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(54) Title: NEURAMINIDASE INHIBITORS AND USES THEREOF

(57) Abstract: The invention is related to various methods for inhibiting or reducing biofilm formation, treating a biofilm production-related disorder, preventing biofilm formation, and screening for neuraminidase inhibitors.

NEURAMINIDASE INHIBITORS AND USES THEREOF

[0001] All patents, patent applications and publications cited herein are hereby incorporated by reference in their entirety. The disclosures of these publications in their entireties are hereby incorporated by reference into this application in order to more fully describe the state of the art as known to those skilled therein as of the date of the invention described and claimed herein.

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GOVERNMENT INTERESTS

[0003] The work described herein was supported in whole, or in part, by National Institute of Health Grant No. RO1 DK29693. Thus, the United States Government has certain rights to the invention.

BACKGROUND OF THE INVENTION

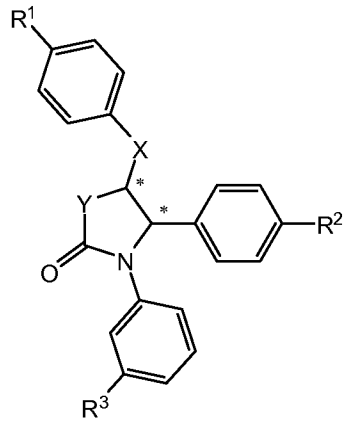
[0004] Many respiratory pathogens including *Hemophilus influenzae* (*H. influenzae*), *Streptococcus pneumoniae* (*S. pneumoniae*), and *Pseudomonas aeruginosa* (*P. aeruginosa*) express neuraminidases that can cleave α-2,3 linked sialic acids from glycoconjugates. As mucosal surfaces are heavily sialylated, neuraminidases have been thought to modify epithelial cells by exposing potential bacterial receptors. However, in contrast to neuraminidase produced by the influenza virus, a role for bacterial neuraminidase in pathogenesis has not been clearly established, especially as it pertains to regulating the formation of biofilms.

SUMMARY OF THE INVENTION

[0005] One aspect of the present invention provides a method for reducing or inhibiting bacterial biofilm formation where a surface is contacted with a bacterial neuraminidase inhibitor for a sufficient time so as to bacterial modulate neuraminidase activity. The neuraminidase inhibitor modulates the activity or the expression of a neuraminidase, thereby resulting in inhibiting or reducing the formation of the biofilm. In one embodiment, the surface comprises a biofilm. A biofilm can be produced by a bacterium, a virus, a protozoan,

a fungus, or by any combination of the organisms mentioned. In one embodiment, the biofilm is a bacterial biofilm. In some embodiments, the neuraminidase is a bacterial neuraminidase. In other embodiments the neuraminidase inhibitor targets bacterial neuraminidases. In some embodiments of the invention, the expression or the activity of the neuraminidase in the biofilm is reduced after the neuraminidase inhibitor is applied to a surface. In one embodiment, the neuraminidase inhibitor is an antibody that specifically binds to the NanA protein of *S. pneumoniae* or a fragment thereof; an antisense RNA or antisense DNA that inhibits expression of a NanA polypeptide; a siRNA that specifically targets a NanA gene, a peptide comprising at least 10 amino acids of SEQ ID NO: 2 wherein the peptide competes with endogenous NanA for ligand binding; or a combination thereof. In specific embodiments, the neuraminidase inhibitor comprises oseltamivir, peramivir, zanamivir, or a variant thereof.

[0006] In further embodiments, he neuraminidase inhibitor is a compound comprising Formula (I):



(I)

wherein,

R^1 is H, halogen, cyano, azido, nitro, C_1-C_6 alkyl, or C_1-C_6 alkoxy;

R^2 is H, halogen, cyano, azido, nitro, C_1-C_6 alkyl, or C_1-C_6 alkoxy;

R^3 is H, $–CO_2R^4$ or $-CON(R^4)_2$;

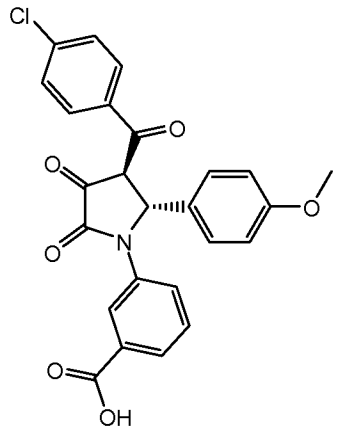
each R^4 is, independently, H or C_1-C_6 alkyl;

X is $-CH_2-$, –(C=O)-, -(C=NH)-, -(C=N-O-C_1-C_6-alkyl)-, or –(C=S)-; and

Y is –(C=O)-, -(C=NH)-, -(C=N-O-C_1-C_6-alkyl)-, or –(C=S)-,

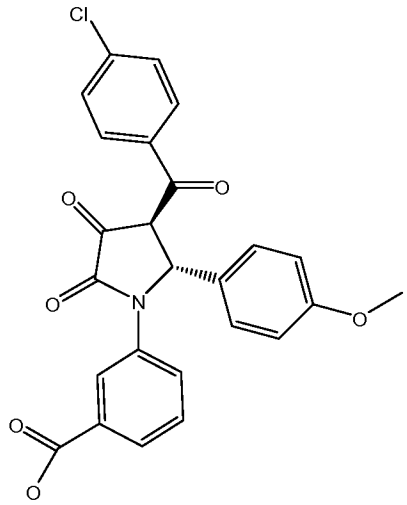
or a pharmaceutically acceptable salt or hydrate thereof.

[0007] In some embodiments, the neuraminidase inhibitor is a compound comprising Formula (A):



Formula (A)

[0008] In some embodiments, the neuraminidase inhibitor is a compound comprising Formula (X):



Formula (X)

[0009] Any biofilm-forming organism can comprise the biofilm mass. In certain embodiments, those organisms are viruses, bacteria, protozoa, and fungi. In various embodiments, the biofilm comprises a Gram-negative bacterium. In other embodiments, the biofilm comprises a Gram-positive bacterium. In some embodiments, the bacterium is *Streptococcus* and in other embodiments the Gram-positive bacteria are *Streptococcus* (e.g., *S. pneumoniae*) while in other embodiments, the Gram-negative bacteria are *Haemophilus*

(e.g., *Haemophilus influenzae*); *Pseudomonas* (*P. aeruginosa*), or *Vibrio* (e.g., *Vibrio cholerae*). A biofilm can be found on various surfaces and such a surface can be contacted with a neuraminidase inhibitor. In one embodiment, the surface comprises a cellular surface of a subject, an *in vitro* surface, or an oral surface of a subject. In some useful embodiments, the surface comprises a prosthetic graft, a catheter, a wound dressing, a wound site, a medical device, a contact lens, an implanted device, an oral device, a pipe, or industrial equipment. In further embodiments of the invention, the contacting comprises administering the neuraminidase inhibitor to a subject via subcutaneous, intra-muscular, intra-peritoneal, or intravenous injection; infusion; oral, nasal, or topical delivery; or a combination thereof. In some embodiments, the subject is a human, mouse, rat, bird, dog, cat, cow, horse, or pig. In another embodiment, the neuraminidase inhibitor is applied to the surface of a prosthetic graft to be introduced into a subject. In other embodiments, the neuraminidase inhibitor is applied to the surface of a catheter to be implanted into a subject. In yet further embodiments, the neuraminidase inhibitor is applied to the surface of a wound dressing to be applied on or in a subject. In other embodiments, the neuraminidase inhibitor is applied to the surface of a wound site on a subject. In additional embodiments, the neuraminidase inhibitor is applied to the surface of a medical device to be implanted or inserted into a subject. The subject in many of these instances can harbor the biofilm or has the propensity to form a biofilm. The neuraminidase inhibitor also can be administered to the subject prior to, or during, or after the implantation or insertion of a prosthetic graft, medical device, or a catheter, the application of the wound dressing or to the wound site.

[0010] The neuraminidase inhibitor according to the method of the invention can be applied to a surface where a biofilm has formed. In one embodiment, the surface comprises a contact lens, an implanted device, an oral device, a pipe, or industrial equipment. In other embodiments, industrial equipment is found in a GMP facility. In some embodiments, the industrial equipment comprises a plumbing system. In other embodiments, the surface where a biofilm has formed comprises an oral surface of a subject. In some embodiments, the biofilm is associated with dental caries while in other embodiments it is associated with periodontal disease. In some embodiments, the neuraminidase inhibitor is in a formulation of a paste, a liquid, a powder, a gel, or a tablet. According to an embodiment of the invention, the neuraminidase inhibitor can be in a paste formulation that can further comprise an abrasive, such as toothpaste. In other embodiments, the neuraminidase inhibitor can be a liquid formulation, such as a mouthwash.

[0011] A second therapeutic composition, different than the neuraminidase inhibitor, can also be administered to a subject. In some embodiments of the invention, administration occurs sequentially while in others administration occurs simultaneously. In various embodiments, the therapeutic composition comprises an antibiotic. In yet additional embodiments, the antibiotic comprises a cephalosporin, a macrolide, a penicillin, a quinolone, a sulfonamide, and a tetracycline, or any combination of the listed antibiotics.

[0012] Another aspect of the current invention provides for methods of treating a biofilm production-related disorder in a subject in need thereof. The method comprises administering to the subject an effective amount of a bacterial neuraminidase inhibitor that reduces biofilm formation in the subject. In one embodiment, the neuraminidase inhibitor is a compound comprising Formula (X), Formula (I), or Formula (A), as described herein. In another embodiment, the neuraminidase inhibitor is an antibody that specifically binds to the NanA protein of *S. pneumoniae* or a fragment thereof; an antisense RNA or antisense DNA that inhibits expression of a NanA polypeptide; a siRNA that specifically targets a NanA gene, a peptide comprising at least 10 amino acids of SEQ ID NO: 2 wherein the peptide competes with endogenous NanA for ligand binding; or a combination thereof. A reduction or inhibition in the growth of biofilm production-related bacteria in the subject can then be determined. A reduction in bacterial growth is indicative of the reduction in or inhibition of biofilm production in the subject. Thus, the method is useful for treating the biofilm production-related disorder. In one embodiment, the subject being treated is a mammal, whereas in other embodiments the subject is a human. In some embodiments, the subject can also be a mouse, rat, bird, dog, cat, cow, horse, or pig. A biofilm production-related disorder of the invention can be a disorder or disease that is characterized by a disease-related growth of bacteria, which can result in the establishment of a biofilm. In other embodiments, the disorder affects an epithelial surface, a mucosal surface, or a combination of those surfaces. In further embodiments of the invention, the surface is a lung surface. In some embodiments, the biofilm production-related disorder is caused by a bacterium, such as a Gram-negative or Gram-positive bacterium. In other embodiments, the bacterium comprises *Streptococcus* (such as *S. pneumoniae*); *Haemophilus* (such as *Haemophilus influenzae*); or *Vibrio* (such as *Vibrio cholerae*). In some embodiments, the bacterium is *S. pneumoniae*. In yet further embodiments, the disorder is pneumonia, cystic fibrosis (CF), otitis media, or chronic obstructive pulmonary disease (COPD). According to the invention, in additional

embodiments, the disorder is a medical device-related bacterial infection. The infection arises from the device being implanted or inserted into the subject.

[0013] The reduction in bacterial growth can be indicative of the reduction in or inhibition of biofilm production in a subject. In some embodiments, the growth of biofilm production-related bacteria can be determined by measuring the biofilm production-related bacteria in a biological sample. In other embodiments, the presence or growth of biofilm production-related bacteria is measured by detecting the presence of antigens of biofilm production-related bacteria in a biological sample. The biological sample can be blood, serum, sputum, lacrimal secretions, semen, urine, vaginal secretions, or a tissue sample. For example, an antibody to *S. pneumoniae* components can be used as a test for colonization/infection in a subject afflicted with a biofilm production-related condition or disorder, wherein the presence of *Streptococcus* antigens is detected in a biological sample, such as blood. These antibodies can be generated according to methods well established in the art or can be obtained commercially (for example, from Abcam, Cambridge, MA; Cell Sciences Canton, MA; Novus Biologicals, Littleton, CO; or GeneTex, San Antonio, TX). The reduction in the growth of biofilm production-related bacteria can also be measured by chest x-rays, or by a pulmonary function test (PFT), such as spirometry or forced expiratory volume (FEV_1) as described below.

[0014] In various embodiments of the invention, the biofilm comprises viruses, protozoa, fungi, or bacteria, such as a *Gram-positive* bacterium and a Gram-negative bacterium. In some embodiments, the bacterium is *Streptococcus* (such as *S. pneumoniae*); *Haemophilus* (such as *Haemophilus influenzae*); or *Vibrio* (such as *Vibrio cholerae*). In other embodiments, the bacterium is *S. pneumoniae*. According to the invention, a neuraminidase inhibitor that is applied to a surface likely to develop a biofilm modulates the activity or expression of a targeted neuraminidase, such as a bacterial neuraminidase. In some embodiments, the expression of the neuraminidase is reduced, while in other embodiments, the activity of the neuraminidase is reduced. In various embodiments, the neuraminidase inhibitor is applied as a formulation comprising a paste, liquid, powder, gel, or tablet. In certain embodiments, the industrial surface to which the neuraminidase inhibitor is applied is part of a plumbing system.

[0015] A useful neuraminidase inhibitor according to the invention can be any compound, small molecule, peptide, protein, aptamer, ribozyme, RNAi, or antisense

oligonucleotide, and the like. In one embodiment, the neuraminidase inhibitor is a viral neuraminidase inhibitor. In other embodiments, the viral neuraminidase inhibitor comprises oseltamivir, peramivir, zanamivir, or a variant thereof.

[0016] Other aspects of the invention provide screening methods for identifying a compound that modulates neuraminidase activity. The method comprises providing an electronic library of test compounds stored on a computer, then providing atomic coordinates for at least twenty amino acid residues of *Streptococcus* neuraminidase listed in **Table 2**, wherein the coordinates have a root mean square deviation therefrom, with respect to at least 50% of the Cα atoms, of not greater than about 2Å, in a computer readable format. The atomic coordinates are then converted into electrical signals readable by a computer processor to generate a three-dimensional model of the neuraminidase. A data processing method is then performed, wherein electronic test compounds from the library are superimposed upon the three-dimensional model of the neuraminidase. Whether a test compound fits into the binding pocket of the three-dimensional model of the neuraminidase is subsequently determined, enabling the identification of which compound would modulate the activity of the neuraminidase.

[0017] In another aspect of the invention, the method for identifying a compound that modulates neuraminidase activity comprises providing an electronic library of test compounds stored on a computer, then providing atomic coordinates listed in **Table 2** in a computer readable format for at least 5, 6, 7, 8, 9, 10, 11, or 12 amino acid residues located within about 10 Å of the *Streptococcus* neuraminidase active site, wherein the residues comprise 5 or more of the following residues: Arg347, Arg366, Asp372, Asp417, Ile442, Phe443, Phe565, Tyr590, Gln602, Glu647, Arg663, Tyr695, Tyr752, or Arg 721. The atomic coordinates are then converted into electrical signals readable by a computer processor to generate a three-dimensional model of the neuraminidase active site. A data processing method is then performed, wherein electronic test compounds from the library are superimposed upon the three-dimensional model of the neuraminidase active site. Whether a test compound fits into the binding pocket of the three-dimensional model of the neuraminidase is subsequently determined, enabling the identification of which compound would modulate the activity of the neuraminidase.

[0018] The methods described above can further comprise obtaining or synthesizing the compound determined to to bind to NanA or modulate the neuraminidase activity;

contacting a bacterium with the compound *in vitro*; and determining whether the compound modulates neuraminidase activity using a biological assay. In one embodiment, the bacterium is a Gram-negative bacterium. In a further embodiment, the bacterium is a Gram-positive bacterium. In another embodiment, the bacterium is *Streptococcus* (i.e., *S. pneumoniae*), *Pseudomonas* (such as *P. aeruginosa*), *Haemophilus*, (i.e *Haemophilus influenzae*), or *Vibrio* (such as *Vibrio cholerae*). In further embodiments, the biological assay comprises a biofilm assay, an adherence assay, or a combination of the two mentioned assays. In one embodiment, the biological assay entails contacting a surface harboring a biofilm (for example, produced by a pathogenic organism, such as a bacterium) *in vitro* with a test neuraminidase inhibitor, and then determining whether the test neuraminidase inhibitor inhibits biofilm formation at the surface. Inhibition of biofilm formation is indicative of the ability of the test neuraminidase inhibitor to inhibit the pathogenic infection, such as a bacterial infection. In one embodiment, the pathogen is a *Gram-positive* bacterium, such as *S. pneumoniae*. Thus, the method can be used for identifying neuraminidase inhibitors that can inhibit a pathogenic infection.

[0019] In a further aspect, the invention provides a compound identified by the screening methods above, wherein the compound binds to the neuraminidase active site, and comes within 10Å of amino acid residues listed in Table 3. In one embodiment, the compound inhibits or reduces biofilm formation. In another embodiment, the compound is a peptide that binds to a neuraminidase, such as an anti-neuraminidase antibody or a binding fragment thereof. In a further embodiment, the peptide interacts with a protein having the amino acid sequence of SEQ ID NO: 2. In some embodiments, the compound interacts with a protein having the amino acid sequence of SEQ ID NO: 2.

[0020] According to the methods of the present invention, a candidate or test neuraminidase inhibitor can be any compound, small molecule, peptide, protein, aptamer, ribozyme, RNAi, or antisense oligonucleotide, and the like. In one embodiment, the test inhibitor is a peptide that binds to a neuraminidase. In further embodiments, the neuraminidase can be a bacterial neuraminidase. In other embodiments, the test inhibitor is an anti-neuraminidase antibody or a binding fragment thereof. In specific embodiments of the invention, the test inhibitor is a peptide that interacts with a protein comprising the amino acid sequence of SEQ ID NO: 2. In various embodiments, the test inhibitor is a viral neuraminidase inhibitor while in other embodiments the viral neuraminidase inhibitor

comprises oseltamivir, peramivir, zanamivir, or a variant thereof. In some embodiments, the neuraminidase inhibitor is compound of Formula (X), Formula (A), or Formula (I), as decribed herein. In further embodiments of the invention, the test inhibitor is a peptide that interacts with a protein having the amino acid sequence of SEQ ID NO: 2.

BRIEF DESCRIPTION OF THE FIGURES

[0021] **FIG. 1** shows schematic representations of the structure of *S. pneumoniae* NanA. **FIG. 1A** depicts the β-strands shown in cyan, α-helices in yellow, and connecting loops in magenta. The inhibitor NANA is shown as a stick model, in black for carbon atoms. **FIG. 1B** depicts the final $2F_o–F_c$ electron density at 1.7 Å resolution for the inhibitor NANA, contoured at 1σ, in a boat conformation. **FIG. 1C** is a stereo drawing showing detailed interactions between NANA (black) or DANA (orange) with the active site of NanA. **FIG. 1D** show the molecular surface of NanA in the active region, colored by electrostatic potential with NANA. The figures were created with Pymol [A76] and Grasp [A77].

[0022] **FIG.2** shows schematic representations of the structure of *P. aeruginosa* NanPs. In **FIG. 2A**, the β-strands are shown in green, α-helices in yellow, and connecting loops in magenta. **FIG. 2B** depicts the molecular surface of NanPs in the active site region, colored by electrostatic potential. The view is the same as that of **FIG. 1D**, and the position of NANA bound to NanA is shown for reference. **FIG. 2C** shows the structural differences between the active site regions NanPs (in green) and NanA (in cyan). Residue numbers in green are for NanPs, and those in blue for NanA.

[0023] **FIG. 3** is a bar graph showing the activity of *P. aeruginosa* neuraminidase mutations. Site-directed mutations were made within the active site of *P. aeruginosa* neuraminidase or truncation in the C-terminus (deleting residues 334-438) and purified protein used to determine neuraminidase activity compared to wild-type enzyme (WT, control) using the fluorogenic substrate 2'-(4-methylumbelliferyl)-α-D-*N*-acetylneuraminic acid. *p-value <0.05.

[0024] **FIG. 4** is a schematic representation showing the phylogenetic analysis of neuraminidases. Shown is the unrooted phylogenetic network for our broad survey of the neuraminidase phylogeny. It is the strict consensus of 3 most parsimonious trees (steps=45885, consistency index=0.326, retention index=0.385, rescaled consistency=0.125).

Solid circles indicate branches with bootstrap values greater than 80%. Grey circles indicate bootstrap values between 50-80%. Open circles indicate bootstrap values for nodes with less than 50% that agreed with the consensus bootstrap tree. Branches without bootstrap designation are found in the maximum parsimony tree but not the bootstrap tree.

[0025] **FIG. 5** shows bar graphs of the activity of *S. pneumoniae* neuraminidase. **FIG. 5A** respresents the titration of activity using concentrations of purified NanA as labeled. **FIG. 5B** demonstrates the effect of divalent cations on activity purified NanA relative to wild-type enzyme (control). Assay was performed using 2'-(4-methylumbelliferyl)-α-D-*N*-acetylneuraminic acid (MNN). *p-value <0.05.

[0026] **FIG. 6** shows bar graphs of the inhibition of *S. pneumoniae* NanA neuraminidase activity by sialic acid compounds NANA and DANA. Activity is shown as a percentage of activity of NanA without inhibitor (control). Assay was performed using 2'-(4-methylumbelliferyl)-α-D-*N*-acetylneuraminic acid. *p-value <0.05.

[0027] **FIG. 7** shows bar graphs of the release of sialic acid from the surface of airway epithelial cells by *S. pneumoniae*. **FIG. 7A** represents exposure of aGM1 by concentrated supernatant from wild-type and *nanA* strains. **FIG. 7B** shows exposure of aGM1 with purified NanA. Cells were stained with antibody to aGM1 and quantified by flow cytometry and are shown as the fold change compared to media only control. *p-value <0.05.

[0028] **FIG. 8** shows graphs of biological activities of *S. pneumoniae* WT and *nanA* mutant. **FIG. 8A** demonstrates adherence to 16HBE airway epithelial cells. **FIG. 8B** depicts mouse colonization data. Mice were infected with 10^5 cfu bacteria and cfu bacteria in the lung determined and Polymorphonuclear monocytes (PMNs) (**FIG. 8C**) were quantified by flow cytometry. For **FIGS. 8B-C**, n=5 for both groups, data not statistically significant (Mann Whitney non-parametric test).

[0029] **FIG. 9** is a bar graph depicting *S. pneumoniae* biofilm formation. Encapsulated (D39 background) strains were grown in microtitre trays without (solid bars) or with (striped bars) previous epithelial cell exposure. Unencapsulated R6 strains were grown in microtitre trays without epithelial cell exposure. Biofilms were measured by crystal violet (CV) staining. Representative experiments are shown * p-value <0.05.

[0030] **FIG. 10** is a bar graph showing inhibition of neuraminidases by oseltamivir. Activity is expressed as a percentage of activity without inhibitor. Assay was performed using 2'-(4-methylumbelliferyl)-α-D-*N*-acetylneuraminic acid. *p-value <0.05.

[0031] **FIG. 11** depicts graphs demonstrating inhibitory activity of candidate neuraminidase inhibitors. **FIG. 11A** is a graphing showing the screening of candidate inhibitors performed with NanA (black bars) and NanPs (gray bars) and inhibitors at 100μM concentration in the neuraminidase assay. **FIGS. 11 B-C** are dose response curves for NanPs and NanA neuraminidases with lead compound XX1. Data was fitted with a power-based trend line. Shown is percentage activity compared to the vehicle (DMSO) only control.

[0032] **FIG. 12** are graphs that depict *S. pneumoniae* biofilm formation. **FIG. 12A** is a graph showing biofilm formation using encapsulated (D39 background) strains that were grown in microtitre trays without (solid bars) or with (striped bars) previous epithelial cell exposure. Unencapsulated R6 strains were grown in microtitre trays without epithelial cell exposure. **FIG. 12B** is a graph showing incubation with NANA results in reduced biofilm formation of the wild-type (D39) strain. Biofilms were measured by crystal violet (CV) staining. Biofilm formation was normalized to growth and expressed as a percentage when compared to the R6 wild-type strain. * p-value <0.05.

[0033] **FIG. 13** are photgraphs showing imaging of *S. pneumoniae* biofilms. **FIG. 13A** are images of CV stained biofilms in microtitre wells of WT and *nanA* strains in D39 (after epithelial cell exposure) and R6 backgrounds. **FIG. 13B** are photographic images of fluorescence microscopy of D39 WT and *nanA* biofilms grown in microtitre trays after epithelial cell exposure and stained with live/dead BacLight stain. Magnification was 200X. **FIG. 13C** is an image of a 3D reconstruction of biofilm structure seen with the WT strain in **FIG. 13B**. **FIG. 13D** is an image of a 3D reconstruction of cells seen with the *nanA* strain in **FIG. 13B**.

[0034] **FIG. 14** depicts the inhibitory activity of NanA inhibitors. **FIG. 14A** is a graphs showing the screening of candidate inhibitors that was performed with NanA and inhibitors at 100μM concentration in the neuraminidase assay. **FIG. 14B** is a dose response curve for NanA with lead compound XX1. Data was fitted with a logarithmic-based trend line. Shown is percentage activity compared to the vehicle (DMSO) only control. **FIG. 14C** is a bar graph that shows biofilm formation of wild-type D39 grown in the presence of XX1 during

epithelial cell exposure and growth in microtitre trays. The *nanA* strain is shown as a reference. Biofilm formation was normalized to growth and expressed as a percentage when compared to the wild-type control. **FIG. 14D** is a schematic of the chemical structure of XX1. *p-value <0.05.

[0035] **FIG. 15** is a schematic showing the synthesis of compounds of Formula I (Scheme 1)

[0036] **FIG. 16** is a diagram of a synthetic scheme showing that compounds of the invention can be tautomerized (Scheme 2).

DETAILED DESCRIPTION OF THE INVENTION

[0037] The invention is related to various methods for inhibiting biofilm formation, treating a biofilm production-related disorder, preventing biofilm formation, and screening for neuraminidase inhibitors. The invention also encompasses a mutant bacterial strain with a deletion in a neuraminidase gene.

[0038] Definitions

[0039] All scientific and technical terms used in this application have meanings commonly used in the art unless otherwise specified. As used in this application, the following words or phrases have the meanings specified.

[0040] As used herein, the term "inhibitor of biofilm formation," or "biofilm synthesis inhibitor" (such as a neuraminidase inhibitor) encompasses an agent that inhibits (e.g., disrupts) the attachment of microorganisms onto a surface, to the biofilm matrix itself, to other cells comprising the biofilm, or a combination thereof, and/or inhibits the ability of such microorganisms to produce, synthesize and/or accumulate biofilm on a surface.

[0041] The terms "disorder" and "disease" are used herein interchangeably for a condition in a subject. A disorder is a disturbance or derangement that affects the normal function of the body of a subject. A disease is a pathological condition of an organ, a body part, or a system resulting from various causes, such as infection, genetic defect, or environmental stress that is characterized by an identifiable group of symptoms. A disorder or disease can refer to a biofilm production-related disorder of the invention that is characterized by a disease-related growth of bacteria in that a biofilm is established.

[0042] The terms "prevent," "preventing," and "prevention" refer herein to the inhibition of the development or onset of a disorder or the prevention of the recurrence, onset, or development of one or more symptoms of a disorder in a subject resulting from the administration of a therapy (e.g., a prophylactic or therapeutic agent), or the administration of a combination of therapies (e.g., a combination of prophylactic or therapeutic agents).

[0043] As used herein, to "block" or "inhibit" a molecule, signal, or a receptor means to interfere with the binding of, or activation of the molecule, signal, or a receptor as detected by a test recognized in the art (such as binding assays). Blockage or inhibition can be partial or total, resulting in a reduction, increase, or modulation in the activation of the molecule, signal, or a receptor as detected by a test recognized in the art.

[0044] "Binding" refers to the interaction or association of a molecule with another entity, such as its target. This interaction can be covalent or noncovalent. The interaction of a molecule and its target site can be regulated by compositions of the invention. For example, administration of a neuraminidase inhibitor or a derivative thereof can block the action of its target, a neuraminidase.

[0045] As used herein, a "fragment" or "portion" is any part or segment of a molecule. For example, a fragment of a molecule includes that part that recognizes and binds its natural target. In the case of an antibody, the fragment is a binding portion of the whole antibody; in the case of a neuraminidase inhibitor, the fragment is that smaller portion of the entire inhibitor.

[0046] A "plumbing system" encompasses the faucets, valves, plumbing fixtures, piping (metal, plastic, and the like), water storage tanks, water recylcers, coils, bilges, hoses, tubing, and backflow preventers as well as their respective interior and exterior surfaces.

[0047] Aspects of the invention are related to methods of inhibiting biofilm formation. The method entails applying a neuraminidase inhibitor to the biofilm and measuring a reduction in the formation of a biofilm. The neuraminidase inhibitor modulates the activity or the expression of the neuraminidase (for example, a bacterial neuraminidase), thereby inhibiting biofilm formation.

[0048] Neuraminidases (sialidases) are produced by a wide variety of mucosal pathogens, ranging from *S. pneumoniae* in the airway to *Vibrio cholerae* in the gut (Vimr et al., (2004) *Microbiol. Mo.l Biol. Rev.* 68:132-153). While the central role of viral

neuraminidase in pathogenesis of influenza is established (Colman (1994) *Protein. Sci.* 3:1687-1696) and provides a target for both vaccines and chemotherapy, the contribution of bacterial neuraminidase to the pathogenesis of infection is not as clearly defined. Neuraminidase producing species such as *Hemophilus* (Vimr et al., (2002) *Trends. Microbiol.* 10:254-257), *Streptococcus pneumoniae* (Camara et al., (1994) *Infect. Immun.* 62:3688-3695; King et al., (2004) *Mol. Microbiol.* 54:159-171), and *P. aeruginosa* (Cacalano et al., (1992) *J. Clin. Invest.* 89:1866-1874) share a common ecological niche, colonizing the heavily sialylated secretions and surfaces of the upper respiratory tract. Although each can bind to asialylated glycolipids exposed by neuraminidase activity (Krivan et al., (1988) *Proc. Natl. Acad. Sci. U.S.A.* 85:6157-6161), they differ substantially in their ability to either metabolize (Godoy et al., (1993) *Infect. Immun.* 61:4415-4426) or incorporate sialic acid into surface structures (Bouchet et al., (2003) *Proc. Natl. Acad. Sci. U.S.A.* 100:8898-8903). Thus, bacterial neuraminidases can interact with both microbial as well as eukaryotic glycoconjugates (Vimr et al., (2004) *Microbiol. Mol. Biol. Rev.* 68:132-153).

[0049] Viral neuraminidase inhibitors have been very useful in the prevention and treatment of influenza, targeting similar high-risk patient populations, such as those patients afflicted with pneumonia, CF, or chronic obstructive pulmonary disease (COPD). The NanPs neuraminidase, for example, of *P. aeruginosa* shares many conserved elements and folds in the manner predicted for other microbial neuraminidases (Roggentin et al., (1989) *Glycoconj. J.* 6:349-353; Rothe et al., (1991) *Mol. Gen. Genet.* 226:190-197).

[0050] *P. aeruginosa* (a Gram-negative bacterium) is a major opportunistic pathogen, an important cause of nosocomial pneumonia as well as the chief cause of lung infection in cystic fibrosis (CF), and is the most common lethal genetic disease of Caucasians. Over two decades ago, neuraminidase production in isolates of *P. aeruginosa* from CF patients was described and indicated to contribute to pulmonary infection (Leprat et al., (1980) *Ann. Microbiol. (Paris)* 131B:209-222).

[0051] *Streptococcus pneumoniae*, or pneumococcus, is a Gram-positive, diplococcus, alpha-hemolytic anaerobe that is a common inhabitant of the nasopharyngeal region. *S. pneumoniae* causes many types of infection other than pneumonia, including, but not limited to, meningitis, bacteremia (or septicaemia), acute sinusitis, otitis media, endocarditis, peritonitis, osteomyelitis, septic arthritis, pericarditis, cellulitis, and brain abscess. *S. pneumoniae* is the most common cause of bacterial meningitis in adults and children, and is

one of the top two isolates found in ear infection, otitis media. Pneumococcal pneumonia is more common in the elderly and very young.

[0052] The capusle of *S. pneumoniae* is the most important element in its pathogenicity. Furthermore, nearly all *S. pneumoniae* clinical isolates have prominent sialidase activities. For example, the organism has been shown to encode 3 different neuraminidases: NanA, NanB, and NanC. For a further discussion, see Henriques-Normark et al., (2008) *Nat Rev Microbiol.* 6(11):827-37; and see Yao KH and Yang YH., (2008) *Vaccine*, 26(35):4425-33.

[0053] The nucleotide sequence of *S. pneumoniae* neuraminidase (sialidase A; NanA) is shown in SEQ ID NO: 1. The polypeptide sequence of *S. pneumoniae* neuraminidase is depicted in SEQ ID NO:2. Sequence information related to NanA is accessible in public databases by GenBank Accession numbers NC_008533 (for mRNA) and YP_816960 (for protein).

[0054] SEQ ID NO: 1 is the *S. pneumoniae* wild type nucleotide sequence corresponding to the NanA (nucleotides 1-2994):

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   1 atgattgtag gagcagtggt atttggaacg tctcctgttt tagctcaaga aggggcaagt
  61 gagcaacctc tggcaaatga aactcaactt tcgggggaga gctcaaccct aactgataca
 121 gaaaagagcc agccttcttc agagactgaa ctttctggca ataagcaaga acaagaaagg
 181 aaagataagc aagaagaaaa aattccaaga gattactatg cacgagattt ggaaaatgtc
 241 gaaacagtga tagaaaaaga agatgttgaa accaatgctt caaatggtca gagagttgat
 301 ttatcaagtg aactagataa actaaagaaa cttgaaaacg caacagttca catggagttt
 361 aagccagatg ccaaggcccc agcattctat aatctctttt ctgtgtcaag tgctactaaa
 421 aaagatgagt acttcactat ggcagtttac aataatactg ctactctaga ggggcgtggt
 481 tcggatggga aacagtttta caataattac aacgatgcac ccttaaaagt taaaccaggt
 541 cagtggaatt ctgtgacttt cacagttgaa aaaccgacag cagaactacc taaaggccga
 601 gtgcgcctct acgtaaacgg ggtattatct cgaacaagtc tgagatctgg caatttcatt
 661 aaagatatgc cagatgtaac gcatgtgcaa atcggagcaa ccaagcgtgc caacaatacg
 721 gtttgggggt caaatctaca gattcggaat ctcactgtgt ataatcgtgc tttaacacca
 781 gaagaggtac aaaaacgtag tcaacttttt aaacgctcag atttagaaaa aaaactacct
 841 gaaggagcgg ctttaacaga gaaaacggac atattcgaaa gcgggcgtaa cggtaaacca
 901 aataaagatg gaatcaagag ttatcgtatt ccagcacttc tcaagacaga taaaggaact
 961 ttgatcgcag gtgcagatga acgccgtctc cattcgagtg actggggtga tatcggtatg
1021 gtcatcagac gtagtgaaga taatggtaaa acttggggtg accgagtaac cattaccaac
1081 ttacgtgaca atccaaaagc ttctgaccca tcgatcggtt caccagtgaa tatcgatatg
1141 gtgttggttc aagatcctga aaccaaacga atcttttcta tctatgacat gttcccagaa
1201 gggaagggaa tctttggaat gtcttcacaa aaagaagaag cctacaaaaa aatcgatgga
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1261 aaaacctatc aaatcctcta tcgtgaagga gaaaagggag cttataccat tcgagaaaat
1321 ggtactgtct atacaccaga tggtaaggcg acagactatc gcgttgttgt agatcctgtt
1381 aaaccagcct atagcgacaa gggggatcta tacaagggta accaattact aggcaatatc
1441 tacttcacaa caaacaaaac ttctccattt agaattgcca aggatagcta tctatggatg
1501 tcctacagtg atgacgacgg gaagacatgg tcagcgcctc aagatattac tccgatggtc
1561 aaagccgatt ggatgaaatt cttgggtgta ggtcctggaa caggaattgt acttcggaat
1621 gggcctcaca agggacggat tttgataccg gtttatacga ctaataatgt atctcactta
1681 aatggctcgc aatcttctcg tatcatctat tcagatgatc atggaaaaac ttggcatgct
1741 ggagaagcgg tcaacgataa ccgtcaggta gacggtcaaa agatccactc ttctacgatg
1801 aacaatagac gtgcgcaaaa tacagaatca acggtggtac aactaaacaa tggagatgtt
1861 aaactcttta tgcgtggttt gactggagat cttcaggttg ctacaagtaa agacggagga
1921 gtgacttggg agaaggatat caaacgttat ccacaggtta aagatgtcta tgttcaaatg
1981 tctgctatcc atacgatgca cgaaggaaaa gaatacatca tcctcagtaa tgcaggtgga
2041 ccgaaacgtg aaaatgggat ggtccacttg gcacgtgtcg aagaaaatgg tgagttgact
2101 tggctcaaac acaatccaat tcaaaaagga gagtttgcct ataattcgct ccaagaatta
2161 ggaaatgggg agtatggcat cttgtatgaa catactgaaa aaggacaaaa tgcctatacc
2221 ctatcattta gaaaatttaa ttgggacttt ttgagcaaag atctgatttc tcctaccgaa
2281 gcgaaagtga agcgaactag agagatgggc aaaggagtta ttggcttgga gttcgactca
2341 gaagtattgg tcaacaaggc tccaaccctt caattggcaa atggtaaaac agcacgcttc
2401 atgacccagt atgatacaaa aaccctccta tttacagtgg attcagagga tatgggtcaa
2461 aaagttacag gtttggcaga aggtgcaatt gaaagtatgc ataatttacc agtctctgtg
2521 gcgggcacta agctttcgaa tggaatgaac ggaagtgaag ctgctgttca tgaagtgcca
2581 gaatacacag gcccattagg gacatccggc gaagagccag ctccaacagt cgagaagcca
2641 gaatacacag gcccactagg gacatccggc gaagagccag ccccgacagt cgagaagcca
2701 gaatacacag gcccactagg gacagctggt gaagaagcag ctccaacagt cgagaagcca
2761 gaatttacag ggggagttaa tggtacagag ccagctgttc atgaaatcgc agagtataag
2821 ggatctgatt cgcttgtaac tcttactaca aaagaagatt atacttacaa agctcctctt
2881 gctcagcagg cacttcctga aacaggaaac aaggagagtg acctcctagc ttcactagga
2941 ctaacagctt tcttccttgg tctgtttacg ctagggaaaa agagagaaca ataa
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[0055] SEQ ID NO: 2 is the *S. pneumoniae* wild type amino acid sequence corresponding to NanA (residues 1-997):

MIVGAVVFGTSPVLAQEGASEQPLANETQLSGESSTLTDTEKSQPSSETELSGNKQEQ
ERKDKQEEKIPRDYYARDLENVETVIEKEDVETNASNGQRVDLSSELDKLKKLENAT
VHMEFKPDAKAPAFYNLFSVSSATKKDEYFTMAVYNNTATLEGRGSDGKQFYNNY
NDAPLKVKPGQWNSVTFTVEKPTAELPKGRVRLYVNGVLSRTSLRSGNFIKDMPDV
THVQIGATKRANNTVWGSNLQIRNLTVYNRALTPEEVQKRSQLFKRSDLEKKLPEG
AALTEKTDIFESGRNGKPNKDGIKSYRIPALLKTDKGTLIAGADERRLHSSDWGDIGM

VIRRSEDNGKTWGDRVTITNLRDNPKASDPSIGSPVNIDMVLVQDPETKRIFSIYDMF
PEGKGIFGMSSQKEEAYKKIDGKTYQILYREGEKGAYTIRENGTVYTPDGKATDYRV
VVDPVKPAYSDKGDLYKGNQLLGNIYFTTNKTSPFRIAKDSYLWMSYSDDDGKTWS
APQDITPMVKADWMKFLGVGPGTGIVLRNGPHKGRILIPVYTTNNVSHLNGSQSSRII
YSDDHGKTWHAGEAVNDNRQVDGQKIHSSTMNNRRAQNTESTVVQLNNGDVKLF
MRGLTGDLQVATSKDGGVTWEKDIKRYPQVKDVYVQMSAIHTMHEGKEYIILSNA
GGPKRENGMVHLARVEENGELTWLKHNPIQKGEFAYNSLQELGNGEYGILYEHTEK
GQNAYTLSFRKFNWDFLSKDLISPTEAKVKRTREMGKGVIGLEFDSEVLVNKAPTLQ
LANGKTARFMTQYDTKTLLFTVDSEDMGQKVTGLAEGAIESMHNLPVSVAGTKLSN
GMNGSEAAVHEVPEYTGPLGTSGEEPAPTVEKPEYTGPLGTSGEEPAPTVEKPEYTG
PLGTAGEEAAPTVEKPEFTGGVNGTEPAVHEIAEYKGSDSLVTLTTKEDYTYKAPLA
QQALPETGNKESDLLASLGLTAFFLGLFTLGKKREQ

[0056] Many pulmonary pathogens, including *P. aeruginosa*, bind to the GalNAcβ1-4Gal moiety exposed on asialylated glycolipids (Krivan et al., (1988) *Proc. Natl. Acad. Sci. U.S.A.* 85:6157-6161). Therefore, the ability to de-sialylate mucosal surfaces can contribute to bacterial colonization of the airways. The *P. aeruginosa* neuraminidase was shown to be osmo-regulated, and accordingly, to be consistent with expression in the milieu of the CF lung (Cacalano et al., (1992) *J. Clin. Invest.* 89:1866-1874). This neuraminidase is capable of exposing the receptor asialoganglioside gangliotetraosylceramide (asialoGM1) (Galβ1,2GalNAcβ1,4Galβ1,4Glcβ1,1Cer) on the surface of CF airway cells *in vitro* (Saiman et al., (1993) *J. Clin. Invest.* 92:1875-1880). However, data to document *P. aeruginosa* adherence to the airway surface in CF patients has been lacking (Baltimore et al., (1989) *Am. Rev. Respir. Dis.* 140:1650-1661). The current consensus is that organisms are predominantly entrapped in dehydrated secretions of the lung and by shedding proinflammatory products activate airway inflammation, a model that does not require direct attachment of organisms to the epithelial surface (Boucher (2004) *Eur. Respir. J.* 23:146-158). Nonetheless, analyses of *P. aeruginosa* gene expression in CF patients document that the NanPs (also referred to as PA2794) neuraminidase locus is one of the most highly expressed genes in this patient population *in vivo* (Lanotte et al., (2004) *J. Med. Microbiol.* 53:73-81). Unlike other respiratory pathogens, *P. aeruginosa* cannot use sialic acid as a carbon source nor does it contain sialic acid as a component of its LPS (Knirel et al., (1988) *Acta. Microbiol. Hung.* 35:3-24).

[0057] Gram-negative bacteria and Gram-positive bacteria, in addition to other unicellular organisms, can produce biofilms. Bacterial biofilms are surface-attached communities of cells that are encased within an extracellular polysaccharide matrix produced by the colonizing cells. Biofilm development occurs via a series of programmed steps, which include an initial attachment to a surface, formation of three-dimensional microcolonies, and the subsequent development of a mature biofilm. Biofilms can be composed of various microorganisms (such as viruses, bacteria, protozoa, and fungi) co-existing within the community and a particular cellular type can predominate. The more deeply a cell is located within a biofilm (such as, the closer the cell is to the solid surface to which the biofilm is attached to, thus being more shielded and protected by the bulk of the biofilm matrix), the more metabolically inactive the cells are. The consequences of this physiologic variation and gradient create a collection of bacterial communities where there is an efficient system established whereby microorganisms have diverse functional traits. A biofilm also is made up of various and diverse non-cellular components and can include, but are not limited to carbohydrates (simple and complex), lipids, proteins (including polypeptides), and lipid complexes of sugars and proteins (lipopolysaccharides and lipoproteins).

[0058] Bacterial biofilms exist in nature as well as in medical and industrial environments, such as a GMP facility. The biofilm can allow bacteria to exist in a dormant state for a certain amount of time until suitable growth conditions arise thus offering the microorganism a selective advantage to ensure its survival. However, this selection can pose serious threats to human health in that biofilms have been observed to be involved in about 65% of human bacterial infections (Smith (2005) *Adv. Drug Deliv. Rev.* 57:1539-1550; Hall-Stoodley et al., (2004) *Nat. Rev. Microbiol.* 2: 95-108). In fact, the majority of infections that occur in animals are biofilm-based. Biofilms are problematic with respect to respiratory conditions and diseases. Cystic Fibrosis (CF), one of the most common fatal genetic disorders in the United States, is most prevalent in Caucasians. It occurs on an average of one in every 3,300 live births, and causes the death of patients inflicted with CF by the age of 30. A mutation in a gene that encodes a chloride transport channel produces partially functional or completely dysfunctional transport channels. CF patients develop thick mucus secretions, which result from disruption of physiological salt/water balance due to the defective transport channel. The secretions clog bronchial tubes in the lungs and can additionally block exit passages of the pancreas and intestines, which lead to loss of function of these organs.

[0059] The mucus secretions are depleted of oxygen due to the metabolic activity of neutrophils, aerobic bacteria, and even epithelial cells. Within this mucus, *P. aeruginosa*, for

example, is found to thrive. *P. aeruginosa* also is an important cause of nosocomial pneumonia. It infects the elderly, cancer chemotherapy patients, and immuno-compromised individuals.

[0060] Other medical conditions and treatments resulting in the development of undesirable biofilms include, but are not limited to, medical device-related infections, catheter-related infection (kidney, vascular, peritoneal), chronic otitis media, prostatitis, dental caries, wounds, acne, chronic obstructive pulmonary disease, infectious kidney stones, orthopedic implant infection, cystitis, bronchiectasis, bacterial endocarditis, Legionnaire's disease, osteomyelitis, and biliary stents (see US Appln. Pub. No. 20050158253). Thus, there is a need in the art for improved therapeutic approaches for the inhibition of biofilm formation and/or the reduction or elimination of biofilms.

[0061] Harsh treatments (such as chemicals and abrasives) have been used to reduce, prevent, or control biofilm formation. However, biological environments (for example, airways, the urinary tract, wound sites, etc) are sensitive to such harsh treatments. Thus, better methods are needed to control biofilm formation.

[0062] In industrial settings, biofilms (comprised of viruses, bacteria, protozoa, fungi, and the like) can adhere to surfaces, such as pipes and filters. Biofilms are problematic in industrial settings because they cause biocorrosion and biofouling in industrial systems, such as heat exchangers, oil pipelines, water systems, filters, and the like (Coetser et al., (2005) *Crit. Rev. Micro.* 31: 212-32). Thus, biofilms can inhibit fluid flow-through in pipes, clog water and other fluid systems, as well as serve as reservoirs for pathogenic bacteria, protozoa, and fungi. As such, industrial biofilms are an important cause of economic inefficiency in industrial processing systems.

[0063] Biofilms (also referred to as "slime residues") can affect a wide variety of commercial, industrial, and processing operations (such as Good Manufacturing Practices (GMP) facilities). Since biofilms are ubiquitous in water handling systems, *S. pneumoniae* a gram-positive, ovoid bacterium (and/or other bacteria, protozoa, fungi and some viruses) can be associated with these biofilms. In many instances, *S. pneumoniae* is a substantial microbial component. Thus, there is a need for compositions and methods for controlling biofilms in commercial settings as well as biological environments.

[0064] The biofilm to be inhibited can be harbored by a subject, can be *in vitro*, or can be on the surface of an implantable/insertable device to be inserted into a subject.

[0065] For example, the terms can refer to a mammal including, but not limited to, and a primate (e.g., a monkey, such as a cynomolgous monkey, a chimpanzee, and a human). For example, the subject can be a non-human animal such as a bird (e.g., a quail, chicken, or turkey), a farm animal (e.g., a cow, goat, horse, pig, or sheep), a pet (e.g., a cat, dog, or guinea pig, rat, or mouse), or laboratory animal (e.g., an animal model for a disorder). The subject according to the invention is a human (e.g., an infant, child, adult, or senior citizen).

[0066] For example, the subject according to the invention can be an animal, such as a mammal. The mammal can be a non-primate (for example, a cow, pig, bird, sheep, goat, horse, cat, dog, rat, rabbit, mouse, and the like) or a primate (for example, a monkey, such as a cynomolgous monkey, a chimpanzee, a human). Non-limiting representative subjects according to the invention can be a human infant, a pre-adolescent child, an adolescent, an adult, or a senior/elderly adult.

[0067] A neuraminidase is an enzyme protein (for example, bacterial, viral, and the like) that cleaves terminal sialic acid residues from carbohydrate moieties on the surfaces of cells infected with such pathogens (for example, bacteria or viruses). This cleavage can result in the release of progeny pathogens from infected cells. Thus, administration of neuraminidase inhibitors can serve as a treatment that limits the severity and spread of pathogenic infections. The neuraminidase inhibitor can also modulate the expression of a neuraminidase via reducing the expression of the neuraminidase. The modulation of neuraminidase activity and/or expression (for example, its reduction) can be due to decreased transcription and /or translation of the neuraminidase molecule, which results in reduced amounts of neuraminidase synthesized by the cell.

[0068] Initial studies of the *P. aeruginosa* neuraminidase performed with purified enzyme, and *in vitro* analyses were consistent with a role for the enzyme in modifying airway epithelial cell surfaces to facilitate bacterial attachment (Cacalano et al., (1992) *J. Clin. Invest.* 89:1866-1874). Moreover, as CF airways were more readily modified than were normal airway cells, the *Pseudomonas* enzyme seemed to be important in that disease (Saiman et al., (1993) *J. Clin. Invest.* 92:1875-1880). However, it has been determined with tests performed under more physiological conditions *in vivo* using isogenic mutants that the *P. aeruginosa* neuraminidase has a different function. The neuraminidase, in addition to other bacterial neuraminidases, is important for biofilm production, as well as the cell-cell interactions that were critical in the initial colonization process. Recent studies indicate that there are significant homologies between the genes involved in sialic acid O-acetylation in many bacterial species (Lewis et al., (2006) *J. Biol. Chem.* 281:11186-11192). Just as

autolysins are necessary for cell wall biosynthesis, enzymes that cleave carbohydrate linkages are necessary for the growth and modification of extracellular polysaccharides during biofilm biosynthesis (Vuong et al., (2004) *J. Biol. Chem.* 279:54881-54886). The invention provides for methods for inhibiting or reducing biofilm formation using neuraminidase inhibitors.

[0069] A neuraminidase inhibitor according to the invention can be used to inhibit the formation of a biofilm by any biofilm-forming organism, such as viruses, bacteria, protozoa, and fungi. Biofilms are comprised of various microorganisms, such as viruses, bacteria, protozoa, and fungi, (e.g., *Borrelia* sp., *Streptococcus* sp., *Neisseria* sp., *Pseudomonas* sp., *Haemophilus* sp., *Vibrio* sp., *Bacillus* sp., *Klebsiella* sp., *Burkholderia* sp., *Salmonella* sp., *Legionella* sp., *P. aeruginosa*, *H. influenzae, V. cholerae*, *Yersinia pestis, Escherichia coli*, *Streptococcus pneumoniae*, *Proteus mirablis*, and *Francisella tularensis*) and can be found in a live subject, *in vitro,* or on a surface, such as on or in the pipes of a plumbing system or industrial equipment.

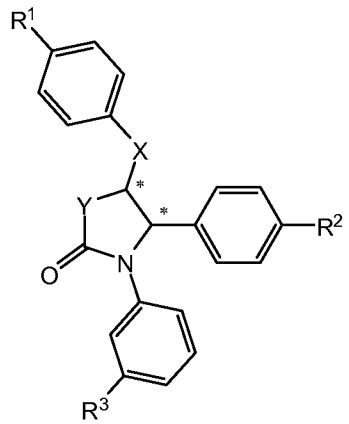
[0070] The neuraminidase inhibitor to be used to inhibit biofilm formation in the method of the invention can be any compound, small molecule, peptide, protein, aptamer, ribozyme, RNAi, or antisense oligonucleotide and the like.

[0071] For example, a neuraminidase inhibitor according to the invention can be a protein, such as an antibody (monoclonal, polyclonal, humanized, and the like), or a binding fragment thereof, directed against a neuraminidase protein, such as a viral, protozoan, fungal, or bacterial neuraminidase (such as *S. pneumoniae*, *H. influenzae,* or *V. cholerae*). An antibody fragment can be a form of an antibody other than the full-length form and includes portions or components that exist within full-length antibodies, in addition to antibody fragments that have been engineered. Antibody fragments can include, but are not limited to, single chain Fv (scFv), diabodies, Fv, and $(Fab')_2$, triabodies, Fc, Fab, CDR1, CDR2, CDR3, combinations of CDR's, variable regions, tetrabodies, bifunctional hybrid antibodies, framework regions, constant regions, and the like (*see,* Maynard et al., (2000) *Ann. Rev. Biomed. Eng.* 2:339-76; Hudson (1998) *Curr. Opin. Biotechnol.* 9:395-402). Antibodies can be obtained commercially, custom generated, or synthesized against an antigen of interest according to methods established in the art (Janeway et al., (2001) Immunobiology, 5th ed., Garland Publishing).

[0072] Additionally, a neuraminidase inhibitor can be a non-antibody peptide or polypeptide that binds to a bacterial neuraminidase. A peptide or polypeptide can be a portion of a protein molecule of interest other than the full-length form, and includes peptides that are smaller constituents that exist within the full-length amino acid sequence of a protein

molecule of interest. These peptides can be obtained commercially or synthesized via liquid phase or solid phase synthesis methods (Atherton et al., (1989) Solid Phase Peptide Synthesis: a Practical Approach. IRL Press, Oxford, England). For example, the neuraminidase inhibitor can be a peptide that interacts with a *Streptococcus* neuraminidase, such as the protein encoded by the NanA gene (*e.g.,* a protein comprising the amino acid sequence of SEQ ID NO:2). The peptide or protein-related neuraminidase inhibitors can be isolated from a natural source, genetically engineered or chemically prepared. These methods are well known in the art.

[0073] A neuraminidase inhibitor can also be a small molecule that binds to a neuraminidase and disrupts its function. Small molecules are a diverse group of synthetic and natural substances generally having low molecular weights. They are isolated from natural sources (for example, plants, fungi, microbes and the like), are obtained commercially and/or available as libraries or collections, or synthesized. Candidate neuramindase inhibitor small molecules can be identified via *in silico* screening or high-through-put (HTP) screening of combinatorial libraries. Most conventional pharmaceuticals, such as aspirin, penicillin, and many chemotherapeutics, are small molecules, can be obtained commercially, can be chemically synthesized, or can be obtained from random or combinatorial libraries as described below (Werner et al., (2006) *Brief Funct. Genomic Proteomic* 5(1):32-6). In one embodiment, the neuraminidase inhibitor is a compound of the Formula I:



(I)

wherein,

R^1 is H, halogen, cyano, azido, nitro, C_1-C_6 alkyl, or C_1-C_6 alkoxy;

R^2 is H, halogen, cyano, azido, nitro, C_1-C_6 alkyl, or C_1-C_6 alkoxy;

R^3 is H, $-CO_2R^4$ or $-CON(R^4)_2$;

each R^4 is, independently, H or C_1-C_6 alkyl;

X is $-CH_2-$, –(C=O)-, -(C=NH)-, -(C=N-O-C_1-C_6-alkyl)-, or –(C=S)-; and

Y is –(C=O)-, -(C=NH)-, -(C=N-O-C_1-C_6-alkyl)-, or –(C=S)-,

or a pharmaceutically acceptable salt or hydrate thereof.

[0074] In one embodiment, R^1 is a halogen. In a specific embodiment, R^1 is chlorine.

[0075] In one embodiment, R^2 is a C_1-C_6 alkoxy group. In specific embodiments, R^2 is methoxy or ethoxy. In a specific embodiment, R^2 is methoxy.

[0076] In one embodiment, R^3 is $-CONH_2$. In another embodiment, R^3 is $-CO_2H$.

