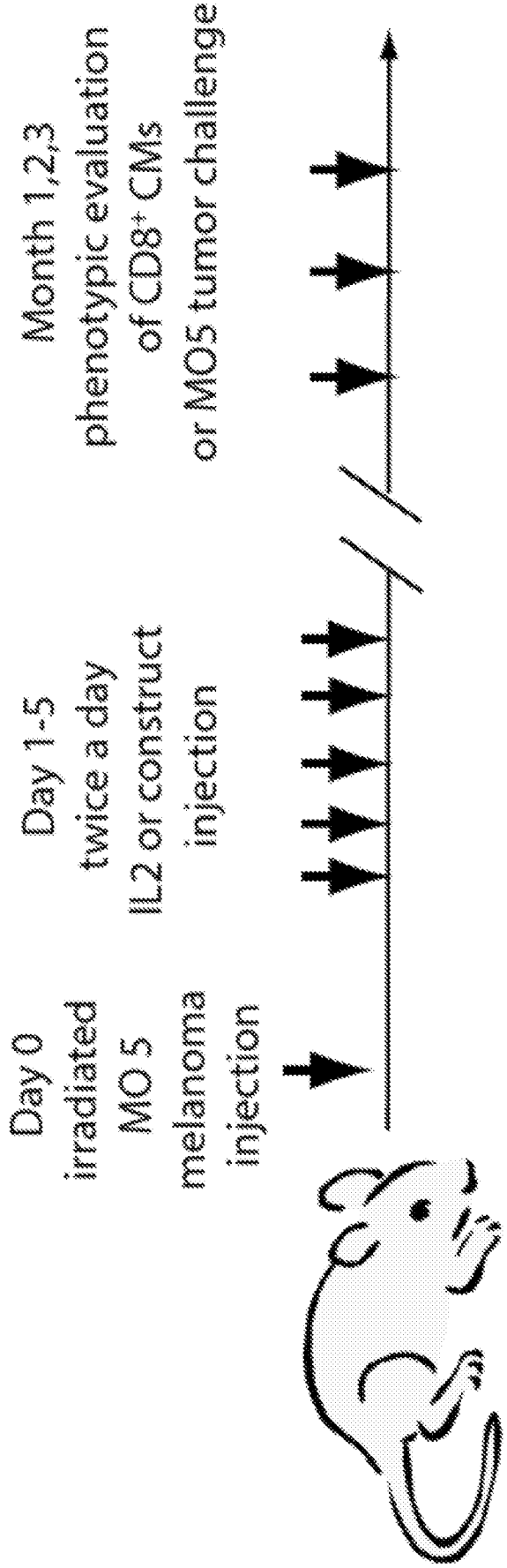

Day 0
irradiated
MO 5
melanoma
injection
Day 1-5
twice a day
IL2 or construct
injection
Month 1,2,3
phenotypic evaluation
of CD8+ CMs
or MO5 tumor challenge

FIG. 13

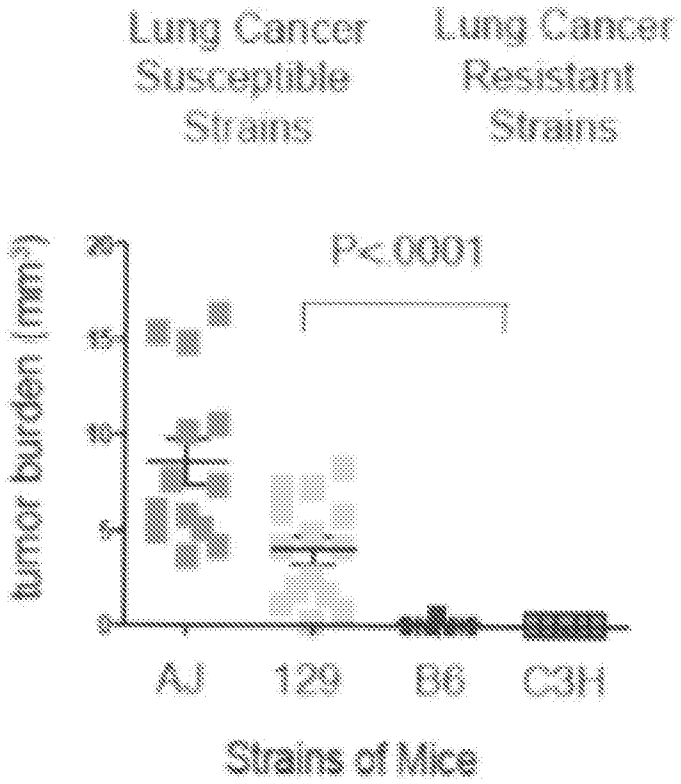


FIG. 14A

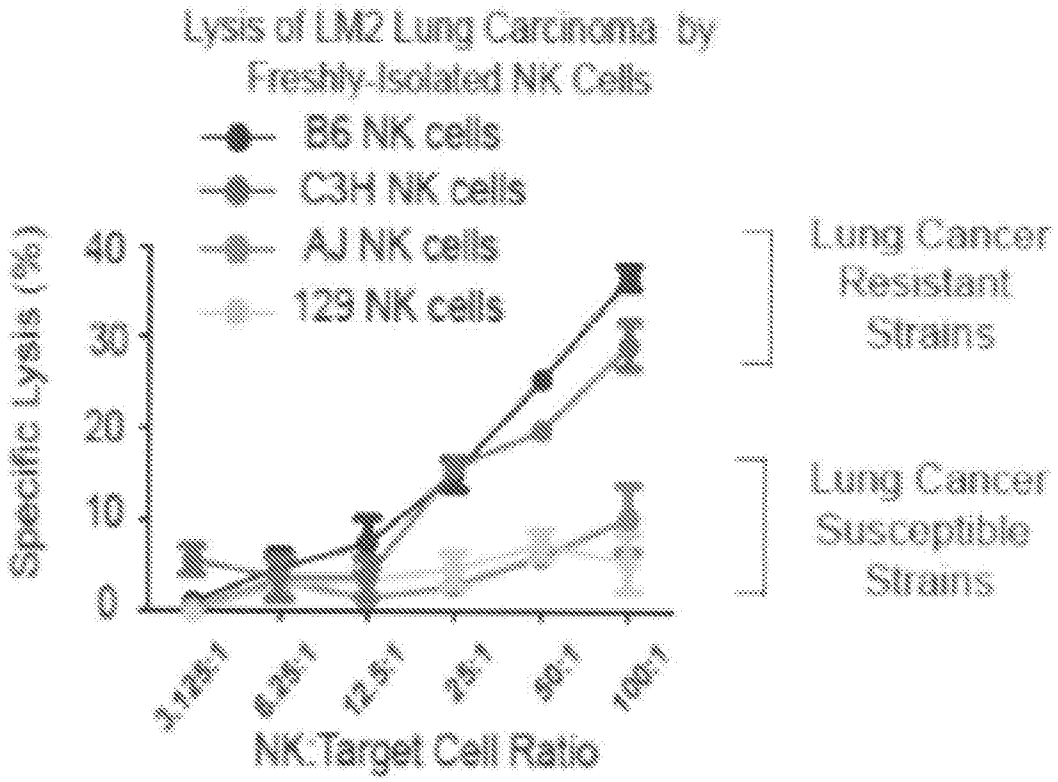


FIG. 14B

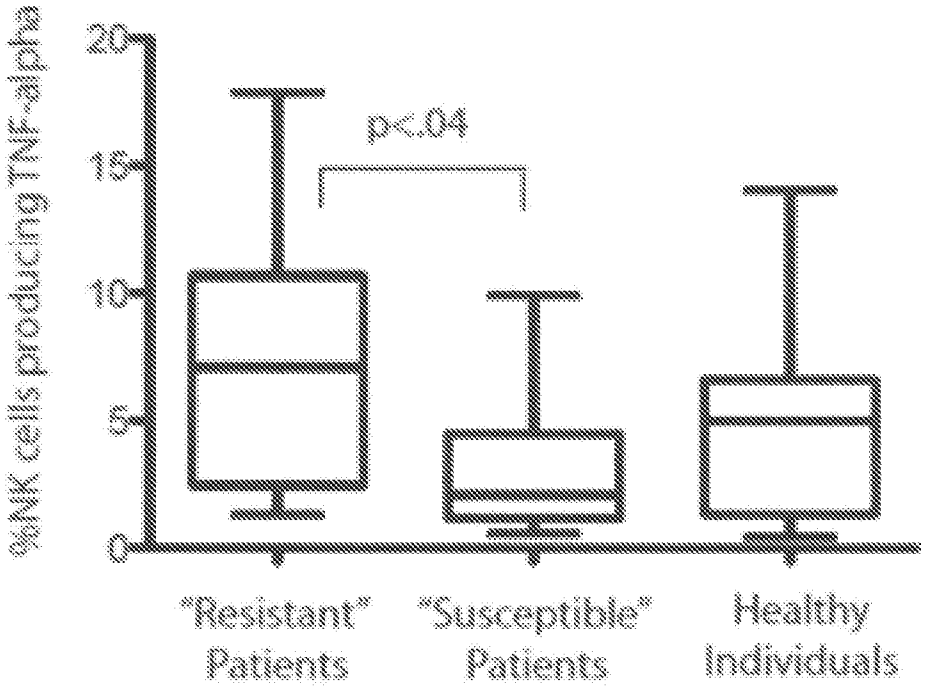

%NK cells producing TNF-alpha
20
15
10
5
0
p<.04
"Resistant" Patients
"Susceptible" Patients
Healthy Individuals

FIG. 15

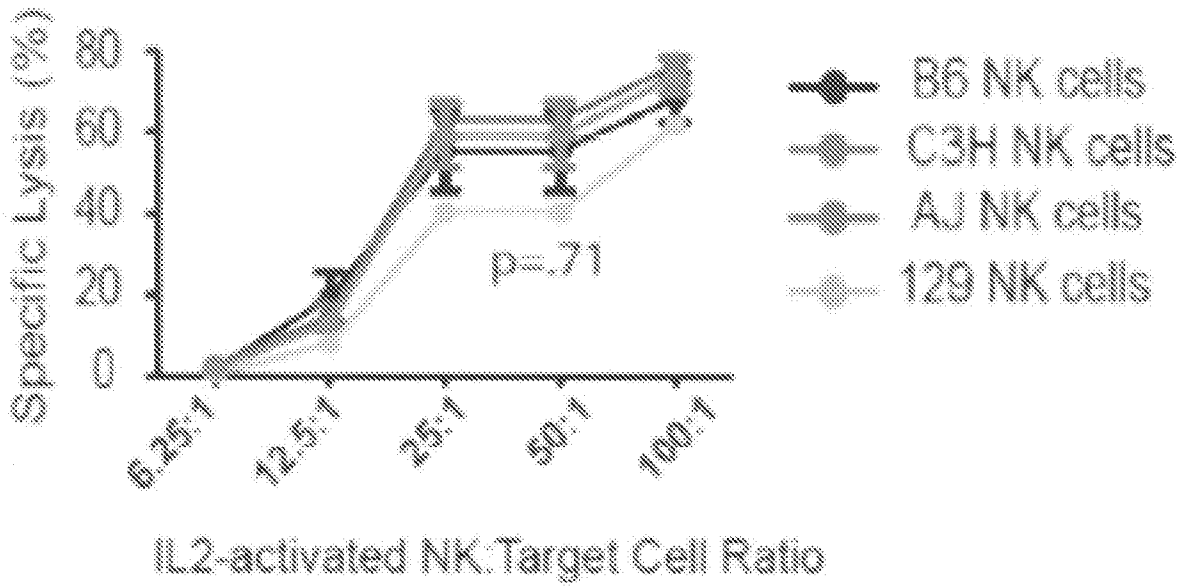

Specific Lysis (%)
80
60
40
20
0
p=.71
6.25:1
12.5:1
25:1
50:1
100:1
IL2-activated NK:Target Cell Ratio
B6 NK cells
C3H NK cells
AJ NK cells
129 NK cells