[0077] In one embodiment, X is –(C=NH)-, –(C=NOH)-, –(C=NOMe)-, –(C=O)-, or –C(=S)-. In a specific embodiment, X is -(C=O)-.

[0078] In one embodiment, Y is –(C=NH)-, –(C=NOH)-, –(C=NOMe)-, –(C=O)-, or –C(=S)-. In a specific embodiment, Y is -(C=O)-.

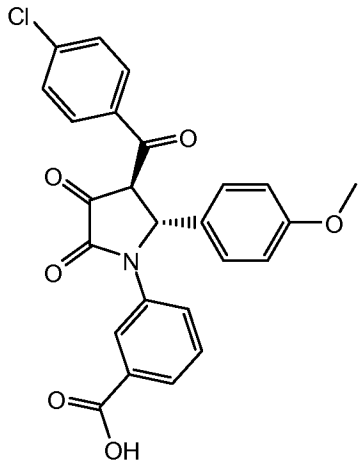
[0079] In one embodiment, R^1, R^2, and R^3 are not H.

[0080] Pharmaceutically acceptable salts are known in the art, and may be selected from those listed in Berge, et al. ["Pharmaceutical Salts," J. Pharm. Sci., 66(1):1-19 (Jan. 1977)]. In one embodiment, a pharmaceutically acceptable salt of a compound of Formula (I) is an acid addition salt, for example a hydrochloride, sulfate, or phosphate salt. In another embodiment, a pharmaceutically acceptable salt of a compound of Formula (I) is a base addition salt, for example a sodium, potassium, calcium, or ammonium salt. In another embodiment, the base addition salt is a tetrafluoroboro salt.

[0081] In one embodiment, a compound of Formula (I) is a zwitterion.

[0082] In one embodiment, the chiral centers marked by asterix in Formula (I) are both *R*.

[0083] In one embodiment, a Compound of Formula (I) is Compound A:

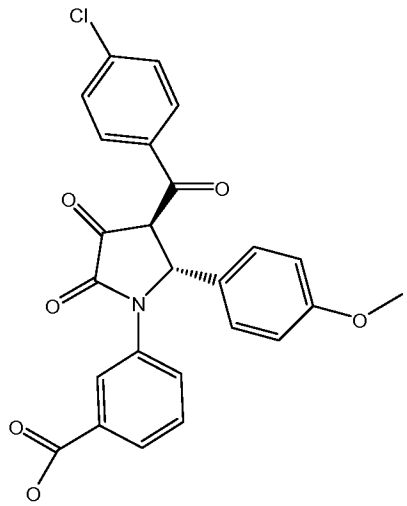


A,

or a pharmaceutically acceptable salt or hydrate thereof.

[0084] Compound A is alternatively known by the chemical name, 3-((2R,3R)-3-(4-chlorobenzoyl)-2-(4-methoxyphenyl)-4,5-dioxopyrrolidin-1-yl)benzoic acid.

[0085] In some embodiments, the neuraminidase inhibitor is a compound comprising Formula (X):



Formula (X)

[0086] In specific embodiments, the compound comprising Formula (X) is compound XX1 (see Examples 1 and 3, and **FIGS. 11** and **14**). The compound of XX1 is available from Schrödinger LLC, (Portland, OR, USA).

[0087] Compounds of Formula I can be made by methods known in the art, such as that in Scheme 1 (see **FIG. 15**).

[0088] Compounds of Formula I can be made by protecting a commercially-available benzyl maleate derivative, for example using the chlorobenzyl derivative to yield compound

3. Protecting group P^1 can be groups capable of forming an amide with amines, for examples esters such as methyl, or ethyl, or others suitable to accomplish the ring closure yielding compound 2. The ketones of resultant pyrrolidone derivative, e.g. 2, can be protected from the nucleophilic aromatic substitution reaction, for example as oxolanes, using standard techniques. Next, the benzoic acid group can be installed using nucleophilic aromatic substitution techniques on a suitably protected iodo-benzoic acid derivative. The nucleophilic aromatic substitution conditions can use an activating agent such as a metal cation complex as known in the art. Alternatively, the aromatic substitution can be accomplished with activated benzoic acid derivatives using a Stille coupling, a Suzuki cross-coupling, or a Buchwald-Hartwig cross-coupling. The substituent "X" is selected according to the coupling reaction conditions chosen. In one example of Stille conditions, X is SnR_3, such as $SnBu_3$. X can also be OTf, I, or $B(OR)_3$, where R is lower alkyl. The carboxylate and ketone groups can be protected before the nucleophilic aromatic substitution step as taught in Greene's Protective Groups in Organic Synthesis, 4th Ed. Wuts and Greene, Eds. Wiley, 2007, which is incorporated herein by reference in its entirety. The product compound, e.g. 3, can be achiral or racemic. If such is the case, the chiral version can be obtained by chiral HPLC purification using techniques known to one skilled in the art.

[0089] Standard protection and deprotection techniques are known to one skilled in the art, and taught in Greene's Protective Groups in Organic Synthesis, 4th Ed. Wuts and Greene, Eds. Wiley, 2007. Solvent and reaction conditions can be chosen as apparent to one skilled in the art in order to accomplish the depicted synthetic transformations. Such conditions can also be found in March, Advanced Organic Chemistry, 4th Ed. Wiley (1992) and references cited therein, which is incorporated herein by reference in its entirety.

[0090] Compounds of the invention may also tautomerize, for example, as shown in Scheme 2 (see **FIG. 16**).

[0091] According to this invention, the neuraminidase inhibitor can also be an FDA approved viral neuraminidase inhibitor, such as the viral neuraminidase inhibitor oseltamivir (Tamiflu), zanamivir (Relenza; Glaxo Smith Kline, Research Triangle Park, NC), peramivir (BioCryst, Birmingham, AL), or a variant thereof. For example, the viral neuraminidase inhibitor, oseltamivir is an ethyl ester prodrug that can be purchased from Roche Laboratories (Nutley, NJ). Amino acid sequences of FDA approved viral neuraminidase inhibitors can also be derivatized, for example, bearing modifications other than insertion, deletion, or substitution of amino acid residues, thus resulting in a variation of the original product (a variant). These modifications can be covalent in nature, and include for example, chemical

bonding with lipids, other organic moieties, inorganic moieties, and polymers. For reviews on viral neuraminidase inhibitors, please see Klumpp et al., (2006) *Curr. Top. Med. Chem.* 6(5):423-34; Zhang et al., (2006) *Mini Rev. Med. Chem.* 6(4):429-48; Jefferson et al., (2006) *Lancet* 367(9507):303-13; Alymova et al., (2005) *Curr Drug Targets Infect. Disord.* 5(4):401-9; Moscona (2005) *N. Engl. J. Med.* 353(13):1363-73; De Clercq (2004) *J. Clin. Virol.* 30(2):115-33; Stiver (2003) *CMAJ* 168(1):49-56; Oxford et al., (2003) *Expert Rev. Anti. Infect. Ther.* 1(2):337-42; Cheer et al., (2002) *Am. J. Respir. Med.* 1(2):147-52; Sidewell et al., (2002) *Expert Opin. Investig. Drugs.* 11(6):859-69; Doucette et al., (2001) *Expert Opin. Pharmacother.* 2(10):1671-83; Young et al., (2001) *Philos. Trans. R. Soc. Lond. B. Biol. Sci.* 356(1416):1905-13; Lew et al., (2000) *Curr. Med. Chem.* 7(6):663-72); Taylor et al., (1996) *Curr. Opin. Struct. Biol.* 1996 6(6):830-7; and U.S. Patent Appln. Nos. 20060057658 and 20040062801.

[0092] Inhibition of RNA can effectively inhibit expression of a gene from which the RNA is transcribed. Inhibitors are selected from the group comprising: siRNA, interfering RNA or RNAi; dsRNA; RNA Polymerase III transcribed DNAs; ribozymes; and antisense nucleic acid, which can be RNA, DNA, or artificial nucleic acid. Also within the scope of the present invention are oligonucleotide sequences that include antisense oligonucleotides and ribozymes that function to bind to, degrade and/or inhibit the translation of an mRNA encoding a neuraminidase, such as a bacterial neuraminidase.

[0093] Antisense oligonucleotides, including antisense DNA, RNA, and DNA/RNA molecules, act to directly block the translation of mRNA by binding to targeted mRNA and preventing protein translation. For example, antisense oligonucleotides of at least about 15 bases and complementary to unique regions of the DNA sequence encoding a neuraminidase polypeptide can be synthesized, e.g., by conventional phosphodiester techniques (Dallas et al., (2006) *Med. Sci. Monit.*12(4):RA67-74; Kalota et al., (2006) *Handb. Exp. Pharmacol.* 173:173-96; Lutzelburger et al., (2006) *Handb. Exp. Pharmacol.* 173:243-59).

[0094] siRNA comprises a double stranded structure containing 15 to 50 base pairs, and having a nucleotide sequence identical or nearly identical to an expressed target gene or RNA within the cell. In one embodiment, an siRNA comprises a double stranded structure containing 21 to 25 base pairs. Antisense polynucleotides include, but are not limited to: morpholinos, 2'-O-methyl polynucleotides, DNA, RNA and the like. RNA polymerase III transcribed DNAs contain promoters, such as the U6 promoter. These DNAs can be transcribed to produce small hairpin RNAs in the cell that can function as siRNA or linear RNAs that can function as antisense RNA. The inhibitor can be polymerized in vitro,

recombinant RNA, contain chimeric sequences, or derivatives of these groups. The inhibitor can contain ribonucleotides, deoxyribonucleotides, synthetic nucleotides, or any suitable combination such that the target RNA and/or gene is inhibited. In addition, these forms of nucleic acid can be single, double, triple, or quadruple stranded. (see for example Bass (2001) *Nature*, 411, 428 429; Elbashir et al., (2001) *Nature*, 411, 494 498; and PCT Publication Nos. WO 00/44895, WO 01/36646, WO 99/32619, WO 00/01846, WO 01/29058, WO 99/07409, WO 00/44914).

[0095] Ribozymes are enzymatic RNA molecules that catalyze the specific cleavage of RNA. The mechanism of ribozyme action involves sequence specific hybridization of the ribozyme molecule to complementary target RNA encoding the neuraminidase, followed by endonucleolytic cleavage. Engineered hammerhead motif ribozyme molecules that specifically and efficiently catalyze endonucleolytic cleavage of mRNA sequences encoding a neuraminidase inhibitor, such as a bacterial neuraminidase inhibitor, are also within the scope of the present invention. Scanning the target molecule for ribozyme cleavage sites that include the following sequences, GUA, GUU, and GUC initially identifies specific ribozyme cleavage sites within any potential RNA target. Once identified, short RNA sequences of between about 15 and 20 ribonucleotides corresponding to the region of the target gene containing the cleavage site can be evaluated for predicted structural features such as secondary structure that can render the oligonucleotide sequence unsuitable. The suitability of candidate targets can also be evaluated by testing their accessibility to hybridization with complementary oligonucleotides using, e.g., ribonuclease protection assays.

[0096] Both the antisense oligonucleotides and ribozymes of the present invention can be prepared by known methods. These include techniques for chemical synthesis such as, e.g., by solid phase phosphoamite chemical synthesis. Alternatively, antisense RNA molecules can be generated by in vitro or in vivo transcription of DNA sequences encoding the RNA molecule. Such DNA sequences can be incorporated into a wide variety of vectors that incorporate suitable RNA polymerase promoters such as the T7 or SP6 polymerase promoters.

[0097] Various modifications to the oligonucleotides of the present invention can be introduced as a means of increasing intracellular stability and half-life. Possible modifications include but are not limited to the addition of flanking sequences of ribonucleotides or deoxyribonucleotides to the 5′ and/or 3′ ends of the molecule, or the use of phosphorothioate or 2′-O-methyl rather than phosphodiesterase linkages within the oligonucleotide backbone.

[0098] An aptamer can be nucleic acid ligand that, through its ability to adopt a specific three-dimensional conformation, binds to and has an antagonizing (*i.e.,* inhibitory) effect on a target. The target of the present invention is neuraminidase, and hence the term neuraminidase aptamer or nucleic acid ligand or neuraminidase aptamer or nucleic acid ligand is used. Inhibition of the target by the aptamer can occur by binding of the target, by catalytically altering the target, by reacting with the target in a way which modifies/alters the target or the functional activity of the target, by covalently attaching to the target as in a suicide inhibitor, by facilitating the reaction between the target and another molecule. Aptamers can be comprised of multiple ribonucleotide units, deoxyribonucleotide units, or a mixture of both types of nucleotide residues. Aptamers can further comprise one or more modified bases, sugars or phosphate backbone units as described in further detail herein.

[0099] Aptamers nucleic acid sequences are readily made that bind to a wide variety of target molecules. The aptamer nucleic acid sequences of the invention can be comprised entirely of RNA or partially of RNA, or entirely or partially of DNA and/or other nucleotide analogs. Aptamers are developed to bind particular ligands by employing known *in vivo* or *in vitro* (more often, *in vitro*) selection techniques known as SELEX (Systematic Evolution of Ligands by Exponential Enrichment). Methods of making aptamers are described in, for example, Ellington and Szostak (1990) *Nature* 346:818, Tuerk and Gold (1990) *Science* 249:505, U.S. Patent No. 5,582,981; PCT Publication No. WO 00/20040; U.S. Patent No. 5,270,163; Lorsch and Szostak (1994) *Biochem.* 33:973; Mannironi *et al.*, (1997) *Biochem.* 36:9726; Blind (1999) *Proc. Nat'l. Acad. Sci. USA* 96:3606-3610; Huizenga and Szostak (1995) *Biochem.* 34:656-665; PCT Publication Nos. WO 99/54506, WO 99/27133, and WO 97/42317; and U.S. Patent No. 5,756,291.

[00100] Generally, in their most basic form, *in vitro* selection techniques for identifying RNA aptamers involve first preparing a large pool of DNA molecules of the desired length that contain at least some region that is randomized or mutagenized. For instance, a common oligonucleotide pool for aptamer selection can contain a region of 20-100 randomized nucleotides flanked on both ends by an about 15-25 nucleotide long region of defined sequence useful for the binding of PCR primers. The oligonucleotide pool is amplified using standard PCR techniques. The DNA pool is then transcribed *in vitro*. The RNA transcripts are then subjected to affinity chromatography. The transcripts are passed through a column or contacted with magnetic beads or the like on which the target ligand has been immobilized. RNA molecules in the pool, which bind to the ligand, are retained on the column or bead, while nonbinding sequences are washed away. The RNA molecules, which bind the ligand,

are then reverse transcribed and amplified again by PCR (usually after elution). The selected pool sequences are then put through another round of the same type of selection. The pool sequences are put through a total of about three to ten iterative rounds of the selection procedure. The cDNA is then amplified, cloned, and sequenced using standard procedures to identify the sequence of the RNA molecules that act as aptamers for the target ligand.

[00101] One can generally choose a suitable ligand without reference to whether an aptamer is yet available. In most cases, an aptamer can be obtained which binds the small, organic molecule of choice by someone of ordinary skill in the art. The unique nature of the *in vitro* selection process allows for the isolation of a suitable aptamer that binds a desired ligand despite a complete dearth of prior knowledge as to what type of structure can bind the desired ligand.

[00102] The association constant for the aptamer and associated ligand is, for example, such that the ligand functions to bind to the aptamer and have the desired effect at the concentration of ligand obtained upon administration of the ligand. For *in vivo* use, for example, the association constant should be such that binding occurs below the concentration of ligand that can be achieved in the serum or other tissue (such as ocular vitreous fluid). For example, the required ligand concentration for *in vivo* use can have undesired effects on the organism.

[00103] The aptamer nucleic acid sequences, in addition to including RNA, DNA and mixed compositions, can be modified. For example, certain modified nucleotides can confer improved characteristic on high-affinity nucleic acid ligands containing them, such as improved *in vivo* stability or improved delivery characteristics. Examples of such modifications include chemical substitutions at the ribose and/or phosphate and/or base positions. SELEX-identified nucleic acid ligands containing modified nucleotides are described in U.S. Patent No. 5,660,985, entitled "High Affinity Nucleic Acid Ligands Containing Modified Nucleotides," that describes oligonucleotides containing nucleotide derivatives chemically modified at the 5- and 2'-positions of pyrimidines. U.S. Patent No. 5,637,459, supra, describes highly specific nucleic acid ligands containing one or more nucleotides modified with 2'-amino (2'-NH.sub.2), 2'-fluoro (2'-F), and/or 2'-O-methyl (2'-OMe). U.S. Appln. Ser. No. 08/264,029, filed Jun. 22, 1994, entitled "Novel Method of Preparation of Known and Novel 2' Modified Nucleosides by Intramolecular Nucleophilic Displacement," describes oligonucleotides containing various 2'-modified pyrimidines.

[00104] The aptamer nucleic acid sequences of the invention further can be combined with other selected oligonucleotides and/or non-oligonucleotide functional units as described

in U.S. Patent No. 5,637,459, entitled "Systematic Evolution of Ligands by Exponential Enrichment: Chimeric SELEX," and U.S. Patent No. 5,683,867, entitled "Systematic Evolution of Ligands by Exponential Enrichment: Blended SELEX," respectively.

[00105] Diversity libraries, such as random or combinatorial peptide or non-peptide libraries can be screened for small molecules and compounds that specifically bind to a bacterial, viral, yeast, or protozoan neuraminidase. Many libraries are known in the art that can be used such as, e.g., chemically synthesized libraries, recombinant (e.g., phage display) libraries, and *in vitro* translation-based libraries.

[00106] Any screening technique known in the art can be used to screen for agonist or antagonist molecules (such as neuraminidase inhibitors) directed at a target of interest (e.g. a neuraminidase, such as a bacterial neuraminidase). The present invention encompasses screens for small molecule ligands or ligand analogs and mimics, as well as screens for natural ligands that bind to and antagonize neuraminidase inhibitors, such as via examining the degree of biofilm inhibition utilizing previously described biofilm assays. For example, natural products libraries can be screened using assays of the invention for molecules that agonize or antagonize the activity of a molecule of interest, such as a neuraminidase.

[00107] Knowledge of the primary sequence of a molecule of interest, such as a neuraminidase inhibitor, and the similarity of that sequence with proteins of known function (e.g., a viral neuraminidase inhibitor such as Tamiflu), can provide an initial clue as the inhibitors or antagonists of the protein. Identification and screening of antagonists is further facilitated by determining structural features of the protein, e.g., using X-ray crystallography, neutron diffraction, nuclear magnetic resonance spectrometry, and other techniques for structure determination. These techniques provide for the rational design or identification of agonists and antagonists.

[00108] Test compounds, such as test neuraminidase inhibitors, are screened from large libraries of synthetic or natural compounds. Numerous means are currently used for random and directed synthesis of saccharide, peptide, and nucleic acid based compounds. Synthetic compound libraries are commercially available from Maybridge Chemical Co. (Trevillet, Cornwall, UK), Comgenex (Princeton, N.J.), Brandon Associates (Merrimack, N.H.), and Microsource (New Milford, Conn.). A rare chemical library is available from Aldrich (Milwaukee, Wis.). Alternatively, libraries of natural compounds in the form of bacterial, fungal, plant and animal extracts are available from e.g. Pan Laboratories (Bothell, Wash.) or MycoSearch (N.C.), or are readily producible. Additionally, natural and synthetically

produced libraries and compounds are readily modified through conventional chemical, physical, and biochemical means (Blondelle et al., (1996) *Tib Tech* 14:60).

[00109] Methods for preparing libraries of molecules are well known in the art and many libraries are commercially available. Libraries of interest in the invention include peptide libraries, randomized oligonucleotide libraries, synthetic organic combinatorial libraries, and the like. Degenerate peptide libraries can be readily prepared in solution, in immobilized form as bacterial flagella peptide display libraries or as phage display libraries. Peptide ligands can be selected from combinatorial libraries of peptides containing at least one amino acid. Libraries can be synthesized of peptoids and non-peptide synthetic moieties. Such libraries can further be synthesized which contain non-peptide synthetic moieties, which are less subject to enzymatic degradation compared to their naturally-occurring counterparts. Libraries are also meant to include for example but are not limited to peptide-on-plasmid libraries, polysome libraries, aptamer libraries, synthetic peptide libraries, synthetic small molecule libraries and chemical libraries. The libraries can also comprise cyclic carbon or heterocyclic structure and/or aromatic or polyaromatic structures substituted with one or more of the above-identified functional groups. Screening compound libraries listed above [also see EXAMPLES 1 and 2, and U.S. Patent Application Publication No. 2005/0009163, which is hereby incorporated by reference], in combination with biofilm assays described below (such as the one depicted in EXAMPLE 1) can be used to identify neuraminidase inhibitors that disrupt the formation of a biofilm (Lew et al., (2000) *Curr. Med. Chem.* 7(6):663-72; Werner et al., (2006) *Brief Funct. Genomic Proteomic* 5(1):32-6).

[00110] Small molecule combinatorial libraries can also be generated. A combinatorial library of small organic compounds is a collection of closely related analogs that differ from each other in one or more points of diversity and are synthesized by organic techniques using multi-step processes. Combinatorial libraries include a vast number of small organic compounds. One type of combinatorial library is prepared by means of parallel synthesis methods to produce a compound array. A compound array can be a collection of compounds identifiable by their spatial addresses in Cartesian coordinates and arranged such that each compound has a common molecular core and one or more variable structural diversity elements. The compounds in such a compound array are produced in parallel in separate reaction vessels, with each compound identified and tracked by its spatial address. Examples of parallel synthesis mixtures and parallel synthesis methods are provided in U.S. Ser. No. 08/177,497, filed Jan. 5, 1994 and its corresponding PCT published patent application W095/18972, published Jul. 13, 1995 and U.S. Pat. No. 5,712,171 granted Jan. 27, 1998 and

its corresponding PCT published patent application W096/22529, which are hereby incorporated by reference.

[00111] Examples of chemically synthesized libraries are described in Fodor et al., (1991) *Science* 251:767-773; Houghten et al., (1991) *Nature* 354:84-86; Lam et al., (1991) *Nature* 354:82-84; Medynski, (1994) *BioTechnology* 12:709-710; Gallop et al., (1994) *J. Medicinal Chemistry* 37(9):1233-1251; Ohlmeyer et al., (1993) *Proc. Natl. Acad. Sci. USA* 90:10922-10926; Erb et al., (1994) *Proc. Natl. Acad. Sci. USA* 91:11422-11426; Houghten et al., (1992) *Biotechniques* 13:412; Jayawickreme et al., (1994) *Proc. Natl. Acad. Sci. USA* 91:1614-1618; Salmon et al., (1993) *Proc. Natl. Acad. Sci. USA* 90:11708-11712; PCT Publication No. WO 93/20242, dated Oct. 14, 1993; and Brenner et al., (1992) *Proc. Natl. Acad. Sci. USA* 89:5381-5383.

[00112] Examples of phage display libraries are described in Scott et al., (1990) *Science* 249:386-390; Devlin et al., (1990) *Science*, 249:404-406; Christian, et al., (1992) *J. Mol. Biol.* 227:711-718; Lenstra, (1992) *J. Immunol. Meth.* 152:149-157; Kay et al., (1993) *Gene* 128:59-65; and PCT Publication No. WO 94/18318.

[00113] *In vitro* translation-based libraries include but are not limited to those described in PCT Publication No. WO 91/05058; and Mattheakis et al., (1994) *Proc. Natl. Acad. Sci. USA* 91:9022-9026.

[00114] In one non-limiting example, non-peptide libraries, such as a benzodiazepine library (see e.g., Bunin et al., (1994) *Proc. Natl. Acad. Sci. USA* 91:4708-4712), can be screened. Peptoid libraries, such as that described by Simon et al., (1992) *Proc. Natl. Acad. Sci. USA* 89:9367-9371, can also be used. Another example of a library that can be used, in which the amide functionalities in peptides have been permethylated to generate a chemically transformed combinatorial library, is described by Ostresh et al. (1994), *Proc. Natl. Acad. Sci. USA* 91:11138-11142.

[00115] Screening the libraries can be accomplished by any variety of commonly known methods. See, for example, the following references, which disclose screening of peptide libraries: Parmley and Smith, (1989) *Adv. Exp. Med. Biol.* 251:215-218; Scott and Smith, (1990) *Science* 249:386-390; Fowlkes et al., (1992) *BioTechniques* 13:422-427; Oldenburg et al., (1992) *Proc. Natl. Acad. Sci. USA* 89:5393-5397; Yu et al., (1994) *Cell* 76:933-945; Staudt et al., (1988) *Science* 241:577-580; Bock et al., (1992) *Nature* 355:564-566; Tuerk et al., (1992) *Proc. Natl. Acad. Sci. USA* 89:6988-6992; Ellington et al., (1992) *Nature* 355:850-852; U.S. Patent Nos. 5,096,815; 5,223,409; and 5,198,346, all to Ladner et al.; Rebar et al., (1994) *Science* 263:671-673; and PCT Pub. WO 94/18318. Screening methods of the

invention utilizing, for example, the libraries described above, can allow for the identification of candidate neuraminidase inhibitors.

[00116] One of skill in the art will be familiar with methods for predicting the effect on protein conformation of a change in protein sequence, and can thus "design" a variant which functions as an antagonist according to known methods. One example of such a method is described by Dahiyat and Mayo in *Science* (1997) 278:82 87, which describes the design of proteins *de novo*. The method can be applied to a known protein to vary only a portion of the polypeptide sequence. By applying the computational methods of Dahiyat and Mayo, specific variants of neuraminidase inhibitors confined to regions which bind the active site of a neuraminidase (such as bacterial neuraminidase) can be proposed and tested to determine whether the variant retains a desired conformation. Similarly, Blake (U.S. Pat. No. 5,565,325) teaches the use of known ligand structures to predict and synthesize variants with similar or modified function.

[00117] Other methods for preparing or identifying peptides that bind to a particular target are known in the art. Molecular imprinting, for instance, can be used for the de novo construction of macromolecular structures such as peptides that bind to a particular molecule. See, for example, Kenneth J. Shea, Molecular Imprinting of Synthetic Network Polymers: The De Novo synthesis of Macromolecular Binding and Catalytic Sites, TRIP Vol. 2, No. 5, May 1994; Mosbach, (1994) *Trends in Biochem. Sci.*, 19(9); and Wulff, G., in Polymeric Reagents and Catalysts (Ford, W. T., Ed.) ACS Symposium Series No. 308, pp 186-230, American Chemical Society (1986). One method for preparing mimics of neuraminidase inhibitors involves the steps of: (i) polymerization of functional monomers around a known substrate (the template or in this case, the neuraminidase active domain) that exhibits a desired activity; (ii) removal of the template molecule; and then (iii) polymerization of a second class of monomers in, the void left by the template, to provide a new molecule which exhibits one or more desired properties which are similar to that of the template. In addition to preparing peptides in this manner other binding molecules such as polysaccharides, nucleosides, drugs, nucleoproteins, lipoproteins, carbohydrates, glycoproteins, steroids, lipids, and other biologically active materials can also be prepared. This method is useful for designing a wide variety of biological mimics that are more stable than their natural counterparts, because they are prepared by the free radical polymerization of functional monomers, resulting in a compound with a nonbiodegradable backbone. Other methods for designing such molecules include for example drug design based on structure activity

relationships, which require the synthesis and evaluation of a number of compounds and molecular modeling.

[00118] A neuraminidase inhibitor according to the method of the invention modulates the activity of a neuraminidase via either reducing the activity of the neuraminidase in the biofilm after the neuraminidase inhibitor is applied, thus inhibiting formation of the biofilm. For example, a reduction in the formation of the biofilm can be measured by looking at a decrease in the surface area covered by the biofilm, thickness, or consistency (such as the integrity of the biofilm).

[00119] An inhibition or reduction in a biofilm via treatment with a neuraminidase inhibitor composition (such as a bacterial neuraminidase inhibitor) can be measured via techniques established in the art. These techniques enable one to assess bacterial attachment via measuring the staining of the adherent biomass, to view microbes *in vivo* via microscopy methods; or to monitor cell death in the biomass in response to toxic agents. The biofilm can be reduced with respect to the surface area covered by the biofilm, thickness, and consistency (for example, the integrity of the biofilm). Non-limiting examples of biofilm assays include microtiter plate biofilm assays, fluorescence-based biofilm assays, static biofilm assays according to Walker et al., ((2005) *Infect. Immun.* 73(6): 3693–3701), Air-liquid interface assays, colony biofilm assays, and Kadouri Drip-Fed Biofilm assays (Merritt et al., (2005) Current Protocols in Microbiology 1.B.1.1-1.B.1.17). Biofilms (such as their morphology, thickness, and the like) also can be analyzed via confocal microscopy methods (Walker et al., (2005) *Infect. Immun.* 73(6): 3693–3701). Thus, these biofilm assays (such as the one depicted in EXAMPLE 1) in combination with screening compound libraries as described above can be used to identify neuraminidase inhibitors that disrupt the formation of a biofilm (Lew et al., (2000) *Curr. Med. Chem.* 7(6):663-72; Werner et al., (2006) *Brief Funct. Genomic Proteomic* 5(1):32-6).

[00120] A reduction in a biofilm indicates that the neuraminidase inhibitor, inhibited formation of the biofilm as determined by observing that the inhibitor modulated the activity or the expression of the neuraminidase protein, because biofilms are comprised of various microorganisms, thus a neuraminidase inhibitor according to the method of the present invention can inhibit such microorganisms from producing a biofilm. Thus, the formation of biofilm by, *e.g.,* of Gram-negative bacteria, Gram-positive bacteria, or a combination thereof, can be inhibited.

[00121] Application of a neuraminidase inhibitor to a biofilm can be accomplished by any means such as spraying it onto the biofilm, infusing it into the biofilming, or pipetting into the depth of the biofilm, and the like (e.g., as shown in EXAMPLE 1).

[00122] If the neuraminidase inhibitor is to be administered to a subject, it will be in the form of a pharmaceutically acceptable composition or formulation as described below, wherein the composition or formulation is free of toxicity, which satisfies FDA requirements (see Remington: The Science and Practice of Pharmacy, 20th ed., Lippincott Williams & Wilkins, 2000; U.S. Patent No. 6030604). Such a neuraminidase inhibitor composition, comprising compounds or pharmaceutically acceptable salts, can be administered to a subject harboring a biofilm or is at risk of developing a biofilm (for example patient has undergone surgery, implantation, and the like) or is afflicted with a biofilm production-related disorder (discussed below). Administration can occur alone or with other therapeutically effective composition(s) (e.g., antibiotics) either simultaneously or at different times.

[00123] Formulations can include those suitable for oral, nasal, topical (including buccal and sublingual), rectal, vaginal and/or parenteral administration. The formulations can conveniently be presented in unit dosage form and can be prepared by any methods well known in the art of pharmacy. The amount of active ingredient which can be combined with a carrier material to produce a single dosage form will vary depending upon the host being treated, the mode of administration. The amount of active ingredient, which can be combined with a carrier material to produce a single dosage form, will generally be that amount of the compound that produces a therapeutic effect. Generally, out of one hundred percent, this amount will range from about 1 percent to about ninety-nine percent of active ingredient, for example, from about 5% to about 70%, or from about 10% to about 30%.

[00124] Methods of preparing these formulations or compositions include the step of bringing into association a compound of the present invention with the carrier and, optionally, one or more accessory ingredients. In general, the formulations are prepared by uniformly and intimately bringing into association a compound of the present invention with liquid carriers, or finely divided solid carriers, or both, and then, if necessary, shaping the product.

[00125] Formulations of the invention suitable for oral administration can be in the form of capsules, cachets, pills, tablets, lozenges (using a flavored basis, usually sucrose and acacia or tragacanth), powders, granules, or as a solution or a suspension in an aqueous or non-aqueous liquid, or as an oil-in-water or water-in-oil liquid emulsion, or as an elixir or syrup, or as pastilles (using an inert base, such as gelatin and glycerin, or sucrose and acacia) and/or

as mouth washes and the like, each containing a predetermined amount of a compound of the present invention as an active ingredient. A compound of the present invention can also be administered as a bolus, electuary or paste.

[00126] In solid dosage forms of the invention for oral administration (capsules, tablets, pills, dragees, powders, granules and the like), the active ingredient is mixed with one or more pharmaceutically acceptable carriers, such as sodium citrate or dicalcium phosphate, and/or any of the following: (1) fillers or extenders, such as starches, lactose, sucrose, glucose, mannitol, and/or silicic acid; (2) binders, such as, for example, carboxymethylcellulose, alginates, gelatin, polyvinyl pyrrolidone, sucrose and/or acacia; (3) humectants, such as glycerol; (4) disintegrating agents, such as agar-agar, calcium carbonate, potato or tapioca starch, alginic acid, certain silicates, and sodium carbonate; (5) solution retarding agents, such as paraffin; (6) absorption accelerators, such as quaternary ammonium compounds; (7) wetting agents, such as, for example, cetyl alcohol and glycerol monostearate; (8) absorbents, such as kaolin and bentonite clay; (9) lubricants, such a talc, calcium stearate, magnesium stearate, solid polyethylene glycols, sodium lauryl sulfate, and mixtures thereof; and (10) coloring agents. In the case of capsules, tablets and pills, the pharmaceutical compositions can also comprise buffering agents. Solid compositions of a similar type can also be employed as fillers in soft and hard-filled gelatin capsules using such excipients as lactose or milk sugars, as well as high molecular weight polyethylene glycols and the like.

[00127] A tablet can be made by compression or molding, optionally with one or more accessory ingredients. Compressed tablets can be prepared using binder (for example, gelatin or hydroxypropylmethyl cellulose), lubricant, inert diluent, preservative, disintegrant (for example, sodium starch glycolate or cross-linked sodium carboxymethyl cellulose), surface-active or dispersing agent. Molded tablets can be made by molding in a suitable machine a mixture of the powdered compound moistened with an inert liquid diluent.

[00128] The tablets, and other solid dosage forms of the pharmaceutical compositions of the present invention, such as dragees, capsules, pills and granules, can optionally be scored or prepared with coatings and shells, such as enteric coatings and other coatings well known in the pharmaceutical-formulating art. They can also be formulated so as to provide slow or controlled release of the active ingredient therein using, for example, hydroxypropylmethyl cellulose in varying proportions to provide the desired release profile, other polymer matrices, liposomes and/or microspheres. They can be sterilized by, for example, filtration through a bacteria-retaining filter, or by incorporating sterilizing agents in the form of sterile

solid compositions which can be dissolved in sterile water, or some other sterile injectable medium immediately before use. These compositions can also optionally contain opacifying agents and can be of a composition that they release the active ingredient(s) only, or, in a certain portion of the gastrointestinal tract, optionally, in a delayed manner. Examples of embedding compositions which can be used include polymeric substances and waxes. The active ingredient can also be in micro-encapsulated form, if appropriate, with one or more of the above-described excipients.

[00129] Liquid dosage forms for oral administration of the compounds of the invention include pharmaceutically acceptable emulsions, microemulsions, solutions, suspensions, syrups and elixirs. In addition to the active ingredient, the liquid dosage forms can contain inert diluents commonly used in the art, such as, for example, water or other solvents, solubilizing agents and emulsifiers, such as ethyl alcohol, isopropyl alcohol, ethyl carbonate, ethyl acetate, benzyl alcohol, benzyl benzoate, propylene glycol, 1,3-butylene glycol, oils (for example, cottonseed, groundnut, corn, germ, olive, castor and sesame oils), glycerol, tetrahydrofuryl alcohol, polyethylene glycols and fatty acid esters of sorbitan, and mixtures thereof.

[00130] Besides inert diluents, the oral compositions can also include adjuvants such as wetting agents, emulsifying and suspending agents, sweetening, flavoring, coloring, perfuming and preservative agents.

[00131] Suspensions, in addition to the active compounds, can contain suspending agents as, for example, ethoxylated isostearyl alcohols, polyoxyethylene sorbitol and sorbitan esters, microcrystalline cellulose, aluminum metahydroxide, bentonite, agar-agar and tragacanth, and mixtures thereof.

[00132] The neuraminidase inhibitor composition can optionally comprise a suitable amount of a physiologically acceptable excipient. Non-limiting examples of physiologically acceptable excipients can be liquids, such as water and oils, including those of petroleum, animal, vegetable, or synthetic origin, such as peanut oil, soybean oil, mineral oil, sesame oil and the like; saline; gum acacia; gelatin; starch paste; talc; keratin; colloidal silica; urea and the like. In addition, auxiliary, stabilizing, thickening, lubricating, and coloring agents can be used. For example, the neuraminidase inhibitor composition and physiologically acceptable excipient are sterile when administered to a subject (such as an animal; for example a human). The physiologically acceptable excipient should be stable under the conditions of manufacture and storage and should be preserved against the contaminating action of microorganisms.

[00133] Water is a useful excipient when the compound or a pharmaceutically acceptable salt of the compound is administered intravenously. Saline solutions and aqueous dextrose and glycerol solutions can also be employed as liquid excipients, e.g., for injectable solutions. Suitable physiologically acceptable excipients also include starch, glucose, lactose, sucrose, gelatin, malt, rice, flour, chalk, silica gel, sodium stearate, glycerol monostearate, talc, sodium chloride, dried skim milk, glycerol, propylene, glycol, water, ethanol and the like. The present compositions, if desired, can also contain minor amounts of wetting or emulsifying agents, or pH buffering agents.

[00134] The neuraminidase inhibitor composition can be administered to the subject by any effective route, for example, orally, by infusion or bolus injection, by absorption through epithelial or mucocutaneous linings (*e.g.*, oral, rectal, vaginal, and intestinal mucosa, etc.), intradermal, intramuscular, intraperitoneal, intravenous, subcutaneous, infusion, intranasal, epidural, oral, sublingual, intracerebral, intravaginal, transdermal, rectal, by inhalation, or topical, e.g., to the ears, nose, eyes, or skin.

[00135] Pulmonary administration can also be employed, *e.g.*, by use of an inhaler or nebulizer, and formulation with an aerosolizing agent, or via perfusion in a fluorocarbon or synthetic pulmonary surfactant. For example, the neuraminidase inhibitor composition can be formulated as a suppository, with traditional binders and excipients such as triglycerides. Various known delivery systems, including encapsulation in liposomes, microparticles, microcapsules, and capsules, can be used. Thus, the neuraminidase inhibitor composition can be delivered in a vesicle, such as a liposome (see, *e.g.,* Langer (1990) *Science* 249:1527-1533; Treat *et al.*, *Liposomes in the Therapy of Infectious Disease and Cancer* 317-327 and 353-365 (1989)).

[00136] The neuraminidase inhibitor composition also can be delivered in a controlled-release system or sustained-release system (*see*, *e.g.*, Goodson, in *Medical Applications of Controlled Release*, vol. 2, pp. 115-138 (1984)). Other controlled or sustained-release systems previously discussed can be used as well (Langer (1990) *Science* 249:1527-1533). For example, a pump can be used (Langer (1990) *Science* 249:1527-1533; Sefton (1987) *CRC Crit. Ref. Biomed. Eng.* 14:201; Buchwald *et al.*, (1980) *Surgery* 88:507; and Saudek *et al.*, (1989) *N. Engl. J Med.* 321:574); or polymeric materials can be used (see Langer and Wise (1985) Medical Applications of Controlled Release; CRC Press Inc.,U.S.; Smolen and Ball (1984) Controlled Drug Bioavailability, Drug Product Design and Performance; Ranger and Peppas, (1983) *J. Macromol. Sci. Rev. Macromol. Chem.* 2:61; Levy *et al.*, (1985) *Science* 228:190; During *et al.*, (1989) *Ann. Neural.* 25:351; and Howard *et al.*, (1989) *J.*

Neurosurg. 71:105). The controlled- or sustained-release systems can be placed in proximity of a target of the compound or a pharmaceutically acceptable salt of the compound, *e.g.*, the respiratory tract, thus requiring only a fraction of the systemic dose.

[00137] Modulation of neuraminidase activity can also result in the reduction or prevention of the formation of a biofilm on semi-solid and solid surfaces. For example, these surfaces can be the surface of implanted and/or inserted devices (a medical device, a catheter, an infusion set of an insulin pump, a stent, a prosthetic graft); a wound dressing; the oral cavity; the alimentary or vaginal tracts; the ears or eyes; a contact lens, in addition to the cases or containers that hold the lenses when not in use; industrial equipment, or plumbing systems.

[00138] Additionally, a neuraminidase inhibitor according to the method of the invention can be applied to a surface of a contact lens or an implantable/insertable device and other surgical or medical devices (such as a medical device, a catheter, the infusion set of an insulin pump, a stent, a prosthetic graft, a wound dressing) or a wound site via covering, coating, contacting, associating with, filling, or loading the device with a therapeutic amount of a neuraminidase inhibitor in any known manner including, but not limited to the following: (1) directly affixing to the implant, device, or wound site a therapeutic agent or composition of the neuraminidase inhibitor (for example, by either spraying the implant or device with a polymer/ neuraminidase inhibitor film, or by dipping the implant or device into a polymer/ neuraminidase inhibitor solution, or by other covalent or noncovalent means); (2) coating the implant, wound site, or device with a substance, (such as a hydrogel) that will in turn absorb the therapeutic neuraminidase inhibitor composition; (3) interweaving a therapeutic neuraminidase inhibitor composition coated thread (or the polymer itself formed into a thread) into the implant or device or wound site; (4) inserting the implant or device into a sleeve or mesh which is comprised of or coated with a therapeutic neuraminidase inhibitor composition; (5) constructing the implant or device itself with a therapeutic neuraminidase inhibitor composition (or with respect to a wound site, constructing the wound dressing with a therapeutic neuraminidase inhibitor composition; or (6) adapting the implant or device or wound dressing to release the therapeutic neuraminidase inhibitor composition. Specific disease conditions (for example, cystic fibrosis, pneumonia, and the like as described below) that are bacteria-based can also benefit from a treatment that modulates the activity of an enzyme involved in biofilm formation (for example, treatment with a neuraminidase inhibitor).

[00139] For example, application of a neuraminidase inhibitor onto the surface of implanted and/or inserted devices (as described above) in order to reduce or prevent bacterial biofilm formation thus allows for long-term implantation and can diminish the resultant likelihood of premature failure of the device due to encrustation and occlusion by such biofilm. The amount of the neuraminidase inhibitor present in a coating, spray, film, and the like (as described above) applied to the surfaces in order to prevent the formation of a bacterial biofilm is an amount effective to inhibit the attachment of microbes onto the surface and/or the synthesis and/or accumulation of biofilm by attached microbes on such a surface.

[00140] Methods of the invention can further protect a subject from premature failure of an insertable or implantable device due to encrustation and occlusion by a bacterial biofilm. According to this method, the subject is administered a therapeutically effective amount of the neuraminidase inhibitor of the invention prior to, at the same time, or after an insertable or implantable device is introduced. An effective amount of a neuraminidase inhibitor can refer to the amount of a therapy which is sufficient to reduce or ameliorate the severity and/or duration of a disorder or one or more symptoms thereof, prevent the advancement of a disorder, cause regression of a disorder, prevent the recurrence, development, onset or progression of one or more symptoms associated with a disorder, detect a disorder, or enhance or improve the prophylactic or therapeutic effect(s) of another therapy (e.g., prophylactic or therapeutic agent).

[00141] The subject is administered the neuraminidase inhibitor that prevents formation of a bacterial biofilm prior to, at the same time, or after the introduction of the implantable/insertable device. Treatment before or after implantation can take place immediately before or after the implantation or several hours before or after implantation, or at a time or times that the skilled physician deems appropriate. According to the present invention, a subject containing a wound site in addition to those subjects receiving implants can harbor a biofilm. For example, a neuraminidase inhibitor can be administered to the subject prior to, during, or after implantation/insertion of a medical device, catheter, stent, prosthesis, and the like or application of a wound dressing. The neuraminidase inhibitor can be administered to the subject according to routes previously described and can further aid in inhibiting biofilm formation on a surface an/or within a subject.

[00142] In the case of the oral cavity, the alimentary or vaginal tracts, the ears or eyes, or a contact lens, a therapeutic amount of a neuraminidase inhibitor can be applied via coating, contacting, associating with, filling, or loading the region with a formulation comprising a paste, gel, liquid, powder, tablet, and the like. With respect to the cases or containers that

hold the lenses when not in use, industrial equipment, or plumbing systems, an effective amount of a neuraminidase inhibitor can be applied in the same manners as described above. These applications would thus aid in the inhibition of biofilm formation on such surfaces.

[00143] In a subject, a biofilm can form on an oral surface (such as teeth, tongue, back of throat, and the like). These biofilms can be associated with day-to-day bacterial activity of natural flora located in such environments, but can also be associated with oral-related disease(s), such as periodontal disease (for example, gingivitis or periodontitis) or dental carries. Application of the neuraminidase inhibitor (according to methods previously described) onto such oral surfaces can inhibit or prevent bacterial biofilm formation. The amount of the neuraminidase inhibitor that can be applied to the surfaces in order to prevent the formation of a bacterial biofilm is an amount effective to inhibit the attachment of microbes onto the surface and/or the synthesis and/or accumulation of biofilm by attached microbes on such a surface.

[00144] The neuraminidase inhibitor for use on oral surfaces can comprise a paste formulation (such as toothpaste), which can then be directly applied to the biofilm of such a surface in a subject. The paste formulation can further comprise an abrasive. The neuraminidase inhibitor can also exist as a gel formulation or in liquid formulation. For example, the neuraminidase inhibitor in a liquid formulation (such as a mouthwash) can directly come in contact with the biofilm on the oral surface of a subject.

[00145] Other aspects of the invention are directed at methods of treating biofilm production-related disorders in subjects in need thereof. The method entails administering to the subject an effective amount of a neuraminidase inhibitor that reduces biofilm formation in the subject, and then measuring a reduction or inhibition in the growth of biofilm production-related bacteria in the subject. The reduction in bacterial growth is indicative of the reduction in, or inhibition of, biofilm production in the subject, thereby treating the biofilm production-related disorder. For example, the administered neuraminidase inhibitor can reduce the activity of the neuraminidase or alter the expression of the neuraminidase, thereby inhibiting or preventing the formation of a bacterial biofilm.

[00146] According to the present invention, modulation of the neuraminidase enzyme (for example, via reducing enzymatic activity or protein expression as described above) can inhibit or reduce biofilm formation due to diminished adherence of microorganisms to a surface or to increased microorganism death. This therapeutic approach thus can be useful for the treatment of biofilm-production-related disorders/conditions and medical-device related infections associated with the formation of microbial biofilms.

[00147] Non-limiting examples of biofilm production-related disorders include chronic otitis media, prostatitis, cystitis, bronchiectasis, bacterial endocarditis, osteomyelitis, dental caries, periodontal disease, infectious kidney stones, acne, Legionnaire's disease, chronic obstructive pulmonary disease (COPD), and infections from implanted/inserted devices. In one specific example, subjects with CF display an accumulation of biofilm in the lungs and digestive tract. In subjects afflicted with COPD, such as emphysema and chronic bronchitis, patients display a characteristic inflammation of the airways wherein airflow through such airways, and subsequently out of the lungs, is chronically obstructed. The methods of treatment according to the invention can also benefit a subject having chronic otitis media. Otitis media refers to an infection or inflammation in the middle ear area. The inflammation begins when infections (for example, those caused by bacterial or viral infections) that cause sore throats, colds, or other respiratory/breathing problems spread to the middle ear. Acute otitis media is the presence of fluid, typically pus, in the middle ear with symptoms of pain, redness of the eardrum, and possible fever. However the biofilm production-related disorder can be further classified as chronic if fluid is present in the middle ear for six or more weeks.

[00148] Biofilm production-related disorders can also encompass infections derived from implanted/inserted devices (such as those described previously), medical device-related infections, such as infections from biliary stents, orthopedic implant infections, and catheter-related infections (kidney, vascular, peritoneal). An infection can also originate from sites where the integrity of the skin and/or soft tissue has been compromised. Non-limiting examples include dermatitis, ulcers from peripheral vascular disease, a burn injury, and trauma. For example, a Gram-positive bacterium, such as *S. pneumoniae*, can cause opportunistic infections in such tissues. The ability of *S. pneumoniae* to infect burn wound sites, e.g., is enhanced due to the breakdown of the skin, burn-related immune defects, and antibiotic selection.

[00149] A subject in need of treatment (for example those previously described, such as an animal or human) can be one afflicted with the infections or disorders described above. As such, the subject is at risk of developing a biofilm on or in a biologically relevant surface, or already has developed such a biofilm. Such a subject at risk can be a candidate for treatment with a neuraminidase inhibitor in order to inhibit the development or onset of a biofilm-production-related disorder/condition or prevent the recurrence, onset, or development of one or more symptoms of a biofilm-production-related disorder/condition.

[00150] The subject in need can be administered a neuraminidase inhibitor as described above. It can be administered alone or in combination with a second therapeutic, e.g., such as an antibiotic, in order to prevent or inhibit the formation of bacterial biofilms. An antibiotic can be co-administered with the bacterial neuraminidase inhibitor, either sequentially or simultaneously. Upon contacting the cell, the bacterial neuraminidase inhibitor modulates the activity or the expression of the bacterial neuraminidase wherein the inhibitor reduces the activity or the expression of the bacterial neuraminidase, as described above.

[00151] An antibiotic refers to any compound known to one of ordinary skill in the art that will inhibit the growth of, or kill, bacteria. Useful, non-limiting examples of an antibiotic include lincosamides (clindomycin); chloramphenicols; tetracyclines (such as Tetracycline, Chlortetracycline, Demeclocycline, Methacycline, Doxycycline, Minocycline); aminoglycosides (such as Gentamicin, Tobramycin, Netilmicin, Amikacin, Kanamycin, Streptomycin, Neomycin); beta-lactams (such as penicillins, cephalosporins, Imipenem, Aztreonam); vancomycins; bacitracins; macrolides (erythromycins), amphotericins; sulfonamides (such as Sulfanilamide, Sulfamethoxazole, Sulfacetamide, Sulfadiazine, Sulfisoxazole, Sulfacytine, Sulfadoxine, Mafenide, p-Aminobenzoic Acid, Trimethoprim-Sulfamethoxazole); Methenamin; Nitrofurantoin; Phenazopyridine; trimethoprim; rifampicins; metronidazoles; cefazolins; Lincomycin; Spectinomycin; mupirocins; quinolones (such as Nalidixic Acid, Cinoxacin, Norfloxacin, Ciprofloxacin, Perfloxacin, Ofloxacin, Enoxacin, Fleroxacin, Levofloxacin); novobiocins; polymixins; gramicidins; and antipseudomonals (such as Carbenicillin, Carbenicillin Indanyl, Ticarcillin, Azlocillin, Mezlocillin, Piperacillin) or any salts or variants thereof. Such antibiotics can be obtained commercially, e.g., from Daiichi Sankyo, Inc. (Parsipanny, NJ), Merck (Whitehouse Station, NJ), Pfizer (New York, NY), Glaxo Smith Kline (Research Triangle Park, NC), Johnson & Johnson (New Brunswick, NJ), AstraZeneca (Wilmington, DE), Novartis (East Hanover, NJ), and Sanofi-Aventis (Bridgewater, NJ). The antibiotic used will depend on the type of bacterial infection.

[00152] Administration of neuraminidase inhibitors to a subject can serve as a treatment that limits the severity and spread of pathogenic infections, such as bacterial infections. Neuraminidase inhibitors intended for human use must be efficacious and function in inhibiting the formation of biofilms, but must also not be toxic. The skilled physician via clinical trials can determine efficacy and toxicity.

[00153] An effective amount of a neuraminidase inhibitor refers to the amount of a therapy sufficient to reduce or ameliorate the severity and/or duration of a disorder, such as a

biofilm production-related disorder (for example, pneumonia, meningitis, CF, COPD, otitis media, and others described above). An effective amount of a neuraminidase inhibitor can also be sufficient to reduce the degree and time-span of one or more symptoms associated with a biofilm production-related disorder. Additionally, this amount can prevent the advancement of a biofilm production-related disorder, cause regression of such a disorder, prevent the recurrence, development, onset or progression of one or more symptoms associated with a biofilm production-related disorder. The skilled physician can determine a therapeutic dose of a neuraminidase inhibitor that inhibits biofilm formation and/or reduces the duration of a disorder or symptoms thereof. Methods of administration of a neuraminidase inhibitor composition have been described above.

[00154] A neuraminidase inhibitor according to the methods of the invention can reduce biofilms associated with a biofilm production-related disorder with respect to the surface area the biofilm covers, thickness, and/or consistency (for example, the integrity of the biofilm). This reduction can be assessed via measuring the growth of bacteria associated with biofilm-production-related disorders, conditions, or diseases. For example, the growth of bacteria of a biofilm-production-related disease can be quantified via measuring the density of bacteria of a biofilm-production-related-disease in a biological sample. Non-limiting examples of biological samples include blood, serum, sputum, lacrimal secretions, semen, urine, vaginal secretions, and tissue samples. The reduction in the growth of bacteria of a biofilm-production-related disease can also be measured by chest x-rays or by a pulmonary function test (PFT) (for example, spirometry or forced expiratory volume (FEV_1)).

[00155] In another non-limiting example, the presence or growth of biofilm production-related bacteria can be measured by detecting the presence of antigens of biofilm production-related bacteria in a biological sample, such as those described above. For example, an antibody to *S. pneumoniae* components can be used as a test for colonization/infection in a subject afflicted with a biofilm production-related condition or disorder, wherein the presence of *Streptococcus* antigens is detected in a biological sample, such as blood. These antibodies can be generated according to methods well established in the art or can be obtained commercially (for example, from Abcam, Cambridge, MA; Cell Sciences Canton, MA; Novus Biologicals, Littleton, CO; or GeneTex, San Antonio, TX).

[00156] Spirometry measures lung function, for example, the volume and/or flow of air that can be inhaled and exhaled. The FEV1 is a measurement of the volume exhaled during the first second of a forced expiratory maneuver started from the level of total lung capacity. FEV_1 is the most frequently used index for evaluating bronchoconstriction, airway

obstruction, or bronchodilatation. These methods are important for assessing biofilm production-related conditions, such as pneumonia, cystic fibrosis, and COPD. A reduction in the growth of bacteria associated with biofilm production-related disorders and/or conditions is indicative of a reduction in or inhibiton of biofilm production.

[00157] Methods of the invention are provided that can prevent or reduce biofilm formation (such as a bacterial biofilm) on a biologically relevant surface, wherein a neuraminidase inhibitor is administered to a subject (such as a mammal, for example a human) in order to prevent or reduce the formation of bacterial biofilms. These surfaces include, but are not limited to, an epithelial or mucosal surface of the respiratory tract, lungs, the oral cavity, the alimentary and vaginal tracts, in the ear or the surface of the eye, and the urinary tract. For example, a biofilm can affect the surface of a lung (such as the lung of a subject with pneumonia, CF, or COPD), which is comprised of epithelial cells.

[00158] Epithelial cells are named on the basis of their cell type: simple squamous, simple cuboidal, simple columnar, stratified squamous, stratified cuboidal, or stratified columnar epithelia. Such epithelial cells can be obtained from any tissue organ having such cells, for example from the lining of cavities such as the mouth, blood vessels, heart and lungs; from the outer layers of the skin; from the lining of the air passages, stomach, and intestines; in the nose, ears and the taste buds of the tongue; from the lining of the vaginal and urinary tracts, rectum, uterus, and oviducts, and from the larger ducts of certain glands and the papillary ducts of the kidneys. Epithelial cells can also be obtained from *in vitro* epithelial cell culture systems well known in the art (see, e.g., Harris, A. (ed.), (1996) Epithelial Cell Culture, Cambridge University Press). Such cell lines can be available commercially or can be generated via standard cell culturing techniques (see e.g. Harris, supra).

[00159] Other aspects of the current invention are directed to methods that are useful for treating a subject (such as an animal or human) that has, is developing, or is at risk of developing a biofilm-production-related disorder/condition. A subject who is developing a biofilm-production-related disorder/condition is an individual harboring an immature biofilm clinically evident or detectable to the skilled artisan, but that has not yet fully formed. A subject at risk of developing a biofilm can be one in which the introduction of a medical device, a graft implantation, and the like is scheduled. The risk of developing a biofilm can also be due to a biofilm production-related disease (such as the channel transporter mutation associated with CF) that is in its earlier stages, e.g., no bacterial infection and/or biofilm formation is yet detected.