FIG. 16

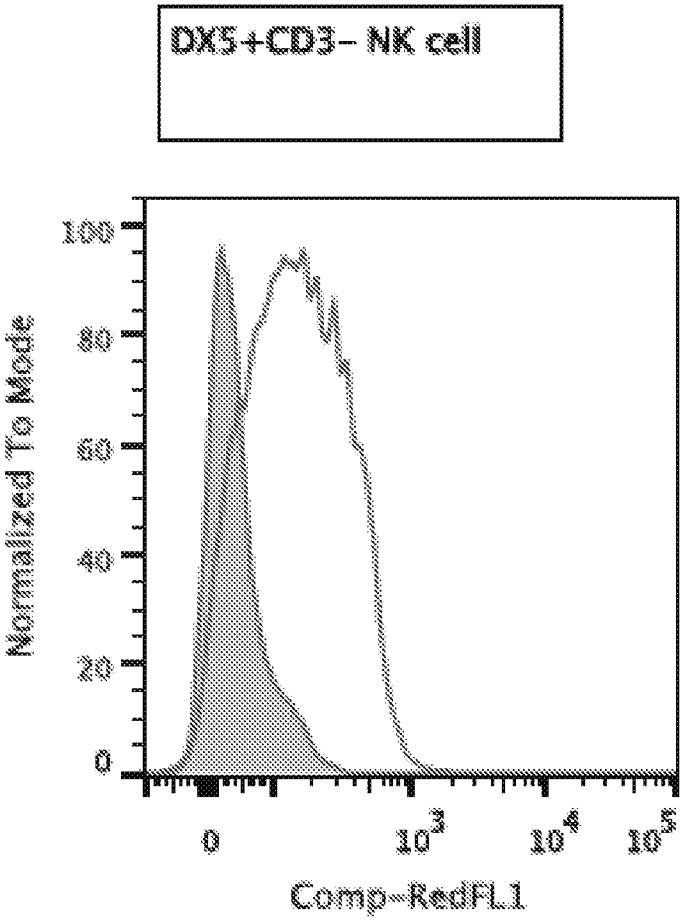


FIG. 17A

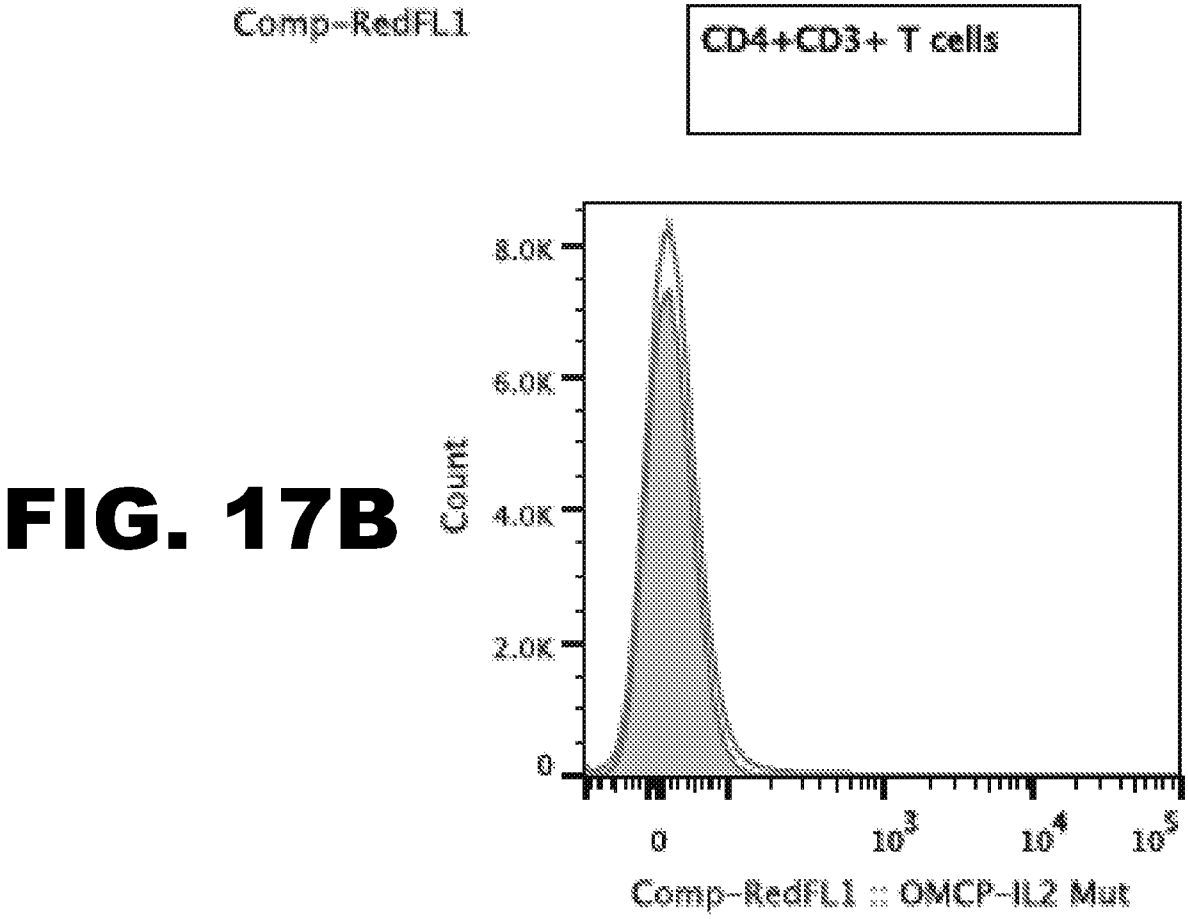


FIG. 17B

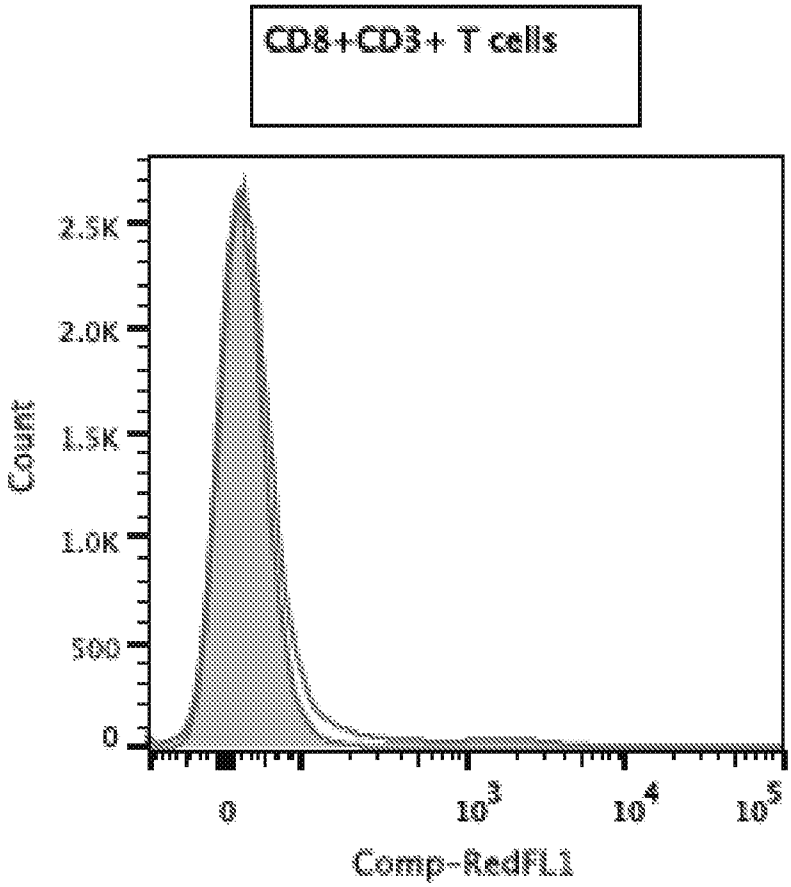


FIG. 17C

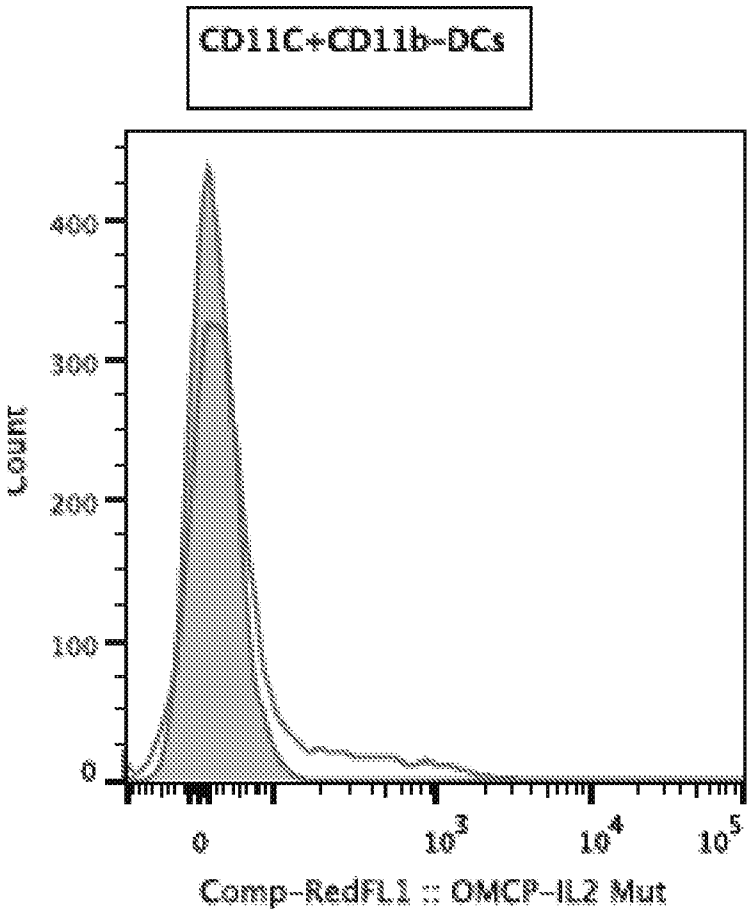


FIG. 17D

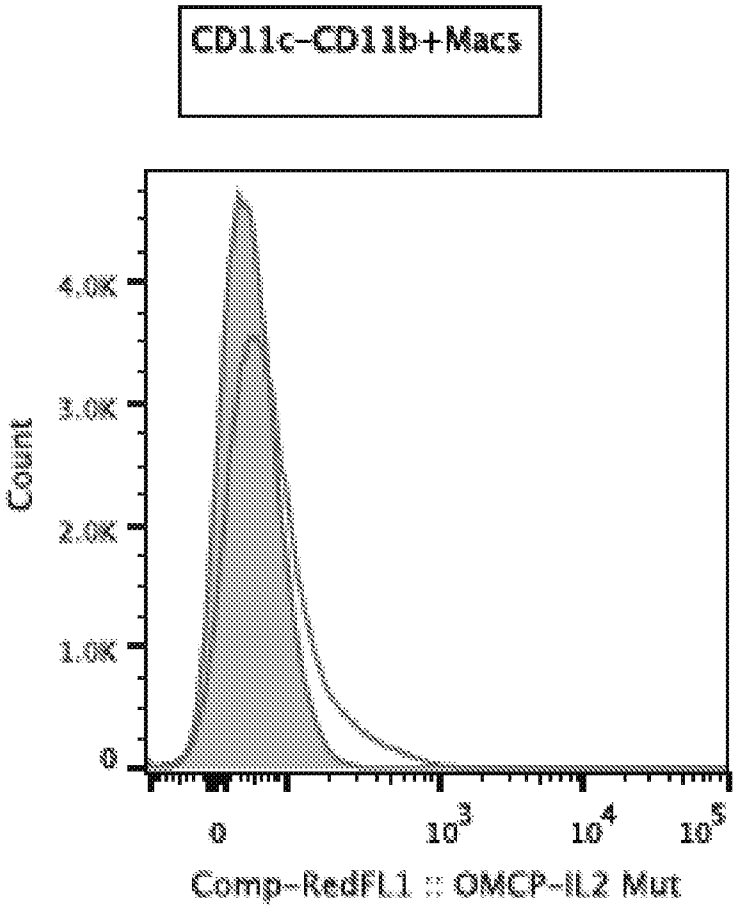


FIG. 17E

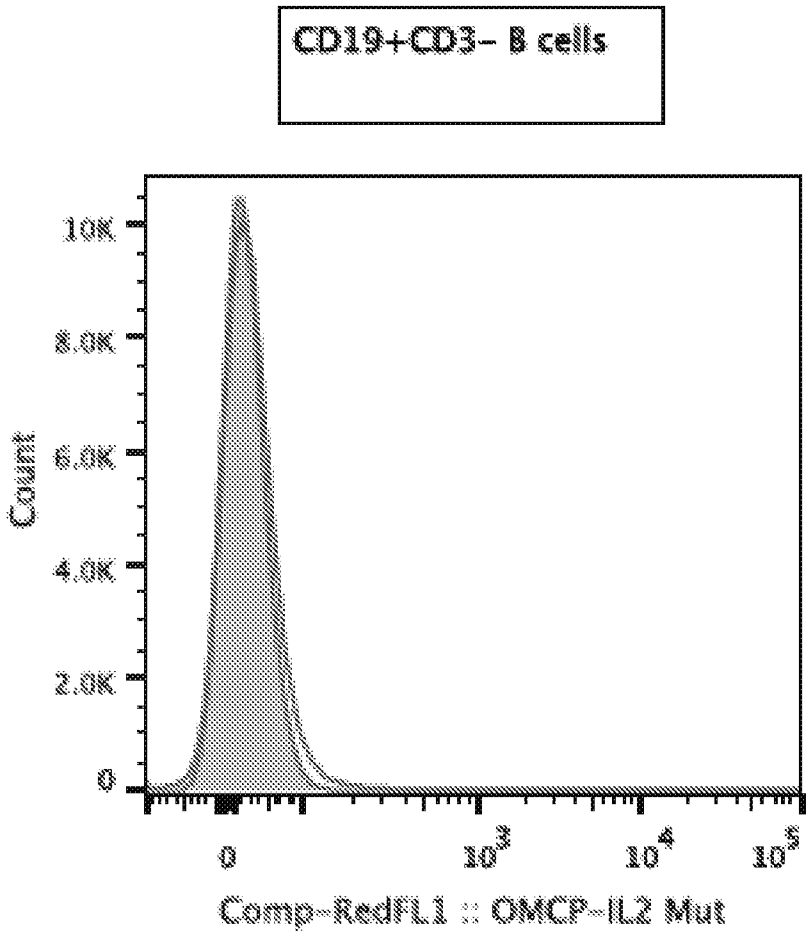


FIG. 17F

daily IL2 or construct injection i.p X 5 doses
sacrifice to evaluate
systemic side effects and
immunologic changes

FIG. 18

Day 0
irradiation
Day 5 start IL2 injections for 5 days
Day 2
10³ RMA-S i.p.
follow long-term
for survival