[00160] In a specific example, methods are provided for preventing biofilm formation in the airways of cystic fibrosis patients who are free of bacterial infection of the airways. Such patients are at risk of developing a biofilm, and as such, are "in need thereof." The method entails administering to the subject an effective amount of a neuraminidase inhibitor, which prevents growth of bacteria associated with a biofilm production-related disorder in the airways of a subject, and detecting the absence of such bacterial growth in the airways of the subject. The absence of bacterial growth is indicative of the lack of biofilm formation in the airways of the subject. For example, the subject can be one afflicted with CF and is a human (such as an individual of 5 years of age or less) that has not yet developed a bacterial infection of the airways indicating that *P. aeruginosa* and/or *S. pneumoniae* has not yet colonized the epithelial cells of the lung airways. Airways of the lung include bronchii, bronchioles, aleveolar ducts, alveolar sacs, and alveoili.

[00161] The growth of bacteria associated with a biofilm-production-related disorder can be quantified by detecting the presence of *S. pneumoniae* (e.g. by measuring the density of the bacteria) in a biological sample according to methods practiced in the art. Non-limiting examples of biological samples include blood, serum, sputum, lacrimal secretions, sweat, semen, urine, vaginal secretions, and tissue samples. For example, the presence or absence of bacteria can be measured via detecting the presence of bacterial in a biological sample, such as those described above. An antibody to *S. pneumoniae* components can be used as a test for colonization/infection in a subject afflicted with a biofilm production-related condition or disorder (such as pneumonia or CF), wherein the presence of *Streptococcus* antigens is detected in a biological sample, such as blood. These antibodies can be generated according to methods well established in the art or can be obtained commercially (for example, from Abcam, Cambridge, MA; Cell Sciences Canton, MA; Novus Biologicals, Littleton, CO; or GeneTex, San Antonio, TX). The absence of bacterial growth and its associated biofilm can also be measured, e.g., by chest x-rays or by a pulmonary function test (PFT) (for example, spirometry or FEV_1, methods described above).

[00162] According to the invention, administration of neuraminidase inhibitors to a subject (for example, one afflicted with CF who is free of bacterial infection in the airways) can serve as a preventive means by which to deter the development of pathogenic infections, such as bacterial infections (eg. *P. aeruginosa* and /or *S. pneumoniae*).

[00163] An effective amount of a neuraminidase inhibitor to be administered can be the amount sufficient to prevent the onset or development of a pathogenic infection associated with a biofilm production-related disease or disorder (for example, pneumonia, COPD, or

CF). The skilled physician can determine a therapeutic dose of a neuraminidase inhibitor that prevents pathogenic infection in addition to biofilm formation. An effective amount of a neuraminidase inhibitor, for example, one directed at the *Streptococcus* enzyme, can be administered according to methods of this invention. Methods of administration of a neuraminidase inhibitor composition have been described above.

[00164] Aspects of the present invention also provide methods of preventing or reducing biofilm formation associated with a wide variety of commercial, industrial, and processing operations, such as those found in water handling/processing industries. The method for inhibiting biofilm formation on an industrial/commercial surface entails applying a neuraminidase inhibitor to the biofilm found on such surfaces. The neuraminidase inhibitor modulated activity or expression of the neuraminidase protein can then be measured. A reduction in the neuraminidase inhibitor modulated activity or expression of the neuraminidase protein is indicative of the inhibition of biofilm formation. The neuraminidase inhibitor can be directed at any neuraminidase produced by organisms in the biofilm. These have been described above.

[00165] The neuraminidase inhibitors useful in the invention that prevent or reduce the formation of bacterial biofilms can be utilized in order to prevent microorganisms from adhering to surfaces. These surfaces can be hard, semi-hard, porous, soft, semi-soft, regenerating, or non-regenerating; and can include, but are not limited to, metal, alloy, polyurethane, water, polymeric surfaces of implantable/insertable devices (such as medical devices or catheters), the enamel of teeth, and surfaces of mammalian cellular membranes.

[00166] For example, some surfaces can be the surfaces of industrial equipment (such as, equipment located in Good Manufacturing Practice (GMP) facilities, food processing plants, photo processing venues, and the like), the surfaces of plumbing systems, or the surfaces bodies of water (such as lakes, swimming pools, oceans, and the like). Embodiments of the invention further provide methods for inhibiting and/or reducing biofilm formation within a plumbing system.

[00167] The surfaces can be coated, sprayed, or impregnated with a neuraminidase inhibitor prior to use to prevent the formation of bacterial biofilms. Surfaces also can be treated with a neuraminidase inhibitor to reduce, control, or eradicate microorganisms (such as those described above) adhering to such surfaces. In a specific example, the method can be used in an open re-circulating water system used for cooling to control the temperature of fermentation tanks. In such a system, the water circulates through coils and jackets in the tank, over an induced draft-cooling tower, and then is pumped back from the sump. Biofilm-

producing microorganisms can flourish in the cooling water system due to contamination and highly nutritive substances from the surrounding environment (Coetser et al., (2005) *Crit. Rev. Micro.* 31: 212-32). This biofilm can form on the cooling tower water distribution elements, its support components, and on the heat transfer surfaces of the system resulting in poor cooling efficiency. Thus, to prevent formation of the biofilm, a neuraminidase inhibitor is applied to treat the water-cooling system. Not only is the treatment suitable for the water-cooling system of a fermentation tank, but can also be applicable to air conditioning condensers, (such as those found in hospitals or industrial plants), that are served by a rooftop open-deck cooling tower (described in U.S. Patent No. 6,395,189 and U.S. Appln. Pub. No. 2005/0158253).

[00168] The neuraminidase inhibitor can be added directly to a water handling or collection system (such as the systems described above). Alternatively, the bacterial neuraminidase inhibitor can be applied to the biofilm, itself, or to the bacteria within, or the producers of the biofilm or which can produce the biofilm. It can be applied as a formulation comprising a paste, liquid, powder, gel, or tablet. The neuraminidase inhibitor functions via modulating the activity or the expression of a bacterial neuraminidase protein. Upon the neuraminidase inhibitor contacting the bacterial cell, the activity or expression of the bacterial neuraminidase is reduced, thereby preventing or reducing the formation of a bacterial biofilm. For example, the biofilm formed on the surfaces of systems (which include but are not limited to plumbing, tubing, and support components) involved with water condensate collections, sewerage discharges, paper pulping operations, re-circulating water systems (such as air conditioning systems, a cooling tower, and the like), and, in water bearing, handling, processing, collection systems of an industrial setting can be formed by a Gram-negative or Gram-positive bacterium (as described above), or a combination thereof.

[00169] Adding the neuraminidase inhibitor prevents or reduces formation of biofilms on the surface of the water or on the surfaces of the pipes or plumbing of water-handling systems, or other surfaces of the collection and/or operation systems that the water contacts.

[00170] Also provided are methods for identifying or screening for inhibitors of a neuraminidase protein useful in preventing or inhibiting the formation of biofilms. The method entails contacting a cell infected with a biofilm-producing microbe, such as a protozoa, yeast, virus, or bacterium, (e.g., *Sreptococcus*) with a test (or candidate) neuraminidase inhibitor, and then determining whether the test neuraminidase inhibitor inhibits biofilm formation. Inhibition of biofilm formation thus is indicative of the ability of the test neuraminidase inhibitor to prevent or inhibit microbial infection.

[00171] Inhibition of biofilm formation can be determined by any known method, such as a visual method performed with the aid of a microscope, colorimterically via densitometry, and the like. Neuraminidase inhibitors that reduce or prevent the formation of a biofilm on surfaces are described or can be identified via biofilm assays as described above (see, e.g., EXAMPLE 1). Thus, one skilled in the art can carry out any known biofilm assay, such as those previously described.

[00172] Neuraminidase gene products, including polynucleotides, oligonucleotides and polypeptides, can be used in screening assays to identify compounds that specifically bind to bacterial, viral, yeast, or protozoan neuraminidase gene products and thus have potential use as agonists, or antagonists of such neuraminidases. In one embodiment, the bacterial, viral, yeast, or protozoan neuraminidase polynucleotides and polypeptides of the invention are useful to screen for compounds that affect the sialidase or biofilm formation activities of bacterial, viral, yeast, or protozoan neuraminidase gene products.

[00173] The invention thus provides assays to detect molecules that specifically bind to bacterial, viral, yeast, or protozoan neuraminidases. For example, recombinant cells expressing a gene encoding bacterial, viral, yeast, or protozoan neuraminidase can be used to recombinantly produce a bacterial, viral, yeast, or protozoan neuraminidases polypeptide, respectively, and to screen for molecules that bind to a bacterial, viral, yeast, or protozoan neuraminidases polypeptide, respectively. Methods that can be used to carry out the foregoing are commonly known in the art.

[00174] A neuraminidase inhibitor that can be used according to the invention has been described above.

[00175] Non-limiting examples of cells to be contacted with the neuraminidase inhibitor include bacterial cells, yeast cells, protozoan cells, and cells infected with a viral or other pathogen. Representative bacteria include but are not limited to *Legionella* sp., *P. aeruginosa*, *H. influenzae, V. cholerae*, *Yersinia pestis, Escherichia coli*, and *Streptococcus pneumoniae*. Alternatively, the cell to be contacted is an animal cell, such as a mammalian cell, or more specifically, a human cell. The cell can be from a particular tissue or cell line, such as an epithelial cell.

[00176] Another aspect of the invention is directed to a mutant *S. pneumoniae* strain having a deletion in the gene encoding a neuraminidase protein. Deleting a portion of the gene so that the gene cannot function can be accomplished by mutation or insertion of another DNA in the base sequence of the gene (also referred to as a gene disruption). As a result, the gene cannot be transcribed into mRNA, the structural gene is not translated, and

the transcription product mRNA becomes incomplete. A mutation or deletion occurs in the amino acid sequence of the translation product or structural protein, rendering the protein unable to perform its original function.

[00177] Any method known in the art can be used for constructing a gene-disrupted strain, such as a strain wherein the gene encodes a neuraminidase protein. For example, the gene disruption can occur via homologous recombination or other methods described in Nickoloff (ed.), (1995) *Methods in Molecular Biology* 47: 291-302, Humana Press Inc., Totowa, N.J.; or in Sambrook et al. (eds.), Molecular Cloning: A Laboratory Manual, Second Edition (1989) Cold Spring Harbor Laboratory Press.

EXAMPLES

[00178] Examples are provided below to facilitate a more complete understanding of the present invention. The following examples illustrate the exemplary modes of making and practicing the present invention. However, the scope of the invention is not limited to specific embodiments disclosed in these Examples, which are for purposes of illustration only, since alternative methods can be utilized to obtain similar results.

EXAMPLE 1 - *Structural Analysis and Inhibitor Identification of Respiratory Pathogen Neuraminidases.*

[00179] There is a need to develop therapeutic agents for the treatment of infections by the human respiratory pathogens *Pseudomonas aeruginosa* and *Streptococcus pneumoniae*. *P. aeruginosa* causes significant morbidity and mortality for cystic fibrosis patients and is a leading nosocomial pathogen. *S. pneumoniae* is the most common cause of bacterial pneumonia and otitis media leading to substantial economic burden. The neuraminidases of *P. aeruginosa* and *S. pneumoniae*, which catalyze the release of terminal sialic acid residues from glycoconjugates, are involved in host colonization in animal models of infection. We demonstrate that the *S. pneumoniae* neuraminidase (NanA), like that of *P. aeruginosa* (NanPs), contributes to biofilm formation. To help identify compounds that inhibit these neuraminidases, the crystal structures of the *P. aeruginosa* and *S. pneumoniae* enzymes were soved at 1.6 and 1.7 Å resolution, respectively. The active site regions of the two enzymes are strikingly different: NanA contains a deep pocket that is similar to that in canonical neuraminidases, while the NanPs active site is much more open. The structural information was used to undertake a ligand-receptor docking screen and a lead compound that shows inhibition against both enzymes was identified. This work can be the basis for developing drugs to prevent colonization of the respiratory tract by these two important pathogens.

[00180] *P. aeruginosa* and *S. pneumoniae* are important human respiratory pathogens. The neuraminidase enzyme, which cleaves sialic acid residues, plays an important role in the pathogenesis of respiratory infection. We demonstrate that the NanA neuraminidase of *S. pneumoniae* like the NanPs enzyme of *P. aeruginosa* is involved in biofilm formation, which enhances airway colonization. We determined the three-dimensional structures of the neuraminidase from these two organisms and show that although they possess similar overall structure, their active sites are vastly different. Using this structural information we identified candidate inhibitory compounds. The information derived from the structures of the two

enzymes and the subsequent identification of inhibitory compounds represents a first step in the development of therapeutics against these two significant human pathogens.

[00181] The production of neuraminidase/sialidase by mucosal pathogens has long been associated with the pathogens of respiratory tract infection [A1]. Neuraminidases are widespread among animals and microorganisms, catalyzing the release of terminal sialic acid residues from glycoconjugates [A2]. The influenza neuraminidase is required to facilitate spread of the virus, cleaving it from its sialic acid receptor. The influenza neuraminidase is not only a key antigen for the highly successful influenza vaccine, it is also the target for the drugs zanamivir and oseltamivir that are widely used to prevent and ameliorate influenza infection [A3]. The analysis of the structure/ function relationships of the influenza neuraminidase and its substrate provides a paradigm for the development of antimicrobial therapy directed at critical virulence factors. These neuraminidases are recognized in most sequence analysis programs by their common elements, often conserved "ASP" boxes, sites in the predicted amino acid sequence that are predicted to interact with sialic acid residues [A2,A4]. Neuraminidases are produced by respiratory pathogens with very different metabolic requirements and highly variable potential for virulence. As neuraminidases are highly conserved virulence factors that appear to be critical for colonization and infection of the respiratory tract by such diverse pathogens, the development of anti-bacterial neuraminidase inhibitors would appear to be a realistic therapeutic target.

[00182] *S. pneumoniae* is the most common cause of bacterial pneumonia and a significant cause of otitis media, a major clinical problem in pediatrics [A5,A6]. There are at least 90 serotypes of *S. pneumoniae*, with the current pediatric vaccine covering seven common and the adult vaccine covering 23 serotypes [A5,A7]. There is a need for therapeutic strategies active against all serotypes as those serotypes not covered by the vaccines are rising in prevalence by genetic recombination and are increasingly associated with invasive disease [A8, A9]. In addition, antibiotic resistance amongst *S. pneumoniae* is a growing problem. *S. pneumoniae* produces at least three distinct neuraminidases [A10]; NanA being the most expressed and active [A11, A12] that is conserved in all strains [A10, A13, A14]. Production of NanA can be detected *in vivo*, and its expression is upregulated upon interaction with host cells [A15-A18]. The pneumococcal neuraminidase modifies host glycoconjugates [A19, A20] and exposes potential binding receptors [A21-A25]. Without being bound by theory, a role in survival has also been indicated as desialylation of other organisms has been

demonstrated [A26]. Pneumococcal neuraminidase activity also provides a source of carbohydrates for bacterial metabolism, cleaving sugars from the mucosal surface [A20, A27, A28], but whether this significantly contributes to bacterial growth *in vivo* is not clearly established. Several studies have stated that *nanA* mutants colonize the rodent respiratory tract less efficiently than wild type strains [A11, A29, A30] and vaccination with purified NanA affords some protection against nasopharyngeal colonization and otitis media [A31-A33]. However, these differences can be mouse strain and animal model dependent [A19, A20, A34, A35].

[00183] *P. aeruginosa,* also a neuraminidase producer, is an opportunistic pathogen which is the most common cause of respiratory tract infection in patients with cystic fibrosis and rarely a cause of infection in otherwise healthy subjects [A36]. The neuraminidase of *P. aeruginosa* (NanPs) has been characterized and found to be important in the pathogenesis of pneumonia in a mouse model of infection [A37]. Its expression is correlative with initial airway colonization, particularly in isolates from young patients recently infected with the organism [A38]. In contrast to the pneumococcal enzyme, the *P. aeruginosa* neuraminidase does not appear to target host glycoconjugates but instead is involved in the biosynthesis of the extracellular polysaccharides on the bacterial surface that are involved in cell-cell interaction, agglutination and biofilm formation [A37]. *P. aeruginosa* does not ferment the sugars that are released through neuraminidase activity and expression of the enzyme does not enhance bacterial growth rates [A37]. Nonetheless, the *P. aeruginosa* neuraminidase mutant is significantly less proficient in colonizing and infecting the lungs of mice and can provide a target for prevention of *P. aeruginosa* infection in susceptible patients.

[00184] Neuraminidase expression by both *S. pneumoniae* and *P. aeruginosa* facilitates their respective abilities to colonize and infect respiratory tract in animal models. We show that *S. pneumoniae,* like *P. aeruginosa,* uses the neuraminidase in biofilm formation. Without being bound by theory, differences in structures of these enzymes can explain their functional differences and their distinctive roles in pathogenesis. We report here the crystal structures of *P. aeruginosa* and *S. pneumoniae* neuraminidases at the 1.6 and 1.7Å level and using this information have identified a number of compounds that were shown to inhibit the enzymes.

[00185] RESULTS

[00186] ***Structure of the NanA neuraminidase from S. pneumoniae***. The crystal structure of the free enzyme of *S. pneumoniae* NanA has been determined at 1.7 Å resolution (Table 1). The bacterial expression construct contained residues 116-1035 and *in situ* proteolysis with trypsin was essential for the crystallization. The current atomic model contains residues 320-793 and 317-793 for the two NanA molecules in the crystallographic asymmetric unit, respectively. Roughly 200 residues from both the N and C termini of the recombinant protein were removed by trypsin during crystallization. The two NanA molecules have essentially the same conformation, with an rms distance of 0.25 Å for their equivalent Cα atoms. Purified NanA is monomeric in solution, based on gel-filtration chromatography.

[00187] The NanA structure contains a six-bladed β-propeller domain, with an insertion (residues 437-535) between the second and the third β-strands of the second blade (**FIG. 1A**). This insertion forms a distinct domain located next to the catalytic β-propeller domain. The overall structure of NanA shares high structural similarity with other bacterial neuraminidases, including the *Salmonella typhimurium* LT2 neuraminidase [A39], *Vibrio cholerae* neuraminidase [A40], *Clostridium perfringens* sialidase NanI [A41], and *Micromonospora viridifaciens* sialidase [A42]. The structures of *S. pneumoniae* NanA in complex with the transition state analog 2,3-dehydro-2-deoxy-*N*-acetylneuraminic acid (DANA) at 2.5 Å resolution [A43] and NanB [A44] were recently reported. The published NanA structure [A43] is based on an expression construct that contains residues 319-822, although only residues 322-791 are observed in the structure and the crystals are in a different space group. Nonetheless, the overall structure and the interactions with DANA are similar to observations based on our structures. The overall rms distance in equivalent Cα positions is 0.4 Å.

[00188] To reveal the molecular mechanism for substrate/inhibitor recognition, we have determined the structures of NanA in complex with the sialic acid compound *N*-acetylneuraminic acid (NANA) and the transition state analog DANA at 1.7 Å resolution (**Table 1**). There is essentially no conformational change in the protein upon the binding of these inhibitors. The rms distance in equivalent Cα atoms among the structures of the free enzyme, the NANA complex, and the DANA complex is about 0.15 Å. In addition, there is essentially no conformational change in the active site of the enzyme, where the inhibitors bind.

[00189] Table 1. *Summary of crystallographic information*

	NanPs free enzyme	**NanA free enzyme**	**NanA in complex with DANA**	**NanA in complex with NANA**
Resolution range (Å)	30-1.6	30-1.7	30-1.7	30-1.7
Number of observations	377,554	636,912	279,534	251,113
R_{merge} (%)[a]	8.8 (36.5)	4.1 (9.4)	3.0 (7.3)	6.0 (14.2)
I/σI	26.2 (4.9)	38.8 (10.7)	31.1 (11.5)	25.3 (6.6)
Redundancy	4.3 (3.9)	3.4 (3.2)	3.0 (2.5)	2.8 (2.5)
Number of reflections	85,363	183,283	93,563	86,772
Completeness (%)	96 (91)	92 (90)	93 (86)	87 (70)
R factor (%)	17.2 (21.7)	17.2 (20.4)	17.8 (20.5)	17.5 (20.8)
Free *R* factor (%)	19.1 (23.7)	19.8 (23.4)	20.9 (24.7)	20.9 (24.8)
Residues in most favored region of the Ramachandran plot (%)	86	86	86	86
rmsd in bond lengths (Å)	0.005	0.005	0.007	0.005
rmsd in bond angles (°)	1.4	1.4	1.3	1.4
Protein Data Bank entry code				

a. The numbers in parenthesis are for the highest resolution shell.

[00190] Clear electron density was observed for the NANA inhibitor, which is bound to NanA in a boat conformation (**FIG. 1B**). As observed in structures of NANA in complex with other neuraminidases, the compound is involved in a large network of ionic and hydrogen-bonding interactions with the active site of NanA (**FIG. 1C**; see also **Table 3**). The carboxyl group of NANA interacts with three Arg residues (Arg347, Arg663 and Arg721), and the amide nitrogen of NANA is hydrogen-bonded to the side chain of Asp417. The two hydroxyl groups on the ring of NANA interact with the side chains of Arg366, Asp417 and Asp372, the last of which is also hydrogen-bonded to one of the hydroxyls on the glycerol group. In addition to the polar interactions, several hydrophobic side chains are located near the inhibitor. Most importantly, residues Ile442 and Phe443 in the long loop at the beginning of the insertion in blade 2 (**FIG. 1A**) cover up part of the inhibitor and greatly reduce the size of the active site pocket, producing a tight fit between the inhibitor and the enzyme (**FIG. 1D**). DANA was bound in the same position as NANA, showing the same interactions with

the enzyme except for the loss of the hydrogen-bond with Asp372 due to the absence of the hydroxyl group on the ring (**FIG. 1C**).

[00191] **Table 3**. *Amino acid residues corresponding to the putative active site/ neuraminidase inhibitor-binding site (residues within 10 Å).*

Arg347	Arg366	Asp372	Asp417	Ile442	Phe443	Phe565	Tyr590
Gln602	Glu647	Arg663	Tyr695	Tyr752	Arg 721		

[00192] ***Structure of the P. aeruginosa neuraminidase reveals exposed active site.*** The structure of the *P. aeruginosa* neuraminidase (NanPs) at 1.6 Å resolution was also determined (**Table 1**). The enzyme, previously referred to as NanA [A37], product of PA2794, has been renamed to reflect its differences to typical bacterial neuraminidases. The structure contains a six-bladed β-propeller in the N-terminal region (residues 1-334, **FIG. 2A**) and a C-terminal domain (C domain, residues 335-438) that belongs to the immuno-globulin superfamily, based on comparisons with other structures in the Protein Data Bank using the SSM server [A45]. A close structural homolog of the C domain is the immuno-globulin superfamily domain of the muscle protein twitchin [A46]. The rms distance among equivalent Cα atoms of the two structures is 3 Å, although the amino acid sequence identity is only 6%. This domain is located about 50 Å away from the active site of the enzyme (**FIG. 2A**); although our mutagenesis studies showed that it is important for the catalytic activity (**FIG. 3**). The domain mediates the formation of a trimer in the crystal, although the protein is monomeric in solution, based on gel-filtration and light scattering experiments.

[00193] The β-propeller domain of *P. aeruginosa* NanPs has the same overall structure as that of canonical neuraminidases. The rms distance among equivalent Cα atoms in *P. aeruginosa* NanPs and these other structures is 2.5-3 Å, but the amino acid sequence identity is 7-19%. Some of the important residues in the active site are also conserved in NanPs, consistent with our observation that it confers some neuraminidase activity [A47]. We constructed Asp79Ala (Asp417 in NanA) and Arg260Ala (Arg721 in NanA) mutations in the active site of NanPs and found these residues to be important for activity (**FIG. 3**). The mutation of Arg292 in the influenza neuraminidase, equivalent to Arg198 in NanPs and Arg663 in NanA, to a lysine confers resistance to the inhibitor oseltamivir [A48]. However, the Arg198Lys mutant of NanPs showed loss of activity (**FIG. 3**).

[00194] There are dramatic differences in the shape of the active site region between NanPs and the other neuraminidases. Compared to NanA (**FIG. 1D**), the active site region of NanPs is much more open (**FIG. 2B**). An important cause of this difference is the lack of the insertion in the second blade of the propeller. The long loop at the beginning of this insertion, especially the side chains of Ile442 and Phe443 (**FIG. 1C**), is absent in NanPs (**FIG. 2C**), leading to a much more exposed active site. Additionally, variations at other amino acid residues also contribute to the different active site topography of NanPs. For example, the side chain of Phe129 in NanPs clashes with the bound position of the acetyl group in NANA (**FIG. 2C**), and this is the only recognizable clash between the inhibitor and the NanPs active site (**FIG. 2B**). The equivalent residue in NanA is Gly567.

[00195] Several other residues in the NANA binding site are not conserved in NanPs (**FIG. 2C**). Especially, of the four arginine residues that interact with NANA in NanA, two (Arg347 and Arg366) are replaced with other residues (His23 and Ala42) in NanPs, while the other two assume different conformations in NanPs (**FIG. 2C**). In addition, Asp372 in NanA is replaced by Gly47 in NanPs. The structural information shows that the active site region of NanPs is not a good fit for the NANA inhibitor (**FIG. 2B**), indicating that NanPs is probably not a conventional neuraminidase, and its natural substrate(s) remain to be identified.

[00196] ***Phylogeny of the S. pneumoniae and P. aeruginosa neuraminidases***. To better ascertain the evolutionary relatedness of NanA and NanPs, a phylogenetic analysis of a number bacterial, eukaryotic and viral neuraminidases was conducted (**FIG. 4**). The neuraminidase superfamily is known to be highly divergent [A2, A4], and, NanA and NanPs cluster at separate branches of the tree. NanA was aligned closest to the erysipeloid-causing bacterium *Erysipelothrix rhusiopathiae* [A49] (**FIG. 4**). NanA also clustered closely to the large neuraminidase of *C. perfringens* [A41] and was more closely related to well characterized bacterial neuraminidases than NanPs. NanPs was part of a deeply rooted branch that was closer to the trypanosome *trans*-sialidases than the enteric neuraminidases. NanPs was most closely matched to a putative neuraminidase from the aquatic organism *Blastopirellula marina* [A50].

[00197] ***Biochemical properties of pneumococcal NanA***. The biochemical activity of NanA was assayed using the fluorogenic sialic acid derivative 2'-(4-methylumbelliferyl)-α-D-*N*-acetylneuraminic acid (MNN). NanA was observed to cleave the fluorogenic substrate significantly at low nanomolar and even at picomolar concentrations (**FIG. 5A**). The Km of

NanA for this substrate is about 1.4 mM, which is generally comparable to the Km values reported for other neuraminidases. The neuraminidase from *Vibrio cholerae* requires divalent cations, specifically calcium, to be active [A40, A51]. Although calcium was not essential for NanA activity, an increase in activity of 70% was observed at a Ca^{2+} concentration of 1 mM (**FIG. 5B**). We observed a 50% activity increase in the presence of magnesium ions (**FIG. 5B**) and decreased activity in the presence of iron and copper, presumably due to their larger molecular masses (**FIG. 5B**). The presence of either copper or ferric ions decreased activity by 90% or greater at millimolar levels, indicating that NanA can possess a cation binding site.

[00198] We next tested the ability of sialic acids to competitively inhibit NanA activity. NANA was able to cause 50% inhibition at 600 μM (**FIG. 6**). We observed higher inhibition with the transition state analog DANA compared to NANA. DANA was able to reduce activity by 50% at 200 μM and this inhibitory potency is in the range that is observed for other neuraminidases [A39, A52]. As a comparison, NANA and DANA possess very weak inhibitory activity towards the *P. aeruginosa* neuraminidase, 50% inhibition being achieved in the 10 millimolar range with both compounds [A37].

[00199] ***Biological activity of pneumococcal NanA***. Many lung pathogens are able to bind to the asialylated ganglioside receptor GM1 (aGM1, Galβ1-3GalNAcβ1-4Galβ1-4Glcβ1-1Cer), including *P. aeruginosa* and *S. pneumoniae* [A22]. The neuraminidase from *P. aeruginosa* is able to expose this receptor [A47]; we sought to investigate if this was also the case for *S. pneumoniae*. Either purified NanA or concentrated supernatant from wild-type *S. pneumoniae* strain D39 but not its isogenic *nanA* mutant exposed aGM1 on the surface of 16HBE epithelial cells (**FIG. 7**). We then investigated the biological significance of this sialic acid release (**FIG. 8**). No effect on bacterial adherence was observed (**FIG. 8A**) nor was there a growth advantage in the presence of airway epithelial cells associated with the wild-type strain. Consistent with intratracheal infection studies [A29] and other colonization studies [A20], we did not observe a decrease in the ability for the *nanA* mutant to colonize mouse lungs after infection under anesthesia (**FIG. 8B**), although we did observe a trend towards less inflammation as assessed by neutrophil recruitment to the lung (**FIG. 8C**).

[00200] ***S. pneumoniae neuraminidase is involved in biofilm formation***. A major function of the *P. aeruginosa* neuraminidase is its participation in cell-cell interactions necessary for biofilm formation [A37]. As *S. pneumoniae nanA* expression is upregulated in lung tissue and in biofilm-growing cells [A16] we investigated the contribution of *nanA* to

the formation of biofilms (**FIG. 9**). Exposure of *S. pneumoniae* to airway epithelial cells caused a significant increase in biofilm formation and the *nanA* mutant had significantly reduced capacity to form biofilms. In an *S. pneumoniae* R6, unencapsulated background the *nanA* strain was also significantly reduced in its ability to form biofilms (**FIG. 9**). Of note, no difference in biofilm formation was observed when *S. pneumoniae* was grown on plastic without previous airway cell interaction.

[00201] ***Identification of small molecule inhibitors to the neuraminidases***. Due to their comparable roles in the colonization and infection of the respiratory tract it seemed reasonable to predict that inhibitors targeting neuraminidases can prevent these respiratory infections. Inhibitors against the influenza neuraminidase, zanamivir (GSK) and oseltamivir (Roche) were both developed from structure-based design relying on high-resolution X-ray crystal structures and functional data [A3]. Oseltamivir was found to inhibit NanA in the micromolar to low millimolar range (**FIG. 10**), IC_{50} 2 mM, a similar 50% inhibition was observed with NanPs at around 600 μM concentration (**FIG. 10**).

[00202] In an effort to identify small molecule inhibitors specific to the bacterial neuraminidases, a virtual library screen was performed (Schrödinger LLC, Portland, OR, USA) using the Glide software and the structure of NanPs [A53, A54]. The Glide analysis examines receptor-ligand docking, running a high-throughput screen of candidate compounds against the active site, a process that has been successful in identifying inhibitors of other enzymes [A55]. A number of compounds identified from this screen showed high degrees of inhibition *in vitro*, more-so with the pneumococcal enzyme which appears to behave more like a neuraminidase than *P. aeruginosa* (**FIG. 11A**). A lead compound, designated XX1, with a quinoline-based chemical scaffold that possesses appropriate pharmacokinetic properties for use in humans, such as adherence to the Lipinski rule of 5, was chosen for further analysis [A56]. XX1 was found to inhibit NanPs (**FIG. 11B**) and NanA (**FIG. 11C**) over a range of concentrations and in a dose-dependent manner. Consistent with the differences in the active site between the two enzymes we also observed differences in inhibition by XX1. An IC_{50} of 8.5 μM was determined for the *S. pneumoniae* neuraminidase and 29 μM for the neuraminidase of *P. aeruginosa*. The inhibition afforded by XX1 to NanA is greater than 20, 80 and 200 times more effective than DANA, NANA and oseltamivir, respectively. Analogs of XX1 as well as a number of different chemical scaffolds in the development of effective inhibitors are currently undergoing further testing and development.

[00203] DISCUSSION

[00204] The neuraminidases of *S. pneumoniae* and *P. aeruginosa* share a common role in facilitating bacterial colonization of the respiratory tract [A11, A29, A30, A37]. We extend this observation further, to show that both enzymes, despite differences in phylogeny and structure, also contribute to biofilm formation. For *S. pneumoniae*, the biofilm phenotype is most evident *in vivo* [A57], or as we show, under *in vitro* conditions that favor neuraminidase expression. We were only able to demonstrate a difference in biofilm production after growth on human airway cells, which induces *nanA* expression [A15, A16, A18] and reduces capsule production [A58]. By selecting for organisms on human airway cells, we apparently mimic an *in vivo* process in which encapsulated organisms that are able to avoid mucus entrapment and clearance gradually produce less capsule to facilitate epithelial attachment [A7]. Enhanced biofilm formation was also associated with the R6 strain, which exhibits reduced capsule production, with its *nanA* mutant also displaying reduced propensity for biofilm formation. The *P. aeruginosa* biofilm phenotype is similarly complex, involving several groups of genes involved in motility and the production of extracellular carbohydrates [A59, A60] . Like *S. pneumoniae*, the *P. aeruginosa nanA* mutant forms a minimal biofilm on human airway cells and is readily cleared from the murine upper airway [A37], consistent with a major role for the enzyme in the colonization process. As organisms enmeshed in extracellular carbohydrates are significantly more difficult to opsonize and phagocytose, the biofilm phenotype even early in pathogenesis appears critical for upper airway colonization.

[00205] Sialic acids represent a major component of the glycolipids that comprise the exposed surface of the respiratory mucosa. While sialic acids provide binding sites for pathogens such as influenza, desialylated glycolipids provide receptors for many of the common bacterial pulmonary pathogens including both *S. pneumoniae* and *P. aeruginosa* [A22], which bind to the exposed GalNAcβ1-4Gal residues when terminal sialic acid is cleaved. The desialylation of airway mucosal cells by the influenza neuraminidase increases susceptibility to secondary infection often caused by *S. pneumoniae* [A61]. We demonstrate that culture supernatant from wild-type but not the *nanA* mutant of *S. pneumoniae* is also capable of exposing asialylated glycolipids on human airway cells. However, the neuraminidase activity associated with intact organisms, either *S. pneumoniae* or *P. aeruginosa* was not associated with increased bacterial attachment, indicating that the neuraminidase activity has a different biological role in pathogenesis. For *S. pneumoniae*, which is able to

metabolize the carbohydrates released from airway mucins, neuraminidase activity can provide a growth advantage *in vivo*, although this has only been demonstrated *in vitro* [A27, A28]. Despite these differences, the observation that NanA and NanPs are both involved in biofilm formation highlights a common strategy of these two respiratory pathogens which need to persist in the same ecological niche. Despite their differences in structure, and different substrates, both neuraminidases possess similar functions in pathogenesis.

[00206] The structure of NanA shows that it is similar to canonical neuraminidases, with an active site that is a good fit for the NANA substrate. Thus, without being bound by theory, NanA behaves like a typical neuraminidase, and this is supported by our biochemical data. Experiences with developing inhibitors against other bacterial and viral neuraminidases can be beneficial for developing NanA inhibitors. In contrast, the structure of NanPs shows a distinct active site surface, such that NANA can no longer be tightly accommodated in it. Therefore, the biochemical function of NanPs can be different from that of NanA, and NanPs can also have a different inhibitor sensitivity profile as compared to NanA, as confirmed from our studies. Even subtle differences in neuraminidase structure can change the specificity for substrates, as seen with the Trypanosome enzymes [A62]. This is also consistent with our phylogenetic analysis, showing large evolutionary separation between NanPs and NanA. Moreover, NanPs contains a unique C-terminal domain, which also appears to be essential for its catalytic activity. The exact biological function of this domain, and in fact of NanPs, remains to be established.

[00207] The current inhibitors against influenza neuraminidase were developed through structure-function studies. We adapted this approach to identify a common inhibitor for the neuraminidases of *P. aeruginosa* and *S. pneumoniae*. Instead of starting with a base scaffold we undertook *in silico* ligand-receptor docking studies to identify putative inhibitors using high-resolution crystal structures before screening in our *in vitro* neuraminidase assays. This allowed us to screen and subsequently identify a range of chemical scaffolds that showed inhibition. The neuraminidase superfamily is quite divergent with low sequence identities, yet still retains tertiary structure similarities like those we have observed between these two neuraminidases [A4]. The differences in active site and probable differences in substrate between NanA and NanPs are also consistent with their divergent family clustering. While the differences between *P. aeruginosa* and *S. pneumoniae* were apparent in inhibitor screening as was the inhibition profile to oseltamivir, several inhibitors provided analogous

levels of inhibition. This enabled us to develop a lead compound that shows significant inhibition against the two enzymes. We should be able to reduce the IC_{50} for both enzymes further once we have conducted structure activity relationship studies or alternatively, develop the other chemical scaffolds that showed promise in the initial screen. Due to the active site differences between the two enzymes, individual compounds specific to each enzymes active site to increase efficacy need to be developed.

[00208] Although these enzymes are distant relatives on the phylogenetic tree, have different active site conformations and have relatively major differences in the affinities of their respective active sites for sialic acid, they share a common function in pathogenesis and the formation of biofilms. Based upon the structural data now available, we have begun to develop highly active neuraminidase inhibitors to prevent bacterial infection in the target populations at increased risk.

[00209] MATERIALS AND METHODS

[00210] ***Bacterial strains and media***. *S. pneumoniae* strains D39 [A63], D39 *nanA* [A19] and R6 [A64] and R6 *nanA* [A20] were grown on trypticase-soy (TS) agar or broth supplemented with 200U/ml catalase (Worthington) and 1μg/ml of chloramphenicol for *nanA* strains. Plate cultures were grown at 37°C in the presence of carbon dioxide (5%). *Escherichia coli* strains were grown on Luria-Bertani (LB) media at 37°C, when required ampicillin was used at 100μg/ml. All chemicals were purchased from Sigma unless otherwise stated.

[00211] ***Epithelial cell culture.*** Human bronchial epithelial cells, 16HBE and human airway cells, 1HAEo$^-$ (Originally from D. Gruenert California Pacific Medical Center Research Institute, San Francisco, California, USA), were grown in minimum essential medium with Earle's salts (Cellgro and Gibco respectively) supplemented with 10% fetal bovine serum (Cambrex and Gibco respectively), 100U/ml penicillin and 100ug/ml streptomycin. 16HBE cells were additionally supplemented with 2 mM glutamine (Invitrogen). Cells were grown at 37°C with 5% CO_2 in a humidified incubator.

[00212] ***Protein expression and purification.*** Full-length (residues 1-438) *P. aeruginosa* NanPs or residues 116–1035 of *S. pneumoniae* D39 sialidase A precursor (NanA) were sub-cloned into the pET28a vector (Novagen) and over-expressed in *E. coli* BL21(DE3) at 20°C as N-terminal hexa-histidine tagged proteins. Site-directed mutations of the *P.*

aeruginosa gene were performed using QuikChange (Stratagene), while the C-terminal truncated protein represents residues 1-333 (of 438). The soluble protein was purified by nickel-agarose, anion exchange and gel filtration chromatography. The *P. aeruginosa* protein was concentrated to 37 mg/ml, and *S. pneumoniae* protein to 30 mg/ml, in a solution containing 20 mM Tris (pH 8.5) and 200 mM NaCl, flash-frozen in liquid nitrogen in the presence of 5% (v/v) glycerol, and stored at –80°C. The N-terminal His-tag was not removed for crystallization. For the production of selenomethionyl proteins, the expression construct was transformed into B834 (DE3) cells (Novagen). The bacterial growth was carried out in defined LeMaster media supplemented with selenomethionine [A65] proteins purified following the same protocol as that for the native protein.

[00213] ***Protein crystallization.*** Crystals of NanPs free enzyme were obtained at 21 °C by the sitting-drop vapor diffusion method. The reservoir solution contained 100 mM Hepes (pH 7.0), 5% Tacsimate, 7% (w/v) PEG 5000MME, and the protein was at 10 mg/ml concentration. Selenomethionine-labeled protein was cross-microseeded with crystals from native protein to obtain adequate crystals. For data collection, the crystals were cryoprotected with the introduction of 20% (v/v) ethylene glycol, and flash-frozen in liquid nitrogen.

[00214] The initial crystallization screen of NanA did not produce any hits. We therefore performed limited proteolysis to search for a stable fragment. By treating NanA with trypsin at 1000:1 (protein:trypsin) ratio, a stable fragment of ~50 kDa molecular weight was observed, indicating that approximately 50 kDa was removed from the recombinant protein by the trypsin treatment. Crystals of NanA were obtained by the sitting-drop vapor diffusion method. The reservoir solution contained 100 mM Hepes (pH 7.0) and 30% Jeffamine ED-2001 (pH 7.0), the protein was at 30 mg/ml and the drops also contained trypsin (at 5000:1 protein:trypsin ratio). Similar to our previous experiences with other proteins [A66, A67], *in situ* proteolysis was essential for the crystallization of this recombinant protein. We confirmed that the protein in the crystal showed smaller molecular weight (~50 kDa) than the original expression construct (~101 kDa) by SDS-PAGE, in agreement with our results from limited proteolysis with trypsin. For the complexes of NanA with NANA and DANA, crystals of the free enzyme were soaked overnight in a solution containing 100 mM Hepes (pH 7.0), 35% Jeffamine ED-2001 (pH 7.0), and 5 mM of each compound (NANA or DANA).

[00215] ***Data collection and processing.*** X-ray diffraction data were collected at the National Synchrotron Light Source (NSLS; Upton, NY, USA). Selenomethionyl single-wavelength anomalous diffraction (SAD) data sets at 1.9 Å and 1.7 Å resolution were collected for NanPs and NanA respectively. Native data sets at 1.6 Å resolution for NanPs and at 1.7 Å resolution for the NANA and DANA complexes of NanA were collected at the X4C beamline. The diffraction images were processed and scaled with the HKL package [A68]. The NanPs crystals belong to space group $P2_13$, with cell parameters of $a=b=c=125.6$ Å. There is one molecule in the crystallographic asymmetric unit. The NanA crystals belong to the space group $C2$, with cell parameters of $a=158.0$ Å, $b=47.7$ Å, $c=137.3$ Å, and $\beta=116.6$ °. There are two molecules in the crystallographic asymmetric unit.

[00216] ***Structure determination and refinement.*** The positions of Se atoms were determined with program BnP [A69]. Reflection phases were calculated based on the SAD data and improved with the program SOLVE/RESOLVE [A70], which also automatically located a large percentage of the residues in the molecule. The atomic model was fit into the electron density with the program O [A71]. The structure refinement was carried out with the program CNS [A72]. The crystallographic information is summarized in Table 1.

[00217] ***Neuraminidase assay.*** Neuraminidase activity of NanA was detected using the fluorogenic substrate 2'-(4-methylumbelliferyl)-α-D-*N*-acetylneuraminic acid (MNN, Sigma). Reactions contained 1.5 mM MNN, 1 nM of NanA in 2.5 mM sodium phosphate buffer (pH 5). Reactions were allowed to incubate for 2 h at 37°C before fluorescence intensity was measured at excitation and emission wavelengths of 360 nm and 465 nm in a Tecan microplate reader (Männedorf, Switzerland). NanPs was assayed as above with 1 mM of enzyme in 7.5 mM sodium chloride and 4 mM calcium chloride. Compounds were screened at a concentration of 100 μM before dose-dependence was established. Compounds were obtained from a variety of sources (Otava, Kyiv, Ukraine; Interbioscreen, Moscow, Russia; Chembridge San Diego, USA; Maybridge, Cornwell, UK; Sigma, St Louis, USA; Princeton, Princeton, USA; Lifechem, Burlington, Canada; Enamine, Kiev, Ukraine). Neuraminidase assays with oseltamivir were performed using the hydrolyzed version of the compound. Divalent cations were supplied in the form of calcium, magnesium, ferric and copper chloride. All neuraminidase assays were performed at least in triplicate.

[00218] ***Quantification of asialoGM1 exposure by flow cytometry.*** 16HBE cells were grown in 24-well plates to confluence and exposed to bacterial supernatants for 3 h followed

by three PBS washes. Supernatants were concentrated approximately 30-fold (Amicon Ultra, Millipore) and adjusted for protein quantity. As a control media alone was also concentrated. Cells were stained with rabbit polyclonal anti aGM1 antibody (Wako) followed by Alexa Fluor 488 donkey anti-rabbit IgG (Molecular Probes). Cells were detached from the plates using 0.02% EGTA in HBSS (Hanks buffered saline solution), fixed with 1% paraformaldehyde and analyzed on a FACSCalibur using CellQuest software (version 3.3; BD). Data were analyzed using WinMDI (version 2.8, Joseph Trotter).

[00219] ***Adherence assay.*** Adherence assays were performed using 16HBE cells. Bacterial strains were grown to mid-log phase, washed with PBS and 0.7-2x10^7 cfu of bacterial cells were added to confluent monolayers in 24-well plates. Bacterial cells were allowed to adhere for 1 h at 37°C before three washes with PBS. Bacteria were dissociated from epithelial cells using TrypLE Express (Gibco) and plated out to determine adherent numbers. The assay was performed with three biological replicates with duplicate technical replicates over two separate experiments.

[00220] ***Biofilm assay.*** Bacterial strains were grown to mid-log phase before being diluted 1:100 in TS broth and catalase. 100 µl of diluted culture was added in triplicate to 96-well flat bottom tissue culture treated plates (Falcon) and left for 18-24 h at 37°C with 5% CO_2. Plates were read at 600 nm to determine levels of growth before being washed in water. Adherent biofilm-forming cells were then stained with 125 µL of 1% crystal violet for 15 min before two further washes in water and allowed to dry. Bound crystal violet was then suspended in 200 µL of ethanol, shaken for 15 min and read at 540 nm.

[00221] ***Biofilm formation after epithelial cell interaction.*** Bacterial strains were grown and inoculated onto 1HAEo$^-$ cells as per adherence assay. After the initial PBS washes fresh MEM media was applied before a further 1h incubation. This removal and addition of fresh media was repeated a further four times before detachment of adherent bacteria using TrypLE Express (Gibco). The detached bacteria were then diluted 1:100 in TS broth and catalase and assayed as per the biofilm assay. Samples were repeated four times, each time in sextuplicate using epithelial cells without bacteria as a negative control.

[00222] ***Mouse model of pneumonia.*** Six-week-old C57Bl/6J mice (Jackson Laboratories) were anaesthetized with ketamine (100 mg/kg) and xylazine (5 mg/kg) before intranasal inoculation with bacteria. Bacteria were grown to mid-log phase, washed with PBS

and 3-4x10^5 cfu inoculated down the nare in a 10 μL volume. The infection persisted for 24 h before euthanasia with pentobarbital. Lungs were removed, homogenized, and plated out to determine bacterial numbers representative of pneumonia and bacteremia respectively. A portion of the lung homogenate was double-stained with phycoerythrin-labeled anti-CD45 and FITC-labeled anti-Ly6G antibodies to determine neutrophil influx into the lung by flow cytometry. Irrelevant, matched isotope antibodies were used as controls. Cells were gated based on forward and site scatter with neutrophils expressed as the Ly6G positive population within CD45 positive cells.

[00223] ***Phylogenetic analysis.*** Our sampling strategy was aimed at maximizing phylogenetic breadth in order to understand the overall pattern of evolution in the neuraminidase/sialidase gene family. We began with a list of well-known neuraminidases including those from *V. cholerae*, *S. typhimurium*, *C. perfringens*, *S. pneumoniae*, *T. cruzi*, and *P. aeruginosa*. For each sequence we did a standard BLAST search and collected one sequence from each genus in the list of hits that had an e-value score of 1x10^{-5} or lower. Duplicates were deleted. We also included sequences that have been included in other prior publications on the evolution of sialidases [A4]. A list of sequences and gene identification numbers is included as supplemental information. Sequences were aligned using the ClustalW algorithm as implemented in the program BioEdit using default settings. Sequences were aligned as amino acids and then transposed back to the original nucleotide sequences maintaining the gaps determined by the initial alignment (5394 characters total, 4124 parsimony informative characters with gaps as a fifth state, 3766 parsimony informative characters with gaps as treated as missing).

[00224] A rigorous phylogenetic analysis was undertaken using maximum parsimony (MP) algorithm implemented in PAUP* [A73]. 1000 replicates of random addition (RA) was performed followed by the tree branch reconnection (TBR) algorithm using the "multrees" option to save more than one optimal tree if discovered in the search. All characters and state transformations were given equal weight. Terminal gaps were scored as missing data in all analyses. We performed two analyses designating internal gaps as a fifth character state in one and as missing data in the other. Although the trees had many nodes in agreement there were major differences between the structures of the 2 trees. Since gaps can be informative characters [A74, A75], analysis in which internal gaps are counted as character states were

used. Nonparametric bootstrap analyses was performed with 100 iterations consisting of 100 RA replicates followed by TBR to gauge the robustness of the tree.

[00225] ***Statistics.*** Significance of data was determined either using a students *t*-test or non-parametric Mann-Whitney test using GraphPad Prism software.

[00226] ***Accession numbers***. The GenBank (www.ncbi.nlm.nih.gov/Entrez/) accession numbers utilized for phylogenetic analysis are: *Verrucomicrobium spinosum* gi|164421336:353068-354225, *Blastopirellula marina* gi|87311313:89394-90503, *Lentisphaera araneosa* gi|149198907:89577-90743, *Propionibacterium acnes* gi|50841496:752060-754375, *Ruminococcus lactaris* gi|197302028:32228-35857, *Erysipelothrix rhusiopathiae* gi|13516389:295-3807, *Pasteurella multocida* gi|15601865:1176085-1179327, *Actinomyces odontolyticus* gi|145845834:308755-310992, *Mannheimia haemolytica* gi|125433996:1-2376, *Haemophilus parasuis* gi|167854877:54475-56886, *Bacteroides fragilis* gi|53711291:4836372-4838006, *Akkermansia muciniphila* gi|187734516:2229943-2231967, *Capnocytophaga canimorsus* gi|194454827:2197-3765, *Parabacteroides distasonis* gi|150006674:3525685-3527310, *Shewanella pealeana* gi|157959830:1838982-1841831, *Flavobacteriales bacterium* gi|88710837:680637-681797, *Rhodopirellula baltica* gi|32470666:1724290-1725519, *Opitutaceae bacterium* gi|153892517:3249-4847, *Sassharopolyspora erythraea* gi|134096620:5769332-5771182, *Pseudoalteromonas haloplanktis* gi|77361923:196316-197458, *Chthoniobacter flavus* gi|196231426:66519-67730, *Janibacter sp.* gi|84494251:767782-770736, *Monosiga brevicollis* gi|167534964:1-984, *Strongylocentrotus purpuratus* gi|115616575:1-719, *Planctomyces maris* gi|149177549:10030-11205, *Acinetobacter baumannii* gi|169632029:647539-649371, *Opitutaceae bacterium* gi|153890920:5481-6641, *Danio rerio* gi|148539964:69-1220, *Corynebacterium diptheriae* gi|38232642:512872-515037, *Gemmata obscuriglobus* gi|163804184:63331-64515, *Streptomyces coelicolor* gi|32141095:7255596-7257542, *Takifugu rubripes* gi|148372013:1-87, *V. cholerae* gi|12057212:1933231-1935654, *C. perfringens nanI* gi|18308982:900997-903081, *C. perfringens nanH* gi|18308982:904693-905499, *P. aeruginosa* gi|110227054:3150886-3152202, *C. septicum* gi|40662, *C. sordellii* gi|1710442, *A. viscosus* gi|39254, *Trypanosoma rangeli* gi|2894809, *T. cruzi* gi|162265, *T. cruzi* SAPA (shed-acute-phase-antigen) gi|10943, *Micromonosporta viridifaciens* gi|216782:816-2759, *Arthrobacter ureafaciens* gi|60544840, *Influenzae* A H5N1 gi|108671038, *Macrobdella decora* gi|1353880, *Salmonella typhimurium*

gi|16763390:1002088-1003326, *S. pneumoniae* gi|116515308:1522475-1525468, *Arcanobacterium pyogenes* gi|18146340:1026-6239, *Xenopus laevis* gi|148228846:180-1376, *Trichomonas vaginalis* gi|123473002:1-1050, *Rattus norvegicus* gi|71896601:59-1288, *Bos taurus* gi|149676185:61-219, 650-842, 1541-1803, 2490-2672, 2849-3071, 3185-3411, and *Monodelphis domestica* gi|126309689:1-1404.

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EXAMPLE 2 – *In silico Screening*

[00228] *In silico screening*. To demonstrate the feasibility of identifying candidate molecule inhibitors, *in silico*, computational modeling software can be utilized in conjunction with high-resolution crystal structure results (for example, using the X-ray coordinates of **Table 2**) to screen databases for existing compounds that would bind to the active site of the *Streptococcus* neuraminidase (see Sherman et al., (2006) *Chem Biol Drug Des* 67(1): 83-4). The atomic coordinates for residues of a *S. pneumoniae* neuraminidase crystal were obtained from PDB Structure No. 2vvZ (available at, http://www.pdb.org/pdb/explore.do?structureId=2VVZ).

[00229] **Table 2**. Atomic Coordinates for S. pneumoniae Neuraminidase Crystal. Table 2 discloses SEQ ID NOS: 3 and 4, respectively.

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CRYST1   49.206   95.626  226.596  90.00  90.00  90.00 P 21 21 21    8

ATOM      1  N   ALA A 322      16.926  39.763  36.357  1.00 30.98           N
ATOM      2  CA  ALA A 322      18.021  40.720  36.692  1.00 31.11           C
ATOM      3  C   ALA A 322      18.342  40.708  38.189  1.00 31.33           C
ATOM      4  O   ALA A 322      17.520  40.297  39.013  1.00 31.21           O
ATOM      5  CB  ALA A 322      17.669  42.134  36.222  1.00 31.03           C
ATOM      6  N   LEU A 323      19.546  41.175  38.517  1.00 31.48           N
ATOM      7  CA  LEU A 323      20.086  41.158  39.870  1.00 31.45           C
ATOM      8  C   LEU A 323      20.926  42.428  40.038  1.00 31.70           C
ATOM      9  O   LEU A 323      21.666  42.800  39.128  1.00 31.75           O
ATOM     10  CB  LEU A 323      20.941  39.896  40.060  1.00 31.28           C
ATOM     11  CG  LEU A 323      21.781  39.620  41.314  1.00 31.31           C
ATOM     12  CD1 LEU A 323      20.920  39.323  42.525  1.00 29.41           C
ATOM     13  CD2 LEU A 323      22.738  38.460  41.055  1.00 31.25           C
ATOM     14  N   THR A 324      20.804  43.098  41.182  1.00 31.95           N
ATOM     15  CA  THR A 324      21.581  44.320  41.430  1.00 32.37           C
ATOM     16  C   THR A 324      23.043  44.005  41.748  1.00 32.57           C
ATOM     17  O   THR A 324      23.379  42.879  42.113  1.00 32.43           O
ATOM     18  CB  THR A 324      20.982  45.190  42.567  1.00 32.46           C
ATOM     19  OG1 THR A 324      20.949  44.444  43.796  1.00 32.85           O
ATOM     20  CG2 THR A 324      19.580  45.667  42.203  1.00 32.29           C
ATOM     21  N   GLU A 325      23.914  44.997  41.583  1.00 32.98           N
ATOM     22  CA  GLU A 325      25.307  44.854  42.004  1.00 33.36           C
ATOM     23  C   GLU A 325      25.321  44.853  43.524  1.00 32.91           C
ATOM     24  O   GLU A 325      24.356  45.293  44.160  1.00 32.79           O
ATOM     25  CB  GLU A 325      26.194  45.986  41.463  1.00 33.55           C
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ATOM     26  CG  GLU A 325      25.966  46.359  39.991  1.00 35.86           C
ATOM     27  CD  GLU A 325      25.949  45.156  39.048  1.00 38.13           C
ATOM     28  OE1 GLU A 325      26.927  44.374  39.044  1.00 39.16           O
ATOM     29  OE2 GLU A 325      24.957  45.002  38.300  1.00 38.96           O
ATOM     30  N   LYS A 326      26.400  44.347  44.109  1.00 32.46           N
ATOM     31  CA  LYS A 326      26.471  44.286  45.560  1.00 32.04           C
ATOM     32  C   LYS A 326      26.632  45.671  46.184  1.00 31.69           C
ATOM     33  O   LYS A 326      27.401  46.506  45.706  1.00 31.56           O
ATOM     34  CB  LYS A 326      27.534  43.280  46.048  1.00 31.93           C
ATOM     35  CG  LYS A 326      28.980  43.619  45.753  1.00 32.00           C
ATOM     36  CD  LYS A 326      29.899  42.521  46.273  1.00 32.02           C
ATOM     37  CE  LYS A 326      31.350  42.984  46.340  1.00 31.95           C
ATOM     38  NZ  LYS A 326      31.616  43.884  47.501  1.00 31.51           N
ATOM     39  N   THR A 327      25.841  45.919  47.220  1.00 31.37           N
ATOM     40  CA  THR A 327      25.969  47.110  48.040  1.00 30.95           C
ATOM     41  C   THR A 327      26.493  46.624  49.387  1.00 30.70           C
ATOM     42  O   THR A 327      25.834  45.830  50.063  1.00 30.83           O
ATOM     43  CB  THR A 327      24.611  47.824  48.191  1.00 30.88           C
ATOM     44  OG1 THR A 327      24.012  47.976  46.900  1.00 31.31           O
ATOM     45  CG2 THR A 327      24.771  49.194  48.818  1.00 30.55           C
ATOM     46  N   ASP A 328      27.693  47.068  49.752  1.00 30.24           N
ATOM     47  CA  ASP A 328      28.331  46.641  50.999  1.00 29.79           C
ATOM     48  C   ASP A 328      27.777  47.416  52.192  1.00 29.68           C
ATOM     49  O   ASP A 328      27.874  48.642  52.253  1.00 29.82           O
ATOM     50  CB  ASP A 328      29.857  46.776  50.911  1.00 29.49           C
ATOM     51  CG  ASP A 328      30.466  45.925  49.797  1.00 28.84           C
ATOM     52  OD1 ASP A 328      29.844  44.938  49.350  1.00 27.94           O
ATOM     53  OD2 ASP A 328      31.587  46.240  49.364  1.00 29.00           O
ATOM     54  N   ILE A 329      27.196  46.687  53.137  1.00 29.47           N
ATOM     55  CA  ILE A 329      26.494  47.288  54.267  1.00 29.07           C
ATOM     56  C   ILE A 329      27.360  47.296  55.518  1.00 28.81           C
ATOM     57  O   ILE A 329      27.310  48.232  56.312  1.00 28.75           O
ATOM     58  CB  ILE A 329      25.163  46.557  54.527  1.00 29.19           C
ATOM     59  CG1 ILE A 329      24.320  46.574  53.249  1.00 29.38           C
ATOM     60  CG2 ILE A 329      24.403  47.188  55.704  1.00 29.20           C
ATOM     61  CD1 ILE A 329      22.992  45.930  53.392  1.00 31.12           C
ATOM     62  N   PHE A 330      28.148  46.243  55.691  1.00 28.67           N
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ATOM     65  O   PHE A 330      30.736  44.737  55.768  1.00 28.31           O
ATOM     66  CB  PHE A 330      28.686  45.175  57.843  1.00 28.25           C
ATOM     67  CG  PHE A 330      27.335  45.451  58.434  1.00 27.52           C
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ATOM     69  CD2 PHE A 330      26.229  44.712  58.040  1.00 26.97           C
ATOM     70  CE1 PHE A 330      25.910  46.706  59.933  1.00 26.69           C
ATOM     71  CE2 PHE A 330      24.978  44.962  58.584  1.00 26.68           C
ATOM     72  CZ  PHE A 330      24.820  45.964  59.532  1.00 26.63           C
ATOM     73  N   GLU A 331      31.352  46.869  56.178  1.00 29.24           N
ATOM     74  CA  GLU A 331      32.663  46.789  55.536  1.00 29.53           C
ATOM     75  C   GLU A 331      33.765  46.450  56.531  1.00 29.79           C
ATOM     76  O   GLU A 331      34.145  47.264  57.373  1.00 29.56           O
ATOM     77  CB  GLU A 331      32.978  48.099  54.806  1.00 29.60           C
ATOM     78  CG  GLU A 331      32.340  48.199  53.422  1.00 30.13           C
ATOM     79  CD  GLU A 331      32.114  49.631  52.963  1.00 30.75           C
ATOM     80  OE1 GLU A 331      31.891  50.513  53.825  1.00 30.82           O
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ATOM     84  C   SER A 332      36.671  45.340  56.765  1.00 31.94           C
ATOM     85  O   SER A 332      36.772  45.795  55.624  1.00 31.94           O
ATOM     86  CB  SER A 332      35.439  43.238  57.128  1.00 31.01           C
ATOM     87  OG  SER A 332      35.598  42.890  55.764  1.00 30.34           O
ATOM     88  N   GLY A 333      37.683  45.299  57.626  1.00 32.89           N
ATOM     89  CA  GLY A 333      39.024  45.747  57.270  1.00 34.20           C
ATOM     90  C   GLY A 333      39.639  44.943  56.139  1.00 35.07           C
ATOM     91  O   GLY A 333      38.975  44.135  55.489  1.00 35.10           O
ATOM     92  N   ARG A 334      40.926  45.155  55.910  1.00 36.11           N
ATOM     93  CA  ARG A 334      41.588  44.555  54.763  1.00 37.10           C
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ATOM     96  CB  ARG A 334      41.694  45.591  53.646  1.00 37.10           C
ATOM     97  CG  ARG A 334      41.622  45.022  52.252  1.00 38.09           C
ATOM     98  CD  ARG A 334      41.571  46.140  51.223  1.00 40.06           C
ATOM     99  NE  ARG A 334      40.205  46.614  50.985  1.00 41.41           N
ATOM    100  CZ  ARG A 334      39.393  46.132  50.044  1.00 42.25           C
ATOM    101  NH1 ARG A 334      39.799  45.146  49.250  1.00 42.54           N
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ATOM    103  N   ASN A 335      43.287  42.816  54.702  1.00 38.00           N
ATOM    104  CA  ASN A 335      44.598  42.185  54.940  1.00 38.53           C
ATOM    105  C   ASN A 335      44.981  42.033  56.420  1.00 38.73           C
ATOM    106  O   ASN A 335      46.141  42.228  56.797  1.00 38.87           O
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ATOM    108  CG  ASN A 335      45.397  43.047  52.692  1.00 39.10           C
ATOM    109  OD1 ASN A 335      45.242  42.041  51.992  1.00 39.31           O
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ATOM    113  C   GLY A 336      44.160  42.735  59.486  1.00 39.17           C
ATOM    114  O   GLY A 336      44.228  42.692  60.715  1.00 39.17           O
ATOM    115  N   LYS A 337      44.022  43.867  58.799  1.00 39.32           N
ATOM    116  CA  LYS A 337      44.107  45.185  59.426  1.00 39.69           C
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ATOM    118  O   LYS A 337      41.761  45.425  58.989  1.00 39.89           O
ATOM    119  CB  LYS A 337      44.952  46.125  58.551  1.00 39.94           C
ATOM    120  CG  LYS A 337      46.244  45.483  58.017  1.00 40.83           C
ATOM    121  CD  LYS A 337      47.322  46.512  57.697  1.00 42.53           C
ATOM    122  CE  LYS A 337      48.675  45.833  57.486  1.00 43.32           C
ATOM    123  NZ  LYS A 337      49.826  46.788  57.564  1.00 43.60           N
ATOM    124  N   PRO A 338      42.585  46.669  60.695  1.00 39.49           N
ATOM    125  CA  PRO A 338      41.265  47.234  60.990  1.00 39.39           C
ATOM    126  C   PRO A 338      40.805  48.174  59.890  1.00 39.40           C
ATOM    127  O   PRO A 338      41.629  48.672  59.123  1.00 39.58           O
ATOM    128  CB  PRO A 338      41.493  48.028  62.288  1.00 39.41           C
ATOM    129  CG  PRO A 338      42.826  47.590  62.809  1.00 39.36           C
ATOM    130  CD  PRO A 338      43.616  47.206  61.600  1.00 39.38           C
ATOM    131  N   ASN A 339      39.500  48.407  59.808  1.00 39.36           N
ATOM    132  CA  ASN A 339      38.961  49.373  58.862  1.00 39.08           C
ATOM    133  C   ASN A 339      39.037  50.792  59.424  1.00 39.21           C
ATOM    134  O   ASN A 339      39.694  51.028  60.440  1.00 39.20           O
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ATOM    136  CG  ASN A 339      36.486  49.158  59.536  1.00 38.50           C
ATOM    137  OD1 ASN A 339      36.751  49.736  60.592  1.00 38.54           O
ATOM    138  ND2 ASN A 339      35.284  48.651  59.283  1.00 36.87           N
ATOM    139  N   LYS A 340      38.347  51.723  58.769  1.00 39.27           N
ATOM    140  CA  LYS A 340      38.376  53.142  59.128  1.00 39.37           C
ATOM    141  C   LYS A 340      37.870  53.437  60.539  1.00 39.02           C
ATOM    142  O   LYS A 340      38.248  54.448  61.130  1.00 39.12           O
ATOM    143  CB  LYS A 340      37.583  53.950  58.097  1.00 39.58           C
ATOM    144  CG  LYS A 340      38.269  53.978  56.750  1.00 41.13           C
ATOM    145  CD  LYS A 340      37.355  53.536  55.610  1.00 42.86           C
ATOM    146  CE  LYS A 340      38.194  52.959  54.475  1.00 43.62           C
ATOM    147  NZ  LYS A 340      37.589  53.198  53.138  1.00 45.04           N
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ATOM    150  C   ASP A 341      37.210  51.950  63.490  1.00 37.55           C
ATOM    151  O   ASP A 341      36.918  52.109  64.675  1.00 37.75           O
ATOM    152  CB  ASP A 341      34.977  52.315  62.409  1.00 38.13           C
ATOM    153  CG  ASP A 341      34.138  53.167  61.466  1.00 38.60           C
ATOM    154  OD1 ASP A 341      34.677  54.131  60.876  1.00 39.05           O
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ATOM    156  N   GLY A 342      38.176  51.128  63.082  1.00 37.00           N
ATOM    157  CA  GLY A 342      38.928  50.275  64.014  1.00 36.18           C
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ATOM    159  O   GLY A 342      38.748  48.101  65.021  1.00 35.59           O
ATOM    160  N   ILE A 343      37.567  48.474  63.137  1.00 35.12           N
ATOM    161  CA  ILE A 343      36.891  47.181  63.136  1.00 34.44           C
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ATOM    162  C   ILE A 343      37.482  46.258  62.072  1.00 33.85           C
ATOM    163  O   ILE A 343      37.526  46.609  60.893  1.00 33.74           O
ATOM    164  CB  ILE A 343      35.358  47.362  62.936  1.00 34.51           C
ATOM    165  CG1 ILE A 343      34.752  48.069  64.155  1.00 34.45           C
ATOM    166  CG2 ILE A 343      34.663  46.019  62.705  1.00 34.60           C
ATOM    167  CD1 ILE A 343      33.600  48.974  63.828  1.00 34.27           C
ATOM    168  N   LYS A 344      37.932  45.083  62.502  1.00 33.13           N
ATOM    169  CA  LYS A 344      38.519  44.095  61.597  1.00 32.92           C
ATOM    170  C   LYS A 344      37.474  43.267  60.859  1.00 32.63           C
ATOM    171  O   LYS A 344      37.668  42.919  59.698  1.00 32.83           O
ATOM    172  CB  LYS A 344      39.473  43.146  62.341  1.00 32.80           C
ATOM    173  CG  LYS A 344      40.778  43.781  62.767  1.00 32.92           C
ATOM    174  CD  LYS A 344      41.797  42.749  63.204  1.00 32.67           C
ATOM    175  CE  LYS A 344      42.870  43.415  64.045  1.00 33.04           C
ATOM    176  NZ  LYS A 344      44.179  42.735  63.903  1.00 33.16           N
ATOM    177  N   SER A 345      36.374  42.944  61.531  1.00 32.16           N
ATOM    178  CA  SER A 345      35.434  41.964  60.998  1.00 31.66           C
ATOM    179  C   SER A 345      33.976  42.293  61.267  1.00 30.99           C
ATOM    180  O   SER A 345      33.632  42.812  62.323  1.00 31.06           O
ATOM    181  CB  SER A 345      35.751  40.579  61.569  1.00 31.68           C
ATOM    182  OG  SER A 345      34.727  39.647  61.259  1.00 32.06           O
ATOM    183  N   TYR A 346      33.138  41.993  60.279  1.00 30.39           N
ATOM    184  CA  TYR A 346      31.691  41.878  60.458  1.00 29.86           C
ATOM    185  C   TYR A 346      31.294  40.471  60.073  1.00 29.67           C
ATOM    186  O   TYR A 346      31.998  39.809  59.300  1.00 29.73           O
ATOM    187  CB  TYR A 346      30.939  42.893  59.607  1.00 29.70           C
ATOM    188  CG  TYR A 346      30.993  44.280  60.178  1.00 29.05           C
ATOM    189  CD1 TYR A 346      30.108  44.668  61.177  1.00 28.28           C
ATOM    190  CD2 TYR A 346      31.936  45.203  59.728  1.00 28.45           C
ATOM    191  CE1 TYR A 346      30.147  45.939  61.713  1.00 28.72           C
ATOM    192  CE2 TYR A 346      31.985  46.485  60.259  1.00 28.98           C
ATOM    193  CZ  TYR A 346      31.086  46.844  61.256  1.00 28.89           C
ATOM    194  OH  TYR A 346      31.118  48.103  61.797  1.00 28.99           O
ATOM    195  N   ARG A 347      30.173  39.998  60.601  1.00 29.19           N
ATOM    196  CA  ARG A 347      29.931  38.574  60.515  1.00 28.81           C
ATOM    197  C   ARG A 347      28.497  38.119  60.244  1.00 28.49           C
ATOM    198  O   ARG A 347      28.126  37.934  59.091  1.00 29.41           O
ATOM    199  CB  ARG A 347      30.533  37.884  61.736  1.00 28.82           C
ATOM    200  CG  ARG A 347      30.863  36.432  61.525  1.00 29.29           C
ATOM    201  CD  ARG A 347      31.917  36.202  60.452  1.00 28.12           C
ATOM    202  NE  ARG A 347      32.466  34.860  60.581  1.00 26.79           N
ATOM    203  CZ  ARG A 347      31.842  33.735  60.239  1.00 25.34           C
ATOM    204  NH1 ARG A 347      30.620  33.755  59.726  1.00 24.11           N
ATOM    205  NH2 ARG A 347      32.456  32.578  60.417  1.00 25.06           N
ATOM    206  N   ILE A 348      27.694  37.936  61.281  1.00 27.51           N
ATOM    207  CA  ILE A 348      26.475  37.125  61.157  1.00 26.38           C
ATOM    208  C   ILE A 348      25.240  37.916  60.699  1.00 25.66           C
ATOM    209  O   ILE A 348      24.578  38.548  61.513  1.00 25.60           O
ATOM    210  CB  ILE A 348      26.174  36.395  62.488  1.00 26.24           C
ATOM    211  CG1 ILE A 348      27.458  35.795  63.082  1.00 25.88           C
ATOM    212  CG2 ILE A 348      25.093  35.358  62.293  1.00 26.28           C
ATOM    213  CD1 ILE A 348      28.075  34.649  62.278  1.00 25.29           C
ATOM    214  N   PRO A 349      24.902  37.843  59.401  1.00 25.14           N
ATOM    215  CA  PRO A 349      23.852  38.696  58.857  1.00 24.90           C
ATOM    216  C   PRO A 349      22.427  38.279  59.235  1.00 24.60           C
ATOM    217  O   PRO A 349      22.101  37.088  59.273  1.00 24.31           O
ATOM    218  CB  PRO A 349      24.048  38.564  57.343  1.00 24.88           C
ATOM    219  CG  PRO A 349      24.622  37.222  57.153  1.00 24.93           C
ATOM    220  CD  PRO A 349      25.458  36.942  58.373  1.00 25.22           C
ATOM    221  N   ALA A 350      21.600  39.281  59.514  1.00 24.17           N
ATOM    222  CA  ALA A 350      20.160  39.106  59.617  1.00 23.78           C
ATOM    223  C   ALA A 350      19.497  40.271  58.895  1.00 23.54           C
ATOM    224  O   ALA A 350      19.963  41.412  58.978  1.00 23.18           O
ATOM    225  CB  ALA A 350      19.721  39.049  61.072  1.00 23.76           C
ATOM    226  N   LEU A 351      18.418  39.969  58.179  1.00 23.31           N
ATOM    227  CA  LEU A 351      17.697  40.965  57.405  1.00 23.13           C
ATOM    228  C   LEU A 351      16.202  40.907  57.702  1.00 23.39           C
ATOM    229  O   LEU A 351      15.585  39.836  57.647  1.00 22.95           O
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ATOM    230  CB  LEU A 351      17.956  40.755  55.908  1.00 23.17           C
ATOM    231  CG  LEU A 351      17.296  41.681  54.879  1.00 22.81           C
ATOM    232  CD1 LEU A 351      17.969  43.055  54.855  1.00 22.43           C
ATOM    233  CD2 LEU A 351      17.340  41.032  53.497  1.00 22.62           C
ATOM    234  N   LEU A 352      15.627  42.069  58.000  1.00 23.74           N
ATOM    235  CA  LEU A 352      14.204  42.164  58.315  1.00 24.04           C
ATOM    236  C   LEU A 352      13.492  43.266  57.531  1.00 24.38           C
ATOM    237  O   LEU A 352      13.972  44.394  57.444  1.00 24.28           O
ATOM    238  CB  LEU A 352      14.009  42.376  59.820  1.00 24.03           C
ATOM    239  CG  LEU A 352      12.602  42.258  60.418  1.00 23.64           C
ATOM    240  CD1 LEU A 352      11.988  40.900  60.139  1.00 22.93           C
ATOM    241  CD2 LEU A 352      12.663  42.521  61.916  1.00 23.76           C
ATOM    242  N   LYS A 353      12.343  42.917  56.962  1.00 24.93           N
ATOM    243  CA  LYS A 353      11.482  43.878  56.289  1.00 25.51           C
ATOM    244  C   LYS A 353      10.321  44.207  57.223  1.00 25.92           C
ATOM    245  O   LYS A 353       9.479  43.349  57.505  1.00 26.10           O
ATOM    246  CB  LYS A 353      10.992  43.310  54.951  1.00 25.43           C
ATOM    247  CG  LYS A 353       9.844  44.078  54.290  1.00 26.24           C
ATOM    248  CD  LYS A 353      10.319  45.283  53.506  1.00 26.71           C
ATOM    249  CE  LYS A 353       9.299  45.663  52.445  1.00 27.33           C
ATOM    250  NZ  LYS A 353       9.793  46.747  51.545  1.00 28.34           N
ATOM    251  N   THR A 354      10.290  45.446  57.707  1.00 26.34           N
ATOM    252  CA  THR A 354       9.312  45.856  58.713  1.00 26.83           C
ATOM    253  C   THR A 354       7.991  46.286  58.094  1.00 27.05           C
ATOM    254  O   THR A 354       7.927  46.640  56.913  1.00 27.14           O
ATOM    255  CB  THR A 354       9.835  47.017  59.594  1.00 27.06           C
ATOM    256  OG1 THR A 354       9.667  48.263  58.904  1.00 27.15           O
ATOM    257  CG2 THR A 354      11.307  46.818  59.956  1.00 26.85           C
ATOM    258  N   ASP A 355       6.943  46.276  58.913  1.00 27.35           N
ATOM    259  CA  ASP A 355       5.617  46.725  58.496  1.00 27.71           C
ATOM    260  C   ASP A 355       5.641  48.118  57.851  1.00 27.68           C
ATOM    261  O   ASP A 355       4.872  48.382  56.932  1.00 27.74           O
ATOM    262  CB  ASP A 355       4.660  46.716  59.685  1.00 27.94           C
ATOM    263  CG  ASP A 355       4.905  47.867  60.637  1.00 29.40           C
ATOM    264  OD1 ASP A 355       6.036  47.986  61.160  1.00 31.07           O
ATOM    265  OD2 ASP A 355       3.966  48.661  60.859  1.00 31.22           O
ATOM    266  N   LYS A 356       6.536  48.990  58.323  1.00 27.51           N
ATOM    267  CA  LYS A 356       6.687  50.340  57.774  1.00 27.35           C
ATOM    268  C   LYS A 356       7.400  50.361  56.417  1.00 27.10           C
ATOM    269  O   LYS A 356       7.531  51.422  55.809  1.00 27.21           O
ATOM    270  CB  LYS A 356       7.418  51.262  58.768  1.00 27.53           C
ATOM    271  CG  LYS A 356       6.581  51.769  59.965  1.00 28.45           C
ATOM    272  CD  LYS A 356       5.491  52.772  59.537  1.00 30.42           C
ATOM    273  CE  LYS A 356       5.221  53.838  60.618  1.00 32.33           C
ATOM    274  NZ  LYS A 356       4.313  53.411  61.736  1.00 31.55           N
ATOM    275  N   GLY A 357       7.859  49.199  55.949  1.00 26.67           N
ATOM    276  CA  GLY A 357       8.560  49.094  54.665  1.00 25.88           C
ATOM    277  C   GLY A 357      10.072  49.196  54.787  1.00 25.51           C
ATOM    278  O   GLY A 357      10.798  49.009  53.810  1.00 25.31           O
ATOM    279  N   THR A 358      10.538  49.486  55.997  1.00 25.09           N
ATOM    280  CA  THR A 358      11.956  49.614  56.308  1.00 24.94           C
ATOM    281  C   THR A 358      12.716  48.281  56.214  1.00 24.92           C
ATOM    282  O   THR A 358      12.170  47.220  56.524  1.00 24.85           O
ATOM    283  CB  THR A 358      12.101  50.183  57.721  1.00 25.01           C
ATOM    284  OG1 THR A 358      11.295  51.364  57.833  1.00 25.55           O
ATOM    285  CG2 THR A 358      13.553  50.499  58.067  1.00 24.51           C
ATOM    286  N   LEU A 359      13.969  48.342  55.772  1.00 24.81           N
ATOM    287  CA  LEU A 359      14.850  47.181  55.832  1.00 25.03           C
ATOM    288  C   LEU A 359      15.843  47.343  56.972  1.00 25.15           C
ATOM    289  O   LEU A 359      16.519  48.375  57.086  1.00 25.24           O
ATOM    290  CB  LEU A 359      15.587  46.957  54.509  1.00 25.21           C
ATOM    291  CG  LEU A 359      14.781  46.468  53.299  1.00 25.20           C
ATOM    292  CD1 LEU A 359      15.661  46.440  52.055  1.00 25.07           C
ATOM    293  CD2 LEU A 359      14.151  45.094  53.553  1.00 25.61           C
ATOM    294  N   ILE A 360      15.907  46.325  57.825  1.00 24.95           N
ATOM    295  CA  ILE A 360      16.827  46.310  58.954  1.00 24.62           C
ATOM    296  C   ILE A 360      17.867  45.226  58.729  1.00 24.61           C
ATOM    297  O   ILE A 360      17.532  44.063  58.479  1.00 24.37           O
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ATOM    298  CB  ILE A 360      16.089  46.100  60.301  1.00 24.63           C
ATOM    299  CG1 ILE A 360      15.068  47.225  60.514  1.00 24.76           C
ATOM    300  CG2 ILE A 360      17.078  46.056  61.462  1.00 24.01           C
ATOM    301  CD1 ILE A 360      14.451  47.273  61.894  1.00 24.77           C
ATOM    302  N   ALA A 361      19.130  45.627  58.808  1.00 24.60           N
ATOM    303  CA  ALA A 361      20.238  44.723  58.591  1.00 24.94           C
ATOM    304  C   ALA A 361      21.066  44.586  59.861  1.00 25.18           C
ATOM    305  O   ALA A 361      21.652  45.561  60.344  1.00 25.18           O
ATOM    306  CB  ALA A 361      21.102  45.211  57.421  1.00 24.77           C
ATOM    307  N   GLY A 362      21.109  43.370  60.395  1.00 25.45           N
ATOM    308  CA  GLY A 362      21.837  43.090  61.629  1.00 25.87           C
ATOM    309  C   GLY A 362      23.137  42.354  61.380  1.00 26.22           C
ATOM    310  O   GLY A 362      23.284  41.679  60.359  1.00 26.25           O
ATOM    311  N   ALA A 363      24.075  42.479  62.319  1.00 26.41           N
ATOM    312  CA  ALA A 363      25.381  41.818  62.222  1.00 26.59           C
ATOM    313  C   ALA A 363      26.126  41.768  63.555  1.00 26.72           C
ATOM    314  O   ALA A 363      25.861  42.559  64.461  1.00 26.55           O
ATOM    315  CB  ALA A 363      26.249  42.524  61.174  1.00 26.57           C
ATOM    316  N   ASP A 364      27.056  40.824  63.659  1.00 27.32           N
ATOM    317  CA  ASP A 364      28.113  40.872  64.670  1.00 27.96           C
ATOM    318  C   ASP A 364      29.148  41.914  64.252  1.00 28.25           C
ATOM    319  O   ASP A 364      29.701  41.834  63.153  1.00 28.09           O
ATOM    320  CB  ASP A 364      28.823  39.523  64.769  1.00 28.03           C
ATOM    321  CG  ASP A 364      28.051  38.499  65.580  1.00 28.42           C
ATOM    322  OD1 ASP A 364      26.808  38.599  65.703  1.00 28.94           O
ATOM    323  OD2 ASP A 364      28.711  37.568  66.085  1.00 28.84           O
ATOM    324  N   GLU A 365      29.402  42.889  65.116  1.00 28.82           N
ATOM    325  CA  GLU A 365      30.506  43.825  64.902  1.00 29.60           C
ATOM    326  C   GLU A 365      31.732  43.329  65.671  1.00 29.82           C
ATOM    327  O   GLU A 365      31.867  43.586  66.872  1.00 29.92           O
ATOM    328  CB  GLU A 365      30.113  45.237  65.343  1.00 29.43           C
ATOM    329  CG  GLU A 365      31.176  46.299  65.088  1.00 30.08           C
ATOM    330  CD  GLU A 365      30.750  47.681  65.553  1.00 30.47           C
ATOM    331  OE1 GLU A 365      30.573  47.879  66.801  1.00 31.38           O
ATOM    332  OE2 GLU A 365      30.597  48.577  64.661  1.00 32.02           O
ATOM    333  N   ARG A 366      32.609  42.604  64.979  1.00 30.14           N
ATOM    334  CA  ARG A 366      33.786  42.000  65.610  1.00 30.64           C
ATOM    335  C   ARG A 366      35.027  42.888  65.433  1.00 31.44           C
ATOM    336  O   ARG A 366      35.735  42.794  64.422  1.00 31.37           O
ATOM    337  CB  ARG A 366      34.010  40.577  65.077  1.00 30.44           C
ATOM    338  CG  ARG A 366      32.838  39.628  65.330  1.00 30.23           C
ATOM    339  CD  ARG A 366      33.048  38.251  64.723  1.00 30.14           C
ATOM    340  NE  ARG A 366      31.859  37.412  64.884  1.00 30.01           N
ATOM    341  CZ  ARG A 366      31.818  36.092  64.690  1.00 29.73           C
ATOM    342  NH1 ARG A 366      32.904  35.422  64.317  1.00 29.14           N
ATOM    343  NH2 ARG A 366      30.678  35.437  64.867  1.00 28.73           N
ATOM    344  N   ARG A 367      35.274  43.743  66.432  1.00 32.27           N
ATOM    345  CA  ARG A 367      36.270  44.828  66.350  1.00 33.32           C
ATOM    346  C   ARG A 367      37.701  44.372  66.026  1.00 33.71           C
ATOM    347  O   ARG A 367      38.281  44.799  65.029  1.00 33.82           O
ATOM    348  CB  ARG A 367      36.244  45.687  67.626  1.00 33.36           C
ATOM    349  CG  ARG A 367      37.319  46.769  67.688  1.00 33.75           C
ATOM    350  CD  ARG A 367      37.065  47.780  68.801  1.00 34.04           C
ATOM    351  NE  ARG A 367      36.038  48.758  68.436  1.00 36.56           N
ATOM    352  CZ  ARG A 367      36.251  49.861  67.712  1.00 37.62           C
ATOM    353  NH1 ARG A 367      37.465  50.156  67.255  1.00 38.38           N
ATOM    354  NH2 ARG A 367      35.239  50.676  67.438  1.00 37.68           N
ATOM    355  N   LEU A 368      38.258  43.507  66.865  1.00 34.18           N
ATOM    356  CA  LEU A 368      39.621  43.013  66.690  1.00 34.76           C
ATOM    357  C   LEU A 368      39.618  41.567  67.136  1.00 34.62           C
ATOM    358  O   LEU A 368      40.381  41.211  68.055  1.00 35.34           O
ATOM    359  CB  LEU A 368      40.577  43.815  67.604  1.00 35.04           C
ATOM    360  CG  LEU A 368      40.255  44.215  69.076  1.00 35.47           C
ATOM    361  CD1 LEU A 368      39.579  43.129  69.942  1.00 35.53           C
ATOM    362  CD2 LEU A 368      41.515  44.703  69.783  1.00 35.36           C
ATOM    363  N   HIS A 369      38.929  40.666  66.436  1.00 33.93           N
ATOM    364  CA  HIS A 369      39.323  40.134  65.150  1.00 32.84           C
ATOM    365  C   HIS A 369      38.123  39.426  64.500  1.00 32.11           C
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ATOM    366  O   HIS A 369      36.996  39.907  64.578  1.00 32.24           O
ATOM    367  CB  HIS A 369      40.279  39.017  65.536  1.00 32.98           C
ATOM    368  CG  HIS A 369      39.838  38.310  66.786  1.00 32.77           C
ATOM    369  ND1 HIS A 369      38.788  37.416  66.803  1.00 32.94           N
ATOM    370  CD2 HIS A 369      40.230  38.448  68.075  1.00 32.59           C
ATOM    371  CE1 HIS A 369      38.588  36.995  68.039  1.00 32.76           C
ATOM    372  NE2 HIS A 369      39.449  37.608  68.831  1.00 32.77           N
ATOM    373  N   SER A 370      38.364  38.249  63.923  1.00 30.95           N
ATOM    374  CA  SER A 370      37.355  37.536  63.129  1.00 29.97           C
ATOM    375  C   SER A 370      36.725  36.290  63.787  1.00 29.37           C
ATOM    376  O   SER A 370      35.760  35.730  63.270  1.00 29.13           O
ATOM    377  CB  SER A 370      37.955  37.165  61.770  1.00 29.69           C
ATOM    378  OG  SER A 370      36.954  36.752  60.872  1.00 29.06           O
ATOM    379  N   SER A 371      37.258  35.858  64.924  1.00 28.82           N
ATOM    380  CA  SER A 371      36.833  34.589  65.513  1.00 28.07           C
ATOM    381  C   SER A 371      35.525  34.698  66.298  1.00 27.81           C
ATOM    382  O   SER A 371      34.994  35.797  66.498  1.00 27.91           O
ATOM    383  CB  SER A 371      37.951  33.989  66.366  1.00 28.06           C
ATOM    384  OG  SER A 371      39.005  33.512  65.544  1.00 28.00           O
ATOM    385  N   ASP A 372      35.016  33.555  66.742  1.00 26.99           N
ATOM    386  CA  ASP A 372      33.728  33.490  67.413  1.00 26.46           C
ATOM    387  C   ASP A 372      33.764  33.941  68.885  1.00 26.44           C
ATOM    388  O   ASP A 372      33.114  33.342  69.742  1.00 26.31           O
ATOM    389  CB  ASP A 372      33.143  32.080  67.264  1.00 26.30           C
ATOM    390  CG  ASP A 372      32.797  31.740  65.812  1.00 25.70           C
ATOM    391  OD1 ASP A 372      32.637  32.676  65.000  1.00 23.97           O
ATOM    392  OD2 ASP A 372      32.680  30.538  65.485  1.00 24.88           O
ATOM    393  N   TRP A 373      34.518  35.006  69.162  1.00 26.28           N
ATOM    394  CA  TRP A 373      34.634  35.579  70.514  1.00 26.40           C
ATOM    395  C   TRP A 373      35.249  36.979  70.455  1.00 26.58           C
ATOM    396  O   TRP A 373      35.599  37.464  69.373  1.00 26.63           O
ATOM    397  CB  TRP A 373      35.470  34.681  71.442  1.00 26.12           C
ATOM    398  CG  TRP A 373      36.812  34.285  70.878  1.00 26.06           C
ATOM    399  CD1 TRP A 373      37.965  35.016  70.918  1.00 25.93           C
ATOM    400  CD2 TRP A 373      37.135  33.062  70.194  1.00 26.02           C
ATOM    401  NE1 TRP A 373      38.988  34.330  70.299  1.00 26.45           N
ATOM    402  CE2 TRP A 373      38.508  33.128  69.846  1.00 26.76           C
ATOM    403  CE3 TRP A 373      36.401  31.921  69.840  1.00 25.43           C
ATOM    404  CZ2 TRP A 373      39.165  32.089  69.160  1.00 26.16           C
ATOM    405  CZ3 TRP A 373      37.052  30.887  69.156  1.00 26.22           C
ATOM    406  CH2 TRP A 373      38.423  30.982  68.822  1.00 26.10           C
ATOM    407  N   GLY A 374      35.371  37.622  71.616  1.00 26.49           N
ATOM    408  CA  GLY A 374      36.062  38.903  71.711  1.00 26.73           C
ATOM    409  C   GLY A 374      35.142  40.085  71.940  1.00 26.85           C
ATOM    410  O   GLY A 374      34.050  39.943  72.489  1.00 26.64           O
ATOM    411  N   ASP A 375      35.608  41.263  71.537  1.00 27.07           N
ATOM    412  CA  ASP A 375      34.787  42.460  71.569  1.00 27.15           C
ATOM    413  C   ASP A 375      33.867  42.383  70.361  1.00 27.15           C
ATOM    414  O   ASP A 375      34.283  42.602  69.221  1.00 27.30           O
ATOM    415  CB  ASP A 375      35.658  43.720  71.538  1.00 27.22           C
ATOM    416  CG  ASP A 375      34.857  45.000  71.746  1.00 27.62           C
ATOM    417  OD1 ASP A 375      33.613  44.934  71.865  1.00 28.63           O
ATOM    418  OD2 ASP A 375      35.477  46.084  71.789  1.00 27.44           O
ATOM    419  N   ILE A 376      32.622  42.006  70.624  1.00 27.16           N
ATOM    420  CA  ILE A 376      31.613  41.896  69.592  1.00 26.89           C
ATOM    421  C   ILE A 376      30.377  42.642  70.057  1.00 26.85           C
ATOM    422  O   ILE A 376      29.910  42.447  71.177  1.00 27.03           O
ATOM    423  CB  ILE A 376      31.254  40.427  69.271  1.00 26.88           C
ATOM    424  CG1 ILE A 376      32.512  39.608  68.969  1.00 26.64           C
ATOM    425  CG2 ILE A 376      30.290  40.365  68.084  1.00 26.87           C
ATOM    426  CD1 ILE A 376      32.265  38.120  68.769  1.00 26.87           C
ATOM    427  N   GLY A 377      29.871  43.517  69.196  1.00 26.82           N
ATOM    428  CA  GLY A 377      28.616  44.218  69.455  1.00 26.46           C
ATOM    429  C   GLY A 377      27.549  43.758  68.486  1.00 26.10           C
ATOM    430  O   GLY A 377      27.861  43.285  67.387  1.00 25.96           O
ATOM    431  N   MET A 378      26.291  43.867  68.904  1.00 26.01           N
ATOM    432  CA  MET A 378      25.154  43.602  68.018  1.00 25.87           C
ATOM    433  C   MET A 378      24.736  44.936  67.420  1.00 25.89           C
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ATOM    434  O   MET A 378      24.327  45.850  68.148  1.00 25.93           O
ATOM    435  CB  MET A 378      23.982  42.976  68.775  1.00 25.73           C
ATOM    436  CG  MET A 378      24.317  41.738  69.586  1.00 26.06           C
ATOM    437  SD  MET A 378      24.606  40.270  68.578  1.00 26.92           S
ATOM    438  CE  MET A 378      26.378  40.361  68.337  1.00 25.08           C
ATOM    439  N   VAL A 379      24.867  45.049  66.100  1.00 25.62           N
ATOM    440  CA  VAL A 379      24.628  46.309  65.400  1.00 25.63           C
ATOM    441  C   VAL A 379      23.557  46.144  64.333  1.00 25.64           C
ATOM    442  O   VAL A 379      23.428  45.077  63.735  1.00 25.94           O
ATOM    443  CB  VAL A 379      25.933  46.860  64.723  1.00 25.51           C
ATOM    444  CG1 VAL A 379      26.968  47.233  65.755  1.00 25.29           C
ATOM    445  CG2 VAL A 379      26.524  45.848  63.743  1.00 25.59           C
ATOM    446  N   ILE A 380      22.788  47.197  64.091  1.00 25.68           N
ATOM    447  CA  ILE A 380      21.940  47.234  62.900  1.00 25.87           C
ATOM    448  C   ILE A 380      22.167  48.491  62.068  1.00 26.24           C
ATOM    449  O   ILE A 380      22.762  49.465  62.535  1.00 26.21           O
ATOM    450  CB  ILE A 380      20.405  47.030  63.195  1.00 25.77           C
ATOM    451  CG1 ILE A 380      19.844  48.126  64.101  1.00 24.95           C
ATOM    452  CG2 ILE A 380      20.116  45.627  63.740  1.00 25.80           C
ATOM    453  CD1 ILE A 380      19.191  49.270  63.342  1.00 25.56           C
ATOM    454  N   ARG A 381      21.711  48.430  60.822  1.00 26.76           N
ATOM    455  CA  ARG A 381      21.576  49.593  59.957  1.00 27.12           C
ATOM    456  C   ARG A 381      20.183  49.553  59.337  1.00 27.37           C
ATOM    457  O   ARG A 381      19.595  48.479  59.189  1.00 27.09           O
ATOM    458  CB  ARG A 381      22.640  49.587  58.866  1.00 27.08           C
ATOM    459  CG  ARG A 381      24.045  49.867  59.369  1.00 27.23           C
ATOM    460  CD  ARG A 381      25.014  50.059  58.210  1.00 27.34           C
ATOM    461  NE  ARG A 381      24.865  51.367  57.578  1.00 27.64           N
ATOM    462  CZ  ARG A 381      25.474  51.743  56.454  1.00 28.85           C
ATOM    463  NH1 ARG A 381      26.281  50.905  55.806  1.00 28.43           N
ATOM    464  NH2 ARG A 381      25.264  52.964  55.967  1.00 28.40           N
ATOM    465  N   ARG A 382      19.665  50.729  58.988  1.00 27.77           N
ATOM    466  CA  ARG A 382      18.313  50.866  58.451  1.00 28.21           C
ATOM    467  C   ARG A 382      18.303  51.440  57.039  1.00 28.60           C
ATOM    468  O   ARG A 382      19.079  52.343  56.722  1.00 28.73           O
ATOM    469  CB  ARG A 382      17.479  51.774  59.353  1.00 28.02           C
ATOM    470  CG  ARG A 382      17.141  51.194  60.697  1.00 27.54           C
ATOM    471  CD  ARG A 382      16.434  52.213  61.580  1.00 27.37           C
ATOM    472  NE  ARG A 382      15.061  52.486  61.147  1.00 27.63           N
ATOM    473  CZ  ARG A 382      14.679  53.564  60.462  1.00 27.60           C
ATOM    474  NH1 ARG A 382      15.562  54.494  60.112  1.00 26.94           N
ATOM    475  NH2 ARG A 382      13.407  53.712  60.124  1.00 27.55           N
ATOM    476  N   SER A 383      17.413  50.924  56.198  1.00 29.07           N
ATOM    477  CA  SER A 383      17.168  51.525  54.895  1.00 29.40           C
ATOM    478  C   SER A 383      15.696  51.844  54.722  1.00 29.69           C
ATOM    479  O   SER A 383      14.834  51.027  55.037  1.00 29.57           O
ATOM    480  CB  SER A 383      17.627  50.617  53.763  1.00 29.44           C
ATOM    481  OG  SER A 383      17.447  51.262  52.510  1.00 29.80           O
ATOM    482  N   GLU A 384      15.423  53.036  54.204  1.00 30.22           N
ATOM    483  CA  GLU A 384      14.058  53.467  53.937  1.00 30.89           C
ATOM    484  C   GLU A 384      13.771  53.506  52.439  1.00 30.86           C
ATOM    485  O   GLU A 384      12.621  53.431  52.023  1.00 31.24           O
ATOM    486  CB  GLU A 384      13.781  54.821  54.597  1.00 30.80           C
ATOM    487  CG  GLU A 384      14.126  54.850  56.088  1.00 31.30           C
ATOM    488  CD  GLU A 384      13.552  56.051  56.820  1.00 31.86           C
ATOM    489  OE1 GLU A 384      13.309  57.095  56.174  1.00 33.40           O
ATOM    490  OE2 GLU A 384      13.346  55.950  58.052  1.00 33.27           O
ATOM    491  N   ASP A 385      14.818  53.606  51.628  1.00 31.13           N
ATOM    492  CA  ASP A 385      14.658  53.556  50.172  1.00 31.34           C
ATOM    493  C   ASP A 385      14.805  52.123  49.664  1.00 31.26           C
ATOM    494  O   ASP A 385      15.277  51.879  48.550  1.00 31.16           O
ATOM    495  CB  ASP A 385      15.618  54.522  49.460  1.00 31.18           C
ATOM    496  CG  ASP A 385      17.071  54.332  49.874  1.00 32.28           C
ATOM    497  OD1 ASP A 385      17.382  53.392  50.644  1.00 33.22           O
ATOM    498  OD2 ASP A 385      17.912  55.135  49.414  1.00 32.58           O
ATOM    499  N   ASN A 386      14.383  51.185  50.507  1.00 31.44           N
ATOM    500  CA  ASN A 386      14.347  49.765  50.177  1.00 31.44           C
ATOM    501  C   ASN A 386      15.694  49.228  49.673  1.00 31.55           C
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ATOM    502  O   ASN A 386      15.761  48.587  48.631  1.00 31.54           O
ATOM    503  CB  ASN A 386      13.220  49.488  49.172  1.00 31.30           C
ATOM    504  CG  ASN A 386      12.712  48.063  49.242  1.00 31.04           C
ATOM    505  OD1 ASN A 386      12.336  47.576  50.309  1.00 31.42           O
ATOM    506  ND2 ASN A 386      12.687  47.390  48.102  1.00 29.95           N
ATOM    507  N   GLY A 387      16.765  49.519  50.408  1.00 31.77           N
ATOM    508  CA  GLY A 387      18.075  48.931  50.132  1.00 32.05           C
ATOM    509  C   GLY A 387      19.057  49.724  49.286  1.00 32.33           C
ATOM    510  O   GLY A 387      20.197  49.292  49.098  1.00 32.56           O
ATOM    511  N   LYS A 388      18.636  50.879  48.776  1.00 32.47           N
ATOM    512  CA  LYS A 388      19.522  51.715  47.961  1.00 32.65           C
ATOM    513  C   LYS A 388      20.579  52.404  48.822  1.00 32.41           C
ATOM    514  O   LYS A 388      21.776  52.251  48.577  1.00 32.31           O
ATOM    515  CB  LYS A 388      18.729  52.744  47.148  1.00 32.87           C
ATOM    516  CG  LYS A 388      17.852  52.130  46.071  1.00 34.42           C
ATOM    517  CD  LYS A 388      16.941  53.165  45.423  1.00 36.60           C
ATOM    518  CE  LYS A 388      16.009  52.500  44.416  1.00 37.43           C
ATOM    519  NZ  LYS A 388      15.032  53.461  43.836  1.00 38.43           N
ATOM    520  N   THR A 389      20.122  53.164  49.818  1.00 32.11           N
ATOM    521  CA  THR A 389      21.004  53.819  50.785  1.00 31.69           C
ATOM    522  C   THR A 389      20.696  53.306  52.186  1.00 31.24           C
ATOM    523  O   THR A 389      19.598  52.811  52.448  1.00 31.38           O
ATOM    524  CB  THR A 389      20.877  55.366  50.759  1.00 31.91           C
ATOM    525  OG1 THR A 389      19.557  55.757  51.162  1.00 31.95           O
ATOM    526  CG2 THR A 389      21.183  55.926  49.368  1.00 31.62           C
ATOM    527  N   TRP A 390      21.670  53.418  53.082  1.00 30.59           N
ATOM    528  CA  TRP A 390      21.539  52.867  54.419  1.00 30.15           C
ATOM    529  C   TRP A 390      22.022  53.888  55.431  1.00 30.11           C
ATOM    530  O   TRP A 390      23.006  54.587  55.182  1.00 29.99           O
ATOM    531  CB  TRP A 390      22.319  51.550  54.542  1.00 29.91           C
ATOM    532  CG  TRP A 390      21.814  50.459  53.621  1.00 29.72           C
ATOM    533  CD1 TRP A 390      22.061  50.337  52.281  1.00 29.74           C
ATOM    534  CD2 TRP A 390      20.975  49.346  53.974  1.00 29.99           C
ATOM    535  NE1 TRP A 390      21.425  49.224  51.776  1.00 30.06           N
ATOM    536  CE2 TRP A 390      20.753  48.597  52.793  1.00 29.99           C
ATOM    537  CE3 TRP A 390      20.393  48.905  55.175  1.00 29.73           C
ATOM    538  CZ2 TRP A 390      19.976  47.430  52.777  1.00 29.68           C
ATOM    539  CZ3 TRP A 390      19.616  47.749  55.156  1.00 29.62           C
ATOM    540  CH2 TRP A 390      19.419  47.024  53.964  1.00 29.94           C
ATOM    541  N   GLY A 391      21.322  53.969  56.563  1.00 29.91           N
ATOM    542  CA  GLY A 391      21.615  54.951  57.608  1.00 29.89           C
ATOM    543  C   GLY A 391      22.840  54.619  58.442  1.00 29.93           C
ATOM    544  O   GLY A 391      23.709  53.862  58.009  1.00 29.81           O
ATOM    545  N   ASP A 392      22.908  55.195  59.641  1.00 29.99           N
ATOM    546  CA  ASP A 392      24.019  54.959  60.563  1.00 30.27           C
ATOM    547  C   ASP A 392      23.923  53.598  61.241  1.00 30.61           C
ATOM    548  O   ASP A 392      22.838  53.034  61.376  1.00 30.75           O
ATOM    549  CB  ASP A 392      24.068  56.051  61.640  1.00 30.30           C
ATOM    550  CG  ASP A 392      24.459  57.414  61.085  1.00 30.07           C
ATOM    551  OD1 ASP A 392      25.231  57.472  60.108  1.00 29.41           O
ATOM    552  OD2 ASP A 392      23.994  58.435  61.631  1.00 30.16           O
ATOM    553  N   ARG A 393      25.067  53.078  61.672  1.00 30.83           N
ATOM    554  CA  ARG A 393      25.100  51.872  62.485  1.00 31.07           C
ATOM    555  C   ARG A 393      24.545  52.195  63.869  1.00 30.97           C
ATOM    556  O   ARG A 393      25.058  53.078  64.564  1.00 31.12           O
ATOM    557  CB  ARG A 393      26.529  51.322  62.592  1.00 30.93           C
ATOM    558  CG  ARG A 393      27.152  50.940  61.259  1.00 31.32           C
ATOM    559  CD  ARG A 393      28.628  50.574  61.387  1.00 31.99           C
ATOM    560  NE  ARG A 393      29.465  51.745  61.645  1.00 34.32           N
ATOM    561  CZ  ARG A 393      30.217  51.911  62.728  1.00 35.30           C
ATOM    562  NH1 ARG A 393      30.268  50.974  63.663  1.00 36.31           N
ATOM    563  NH2 ARG A 393      30.933  53.016  62.874  1.00 36.01           N
ATOM    564  N   VAL A 394      23.478  51.493  64.248  1.00 30.78           N
ATOM    565  CA  VAL A 394      22.910  51.594  65.589  1.00 30.37           C
ATOM    566  C   VAL A 394      23.353  50.365  66.379  1.00 30.14           C
ATOM    567  O   VAL A 394      23.014  49.242  66.030  1.00 30.25           O
ATOM    568  CB  VAL A 394      21.350  51.697  65.559  1.00 30.44           C
ATOM    569  CG1 VAL A 394      20.762  51.531  66.950  1.00 30.63           C
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ATOM    570  CG2 VAL A 394      20.901  53.026  64.964  1.00 29.99           C
ATOM    571  N   THR A 395      24.129  50.589  67.432  1.00 30.03           N
ATOM    572  CA  THR A 395      24.567  49.511  68.308  1.00 29.72           C
ATOM    573  C   THR A 395      23.466  49.164  69.305  1.00 29.69           C
ATOM    574  O   THR A 395      23.027  50.012  70.089  1.00 29.73           O
ATOM    575  CB  THR A 395      25.858  49.885  69.065  1.00 29.76           C
ATOM    576  OG1 THR A 395      26.867  50.265  68.122  1.00 29.58           O
ATOM    577  CG2 THR A 395      26.365  48.696  69.894  1.00 29.36           C
ATOM    578  N   ILE A 396      23.015  47.915  69.260  1.00 29.40           N
ATOM    579  CA  ILE A 396      21.982  47.445  70.166  1.00 29.08           C
ATOM    580  C   ILE A 396      22.631  47.128  71.512  1.00 28.98           C
ATOM    581  O   ILE A 396      22.198  47.618  72.555  1.00 28.73           O
ATOM    582  CB  ILE A 396      21.245  46.199  69.604  1.00 29.20           C
ATOM    583  CG1 ILE A 396      20.733  46.460  68.177  1.00 29.44           C
ATOM    584  CG2 ILE A 396      20.109  45.782  70.537  1.00 28.85           C
ATOM    585  CD1 ILE A 396      20.025  45.270  67.519  1.00 28.92           C
ATOM    586  N   THR A 397      23.676  46.307  71.474  1.00 29.01           N
ATOM    587  CA  THR A 397      24.390  45.905  72.678  1.00 29.06           C
ATOM    588  C   THR A 397      25.857  45.710  72.365  1.00 29.29           C
ATOM    589  O   THR A 397      26.204  45.037  71.398  1.00 29.42           O
ATOM    590  CB  THR A 397      23.844  44.573  73.277  1.00 29.04           C
ATOM    591  OG1 THR A 397      22.411  44.585  73.292  1.00 28.28           O
ATOM    592  CG2 THR A 397      24.366  44.367  74.694  1.00 28.30           C
ATOM    593  N   ASN A 398      26.706  46.332  73.174  1.00 29.71           N
ATOM    594  CA  ASN A 398      28.119  45.987  73.234  1.00 30.16           C
ATOM    595  C   ASN A 398      28.574  46.089  74.676  1.00 30.41           C
ATOM    596  O   ASN A 398      28.649  47.182  75.229  1.00 30.44           O
ATOM    597  CB  ASN A 398      28.968  46.892  72.336  1.00 29.97           C
ATOM    598  CG  ASN A 398      30.362  46.316  72.061  1.00 30.47           C
ATOM    599  OD1 ASN A 398      30.812  45.359  72.706  1.00 29.87           O
ATOM    600  ND2 ASN A 398      31.052  46.908  71.094  1.00 30.90           N
ATOM    601  N   LEU A 399      28.846  44.941  75.285  1.00 31.04           N
ATOM    602  CA  LEU A 399      29.321  44.891  76.664  1.00 31.74           C
ATOM    603  C   LEU A 399      30.771  45.348  76.715  1.00 32.40           C
ATOM    604  O   LEU A 399      31.552  45.038  75.815  1.00 32.19           O
ATOM    605  CB  LEU A 399      29.171  43.476  77.233  1.00 31.69           C