FIG. 19

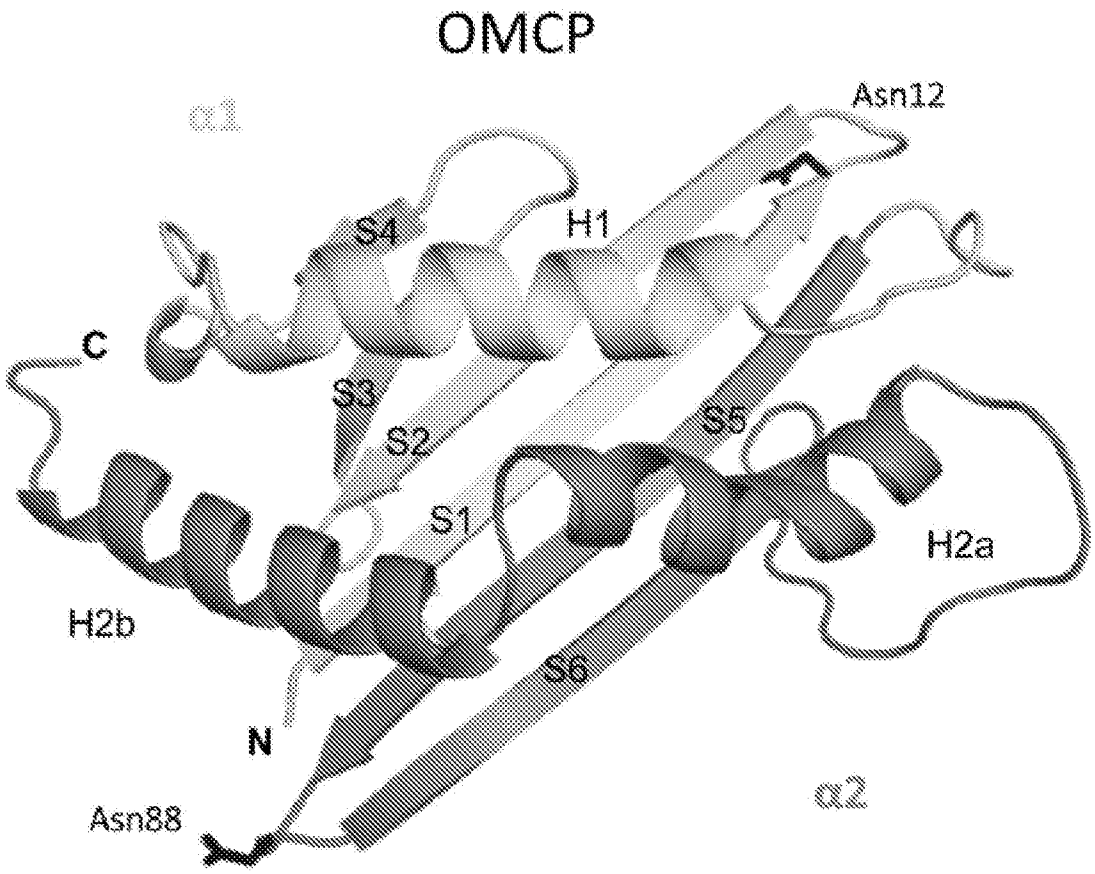


FIG. 20A

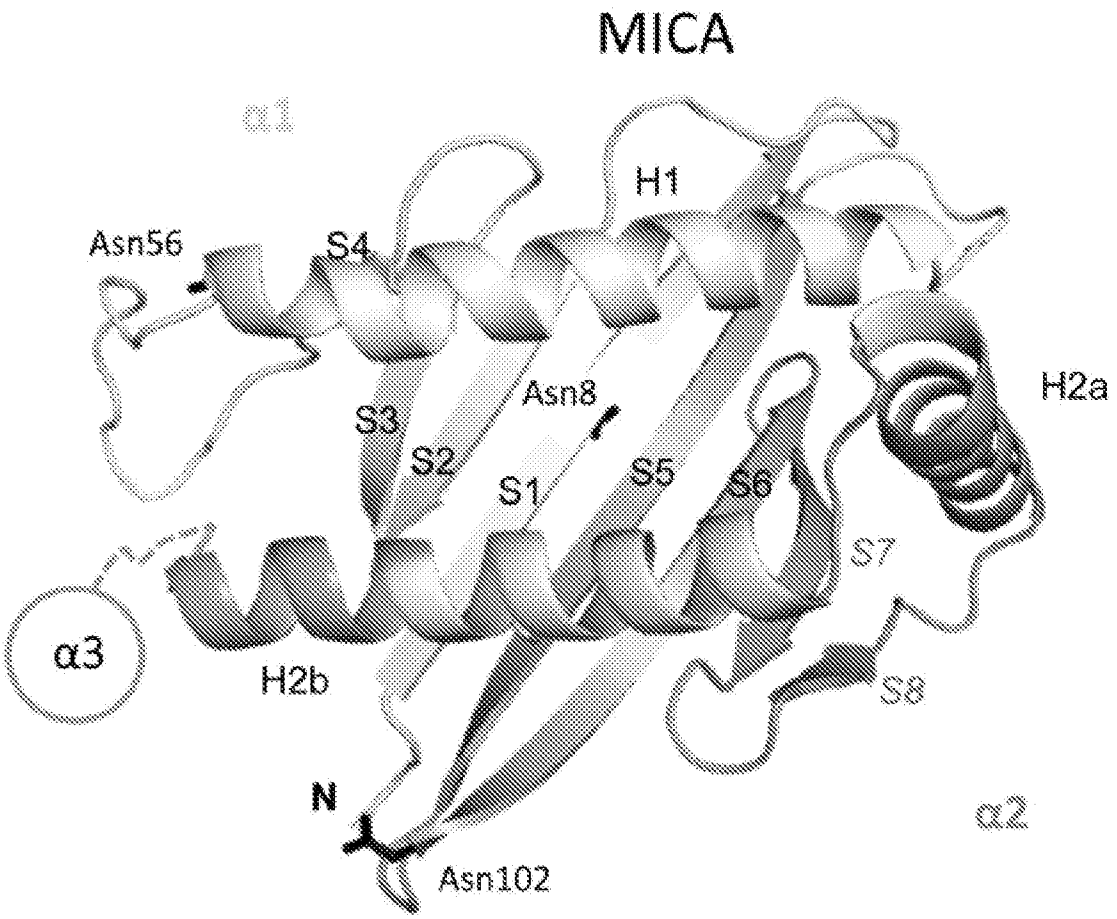

MICA
α1
H1
Asn56
S4
Asn8
H2a
S3
S2
S1
S5
S6
S7
α3
H2b
S8
N
α2
Asn102

FIG. 20B

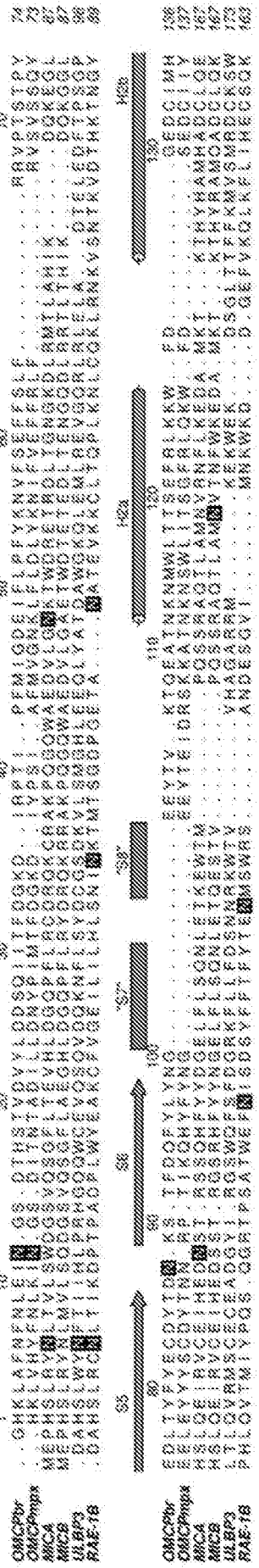


FIG. 20C

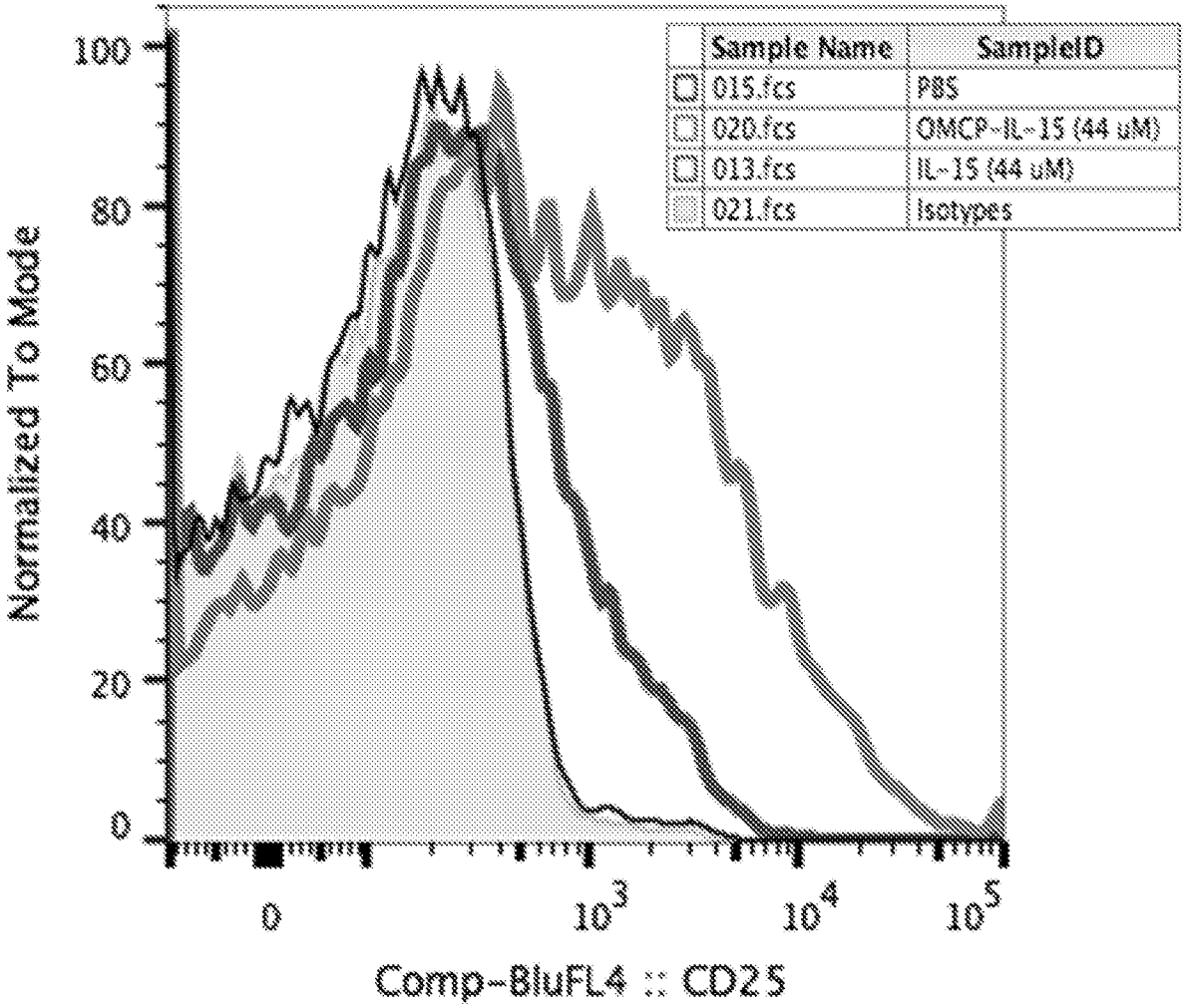

Sample Name
SampleID
015.fcs
PBS
020.fcs
OMCP-IL-15 (44 uM)
013.fcs
IL-15 (44 uM)
021.fcs
Isotypes
Normalized To Mode
100
80
60
40
20
0
0
10^3
10^4
10^5
Comp-BluFL4 :: CD25

FIG. 21

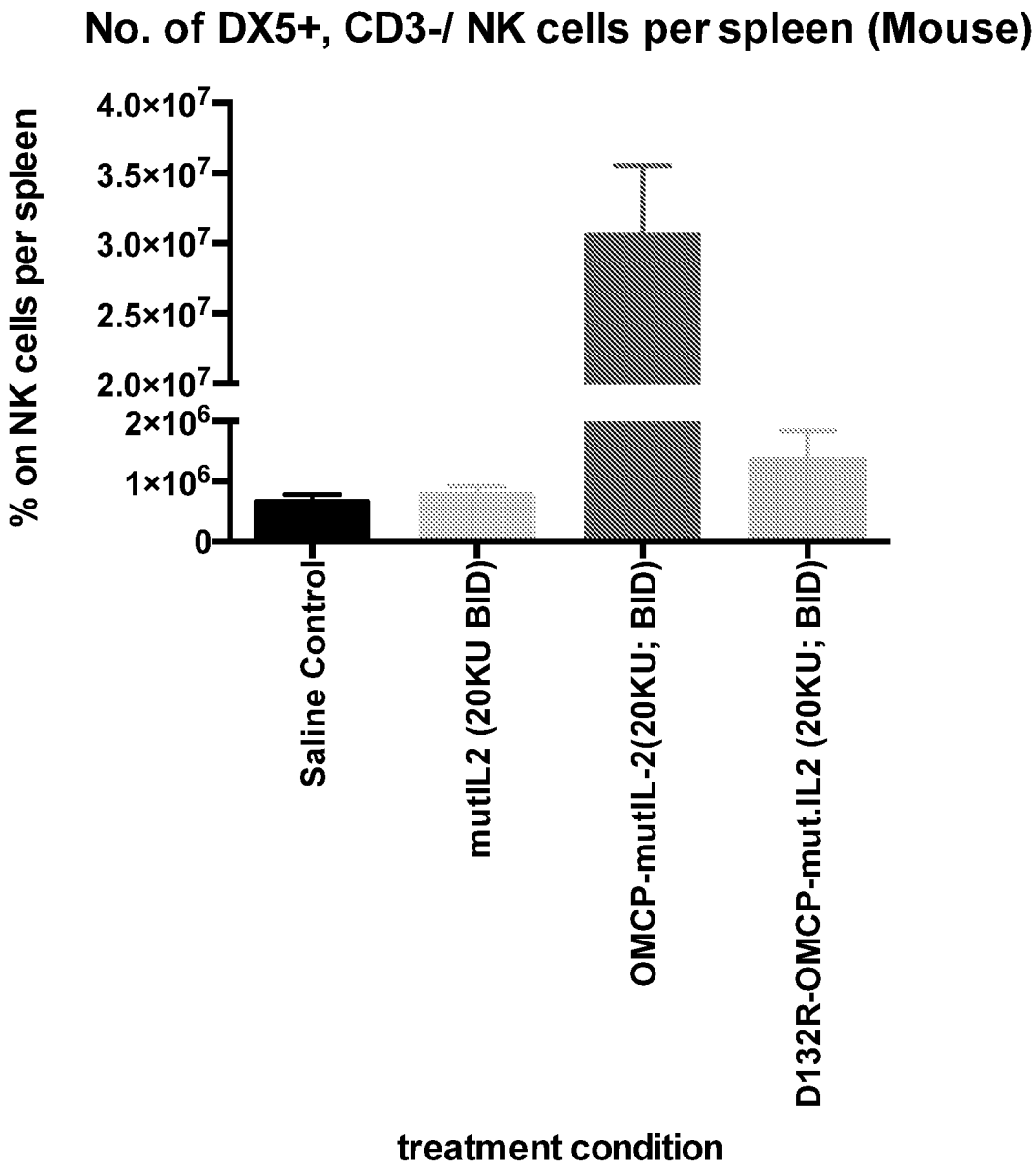

No. of DX5+, CD3-/ NK cells per spleen (Mouse)
% on NK cells per spleen
4.0×10^7
3.5×10^7
3.0×10^7
2.5×10^7
2.0×10^7
2×10^6
1×10^6
0
Saline Control
mutIL2 (20KU BID)
OMCP-mutIL-2(20KU; BID)
D132R-OMCP-mut.IL2 (20KU; BID)
treatment condition

FIG. 22

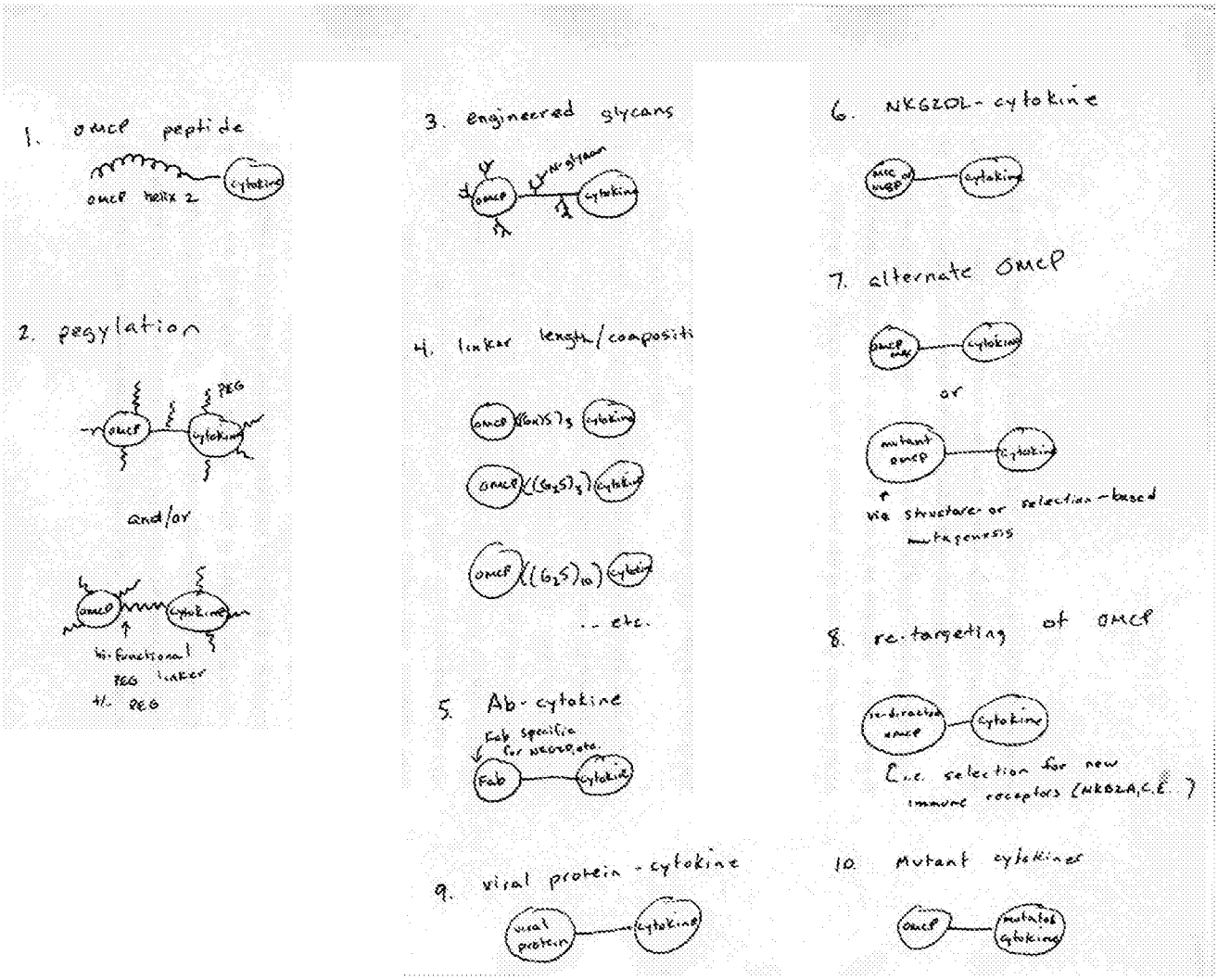

1. OMCP peptide
OMCP helix 2
cytokine
2. pegylation
PEG
OMCP
cytokine
and/or
bi-functional PEG linker
+/- PEG
3. engineered glycans
N-glycan
4. linker length/composition
(G4S)3
(G2S)3
(G2S)10
... etc.
5. Ab-cytokine
Fab specific for receptor
Fab
6. NKG2DL-cytokine
7. alternate OMCP
or
mutant OMCP
via structure or selection-based mutagenesis
8. re-targeting of OMCP
re-directed OMCP
i.e. selection for new immune receptors (NKG2A, C, E, ...)
9. viral protein-cytokine
viral protein
10. Mutant cytokines
mutated cytokine