ATOM    606  CG  LEU A 399      27.756  42.873  77.184  1.00 31.25           C
ATOM    607  CD1 LEU A 399      27.756  41.393  77.562  1.00 29.67           C
ATOM    608  CD2 LEU A 399      26.785  43.668  78.056  1.00 29.66           C
ATOM    609  N   ARG A 400      31.123  46.101  77.754  1.00 33.41           N
ATOM    610  CA  ARG A 400      32.475  46.651  77.858  1.00 34.49           C
ATOM    611  C   ARG A 400      33.505  45.566  78.147  1.00 35.22           C
ATOM    612  O   ARG A 400      33.221  44.611  78.874  1.00 35.31           O
ATOM    613  CB  ARG A 400      32.545  47.772  78.895  1.00 34.35           C
ATOM    614  CG  ARG A 400      32.412  47.330  80.338  1.00 34.53           C
ATOM    615  CD  ARG A 400      32.211  48.542  81.231  1.00 34.00           C
ATOM    616  NE  ARG A 400      32.393  48.217  82.639  1.00 33.98           N
ATOM    617  CZ  ARG A 400      33.568  48.196  83.260  1.00 33.20           C
ATOM    618  NH1 ARG A 400      34.683  48.475  82.598  1.00 32.29           N
ATOM    619  NH2 ARG A 400      33.624  47.888  84.547  1.00 32.93           N
ATOM    620  N   ASP A 401      34.690  45.715  77.560  1.00 36.17           N
ATOM    621  CA  ASP A 401      35.758  44.734  77.734  1.00 37.21           C
ATOM    622  C   ASP A 401      36.334  44.773  79.146  1.00 37.58           C
ATOM    623  O   ASP A 401      36.162  45.756  79.868  1.00 37.55           O
ATOM    624  CB  ASP A 401      36.867  44.931  76.688  1.00 37.32           C
ATOM    625  CG  ASP A 401      37.592  46.265  76.826  1.00 38.42           C
ATOM    626  OD1 ASP A 401      37.111  47.164  77.553  1.00 39.60           O
ATOM    627  OD2 ASP A 401      38.654  46.421  76.188  1.00 40.20           O
ATOM    628  N   ASN A 402      36.990  43.683  79.534  1.00 38.33           N
ATOM    629  CA  ASN A 402      37.743  43.634  80.773  1.00 39.07           C
ATOM    630  C   ASN A 402      39.088  44.332  80.572  1.00 39.53           C
ATOM    631  O   ASN A 402      39.987  43.765  79.940  1.00 39.49           O
ATOM    632  CB  ASN A 402      37.938  42.185  81.222  1.00 39.26           C
ATOM    633  CG  ASN A 402      38.651  42.071  82.560  1.00 39.57           C
ATOM    634  OD1 ASN A 402      39.394  42.967  82.968  1.00 40.75           O
ATOM    635  ND2 ASN A 402      38.433  40.960  83.246  1.00 39.63           N
ATOM    636  N   PRO A 403      39.238  45.552  81.127  1.00 39.98           N
ATOM    637  CA  PRO A 403      40.410  46.394  80.866  1.00 40.36           C
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ATOM    638  C   PRO A 403      41.695  45.803  81.439  1.00 40.65           C
ATOM    639  O   PRO A 403      42.784  46.239  81.071  1.00 40.74           O
ATOM    640  CB  PRO A 403      40.076  47.707  81.591  1.00 40.33           C
ATOM    641  CG  PRO A 403      38.597  47.649  81.865  1.00 40.40           C
ATOM    642  CD  PRO A 403      38.314  46.200  82.075  1.00 40.12           C
ATOM    643  N   LYS A 404      41.557  44.816  82.323  1.00 40.93           N
ATOM    644  CA  LYS A 404      42.700  44.216  83.008  1.00 41.05           C
ATOM    645  C   LYS A 404      42.965  42.786  82.547  1.00 40.93           C
ATOM    646  O   LYS A 404      43.735  42.054  83.177  1.00 40.95           O
ATOM    647  CB  LYS A 404      42.515  44.285  84.532  1.00 41.18           C
ATOM    648  CG  LYS A 404      42.646  45.697  85.113  1.00 41.88           C
ATOM    649  CD  LYS A 404      44.114  46.074  85.350  1.00 43.64           C
ATOM    650  CE  LYS A 404      44.364  47.574  85.165  1.00 44.41           C
ATOM    651  NZ  LYS A 404      43.522  48.428  86.052  1.00 45.12           N
ATOM    652  N   ALA A 405      42.335  42.398  81.440  1.00 40.71           N
ATOM    653  CA  ALA A 405      42.599  41.100  80.828  1.00 40.53           C
ATOM    654  C   ALA A 405      43.935  41.142  80.093  1.00 40.40           C
ATOM    655  O   ALA A 405      44.244  42.124  79.405  1.00 40.42           O
ATOM    656  CB  ALA A 405      41.478  40.719  79.877  1.00 40.55           C
ATOM    657  N   SER A 406      44.722  40.081  80.246  1.00 40.10           N
ATOM    658  CA  SER A 406      46.044  39.993  79.619  1.00 39.82           C
ATOM    659  C   SER A 406      45.986  39.793  78.096  1.00 39.72           C
ATOM    660  O   SER A 406      46.813  40.347  77.366  1.00 39.83           O
ATOM    661  CB  SER A 406      46.879  38.893  80.276  1.00 39.85           C
ATOM    662  OG  SER A 406      46.173  37.668  80.309  1.00 39.28           O
ATOM    663  N   ASP A 407      45.017  39.002  77.630  1.00 39.22           N
ATOM    664  CA  ASP A 407      44.792  38.790  76.196  1.00 38.46           C
ATOM    665  C   ASP A 407      43.480  39.458  75.784  1.00 38.10           C
ATOM    666  O   ASP A 407      42.400  38.931  76.063  1.00 38.19           O
ATOM    667  CB  ASP A 407      44.779  37.287  75.867  1.00 38.37           C
ATOM    668  CG  ASP A 407      44.613  36.993  74.368  1.00 37.98           C
ATOM    669  OD1 ASP A 407      44.326  37.920  73.571  1.00 37.46           O
ATOM    670  OD2 ASP A 407      44.762  35.809  73.991  1.00 37.17           O
ATOM    671  N   PRO A 408      43.569  40.614  75.096  1.00 37.68           N
ATOM    672  CA  PRO A 408      42.379  41.430  74.851  1.00 37.23           C
ATOM    673  C   PRO A 408      41.490  40.870  73.744  1.00 36.84           C
ATOM    674  O   PRO A 408      40.331  41.266  73.633  1.00 37.06           O
ATOM    675  CB  PRO A 408      42.954  42.796  74.435  1.00 37.30           C
ATOM    676  CG  PRO A 408      44.462  42.655  74.469  1.00 37.42           C
ATOM    677  CD  PRO A 408      44.770  41.199  74.473  1.00 37.68           C
ATOM    678  N   SER A 409      42.030  39.960  72.935  1.00 36.22           N
ATOM    679  CA  SER A 409      41.273  39.328  71.862  1.00 35.40           C
ATOM    680  C   SER A 409      40.288  38.308  72.427  1.00 34.95           C
ATOM    681  O   SER A 409      39.351  37.893  71.741  1.00 34.89           O
ATOM    682  CB  SER A 409      42.215  38.668  70.846  1.00 35.37           C
ATOM    683  OG  SER A 409      42.730  37.442  71.329  1.00 35.18           O
ATOM    684  N   ILE A 410      40.517  37.905  73.676  1.00 34.22           N
ATOM    685  CA  ILE A 410      39.608  37.017  74.403  1.00 33.59           C
ATOM    686  C   ILE A 410      39.131  37.661  75.709  1.00 33.24           C
ATOM    687  O   ILE A 410      38.567  36.985  76.575  1.00 33.12           O
ATOM    688  CB  ILE A 410      40.252  35.620  74.694  1.00 33.66           C
ATOM    689  CG1 ILE A 410      41.502  35.753  75.576  1.00 33.32           C
ATOM    690  CG2 ILE A 410      40.565  34.878  73.385  1.00 33.85           C
ATOM    691  CD1 ILE A 410      41.953  34.459  76.234  1.00 33.17           C
ATOM    692  N   GLY A 411      39.345  38.973  75.829  1.00 32.68           N
ATOM    693  CA  GLY A 411      39.169  39.684  77.096  1.00 31.89           C
ATOM    694  C   GLY A 411      37.936  40.555  77.206  1.00 31.32           C
ATOM    695  O   GLY A 411      37.949  41.594  77.872  1.00 31.07           O
ATOM    696  N   SER A 412      36.861  40.122  76.558  1.00 30.95           N
ATOM    697  CA  SER A 412      35.594  40.840  76.604  1.00 30.25           C
ATOM    698  C   SER A 412      34.445  39.849  76.779  1.00 29.72           C
ATOM    699  O   SER A 412      34.501  38.740  76.241  1.00 29.82           O
ATOM    700  CB  SER A 412      35.401  41.674  75.332  1.00 30.16           C
ATOM    701  OG  SER A 412      34.274  42.530  75.440  1.00 30.49           O
ATOM    702  N   PRO A 413      33.421  40.226  77.572  1.00 29.10           N
ATOM    703  CA  PRO A 413      32.151  39.500  77.543  1.00 28.57           C
ATOM    704  C   PRO A 413      31.594  39.541  76.126  1.00 27.90           C
ATOM    705  O   PRO A 413      31.804  40.520  75.414  1.00 27.64           O
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ATOM    706  CB  PRO A 413      31.262  40.304  78.496  1.00 28.54           C
ATOM    707  CG  PRO A 413      32.214  41.008  79.400  1.00 28.65           C
ATOM    708  CD  PRO A 413      33.408  41.322  78.559  1.00 28.96           C
ATOM    709  N   VAL A 414      30.899  38.484  75.720  1.00 27.49           N
ATOM    710  CA  VAL A 414      30.558  38.296  74.311  1.00 26.85           C
ATOM    711  C   VAL A 414      29.055  38.322  74.042  1.00 26.29           C
ATOM    712  O   VAL A 414      28.283  37.676  74.743  1.00 26.49           O
ATOM    713  CB  VAL A 414      31.149  36.963  73.757  1.00 26.98           C
ATOM    714  CG1 VAL A 414      30.959  36.872  72.246  1.00 26.71           C
ATOM    715  CG2 VAL A 414      32.629  36.822  74.118  1.00 26.56           C
ATOM    716  N   ASN A 415      28.660  39.098  73.036  1.00 25.59           N
ATOM    717  CA  ASN A 415      27.382  38.916  72.351  1.00 24.74           C
ATOM    718  C   ASN A 415      27.679  38.409  70.941  1.00 24.22           C
ATOM    719  O   ASN A 415      28.611  38.886  70.301  1.00 23.92           O
ATOM    720  CB  ASN A 415      26.597  40.228  72.299  1.00 24.63           C
ATOM    721  CG  ASN A 415      26.042  40.639  73.658  1.00 24.21           C
ATOM    722  OD1 ASN A 415      26.264  41.762  74.112  1.00 23.56           O
ATOM    723  ND2 ASN A 415      25.308  39.734  74.308  1.00 22.62           N
ATOM    724  N   ILE A 416      26.903  37.438  70.462  1.00 23.84           N
ATOM    725  CA  ILE A 416      27.221  36.742  69.207  1.00 22.95           C
ATOM    726  C   ILE A 416      25.994  36.065  68.589  1.00 23.06           C
ATOM    727  O   ILE A 416      25.214  35.426  69.303  1.00 23.14           O
ATOM    728  CB  ILE A 416      28.384  35.719  69.421  1.00 22.83           C
ATOM    729  CG1 ILE A 416      28.725  34.966  68.128  1.00 22.48           C
ATOM    730  CG2 ILE A 416      28.071  34.767  70.578  1.00 22.00           C
ATOM    731  CD1 ILE A 416      30.097  34.308  68.133  1.00 22.63           C
ATOM    732  N   ASP A 417      25.836  36.209  67.267  1.00 22.91           N
ATOM    733  CA  ASP A 417      24.730  35.603  66.498  1.00 22.74           C
ATOM    734  C   ASP A 417      23.358  36.188  66.862  1.00 22.69           C
ATOM    735  O   ASP A 417      22.872  35.973  67.965  1.00 22.74           O
ATOM    736  CB  ASP A 417      24.705  34.071  66.681  1.00 22.68           C
ATOM    737  CG  ASP A 417      25.959  33.379  66.140  1.00 22.73           C
ATOM    738  OD1 ASP A 417      26.776  34.034  65.463  1.00 22.83           O
ATOM    739  OD2 ASP A 417      26.117  32.165  66.380  1.00 21.41           O
ATOM    740  N   MET A 418      22.724  36.917  65.949  1.00 22.62           N
ATOM    741  CA  MET A 418      21.377  37.435  66.238  1.00 22.84           C
ATOM    742  C   MET A 418      20.276  36.870  65.339  1.00 22.23           C
ATOM    743  O   MET A 418      20.518  36.501  64.196  1.00 22.31           O
ATOM    744  CB  MET A 418      21.336  38.974  66.243  1.00 22.47           C
ATOM    745  CG  MET A 418      21.133  39.628  64.890  1.00 23.35           C
ATOM    746  SD  MET A 418      21.324  41.425  64.918  1.00 24.58           S
ATOM    747  CE  MET A 418      19.665  41.959  65.158  1.00 25.04           C
ATOM    748  N   VAL A 419      19.071  36.790  65.893  1.00 21.95           N
ATOM    749  CA  VAL A 419      17.866  36.540  65.120  1.00 21.49           C
ATOM    750  C   VAL A 419      16.988  37.791  65.198  1.00 21.50           C
ATOM    751  O   VAL A 419      16.809  38.365  66.274  1.00 21.03           O
ATOM    752  CB  VAL A 419      17.088  35.287  65.625  1.00 21.51           C
ATOM    753  CG1 VAL A 419      15.688  35.212  64.997  1.00 20.57           C
ATOM    754  CG2 VAL A 419      17.862  34.027  65.321  1.00 20.60           C
ATOM    755  N   LEU A 420      16.473  38.219  64.047  1.00 21.40           N
ATOM    756  CA  LEU A 420      15.499  39.300  63.986  1.00 21.44           C
ATOM    757  C   LEU A 420      14.096  38.780  63.683  1.00 21.50           C
ATOM    758  O   LEU A 420      13.940  37.803  62.952  1.00 21.66           O
ATOM    759  CB  LEU A 420      15.908  40.329  62.932  1.00 21.44           C
ATOM    760  CG  LEU A 420      17.082  41.224  63.311  1.00 20.77           C
ATOM    761  CD1 LEU A 420      17.558  42.058  62.119  1.00 20.39           C
ATOM    762  CD2 LEU A 420      16.676  42.103  64.475  1.00 20.58           C
ATOM    763  N   VAL A 421      13.088  39.433  64.262  1.00 21.66           N
ATOM    764  CA  VAL A 421      11.681  39.183  63.929  1.00 21.69           C
ATOM    765  C   VAL A 421      10.826  40.381  64.343  1.00 22.17           C
ATOM    766  O   VAL A 421      11.125  41.037  65.342  1.00 22.32           O
ATOM    767  CB  VAL A 421      11.150  37.851  64.557  1.00 21.68           C
ATOM    768  CG1 VAL A 421      11.107  37.917  66.094  1.00 20.68           C
ATOM    769  CG2 VAL A 421       9.786  37.475  63.970  1.00 21.48           C
ATOM    770  N   GLN A 422       9.791  40.687  63.563  1.00 22.68           N
ATOM    771  CA  GLN A 422       8.788  41.666  63.985  1.00 23.56           C
ATOM    772  C   GLN A 422       7.463  40.992  64.291  1.00 24.26           C
ATOM    773  O   GLN A 422       6.983  40.166  63.516  1.00 24.71           O
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ATOM    774  CB  GLN A 422       8.572  42.779  62.948  1.00 23.41           C
ATOM    775  CG  GLN A 422       7.658  43.902  63.472  1.00 23.31           C
ATOM    776  CD  GLN A 422       7.566  45.110  62.561  1.00 23.70           C
ATOM    777  OE1 GLN A 422       7.415  44.985  61.348  1.00 25.43           O
ATOM    778  NE2 GLN A 422       7.646  46.294  63.150  1.00 23.70           N
ATOM    779  N   ASP A 423       6.876  41.343  65.430  1.00 25.21           N
ATOM    780  CA  ASP A 423       5.506  40.944  65.730  1.00 26.08           C
ATOM    781  C   ASP A 423       4.573  41.827  64.896  1.00 26.61           C
ATOM    782  O   ASP A 423       4.559  43.048  65.079  1.00 26.62           O
ATOM    783  CB  ASP A 423       5.216  41.092  67.229  1.00 26.03           C
ATOM    784  CG  ASP A 423       3.847  40.558  67.619  1.00 26.26           C
ATOM    785  OD1 ASP A 423       2.824  41.145  67.199  1.00 27.37           O
ATOM    786  OD2 ASP A 423       3.794  39.557  68.363  1.00 25.65           O
ATOM    787  N   PRO A 424       3.791  41.215  63.979  1.00 27.09           N
ATOM    788  CA  PRO A 424       2.919  41.993  63.084  1.00 27.35           C
ATOM    789  C   PRO A 424       1.764  42.710  63.802  1.00 27.68           C
ATOM    790  O   PRO A 424       1.277  43.723  63.299  1.00 27.77           O
ATOM    791  CB  PRO A 424       2.390  40.944  62.093  1.00 27.13           C
ATOM    792  CG  PRO A 424       2.511  39.654  62.788  1.00 26.70           C
ATOM    793  CD  PRO A 424       3.670  39.764  63.740  1.00 26.91           C
ATOM    794  N   GLU A 425       1.342  42.206  64.962  1.00 28.22           N
ATOM    795  CA  GLU A 425       0.293  42.879  65.745  1.00 28.91           C
ATOM    796  C   GLU A 425       0.847  44.098  66.467  1.00 28.65           C
ATOM    797  O   GLU A 425       0.370  45.210  66.266  1.00 28.92           O
ATOM    798  CB  GLU A 425      -0.368  41.939  66.765  1.00 29.19           C
ATOM    799  CG  GLU A 425      -1.151  40.776  66.173  1.00 31.37           C
ATOM    800  CD  GLU A 425      -2.114  41.202  65.078  1.00 33.90           C
ATOM    801  OE1 GLU A 425      -2.989  42.062  65.350  1.00 35.91           O
ATOM    802  OE2 GLU A 425      -1.993  40.670  63.950  1.00 33.42           O
ATOM    803  N   THR A 426       1.862  43.884  67.297  1.00 28.46           N
ATOM    804  CA  THR A 426       2.388  44.948  68.154  1.00 28.45           C
ATOM    805  C   THR A 426       3.330  45.900  67.425  1.00 27.97           C
ATOM    806  O   THR A 426       3.564  47.008  67.889  1.00 27.99           O
ATOM    807  CB  THR A 426       3.102  44.369  69.388  1.00 28.38           C
ATOM    808  OG1 THR A 426       2.326  43.291  69.917  1.00 28.44           O
ATOM    809  CG2 THR A 426       3.253  45.436  70.472  1.00 29.45           C
ATOM    810  N   LYS A 427       3.851  45.461  66.280  1.00 27.76           N
ATOM    811  CA  LYS A 427       4.873  46.191  65.511  1.00 27.33           C
ATOM    812  C   LYS A 427       6.201  46.256  66.274  1.00 26.88           C
ATOM    813  O   LYS A 427       7.060  47.106  65.990  1.00 26.96           O
ATOM    814  CB  LYS A 427       4.399  47.600  65.088  1.00 27.67           C
ATOM    815  CG  LYS A 427       2.959  47.695  64.538  1.00 28.12           C
ATOM    816  CD  LYS A 427       2.722  46.795  63.320  1.00 28.71           C
ATOM    817  CE  LYS A 427       1.463  47.191  62.540  1.00 29.13           C
ATOM    818  NZ  LYS A 427       0.209  47.155  63.350  1.00 29.68           N
ATOM    819  N   ARG A 428       6.366  45.356  67.242  1.00 25.78           N
ATOM    820  CA  ARG A 428       7.591  45.300  68.019  1.00 24.94           C
ATOM    821  C   ARG A 428       8.640  44.432  67.323  1.00 24.48           C
ATOM    822  O   ARG A 428       8.339  43.338  66.849  1.00 24.34           O
ATOM    823  CB  ARG A 428       7.320  44.803  69.437  1.00 24.89           C
ATOM    824  CG  ARG A 428       8.563  44.740  70.312  1.00 24.28           C
ATOM    825  CD  ARG A 428       8.206  44.533  71.765  1.00 24.09           C
ATOM    826  NE  ARG A 428       7.825  45.783  72.410  1.00 23.84           N
ATOM    827  CZ  ARG A 428       7.575  45.910  73.707  1.00 24.39           C
ATOM    828  NH1 ARG A 428       7.657  44.854  74.510  1.00 24.65           N
ATOM    829  NH2 ARG A 428       7.243  47.096  74.201  1.00 24.36           N
ATOM    830  N   ILE A 429       9.866  44.944  67.268  1.00 23.80           N
ATOM    831  CA  ILE A 429      10.972  44.250  66.633  1.00 23.40           C
ATOM    832  C   ILE A 429      11.899  43.669  67.689  1.00 23.09           C
ATOM    833  O   ILE A 429      12.382  44.379  68.572  1.00 22.96           O
ATOM    834  CB  ILE A 429      11.755  45.181  65.667  1.00 23.39           C
ATOM    835  CG1 ILE A 429      10.875  45.555  64.468  1.00 23.36           C
ATOM    836  CG2 ILE A 429      13.033  44.506  65.187  1.00 22.89           C
ATOM    837  CD1 ILE A 429      11.206  46.894  63.845  1.00 23.02           C
ATOM    838  N   PHE A 430      12.138  42.368  67.582  1.00 22.75           N
ATOM    839  CA  PHE A 430      12.982  41.655  68.523  1.00 22.29           C
ATOM    840  C   PHE A 430      14.305  41.279  67.891  1.00 22.18           C
ATOM    841  O   PHE A 430      14.356  40.834  66.743  1.00 22.04           O
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ATOM    842  CB  PHE A 430      12.289  40.380  69.002  1.00 22.18           C
ATOM    843  CG  PHE A 430      10.974  40.621  69.670  1.00 22.06           C
ATOM    844  CD1 PHE A 430      10.910  40.861  71.038  1.00 22.00           C
ATOM    845  CD2 PHE A 430       9.796  40.599  68.935  1.00 21.34           C
ATOM    846  CE1 PHE A 430       9.683  41.088  71.668  1.00 22.14           C
ATOM    847  CE2 PHE A 430       8.569  40.823  69.554  1.00 22.24           C
ATOM    848  CZ  PHE A 430       8.513  41.067  70.926  1.00 21.79           C
ATOM    849  N   SER A 431      15.374  41.466  68.654  1.00 21.99           N
ATOM    850  CA  SER A 431      16.661  40.883  68.325  1.00 21.70           C
ATOM    851  C   SER A 431      17.085  39.958  69.462  1.00 21.43           C
ATOM    852  O   SER A 431      17.281  40.393  70.591  1.00 21.70           O
ATOM    853  CB  SER A 431      17.705  41.970  68.092  1.00 21.69           C
ATOM    854  OG  SER A 431      19.001  41.404  67.999  1.00 21.91           O
ATOM    855  N   ILE A 432      17.204  38.677  69.156  1.00 21.28           N
ATOM    856  CA  ILE A 432      17.612  37.680  70.139  1.00 21.08           C
ATOM    857  C   ILE A 432      18.994  37.153  69.760  1.00 20.93           C
ATOM    858  O   ILE A 432      19.267  36.880  68.589  1.00 20.68           O
ATOM    859  CB  ILE A 432      16.553  36.555  70.273  1.00 21.11           C
ATOM    860  CG1 ILE A 432      15.202  37.178  70.651  1.00 21.17           C
ATOM    861  CG2 ILE A 432      16.988  35.509  71.306  1.00 20.95           C
ATOM    862  CD1 ILE A 432      14.020  36.256  70.594  1.00 21.89           C
ATOM    863  N   TYR A 433      19.871  37.057  70.753  1.00 20.88           N
ATOM    864  CA  TYR A 433      21.285  36.771  70.518  1.00 20.89           C
ATOM    865  C   TYR A 433      21.920  36.111  71.727  1.00 20.88           C
ATOM    866  O   TYR A 433      21.401  36.201  72.838  1.00 20.75           O
ATOM    867  CB  TYR A 433      22.041  38.055  70.155  1.00 21.09           C
ATOM    868  CG  TYR A 433      21.738  39.214  71.072  1.00 21.23           C
ATOM    869  CD1 TYR A 433      20.721  40.117  70.771  1.00 21.42           C
ATOM    870  CD2 TYR A 433      22.459  39.403  72.249  1.00 21.70           C
ATOM    871  CE1 TYR A 433      20.425  41.180  71.620  1.00 21.58           C
ATOM    872  CE2 TYR A 433      22.169  40.465  73.106  1.00 22.32           C
ATOM    873  CZ  TYR A 433      21.149  41.343  72.783  1.00 21.42           C
ATOM    874  OH  TYR A 433      20.858  42.387  73.624  1.00 22.09           O
ATOM    875  N   ASP A 434      23.046  35.446  71.500  1.00 21.07           N
ATOM    876  CA  ASP A 434      23.740  34.712  72.549  1.00 21.21           C
ATOM    877  C   ASP A 434      24.471  35.661  73.489  1.00 21.46           C
ATOM    878  O   ASP A 434      24.738  36.807  73.142  1.00 21.64           O
ATOM    879  CB  ASP A 434      24.745  33.730  71.940  1.00 21.08           C
ATOM    880  CG  ASP A 434      24.112  32.765  70.964  1.00 20.98           C
ATOM    881  OD1 ASP A 434      22.874  32.783  70.816  1.00 20.98           O
ATOM    882  OD2 ASP A 434      24.857  31.979  70.340  1.00 21.05           O
ATOM    883  N   MET A 435      24.791  35.168  74.678  1.00 21.97           N
ATOM    884  CA  MET A 435      25.652  35.883  75.606  1.00 22.48           C
ATOM    885  C   MET A 435      26.574  34.912  76.352  1.00 23.01           C
ATOM    886  O   MET A 435      26.131  33.881  76.874  1.00 22.98           O
ATOM    887  CB  MET A 435      24.829  36.738  76.580  1.00 22.40           C
ATOM    888  CG  MET A 435      25.663  37.680  77.450  1.00 22.17           C
ATOM    889  SD  MET A 435      26.263  36.904  78.973  1.00 22.48           S
ATOM    890  CE  MET A 435      27.561  38.050  79.457  1.00 22.12           C
ATOM    891  N   PHE A 436      27.861  35.246  76.359  1.00 23.51           N
ATOM    892  CA  PHE A 436      28.872  34.555  77.162  1.00 24.26           C
ATOM    893  C   PHE A 436      29.616  35.626  77.939  1.00 24.65           C
ATOM    894  O   PHE A 436      29.858  36.712  77.405  1.00 25.02           O
ATOM    895  CB  PHE A 436      29.901  33.830  76.280  1.00 24.06           C
ATOM    896  CG  PHE A 436      29.343  32.688  75.485  1.00 24.12           C
ATOM    897  CD1 PHE A 436      29.376  31.390  75.993  1.00 23.57           C
ATOM    898  CD2 PHE A 436      28.815  32.899  74.209  1.00 23.69           C
ATOM    899  CE1 PHE A 436      28.870  30.322  75.255  1.00 23.42           C
ATOM    900  CE2 PHE A 436      28.310  31.833  73.462  1.00 23.61           C
ATOM    901  CZ  PHE A 436      28.339  30.540  73.989  1.00 23.28           C
ATOM    902  N   PRO A 437      29.984  35.337  79.200  1.00 25.06           N
ATOM    903  CA  PRO A 437      30.945  36.214  79.868  1.00 25.30           C
ATOM    904  C   PRO A 437      32.326  36.107  79.213  1.00 25.67           C
ATOM    905  O   PRO A 437      32.504  35.321  78.271  1.00 25.50           O
ATOM    906  CB  PRO A 437      30.971  35.678  81.305  1.00 25.32           C
ATOM    907  CG  PRO A 437      30.510  34.267  81.209  1.00 25.01           C
ATOM    908  CD  PRO A 437      29.527  34.238  80.074  1.00 25.10           C
ATOM    909  N   GLU A 438      33.280  36.899  79.703  1.00 26.34           N
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ATOM    910  CA  GLU A 438      34.667  36.892  79.213  1.00 26.89           C
ATOM    911  C   GLU A 438      35.171  35.463  78.993  1.00 27.13           C
ATOM    912  O   GLU A 438      35.102  34.628  79.897  1.00 27.06           O
ATOM    913  CB  GLU A 438      35.580  37.654  80.198  1.00 27.05           C
ATOM    914  CG  GLU A 438      37.092  37.651  79.870  1.00 27.00           C
ATOM    915  CD  GLU A 438      37.968  38.247  80.985  1.00 27.15           C
ATOM    916  OE1 GLU A 438      37.438  38.657  82.043  1.00 27.17           O
ATOM    917  OE2 GLU A 438      39.200  38.305  80.800  1.00 27.28           O
ATOM    918  N   GLY A 439      35.663  35.190  77.786  1.00 27.38           N
ATOM    919  CA  GLY A 439      36.186  33.869  77.437  1.00 27.69           C
ATOM    920  C   GLY A 439      36.187  33.655  75.937  1.00 28.01           C
ATOM    921  O   GLY A 439      36.276  34.618  75.175  1.00 27.99           O
ATOM    922  N   LYS A 440      36.070  32.398  75.515  1.00 28.29           N
ATOM    923  CA  LYS A 440      36.070  32.055  74.091  1.00 28.86           C
ATOM    924  C   LYS A 440      34.708  31.562  73.572  1.00 28.91           C
ATOM    925  O   LYS A 440      34.643  30.751  72.646  1.00 28.81           O
ATOM    926  CB  LYS A 440      37.189  31.056  73.771  1.00 28.79           C
ATOM    927  CG  LYS A 440      38.573  31.669  73.788  1.00 29.25           C
ATOM    928  CD  LYS A 440      39.671  30.647  73.514  1.00 29.58           C
ATOM    929  CE  LYS A 440      41.025  31.181  73.981  1.00 32.26           C
ATOM    930  NZ  LYS A 440      42.210  30.475  73.387  1.00 34.61           N
ATOM    931  N   GLY A 441      33.635  32.066  74.182  1.00 29.22           N
ATOM    932  CA  GLY A 441      32.247  31.837  73.751  1.00 29.39           C
ATOM    933  C   GLY A 441      31.902  30.624  72.898  1.00 29.74           C
ATOM    934  O   GLY A 441      31.804  30.723  71.664  1.00 30.16           O
ATOM    935  N   ILE A 442      31.692  29.495  73.570  1.00 29.48           N
ATOM    936  CA  ILE A 442      31.331  28.183  72.982  1.00 29.24           C
ATOM    937  C   ILE A 442      32.529  27.260  72.835  1.00 29.30           C
ATOM    938  O   ILE A 442      32.421  26.060  73.087  1.00 29.36           O
ATOM    939  CB  ILE A 442      30.471  28.218  71.676  1.00 29.23           C
ATOM    940  CG1 ILE A 442      29.521  27.013  71.663  1.00 28.90           C
ATOM    941  CG2 ILE A 442      31.342  28.223  70.406  1.00 29.20           C
ATOM    942  CD1 ILE A 442      28.568  26.969  70.500  1.00 28.87           C
ATOM    943  N   PHE A 443      33.666  27.827  72.441  1.00 29.29           N
ATOM    944  CA  PHE A 443      34.917  27.082  72.423  1.00 29.35           C
ATOM    945  C   PHE A 443      35.681  27.286  73.730  1.00 29.62           C
ATOM    946  O   PHE A 443      36.812  26.820  73.869  1.00 29.85           O
ATOM    947  CB  PHE A 443      35.779  27.487  71.226  1.00 29.12           C
ATOM    948  CG  PHE A 443      35.159  27.170  69.898  1.00 28.46           C
ATOM    949  CD1 PHE A 443      35.135  25.864  69.421  1.00 27.52           C
ATOM    950  CD2 PHE A 443      34.608  28.183  69.117  1.00 28.14           C
ATOM    951  CE1 PHE A 443      34.567  25.569  68.190  1.00 27.35           C
ATOM    952  CE2 PHE A 443      34.038  27.897  67.882  1.00 28.03           C
ATOM    953  CZ  PHE A 443      34.018  26.585  67.418  1.00 27.93           C
ATOM    954  N   GLY A 444      35.051  27.974  74.682  1.00 29.88           N
ATOM    955  CA  GLY A 444      35.673  28.271  75.969  1.00 30.23           C
ATOM    956  C   GLY A 444      34.792  27.965  77.165  1.00 30.47           C
ATOM    957  O   GLY A 444      34.915  28.599  78.215  1.00 30.75           O
ATOM    958  N   MET A 445      33.903  26.993  77.008  1.00 30.69           N
ATOM    959  CA  MET A 445      32.998  26.609  78.080  1.00 30.93           C
ATOM    960  C   MET A 445      33.650  25.617  79.045  1.00 31.23           C
ATOM    961  O   MET A 445      34.426  24.744  78.636  1.00 31.25           O
ATOM    962  CB  MET A 445      31.713  26.021  77.505  1.00 30.86           C
ATOM    963  CG  MET A 445      30.912  26.994  76.638  1.00 31.34           C
ATOM    964  SD  MET A 445      29.299  26.331  76.177  1.00 31.05           S
ATOM    965  CE  MET A 445      28.417  26.465  77.738  1.00 32.17           C
ATOM    966  N   SER A 446      33.322  25.766  80.327  1.00 31.49           N
ATOM    967  CA  SER A 446      33.792  24.870  81.376  1.00 31.67           C
ATOM    968  C   SER A 446      33.178  23.492  81.197  1.00 31.55           C
ATOM    969  O   SER A 446      32.053  23.370  80.706  1.00 31.82           O
ATOM    970  CB  SER A 446      33.415  25.426  82.750  1.00 31.84           C
ATOM    971  OG  SER A 446      33.575  24.444  83.765  1.00 32.86           O
ATOM    972  N   SER A 447      33.917  22.459  81.597  1.00 31.13           N
ATOM    973  CA  SER A 447      33.421  21.090  81.501  1.00 30.68           C
ATOM    974  C   SER A 447      32.562  20.718  82.710  1.00 30.22           C
ATOM    975  O   SER A 447      31.979  19.638  82.746  1.00 30.35           O
ATOM    976  CB  SER A 447      34.579  20.100  81.334  1.00 30.68           C
ATOM    977  OG  SER A 447      35.318  19.974  82.535  1.00 31.08           O
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ATOM    978  N   GLN A 448      32.502  21.607  83.700  1.00 29.73           N
ATOM    979  CA  GLN A 448      31.628  21.417  84.863  1.00 29.21           C
ATOM    980  C   GLN A 448      30.566  22.515  84.954  1.00 29.04           C
ATOM    981  O   GLN A 448      30.813  23.670  84.591  1.00 29.02           O
ATOM    982  CB  GLN A 448      32.431  21.351  86.164  1.00 29.09           C
ATOM    983  CG  GLN A 448      33.414  20.180  86.264  1.00 28.72           C
ATOM    984  CD  GLN A 448      32.736  18.822  86.323  1.00 27.71           C
ATOM    985  OE1 GLN A 448      31.738  18.635  87.015  1.00 27.04           O
ATOM    986  NE2 GLN A 448      33.288  17.864  85.598  1.00 27.56           N
ATOM    987  N   LYS A 449      29.386  22.140  85.437  1.00 28.75           N
ATOM    988  CA  LYS A 449      28.260  23.056  85.547  1.00 28.13           C
ATOM    989  C   LYS A 449      28.364  23.905  86.803  1.00 28.03           C
ATOM    990  O   LYS A 449      28.642  23.401  87.890  1.00 27.89           O
ATOM    991  CB  LYS A 449      26.935  22.281  85.551  1.00 28.13           C
ATOM    992  CG  LYS A 449      25.683  23.146  85.666  1.00 27.71           C
ATOM    993  CD  LYS A 449      24.433  22.287  85.687  1.00 27.89           C
ATOM    994  CE  LYS A 449      23.158  23.122  85.668  1.00 27.72           C
ATOM    995  NZ  LYS A 449      22.887  23.694  84.328  1.00 27.00           N
ATOM    996  N   GLU A 450      28.149  25.203  86.631  1.00 27.87           N
ATOM    997  CA  GLU A 450      27.903  26.104  87.740  1.00 27.86           C
ATOM    998  C   GLU A 450      26.457  26.551  87.580  1.00 27.60           C
ATOM    999  O   GLU A 450      26.071  26.999  86.508  1.00 27.70           O
ATOM   1000  CB  GLU A 450      28.853  27.312  87.693  1.00 27.98           C
ATOM   1001  CG  GLU A 450      30.340  26.969  87.573  1.00 27.79           C
ATOM   1002  CD  GLU A 450      31.243  28.200  87.508  1.00 28.15           C
ATOM   1003  OE1 GLU A 450      30.733  29.320  87.274  1.00 27.29           O
ATOM   1004  OE2 GLU A 450      32.475  28.042  87.693  1.00 28.47           O
ATOM   1005  N   GLU A 451      25.653  26.404  88.629  1.00 27.58           N
ATOM   1006  CA  GLU A 451      24.268  26.881  88.609  1.00 27.46           C
ATOM   1007  C   GLU A 451      24.236  28.372  88.260  1.00 27.42           C
ATOM   1008  O   GLU A 451      24.937  29.177  88.885  1.00 27.25           O
ATOM   1009  CB  GLU A 451      23.593  26.656  89.968  1.00 27.50           C
ATOM   1010  CG  GLU A 451      23.557  25.206  90.466  1.00 28.34           C
ATOM   1011  CD  GLU A 451      22.642  24.295  89.650  1.00 30.83           C
ATOM   1012  OE1 GLU A 451      21.708  24.795  88.967  1.00 31.10           O
ATOM   1013  OE2 GLU A 451      22.861  23.061  89.698  1.00 31.27           O
ATOM   1014  N   ALA A 452      23.440  28.740  87.258  1.00 27.16           N
ATOM   1015  CA  ALA A 452      23.347  30.144  86.857  1.00 27.28           C
ATOM   1016  C   ALA A 452      22.192  30.905  87.520  1.00 27.29           C
ATOM   1017  O   ALA A 452      22.262  32.121  87.680  1.00 27.18           O
ATOM   1018  CB  ALA A 452      23.297  30.273  85.332  1.00 27.02           C
ATOM   1019  N   TYR A 453      21.147  30.181  87.913  1.00 27.68           N
ATOM   1020  CA  TYR A 453      19.911  30.785  88.422  1.00 28.01           C
ATOM   1021  C   TYR A 453      19.380  30.015  89.623  1.00 28.98           C
ATOM   1022  O   TYR A 453      19.600  28.803  89.746  1.00 29.02           O
ATOM   1023  CB  TYR A 453      18.831  30.840  87.324  1.00 27.18           C
ATOM   1024  CG  TYR A 453      19.238  31.623  86.092  1.00 26.04           C
ATOM   1025  CD1 TYR A 453      19.073  33.010  86.032  1.00 24.87           C
ATOM   1026  CD2 TYR A 453      19.791  30.976  84.989  1.00 24.60           C
ATOM   1027  CE1 TYR A 453      19.456  33.728  84.906  1.00 24.60           C
ATOM   1028  CE2 TYR A 453      20.176  31.680  83.862  1.00 23.78           C
ATOM   1029  CZ  TYR A 453      20.011  33.051  83.826  1.00 24.97           C
ATOM   1030  OH  TYR A 453      20.402  33.740  82.706  1.00 25.06           O
ATOM   1031  N   LYS A 454      18.678  30.726  90.504  1.00 30.08           N
ATOM   1032  CA  LYS A 454      18.076  30.121  91.689  1.00 31.15           C
ATOM   1033  C   LYS A 454      16.626  30.589  91.862  1.00 31.82           C
ATOM   1034  O   LYS A 454      16.318  31.760  91.623  1.00 31.94           O
ATOM   1035  CB  LYS A 454      18.909  30.455  92.934  1.00 31.33           C
ATOM   1036  CG  LYS A 454      18.583  29.601  94.152  1.00 31.98           C
ATOM   1037  CD  LYS A 454      19.606  29.749  95.254  1.00 32.85           C
ATOM   1038  CE  LYS A 454      19.384  28.677  96.311  1.00 34.21           C
ATOM   1039  NZ  LYS A 454      20.418  28.710  97.385  1.00 35.38           N
ATOM   1040  N   LYS A 455      15.743  29.672  92.266  1.00 32.56           N
ATOM   1041  CA  LYS A 455      14.345  30.012  92.541  1.00 33.36           C
ATOM   1042  C   LYS A 455      14.082  30.168  94.045  1.00 33.80           C
ATOM   1043  O   LYS A 455      13.848  29.182  94.758  1.00 33.99           O
ATOM   1044  CB  LYS A 455      13.392  28.981  91.918  1.00 33.32           C
ATOM   1045  CG  LYS A 455      11.947  29.478  91.778  1.00 33.38           C
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ATOM   1046  CD  LYS A 455      11.103  28.551  90.915  1.00 33.73           C
ATOM   1047  CE  LYS A 455      11.440  28.708  89.431  1.00 35.53           C
ATOM   1048  NZ  LYS A 455      10.645  27.794  88.554  1.00 35.83           N
ATOM   1049  N   ILE A 456      14.132  31.413  94.518  1.00 34.33           N
ATOM   1050  CA  ILE A 456      13.875  31.723  95.921  1.00 34.64           C
ATOM   1051  C   ILE A 456      12.438  32.204  96.078  1.00 35.06           C
ATOM   1052  O   ILE A 456      12.077  33.286  95.596  1.00 35.06           O
ATOM   1053  CB  ILE A 456      14.884  32.764  96.483  1.00 34.86           C
ATOM   1054  CG1 ILE A 456      16.275  32.128  96.613  1.00 34.65           C
ATOM   1055  CG2 ILE A 456      14.419  33.311  97.846  1.00 34.84           C
ATOM   1056  CD1 ILE A 456      17.398  33.111  96.824  1.00 33.67           C
ATOM   1057  N   ASP A 457      11.624  31.373  96.734  1.00 35.43           N
ATOM   1058  CA  ASP A 457      10.211  31.667  96.999  1.00 35.68           C
ATOM   1059  C   ASP A 457       9.441  31.994  95.714  1.00 35.54           C
ATOM   1060  O   ASP A 457       8.719  32.997  95.634  1.00 35.36           O
ATOM   1061  CB  ASP A 457      10.075  32.796  98.036  1.00 36.00           C
ATOM   1062  CG  ASP A 457       8.673  32.903  98.611  1.00 37.06           C
ATOM   1063  OD1 ASP A 457       8.129  31.869  99.069  1.00 38.08           O
ATOM   1064  OD2 ASP A 457       8.119  34.027  98.609  1.00 37.98           O
ATOM   1065  N   GLY A 458       9.615  31.140  94.708  1.00 35.45           N
ATOM   1066  CA  GLY A 458       8.890  31.266  93.444  1.00 35.31           C
ATOM   1067  C   GLY A 458       9.391  32.320  92.467  1.00 35.17           C
ATOM   1068  O   GLY A 458       8.835  32.461  91.379  1.00 35.36           O
ATOM   1069  N   LYS A 459      10.426  33.065  92.844  1.00 34.83           N
ATOM   1070  CA  LYS A 459      11.026  34.048  91.943  1.00 34.52           C
ATOM   1071  C   LYS A 459      12.431  33.620  91.551  1.00 34.05           C
ATOM   1072  O   LYS A 459      13.197  33.146  92.396  1.00 34.34           O
ATOM   1073  CB  LYS A 459      11.059  35.444  92.575  1.00 34.73           C
ATOM   1074  CG  LYS A 459       9.725  36.175  92.571  1.00 35.27           C
ATOM   1075  CD  LYS A 459       9.925  37.690  92.527  1.00 36.81           C
ATOM   1076  CE  LYS A 459       8.635  38.434  92.884  1.00 37.56           C
ATOM   1077  NZ  LYS A 459       8.645  39.850  92.410  1.00 37.55           N
ATOM   1078  N   THR A 460      12.758  33.797  90.271  1.00 33.21           N
ATOM   1079  CA  THR A 460      14.049  33.402  89.715  1.00 32.58           C
ATOM   1080  C   THR A 460      15.046  34.570  89.731  1.00 32.18           C
ATOM   1081  O   THR A 460      14.779  35.640  89.180  1.00 32.07           O
ATOM   1082  CB  THR A 460      13.886  32.834  88.267  1.00 32.65           C
ATOM   1083  OG1 THR A 460      13.015  31.695  88.291  1.00 32.79           O
ATOM   1084  CG2 THR A 460      15.228  32.410  87.673  1.00 32.25           C
ATOM   1085  N   TYR A 461      16.190  34.362  90.377  1.00 31.76           N
ATOM   1086  CA  TYR A 461      17.275  35.352  90.366  1.00 31.46           C
ATOM   1087  C   TYR A 461      18.567  34.737  89.828  1.00 31.03           C
ATOM   1088  O   TYR A 461      18.869  33.573  90.097  1.00 30.81           O
ATOM   1089  CB  TYR A 461      17.528  35.929  91.766  1.00 31.44           C
ATOM   1090  CG  TYR A 461      16.314  36.501  92.475  1.00 31.69           C
ATOM   1091  CD1 TYR A 461      15.691  37.661  92.014  1.00 31.59           C
ATOM   1092  CD2 TYR A 461      15.807  35.896  93.629  1.00 32.41           C
ATOM   1093  CE1 TYR A 461      14.585  38.195  92.667  1.00 31.82           C
ATOM   1094  CE2 TYR A 461      14.692  36.423  94.298  1.00 32.05           C
ATOM   1095  CZ  TYR A 461      14.089  37.574  93.807  1.00 32.14           C
ATOM   1096  OH  TYR A 461      12.992  38.112  94.447  1.00 31.78           O
ATOM   1097  N   GLN A 462      19.323  35.520  89.065  1.00 30.90           N
ATOM   1098  CA  GLN A 462      20.641  35.086  88.610  1.00 30.97           C
ATOM   1099  C   GLN A 462      21.596  34.949  89.800  1.00 31.28           C
ATOM   1100  O   GLN A 462      21.537  35.733  90.752  1.00 31.18           O
ATOM   1101  CB  GLN A 462      21.218  36.031  87.544  1.00 30.83           C
ATOM   1102  CG  GLN A 462      22.506  35.512  86.898  1.00 30.35           C
ATOM   1103  CD  GLN A 462      22.924  36.274  85.654  1.00 30.59           C
ATOM   1104  OE1 GLN A 462      22.653  37.468  85.505  1.00 30.10           O
ATOM   1105  NE2 GLN A 462      23.605  35.583  84.756  1.00 30.48           N
ATOM   1106  N   ILE A 463      22.455  33.936  89.732  1.00 31.51           N
ATOM   1107  CA  ILE A 463      23.425  33.639  90.776  1.00 31.87           C
ATOM   1108  C   ILE A 463      24.729  34.424  90.572  1.00 32.48           C
ATOM   1109  O   ILE A 463      25.079  34.784  89.442  1.00 32.35           O
ATOM   1110  CB  ILE A 463      23.691  32.107  90.851  1.00 31.66           C
ATOM   1111  CG1 ILE A 463      22.452  31.392  91.404  1.00 31.56           C
ATOM   1112  CG2 ILE A 463      24.926  31.790  91.703  1.00 31.59           C
ATOM   1113  CD1 ILE A 463      22.508  29.881  91.330  1.00 31.58           C
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ATOM   1114  N   LEU A 464      25.418  34.707  91.679  1.00 33.20           N
ATOM   1115  CA  LEU A 464      26.769  35.267  91.651  1.00 33.99           C
ATOM   1116  C   LEU A 464      27.719  34.414  92.488  1.00 34.80           C
ATOM   1117  O   LEU A 464      27.342  33.913  93.546  1.00 35.10           O
ATOM   1118  CB  LEU A 464      26.777  36.715  92.156  1.00 33.79           C
ATOM   1119  CG  LEU A 464      26.077  37.800  91.325  1.00 33.47           C
ATOM   1120  CD1 LEU A 464      25.934  39.075  92.145  1.00 33.53           C
ATOM   1121  CD2 LEU A 464      26.799  38.088  90.011  1.00 32.46           C
ATOM   1122  N   TYR A 465      28.950  34.244  92.019  1.00 35.71           N
ATOM   1123  CA  TYR A 465      29.946  33.497  92.786  1.00 36.81           C
ATOM   1124  C   TYR A 465      31.054  34.400  93.309  1.00 37.67           C
ATOM   1125  O   TYR A 465      31.750  35.059  92.529  1.00 37.90           O
ATOM   1126  CB  TYR A 465      30.519  32.348  91.958  1.00 36.45           C
ATOM   1127  CG  TYR A 465      29.486  31.298  91.633  1.00 36.63           C
ATOM   1128  CD1 TYR A 465      29.124  30.335  92.577  1.00 36.31           C
ATOM   1129  CD2 TYR A 465      28.854  31.274  90.389  1.00 35.95           C
ATOM   1130  CE1 TYR A 465      28.171  29.373  92.289  1.00 35.78           C
ATOM   1131  CE2 TYR A 465      27.901  30.312  90.092  1.00 35.68           C
ATOM   1132  CZ  TYR A 465      27.562  29.367  91.047  1.00 35.72           C
ATOM   1133  OH  TYR A 465      26.617  28.410  90.763  1.00 35.88           O
ATOM   1134  N   ARG A 466      31.193  34.440  94.634  1.00 38.77           N
ATOM   1135  CA  ARG A 466      32.236  35.234  95.283  1.00 39.86           C
ATOM   1136  C   ARG A 466      33.581  34.514  95.260  1.00 40.53           C
ATOM   1137  O   ARG A 466      33.645  33.288  95.360  1.00 40.57           O
ATOM   1138  CB  ARG A 466      31.857  35.597  96.723  1.00 39.72           C
ATOM   1139  CG  ARG A 466      32.639  36.797  97.254  1.00 40.77           C
ATOM   1140  CD  ARG A 466      32.776  36.805  98.767  1.00 41.70           C
ATOM   1141  NE  ARG A 466      31.675  37.514  99.415  1.00 42.18           N
ATOM   1142  CZ  ARG A 466      31.712  38.791  99.786  1.00 41.94           C
ATOM   1143  NH1 ARG A 466      32.801  39.520  99.575  1.00 42.15           N
ATOM   1144  NH2 ARG A 466      30.653  39.340 100.367  1.00 41.42           N
ATOM   1145  N   GLU A 467      34.650  35.296  95.125  1.00 41.52           N
ATOM   1146  CA  GLU A 467      36.018  34.783  95.150  1.00 42.71           C
ATOM   1147  C   GLU A 467      36.284  33.988  96.427  1.00 42.58           C
ATOM   1148  O   GLU A 467      35.961  34.439  97.529  1.00 42.43           O
ATOM   1149  CB  GLU A 467      37.026  35.934  95.013  1.00 42.52           C
ATOM   1150  CG  GLU A 467      36.793  36.815  93.779  1.00 43.91           C
ATOM   1151  CD  GLU A 467      37.848  37.911  93.586  1.00 44.52           C
ATOM   1152  OE1 GLU A 467      38.401  38.426  94.596  1.00 45.70           O
ATOM   1153  OE2 GLU A 467      38.107  38.264  92.406  1.00 46.43           O
ATOM   1154  N   GLY A 468      36.839  32.791  96.260  1.00 42.99           N
ATOM   1155  CA  GLY A 468      37.223  31.935  97.382  1.00 43.41           C
ATOM   1156  C   GLY A 468      36.083  31.287  98.148  1.00 43.72           C
ATOM   1157  O   GLY A 468      36.264  30.225  98.740  1.00 43.91           O
ATOM   1158  N   GLU A 469      34.913  31.924  98.131  1.00 43.84           N
ATOM   1159  CA  GLU A 469      33.741  31.476  98.891  1.00 43.93           C
ATOM   1160  C   GLU A 469      32.773  30.613  98.064  1.00 43.78           C
ATOM   1161  O   GLU A 469      32.518  30.890  96.888  1.00 43.77           O
ATOM   1162  CB  GLU A 469      33.012  32.701  99.446  1.00 43.93           C
ATOM   1163  CG  GLU A 469      31.947  32.426 100.496  1.00 44.20           C
ATOM   1164  CD  GLU A 469      31.289  33.709 100.977  1.00 44.52           C
ATOM   1165  OE1 GLU A 469      32.020  34.704 101.199  1.00 45.61           O
ATOM   1166  OE2 GLU A 469      30.048  33.728 101.131  1.00 44.33           O
ATOM   1167  N   LYS A 470      32.242  29.568  98.692  1.00 43.64           N
ATOM   1168  CA  LYS A 470      31.237  28.706  98.076  1.00 43.38           C
ATOM   1169  C   LYS A 470      29.845  29.144  98.527  1.00 43.57           C
ATOM   1170  O   LYS A 470      29.628  29.407  99.716  1.00 43.58           O
ATOM   1171  CB  LYS A 470      31.478  27.244  98.466  1.00 43.10           C
ATOM   1172  CG  LYS A 470      30.372  26.284  98.048  1.00 42.93           C
ATOM   1173  CD  LYS A 470      30.552  24.908  98.672  1.00 43.10           C
ATOM   1174  CE  LYS A 470      29.463  23.940  98.218  1.00 42.35           C
ATOM   1175  NZ  LYS A 470      29.695  22.557  98.730  1.00 41.88           N
ATOM   1176  N   GLY A 471      28.907  29.226  97.584  1.00 43.45           N
ATOM   1177  CA  GLY A 471      27.521  29.509  97.938  1.00 43.50           C
ATOM   1178  C   GLY A 471      26.746  30.403  96.992  1.00 43.60           C
ATOM   1179  O   GLY A 471      27.325  31.072  96.132  1.00 43.40           O
ATOM   1180  N   ALA A 472      25.426  30.403  97.189  1.00 43.70           N
ATOM   1181  CA  ALA A 472      24.447  31.134  96.374  1.00 43.79           C
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ATOM   1182  C   ALA A 472      24.861  32.539  95.941  1.00 43.90           C
ATOM   1183  O   ALA A 472      25.612  32.680  94.984  1.00 44.39           O
ATOM   1184  CB  ALA A 472      23.082  31.167  97.086  1.00 43.83           C
ATOM   1185  N   TYR A 473      24.382  33.564  96.646  1.00 43.76           N
ATOM   1186  CA  TYR A 473      24.408  34.964  96.173  1.00 43.85           C
ATOM   1187  C   TYR A 473      23.495  35.144  94.959  1.00 43.83           C
ATOM   1188  O   TYR A 473      23.697  34.517  93.917  1.00 43.65           O
ATOM   1189  CB  TYR A 473      25.827  35.465  95.844  1.00 43.88           C
ATOM   1190  CG  TYR A 473      26.710  35.768  97.038  1.00 43.94           C
ATOM   1191  CD1 TYR A 473      26.581  36.965  97.744  1.00 43.71           C
ATOM   1192  CD2 TYR A 473      27.693  34.866  97.443  1.00 43.92           C
ATOM   1193  CE1 TYR A 473      27.397  37.245  98.838  1.00 43.70           C
ATOM   1194  CE2 TYR A 473      28.512  35.135  98.528  1.00 44.09           C
ATOM   1195  CZ  TYR A 473      28.360  36.324  99.223  1.00 44.20           C
ATOM   1196  OH  TYR A 473      29.178  36.582 100.301  1.00 43.91           O
ATOM   1197  N   THR A 474      22.490  36.003  95.099  1.00 43.97           N
ATOM   1198  CA  THR A 474      21.526  36.237  94.023  1.00 44.30           C
ATOM   1199  C   THR A 474      21.522  37.696  93.569  1.00 44.53           C
ATOM   1200  O   THR A 474      22.269  38.503  94.108  1.00 44.67           O
ATOM   1201  CB  THR A 474      20.108  35.793  94.429  1.00 44.25           C
ATOM   1202  OG1 THR A 474      19.760  36.379  95.690  1.00 44.06           O
ATOM   1203  CG2 THR A 474      20.038  34.274  94.524  1.00 43.92           C
ATOM   1204  N   ILE A 475      20.714  38.021  92.558  1.00 44.83           N
ATOM   1205  CA  ILE A 475      20.557  39.406  92.090  1.00 45.16           C
ATOM   1206  C   ILE A 475      19.078  39.760  92.080  1.00 45.58           C
ATOM   1207  O   ILE A 475      18.317  39.248  91.258  1.00 45.86           O
ATOM   1208  CB  ILE A 475      21.143  39.634  90.673  1.00 45.04           C
ATOM   1209  CG1 ILE A 475      22.626  39.254  90.627  1.00 44.87           C
ATOM   1210  CG2 ILE A 475      20.947  41.092  90.243  1.00 45.27           C
ATOM   1211  CD1 ILE A 475      23.206  39.163  89.230  1.00 44.94           C
ATOM   1212  N   ARG A 476      18.676  40.642  92.989  1.00 46.07           N
ATOM   1213  CA  ARG A 476      17.262  40.925  93.205  1.00 46.46           C
ATOM   1214  C   ARG A 476      16.931  42.393  92.960  1.00 47.15           C
ATOM   1215  O   ARG A 476      17.814  43.190  92.646  1.00 47.38           O
ATOM   1216  CB  ARG A 476      16.855  40.523  94.630  1.00 46.53           C
ATOM   1217  CG  ARG A 476      17.318  39.130  95.073  1.00 46.02           C
ATOM   1218  CD  ARG A 476      16.674  38.721  96.393  1.00 45.61           C
ATOM   1219  NE  ARG A 476      17.381  37.617  97.048  1.00 43.22           N
ATOM   1220  CZ  ARG A 476      16.890  36.897  98.055  1.00 41.95           C
ATOM   1221  NH1 ARG A 476      15.677  37.147  98.532  1.00 41.15           N
ATOM   1222  NH2 ARG A 476      17.612  35.921  98.586  1.00 41.08           N
ATOM   1223  N   GLU A 477      15.644  42.718  93.070  1.00 47.83           N
ATOM   1224  CA  GLU A 477      15.145  44.097  93.210  1.00 48.66           C
ATOM   1225  C   GLU A 477      15.764  45.147  92.277  1.00 48.96           C
ATOM   1226  O   GLU A 477      15.403  45.216  91.099  1.00 49.26           O
ATOM   1227  CB  GLU A 477      15.246  44.540  94.673  1.00 48.88           C
ATOM   1228  CG  GLU A 477      14.525  43.606  95.644  1.00 49.75           C
ATOM   1229  CD  GLU A 477      15.094  43.654  97.047  1.00 50.82           C
ATOM   1230  OE1 GLU A 477      16.171  44.264  97.244  1.00 51.19           O
ATOM   1231  OE2 GLU A 477      14.462  43.073  97.956  1.00 51.58           O
ATOM   1232  N   ASN A 478      16.670  45.970  92.803  1.00 49.16           N
ATOM   1233  CA  ASN A 478      17.307  47.019  92.002  1.00 49.60           C
ATOM   1234  C   ASN A 478      18.776  46.694  91.739  1.00 49.57           C
ATOM   1235  O   ASN A 478      19.636  47.579  91.715  1.00 49.52           O
ATOM   1236  CB  ASN A 478      17.162  48.393  92.677  1.00 49.75           C
ATOM   1237  CG  ASN A 478      17.332  49.562  91.694  1.00 50.95           C
ATOM   1238  OD1 ASN A 478      16.850  49.520  90.554  1.00 51.93           O
ATOM   1239  ND2 ASN A 478      18.013  50.617  92.143  1.00 51.48           N
ATOM   1240  N   GLY A 479      19.052  45.409  91.544  1.00 49.58           N
ATOM   1241  CA  GLY A 479      20.420  44.932  91.399  1.00 49.48           C
ATOM   1242  C   GLY A 479      21.101  44.677  92.727  1.00 49.41           C
ATOM   1243  O   GLY A 479      22.273  44.296  92.760  1.00 49.20           O
ATOM   1244  N   THR A 480      20.366  44.897  93.820  1.00 49.52           N
ATOM   1245  CA  THR A 480      20.839  44.590  95.171  1.00 49.47           C
ATOM   1246  C   THR A 480      21.220  43.116  95.210  1.00 49.49           C
ATOM   1247  O   THR A 480      20.402  42.254  94.879  1.00 49.41           O
ATOM   1248  CB  THR A 480      19.749  44.867  96.233  1.00 49.46           C
ATOM   1249  OG1 THR A 480      19.269  46.209  96.096  1.00 49.58           O
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ATOM   1250  CG2 THR A 480      20.299  44.678  97.636  1.00 49.27           C
ATOM   1251  N   VAL A 481      22.463  42.837  95.600  1.00 49.60           N
ATOM   1252  CA  VAL A 481      23.004  41.477  95.530  1.00 49.75           C
ATOM   1253  C   VAL A 481      22.244  40.482  96.422  1.00 50.03           C
ATOM   1254  O   VAL A 481      21.356  39.791  95.923  1.00 50.33           O
ATOM   1255  CB  VAL A 481      24.545  41.437  95.725  1.00 49.65           C
ATOM   1256  CG1 VAL A 481      25.062  40.001  95.770  1.00 49.63           C
ATOM   1257  CG2 VAL A 481      25.227  42.189  94.591  1.00 49.47           C
ATOM   1258  N   TYR A 482      22.559  40.430  97.718  1.00 50.05           N
ATOM   1259  CA  TYR A 482      21.996  39.426  98.644  1.00 50.04           C
ATOM   1260  C   TYR A 482      22.929  38.237  98.854  1.00 50.23           C
ATOM   1261  O   TYR A 482      23.433  37.650  97.894  1.00 50.16           O
ATOM   1262  CB  TYR A 482      20.610  38.922  98.204  1.00 49.83           C
ATOM   1263  CG  TYR A 482      19.457  39.809  98.616  1.00 49.68           C
ATOM   1264  CD1 TYR A 482      18.632  39.454  99.682  1.00 49.36           C
ATOM   1265  CD2 TYR A 482      19.190  41.004  97.942  1.00 49.42           C
ATOM   1266  CE1 TYR A 482      17.568  40.263 100.067  1.00 49.38           C
ATOM   1267  CE2 TYR A 482      18.132  41.820  98.319  1.00 49.59           C
ATOM   1268  CZ  TYR A 482      17.324  41.443  99.382  1.00 49.70           C
ATOM   1269  OH  TYR A 482      16.274  42.249  99.763  1.00 49.75           O
ATOM   1270  N   THR A 483      23.136  37.895 100.124  1.00 50.47           N
ATOM   1271  CA  THR A 483      23.974  36.772 100.545  1.00 50.90           C
ATOM   1272  C   THR A 483      23.199  35.444 100.427  1.00 51.05           C
ATOM   1273  O   THR A 483      21.969  35.465 100.341  1.00 51.11           O
ATOM   1274  CB  THR A 483      24.499  37.012 102.002  1.00 50.89           C
ATOM   1275  OG1 THR A 483      25.339  35.932 102.421  1.00 51.63           O
ATOM   1276  CG2 THR A 483      23.361  37.151 102.981  1.00 50.61           C
ATOM   1277  N   PRO A 484      23.908  34.290 100.388  1.00 51.21           N
ATOM   1278  CA  PRO A 484      23.226  32.993 100.495  1.00 51.51           C
ATOM   1279  C   PRO A 484      22.342  32.841 101.743  1.00 52.04           C
ATOM   1280  O   PRO A 484      21.564  31.892 101.820  1.00 52.25           O
ATOM   1281  CB  PRO A 484      24.382  31.991 100.557  1.00 51.32           C
ATOM   1282  CG  PRO A 484      25.497  32.661  99.879  1.00 51.09           C
ATOM   1283  CD  PRO A 484      25.360  34.119 100.191  1.00 51.11           C
ATOM   1284  N   ASP A 485      22.468  33.760 102.702  1.00 52.65           N
ATOM   1285  CA  ASP A 485      21.617  33.788 103.898  1.00 53.28           C
ATOM   1286  C   ASP A 485      20.230  34.359 103.611  1.00 53.70           C
ATOM   1287  O   ASP A 485      19.280  34.110 104.357  1.00 53.74           O
ATOM   1288  CB  ASP A 485      22.265  34.629 105.008  1.00 53.34           C
ATOM   1289  CG  ASP A 485      23.160  33.818 105.930  1.00 53.68           C
ATOM   1290  OD1 ASP A 485      23.146  32.570 105.859  1.00 54.20           O
ATOM   1291  OD2 ASP A 485      23.876  34.440 106.745  1.00 54.15           O
ATOM   1292  N   GLY A 486      20.123  35.140 102.540  1.00 54.20           N
ATOM   1293  CA  GLY A 486      18.902  35.880 102.244  1.00 54.87           C
ATOM   1294  C   GLY A 486      18.923  37.262 102.871  1.00 55.36           C
ATOM   1295  O   GLY A 486      17.933  37.992 102.815  1.00 55.25           O
ATOM   1296  N   LYS A 487      20.056  37.618 103.474  1.00 56.00           N
ATOM   1297  CA  LYS A 487      20.240  38.938 104.072  1.00 56.75           C
ATOM   1298  C   LYS A 487      20.544  39.941 102.978  1.00 57.05           C
ATOM   1299  O   LYS A 487      21.427  39.720 102.147  1.00 56.96           O
ATOM   1300  CB  LYS A 487      21.367  38.935 105.115  1.00 56.57           C
ATOM   1301  CG  LYS A 487      21.052  38.146 106.380  1.00 57.10           C
ATOM   1302  CD  LYS A 487      22.250  38.073 107.318  1.00 57.24           C
ATOM   1303  CE  LYS A 487      21.909  37.278 108.574  1.00 58.10           C
ATOM   1304  NZ  LYS A 487      23.053  37.209 109.523  1.00 58.35           N
ATOM   1305  N   ALA A 488      19.795  41.038 102.976  1.00 57.66           N
ATOM   1306  CA  ALA A 488      20.016  42.116 102.024  1.00 58.21           C
ATOM   1307  C   ALA A 488      21.345  42.791 102.321  1.00 58.52           C
ATOM   1308  O   ALA A 488      21.388  43.868 102.919  1.00 58.69           O
ATOM   1309  CB  ALA A 488      18.871  43.126 102.080  1.00 58.23           C
ATOM   1310  N   THR A 489      22.434  42.134 101.927  1.00 58.91           N
ATOM   1311  CA  THR A 489      23.758  42.720 102.064  1.00 59.21           C
ATOM   1312  C   THR A 489      23.867  43.829 101.039  1.00 59.31           C
ATOM   1313  O   THR A 489      24.367  43.625  99.926  1.00 59.47           O
ATOM   1314  CB  THR A 489      24.897  41.697 101.867  1.00 59.35           C
ATOM   1315  OG1 THR A 489      24.732  41.024 100.610  1.00 59.36           O
ATOM   1316  CG2 THR A 489      24.925  40.684 103.016  1.00 59.44           C
ATOM   1317  N   ASP A 490      23.354  44.995 101.428  1.00 59.49           N
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ATOM   1318  CA  ASP A 490      23.426  46.208 100.627  1.00 59.47           C
ATOM   1319  C   ASP A 490      24.878  46.589 100.392  1.00 59.15           C
ATOM   1320  O   ASP A 490      25.767  45.732 100.415  1.00 59.07           O
ATOM   1321  CB  ASP A 490      22.670  47.362 101.306  1.00 59.79           C
ATOM   1322  CG  ASP A 490      21.195  47.413 100.923  1.00 60.56           C
ATOM   1323  OD1 ASP A 490      20.836  46.996  99.797  1.00 61.32           O
ATOM   1324  OD2 ASP A 490      20.392  47.889 101.754  1.00 61.61           O
ATOM   1325  N   TYR A 491      25.121  47.881 100.192  1.00 58.80           N
ATOM   1326  CA  TYR A 491      26.371  48.340  99.612  1.00 58.40           C
ATOM   1327  C   TYR A 491      26.392  47.820  98.160  1.00 57.75           C
ATOM   1328  O   TYR A 491      26.462  48.607  97.216  1.00 57.86           O
ATOM   1329  CB  TYR A 491      27.596  47.847 100.417  1.00 58.72           C
ATOM   1330  CG  TYR A 491      27.702  48.334 101.862  1.00 59.19           C
ATOM   1331  CD1 TYR A 491      28.821  49.054 102.294  1.00 59.58           C
ATOM   1332  CD2 TYR A 491      26.701  48.050 102.804  1.00 59.90           C
ATOM   1333  CE1 TYR A 491      28.935  49.494 103.624  1.00 59.77           C
ATOM   1334  CE2 TYR A 491      26.801  48.486 104.133  1.00 59.88           C
ATOM   1335  CZ  TYR A 491      27.920  49.208 104.537  1.00 60.00           C
ATOM   1336  OH  TYR A 491      28.021  49.636 105.848  1.00 59.47           O
ATOM   1337  N   ARG A 492      26.268  46.500  98.004  1.00 56.87           N
ATOM   1338  CA  ARG A 492      26.362  45.797  96.714  1.00 55.99           C
ATOM   1339  C   ARG A 492      25.170  46.005  95.772  1.00 55.30           C
ATOM   1340  O   ARG A 492      24.038  45.624  96.097  1.00 55.16           O
ATOM   1341  CB  ARG A 492      26.530  44.291  96.955  1.00 56.02           C
ATOM   1342  CG  ARG A 492      27.615  43.899  97.936  1.00 55.82           C
ATOM   1343  CD  ARG A 492      28.978  44.160  97.347  1.00 55.09           C
ATOM   1344  NE  ARG A 492      30.038  43.774  98.264  1.00 54.67           N
ATOM   1345  CZ  ARG A 492      31.307  44.130  98.118  1.00 54.88           C
ATOM   1346  NH1 ARG A 492      31.667  44.886  97.088  1.00 55.12           N
ATOM   1347  NH2 ARG A 492      32.214  43.736  99.003  1.00 54.34           N
ATOM   1348  N   VAL A 493      25.436  46.602  94.609  1.00 54.40           N
ATOM   1349  CA  VAL A 493      24.464  46.652  93.505  1.00 53.50           C
ATOM   1350  C   VAL A 493      25.100  46.302  92.158  1.00 52.84           C
ATOM   1351  O   VAL A 493      26.219  46.722  91.853  1.00 52.57           O
ATOM   1352  CB  VAL A 493      23.677  48.008  93.393  1.00 53.56           C
ATOM   1353  CG1 VAL A 493      22.510  48.056  94.378  1.00 53.58           C
ATOM   1354  CG2 VAL A 493      24.593  49.226  93.550  1.00 53.62           C
ATOM   1355  N   VAL A 494      24.376  45.504  91.379  1.00 52.22           N
ATOM   1356  CA  VAL A 494      24.689  45.246  89.979  1.00 51.43           C
ATOM   1357  C   VAL A 494      23.725  46.093  89.169  1.00 51.11           C
ATOM   1358  O   VAL A 494      22.545  46.183  89.508  1.00 50.94           O
ATOM   1359  CB  VAL A 494      24.469  43.757  89.609  1.00 51.44           C
ATOM   1360  CG1 VAL A 494      24.589  43.542  88.100  1.00 51.30           C
ATOM   1361  CG2 VAL A 494      25.442  42.859  90.356  1.00 50.97           C
ATOM   1362  N   VAL A 495      24.210  46.724  88.109  1.00 50.70           N
ATOM   1363  CA  VAL A 495      23.318  47.522  87.280  1.00 50.49           C
ATOM   1364  C   VAL A 495      22.611  46.635  86.256  1.00 50.33           C
ATOM   1365  O   VAL A 495      23.245  45.812  85.588  1.00 50.33           O
ATOM   1366  CB  VAL A 495      24.035  48.701  86.569  1.00 50.59           C
ATOM   1367  CG1 VAL A 495      23.036  49.816  86.276  1.00 50.69           C
ATOM   1368  CG2 VAL A 495      25.177  49.253  87.414  1.00 50.31           C
ATOM   1369  N   ASP A 496      21.292  46.789  86.166  1.00 50.04           N
ATOM   1370  CA  ASP A 496      20.503  46.186  85.085  1.00 49.87           C
ATOM   1371  C   ASP A 496      19.498  47.131  84.418  1.00 49.79           C
ATOM   1372  O   ASP A 496      19.067  46.859  83.298  1.00 50.24           O
ATOM   1373  CB  ASP A 496      19.841  44.863  85.497  1.00 49.91           C
ATOM   1374  CG  ASP A 496      19.632  44.746  86.987  1.00 49.64           C
ATOM   1375  OD1 ASP A 496      18.747  45.446  87.528  1.00 49.69           O
ATOM   1376  OD2 ASP A 496      20.349  43.938  87.612  1.00 48.95           O
ATOM   1377  N   PRO A 497      19.089  48.220  85.102  1.00 49.61           N
ATOM   1378  CA  PRO A 497      18.498  49.306  84.330  1.00 49.37           C
ATOM   1379  C   PRO A 497      19.569  50.317  83.869  1.00 49.09           C
ATOM   1380  O   PRO A 497      19.712  51.401  84.445  1.00 49.14           O
ATOM   1381  CB  PRO A 497      17.493  49.935  85.313  1.00 49.36           C
ATOM   1382  CG  PRO A 497      17.737  49.253  86.664  1.00 49.79           C
ATOM   1383  CD  PRO A 497      19.037  48.515  86.543  1.00 49.76           C
ATOM   1384  N   VAL A 498      20.314  49.929  82.838  1.00 48.56           N
ATOM   1385  CA  VAL A 498      21.325  50.767  82.184  1.00 48.25           C
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ATOM   1386  C   VAL A 498      20.712  51.380  80.912  1.00 47.87           C
ATOM   1387  O   VAL A 498      19.615  50.957  80.541  1.00 47.91           O
ATOM   1388  CB  VAL A 498      22.510  49.865  81.757  1.00 48.37           C
ATOM   1389  CG1 VAL A 498      23.269  49.381  82.967  1.00 48.71           C
ATOM   1390  CG2 VAL A 498      22.011  48.645  80.973  1.00 47.94           C
ATOM   1391  N   LYS A 499      21.303  52.394  80.251  1.00 47.45           N
ATOM   1392  CA  LYS A 499      21.910  53.668  80.760  1.00 46.98           C
ATOM   1393  C   LYS A 499      22.723  54.484  79.707  1.00 46.12           C
ATOM   1394  O   LYS A 499      22.172  55.438  79.153  1.00 46.15           O
ATOM   1395  CB  LYS A 499      22.474  53.650  82.189  1.00 47.26           C
ATOM   1396  CG  LYS A 499      21.515  54.396  83.127  1.00 47.49           C
ATOM   1397  CD  LYS A 499      21.848  54.249  84.613  1.00 47.72           C
ATOM   1398  CE  LYS A 499      20.859  55.117  85.430  1.00 48.69           C
ATOM   1399  NZ  LYS A 499      20.973  54.934  86.913  1.00 49.29           N
ATOM   1400  N   PRO A 500      24.017  54.167  79.459  1.00 45.38           N
ATOM   1401  CA  PRO A 500      24.596  54.413  78.118  1.00 44.83           C
ATOM   1402  C   PRO A 500      24.112  53.359  77.105  1.00 44.17           C
ATOM   1403  O   PRO A 500      22.981  52.885  77.227  1.00 44.27           O
ATOM   1404  CB  PRO A 500      26.113  54.292  78.350  1.00 44.82           C
ATOM   1405  CG  PRO A 500      26.300  54.334  79.837  1.00 45.03           C
ATOM   1406  CD  PRO A 500      25.053  53.724  80.401  1.00 45.46           C
ATOM   1407  N   ALA A 501      24.932  52.988  76.119  1.00 43.29           N
ATOM   1408  CA  ALA A 501      24.521  51.941  75.158  1.00 42.43           C
ATOM   1409  C   ALA A 501      24.677  50.525  75.755  1.00 41.67           C
ATOM   1410  O   ALA A 501      25.008  49.553  75.066  1.00 41.39           O
ATOM   1411  CB  ALA A 501      25.249  52.092  73.819  1.00 42.25           C
ATOM   1412  N   TYR A 502      24.425  50.453  77.062  1.00 40.73           N
ATOM   1413  CA  TYR A 502      24.354  49.214  77.846  1.00 39.80           C
ATOM   1414  C   TYR A 502      25.704  48.520  78.076  1.00 39.34           C
ATOM   1415  O   TYR A 502      25.747  47.387  78.555  1.00 39.10           O
ATOM   1416  CB  TYR A 502      23.271  48.259  77.299  1.00 39.59           C
ATOM   1417  CG  TYR A 502      21.994  48.963  76.867  1.00 39.08           C
ATOM   1418  CD1 TYR A 502      21.276  49.763  77.757  1.00 39.08           C
ATOM   1419  CD2 TYR A 502      21.512  48.838  75.565  1.00 38.95           C
ATOM   1420  CE1 TYR A 502      20.115  50.419  77.364  1.00 38.94           C
ATOM   1421  CE2 TYR A 502      20.346  49.486  75.162  1.00 38.78           C
ATOM   1422  CZ  TYR A 502      19.655  50.275  76.067  1.00 39.16           C
ATOM   1423  OH  TYR A 502      18.501  50.921  75.682  1.00 39.14           O
ATOM   1424  N   SER A 503      26.798  49.221  77.770  1.00 38.77           N
ATOM   1425  CA  SER A 503      28.149  48.731  78.064  1.00 38.23           C
ATOM   1426  C   SER A 503      28.399  48.607  79.570  1.00 37.99           C
ATOM   1427  O   SER A 503      29.287  47.867  80.004  1.00 37.96           O
ATOM   1428  CB  SER A 503      29.208  49.639  77.432  1.00 38.28           C
ATOM   1429  OG  SER A 503      29.057  50.983  77.853  1.00 38.21           O
ATOM   1430  N   ASP A 504      27.599  49.328  80.353  1.00 37.38           N
ATOM   1431  CA  ASP A 504      27.692  49.314  81.810  1.00 36.90           C
ATOM   1432  C   ASP A 504      26.814  48.245  82.482  1.00 36.55           C
ATOM   1433  O   ASP A 504      26.757  48.179  83.716  1.00 36.41           O
ATOM   1434  CB  ASP A 504      27.359  50.703  82.370  1.00 36.92           C
ATOM   1435  CG  ASP A 504      25.976  51.182  81.967  1.00 36.85           C
ATOM   1436  OD1 ASP A 504      25.591  50.997  80.791  1.00 35.69           O
ATOM   1437  OD2 ASP A 504      25.274  51.754  82.826  1.00 37.49           O
ATOM   1438  N   LYS A 505      26.131  47.421  81.683  1.00 36.02           N
ATOM   1439  CA  LYS A 505      25.350  46.302  82.224  1.00 35.44           C
ATOM   1440  C   LYS A 505      26.267  45.331  82.960  1.00 35.34           C
ATOM   1441  O   LYS A 505      27.318  44.952  82.447  1.00 35.26           O
ATOM   1442  CB  LYS A 505      24.561  45.573  81.127  1.00 35.29           C
ATOM   1443  CG  LYS A 505      23.566  44.543  81.664  1.00 34.88           C
ATOM   1444  CD  LYS A 505      22.717  43.927  80.562  1.00 34.92           C
ATOM   1445  CE  LYS A 505      21.958  42.698  81.052  1.00 34.21           C
ATOM   1446  NZ  LYS A 505      20.795  43.023  81.926  1.00 34.41           N
ATOM   1447  N   GLY A 506      25.873  44.954  84.171  1.00 35.37           N
ATOM   1448  CA  GLY A 506      26.664  44.038  84.991  1.00 35.52           C
ATOM   1449  C   GLY A 506      27.775  44.701  85.794  1.00 35.69           C
ATOM   1450  O   GLY A 506      28.508  44.025  86.522  1.00 35.44           O
ATOM   1451  N   ASP A 507      27.912  46.018  85.652  1.00 35.99           N
ATOM   1452  CA  ASP A 507      28.857  46.785  86.458  1.00 36.55           C
ATOM   1453  C   ASP A 507      28.509  46.612  87.927  1.00 37.00           C
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ATOM   1454  O   ASP A 507      27.330  46.637  88.301  1.00 37.00           O
ATOM   1455  CB  ASP A 507      28.834  48.273  86.083  1.00 36.33           C
ATOM   1456  CG  ASP A 507      29.752  48.603  84.911  1.00 36.35           C
ATOM   1457  OD1 ASP A 507      30.431  47.691  84.387  1.00 35.90           O
ATOM   1458  OD2 ASP A 507      29.794  49.788  84.509  1.00 36.31           O
ATOM   1459  N   LEU A 508      29.531  46.415  88.752  1.00 37.44           N
ATOM   1460  CA  LEU A 508      29.306  46.216  90.177  1.00 38.11           C
ATOM   1461  C   LEU A 508      29.794  47.389  91.030  1.00 38.59           C
ATOM   1462  O   LEU A 508      30.950  47.813  90.937  1.00 38.69           O
ATOM   1463  CB  LEU A 508      29.901  44.883  90.648  1.00 37.85           C
ATOM   1464  CG  LEU A 508      29.372  44.443  92.019  1.00 37.85           C
ATOM   1465  CD1 LEU A 508      28.942  42.996  92.002  1.00 36.87           C
ATOM   1466  CD2 LEU A 508      30.382  44.710  93.131  1.00 37.66           C
ATOM   1467  N   TYR A 509      28.884  47.903  91.851  1.00 39.10           N
ATOM   1468  CA  TYR A 509      29.150  49.011  92.755  1.00 39.80           C
ATOM   1469  C   TYR A 509      29.136  48.515  94.201  1.00 40.29           C
ATOM   1470  O   TYR A 509      28.437  47.553  94.515  1.00 40.22           O
ATOM   1471  CB  TYR A 509      28.076  50.088  92.570  1.00 39.71           C
ATOM   1472  CG  TYR A 509      28.226  50.922  91.312  1.00 39.89           C
ATOM   1473  CD1 TYR A 509      28.698  52.234  91.379  1.00 39.75           C
ATOM   1474  CD2 TYR A 509      27.890  50.407  90.054  1.00 39.64           C
ATOM   1475  CE1 TYR A 509      28.840  53.010  90.230  1.00 39.56           C
ATOM   1476  CE2 TYR A 509      28.030  51.174  88.897  1.00 38.87           C
ATOM   1477  CZ  TYR A 509      28.505  52.473  88.995  1.00 39.71           C
ATOM   1478  OH  TYR A 509      28.643  53.244  87.865  1.00 39.86           O
ATOM   1479  N   LYS A 510      29.919  49.159  95.070  1.00 41.14           N
ATOM   1480  CA  LYS A 510      29.775  48.972  96.522  1.00 41.86           C
ATOM   1481  C   LYS A 510      29.113  50.190  97.150  1.00 42.35           C
ATOM   1482  O   LYS A 510      28.266  50.061  98.026  1.00 42.45           O
ATOM   1483  CB  LYS A 510      31.108  48.694  97.217  1.00 41.86           C
ATOM   1484  CG  LYS A 510      30.945  48.005  98.574  1.00 42.23           C
ATOM   1485  CD  LYS A 510      32.194  48.145  99.433  1.00 43.27           C
ATOM   1486  CE  LYS A 510      32.377  46.959 100.382  1.00 43.78           C
ATOM   1487  NZ  LYS A 510      31.374  46.895 101.486  1.00 44.22           N
ATOM   1488  N   GLY A 511      29.507  51.378  96.712  1.00 42.80           N
ATOM   1489  CA  GLY A 511      28.849  52.593  97.172  1.00 43.41           C
ATOM   1490  C   GLY A 511      28.359  53.353  95.968  1.00 43.80           C
ATOM   1491  O   GLY A 511      27.600  52.822  95.150  1.00 43.93           O
ATOM   1492  N   ASN A 512      28.801  54.600  95.866  1.00 44.06           N
ATOM   1493  CA  ASN A 512      28.640  55.381  94.650  1.00 44.35           C
ATOM   1494  C   ASN A 512      29.834  55.156  93.719  1.00 44.19           C
ATOM   1495  O   ASN A 512      29.887  55.697  92.608  1.00 44.04           O
ATOM   1496  CB  ASN A 512      28.495  56.866  94.996  1.00 44.59           C
ATOM   1497  CG  ASN A 512      27.242  57.156  95.804  1.00 45.35           C
ATOM   1498  OD1 ASN A 512      26.153  56.673  95.482  1.00 46.76           O
ATOM   1499  ND2 ASN A 512      27.389  57.953  96.856  1.00 45.71           N
ATOM   1500  N   GLN A 513      30.786  54.352  94.194  1.00 44.07           N
ATOM   1501  CA  GLN A 513      32.001  54.027  93.455  1.00 44.17           C
ATOM   1502  C   GLN A 513      31.863  52.675  92.761  1.00 43.91           C
ATOM   1503  O   GLN A 513      31.132  51.799  93.234  1.00 43.90           O
ATOM   1504  CB  GLN A 513      33.218  54.018  94.387  1.00 44.45           C
ATOM   1505  CG  GLN A 513      33.240  52.863  95.395  1.00 45.29           C
ATOM   1506  CD  GLN A 513      34.648  52.456  95.814  1.00 47.13           C
ATOM   1507  OE1 GLN A 513      35.643  52.826  95.176  1.00 47.20           O
ATOM   1508  NE2 GLN A 513      34.736  51.677  96.890  1.00 47.65           N
ATOM   1509  N   LEU A 514      32.578  52.511  91.647  1.00 43.53           N
ATOM   1510  CA  LEU A 514      32.462  51.313  90.814  1.00 43.01           C
ATOM   1511  C   LEU A 514      33.038  50.078  91.522  1.00 42.63           C
ATOM   1512  O   LEU A 514      32.561  49.712  92.605  1.00 42.80           O
ATOM   1513  CB  LEU A 514      33.092  51.555  89.433  1.00 43.01           C
ATOM   1514  CG  LEU A 514      32.745  50.683  88.215  1.00 43.12           C
ATOM   1515  CD1 LEU A 514      31.290  50.238  88.195  1.00 42.92           C
ATOM   1516  CD2 LEU A 514      33.095  51.421  86.924  1.00 43.05           C
ATOM   1517  N   LEU A 515      34.043  49.449  90.911  1.00 41.83           N
ATOM   1518  CA  LEU A 515      34.692  48.216  91.394  1.00 41.05           C
ATOM   1519  C   LEU A 515      35.069  47.341  90.214  1.00 40.26           C
ATOM   1520  O   LEU A 515      36.246  47.206  89.887  1.00 40.28           O
ATOM   1521  CB  LEU A 515      33.824  47.410  92.373  1.00 41.19           C
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ATOM   1522  CG  LEU A 515      34.149  47.467  93.871  1.00 41.69           C
ATOM   1523  CD1 LEU A 515      32.981  46.934  94.679  1.00 42.03           C
ATOM   1524  CD2 LEU A 515      35.417  46.688  94.197  1.00 42.18           C
ATOM   1525  N   GLY A 516      34.061  46.757  89.571  1.00 39.38           N
ATOM   1526  CA  GLY A 516      34.281  45.882  88.424  1.00 37.96           C
ATOM   1527  C   GLY A 516      33.013  45.540  87.671  1.00 36.96           C
ATOM   1528  O   GLY A 516      32.097  46.362  87.562  1.00 37.01           O
ATOM   1529  N   ASN A 517      32.960  44.317  87.155  1.00 35.84           N
ATOM   1530  CA  ASN A 517      31.839  43.868  86.335  1.00 34.59           C
ATOM   1531  C   ASN A 517      31.652  42.356  86.448  1.00 34.17           C
ATOM   1532  O   ASN A 517      32.616  41.593  86.343  1.00 33.85           O
ATOM   1533  CB  ASN A 517      32.046  44.303  84.878  1.00 34.41           C
ATOM   1534  CG  ASN A 517      30.852  44.008  83.996  1.00 32.96           C
ATOM   1535  OD1 ASN A 517      30.587  42.859  83.658  1.00 31.49           O
ATOM   1536  ND2 ASN A 517      30.138  45.054  83.598  1.00 31.54           N
ATOM   1537  N   ILE A 518      30.404  41.936  86.652  1.00 33.65           N
ATOM   1538  CA  ILE A 518      30.083  40.531  86.941  1.00 33.11           C
ATOM   1539  C   ILE A 518      30.291  39.570  85.766  1.00 32.83           C
ATOM   1540  O   ILE A 518      30.252  38.355  85.945  1.00 32.66           O
ATOM   1541  CB  ILE A 518      28.650  40.371  87.514  1.00 33.12           C
ATOM   1542  CG1 ILE A 518      27.605  40.844  86.496  1.00 33.15           C
ATOM   1543  CG2 ILE A 518      28.529  41.109  88.837  1.00 32.57           C
ATOM   1544  CD1 ILE A 518      26.184  40.446  86.812  1.00 32.82           C
ATOM   1545  N   TYR A 519      30.509  40.116  84.573  1.00 32.73           N
ATOM   1546  CA  TYR A 519      30.821  39.295  83.399  1.00 32.71           C
ATOM   1547  C   TYR A 519      32.336  39.140  83.179  1.00 32.89           C
ATOM   1548  O   TYR A 519      32.762  38.473  82.232  1.00 33.04           O
ATOM   1549  CB  TYR A 519      30.151  39.848  82.129  1.00 32.15           C
ATOM   1550  CG  TYR A 519      28.693  40.221  82.270  1.00 31.53           C
ATOM   1551  CD1 TYR A 519      27.779  39.362  82.886  1.00 30.97           C
ATOM   1552  CD2 TYR A 519      28.220  41.430  81.768  1.00 31.22           C
ATOM   1553  CE1 TYR A 519      26.432  39.709  83.007  1.00 30.51           C
ATOM   1554  CE2 TYR A 519      26.878  41.786  81.886  1.00 30.74           C
ATOM   1555  CZ  TYR A 519      25.993  40.923  82.506  1.00 31.02           C
ATOM   1556  OH  TYR A 519      24.671  41.285  82.619  1.00 31.14           O
ATOM   1557  N   PHE A 520      33.136  39.760  84.046  1.00 33.18           N
ATOM   1558  CA  PHE A 520      34.597  39.650  83.991  1.00 33.68           C
ATOM   1559  C   PHE A 520      35.022  38.331  84.623  1.00 33.97           C
ATOM   1560  O   PHE A 520      34.493  37.941  85.664  1.00 34.03           O
ATOM   1561  CB  PHE A 520      35.262  40.828  84.718  1.00 33.76           C
ATOM   1562  CG  PHE A 520      35.131  42.163  84.004  1.00 34.02           C
ATOM   1563  CD1 PHE A 520      34.382  42.294  82.834  1.00 33.80           C
ATOM   1564  CD2 PHE A 520      35.738  43.300  84.531  1.00 34.57           C
ATOM   1565  CE1 PHE A 520      34.262  43.523  82.192  1.00 34.23           C
ATOM   1566  CE2 PHE A 520      35.623  44.538  83.899  1.00 34.73           C
ATOM   1567  CZ  PHE A 520      34.886  44.649  82.724  1.00 34.63           C
ATOM   1568  N   THR A 521      35.968  37.649  83.986  1.00 34.46           N
ATOM   1569  CA  THR A 521      36.383  36.302  84.392  1.00 35.27           C
ATOM   1570  C   THR A 521      37.821  36.273  84.924  1.00 35.45           C
ATOM   1571  O   THR A 521      38.151  35.467  85.794  1.00 35.52           O
ATOM   1572  CB  THR A 521      36.243  35.309  83.212  1.00 35.33           C
ATOM   1573  OG1 THR A 521      34.940  35.447  82.632  1.00 36.70           O
ATOM   1574  CG2 THR A 521      36.421  33.862  83.668  1.00 35.85           C
ATOM   1575  N   THR A 522      38.658  37.170  84.407  1.00 35.73           N
ATOM   1576  CA  THR A 522      40.078  37.200  84.738  1.00 35.92           C
ATOM   1577  C   THR A 522      40.465  38.536  85.377  1.00 36.02           C
ATOM   1578  O   THR A 522      39.880  39.574  85.055  1.00 35.77           O
ATOM   1579  CB  THR A 522      40.932  36.948  83.471  1.00 35.96           C
ATOM   1580  OG1 THR A 522      40.454  35.775  82.801  1.00 35.53           O
ATOM   1581  CG2 THR A 522      42.395  36.745  83.825  1.00 36.58           C
ATOM   1582  N   ASN A 523      41.439  38.488  86.291  1.00 36.10           N
ATOM   1583  CA  ASN A 523      42.035  39.680  86.918  1.00 36.32           C
ATOM   1584  C   ASN A 523      40.999  40.682  87.426  1.00 36.45           C
ATOM   1585  O   ASN A 523      41.085  41.884  87.152  1.00 36.54           O
ATOM   1586  CB  ASN A 523      43.037  40.359  85.968  1.00 36.25           C
ATOM   1587  CG  ASN A 523      44.072  39.385  85.408  1.00 36.56           C
ATOM   1588  OD1 ASN A 523      44.394  38.371  86.031  1.00 37.31           O
ATOM   1589  ND2 ASN A 523      44.592  39.691  84.224  1.00 36.35           N
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ATOM   1590  N   LYS A 524      40.031  40.168  88.177  1.00 36.46           N
ATOM   1591  CA  LYS A 524      38.869  40.938  88.588  1.00 36.48           C
ATOM   1592  C   LYS A 524      39.200  41.961  89.661  1.00 36.87           C
ATOM   1593  O   LYS A 524      39.984  41.693  90.570  1.00 36.78           O
ATOM   1594  CB  LYS A 524      37.758  40.006  89.074  1.00 36.52           C
ATOM   1595  CG  LYS A 524      37.164  39.116  87.979  1.00 36.16           C
ATOM   1596  CD  LYS A 524      36.205  38.074  88.556  1.00 35.90           C
ATOM   1597  CE  LYS A 524      34.956  38.714  89.151  1.00 34.47           C
ATOM   1598  NZ  LYS A 524      34.193  39.535  88.162  1.00 33.84           N
ATOM   1599  N   THR A 525      38.587  43.134  89.533  1.00 37.24           N
ATOM   1600  CA  THR A 525      38.709  44.212  90.511  1.00 37.48           C
ATOM   1601  C   THR A 525      37.523  44.212  91.494  1.00 37.34           C
ATOM   1602  O   THR A 525      37.500  44.989  92.446  1.00 37.42           O
ATOM   1603  CB  THR A 525      38.836  45.580  89.794  1.00 37.67           C
ATOM   1604  OG1 THR A 525      39.767  45.466  88.713  1.00 37.73           O
ATOM   1605  CG2 THR A 525      39.322  46.677  90.755  1.00 38.48           C
ATOM   1606  N   SER A 526      36.549  43.332  91.255  1.00 37.27           N
ATOM   1607  CA  SER A 526      35.387  43.159  92.135  1.00 37.12           C
ATOM   1608  C   SER A 526      35.306  41.699  92.581  1.00 36.73           C
ATOM   1609  O   SER A 526      35.842  40.827  91.903  1.00 37.17           O
ATOM   1610  CB  SER A 526      34.092  43.565  91.415  1.00 37.28           C
ATOM   1611  OG  SER A 526      33.626  42.535  90.551  1.00 37.83           O
ATOM   1612  N   PRO A 527      34.641  41.422  93.718  1.00 36.38           N
ATOM   1613  CA  PRO A 527      34.566  40.028  94.177  1.00 36.04           C
ATOM   1614  C   PRO A 527      33.504  39.141  93.499  1.00 35.63           C
ATOM   1615  O   PRO A 527      33.489  37.931  93.733  1.00 35.58           O
ATOM   1616  CB  PRO A 527      34.263  40.172  95.673  1.00 35.94           C
ATOM   1617  CG  PRO A 527      33.524  41.453  95.789  1.00 36.26           C
ATOM   1618  CD  PRO A 527      33.962  42.347  94.648  1.00 36.37           C
ATOM   1619  N   PHE A 528      32.643  39.720  92.665  1.00 35.27           N
ATOM   1620  CA  PHE A 528      31.503  38.970  92.117  1.00 34.92           C
ATOM   1621  C   PHE A 528      31.518  38.714  90.612  1.00 34.47           C
ATOM   1622  O   PHE A 528      31.792  39.612  89.815  1.00 34.56           O
ATOM   1623  CB  PHE A 528      30.181  39.635  92.500  1.00 34.95           C
ATOM   1624  CG  PHE A 528      29.921  39.660  93.972  1.00 35.46           C
ATOM   1625  CD1 PHE A 528      29.482  38.518  94.633  1.00 35.46           C
ATOM   1626  CD2 PHE A 528      30.110  40.829  94.702  1.00 35.96           C
ATOM   1627  CE1 PHE A 528      29.239  38.538  95.998  1.00 35.79           C
ATOM   1628  CE2 PHE A 528      29.871  40.859  96.070  1.00 35.87           C
ATOM   1629  CZ  PHE A 528      29.433  39.713  96.720  1.00 35.73           C
ATOM   1630  N   ARG A 529      31.197  37.476  90.247  1.00 33.94           N
ATOM   1631  CA  ARG A 529      30.994  37.083  88.854  1.00 33.18           C
ATOM   1632  C   ARG A 529      29.773  36.169  88.727  1.00 32.69           C
ATOM   1633  O   ARG A 529      29.367  35.524  89.695  1.00 32.65           O
ATOM   1634  CB  ARG A 529      32.236  36.379  88.298  1.00 33.17           C
ATOM   1635  CG  ARG A 529      32.566  35.044  88.954  1.00 33.25           C
ATOM   1636  CD  ARG A 529      33.445  34.198  88.048  1.00 34.49           C
ATOM   1637  NE  ARG A 529      33.723  32.882  88.624  1.00 35.65           N
ATOM   1638  CZ  ARG A 529      32.970  31.796  88.453  1.00 36.54           C
ATOM   1639  NH1 ARG A 529      31.865  31.838  87.711  1.00 35.55           N
ATOM   1640  NH2 ARG A 529      33.328  30.653  89.030  1.00 37.41           N
ATOM   1641  N   ILE A 530      29.194  36.115  87.531  1.00 31.91           N
ATOM   1642  CA  ILE A 530      28.122  35.160  87.245  1.00 31.11           C
ATOM   1643  C   ILE A 530      28.706  33.773  86.990  1.00 30.48           C
ATOM   1644  O   ILE A 530      29.925  33.589  87.033  1.00 30.43           O
ATOM   1645  CB  ILE A 530      27.245  35.596  86.043  1.00 31.17           C
ATOM   1646  CG1 ILE A 530      28.090  35.765  84.770  1.00 31.17           C
ATOM   1647  CG2 ILE A 530      26.482  36.871  86.386  1.00 31.14           C
ATOM   1648  CD1 ILE A 530      27.279  35.861  83.468  1.00 31.03           C
ATOM   1649  N   ALA A 531      27.830  32.807  86.734  1.00 29.68           N
ATOM   1650  CA  ALA A 531      28.236  31.450  86.374  1.00 28.82           C
ATOM   1651  C   ALA A 531      28.822  31.394  84.962  1.00 28.17           C
ATOM   1652  O   ALA A 531      28.340  32.071  84.054  1.00 27.87           O
ATOM   1653  CB  ALA A 531      27.054  30.498  86.490  1.00 28.75           C
ATOM   1654  N   LYS A 532      29.858  30.576  84.794  1.00 27.59           N
ATOM   1655  CA  LYS A 532      30.506  30.387  83.503  1.00 27.27           C
ATOM   1656  C   LYS A 532      29.610  29.518  82.620  1.00 26.30           C
ATOM   1657  O   LYS A 532      29.665  28.285  82.655  1.00 26.00           O
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ATOM   1658  CB  LYS A 532      31.889  29.763  83.698  1.00 27.16           C
ATOM   1659  CG  LYS A 532      32.848  29.905  82.515  1.00 27.98           C
ATOM   1660  CD  LYS A 532      34.233  29.327  82.882  1.00 28.75           C
ATOM   1661  CE  LYS A 532      35.103  29.054  81.650  1.00 31.48           C
ATOM   1662  NZ  LYS A 532      35.776  30.286  81.127  1.00 32.73           N
ATOM   1663  N   ASP A 533      28.772  30.184  81.833  1.00 25.57           N
ATOM   1664  CA  ASP A 533      27.760  29.496  81.044  1.00 24.91           C
ATOM   1665  C   ASP A 533      27.406  30.221  79.746  1.00 24.32           C
ATOM   1666  O   ASP A 533      27.838  31.351  79.507  1.00 24.30           O
ATOM   1667  CB  ASP A 533      26.496  29.280  81.885  1.00 24.79           C
ATOM   1668  CG  ASP A 533      25.710  28.057  81.455  1.00 25.30           C
ATOM   1669  OD1 ASP A 533      26.007  27.478  80.388  1.00 25.65           O
ATOM   1670  OD2 ASP A 533      24.783  27.666  82.186  1.00 26.36           O
ATOM   1671  N   SER A 534      26.638  29.529  78.909  1.00 23.67           N
ATOM   1672  CA  SER A 534      25.991  30.087  77.726  1.00 22.96           C
ATOM   1673  C   SER A 534      24.668  30.735  78.150  1.00 22.41           C
ATOM   1674  O   SER A 534      23.948  30.196  78.995  1.00 22.29           O
ATOM   1675  CB  SER A 534      25.759  28.958  76.701  1.00 22.99           C
ATOM   1676  OG  SER A 534      24.743  29.262  75.758  1.00 22.76           O
ATOM   1677  N   TYR A 535      24.360  31.897  77.580  1.00 21.82           N
ATOM   1678  CA  TYR A 535      23.136  32.629  77.925  1.00 21.52           C
ATOM   1679  C   TYR A 535      22.393  33.117  76.685  1.00 21.46           C
ATOM   1680  O   TYR A 535      22.943  33.138  75.579  1.00 21.40           O
ATOM   1681  CB  TYR A 535      23.445  33.825  78.830  1.00 21.12           C
ATOM   1682  CG  TYR A 535      23.998  33.463  80.188  1.00 21.17           C
ATOM   1683  CD1 TYR A 535      23.161  33.360  81.298  1.00 20.69           C
ATOM   1684  CD2 TYR A 535      25.367  33.245  80.372  1.00 20.90           C
ATOM   1685  CE1 TYR A 535      23.667  33.037  82.556  1.00 20.50           C
ATOM   1686  CE2 TYR A 535      25.881  32.917  81.627  1.00 21.33           C
ATOM   1687  CZ  TYR A 535      25.024  32.819  82.712  1.00 20.77           C
ATOM   1688  OH  TYR A 535      25.532  32.493  83.949  1.00 21.04           O
ATOM   1689  N   LEU A 536      21.145  33.527  76.884  1.00 21.26           N
ATOM   1690  CA  LEU A 536      20.302  33.978  75.790  1.00 21.36           C
ATOM   1691  C   LEU A 536      19.622  35.298  76.137  1.00 21.45           C
ATOM   1692  O   LEU A 536      18.857  35.378  77.098  1.00 21.67           O
ATOM   1693  CB  LEU A 536      19.266  32.907  75.437  1.00 21.00           C
ATOM   1694  CG  LEU A 536      18.683  33.018  74.034  1.00 21.29           C
ATOM   1695  CD1 LEU A 536      19.771  32.814  72.980  1.00 21.36           C
ATOM   1696  CD2 LEU A 536      17.551  32.027  73.847  1.00 20.77           C
ATOM   1697  N   TRP A 537      19.910  36.321  75.340  1.00 21.34           N
ATOM   1698  CA  TRP A 537      19.452  37.674  75.596  1.00 21.48           C
ATOM   1699  C   TRP A 537      18.544  38.178  74.488  1.00 21.41           C
ATOM   1700  O   TRP A 537      18.598  37.690  73.364  1.00 21.48           O
ATOM   1701  CB  TRP A 537      20.656  38.608  75.740  1.00 21.74           C
ATOM   1702  CG  TRP A 537      21.345  38.546  77.082  1.00 21.86           C
ATOM   1703  CD1 TRP A 537      21.142  37.627  78.072  1.00 21.36           C
ATOM   1704  CD2 TRP A 537      22.372  39.429  77.557  1.00 21.92           C
ATOM   1705  NE1 TRP A 537      21.964  37.895  79.138  1.00 22.21           N
ATOM   1706  CE2 TRP A 537      22.729  38.995  78.851  1.00 21.85           C
ATOM   1707  CE3 TRP A 537      23.019  40.550  77.016  1.00 21.71           C
ATOM   1708  CZ2 TRP A 537      23.707  39.641  79.618  1.00 21.83           C
ATOM   1709  CZ3 TRP A 537      23.990  41.196  77.779  1.00 21.94           C
ATOM   1710  CH2 TRP A 537      24.324  40.738  79.068  1.00 21.57           C
ATOM   1711  N   MET A 538      17.717  39.165  74.814  1.00 21.49           N
ATOM   1712  CA  MET A 538      16.820  39.768  73.835  1.00 21.88           C
ATOM   1713  C   MET A 538      16.675  41.271  74.057  1.00 21.87           C
ATOM   1714  O   MET A 538      16.595  41.734  75.192  1.00 22.10           O
ATOM   1715  CB  MET A 538      15.453  39.072  73.878  1.00 21.82           C
ATOM   1716  CG  MET A 538      14.382  39.685  72.992  1.00 22.02           C
ATOM   1717  SD  MET A 538      13.535  41.086  73.760  1.00 23.50           S
ATOM   1718  CE  MET A 538      12.470  40.222  74.922  1.00 21.20           C
ATOM   1719  N   SER A 539      16.643  42.027  72.966  1.00 22.06           N
ATOM   1720  CA  SER A 539      16.346  43.460  73.019  1.00 22.23           C
ATOM   1721  C   SER A 539      15.248  43.790  72.005  1.00 22.62           C
ATOM   1722  O   SER A 539      15.156  43.145  70.955  1.00 22.72           O
ATOM   1723  CB  SER A 539      17.602  44.289  72.746  1.00 22.15           C
ATOM   1724  OG  SER A 539      18.669  43.932  73.617  1.00 21.56           O
ATOM   1725  N   TYR A 540      14.416  44.782  72.322  1.00 22.96           N
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ATOM   1726  CA  TYR A 540      13.294  45.142  71.453  1.00 23.35           C
ATOM   1727  C   TYR A 540      13.260  46.609  71.035  1.00 23.56           C
ATOM   1728  O   TYR A 540      13.809  47.477  71.719  1.00 23.63           O
ATOM   1729  CB  TYR A 540      11.951  44.732  72.079  1.00 23.36           C
ATOM   1730  CG  TYR A 540      11.627  45.406  73.399  1.00 23.63           C
ATOM   1731  CD1 TYR A 540      11.150  46.719  73.435  1.00 23.15           C
ATOM   1732  CD2 TYR A 540      11.775  44.721  74.611  1.00 23.64           C
ATOM   1733  CE1 TYR A 540      10.846  47.341  74.639  1.00 23.50           C
ATOM   1734  CE2 TYR A 540      11.470  45.333  75.824  1.00 24.11           C
ATOM   1735  CZ  TYR A 540      11.006  46.648  75.828  1.00 24.09           C
ATOM   1736  OH  TYR A 540      10.706  47.273  77.014  1.00 23.93           O
ATOM   1737  N   SER A 541      12.592  46.868  69.914  1.00 23.89           N
ATOM   1738  CA  SER A 541      12.409  48.217  69.401  1.00 24.33           C
ATOM   1739  C   SER A 541      10.948  48.509  69.068  1.00 24.73           C
ATOM   1740  O   SER A 541      10.296  47.741  68.355  1.00 24.68           O
ATOM   1741  CB  SER A 541      13.264  48.422  68.158  1.00 24.45           C
ATOM   1742  OG  SER A 541      13.055  49.712  67.622  1.00 25.02           O
ATOM   1743  N   ASP A 542      10.443  49.627  69.581  1.00 25.11           N
ATOM   1744  CA  ASP A 542       9.080  50.055  69.280  1.00 25.40           C
ATOM   1745  C   ASP A 542       9.031  51.241  68.321  1.00 25.74           C
ATOM   1746  O   ASP A 542       7.955  51.772  68.035  1.00 25.86           O
ATOM   1747  CB  ASP A 542       8.313  50.365  70.570  1.00 25.32           C
ATOM   1748  CG  ASP A 542       8.018  49.117  71.393  1.00 25.35           C
ATOM   1749  OD1 ASP A 542       7.687  48.063  70.812  1.00 25.13           O
ATOM   1750  OD2 ASP A 542       8.105  49.194  72.633  1.00 26.19           O
ATOM   1751  N   ASP A 543      10.192  51.662  67.824  1.00 26.17           N
ATOM   1752  CA  ASP A 543      10.230  52.741  66.836  1.00 26.68           C
ATOM   1753  C   ASP A 543      10.954  52.329  65.552  1.00 26.94           C
ATOM   1754  O   ASP A 543      11.822  53.050  65.043  1.00 27.13           O
ATOM   1755  CB  ASP A 543      10.805  54.035  67.434  1.00 26.51           C
ATOM   1756  CG  ASP A 543      12.203  53.860  68.007  1.00 27.10           C
ATOM   1757  OD1 ASP A 543      12.841  52.797  67.811  1.00 26.77           O
ATOM   1758  OD2 ASP A 543      12.669  54.811  68.662  1.00 28.02           O
ATOM   1759  N   ASP A 544      10.587  51.157  65.043  1.00 27.29           N
ATOM   1760  CA  ASP A 544      11.036  50.684  63.730  1.00 27.81           C
ATOM   1761  C   ASP A 544      12.555  50.480  63.631  1.00 27.84           C
ATOM   1762  O   ASP A 544      13.132  50.585  62.550  1.00 27.85           O
ATOM   1763  CB  ASP A 544      10.517  51.617  62.614  1.00 27.86           C
ATOM   1764  CG  ASP A 544      10.568  50.977  61.241  1.00 28.21           C
ATOM   1765  OD1 ASP A 544      10.112  49.820  61.093  1.00 29.09           O
ATOM   1766  OD2 ASP A 544      11.060  51.640  60.306  1.00 28.32           O
ATOM   1767  N   GLY A 545      13.190  50.185  64.764  1.00 28.04           N
ATOM   1768  CA  GLY A 545      14.606  49.814  64.787  1.00 28.17           C
ATOM   1769  C   GLY A 545      15.589  50.926  65.114  1.00 28.42           C
ATOM   1770  O   GLY A 545      16.804  50.706  65.116  1.00 28.60           O
ATOM   1771  N   LYS A 546      15.068  52.115  65.400  1.00 28.61           N
ATOM   1772  CA  LYS A 546      15.896  53.289  65.680  1.00 28.73           C
ATOM   1773  C   LYS A 546      16.485  53.274  67.095  1.00 28.87           C
ATOM   1774  O   LYS A 546      17.669  53.558  67.275  1.00 29.14           O
ATOM   1775  CB  LYS A 546      15.096  54.570  65.428  1.00 28.86           C
ATOM   1776  CG  LYS A 546      14.695  54.762  63.965  1.00 29.03           C
ATOM   1777  CD  LYS A 546      13.699  55.894  63.797  1.00 30.05           C
ATOM   1778  CE  LYS A 546      13.745  56.454  62.383  1.00 30.86           C
ATOM   1779  NZ  LYS A 546      12.661  57.440  62.127  1.00 31.61           N
ATOM   1780  N   THR A 547      15.661  52.942  68.090  1.00 28.74           N
ATOM   1781  CA  THR A 547      16.126  52.807  69.475  1.00 28.54           C
ATOM   1782  C   THR A 547      15.737  51.441  70.040  1.00 28.43           C
ATOM   1783  O   THR A 547      14.698  50.882  69.683  1.00 28.29           O
ATOM   1784  CB  THR A 547      15.572  53.922  70.406  1.00 28.80           C
ATOM   1785  OG1 THR A 547      14.136  53.843  70.464  1.00 28.91           O
ATOM   1786  CG2 THR A 547      16.009  55.314  69.927  1.00 28.22           C
ATOM   1787  N   TRP A 548      16.573  50.922  70.933  1.00 28.17           N
ATOM   1788  CA  TRP A 548      16.426  49.566  71.437  1.00 27.97           C
ATOM   1789  C   TRP A 548      16.389  49.544  72.949  1.00 27.97           C
ATOM   1790  O   TRP A 548      16.981  50.404  73.606  1.00 27.87           O
ATOM   1791  CB  TRP A 548      17.576  48.692  70.933  1.00 28.04           C
ATOM   1792  CG  TRP A 548      17.528  48.488  69.463  1.00 28.17           C
ATOM   1793  CD1 TRP A 548      17.988  49.343  68.502  1.00 28.22           C
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ATOM   1794  CD2 TRP A 548      16.964  47.367  68.771  1.00 28.20           C
ATOM   1795  NE1 TRP A 548      17.753  48.818  67.252  1.00 29.06           N
ATOM   1796  CE2 TRP A 548      17.127  47.606  67.387  1.00 28.50           C