FIG. 23

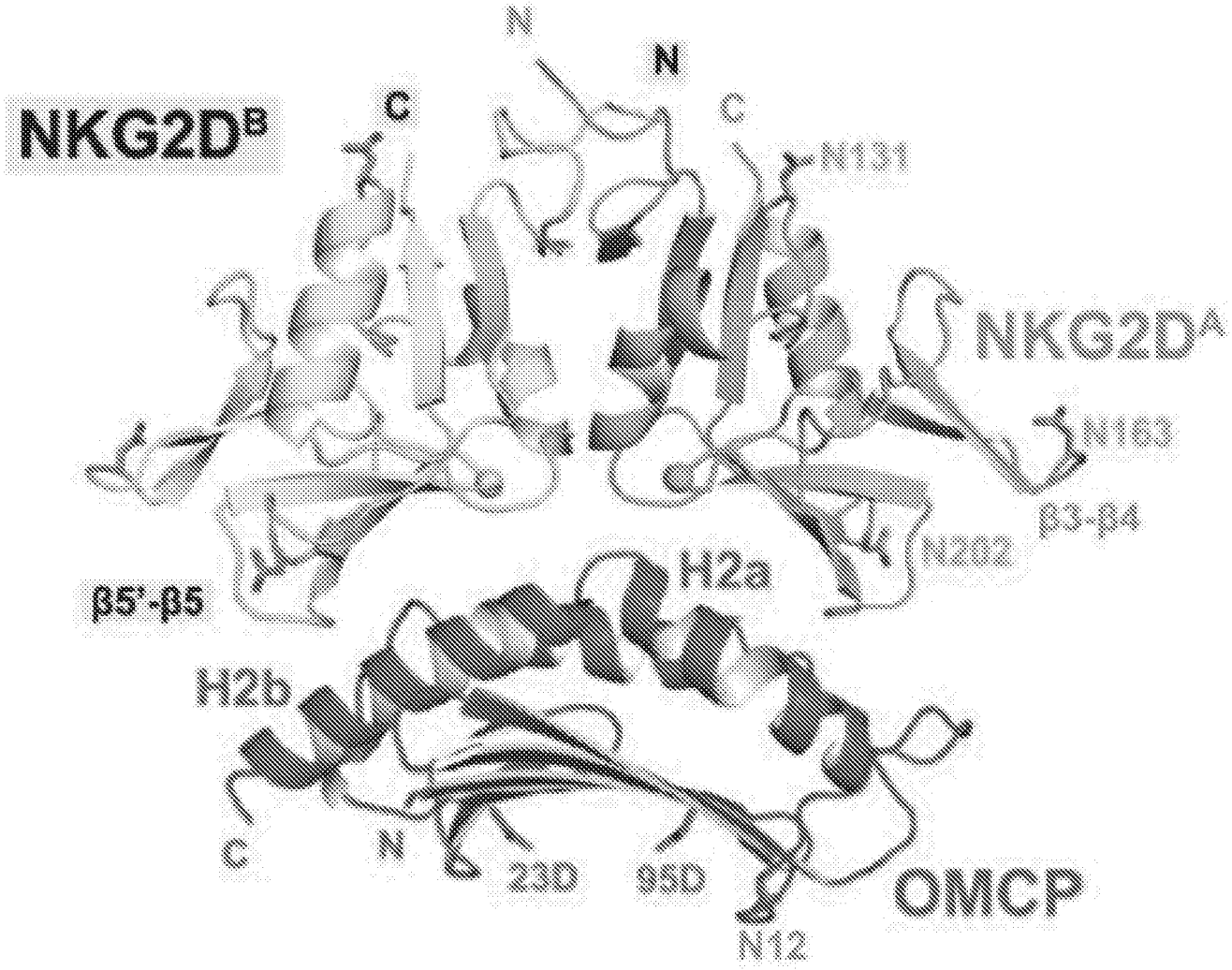

NKG2D^B
N
N
C
C
N131
NKG2D^A
N163
β3-β4
N202
H2a
β5'-β5
H2b
C
N
23D
95D
N12
OMCP

FIG. 24A

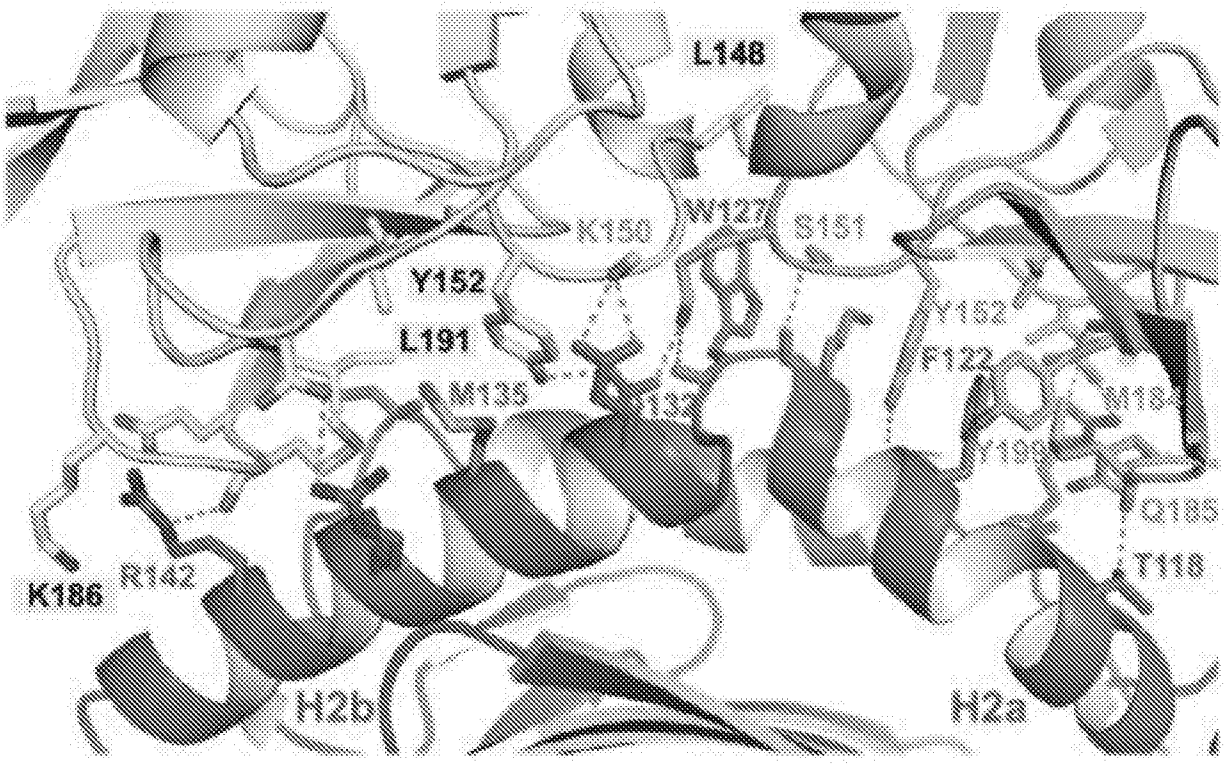

L148
K150
W137
S151
Y152
L191
M139
I137
Y152
F122
M18
Y19
Q185
T118
K186
R142
H2b
H2a

FIG. 24B

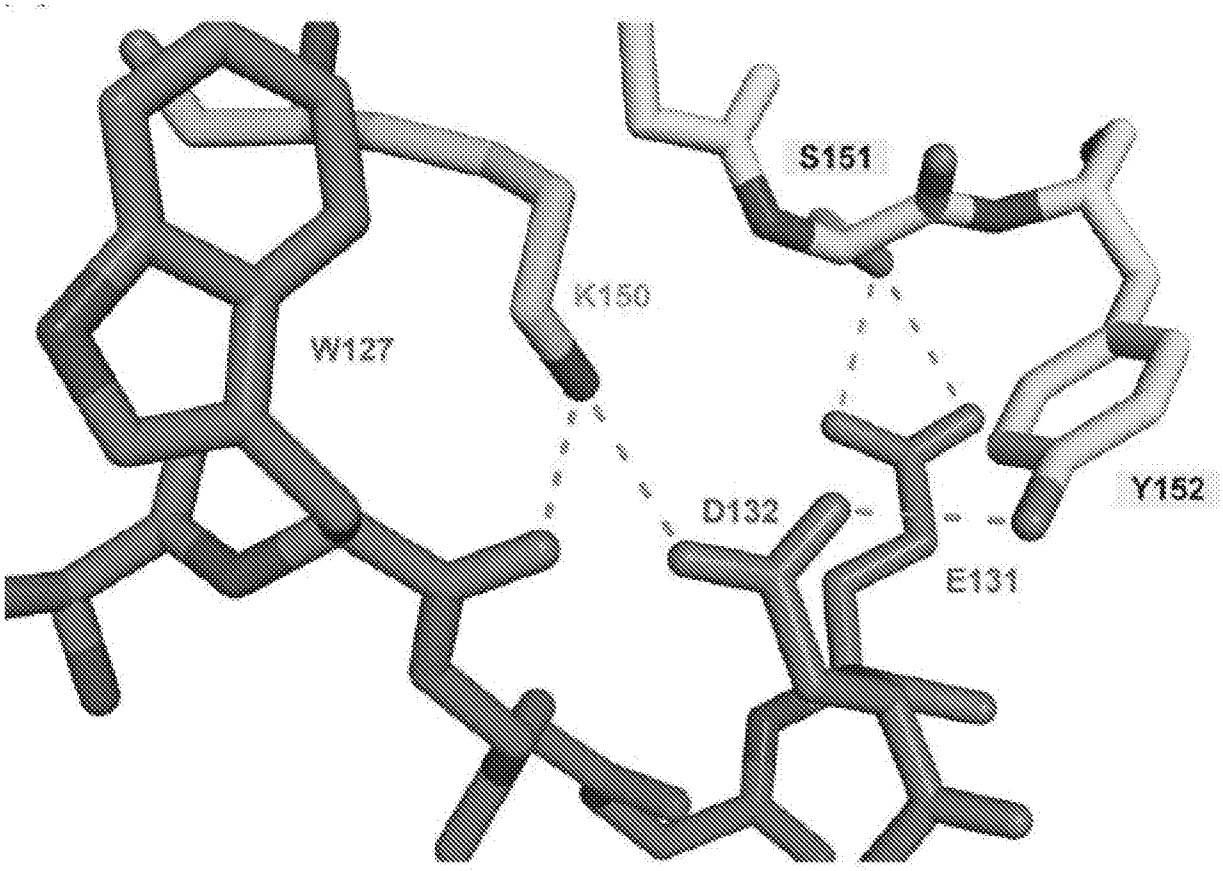


FIG. 25A

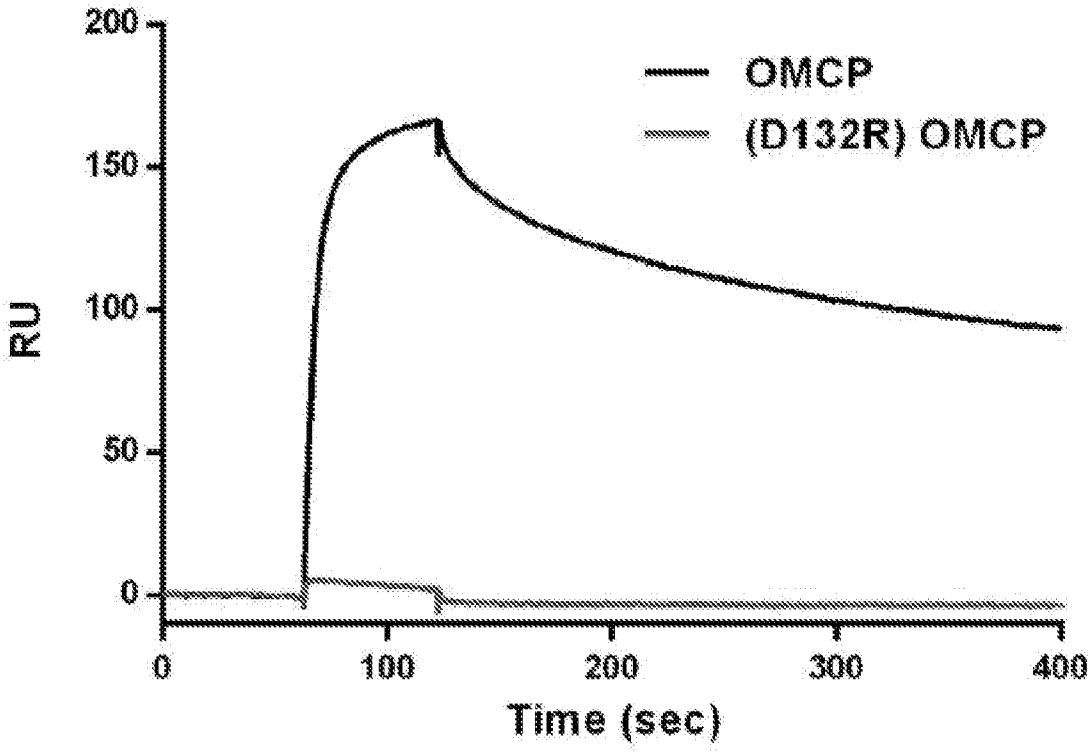


FIG. 25B

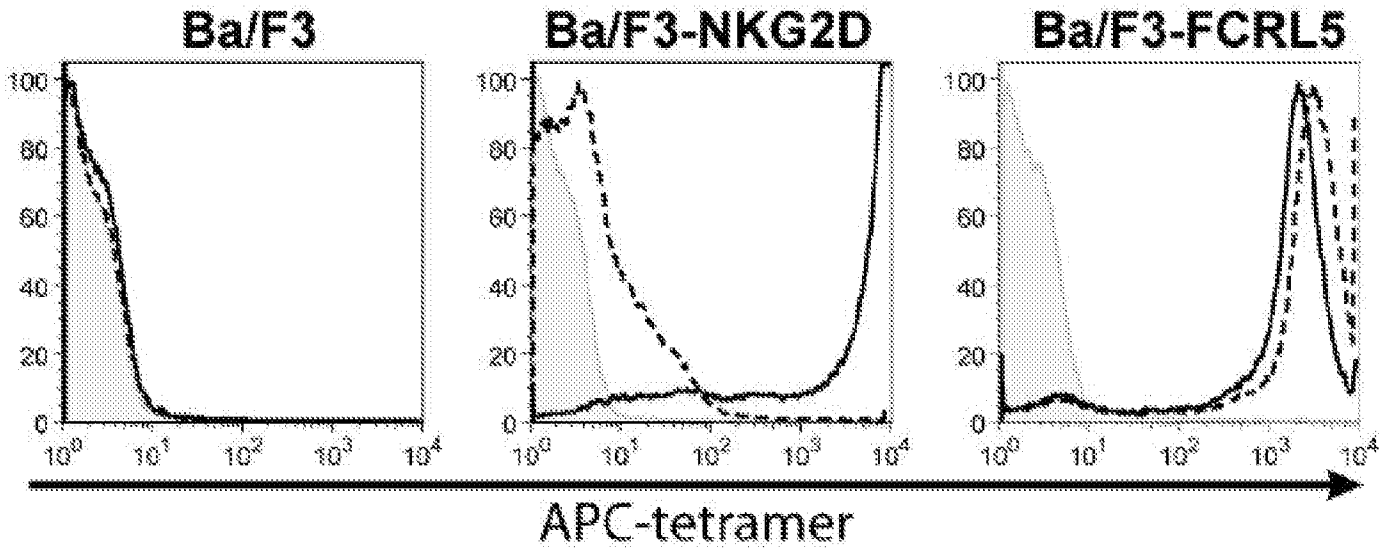


FIG. 25C

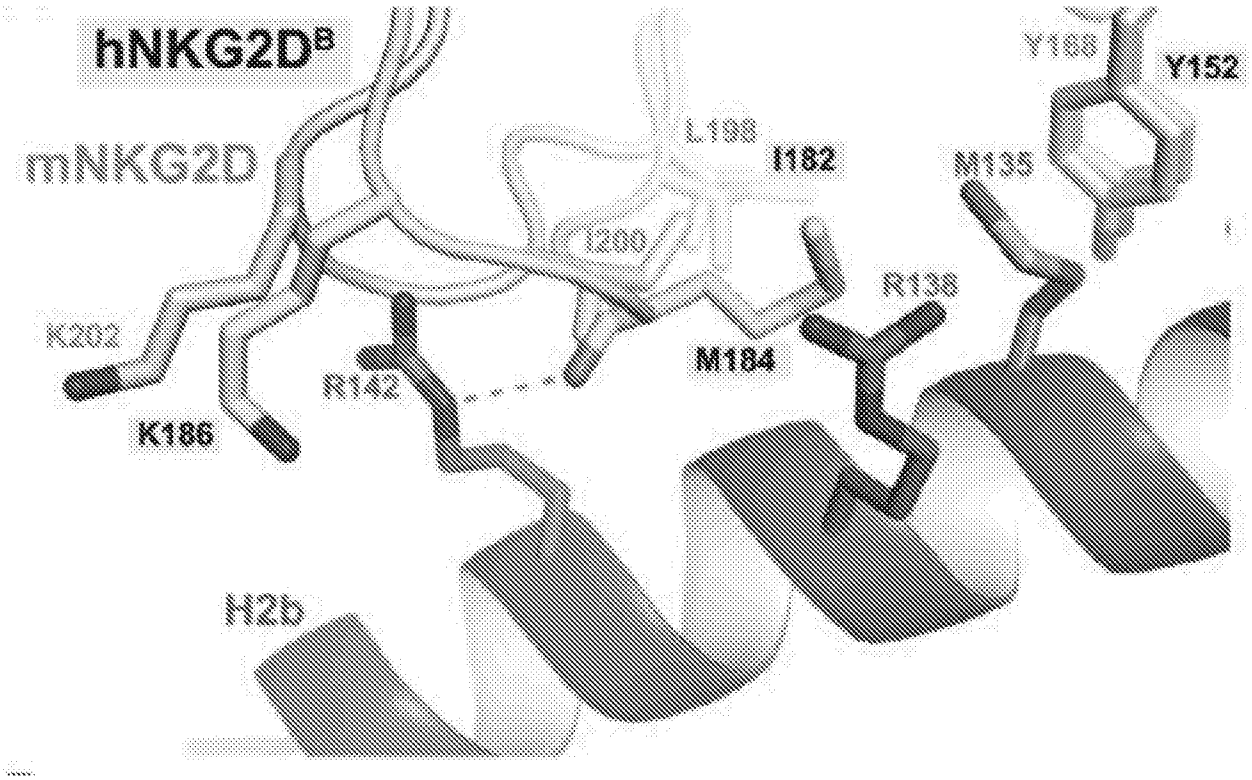

hNKG2D^B
mNKG2D
L198
I182
Y168