ATOM   1797  CE3 TRP A 548      16.342  46.180  69.184  1.00 28.65           C
ATOM   1798  CZ2 TRP A 548      16.684  46.702  66.410  1.00 28.01           C
ATOM   1799  CZ3 TRP A 548      15.906  45.275  68.208  1.00 28.33           C
ATOM   1800  CH2 TRP A 548      16.082  45.545  66.841  1.00 27.91           C
ATOM   1801  N   SER A 549      15.695  48.550  73.495  1.00 27.79           N
ATOM   1802  CA  SER A 549      15.620  48.372  74.936  1.00 27.72           C
ATOM   1803  C   SER A 549      16.931  47.797  75.461  1.00 27.56           C
ATOM   1804  O   SER A 549      17.749  47.284  74.690  1.00 27.59           O
ATOM   1805  CB  SER A 549      14.454  47.448  75.297  1.00 27.62           C
ATOM   1806  OG  SER A 549      14.645  46.150  74.752  1.00 28.57           O
ATOM   1807  N   ALA A 550      17.122  47.905  76.773  1.00 27.43           N
ATOM   1808  CA  ALA A 550      18.213  47.235  77.476  1.00 27.32           C
ATOM   1809  C   ALA A 550      17.996  45.725  77.398  1.00 27.25           C
ATOM   1810  O   ALA A 550      16.849  45.269  77.391  1.00 27.69           O
ATOM   1811  CB  ALA A 550      18.257  47.692  78.924  1.00 27.21           C
ATOM   1812  N   PRO A 551      19.086  44.942  77.339  1.00 26.94           N
ATOM   1813  CA  PRO A 551      18.968  43.493  77.138  1.00 26.66           C
ATOM   1814  C   PRO A 551      18.143  42.784  78.208  1.00 26.35           C
ATOM   1815  O   PRO A 551      18.410  42.939  79.401  1.00 26.41           O
ATOM   1816  CB  PRO A 551      20.425  43.011  77.205  1.00 26.71           C
ATOM   1817  CG  PRO A 551      21.241  44.207  76.874  1.00 26.71           C
ATOM   1818  CD  PRO A 551      20.493  45.366  77.454  1.00 26.95           C
ATOM   1819  N   GLN A 552      17.139  42.025  77.781  1.00 26.07           N
ATOM   1820  CA  GLN A 552      16.425  41.136  78.689  1.00 25.63           C
ATOM   1821  C   GLN A 552      17.076  39.777  78.663  1.00 25.18           C
ATOM   1822  O   GLN A 552      17.300  39.206  77.589  1.00 24.92           O
ATOM   1823  CB  GLN A 552      14.949  41.001  78.320  1.00 26.09           C
ATOM   1824  CG  GLN A 552      14.003  41.803  79.196  1.00 27.73           C
ATOM   1825  CD  GLN A 552      14.043  43.280  78.882  1.00 30.53           C
ATOM   1826  OE1 GLN A 552      14.367  43.678  77.760  1.00 32.40           O
ATOM   1827  NE2 GLN A 552      13.716  44.105  79.869  1.00 31.19           N
ATOM   1828  N   ASP A 553      17.387  39.273  79.854  1.00 24.65           N
ATOM   1829  CA  ASP A 553      17.905  37.931  80.018  1.00 24.03           C
ATOM   1830  C   ASP A 553      16.726  36.974  80.008  1.00 23.59           C
ATOM   1831  O   ASP A 553      15.962  36.915  80.968  1.00 23.64           O
ATOM   1832  CB  ASP A 553      18.660  37.818  81.338  1.00 23.99           C
ATOM   1833  CG  ASP A 553      19.368  36.485  81.500  1.00 24.33           C
ATOM   1834  OD1 ASP A 553      19.552  35.751  80.500  1.00 23.49           O
ATOM   1835  OD2 ASP A 553      19.757  36.176  82.642  1.00 25.83           O
ATOM   1836  N   ILE A 554      16.578  36.228  78.920  1.00 23.09           N
ATOM   1837  CA  ILE A 554      15.449  35.302  78.771  1.00 22.53           C
ATOM   1838  C   ILE A 554      15.846  33.855  79.033  1.00 22.09           C
ATOM   1839  O   ILE A 554      15.003  32.958  78.990  1.00 22.08           O
ATOM   1840  CB  ILE A 554      14.758  35.439  77.384  1.00 22.65           C
ATOM   1841  CG1 ILE A 554      15.726  35.098  76.243  1.00 22.34           C
ATOM   1842  CG2 ILE A 554      14.169  36.847  77.225  1.00 22.31           C
ATOM   1843  CD1 ILE A 554      15.041  34.674  74.949  1.00 23.41           C
ATOM   1844  N   THR A 555      17.131  33.654  79.324  1.00 21.80           N
ATOM   1845  CA  THR A 555      17.732  32.327  79.559  1.00 21.59           C
ATOM   1846  C   THR A 555      16.886  31.367  80.411  1.00 21.45           C
ATOM   1847  O   THR A 555      16.579  30.266  79.949  1.00 21.27           O
ATOM   1848  CB  THR A 555      19.168  32.445  80.164  1.00 21.35           C
ATOM   1849  OG1 THR A 555      19.926  33.415  79.432  1.00 21.97           O
ATOM   1850  CG2 THR A 555      19.903  31.106  80.142  1.00 21.14           C
ATOM   1851  N   PRO A 556      16.498  31.780  81.645  1.00 21.63           N
ATOM   1852  CA  PRO A 556      15.827  30.821  82.541  1.00 21.64           C
ATOM   1853  C   PRO A 556      14.473  30.332  82.036  1.00 21.70           C
ATOM   1854  O   PRO A 556      13.992  29.295  82.485  1.00 21.75           O
ATOM   1855  CB  PRO A 556      15.670  31.601  83.857  1.00 21.58           C
ATOM   1856  CG  PRO A 556      15.732  33.039  83.468  1.00 21.67           C
ATOM   1857  CD  PRO A 556      16.636  33.114  82.274  1.00 21.44           C
ATOM   1858  N   MET A 557      13.870  31.050  81.094  1.00 22.12           N
ATOM   1859  CA  MET A 557      12.574  30.635  80.541  1.00 22.38           C
ATOM   1860  C   MET A 557      12.692  29.412  79.627  1.00 22.10           C
ATOM   1861  O   MET A 557      11.742  28.641  79.483  1.00 22.03           O
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ATOM   1862  CB  MET A 557      11.905  31.780  79.777  1.00 22.16           C
ATOM   1863  CG  MET A 557      11.863  33.109  80.514  1.00 22.83           C
ATOM   1864  SD  MET A 557      10.670  34.245  79.779  1.00 23.61           S
ATOM   1865  CE  MET A 557      11.287  35.833  80.332  1.00 23.16           C
ATOM   1866  N   VAL A 558      13.862  29.232  79.020  1.00 22.14           N
ATOM   1867  CA  VAL A 558      14.007  28.288  77.910  1.00 22.04           C
ATOM   1868  C   VAL A 558      15.125  27.259  78.054  1.00 22.23           C
ATOM   1869  O   VAL A 558      15.138  26.256  77.333  1.00 21.96           O
ATOM   1870  CB  VAL A 558      14.193  29.039  76.570  1.00 22.30           C
ATOM   1871  CG1 VAL A 558      12.923  29.813  76.211  1.00 21.48           C
ATOM   1872  CG2 VAL A 558      15.427  29.970  76.621  1.00 21.72           C
ATOM   1873  N   LYS A 559      16.054  27.502  78.976  1.00 22.46           N
ATOM   1874  CA  LYS A 559      17.221  26.632  79.134  1.00 22.60           C
ATOM   1875  C   LYS A 559      17.074  25.593  80.249  1.00 22.93           C
ATOM   1876  O   LYS A 559      16.975  25.951  81.416  1.00 23.29           O
ATOM   1877  CB  LYS A 559      18.475  27.470  79.378  1.00 22.48           C
ATOM   1878  CG  LYS A 559      19.737  26.674  79.211  1.00 21.49           C
ATOM   1879  CD  LYS A 559      20.961  27.498  79.438  1.00 19.97           C
ATOM   1880  CE  LYS A 559      22.140  26.744  78.902  1.00 19.47           C
ATOM   1881  NZ  LYS A 559      23.324  26.904  79.758  1.00 20.96           N
ATOM   1882  N   ALA A 560      17.100  24.311  79.882  1.00 23.25           N
ATOM   1883  CA  ALA A 560      16.967  23.204  80.844  1.00 23.46           C
ATOM   1884  C   ALA A 560      18.249  22.924  81.648  1.00 23.73           C
ATOM   1885  O   ALA A 560      19.324  23.423  81.307  1.00 23.93           O
ATOM   1886  CB  ALA A 560      16.500  21.940  80.130  1.00 23.36           C
ATOM   1887  N   ASP A 561      18.117  22.115  82.705  1.00 24.04           N
ATOM   1888  CA  ASP A 561      19.216  21.780  83.624  1.00 24.19           C
ATOM   1889  C   ASP A 561      20.381  21.078  82.937  1.00 23.90           C
ATOM   1890  O   ASP A 561      21.529  21.232  83.353  1.00 24.25           O
ATOM   1891  CB  ASP A 561      18.735  20.863  84.758  1.00 24.46           C
ATOM   1892  CG  ASP A 561      17.573  21.437  85.545  1.00 26.44           C
ATOM   1893  OD1 ASP A 561      17.474  22.681  85.673  1.00 29.36           O
ATOM   1894  OD2 ASP A 561      16.754  20.631  86.052  1.00 27.87           O
ATOM   1895  N   TRP A 562      20.085  20.281  81.913  1.00 23.33           N
ATOM   1896  CA  TRP A 562      21.116  19.464  81.264  1.00 22.83           C
ATOM   1897  C   TRP A 562      21.865  20.220  80.174  1.00 22.36           C
ATOM   1898  O   TRP A 562      22.978  19.831  79.801  1.00 22.06           O
ATOM   1899  CB  TRP A 562      20.513  18.188  80.680  1.00 22.60           C
ATOM   1900  CG  TRP A 562      19.403  18.437  79.698  1.00 22.81           C
ATOM   1901  CD1 TRP A 562      18.067  18.453  79.968  1.00 22.92           C
ATOM   1902  CD2 TRP A 562      19.532  18.711  78.292  1.00 22.95           C
ATOM   1903  NE1 TRP A 562      17.354  18.709  78.823  1.00 22.94           N
ATOM   1904  CE2 TRP A 562      18.225  18.867  77.778  1.00 22.62           C
ATOM   1905  CE3 TRP A 562      20.623  18.822  77.415  1.00 22.37           C
ATOM   1906  CZ2 TRP A 562      17.974  19.133  76.428  1.00 22.30           C
ATOM   1907  CZ3 TRP A 562      20.373  19.086  76.069  1.00 22.53           C
ATOM   1908  CH2 TRP A 562      19.057  19.241  75.591  1.00 22.74           C
ATOM   1909  N   MET A 563      21.238  21.285  79.668  1.00 21.57           N
ATOM   1910  CA  MET A 563      21.751  22.029  78.518  1.00 20.97           C
ATOM   1911  C   MET A 563      23.093  22.673  78.838  1.00 20.95           C
ATOM   1912  O   MET A 563      23.258  23.317  79.884  1.00 20.81           O
ATOM   1913  CB  MET A 563      20.730  23.073  78.025  1.00 20.70           C
ATOM   1914  CG  MET A 563      19.489  22.478  77.311  1.00 20.52           C
ATOM   1915  SD  MET A 563      18.203  23.686  76.860  1.00 20.70           S
ATOM   1916  CE  MET A 563      16.977  22.648  76.072  1.00 20.16           C
ATOM   1917  N   LYS A 564      24.063  22.457  77.952  1.00 20.57           N
ATOM   1918  CA  LYS A 564      25.328  23.162  78.039  1.00 20.24           C
ATOM   1919  C   LYS A 564      25.184  24.452  77.238  1.00 19.66           C
ATOM   1920  O   LYS A 564      24.902  25.511  77.802  1.00 19.66           O
ATOM   1921  CB  LYS A 564      26.485  22.299  77.526  1.00 20.36           C
ATOM   1922  CG  LYS A 564      27.862  22.832  77.912  1.00 20.67           C
ATOM   1923  CD  LYS A 564      28.993  21.905  77.470  1.00 20.79           C
ATOM   1924  CE  LYS A 564      30.272  22.261  78.221  1.00 22.25           C
ATOM   1925  NZ  LYS A 564      31.449  21.492  77.743  1.00 24.17           N
ATOM   1926  N   PHE A 565      25.362  24.353  75.926  1.00 18.86           N
ATOM   1927  CA  PHE A 565      25.126  25.476  75.040  1.00 18.48           C
ATOM   1928  C   PHE A 565      23.655  25.578  74.645  1.00 18.46           C
ATOM   1929  O   PHE A 565      23.008  24.572  74.354  1.00 18.37           O
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ATOM   1930  CB  PHE A 565      25.992  25.364  73.780  1.00 18.08           C
ATOM   1931  CG  PHE A 565      25.680  26.402  72.733  1.00 17.18           C
ATOM   1932  CD1 PHE A 565      26.076  27.723  72.901  1.00 16.42           C
ATOM   1933  CD2 PHE A 565      24.985  26.056  71.581  1.00 16.53           C
ATOM   1934  CE1 PHE A 565      25.789  28.686  71.932  1.00 16.62           C
ATOM   1935  CE2 PHE A 565      24.688  27.014  70.606  1.00 17.15           C
ATOM   1936  CZ  PHE A 565      25.098  28.330  70.780  1.00 16.71           C
ATOM   1937  N   LEU A 566      23.140  26.804  74.640  1.00 18.37           N
ATOM   1938  CA  LEU A 566      21.879  27.119  73.977  1.00 18.25           C
ATOM   1939  C   LEU A 566      22.048  28.453  73.272  1.00 18.28           C
ATOM   1940  O   LEU A 566      22.221  29.489  73.924  1.00 18.49           O
ATOM   1941  CB  LEU A 566      20.715  27.182  74.973  1.00 18.09           C
ATOM   1942  CG  LEU A 566      19.424  27.841  74.459  1.00 17.66           C
ATOM   1943  CD1 LEU A 566      18.679  26.951  73.469  1.00 18.03           C
ATOM   1944  CD2 LEU A 566      18.528  28.215  75.614  1.00 17.22           C
ATOM   1945  N   GLY A 567      22.004  28.420  71.944  1.00 18.21           N
ATOM   1946  CA  GLY A 567      22.167  29.630  71.139  1.00 18.37           C
ATOM   1947  C   GLY A 567      21.253  29.676  69.933  1.00 18.34           C
ATOM   1948  O   GLY A 567      20.693  28.661  69.530  1.00 18.16           O
ATOM   1949  N   VAL A 568      21.108  30.864  69.358  1.00 18.41           N
ATOM   1950  CA  VAL A 568      20.221  31.063  68.222  1.00 18.52           C
ATOM   1951  C   VAL A 568      20.773  30.433  66.947  1.00 18.88           C
ATOM   1952  O   VAL A 568      21.996  30.273  66.790  1.00 18.51           O
ATOM   1953  CB  VAL A 568      19.935  32.568  67.954  1.00 18.65           C
ATOM   1954  CG1 VAL A 568      19.030  33.175  69.041  1.00 18.14           C
ATOM   1955  CG2 VAL A 568      21.222  33.354  67.819  1.00 18.61           C
ATOM   1956  N   GLY A 569      19.852  30.050  66.062  1.00 19.03           N
ATOM   1957  CA  GLY A 569      20.164  29.767  64.667  1.00 19.11           C
ATOM   1958  C   GLY A 569      19.998  31.082  63.929  1.00 19.34           C
ATOM   1959  O   GLY A 569      18.893  31.419  63.495  1.00 19.18           O
ATOM   1960  N   PRO A 570      21.100  31.834  63.774  1.00 19.64           N
ATOM   1961  CA  PRO A 570      21.038  33.244  63.381  1.00 19.73           C
ATOM   1962  C   PRO A 570      20.394  33.470  62.022  1.00 19.99           C
ATOM   1963  O   PRO A 570      20.418  32.585  61.157  1.00 19.62           O
ATOM   1964  CB  PRO A 570      22.507  33.659  63.337  1.00 19.84           C
ATOM   1965  CG  PRO A 570      23.258  32.379  63.134  1.00 19.84           C
ATOM   1966  CD  PRO A 570      22.491  31.372  63.924  1.00 19.69           C
ATOM   1967  N   GLY A 571      19.832  34.662  61.851  1.00 20.05           N
ATOM   1968  CA  GLY A 571      19.096  35.010  60.654  1.00 20.46           C
ATOM   1969  C   GLY A 571      17.796  35.670  61.046  1.00 20.88           C
ATOM   1970  O   GLY A 571      17.756  36.425  62.021  1.00 20.87           O
ATOM   1971  N   THR A 572      16.732  35.373  60.298  1.00 21.17           N
ATOM   1972  CA  THR A 572      15.439  36.020  60.496  1.00 21.59           C
ATOM   1973  C   THR A 572      14.352  35.017  60.868  1.00 21.72           C
ATOM   1974  O   THR A 572      14.093  34.066  60.123  1.00 21.78           O
ATOM   1975  CB  THR A 572      15.030  36.832  59.248  1.00 21.77           C
ATOM   1976  OG1 THR A 572      16.008  37.852  59.014  1.00 22.63           O
ATOM   1977  CG2 THR A 572      13.658  37.496  59.431  1.00 21.73           C
ATOM   1978  N   GLY A 573      13.725  35.240  62.025  1.00 21.63           N
ATOM   1979  CA  GLY A 573      12.659  34.365  62.527  1.00 21.49           C
ATOM   1980  C   GLY A 573      11.338  34.645  61.836  1.00 21.48           C
ATOM   1981  O   GLY A 573      11.267  35.518  60.962  1.00 21.46           O
ATOM   1982  N   ILE A 574      10.291  33.912  62.223  1.00 21.21           N
ATOM   1983  CA  ILE A 574       8.959  34.090  61.626  1.00 21.09           C
ATOM   1984  C   ILE A 574       7.836  34.216  62.652  1.00 21.28           C
ATOM   1985  O   ILE A 574       7.971  33.786  63.801  1.00 21.42           O
ATOM   1986  CB  ILE A 574       8.587  32.940  60.639  1.00 20.99           C
ATOM   1987  CG1 ILE A 574       8.234  31.657  61.409  1.00 20.81           C
ATOM   1988  CG2 ILE A 574       9.695  32.739  59.595  1.00 20.50           C
ATOM   1989  CD1 ILE A 574       7.649  30.541  60.573  1.00 20.89           C
ATOM   1990  N   VAL A 575       6.728  34.817  62.222  1.00 21.33           N
ATOM   1991  CA  VAL A 575       5.475  34.772  62.970  1.00 21.17           C
ATOM   1992  C   VAL A 575       4.517  33.868  62.190  1.00 21.11           C
ATOM   1993  O   VAL A 575       4.367  34.031  60.983  1.00 20.97           O
ATOM   1994  CB  VAL A 575       4.885  36.192  63.195  1.00 21.17           C
ATOM   1995  CG1 VAL A 575       3.508  36.129  63.864  1.00 21.09           C
ATOM   1996  CG2 VAL A 575       5.829  37.022  64.041  1.00 20.92           C
ATOM   1997  N   LEU A 576       3.907  32.895  62.864  1.00 21.34           N
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ATOM   1998  CA  LEU A 576       2.966  31.990  62.192  1.00 21.68           C
ATOM   1999  C   LEU A 576       1.737  32.767  61.721  1.00 22.12           C
ATOM   2000  O   LEU A 576       1.121  33.507  62.496  1.00 21.91           O
ATOM   2001  CB  LEU A 576       2.566  30.807  63.087  1.00 21.37           C
ATOM   2002  CG  LEU A 576       3.671  29.884  63.622  1.00 20.82           C
ATOM   2003  CD1 LEU A 576       3.082  28.812  64.518  1.00 19.76           C
ATOM   2004  CD2 LEU A 576       4.488  29.251  62.500  1.00 19.90           C
ATOM   2005  N   ARG A 577       1.409  32.610  60.441  1.00 22.62           N
ATOM   2006  CA  ARG A 577       0.344  33.387  59.809  1.00 23.46           C
ATOM   2007  C   ARG A 577      -1.004  32.660  59.707  1.00 23.61           C
ATOM   2008  O   ARG A 577      -2.019  33.291  59.406  1.00 23.71           O
ATOM   2009  CB  ARG A 577       0.792  33.882  58.430  1.00 23.57           C
ATOM   2010  CG  ARG A 577       1.220  32.771  57.508  1.00 24.18           C
ATOM   2011  CD  ARG A 577       1.674  33.259  56.134  1.00 24.14           C
ATOM   2012  NE  ARG A 577       1.772  32.096  55.251  1.00 25.19           N
ATOM   2013  CZ  ARG A 577       2.807  31.261  55.211  1.00 24.64           C
ATOM   2014  NH1 ARG A 577       3.874  31.463  55.975  1.00 24.29           N
ATOM   2015  NH2 ARG A 577       2.777  30.223  54.394  1.00 25.16           N
ATOM   2016  N   ASN A 578      -1.020  31.352  59.969  1.00 23.82           N
ATOM   2017  CA  ASN A 578      -2.255  30.566  59.874  1.00 24.26           C
ATOM   2018  C   ASN A 578      -2.317  29.348  60.813  1.00 24.58           C
ATOM   2019  O   ASN A 578      -1.302  28.932  61.373  1.00 24.56           O
ATOM   2020  CB  ASN A 578      -2.493  30.137  58.423  1.00 24.09           C
ATOM   2021  CG  ASN A 578      -1.512  29.092  57.960  1.00 24.12           C
ATOM   2022  OD1 ASN A 578      -1.507  27.966  58.463  1.00 25.12           O
ATOM   2023  ND2 ASN A 578      -0.679  29.448  56.990  1.00 23.31           N
ATOM   2024  N   GLY A 579      -3.510  28.773  60.964  1.00 24.89           N
ATOM   2025  CA  GLY A 579      -3.706  27.614  61.836  1.00 25.08           C
ATOM   2026  C   GLY A 579      -3.953  28.038  63.275  1.00 25.66           C
ATOM   2027  O   GLY A 579      -4.004  29.240  63.571  1.00 25.92           O
ATOM   2028  N   PRO A 580      -4.108  27.060  64.186  1.00 25.76           N
ATOM   2029  CA  PRO A 580      -4.485  27.359  65.575  1.00 25.83           C
ATOM   2030  C   PRO A 580      -3.392  28.005  66.439  1.00 25.99           C
ATOM   2031  O   PRO A 580      -3.665  28.376  67.587  1.00 26.04           O
ATOM   2032  CB  PRO A 580      -4.888  25.988  66.137  1.00 25.87           C
ATOM   2033  CG  PRO A 580      -4.175  24.996  65.290  1.00 25.83           C
ATOM   2034  CD  PRO A 580      -3.958  25.613  63.941  1.00 25.80           C
ATOM   2035  N   HIS A 581      -2.180  28.144  65.900  1.00 25.90           N
ATOM   2036  CA  HIS A 581      -1.070  28.768  66.635  1.00 25.74           C
ATOM   2037  C   HIS A 581      -0.619  30.080  65.980  1.00 25.62           C
ATOM   2038  O   HIS A 581       0.438  30.623  66.307  1.00 25.64           O
ATOM   2039  CB  HIS A 581       0.106  27.796  66.771  1.00 25.66           C
ATOM   2040  CG  HIS A 581      -0.269  26.468  67.358  1.00 26.37           C
ATOM   2041  ND1 HIS A 581      -0.164  25.284  66.656  1.00 26.76           N
ATOM   2042  CD2 HIS A 581      -0.746  26.136  68.582  1.00 26.38           C
ATOM   2043  CE1 HIS A 581      -0.568  24.284  67.418  1.00 26.70           C
ATOM   2044  NE2 HIS A 581      -0.924  24.773  68.593  1.00 27.30           N
ATOM   2045  N   LYS A 582      -1.439  30.572  65.052  1.00 25.31           N
ATOM   2046  CA  LYS A 582      -1.219  31.841  64.358  1.00 24.93           C
ATOM   2047  C   LYS A 582      -0.881  32.950  65.346  1.00 24.26           C
ATOM   2048  O   LYS A 582      -1.552  33.107  66.366  1.00 24.34           O
ATOM   2049  CB  LYS A 582      -2.469  32.195  63.542  1.00 24.85           C
ATOM   2050  CG  LYS A 582      -2.434  33.516  62.776  1.00 25.44           C
ATOM   2051  CD  LYS A 582      -3.838  33.829  62.233  1.00 25.80           C
ATOM   2052  CE  LYS A 582      -3.886  35.105  61.390  1.00 27.57           C
ATOM   2053  NZ  LYS A 582      -3.303  36.285  62.075  1.00 28.30           N
ATOM   2054  N   GLY A 583       0.169  33.707  65.043  1.00 23.76           N
ATOM   2055  CA  GLY A 583       0.624  34.783  65.917  1.00 22.91           C
ATOM   2056  C   GLY A 583       1.778  34.356  66.808  1.00 22.58           C
ATOM   2057  O   GLY A 583       2.388  35.192  67.477  1.00 22.36           O
ATOM   2058  N   ARG A 584       2.063  33.052  66.830  1.00 22.27           N
ATOM   2059  CA  ARG A 584       3.231  32.517  67.538  1.00 21.91           C
ATOM   2060  C   ARG A 584       4.535  32.937  66.861  1.00 21.53           C
ATOM   2061  O   ARG A 584       4.687  32.809  65.641  1.00 21.33           O
ATOM   2062  CB  ARG A 584       3.166  30.994  67.622  1.00 21.98           C
ATOM   2063  CG  ARG A 584       4.369  30.351  68.291  1.00 22.52           C
ATOM   2064  CD  ARG A 584       4.218  28.853  68.360  1.00 22.64           C
ATOM   2065  NE  ARG A 584       3.297  28.458  69.421  1.00 23.70           N
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ATOM   2066  CZ  ARG A 584       2.758  27.246  69.530  1.00 23.67           C
ATOM   2067  NH1 ARG A 584       3.039  26.302  68.640  1.00 22.10           N
ATOM   2068  NH2 ARG A 584       1.931  26.982  70.533  1.00 24.49           N
ATOM   2069  N   ILE A 585       5.463  33.435  67.672  1.00 20.94           N
ATOM   2070  CA  ILE A 585       6.784  33.823  67.207  1.00 20.71           C
ATOM   2071  C   ILE A 585       7.712  32.618  67.297  1.00 20.41           C
ATOM   2072  O   ILE A 585       7.761  31.962  68.327  1.00 20.72           O
ATOM   2073  CB  ILE A 585       7.359  34.989  68.049  1.00 20.62           C
ATOM   2074  CG1 ILE A 585       6.416  36.198  68.002  1.00 20.69           C
ATOM   2075  CG2 ILE A 585       8.769  35.355  67.578  1.00 20.07           C
ATOM   2076  CD1 ILE A 585       6.782  37.323  68.971  1.00 21.07           C
ATOM   2077  N   LEU A 586       8.430  32.322  66.217  1.00 20.13           N
ATOM   2078  CA  LEU A 586       9.403  31.229  66.214  1.00 19.91           C
ATOM   2079  C   LEU A 586      10.822  31.743  66.014  1.00 19.80           C
ATOM   2080  O   LEU A 586      11.101  32.484  65.063  1.00 20.11           O
ATOM   2081  CB  LEU A 586       9.071  30.190  65.137  1.00 19.96           C
ATOM   2082  CG  LEU A 586       7.706  29.494  65.164  1.00 19.90           C
ATOM   2083  CD1 LEU A 586       7.648  28.439  64.074  1.00 19.88           C
ATOM   2084  CD2 LEU A 586       7.437  28.874  66.517  1.00 20.06           C
ATOM   2085  N   ILE A 587      11.704  31.351  66.927  1.00 19.17           N
ATOM   2086  CA  ILE A 587      13.117  31.688  66.863  1.00 18.50           C
ATOM   2087  C   ILE A 587      13.894  30.384  66.806  1.00 18.40           C
ATOM   2088  O   ILE A 587      13.836  29.593  67.743  1.00 18.34           O
ATOM   2089  CB  ILE A 587      13.576  32.476  68.120  1.00 18.32           C
ATOM   2090  CG1 ILE A 587      12.623  33.640  68.441  1.00 18.13           C
ATOM   2091  CG2 ILE A 587      15.024  32.918  67.982  1.00 17.75           C
ATOM   2092  CD1 ILE A 587      12.569  34.754  67.398  1.00 17.34           C
ATOM   2093  N   PRO A 588      14.602  30.134  65.696  1.00 18.50           N
ATOM   2094  CA  PRO A 588      15.435  28.927  65.607  1.00 18.31           C
ATOM   2095  C   PRO A 588      16.582  28.971  66.614  1.00 18.11           C
ATOM   2096  O   PRO A 588      17.202  30.028  66.804  1.00 18.36           O
ATOM   2097  CB  PRO A 588      15.989  28.982  64.177  1.00 18.21           C
ATOM   2098  CG  PRO A 588      15.062  29.917  63.433  1.00 18.51           C
ATOM   2099  CD  PRO A 588      14.654  30.932  64.457  1.00 18.57           C
ATOM   2100  N   VAL A 589      16.836  27.840  67.266  1.00 17.61           N
ATOM   2101  CA  VAL A 589      17.930  27.711  68.224  1.00 17.23           C
ATOM   2102  C   VAL A 589      18.545  26.311  68.147  1.00 17.10           C
ATOM   2103  O   VAL A 589      18.024  25.423  67.464  1.00 16.74           O
ATOM   2104  CB  VAL A 589      17.481  27.987  69.693  1.00 17.17           C
ATOM   2105  CG1 VAL A 589      16.866  29.376  69.851  1.00 17.28           C
ATOM   2106  CG2 VAL A 589      16.514  26.927  70.184  1.00 17.84           C
ATOM   2107  N   TYR A 590      19.655  26.122  68.852  1.00 17.03           N
ATOM   2108  CA  TYR A 590      20.240  24.801  69.003  1.00 17.44           C
ATOM   2109  C   TYR A 590      21.027  24.646  70.291  1.00 17.67           C
ATOM   2110  O   TYR A 590      21.468  25.628  70.891  1.00 17.46           O
ATOM   2111  CB  TYR A 590      21.073  24.394  67.777  1.00 17.27           C
ATOM   2112  CG  TYR A 590      22.323  25.194  67.535  1.00 17.42           C
ATOM   2113  CD1 TYR A 590      22.260  26.497  67.018  1.00 17.48           C
ATOM   2114  CD2 TYR A 590      23.575  24.640  67.781  1.00 16.63           C
ATOM   2115  CE1 TYR A 590      23.419  27.233  66.776  1.00 16.90           C
ATOM   2116  CE2 TYR A 590      24.736  25.360  67.537  1.00 17.04           C
ATOM   2117  CZ  TYR A 590      24.652  26.655  67.034  1.00 17.25           C
ATOM   2118  OH  TYR A 590      25.810  27.366  66.795  1.00 18.08           O
ATOM   2119  N   THR A 591      21.188  23.393  70.706  1.00 18.22           N
ATOM   2120  CA  THR A 591      21.793  23.069  71.992  1.00 18.65           C
ATOM   2121  C   THR A 591      22.931  22.063  71.860  1.00 19.26           C
ATOM   2122  O   THR A 591      23.021  21.335  70.866  1.00 19.63           O
ATOM   2123  CB  THR A 591      20.752  22.470  72.969  1.00 18.43           C
ATOM   2124  OG1 THR A 591      20.208  21.269  72.408  1.00 18.34           O
ATOM   2125  CG2 THR A 591      19.627  23.456  73.252  1.00 17.97           C
ATOM   2126  N   THR A 592      23.800  22.039  72.868  1.00 19.51           N
ATOM   2127  CA  THR A 592      24.727  20.938  73.065  1.00 19.73           C
ATOM   2128  C   THR A 592      24.473  20.380  74.457  1.00 20.07           C
ATOM   2129  O   THR A 592      23.892  21.065  75.314  1.00 19.74           O
ATOM   2130  CB  THR A 592      26.210  21.369  72.935  1.00 19.96           C
ATOM   2131  OG1 THR A 592      26.581  22.192  74.049  1.00 20.26           O
ATOM   2132  CG2 THR A 592      26.450  22.130  71.635  1.00 19.54           C
ATOM   2133  N   ASN A 593      24.878  19.131  74.673  1.00 20.44           N
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ATOM   2134  CA  ASN A 593      24.787  18.514  75.992  1.00 20.95           C
ATOM   2135  C   ASN A 593      26.169  18.265  76.582  1.00 21.40           C
ATOM   2136  O   ASN A 593      27.185  18.496  75.918  1.00 21.65           O
ATOM   2137  CB  ASN A 593      23.958  17.224  75.953  1.00 20.88           C
ATOM   2138  CG  ASN A 593      24.593  16.137  75.112  1.00 20.73           C
ATOM   2139  OD1 ASN A 593      25.815  16.024  75.033  1.00 21.63           O
ATOM   2140  ND2 ASN A 593      23.760  15.324  74.479  1.00 19.73           N
ATOM   2141  N   ASN A 594      26.201  17.788  77.823  1.00 21.73           N
ATOM   2142  CA  ASN A 594      27.455  17.592  78.546  1.00 21.83           C
ATOM   2143  C   ASN A 594      28.127  16.264  78.212  1.00 22.25           C
ATOM   2144  O   ASN A 594      29.251  16.004  78.642  1.00 22.47           O
ATOM   2145  CB  ASN A 594      27.224  17.724  80.057  1.00 21.54           C
ATOM   2146  CG  ASN A 594      26.924  19.156  80.486  1.00 21.49           C
ATOM   2147  OD1 ASN A 594      27.625  20.101  80.101  1.00 21.64           O
ATOM   2148  ND2 ASN A 594      25.891  19.322  81.306  1.00 21.20           N
ATOM   2149  N   VAL A 595      27.437  15.427  77.439  1.00 22.76           N
ATOM   2150  CA  VAL A 595      27.965  14.116  77.061  1.00 23.03           C
ATOM   2151  C   VAL A 595      28.971  14.242  75.929  1.00 23.41           C
ATOM   2152  O   VAL A 595      30.038  13.623  75.976  1.00 23.84           O
ATOM   2153  CB  VAL A 595      26.838  13.099  76.694  1.00 23.07           C
ATOM   2154  CG1 VAL A 595      27.423  11.773  76.170  1.00 22.63           C
ATOM   2155  CG2 VAL A 595      25.962  12.826  77.898  1.00 22.53           C
ATOM   2156  N   SER A 596      28.644  15.047  74.921  1.00 23.60           N
ATOM   2157  CA  SER A 596      29.529  15.195  73.761  1.00 23.84           C
ATOM   2158  C   SER A 596      29.772  16.637  73.285  1.00 23.96           C
ATOM   2159  O   SER A 596      30.584  16.858  72.395  1.00 24.21           O
ATOM   2160  CB  SER A 596      29.043  14.316  72.600  1.00 23.74           C
ATOM   2161  OG  SER A 596      27.714  14.631  72.233  1.00 23.37           O
ATOM   2162  N   HIS A 597      29.083  17.605  73.886  1.00 24.27           N
ATOM   2163  CA  HIS A 597      29.221  19.035  73.535  1.00 24.28           C
ATOM   2164  C   HIS A 597      29.168  19.301  72.014  1.00 24.53           C
ATOM   2165  O   HIS A 597      28.119  19.102  71.396  1.00 24.93           O
ATOM   2166  CB  HIS A 597      30.456  19.656  74.208  1.00 24.04           C
ATOM   2167  CG  HIS A 597      30.575  21.136  74.017  1.00 24.17           C
ATOM   2168  ND1 HIS A 597      29.504  21.996  74.152  1.00 24.60           N
ATOM   2169  CD2 HIS A 597      31.642  21.910  73.710  1.00 23.89           C
ATOM   2170  CE1 HIS A 597      29.906  23.235  73.928  1.00 24.14           C
ATOM   2171  NE2 HIS A 597      31.199  23.210  73.658  1.00 24.20           N
ATOM   2172  N   LEU A 598      30.285  19.723  71.418  1.00 24.22           N
ATOM   2173  CA  LEU A 598      30.323  20.075  70.002  1.00 23.93           C
ATOM   2174  C   LEU A 598      30.669  18.895  69.092  1.00 24.07           C
ATOM   2175  O   LEU A 598      30.557  18.997  67.866  1.00 23.97           O
ATOM   2176  CB  LEU A 598      31.290  21.239  69.759  1.00 23.70           C
ATOM   2177  CG  LEU A 598      30.799  22.639  70.152  1.00 23.89           C
ATOM   2178  CD1 LEU A 598      31.941  23.638  70.137  1.00 23.90           C
ATOM   2179  CD2 LEU A 598      29.666  23.119  69.243  1.00 23.37           C
ATOM   2180  N   ASN A 599      31.081  17.779  69.689  1.00 23.95           N
ATOM   2181  CA  ASN A 599      31.466  16.603  68.916  1.00 24.06           C
ATOM   2182  C   ASN A 599      30.305  15.806  68.332  1.00 23.68           C
ATOM   2183  O   ASN A 599      30.387  15.356  67.188  1.00 23.88           O
ATOM   2184  CB  ASN A 599      32.423  15.707  69.705  1.00 24.38           C
ATOM   2185  CG  ASN A 599      33.880  16.134  69.538  1.00 25.66           C
ATOM   2186  OD1 ASN A 599      34.585  15.634  68.655  1.00 27.02           O
ATOM   2187  ND2 ASN A 599      34.323  17.085  70.358  1.00 25.44           N
ATOM   2188  N   GLY A 600      29.229  15.638  69.099  1.00 23.13           N
ATOM   2189  CA  GLY A 600      28.077  14.886  68.621  1.00 22.08           C
ATOM   2190  C   GLY A 600      26.734  15.124  69.285  1.00 21.59           C
ATOM   2191  O   GLY A 600      25.932  14.194  69.378  1.00 21.68           O
ATOM   2192  N   SER A 601      26.462  16.354  69.721  1.00 21.04           N
ATOM   2193  CA  SER A 601      25.170  16.655  70.356  1.00 20.62           C
ATOM   2194  C   SER A 601      24.442  17.895  69.843  1.00 20.40           C
ATOM   2195  O   SER A 601      23.375  18.245  70.361  1.00 20.39           O
ATOM   2196  CB  SER A 601      25.312  16.749  71.876  1.00 20.53           C
ATOM   2197  OG  SER A 601      25.867  17.992  72.267  1.00 20.21           O
ATOM   2198  N   GLN A 602      25.001  18.565  68.844  1.00 20.05           N
ATOM   2199  CA  GLN A 602      24.341  19.750  68.296  1.00 20.01           C
ATOM   2200  C   GLN A 602      22.926  19.411  67.828  1.00 19.79           C
ATOM   2201  O   GLN A 602      22.733  18.530  66.993  1.00 20.05           O
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ATOM   2202  CB  GLN A 602      25.175  20.386  67.190  1.00 19.72           C
ATOM   2203  CG  GLN A 602      26.334  21.208  67.727  1.00 19.95           C
ATOM   2204  CD  GLN A 602      27.285  21.674  66.642  1.00 20.59           C
ATOM   2205  OE1 GLN A 602      27.205  22.816  66.183  1.00 21.19           O
ATOM   2206  NE2 GLN A 602      28.191  20.791  66.224  1.00 19.21           N
ATOM   2207  N   SER A 603      21.936  20.089  68.401  1.00 19.56           N
ATOM   2208  CA  SER A 603      20.533  19.733  68.167  1.00 19.37           C
ATOM   2209  C   SER A 603      19.646  20.949  67.957  1.00 19.29           C
ATOM   2210  O   SER A 603      19.533  21.806  68.838  1.00 19.38           O
ATOM   2211  CB  SER A 603      20.000  18.879  69.319  1.00 19.30           C
ATOM   2212  OG  SER A 603      20.629  17.604  69.340  1.00 18.84           O
ATOM   2213  N   SER A 604      19.023  21.007  66.783  1.00 19.00           N
ATOM   2214  CA  SER A 604      18.105  22.080  66.418  1.00 18.78           C
ATOM   2215  C   SER A 604      16.766  21.994  67.142  1.00 18.70           C
ATOM   2216  O   SER A 604      16.241  20.900  67.395  1.00 18.51           O
ATOM   2217  CB  SER A 604      17.835  22.055  64.912  1.00 18.85           C
ATOM   2218  OG  SER A 604      19.034  22.112  64.167  1.00 18.95           O
ATOM   2219  N   ARG A 605      16.227  23.165  67.471  1.00 18.56           N
ATOM   2220  CA  ARG A 605      14.838  23.306  67.904  1.00 18.27           C
ATOM   2221  C   ARG A 605      14.392  24.749  67.676  1.00 18.52           C
ATOM   2222  O   ARG A 605      15.148  25.557  67.127  1.00 18.41           O
ATOM   2223  CB  ARG A 605      14.653  22.882  69.376  1.00 18.20           C
ATOM   2224  CG  ARG A 605      15.318  23.780  70.422  1.00 17.99           C
ATOM   2225  CD  ARG A 605      14.961  23.349  71.850  1.00 17.59           C
ATOM   2226  NE  ARG A 605      15.634  22.106  72.209  1.00 16.04           N
ATOM   2227  CZ  ARG A 605      15.308  21.317  73.230  1.00 16.40           C
ATOM   2228  NH1 ARG A 605      14.291  21.613  74.034  1.00 14.56           N
ATOM   2229  NH2 ARG A 605      16.014  20.213  73.448  1.00 16.98           N
ATOM   2230  N   ILE A 606      13.167  25.069  68.086  1.00 18.50           N
ATOM   2231  CA  ILE A 606      12.734  26.456  68.146  1.00 18.74           C
ATOM   2232  C   ILE A 606      12.387  26.840  69.581  1.00 18.93           C
ATOM   2233  O   ILE A 606      12.044  25.984  70.396  1.00 19.22           O
ATOM   2234  CB  ILE A 606      11.528  26.755  67.195  1.00 18.61           C
ATOM   2235  CG1 ILE A 606      10.289  25.927  67.567  1.00 19.01           C
ATOM   2236  CG2 ILE A 606      11.909  26.504  65.735  1.00 18.48           C
ATOM   2237  CD1 ILE A 606       9.402  26.540  68.640  1.00 18.43           C
ATOM   2238  N   ILE A 607      12.507  28.126  69.887  1.00 19.08           N
ATOM   2239  CA  ILE A 607      11.836  28.695  71.040  1.00 19.35           C
ATOM   2240  C   ILE A 607      10.726  29.570  70.480  1.00 19.74           C
ATOM   2241  O   ILE A 607      10.815  30.026  69.337  1.00 19.52           O
ATOM   2242  CB  ILE A 607      12.778  29.493  72.008  1.00 19.29           C
ATOM   2243  CG1 ILE A 607      13.474  30.659  71.299  1.00 19.06           C
ATOM   2244  CG2 ILE A 607      13.784  28.558  72.674  1.00 19.19           C
ATOM   2245  CD1 ILE A 607      14.048  31.712  72.243  1.00 19.16           C
ATOM   2246  N   TYR A 608       9.680  29.779  71.276  1.00 20.27           N
ATOM   2247  CA  TYR A 608       8.483  30.468  70.814  1.00 20.83           C
ATOM   2248  C   TYR A 608       7.835  31.353  71.878  1.00 21.25           C
ATOM   2249  O   TYR A 608       8.082  31.186  73.077  1.00 21.22           O
ATOM   2250  CB  TYR A 608       7.469  29.452  70.258  1.00 21.21           C
ATOM   2251  CG  TYR A 608       6.839  28.527  71.290  1.00 21.19           C
ATOM   2252  CD1 TYR A 608       7.448  27.322  71.639  1.00 21.34           C
ATOM   2253  CD2 TYR A 608       5.627  28.850  71.894  1.00 20.57           C
ATOM   2254  CE1 TYR A 608       6.873  26.470  72.582  1.00 21.23           C
ATOM   2255  CE2 TYR A 608       5.042  28.006  72.831  1.00 20.89           C
ATOM   2256  CZ  TYR A 608       5.668  26.820  73.170  1.00 21.45           C
ATOM   2257  OH  TYR A 608       5.087  25.983  74.096  1.00 21.17           O
ATOM   2258  N   SER A 609       7.015  32.302  71.422  1.00 21.74           N
ATOM   2259  CA  SER A 609       6.237  33.173  72.304  1.00 21.86           C
ATOM   2260  C   SER A 609       4.810  33.279  71.789  1.00 22.56           C
ATOM   2261  O   SER A 609       4.586  33.523  70.600  1.00 22.56           O
ATOM   2262  CB  SER A 609       6.865  34.562  72.394  1.00 21.81           C
ATOM   2263  OG  SER A 609       6.124  35.413  73.261  1.00 20.41           O
ATOM   2264  N   ASP A 610       3.849  33.082  72.684  1.00 23.33           N
ATOM   2265  CA  ASP A 610       2.432  33.217  72.334  1.00 24.10           C
ATOM   2266  C   ASP A 610       1.817  34.526  72.855  1.00 24.50           C
ATOM   2267  O   ASP A 610       0.629  34.794  72.635  1.00 24.43           O
ATOM   2268  CB  ASP A 610       1.632  32.012  72.839  1.00 24.02           C
ATOM   2269  CG  ASP A 610       1.882  30.755  72.025  1.00 24.33           C
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ATOM   2270  OD1 ASP A 610       2.239  30.851  70.826  1.00 23.74           O
ATOM   2271  OD2 ASP A 610       1.711  29.660  72.597  1.00 24.37           O
ATOM   2272  N   ASP A 611       2.637  35.339  73.523  1.00 24.83           N
ATOM   2273  CA  ASP A 611       2.169  36.579  74.135  1.00 25.20           C
ATOM   2274  C   ASP A 611       2.961  37.802  73.682  1.00 25.48           C
ATOM   2275  O   ASP A 611       3.212  38.717  74.467  1.00 25.52           O
ATOM   2276  CB  ASP A 611       2.153  36.467  75.664  1.00 25.19           C
ATOM   2277  CG  ASP A 611       3.527  36.160  76.261  1.00 25.85           C
ATOM   2278  OD1 ASP A 611       4.562  36.378  75.597  1.00 25.44           O
ATOM   2279  OD2 ASP A 611       3.562  35.712  77.428  1.00 27.33           O
ATOM   2280  N   HIS A 612       3.340  37.801  72.408  1.00 25.80           N
ATOM   2281  CA  HIS A 612       3.983  38.945  71.766  1.00 26.15           C
ATOM   2282  C   HIS A 612       5.325  39.320  72.396  1.00 26.25           C
ATOM   2283  O   HIS A 612       5.649  40.503  72.524  1.00 26.40           O
ATOM   2284  CB  HIS A 612       3.024  40.146  71.710  1.00 26.40           C
ATOM   2285  CG  HIS A 612       1.667  39.810  71.162  1.00 26.89           C
ATOM   2286  ND1 HIS A 612       1.475  39.337  69.879  1.00 25.90           N
ATOM   2287  CD2 HIS A 612       0.435  39.880  71.723  1.00 26.58           C
ATOM   2288  CE1 HIS A 612       0.187  39.129  69.675  1.00 25.20           C
ATOM   2289  NE2 HIS A 612      -0.467  39.456  70.776  1.00 26.45           N
ATOM   2290  N   GLY A 613       6.095  38.304  72.787  1.00 26.18           N
ATOM   2291  CA  GLY A 613       7.474  38.496  73.225  1.00 25.90           C
ATOM   2292  C   GLY A 613       7.694  38.656  74.716  1.00 25.90           C
ATOM   2293  O   GLY A 613       8.827  38.856  75.155  1.00 25.60           O
ATOM   2294  N   LYS A 614       6.621  38.569  75.498  1.00 25.98           N
ATOM   2295  CA  LYS A 614       6.733  38.696  76.954  1.00 26.22           C
ATOM   2296  C   LYS A 614       7.397  37.468  77.592  1.00 25.55           C
ATOM   2297  O   LYS A 614       8.308  37.611  78.405  1.00 25.86           O
ATOM   2298  CB  LYS A 614       5.365  38.996  77.595  1.00 26.29           C
ATOM   2299  CG  LYS A 614       5.385  39.112  79.128  1.00 27.03           C
ATOM   2300  CD  LYS A 614       4.074  39.661  79.678  1.00 27.15           C
ATOM   2301  CE  LYS A 614       4.125  39.790  81.202  1.00 29.70           C
ATOM   2302  NZ  LYS A 614       2.817  40.248  81.793  1.00 30.30           N
ATOM   2303  N   THR A 615       6.934  36.273  77.233  1.00 24.85           N
ATOM   2304  CA  THR A 615       7.526  35.030  77.740  1.00 24.31           C
ATOM   2305  C   THR A 615       7.947  34.139  76.585  1.00 24.03           C
ATOM   2306  O   THR A 615       7.405  34.237  75.487  1.00 23.91           O
ATOM   2307  CB  THR A 615       6.569  34.221  78.649  1.00 24.22           C
ATOM   2308  OG1 THR A 615       5.377  33.898  77.928  1.00 23.99           O
ATOM   2309  CG2 THR A 615       6.213  34.997  79.911  1.00 24.24           C
ATOM   2310  N   TRP A 616       8.923  33.276  76.842  1.00 23.60           N
ATOM   2311  CA  TRP A 616       9.427  32.368  75.828  1.00 22.94           C
ATOM   2312  C   TRP A 616       9.413  30.945  76.355  1.00 22.75           C
ATOM   2313  O   TRP A 616       9.528  30.719  77.562  1.00 22.77           O
ATOM   2314  CB  TRP A 616      10.829  32.795  75.379  1.00 22.82           C
ATOM   2315  CG  TRP A 616      10.823  34.167  74.785  1.00 22.48           C
ATOM   2316  CD1 TRP A 616      10.945  35.354  75.455  1.00 22.44           C
ATOM   2317  CD2 TRP A 616      10.641  34.501  73.407  1.00 22.15           C
ATOM   2318  NE1 TRP A 616      10.864  36.407  74.576  1.00 22.32           N
ATOM   2319  CE2 TRP A 616      10.680  35.913  73.311  1.00 22.46           C
ATOM   2320  CE3 TRP A 616      10.452  33.747  72.242  1.00 21.85           C
ATOM   2321  CZ2 TRP A 616      10.535  36.587  72.093  1.00 22.13           C
ATOM   2322  CZ3 TRP A 616      10.306  34.417  71.030  1.00 22.39           C
ATOM   2323  CH2 TRP A 616      10.350  35.825  70.967  1.00 22.39           C
ATOM   2324  N   HIS A 617       9.245  29.992  75.444  1.00 22.54           N
ATOM   2325  CA  HIS A 617       9.227  28.577  75.797  1.00 22.35           C
ATOM   2326  C   HIS A 617      10.055  27.774  74.800  1.00 21.96           C
ATOM   2327  O   HIS A 617      10.162  28.140  73.628  1.00 21.60           O
ATOM   2328  CB  HIS A 617       7.790  28.046  75.832  1.00 22.57           C
ATOM   2329  CG  HIS A 617       6.866  28.856  76.685  1.00 23.43           C
ATOM   2330  ND1 HIS A 617       6.673  28.600  78.027  1.00 24.70           N
ATOM   2331  CD2 HIS A 617       6.089  29.926  76.391  1.00 23.60           C
ATOM   2332  CE1 HIS A 617       5.812  29.473  78.520  1.00 24.49           C
ATOM   2333  NE2 HIS A 617       5.446  30.292  77.549  1.00 24.05           N
ATOM   2334  N   ALA A 618      10.639  26.681  75.278  1.00 21.57           N
ATOM   2335  CA  ALA A 618      11.393  25.787  74.428  1.00 21.25           C
ATOM   2336  C   ALA A 618      10.471  24.728  73.859  1.00 21.30           C
ATOM   2337  O   ALA A 618       9.708  24.093  74.598  1.00 21.22           O
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ATOM   2338  CB  ALA A 618      12.518  25.137  75.206  1.00 21.19           C
ATOM   2339  N   GLY A 619      10.539  24.544  72.542  1.00 21.14           N
ATOM   2340  CA  GLY A 619       9.961  23.367  71.905  1.00 21.04           C
ATOM   2341  C   GLY A 619      10.882  22.172  72.099  1.00 20.80           C
ATOM   2342  O   GLY A 619      11.972  22.304  72.653  1.00 20.60           O
ATOM   2343  N   GLU A 620      10.434  21.003  71.654  1.00 21.09           N
ATOM   2344  CA  GLU A 620      11.260  19.785  71.652  1.00 21.16           C
ATOM   2345  C   GLU A 620      12.327  19.862  70.566  1.00 20.91           C
ATOM   2346  O   GLU A 620      12.144  20.543  69.553  1.00 20.92           O
ATOM   2347  CB  GLU A 620      10.395  18.541  71.411  1.00 21.10           C
ATOM   2348  CG  GLU A 620       9.360  18.267  72.503  1.00 21.22           C
ATOM   2349  CD  GLU A 620       8.778  16.850  72.456  1.00 21.67           C
ATOM   2350  OE1 GLU A 620       9.110  16.058  71.538  1.00 21.86           O
ATOM   2351  OE2 GLU A 620       7.973  16.524  73.355  1.00 23.31           O
ATOM   2352  N   ALA A 621      13.443  19.170  70.779  1.00 20.48           N
ATOM   2353  CA  ALA A 621      14.465  19.058  69.750  1.00 20.13           C
ATOM   2354  C   ALA A 621      14.002  18.071  68.691  1.00 20.09           C
ATOM   2355  O   ALA A 621      13.224  17.163  68.987  1.00 20.41           O
ATOM   2356  CB  ALA A 621      15.789  18.618  70.351  1.00 19.93           C
ATOM   2357  N   VAL A 622      14.476  18.258  67.460  1.00 19.87           N
ATOM   2358  CA  VAL A 622      14.234  17.325  66.363  1.00 19.78           C
ATOM   2359  C   VAL A 622      14.849  15.973  66.693  1.00 20.24           C
ATOM   2360  O   VAL A 622      14.348  14.924  66.272  1.00 20.06           O
ATOM   2361  CB  VAL A 622      14.832  17.852  65.032  1.00 19.99           C
ATOM   2362  CG1 VAL A 622      14.748  16.794  63.930  1.00 18.57           C
ATOM   2363  CG2 VAL A 622      14.136  19.154  64.605  1.00 19.53           C
ATOM   2364  N   ASN A 623      15.936  16.012  67.460  1.00 20.61           N
ATOM   2365  CA  ASN A 623      16.625  14.807  67.893  1.00 21.08           C
ATOM   2366  C   ASN A 623      16.016  14.100  69.116  1.00 21.43           C
ATOM   2367  O   ASN A 623      16.483  13.018  69.493  1.00 21.72           O
ATOM   2368  CB  ASN A 623      18.100  15.114  68.142  1.00 21.11           C
ATOM   2369  CG  ASN A 623      18.882  15.292  66.862  1.00 21.28           C
ATOM   2370  OD1 ASN A 623      18.389  15.003  65.773  1.00 21.42           O
ATOM   2371  ND2 ASN A 623      20.118  15.765  66.987  1.00 21.57           N
ATOM   2372  N   ASP A 624      14.990  14.693  69.728  1.00 21.66           N
ATOM   2373  CA  ASP A 624      14.339  14.083  70.902  1.00 22.42           C
ATOM   2374  C   ASP A 624      13.421  12.933  70.513  1.00 23.01           C
ATOM   2375  O   ASP A 624      12.462  13.117  69.755  1.00 23.13           O
ATOM   2376  CB  ASP A 624      13.577  15.126  71.737  1.00 22.11           C
ATOM   2377  CG  ASP A 624      14.508  16.097  72.456  1.00 21.59           C
ATOM   2378  OD1 ASP A 624      15.707  15.787  72.603  1.00 20.84           O
ATOM   2379  OD2 ASP A 624      14.046  17.178  72.874  1.00 21.45           O
ATOM   2380  N   ASN A 625      13.741  11.754  71.043  1.00 23.78           N
ATOM   2381  CA  ASN A 625      13.041  10.489  70.765  1.00 24.64           C
ATOM   2382  C   ASN A 625      12.999  10.130  69.280  1.00 24.87           C
ATOM   2383  O   ASN A 625      12.008   9.607  68.769  1.00 25.24           O
ATOM   2384  CB  ASN A 625      11.644  10.457  71.397  1.00 24.82           C
ATOM   2385  CG  ASN A 625      11.149   9.040  71.651  1.00 26.05           C
ATOM   2386  OD1 ASN A 625      11.934   8.126  71.942  1.00 27.20           O
ATOM   2387  ND2 ASN A 625       9.838   8.851  71.549  1.00 27.88           N
ATOM   2388  N   ARG A 626      14.104  10.420  68.605  1.00 25.07           N
ATOM   2389  CA  ARG A 626      14.257  10.177  67.183  1.00 25.11           C
ATOM   2390  C   ARG A 626      15.064   8.904  66.962  1.00 25.29           C
ATOM   2391  O   ARG A 626      15.986   8.599  67.728  1.00 25.20           O
ATOM   2392  CB  ARG A 626      14.975  11.370  66.561  1.00 25.12           C