Y152
M135
I200
R138
K202
M184
R142
K186
H2b

FIG. 26A

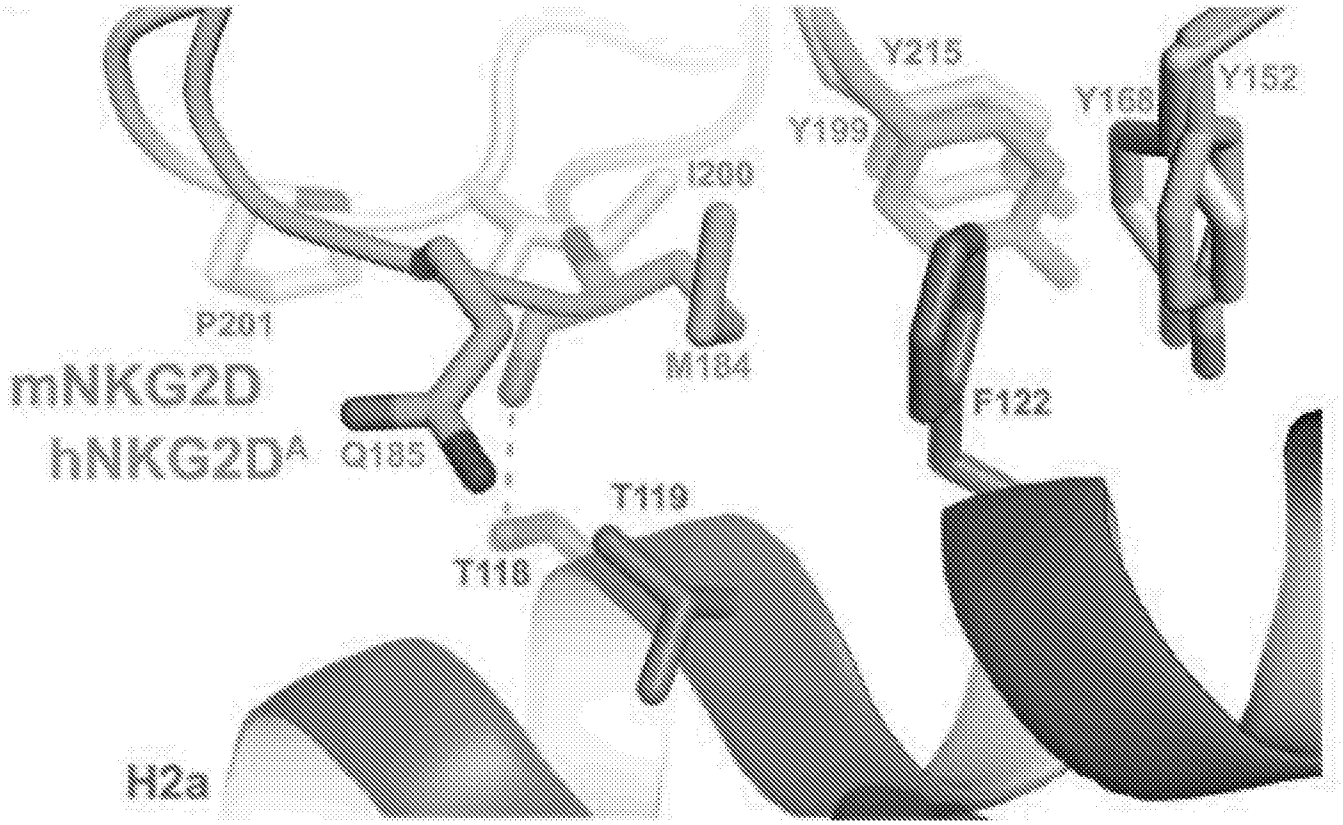

Y215
Y199
Y188
Y152
I200
P201
M184
mNKG2D
hNKG2DA
Q185
F122
T119
T118
H2a

FIG. 26B

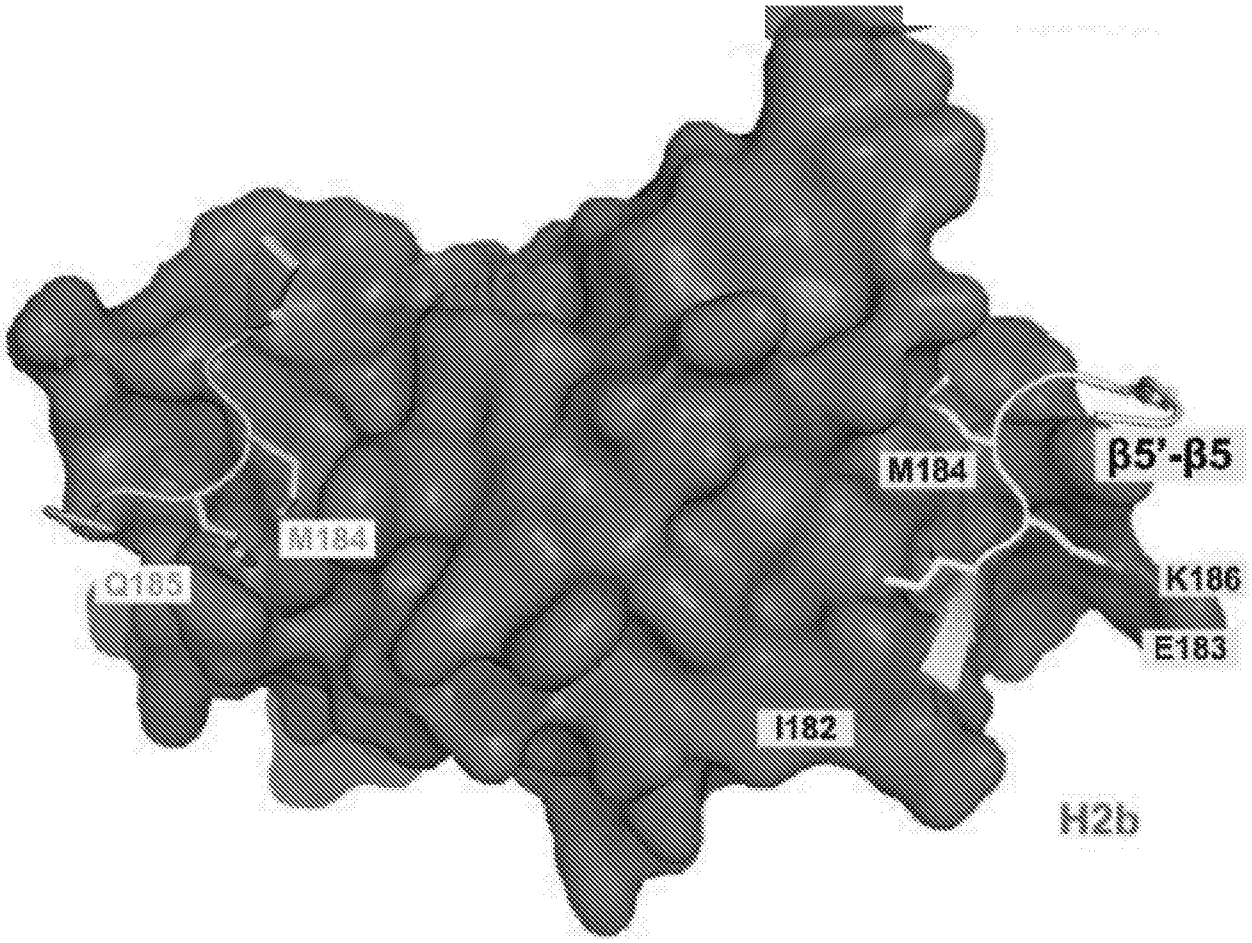


FIG. 26C

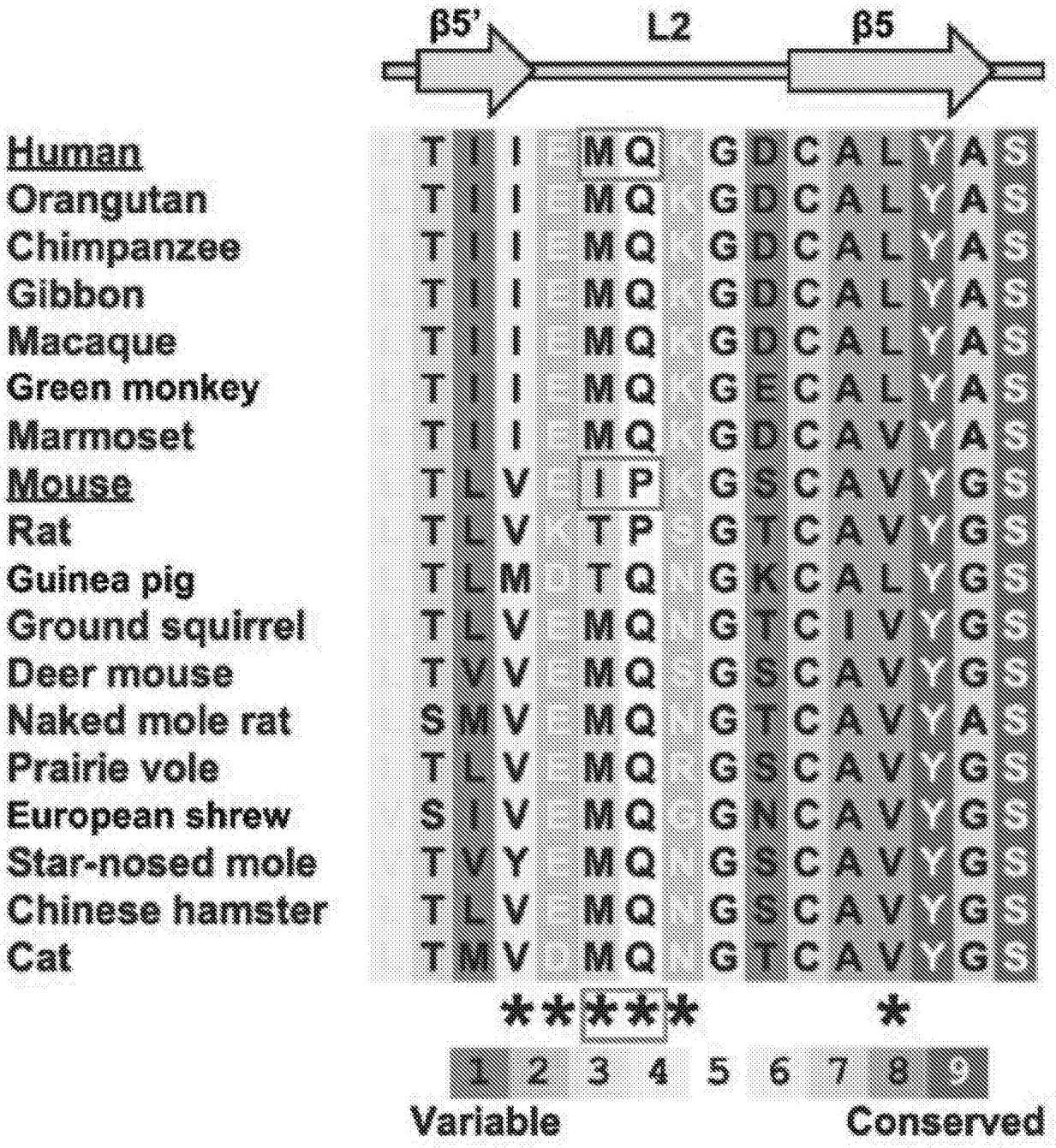

β5'
L2
β5
Human
Orangutan
Chimpanzee
Gibbon
Macaque
Green monkey
Marmoset
Mouse
Rat
Guinea pig
Ground squirrel
Deer mouse
Naked mole rat
Prairie vole
European shrew
Star-nosed mole
Chinese hamster
Cat
1 2 3 4 5 6 7 8 9
Variable
Conserved

FIG. 26D

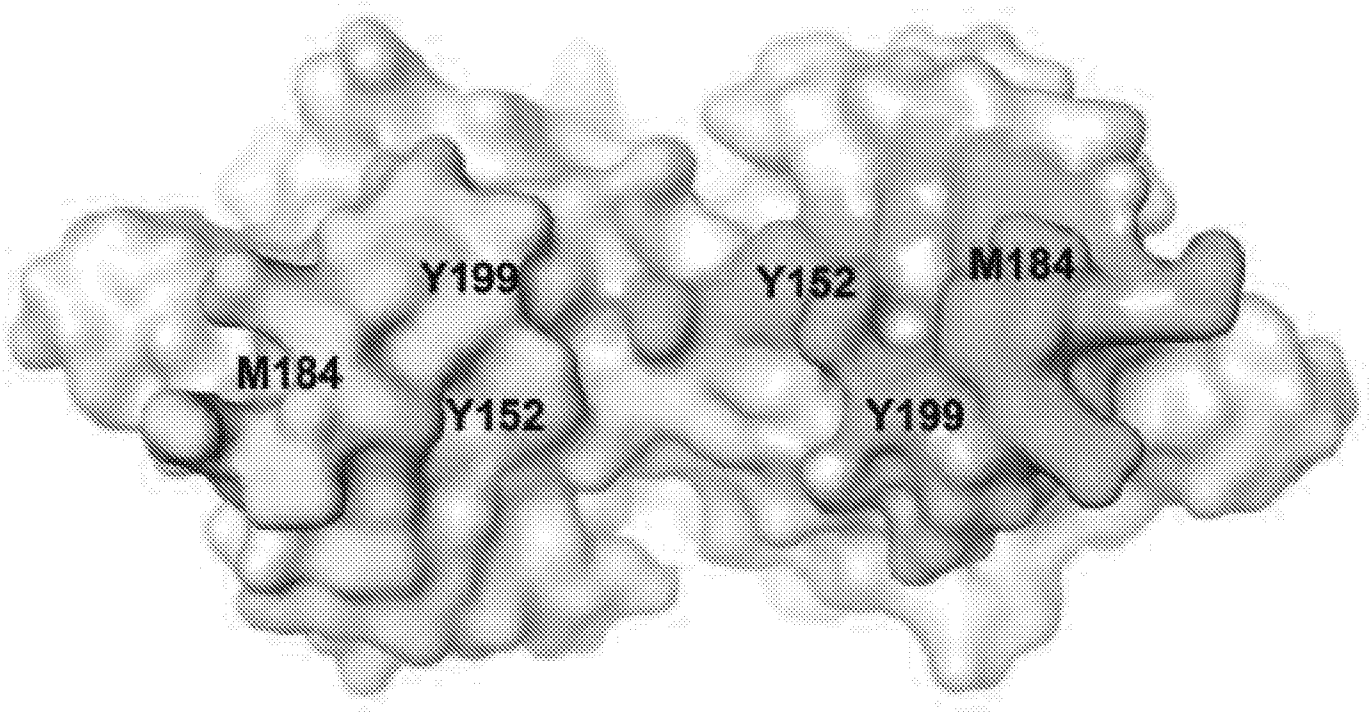


FIG. 27A

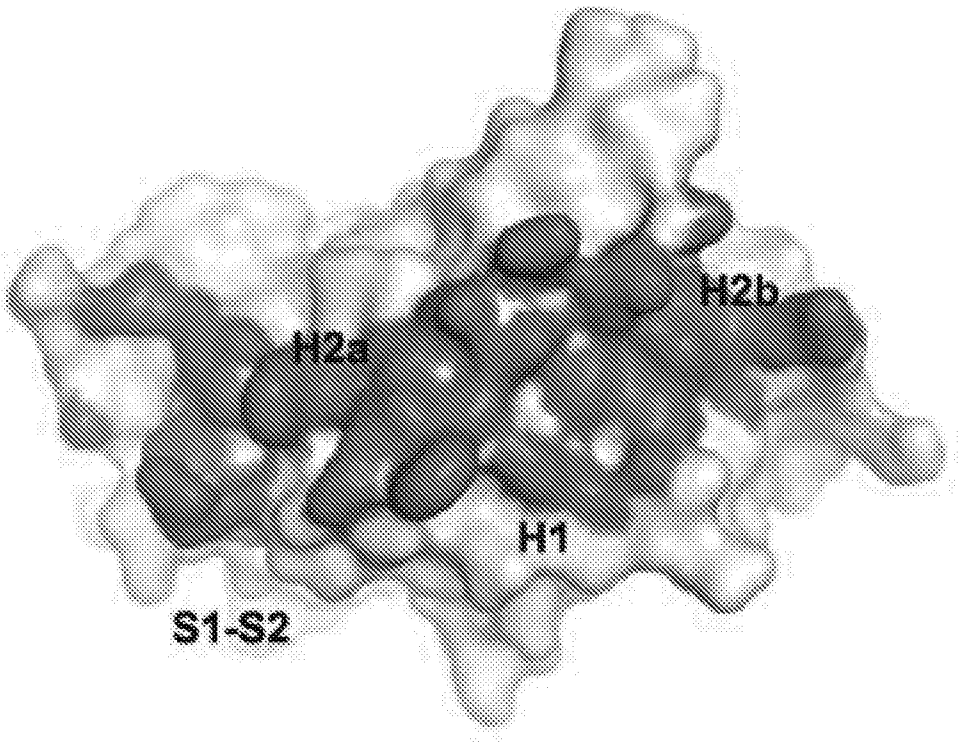


FIG. 27B

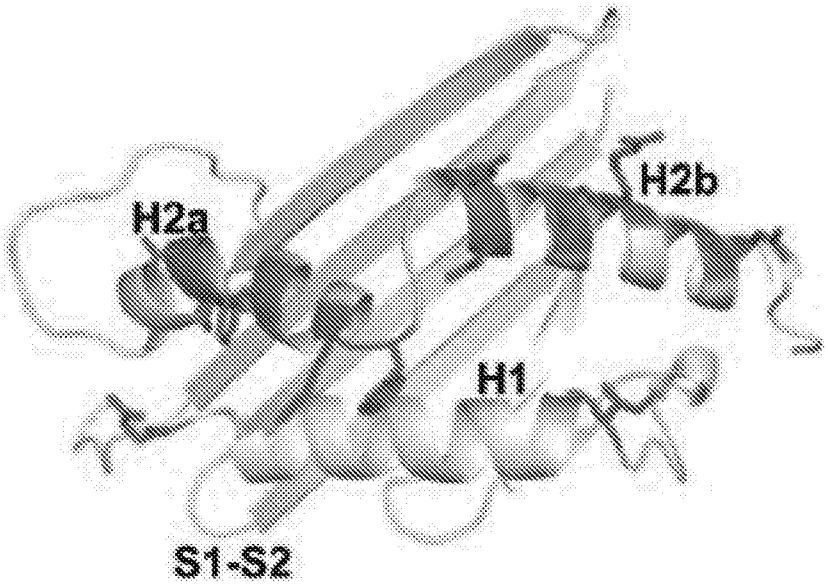


FIG. 27C

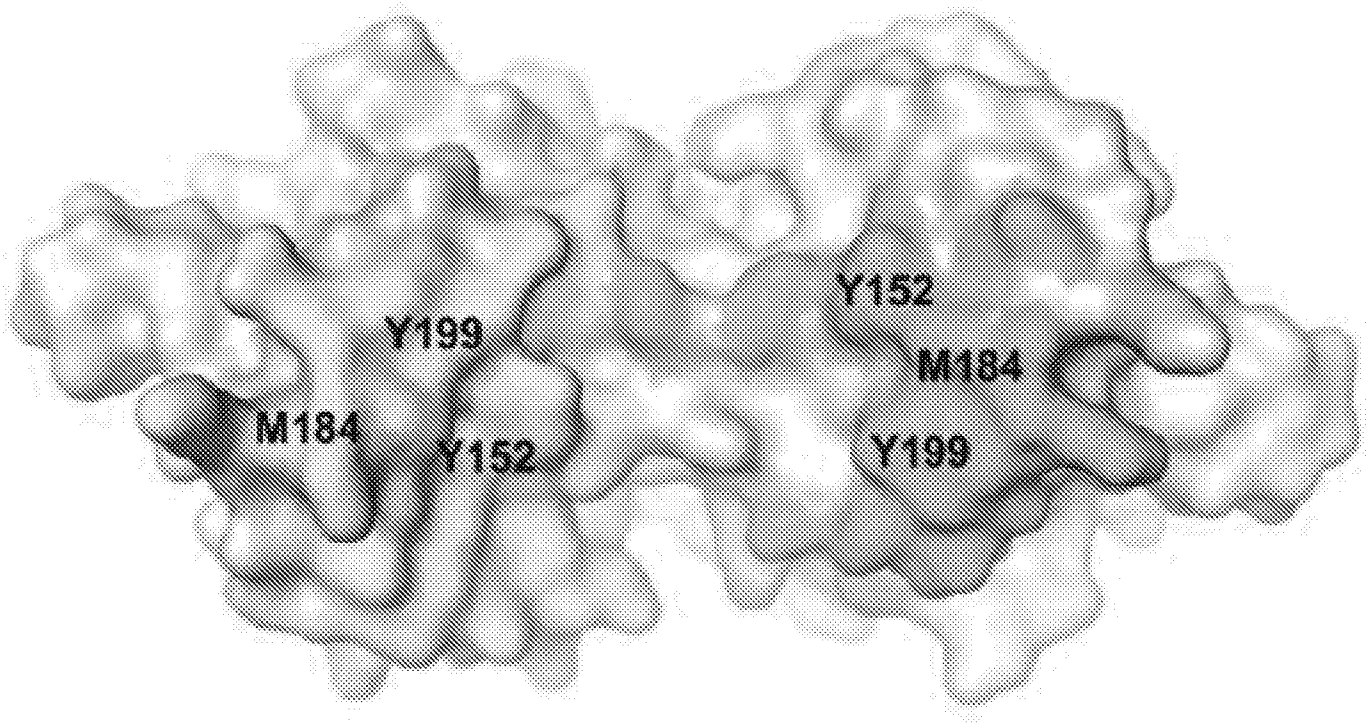


FIG. 27D

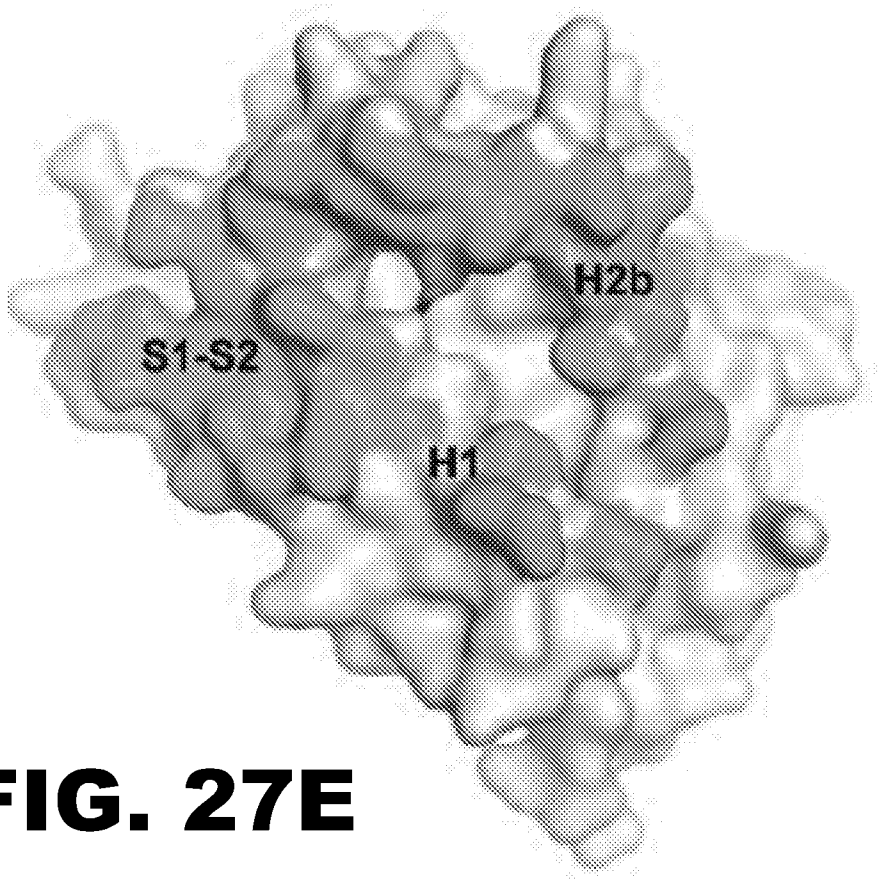


FIG. 27E

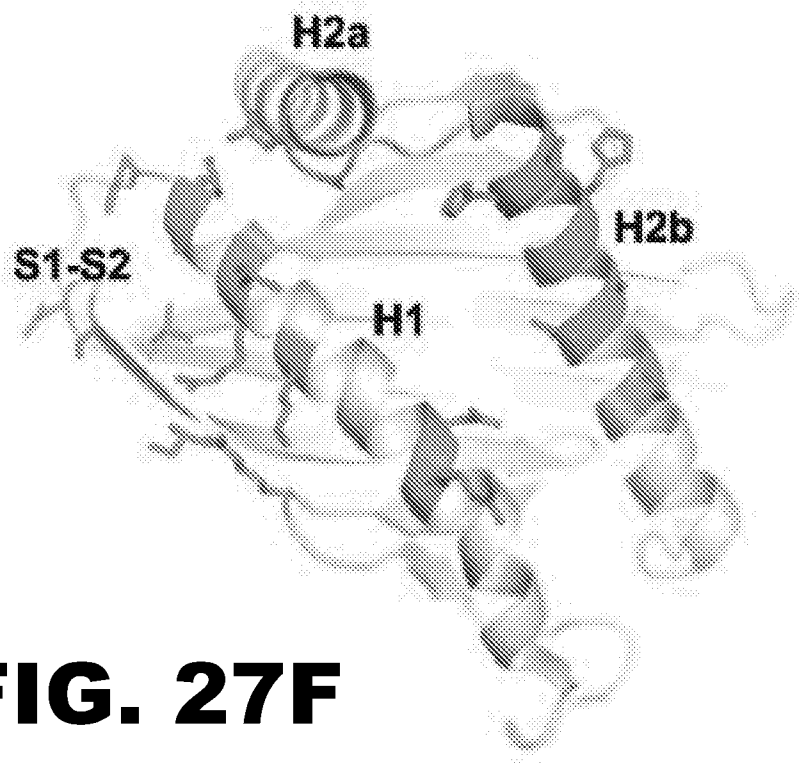


FIG. 27F

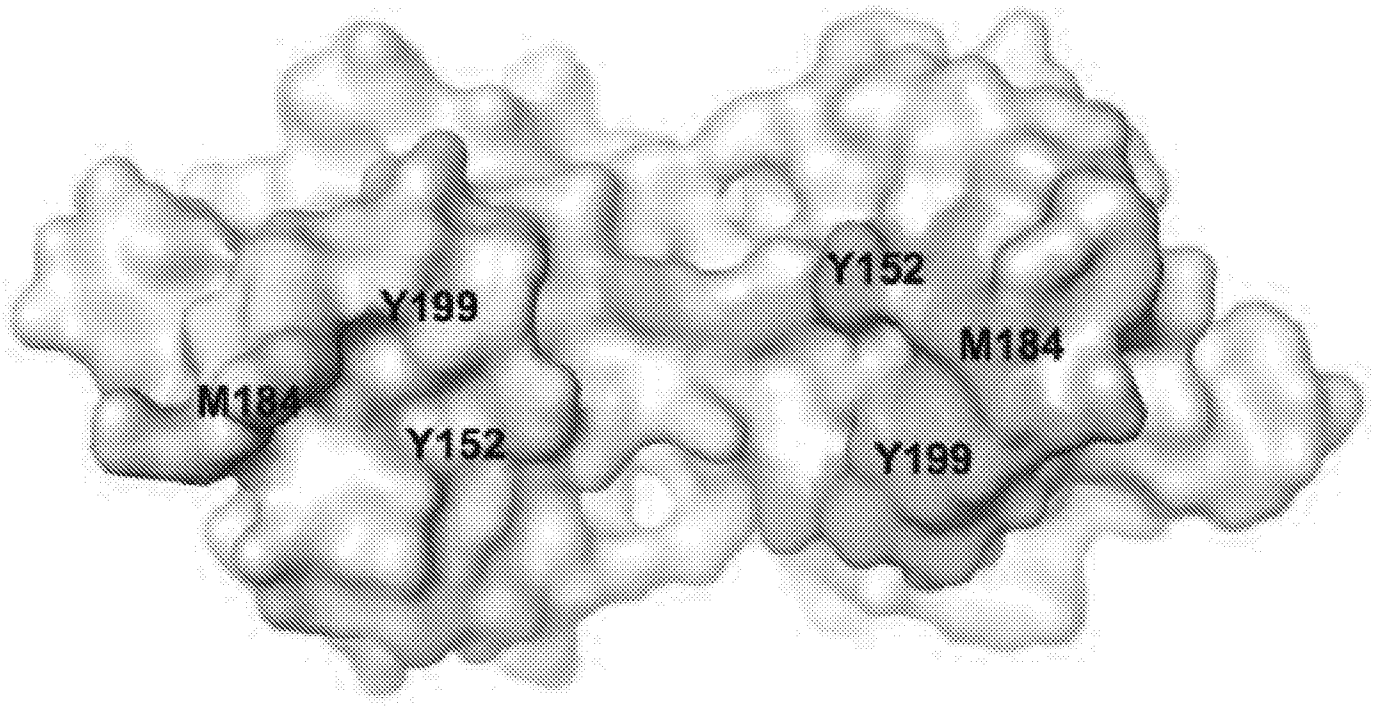


FIG. 27G

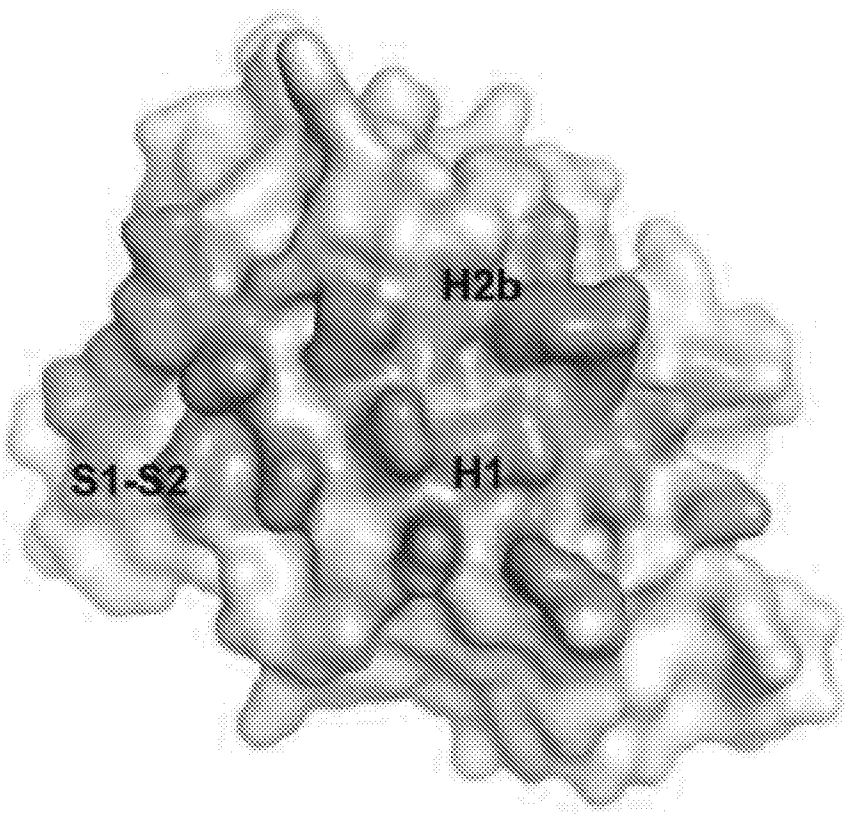


FIG. 27H

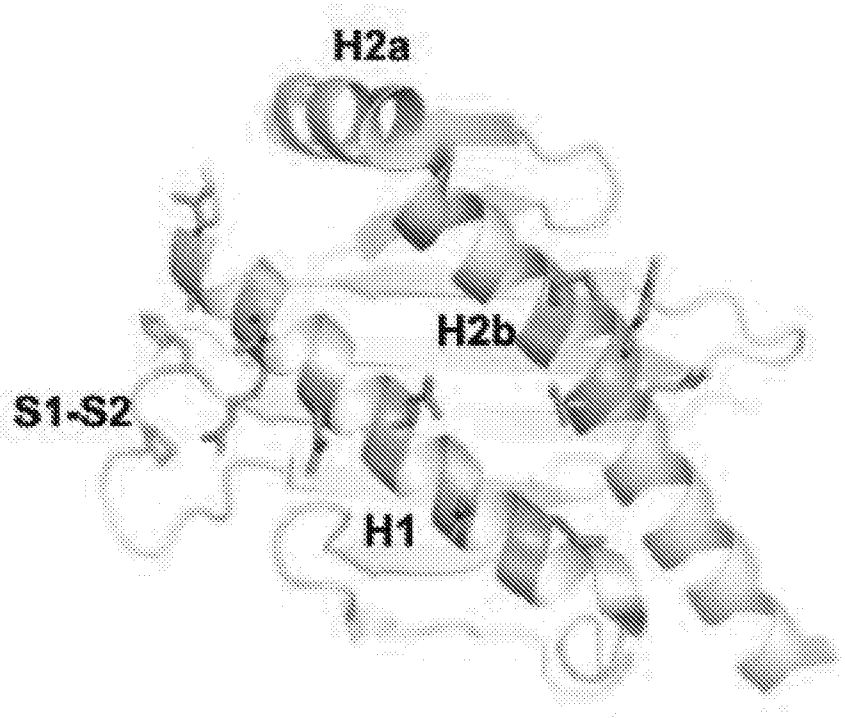


FIG. 27I

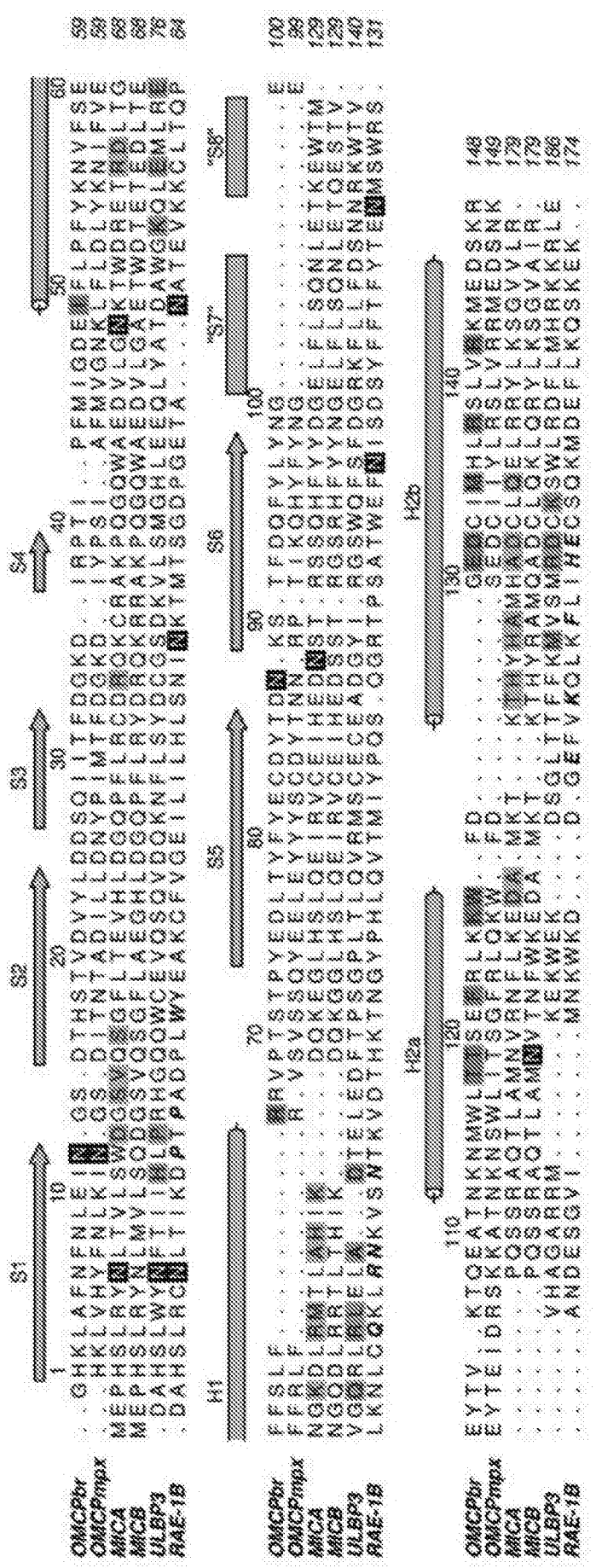

OMCPbr
OMCPmpx
MICA
MICB
ULBP3
RAE-1B
S1
S2
S3
S4
S5
S6
"S7"
"S8"
H1
H2a
H2b

FIG. 27J

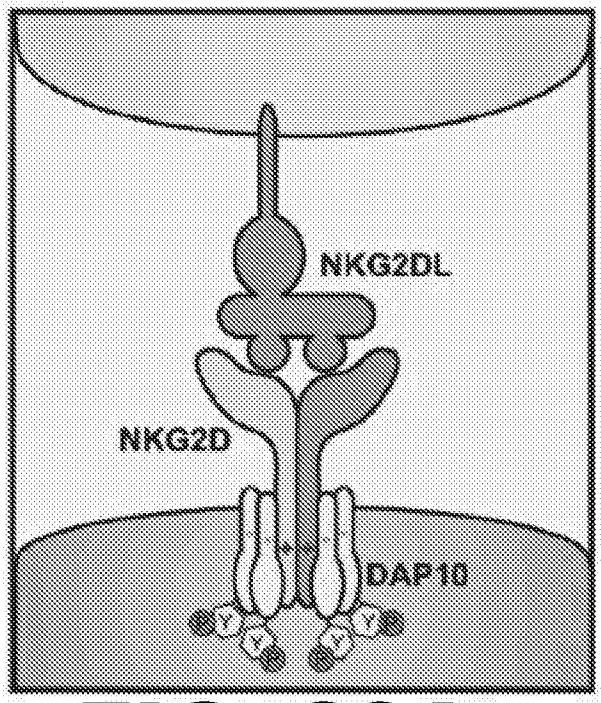


FIG. 28A

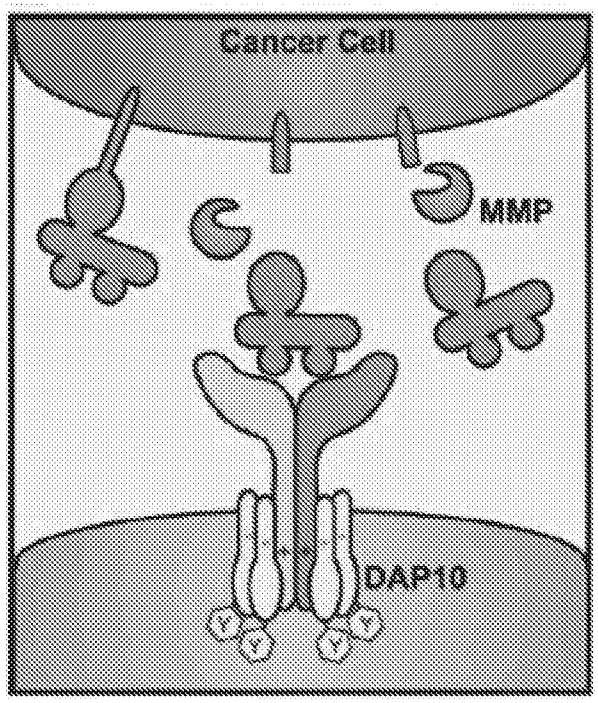


FIG. 28B

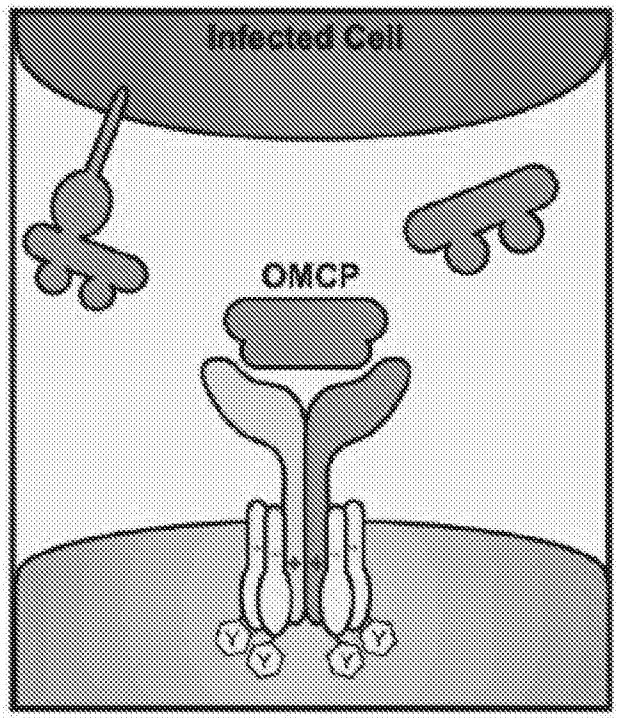


FIG. 28C

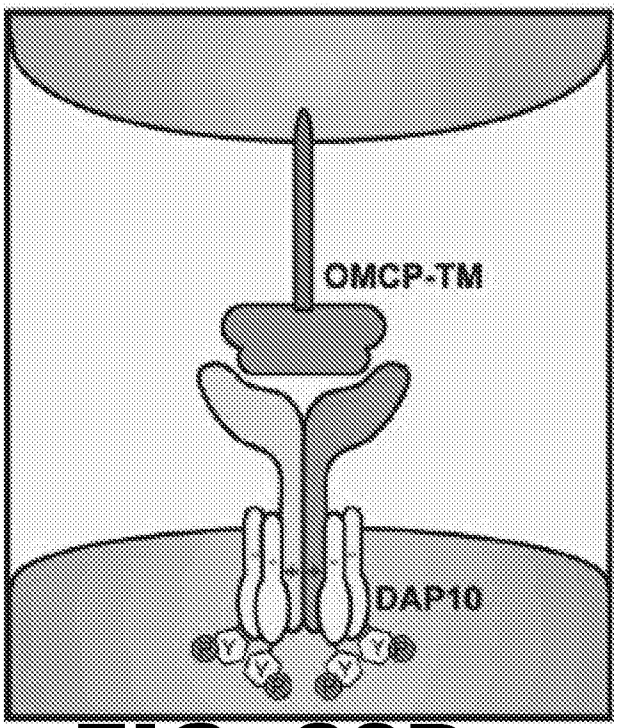


FIG. 28D

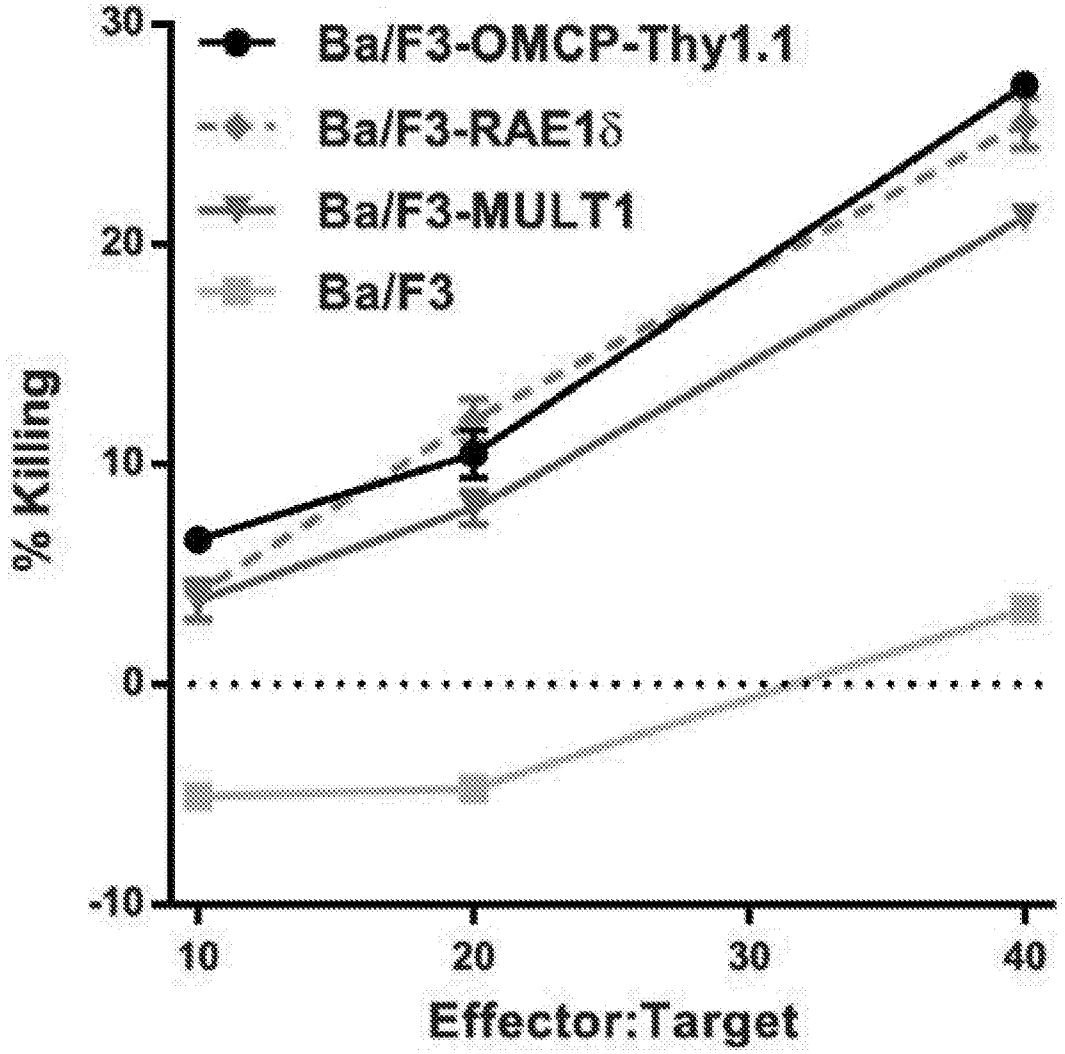

30
20
10
0
-10
% Killing
Ba/F3-OMCP-Thy1.1
Ba/F3-RAE1δ
Ba/F3-MULT1
Ba/F3
10
20
30
40
Effector:Target

FIG. 28E

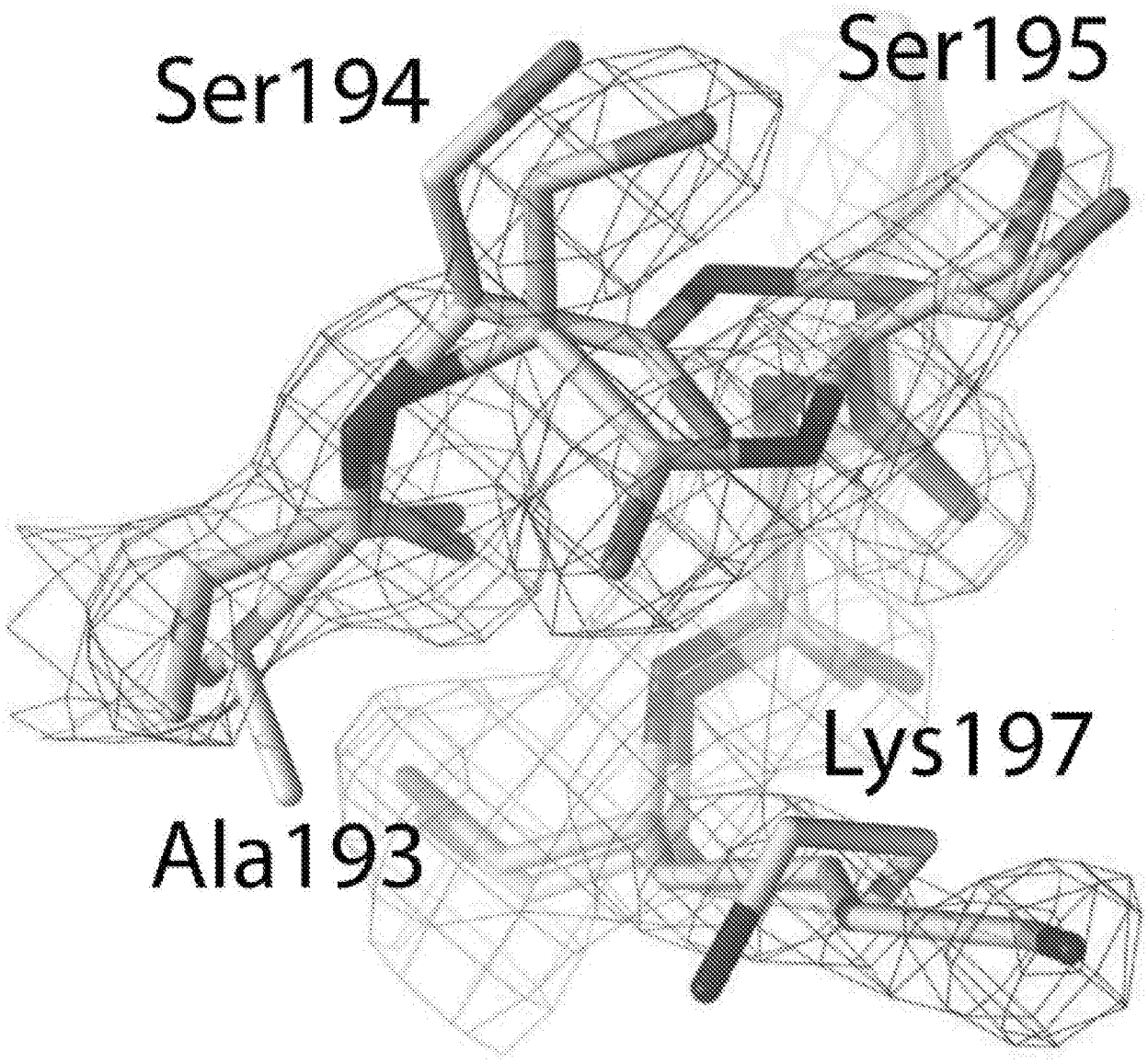


FIG. 29A

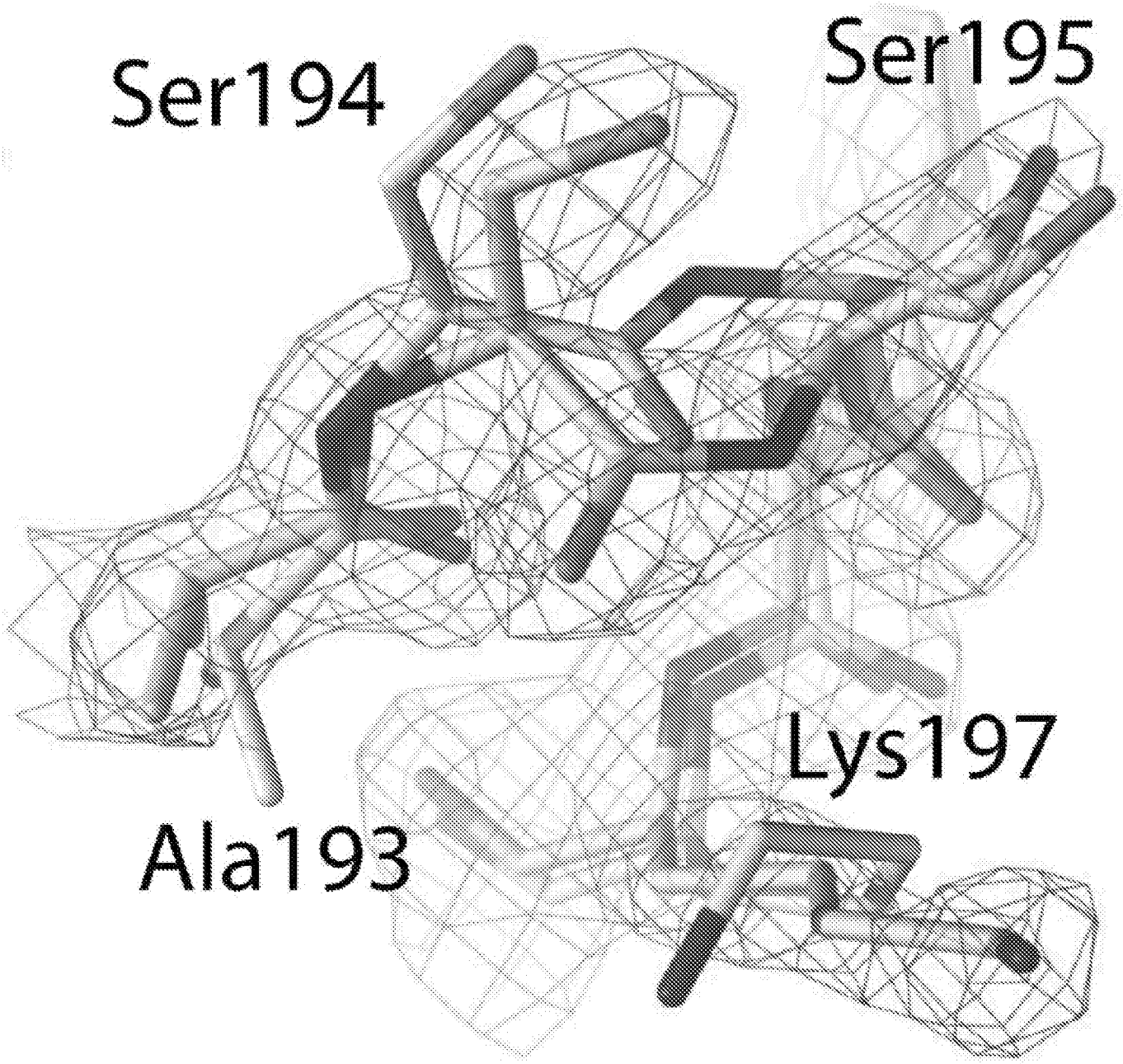


FIG. 29B

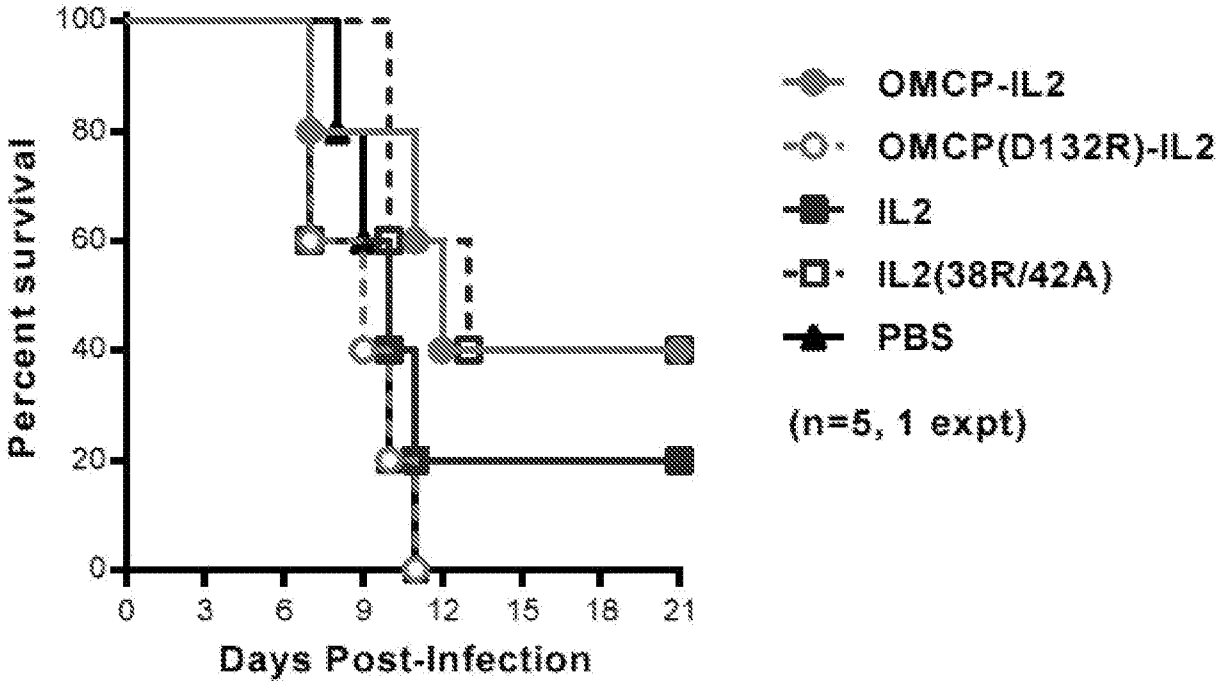


FIG. 30A

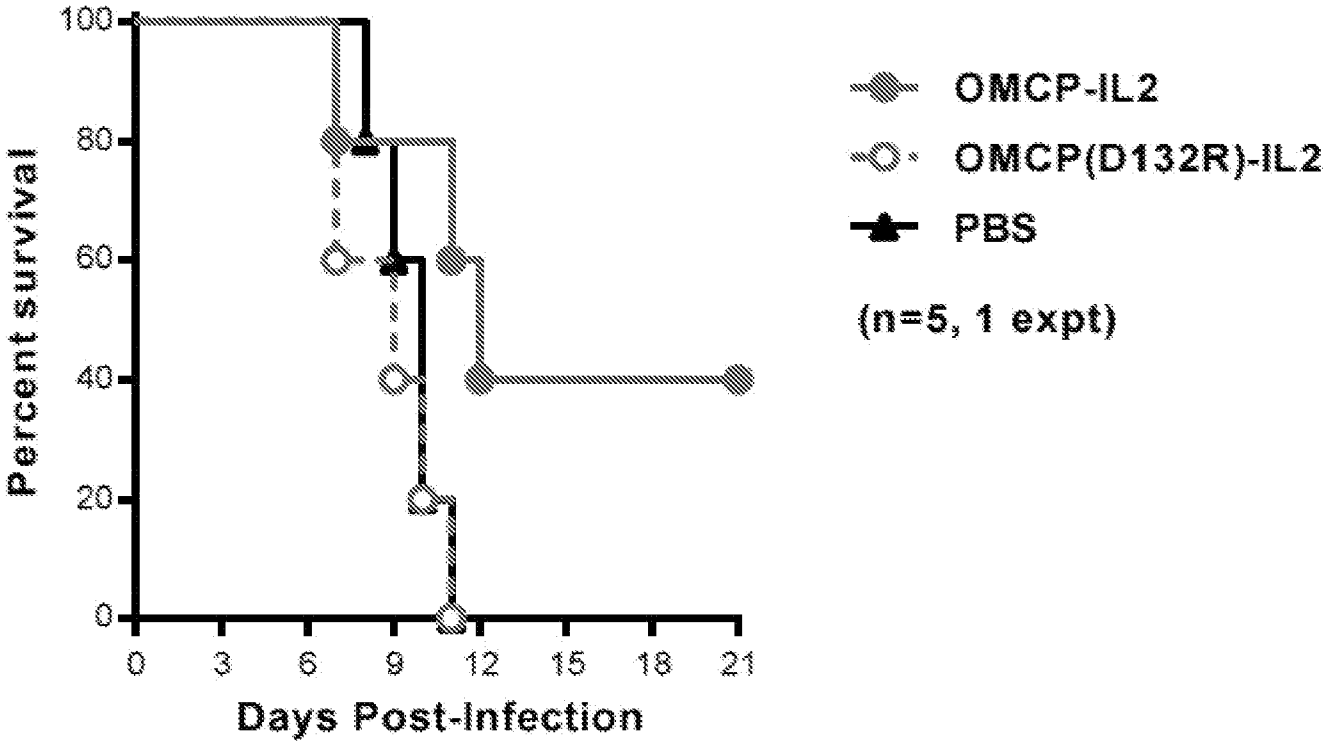


FIG. 30B

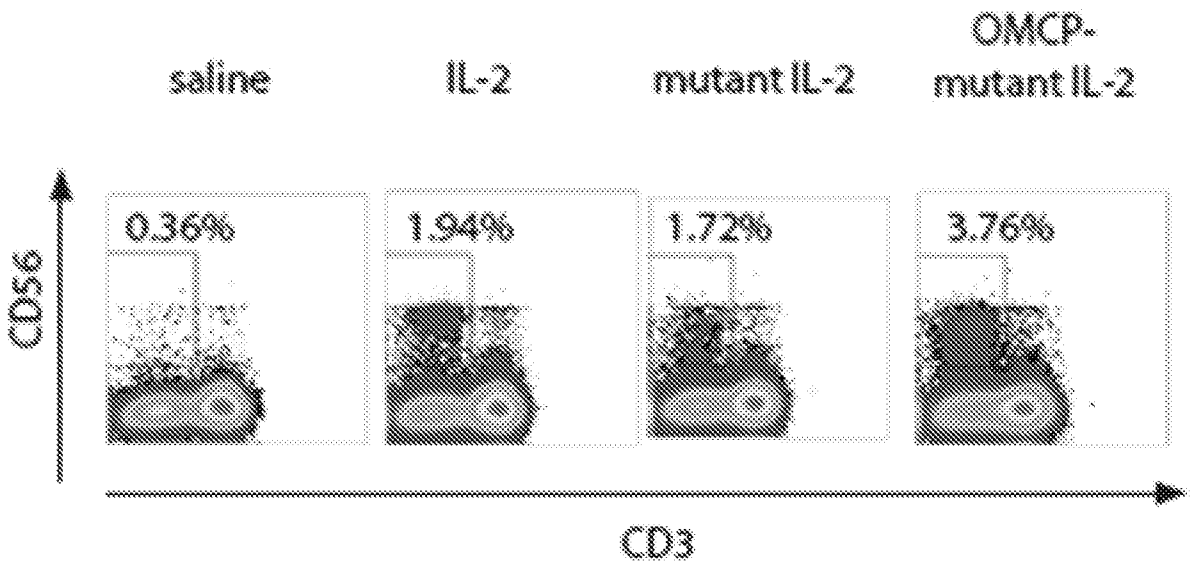


FIG. 31A

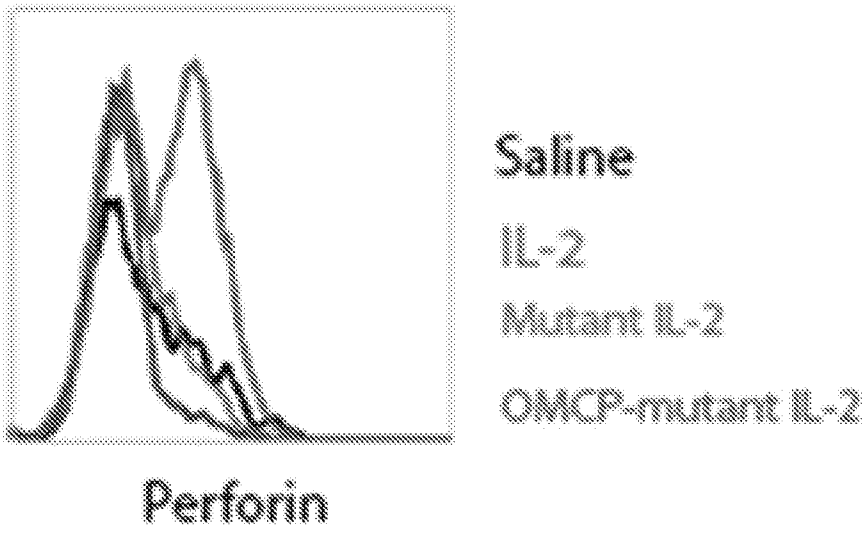


FIG. 31B

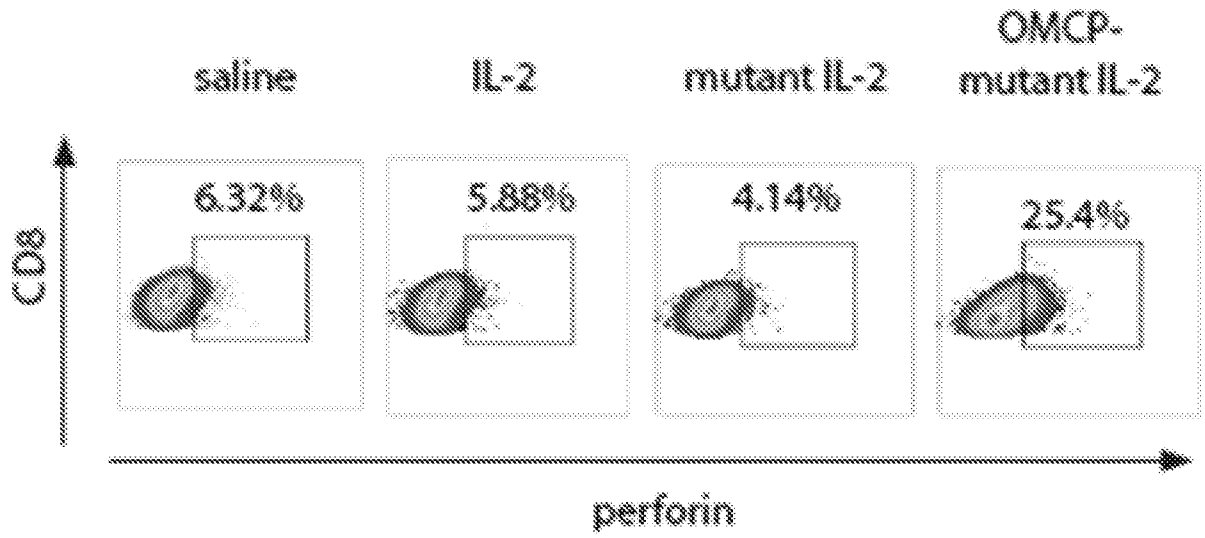


FIG. 31C

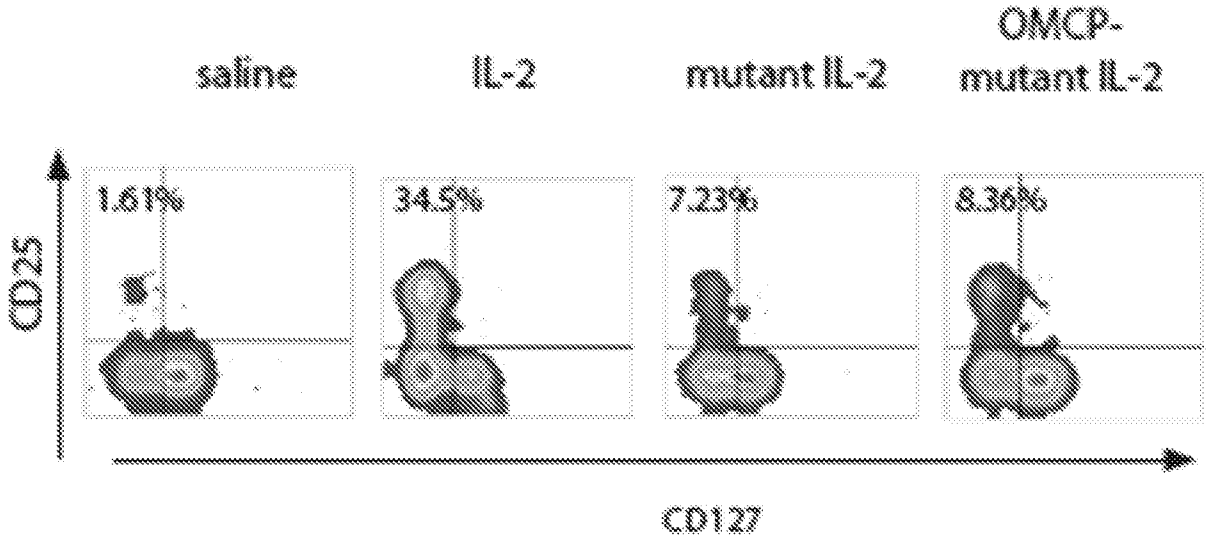


FIG. 31D

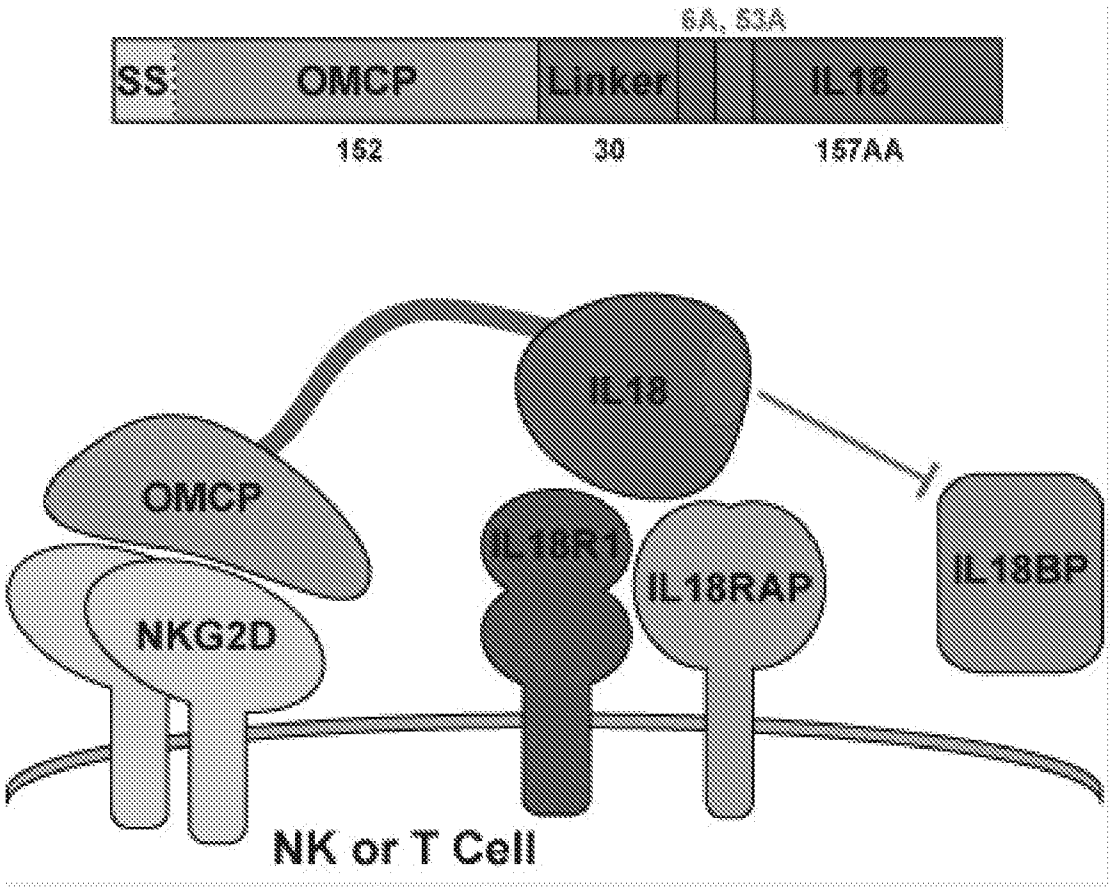
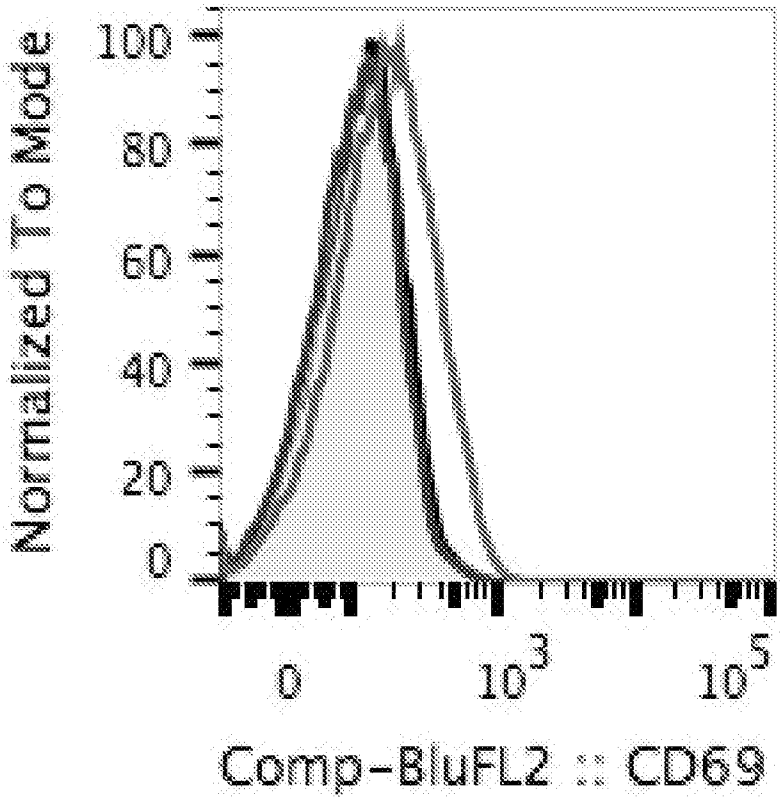

6A, 63A
SS
OMCP
Linker
IL18
162
30
157AA
IL18
OMCP
IL18R1
IL18RAP
IL18BP
NKG2D
NK or T Cell

FIG. 32



	Sample Name	SampleID
☐	021.fcs	OMCP-hIL-18 (4.4)
☐	015.fcs	hIL-18 (4.4)
☐	030.fcs	PBS (Isotype)
☐	009.fcs	PBS#1

FIG. 33