ATOM   2393  CG  ARG A 626      15.282  11.249  65.098  1.00 24.94           C
ATOM   2394  CD  ARG A 626      16.393  12.201  64.754  1.00 25.44           C
ATOM   2395  NE  ARG A 626      16.996  11.889  63.465  1.00 25.40           N
ATOM   2396  CZ  ARG A 626      18.180  12.334  63.070  1.00 25.64           C
ATOM   2397  NH1 ARG A 626      18.906  13.113  63.868  1.00 25.16           N
ATOM   2398  NH2 ARG A 626      18.638  12.005  61.870  1.00 26.15           N
ATOM   2399  N   GLN A 627      14.729   8.163  65.911  1.00 25.46           N
ATOM   2400  CA  GLN A 627      15.436   6.926  65.627  1.00 25.58           C
ATOM   2401  C   GLN A 627      16.548   7.091  64.595  1.00 25.65           C
ATOM   2402  O   GLN A 627      16.310   7.481  63.453  1.00 25.58           O
ATOM   2403  CB  GLN A 627      14.469   5.821  65.220  1.00 25.63           C
ATOM   2404  CG  GLN A 627      14.942   4.452  65.670  1.00 26.15           C
ATOM   2405  CD  GLN A 627      13.865   3.396  65.561  1.00 26.36           C
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ATOM   2406  OE1 GLN A 627      13.144   3.125  66.525  1.00 26.87           O
ATOM   2407  NE2 GLN A 627      13.741   2.799  64.381  1.00 25.79           N
ATOM   2408  N   VAL A 628      17.769   6.802  65.036  1.00 25.97           N
ATOM   2409  CA  VAL A 628      18.946   6.768  64.180  1.00 25.97           C
ATOM   2410  C   VAL A 628      19.500   5.348  64.217  1.00 26.20           C
ATOM   2411  O   VAL A 628      19.906   4.871  65.274  1.00 26.15           O
ATOM   2412  CB  VAL A 628      20.031   7.763  64.674  1.00 25.89           C
ATOM   2413  CG1 VAL A 628      21.336   7.597  63.889  1.00 25.59           C
ATOM   2414  CG2 VAL A 628      19.528   9.190  64.581  1.00 25.81           C
ATOM   2415  N   ASP A 629      19.503   4.677  63.066  1.00 26.67           N
ATOM   2416  CA  ASP A 629      20.043   3.315  62.942  1.00 27.40           C
ATOM   2417  C   ASP A 629      19.442   2.323  63.944  1.00 27.57           C
ATOM   2418  O   ASP A 629      20.165   1.508  64.533  1.00 27.35           O
ATOM   2419  CB  ASP A 629      21.577   3.322  63.059  1.00 27.72           C
ATOM   2420  CG  ASP A 629      22.249   4.124  61.955  1.00 28.52           C
ATOM   2421  OD1 ASP A 629      21.836   3.999  60.781  1.00 28.82           O
ATOM   2422  OD2 ASP A 629      23.194   4.882  62.265  1.00 29.81           O
ATOM   2423  N   GLY A 630      18.124   2.409  64.137  1.00 27.86           N
ATOM   2424  CA  GLY A 630      17.400   1.514  65.042  1.00 28.19           C
ATOM   2425  C   GLY A 630      17.523   1.836  66.522  1.00 28.60           C
ATOM   2426  O   GLY A 630      16.931   1.153  67.352  1.00 28.89           O
ATOM   2427  N   GLN A 631      18.289   2.869  66.863  1.00 28.79           N
ATOM   2428  CA  GLN A 631      18.447   3.282  68.261  1.00 29.24           C
ATOM   2429  C   GLN A 631      17.936   4.700  68.471  1.00 28.48           C
ATOM   2430  O   GLN A 631      18.369   5.624  67.785  1.00 28.59           O
ATOM   2431  CB  GLN A 631      19.913   3.182  68.693  1.00 29.15           C
ATOM   2432  CG  GLN A 631      20.411   1.746  68.908  1.00 30.64           C
ATOM   2433  CD  GLN A 631      21.921   1.660  69.162  1.00 31.20           C
ATOM   2434  OE1 GLN A 631      22.660   2.646  69.015  1.00 32.91           O
ATOM   2435  NE2 GLN A 631      22.382   0.471  69.544  1.00 34.05           N
ATOM   2436  N   LYS A 632      17.013   4.870  69.415  1.00 27.81           N
ATOM   2437  CA  LYS A 632      16.464   6.192  69.711  1.00 27.29           C
ATOM   2438  C   LYS A 632      17.482   7.063  70.435  1.00 26.44           C
ATOM   2439  O   LYS A 632      18.198   6.580  71.305  1.00 26.43           O
ATOM   2440  CB  LYS A 632      15.177   6.085  70.528  1.00 27.27           C
ATOM   2441  CG  LYS A 632      14.027   5.412  69.779  1.00 28.01           C
ATOM   2442  CD  LYS A 632      12.762   5.342  70.630  1.00 28.31           C
ATOM   2443  CE  LYS A 632      11.787   4.286  70.115  1.00 30.01           C
ATOM   2444  NZ  LYS A 632      11.333   4.548  68.714  1.00 31.65           N
ATOM   2445  N   ILE A 633      17.554   8.336  70.047  1.00 25.39           N
ATOM   2446  CA  ILE A 633      18.409   9.312  70.717  1.00 24.44           C
ATOM   2447  C   ILE A 633      17.588  10.413  71.395  1.00 23.93           C
ATOM   2448  O   ILE A 633      16.364  10.484  71.240  1.00 23.85           O
ATOM   2449  CB  ILE A 633      19.454   9.961  69.759  1.00 24.42           C
ATOM   2450  CG1 ILE A 633      18.772  10.618  68.553  1.00 24.76           C
ATOM   2451  CG2 ILE A 633      20.498   8.944  69.328  1.00 25.00           C
ATOM   2452  CD1 ILE A 633      19.696  11.464  67.679  1.00 24.33           C
ATOM   2453  N   HIS A 634      18.280  11.254  72.157  1.00 22.96           N
ATOM   2454  CA  HIS A 634      17.702  12.428  72.772  1.00 22.28           C
ATOM   2455  C   HIS A 634      18.799  13.468  72.775  1.00 22.05           C
ATOM   2456  O   HIS A 634      19.974  13.119  72.896  1.00 22.07           O
ATOM   2457  CB  HIS A 634      17.272  12.120  74.205  1.00 22.30           C
ATOM   2458  CG  HIS A 634      16.469  13.208  74.844  1.00 21.71           C
ATOM   2459  ND1 HIS A 634      17.044  14.240  75.557  1.00 21.42           N
ATOM   2460  CD2 HIS A 634      15.134  13.427  74.879  1.00 21.28           C
ATOM   2461  CE1 HIS A 634      16.099  15.047  76.002  1.00 20.31           C
ATOM   2462  NE2 HIS A 634      14.930  14.576  75.605  1.00 21.37           N
ATOM   2463  N   SER A 635      18.427  14.739  72.646  1.00 21.64           N
ATOM   2464  CA  SER A 635      19.420  15.814  72.545  1.00 21.40           C
ATOM   2465  C   SER A 635      20.261  15.999  73.819  1.00 21.25           C
ATOM   2466  O   SER A 635      21.356  16.564  73.762  1.00 21.25           O
ATOM   2467  CB  SER A 635      18.761  17.131  72.121  1.00 21.27           C
ATOM   2468  OG  SER A 635      17.712  17.497  72.994  1.00 21.38           O
ATOM   2469  N   SER A 636      19.753  15.508  74.950  1.00 20.81           N
ATOM   2470  CA  SER A 636      20.449  15.610  76.232  1.00 20.67           C
ATOM   2471  C   SER A 636      21.491  14.519  76.465  1.00 20.76           C
ATOM   2472  O   SER A 636      22.358  14.673  77.319  1.00 20.42           O
ATOM   2473  CB  SER A 636      19.447  15.617  77.392  1.00 20.58           C
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ATOM   2474  OG  SER A 636      18.786  14.371  77.522  1.00 20.58           O
ATOM   2475  N   THR A 637      21.404  13.426  75.705  1.00 21.05           N
ATOM   2476  CA  THR A 637      22.253  12.252  75.934  1.00 21.37           C
ATOM   2477  C   THR A 637      23.001  11.766  74.685  1.00 21.52           C
ATOM   2478  O   THR A 637      23.775  10.808  74.752  1.00 21.36           O
ATOM   2479  CB  THR A 637      21.428  11.068  76.516  1.00 21.66           C
ATOM   2480  OG1 THR A 637      20.285  10.812  75.683  1.00 21.94           O
ATOM   2481  CG2 THR A 637      20.956  11.370  77.949  1.00 21.43           C
ATOM   2482  N   MET A 638      22.776  12.427  73.551  1.00 21.74           N
ATOM   2483  CA  MET A 638      23.315  11.947  72.280  1.00 21.69           C
ATOM   2484  C   MET A 638      24.821  12.166  72.108  1.00 21.73           C
ATOM   2485  O   MET A 638      25.398  13.115  72.656  1.00 21.51           O
ATOM   2486  CB  MET A 638      22.527  12.514  71.091  1.00 21.79           C
ATOM   2487  CG  MET A 638      22.860  13.945  70.715  1.00 21.58           C
ATOM   2488  SD  MET A 638      21.951  14.519  69.274  1.00 21.85           S
ATOM   2489  CE  MET A 638      22.867  13.792  67.915  1.00 22.09           C
ATOM   2490  N   ASN A 639      25.438  11.261  71.348  1.00 21.83           N
ATOM   2491  CA  ASN A 639      26.846  11.339  70.969  1.00 21.80           C
ATOM   2492  C   ASN A 639      27.021  10.677  69.610  1.00 22.19           C
ATOM   2493  O   ASN A 639      27.470   9.535  69.497  1.00 22.24           O
ATOM   2494  CB  ASN A 639      27.757  10.694  72.022  1.00 21.36           C
ATOM   2495  CG  ASN A 639      29.242  10.811  71.665  1.00 20.90           C
ATOM   2496  OD1 ASN A 639      29.645  11.683  70.891  1.00 19.94           O
ATOM   2497  ND2 ASN A 639      30.055   9.925  72.224  1.00 19.34           N
ATOM   2498  N   ASN A 640      26.638  11.417  68.579  1.00 22.77           N
ATOM   2499  CA  ASN A 640      26.600  10.920  67.219  1.00 23.26           C
ATOM   2500  C   ASN A 640      26.814  12.109  66.305  1.00 23.96           C
ATOM   2501  O   ASN A 640      25.931  12.965  66.171  1.00 23.89           O
ATOM   2502  CB  ASN A 640      25.246  10.257  66.940  1.00 23.03           C
ATOM   2503  CG  ASN A 640      25.149   9.668  65.542  1.00 22.82           C
ATOM   2504  OD1 ASN A 640      25.458  10.323  64.541  1.00 22.96           O
ATOM   2505  ND2 ASN A 640      24.702   8.423  65.468  1.00 22.01           N
ATOM   2506  N   ARG A 641      27.995  12.154  65.689  1.00 24.62           N
ATOM   2507  CA  ARG A 641      28.410  13.276  64.855  1.00 25.23           C
ATOM   2508  C   ARG A 641      27.431  13.531  63.711  1.00 25.17           C
ATOM   2509  O   ARG A 641      27.003  14.675  63.488  1.00 25.40           O
ATOM   2510  CB  ARG A 641      29.816  13.038  64.303  1.00 25.26           C
ATOM   2511  CG  ARG A 641      30.494  14.304  63.823  1.00 26.40           C
ATOM   2512  CD  ARG A 641      31.906  14.066  63.300  1.00 26.66           C
ATOM   2513  NE  ARG A 641      32.303  15.169  62.423  1.00 29.71           N
ATOM   2514  CZ  ARG A 641      32.069  15.208  61.110  1.00 30.42           C
ATOM   2515  NH1 ARG A 641      31.456  14.191  60.506  1.00 29.21           N
ATOM   2516  NH2 ARG A 641      32.450  16.266  60.396  1.00 30.64           N
ATOM   2517  N   ARG A 642      27.067  12.456  63.016  1.00 24.80           N
ATOM   2518  CA  ARG A 642      26.251  12.528  61.810  1.00 24.72           C
ATOM   2519  C   ARG A 642      24.798  12.958  62.068  1.00 24.18           C
ATOM   2520  O   ARG A 642      24.145  13.521  61.183  1.00 24.00           O
ATOM   2521  CB  ARG A 642      26.277  11.170  61.100  1.00 25.06           C
ATOM   2522  CG  ARG A 642      25.582  11.150  59.754  1.00 26.28           C
ATOM   2523  CD  ARG A 642      25.885   9.875  58.986  1.00 27.98           C
ATOM   2524  NE  ARG A 642      25.277   9.892  57.656  1.00 29.07           N
ATOM   2525  CZ  ARG A 642      25.811  10.483  56.589  1.00 29.96           C
ATOM   2526  NH1 ARG A 642      26.977  11.122  56.676  1.00 30.08           N
ATOM   2527  NH2 ARG A 642      25.178  10.434  55.425  1.00 30.47           N
ATOM   2528  N   ALA A 643      24.299  12.691  63.274  1.00 23.32           N
ATOM   2529  CA  ALA A 643      22.886  12.900  63.576  1.00 22.45           C
ATOM   2530  C   ALA A 643      22.599  14.305  64.108  1.00 21.96           C
ATOM   2531  O   ALA A 643      21.452  14.647  64.405  1.00 22.03           O
ATOM   2532  CB  ALA A 643      22.379  11.832  64.537  1.00 22.39           C
ATOM   2533  N   GLN A 644      23.643  15.117  64.208  1.00 21.07           N
ATOM   2534  CA  GLN A 644      23.504  16.490  64.651  1.00 20.46           C
ATOM   2535  C   GLN A 644      22.749  17.349  63.649  1.00 20.36           C
ATOM   2536  O   GLN A 644      22.744  17.081  62.446  1.00 20.22           O
ATOM   2537  CB  GLN A 644      24.873  17.118  64.871  1.00 20.43           C
ATOM   2538  CG  GLN A 644      25.622  16.628  66.086  1.00 20.25           C
ATOM   2539  CD  GLN A 644      27.013  17.197  66.131  1.00 19.57           C
ATOM   2540  OE1 GLN A 644      27.301  18.088  66.918  1.00 18.79           O
ATOM   2541  NE2 GLN A 644      27.881  16.704  65.259  1.00 20.47           N
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ATOM   2542  N   ASN A 645      22.115  18.388  64.170  1.00 20.08           N
ATOM   2543  CA  ASN A 645      21.549  19.449  63.368  1.00 19.92           C
ATOM   2544  C   ASN A 645      21.682  20.715  64.183  1.00 20.00           C
ATOM   2545  O   ASN A 645      21.425  20.713  65.382  1.00 20.06           O
ATOM   2546  CB  ASN A 645      20.098  19.164  62.975  1.00 19.96           C
ATOM   2547  CG  ASN A 645      19.363  18.310  63.989  1.00 19.74           C
ATOM   2548  OD1 ASN A 645      19.009  18.774  65.071  1.00 21.27           O
ATOM   2549  ND2 ASN A 645      19.105  17.061  63.630  1.00 18.29           N
ATOM   2550  N   THR A 646      22.106  21.795  63.541  1.00 20.14           N
ATOM   2551  CA  THR A 646      22.610  22.942  64.288  1.00 20.17           C
ATOM   2552  C   THR A 646      21.773  24.198  64.043  1.00 20.35           C
ATOM   2553  O   THR A 646      20.577  24.229  64.359  1.00 20.31           O
ATOM   2554  CB  THR A 646      24.112  23.175  63.990  1.00 20.10           C
ATOM   2555  OG1 THR A 646      24.264  23.764  62.694  1.00 19.88           O
ATOM   2556  CG2 THR A 646      24.869  21.856  64.020  1.00 19.40           C
ATOM   2557  N   GLU A 647      22.411  25.231  63.501  1.00 20.59           N
ATOM   2558  CA  GLU A 647      21.714  26.416  63.017  1.00 20.79           C
ATOM   2559  C   GLU A 647      20.654  25.957  62.037  1.00 20.46           C
ATOM   2560  O   GLU A 647      20.857  24.995  61.297  1.00 20.49           O
ATOM   2561  CB  GLU A 647      22.679  27.366  62.300  1.00 20.58           C
ATOM   2562  CG  GLU A 647      23.921  27.735  63.093  1.00 20.89           C
ATOM   2563  CD  GLU A 647      24.990  28.405  62.236  1.00 21.39           C
ATOM   2564  OE1 GLU A 647      25.171  28.020  61.062  1.00 21.55           O
ATOM   2565  OE2 GLU A 647      25.659  29.327  62.743  1.00 23.40           O
ATOM   2566  N   SER A 648      19.518  26.639  62.036  1.00 20.32           N
ATOM   2567  CA  SER A 648      18.436  26.256  61.154  1.00 20.16           C
ATOM   2568  C   SER A 648      17.676  27.475  60.687  1.00 19.99           C
ATOM   2569  O   SER A 648      17.863  28.579  61.215  1.00 19.85           O
ATOM   2570  CB  SER A 648      17.494  25.286  61.869  1.00 20.05           C
ATOM   2571  OG  SER A 648      16.943  25.901  63.018  1.00 20.75           O
ATOM   2572  N   THR A 649      16.831  27.274  59.683  1.00 19.80           N
ATOM   2573  CA  THR A 649      15.919  28.315  59.248  1.00 20.07           C
ATOM   2574  C   THR A 649      14.485  27.778  59.171  1.00 20.30           C
ATOM   2575  O   THR A 649      14.249  26.653  58.713  1.00 20.15           O
ATOM   2576  CB  THR A 649      16.391  28.993  57.940  1.00 20.08           C
ATOM   2577  OG1 THR A 649      15.546  30.112  57.650  1.00 20.03           O
ATOM   2578  CG2 THR A 649      16.393  28.017  56.761  1.00 20.04           C
ATOM   2579  N   VAL A 650      13.540  28.587  59.642  1.00 20.57           N
ATOM   2580  CA  VAL A 650      12.167  28.133  59.879  1.00 20.87           C
ATOM   2581  C   VAL A 650      11.173  28.761  58.891  1.00 21.10           C
ATOM   2582  O   VAL A 650      11.257  29.958  58.611  1.00 21.07           O
ATOM   2583  CB  VAL A 650      11.754  28.393  61.370  1.00 20.97           C
ATOM   2584  CG1 VAL A 650      11.632  29.900  61.674  1.00 20.68           C
ATOM   2585  CG2 VAL A 650      10.483  27.646  61.733  1.00 20.39           C
ATOM   2586  N   VAL A 651      10.262  27.944  58.347  1.00 21.38           N
ATOM   2587  CA  VAL A 651       9.205  28.424  57.435  1.00 21.76           C
ATOM   2588  C   VAL A 651       7.855  27.729  57.681  1.00 21.93           C
ATOM   2589  O   VAL A 651       7.808  26.512  57.909  1.00 21.81           O
ATOM   2590  CB  VAL A 651       9.579  28.274  55.914  1.00 21.91           C
ATOM   2591  CG1 VAL A 651      10.995  28.751  55.615  1.00 21.91           C
ATOM   2592  CG2 VAL A 651       9.419  26.852  55.443  1.00 22.76           C
ATOM   2593  N   GLN A 652       6.766  28.497  57.628  1.00 21.99           N
ATOM   2594  CA  GLN A 652       5.422  27.913  57.671  1.00 22.26           C
ATOM   2595  C   GLN A 652       4.812  27.768  56.277  1.00 22.37           C
ATOM   2596  O   GLN A 652       4.913  28.672  55.445  1.00 22.33           O
ATOM   2597  CB  GLN A 652       4.465  28.706  58.582  1.00 22.32           C
ATOM   2598  CG  GLN A 652       3.155  27.940  58.861  1.00 22.11           C
ATOM   2599  CD  GLN A 652       2.193  28.656  59.796  1.00 22.16           C
ATOM   2600  OE1 GLN A 652       2.003  29.869  59.716  1.00 21.85           O
ATOM   2601  NE2 GLN A 652       1.562  27.893  60.679  1.00 21.83           N
ATOM   2602  N   LEU A 653       4.178  26.621  56.039  1.00 22.74           N
ATOM   2603  CA  LEU A 653       3.424  26.376  54.806  1.00 23.06           C
ATOM   2604  C   LEU A 653       2.018  26.960  54.896  1.00 22.97           C
ATOM   2605  O   LEU A 653       1.538  27.291  55.987  1.00 23.10           O
ATOM   2606  CB  LEU A 653       3.332  24.871  54.512  1.00 22.88           C
ATOM   2607  CG  LEU A 653       4.600  24.073  54.208  1.00 23.60           C
ATOM   2608  CD1 LEU A 653       4.231  22.667  53.769  1.00 23.89           C
ATOM   2609  CD2 LEU A 653       5.464  24.747  53.142  1.00 24.70           C
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ATOM   2610  N   ASN A 654       1.358  27.076  53.746  1.00 23.03           N
ATOM   2611  CA  ASN A 654      -0.050  27.480  53.699  1.00 23.03           C
ATOM   2612  C   ASN A 654      -1.002  26.469  54.336  1.00 22.64           C
ATOM   2613  O   ASN A 654      -2.132  26.816  54.678  1.00 22.55           O
ATOM   2614  CB  ASN A 654      -0.482  27.802  52.262  1.00 23.23           C
ATOM   2615  CG  ASN A 654       0.090  29.114  51.772  1.00 23.57           C
ATOM   2616  OD1 ASN A 654       0.359  30.017  52.563  1.00 23.90           O
ATOM   2617  ND2 ASN A 654       0.288  29.226  50.464  1.00 24.45           N
ATOM   2618  N   ASN A 655      -0.533  25.235  54.508  1.00 22.36           N
ATOM   2619  CA  ASN A 655      -1.314  24.196  55.171  1.00 22.27           C
ATOM   2620  C   ASN A 655      -1.059  24.077  56.681  1.00 22.38           C
ATOM   2621  O   ASN A 655      -1.567  23.163  57.332  1.00 22.03           O
ATOM   2622  CB  ASN A 655      -1.146  22.846  54.461  1.00 22.38           C
ATOM   2623  CG  ASN A 655       0.224  22.215  54.674  1.00 23.37           C
ATOM   2624  OD1 ASN A 655       1.078  22.737  55.390  1.00 24.64           O
ATOM   2625  ND2 ASN A 655       0.428  21.066  54.051  1.00 24.33           N
ATOM   2626  N   GLY A 656      -0.271  25.007  57.226  1.00 22.54           N
ATOM   2627  CA  GLY A 656      -0.045  25.088  58.669  1.00 22.40           C
ATOM   2628  C   GLY A 656       1.198  24.373  59.163  1.00 22.46           C
ATOM   2629  O   GLY A 656       1.615  24.552  60.314  1.00 22.39           O
ATOM   2630  N   ASP A 657       1.794  23.558  58.301  1.00 22.33           N
ATOM   2631  CA  ASP A 657       3.000  22.841  58.674  1.00 22.26           C
ATOM   2632  C   ASP A 657       4.168  23.805  58.783  1.00 22.25           C
ATOM   2633  O   ASP A 657       4.215  24.840  58.097  1.00 22.00           O
ATOM   2634  CB  ASP A 657       3.318  21.728  57.675  1.00 22.36           C
ATOM   2635  CG  ASP A 657       2.476  20.480  57.898  1.00 23.55           C
ATOM   2636  OD1 ASP A 657       1.557  20.510  58.753  1.00 24.51           O
ATOM   2637  OD2 ASP A 657       2.741  19.462  57.217  1.00 23.42           O
ATOM   2638  N   VAL A 658       5.090  23.457  59.675  1.00 21.80           N
ATOM   2639  CA  VAL A 658       6.314  24.194  59.873  1.00 21.32           C
ATOM   2640  C   VAL A 658       7.455  23.340  59.363  1.00 21.06           C
ATOM   2641  O   VAL A 658       7.556  22.160  59.700  1.00 21.44           O
ATOM   2642  CB  VAL A 658       6.542  24.513  61.366  1.00 21.44           C
ATOM   2643  CG1 VAL A 658       7.868  25.237  61.567  1.00 20.76           C
ATOM   2644  CG2 VAL A 658       5.387  25.336  61.916  1.00 21.18           C
ATOM   2645  N   LYS A 659       8.309  23.939  58.545  1.00 20.59           N
ATOM   2646  CA  LYS A 659       9.489  23.255  58.044  1.00 20.15           C
ATOM   2647  C   LYS A 659      10.743  23.890  58.629  1.00 19.44           C
ATOM   2648  O   LYS A 659      10.875  25.116  58.668  1.00 18.90           O
ATOM   2649  CB  LYS A 659       9.525  23.277  56.510  1.00 20.26           C
ATOM   2650  CG  LYS A 659       8.336  22.592  55.836  1.00 21.28           C
ATOM   2651  CD  LYS A 659       8.518  21.077  55.765  1.00 23.70           C
ATOM   2652  CE  LYS A 659       7.376  20.412  55.007  1.00 24.90           C
ATOM   2653  NZ  LYS A 659       7.380  18.931  55.217  1.00 26.29           N
ATOM   2654  N   LEU A 660      11.648  23.039  59.101  1.00 19.21           N
ATOM   2655  CA  LEU A 660      12.912  23.489  59.675  1.00 18.87           C
ATOM   2656  C   LEU A 660      14.096  22.978  58.860  1.00 18.78           C
ATOM   2657  O   LEU A 660      14.420  21.791  58.873  1.00 18.71           O
ATOM   2658  CB  LEU A 660      13.021  23.071  61.140  1.00 18.45           C
ATOM   2659  CG  LEU A 660      14.061  23.774  62.015  1.00 18.35           C
ATOM   2660  CD1 LEU A 660      13.700  25.232  62.286  1.00 16.99           C
ATOM   2661  CD2 LEU A 660      14.222  23.015  63.323  1.00 18.65           C
ATOM   2662  N   PHE A 661      14.727  23.894  58.138  1.00 18.91           N
ATOM   2663  CA  PHE A 661      15.892  23.577  57.334  1.00 19.18           C
ATOM   2664  C   PHE A 661      17.131  23.708  58.211  1.00 19.48           C
ATOM   2665  O   PHE A 661      17.438  24.790  58.701  1.00 19.25           O
ATOM   2666  CB  PHE A 661      15.965  24.509  56.129  1.00 19.00           C
ATOM   2667  CG  PHE A 661      14.732  24.489  55.282  1.00 19.11           C
ATOM   2668  CD1 PHE A 661      14.646  23.645  54.181  1.00 19.13           C
ATOM   2669  CD2 PHE A 661      13.644  25.303  55.591  1.00 19.18           C
ATOM   2670  CE1 PHE A 661      13.497  23.615  53.389  1.00 19.04           C
ATOM   2671  CE2 PHE A 661      12.493  25.279  54.807  1.00 19.57           C
ATOM   2672  CZ  PHE A 661      12.423  24.431  53.699  1.00 19.06           C
ATOM   2673  N   MET A 662      17.831  22.594  58.402  1.00 19.92           N
ATOM   2674  CA  MET A 662      18.856  22.498  59.427  1.00 20.59           C
ATOM   2675  C   MET A 662      20.224  22.242  58.839  1.00 20.71           C
ATOM   2676  O   MET A 662      20.404  21.306  58.065  1.00 21.03           O
ATOM   2677  CB  MET A 662      18.521  21.371  60.405  1.00 20.43           C
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ATOM   2678  CG  MET A 662      17.132  21.454  61.032  1.00 20.74           C
ATOM   2679  SD  MET A 662      16.700  19.925  61.885  1.00 21.48           S
ATOM   2680  CE  MET A 662      16.728  18.758  60.523  1.00 19.88           C
ATOM   2681  N   ARG A 663      21.186  23.080  59.215  1.00 20.95           N
ATOM   2682  CA  ARG A 663      22.593  22.836  58.918  1.00 21.28           C
ATOM   2683  C   ARG A 663      23.053  21.526  59.572  1.00 21.63           C
ATOM   2684  O   ARG A 663      22.817  21.290  60.760  1.00 21.66           O
ATOM   2685  CB  ARG A 663      23.441  24.018  59.404  1.00 21.23           C
ATOM   2686  CG  ARG A 663      24.950  23.768  59.456  1.00 21.19           C
ATOM   2687  CD  ARG A 663      25.677  24.975  60.017  1.00 21.11           C
ATOM   2688  NE  ARG A 663      27.062  24.684  60.368  1.00 21.85           N
ATOM   2689  CZ  ARG A 663      27.962  25.608  60.697  1.00 21.81           C
ATOM   2690  NH1 ARG A 663      27.631  26.891  60.713  1.00 21.56           N
ATOM   2691  NH2 ARG A 663      29.200  25.253  61.001  1.00 21.18           N
ATOM   2692  N   GLY A 664      23.708  20.680  58.785  1.00 22.13           N
ATOM   2693  CA  GLY A 664      24.185  19.385  59.262  1.00 22.61           C
ATOM   2694  C   GLY A 664      25.332  18.848  58.439  1.00 22.96           C
ATOM   2695  O   GLY A 664      25.952  19.585  57.674  1.00 22.99           O
ATOM   2696  N   LEU A 665      25.595  17.553  58.580  1.00 23.62           N
ATOM   2697  CA  LEU A 665      26.810  16.942  58.037  1.00 24.16           C
ATOM   2698  C   LEU A 665      26.528  15.739  57.146  1.00 24.59           C
ATOM   2699  O   LEU A 665      27.218  14.717  57.211  1.00 24.72           O
ATOM   2700  CB  LEU A 665      27.762  16.568  59.178  1.00 24.04           C
ATOM   2701  CG  LEU A 665      28.356  17.787  59.885  1.00 24.10           C
ATOM   2702  CD1 LEU A 665      28.753  17.469  61.318  1.00 24.23           C
ATOM   2703  CD2 LEU A 665      29.531  18.344  59.089  1.00 24.60           C
ATOM   2704  N   THR A 666      25.515  15.884  56.302  1.00 25.02           N
ATOM   2705  CA  THR A 666      25.132  14.850  55.353  1.00 25.40           C
ATOM   2706  C   THR A 666      25.509  15.262  53.925  1.00 25.57           C
ATOM   2707  O   THR A 666      25.310  14.496  52.981  1.00 25.91           O
ATOM   2708  CB  THR A 666      23.612  14.594  55.411  1.00 25.43           C
ATOM   2709  OG1 THR A 666      22.916  15.792  55.049  1.00 26.40           O
ATOM   2710  CG2 THR A 666      23.176  14.178  56.809  1.00 25.17           C
ATOM   2711  N   GLY A 667      26.047  16.473  53.775  1.00 25.67           N
ATOM   2712  CA  GLY A 667      26.295  17.076  52.463  1.00 25.62           C
ATOM   2713  C   GLY A 667      25.010  17.471  51.760  1.00 25.70           C
ATOM   2714  O   GLY A 667      25.036  17.989  50.650  1.00 26.03           O
ATOM   2715  N   ASP A 668      23.891  17.237  52.439  1.00 25.81           N
ATOM   2716  CA  ASP A 668      22.544  17.320  51.881  1.00 25.57           C
ATOM   2717  C   ASP A 668      21.704  18.321  52.642  1.00 24.85           C
ATOM   2718  O   ASP A 668      21.990  18.623  53.792  1.00 24.51           O
ATOM   2719  CB  ASP A 668      21.852  15.962  52.039  1.00 25.81           C
ATOM   2720  CG  ASP A 668      22.096  15.049  50.879  1.00 27.43           C
ATOM   2721  OD1 ASP A 668      21.783  15.440  49.743  1.00 29.81           O
ATOM   2722  OD2 ASP A 668      22.590  13.928  51.091  1.00 30.16           O
ATOM   2723  N   LEU A 669      20.634  18.793  52.010  1.00 24.22           N
ATOM   2724  CA  LEU A 669      19.634  19.575  52.715  1.00 23.55           C
ATOM   2725  C   LEU A 669      18.783  18.694  53.629  1.00 23.26           C
ATOM   2726  O   LEU A 669      18.132  17.757  53.174  1.00 23.44           O
ATOM   2727  CB  LEU A 669      18.745  20.346  51.740  1.00 23.26           C
ATOM   2728  CG  LEU A 669      17.776  21.317  52.417  1.00 22.42           C
ATOM   2729  CD1 LEU A 669      18.528  22.433  53.122  1.00 20.50           C
ATOM   2730  CD2 LEU A 669      16.798  21.876  51.408  1.00 21.11           C
ATOM   2731  N   GLN A 670      18.794  19.017  54.917  1.00 22.85           N
ATOM   2732  CA  GLN A 670      18.035  18.278  55.918  1.00 22.37           C
ATOM   2733  C   GLN A 670      16.863  19.117  56.402  1.00 22.15           C
ATOM   2734  O   GLN A 670      17.030  20.274  56.800  1.00 21.78           O
ATOM   2735  CB  GLN A 670      18.927  17.914  57.101  1.00 22.48           C
ATOM   2736  CG  GLN A 670      20.092  16.992  56.762  1.00 22.25           C
ATOM   2737  CD  GLN A 670      20.767  16.456  58.009  1.00 22.43           C
ATOM   2738  OE1 GLN A 670      21.860  16.900  58.377  1.00 22.73           O
ATOM   2739  NE2 GLN A 670      20.111  15.513  58.680  1.00 20.28           N
ATOM   2740  N   VAL A 671      15.675  18.522  56.370  1.00 22.00           N
ATOM   2741  CA  VAL A 671      14.447  19.244  56.682  1.00 21.78           C
ATOM   2742  C   VAL A 671      13.576  18.462  57.669  1.00 21.87           C
ATOM   2743  O   VAL A 671      13.274  17.282  57.448  1.00 21.96           O
ATOM   2744  CB  VAL A 671      13.634  19.549  55.400  1.00 21.71           C
ATOM   2745  CG1 VAL A 671      12.514  20.536  55.704  1.00 21.98           C
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ATOM   2746  CG2 VAL A 671      14.541  20.091  54.292  1.00 21.18           C
ATOM   2747  N   ALA A 672      13.177  19.131  58.752  1.00 21.64           N
ATOM   2748  CA  ALA A 672      12.262  18.556  59.737  1.00 21.69           C
ATOM   2749  C   ALA A 672      10.855  19.139  59.582  1.00 21.84           C
ATOM   2750  O   ALA A 672      10.696  20.280  59.137  1.00 21.55           O
ATOM   2751  CB  ALA A 672      12.783  18.798  61.148  1.00 21.50           C
ATOM   2752  N   THR A 673       9.845  18.359  59.968  1.00 21.95           N
ATOM   2753  CA  THR A 673       8.449  18.778  59.873  1.00 22.19           C
ATOM   2754  C   THR A 673       7.707  18.753  61.220  1.00 22.46           C
ATOM   2755  O   THR A 673       7.771  17.760  61.958  1.00 22.31           O
ATOM   2756  CB  THR A 673       7.690  17.912  58.840  1.00 22.29           C
ATOM   2757  OG1 THR A 673       8.326  18.033  57.558  1.00 21.98           O
ATOM   2758  CG2 THR A 673       6.229  18.353  58.722  1.00 22.10           C
ATOM   2759  N   SER A 674       7.001  19.851  61.516  1.00 22.87           N
ATOM   2760  CA  SER A 674       6.187  19.994  62.731  1.00 23.25           C
ATOM   2761  C   SER A 674       4.712  20.205  62.396  1.00 23.80           C
ATOM   2762  O   SER A 674       4.378  20.992  61.508  1.00 23.85           O
ATOM   2763  CB  SER A 674       6.677  21.178  63.572  1.00 23.29           C
ATOM   2764  OG  SER A 674       5.805  21.444  64.666  1.00 23.16           O
ATOM   2765  N   LYS A 675       3.839  19.526  63.139  1.00 24.35           N
ATOM   2766  CA  LYS A 675       2.396  19.597  62.919  1.00 24.95           C
ATOM   2767  C   LYS A 675       1.693  20.470  63.954  1.00 25.01           C
ATOM   2768  O   LYS A 675       0.595  20.975  63.703  1.00 25.02           O
ATOM   2769  CB  LYS A 675       1.781  18.195  62.944  1.00 25.23           C
ATOM   2770  CG  LYS A 675       2.258  17.254  61.847  1.00 26.53           C
ATOM   2771  CD  LYS A 675       1.666  17.619  60.502  1.00 28.36           C
ATOM   2772  CE  LYS A 675       1.979  16.559  59.458  1.00 29.29           C
ATOM   2773  NZ  LYS A 675       1.822  17.147  58.099  1.00 30.40           N
ATOM   2774  N   ASP A 676       2.324  20.628  65.117  1.00 24.96           N
ATOM   2775  CA  ASP A 676       1.768  21.413  66.217  1.00 24.75           C
ATOM   2776  C   ASP A 676       2.431  22.785  66.372  1.00 24.88           C
ATOM   2777  O   ASP A 676       2.435  23.370  67.462  1.00 25.11           O
ATOM   2778  CB  ASP A 676       1.827  20.623  67.532  1.00 24.72           C
ATOM   2779  CG  ASP A 676       3.233  20.108  67.866  1.00 25.45           C
ATOM   2780  OD1 ASP A 676       4.217  20.456  67.162  1.00 26.18           O
ATOM   2781  OD2 ASP A 676       3.344  19.341  68.849  1.00 24.89           O
ATOM   2782  N   GLY A 677       2.996  23.291  65.281  1.00 24.91           N
ATOM   2783  CA  GLY A 677       3.503  24.658  65.239  1.00 25.05           C
ATOM   2784  C   GLY A 677       4.827  24.888  65.936  1.00 25.13           C
ATOM   2785  O   GLY A 677       5.004  25.891  66.625  1.00 25.22           O
ATOM   2786  N   GLY A 678       5.757  23.957  65.750  1.00 25.28           N
ATOM   2787  CA  GLY A 678       7.123  24.134  66.217  1.00 25.26           C
ATOM   2788  C   GLY A 678       7.489  23.359  67.457  1.00 25.31           C
ATOM   2789  O   GLY A 678       8.670  23.162  67.724  1.00 25.68           O
ATOM   2790  N   VAL A 679       6.484  22.908  68.209  1.00 25.43           N
ATOM   2791  CA  VAL A 679       6.710  22.215  69.484  1.00 25.33           C
ATOM   2792  C   VAL A 679       7.248  20.786  69.309  1.00 25.61           C
ATOM   2793  O   VAL A 679       8.230  20.412  69.951  1.00 25.80           O
ATOM   2794  CB  VAL A 679       5.442  22.221  70.389  1.00 25.26           C
ATOM   2795  CG1 VAL A 679       5.766  21.705  71.790  1.00 24.24           C
ATOM   2796  CG2 VAL A 679       4.848  23.621  70.475  1.00 25.13           C
ATOM   2797  N   THR A 680       6.611  20.004  68.443  1.00 25.77           N
ATOM   2798  CA  THR A 680       6.972  18.599  68.219  1.00 26.08           C
ATOM   2799  C   THR A 680       7.413  18.408  66.772  1.00 25.99           C
ATOM   2800  O   THR A 680       7.019  19.171  65.894  1.00 25.78           O
ATOM   2801  CB  THR A 680       5.780  17.645  68.592  1.00 26.26           C
ATOM   2802  OG1 THR A 680       5.676  17.548  70.019  1.00 26.83           O
ATOM   2803  CG2 THR A 680       5.949  16.233  68.033  1.00 27.03           C
ATOM   2804  N   TRP A 681       8.241  17.393  66.533  1.00 26.13           N
ATOM   2805  CA  TRP A 681       8.744  17.101  65.195  1.00 26.30           C
ATOM   2806  C   TRP A 681       8.414  15.675  64.784  1.00 27.08           C
ATOM   2807  O   TRP A 681       8.415  14.766  65.619  1.00 27.10           O
ATOM   2808  CB  TRP A 681      10.250  17.350  65.128  1.00 25.70           C
ATOM   2809  CG  TRP A 681      10.596  18.753  65.500  1.00 25.23           C
ATOM   2810  CD1 TRP A 681      11.032  19.198  66.713  1.00 23.95           C
ATOM   2811  CD2 TRP A 681      10.492  19.908  64.659  1.00 24.66           C
ATOM   2812  NE1 TRP A 681      11.227  20.556  66.674  1.00 24.01           N
ATOM   2813  CE2 TRP A 681      10.900  21.018  65.427  1.00 24.30           C
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ATOM   2814  CE3 TRP A 681      10.103  20.110  63.325  1.00 23.66           C
ATOM   2815  CZ2 TRP A 681      10.927  22.318  64.909  1.00 25.23           C
ATOM   2816  CZ3 TRP A 681      10.129  21.396  62.812  1.00 24.13           C
ATOM   2817  CH2 TRP A 681      10.538  22.486  63.603  1.00 24.80           C
ATOM   2818  N   GLU A 682       8.123  15.489  63.498  1.00 27.96           N
ATOM   2819  CA  GLU A 682       7.829  14.162  62.950  1.00 28.91           C
ATOM   2820  C   GLU A 682       9.044  13.225  62.981  1.00 29.28           C
ATOM   2821  O   GLU A 682      10.184  13.675  63.076  1.00 29.32           O
ATOM   2822  CB  GLU A 682       7.266  14.278  61.530  1.00 28.96           C
ATOM   2823  CG  GLU A 682       5.876  14.912  61.461  1.00 30.54           C
ATOM   2824  CD  GLU A 682       4.858  14.211  62.357  1.00 32.68           C
ATOM   2825  OE1 GLU A 682       4.516  13.037  62.082  1.00 33.52           O
ATOM   2826  OE2 GLU A 682       4.397  14.837  63.336  1.00 33.25           O
ATOM   2827  N   LYS A 683       8.777  11.923  62.902  1.00 30.07           N
ATOM   2828  CA  LYS A 683       9.791  10.872  63.030  1.00 30.62           C
ATOM   2829  C   LYS A 683      11.050  11.128  62.208  1.00 30.71           C
ATOM   2830  O   LYS A 683      12.169  11.057  62.728  1.00 30.80           O
ATOM   2831  CB  LYS A 683       9.198   9.519  62.616  1.00 30.81           C
ATOM   2832  CG  LYS A 683       8.600   8.701  63.753  1.00 32.31           C
ATOM   2833  CD  LYS A 683       7.543   7.707  63.247  1.00 34.37           C
ATOM   2834  CE  LYS A 683       8.156   6.543  62.459  1.00 35.83           C
ATOM   2835  NZ  LYS A 683       7.128   5.539  62.017  1.00 35.88           N
ATOM   2836  N   ASP A 684      10.849  11.430  60.928  1.00 30.56           N
ATOM   2837  CA  ASP A 684      11.922  11.384  59.945  1.00 30.58           C
ATOM   2838  C   ASP A 684      12.362  12.743  59.410  1.00 30.11           C
ATOM   2839  O   ASP A 684      11.550  13.647  59.201  1.00 29.98           O
ATOM   2840  CB  ASP A 684      11.521  10.467  58.786  1.00 30.74           C
ATOM   2841  CG  ASP A 684      11.360   9.018  59.221  1.00 31.96           C
ATOM   2842  OD1 ASP A 684      12.247   8.504  59.947  1.00 33.01           O
ATOM   2843  OD2 ASP A 684      10.346   8.394  58.835  1.00 31.88           O
ATOM   2844  N   ILE A 685      13.667  12.862  59.201  1.00 29.62           N
ATOM   2845  CA  ILE A 685      14.262  14.033  58.587  1.00 29.16           C
ATOM   2846  C   ILE A 685      14.356  13.753  57.094  1.00 28.90           C
ATOM   2847  O   ILE A 685      15.032  12.807  56.669  1.00 28.84           O
ATOM   2848  CB  ILE A 685      15.660  14.342  59.186  1.00 29.07           C
ATOM   2849  CG1 ILE A 685      15.540  14.663  60.679  1.00 29.10           C
ATOM   2850  CG2 ILE A 685      16.318  15.509  58.460  1.00 29.66           C
ATOM   2851  CD1 ILE A 685      16.869  14.938  61.369  1.00 29.03           C
ATOM   2852  N   LYS A 686      13.647  14.558  56.306  1.00 28.48           N
ATOM   2853  CA  LYS A 686      13.695  14.462  54.848  1.00 28.13           C
ATOM   2854  C   LYS A 686      15.033  15.007  54.340  1.00 27.72           C
ATOM   2855  O   LYS A 686      15.547  15.994  54.862  1.00 27.96           O
ATOM   2856  CB  LYS A 686      12.506  15.214  54.235  1.00 28.14           C
ATOM   2857  CG  LYS A 686      12.456  15.253  52.710  1.00 28.62           C
ATOM   2858  CD  LYS A 686      11.921  13.973  52.087  1.00 28.85           C
ATOM   2859  CE  LYS A 686      11.976  14.058  50.564  1.00 29.14           C
ATOM   2860  NZ  LYS A 686      11.580  12.784  49.911  1.00 28.93           N
ATOM   2861  N   ARG A 687      15.610  14.342  53.347  1.00 27.22           N
ATOM   2862  CA  ARG A 687      16.865  14.790  52.751  1.00 26.84           C
ATOM   2863  C   ARG A 687      16.721  15.030  51.255  1.00 27.11           C
ATOM   2864  O   ARG A 687      16.130  14.217  50.540  1.00 27.10           O
ATOM   2865  CB  ARG A 687      17.994  13.799  53.025  1.00 26.44           C
ATOM   2866  CG  ARG A 687      18.744  14.067  54.315  1.00 25.69           C
ATOM   2867  CD  ARG A 687      19.743  12.971  54.621  1.00 23.73           C
ATOM   2868  NE  ARG A 687      20.773  12.885  53.588  1.00 23.79           N
ATOM   2869  CZ  ARG A 687      21.680  11.916  53.499  1.00 23.09           C
ATOM   2870  NH1 ARG A 687      21.707  10.925  54.381  1.00 23.76           N
ATOM   2871  NH2 ARG A 687      22.563  11.935  52.520  1.00 22.74           N
ATOM   2872  N   TYR A 688      17.263  16.156  50.796  1.00 27.26           N
ATOM   2873  CA  TYR A 688      17.207  16.537  49.390  1.00 27.52           C
ATOM   2874  C   TYR A 688      18.610  16.628  48.783  1.00 27.88           C
ATOM   2875  O   TYR A 688      19.317  17.619  48.992  1.00 27.88           O
ATOM   2876  CB  TYR A 688      16.470  17.872  49.213  1.00 27.16           C
ATOM   2877  CG  TYR A 688      15.005  17.840  49.597  1.00 26.62           C
ATOM   2878  CD1 TYR A 688      14.038  17.389  48.698  1.00 25.45           C
ATOM   2879  CD2 TYR A 688      14.586  18.281  50.855  1.00 25.54           C
ATOM   2880  CE1 TYR A 688      12.684  17.366  49.050  1.00 25.89           C
ATOM   2881  CE2 TYR A 688      13.246  18.264  51.216  1.00 25.60           C
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ATOM   2882  CZ  TYR A 688      12.296  17.805  50.310  1.00 26.63           C
ATOM   2883  OH  TYR A 688      10.963  17.782  50.668  1.00 26.80           O
ATOM   2884  N   PRO A 689      19.019  15.589  48.029  1.00 28.11           N
ATOM   2885  CA  PRO A 689      20.294  15.618  47.304  1.00 28.10           C
ATOM   2886  C   PRO A 689      20.379  16.735  46.247  1.00 28.25           C
ATOM   2887  O   PRO A 689      21.476  17.050  45.770  1.00 28.17           O
ATOM   2888  CB  PRO A 689      20.368  14.229  46.654  1.00 28.12           C
ATOM   2889  CG  PRO A 689      18.952  13.726  46.624  1.00 28.17           C
ATOM   2890  CD  PRO A 689      18.297  14.314  47.839  1.00 28.24           C
ATOM   2891  N   GLN A 690      19.238  17.331  45.900  1.00 28.21           N
ATOM   2892  CA  GLN A 690      19.198  18.448  44.948  1.00 28.24           C
ATOM   2893  C   GLN A 690      19.812  19.731  45.525  1.00 28.12           C
ATOM   2894  O   GLN A 690      20.129  20.661  44.779  1.00 28.20           O
ATOM   2895  CB  GLN A 690      17.761  18.739  44.481  1.00 28.38           C
ATOM   2896  CG  GLN A 690      17.037  17.593  43.773  1.00 29.01           C
ATOM   2897  CD  GLN A 690      16.384  16.611  44.744  1.00 30.57           C
ATOM   2898  OE1 GLN A 690      16.304  16.861  45.952  1.00 30.90           O
ATOM   2899  NE2 GLN A 690      15.930  15.478  44.217  1.00 31.01           N
ATOM   2900  N   VAL A 691      19.962  19.791  46.847  1.00 27.77           N
ATOM   2901  CA  VAL A 691      20.527  20.974  47.490  1.00 27.53           C
ATOM   2902  C   VAL A 691      21.675  20.607  48.424  1.00 27.48           C
ATOM   2903  O   VAL A 691      21.488  19.904  49.420  1.00 27.36           O
ATOM   2904  CB  VAL A 691      19.468  21.800  48.265  1.00 27.50           C
ATOM   2905  CG1 VAL A 691      20.013  23.179  48.580  1.00 27.73           C
ATOM   2906  CG2 VAL A 691      18.180  21.929  47.471  1.00 27.31           C
ATOM   2907  N   LYS A 692      22.860  21.107  48.091  1.00 27.46           N
ATOM   2908  CA  LYS A 692      24.068  20.805  48.838  1.00 27.30           C
ATOM   2909  C   LYS A 692      24.110  21.610  50.117  1.00 27.02           C
ATOM   2910  O   LYS A 692      23.570  22.720  50.177  1.00 27.33           O
ATOM   2911  CB  LYS A 692      25.318  21.110  47.999  1.00 27.52           C
ATOM   2912  CG  LYS A 692      25.509  20.228  46.773  1.00 27.99           C
ATOM   2913  CD  LYS A 692      25.791  18.782  47.170  1.00 29.81           C
ATOM   2914  CE  LYS A 692      26.051  17.912  45.950  1.00 29.90           C
ATOM   2915  NZ  LYS A 692      26.333  16.525  46.372  1.00 30.59           N
ATOM   2916  N   ASP A 693      24.756  21.038  51.131  1.00 26.46           N
ATOM   2917  CA  ASP A 693      25.038  21.724  52.389  1.00 26.08           C
ATOM   2918  C   ASP A 693      26.472  21.404  52.801  1.00 25.73           C
ATOM   2919  O   ASP A 693      26.805  20.260  53.105  1.00 25.62           O
ATOM   2920  CB  ASP A 693      24.022  21.308  53.464  1.00 26.08           C
ATOM   2921  CG  ASP A 693      24.465  21.651  54.882  1.00 26.58           C
ATOM   2922  OD1 ASP A 693      25.171  22.661  55.093  1.00 27.15           O
ATOM   2923  OD2 ASP A 693      24.084  20.899  55.801  1.00 27.65           O
ATOM   2924  N   VAL A 694      27.322  22.424  52.791  1.00 25.49           N
ATOM   2925  CA  VAL A 694      28.745  22.248  53.107  1.00 25.17           C
ATOM   2926  C   VAL A 694      29.037  22.589  54.576  1.00 25.16           C
ATOM   2927  O   VAL A 694      30.163  22.963  54.932  1.00 25.29           O
ATOM   2928  CB  VAL A 694      29.651  23.065  52.144  1.00 25.19           C
ATOM   2929  CG1 VAL A 694      29.335  22.720  50.682  1.00 24.30           C
ATOM   2930  CG2 VAL A 694      29.502  24.566  52.388  1.00 24.85           C
ATOM   2931  N   TYR A 695      28.004  22.448  55.415  1.00 24.76           N
ATOM   2932  CA  TYR A 695      28.067  22.709  56.861  1.00 24.22           C
ATOM   2933  C   TYR A 695      28.224  24.200  57.146  1.00 23.99           C
ATOM   2934  O   TYR A 695      29.211  24.662  57.733  1.00 23.98           O
ATOM   2935  CB  TYR A 695      29.137  21.850  57.554  1.00 24.11           C
ATOM   2936  CG  TYR A 695      29.067  21.849  59.064  1.00 24.22           C
ATOM   2937  CD1 TYR A 695      27.879  21.530  59.733  1.00 24.31           C
ATOM   2938  CD2 TYR A 695      30.193  22.156  59.831  1.00 23.99           C
ATOM   2939  CE1 TYR A 695      27.812  21.525  61.128  1.00 23.96           C
ATOM   2940  CE2 TYR A 695      30.139  22.153  61.226  1.00 23.84           C
ATOM   2941  CZ  TYR A 695      28.949  21.834  61.865  1.00 24.02           C
ATOM   2942  OH  TYR A 695      28.898  21.828  63.239  1.00 23.92           O
ATOM   2943  N   VAL A 696      27.217  24.947  56.711  1.00 23.62           N
ATOM   2944  CA  VAL A 696      27.194  26.394  56.834  1.00 22.96           C
ATOM   2945  C   VAL A 696      25.730  26.837  56.967  1.00 22.54           C
ATOM   2946  O   VAL A 696      24.817  26.106  56.578  1.00 22.03           O
ATOM   2947  CB  VAL A 696      27.936  27.068  55.631  1.00 22.87           C
ATOM   2948  CG1 VAL A 696      27.168  26.878  54.309  1.00 23.20           C
ATOM   2949  CG2 VAL A 696      28.220  28.540  55.903  1.00 22.58           C
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ATOM   2950  N   GLN A 697      25.522  28.018  57.543  1.00 22.28           N
ATOM   2951  CA  GLN A 697      24.184  28.575  57.751  1.00 22.24           C
ATOM   2952  C   GLN A 697      23.454  28.865  56.434  1.00 22.48           C
ATOM   2953  O   GLN A 697      24.079  29.148  55.403  1.00 22.65           O
ATOM   2954  CB  GLN A 697      24.281  29.839  58.615  1.00 22.00           C
ATOM   2955  CG  GLN A 697      22.972  30.572  58.912  1.00 21.27           C
ATOM   2956  CD  GLN A 697      22.686  31.719  57.949  1.00 20.33           C
ATOM   2957  OE1 GLN A 697      23.283  31.822  56.873  1.00 20.66           O
ATOM   2958  NE2 GLN A 697      21.757  32.579  58.332  1.00 19.36           N
ATOM   2959  N   MET A 698      22.129  28.803  56.496  1.00 22.33           N
ATOM   2960  CA  MET A 698      21.271  29.061  55.358  1.00 22.60           C
ATOM   2961  C   MET A 698      20.074  29.880  55.801  1.00 22.71           C
ATOM   2962  O   MET A 698      19.766  29.948  56.988  1.00 23.00           O
ATOM   2963  CB  MET A 698      20.796  27.739  54.750  1.00 22.54           C
ATOM   2964  CG  MET A 698      19.911  26.898  55.667  1.00 22.25           C
ATOM   2965  SD  MET A 698      19.650  25.232  55.036  1.00 23.52           S
ATOM   2966  CE  MET A 698      21.133  24.397  55.613  1.00 20.73           C
ATOM   2967  N   SER A 699      19.406  30.514  54.847  1.00 23.03           N
ATOM   2968  CA  SER A 699      18.124  31.140  55.114  1.00 23.44           C
ATOM   2969  C   SER A 699      17.109  30.716  54.068  1.00 23.69           C
ATOM   2970  O   SER A 699      17.439  30.549  52.895  1.00 23.75           O
ATOM   2971  CB  SER A 699      18.243  32.665  55.183  1.00 23.38           C
ATOM   2972  OG  SER A 699      18.631  33.216  53.944  1.00 23.78           O
ATOM   2973  N   ALA A 700      15.878  30.521  54.514  1.00 23.94           N
ATOM   2974  CA  ALA A 700      14.792  30.143  53.632  1.00 24.25           C
ATOM   2975  C   ALA A 700      13.565  30.960  53.985  1.00 24.58           C
ATOM   2976  O   ALA A 700      13.333  31.269  55.159  1.00 24.28           O
ATOM   2977  CB  ALA A 700      14.493  28.656  53.749  1.00 23.92           C
ATOM   2978  N   ILE A 701      12.790  31.313  52.962  1.00 25.06           N
ATOM   2979  CA  ILE A 701      11.541  32.050  53.151  1.00 25.62           C
ATOM   2980  C   ILE A 701      10.404  31.543  52.267  1.00 26.12           C
ATOM   2981  O   ILE A 701      10.615  31.120  51.127  1.00 26.25           O
ATOM   2982  CB  ILE A 701      11.703  33.588  52.940  1.00 25.70           C
ATOM   2983  CG1 ILE A 701      12.418  33.902  51.618  1.00 25.41           C
ATOM   2984  CG2 ILE A 701      12.398  34.237  54.147  1.00 25.40           C
ATOM   2985  CD1 ILE A 701      12.189  35.310  51.108  1.00 25.45           C
ATOM   2986  N   HIS A 702       9.201  31.581  52.830  1.00 26.55           N
ATOM   2987  CA  HIS A 702       7.967  31.384  52.097  1.00 27.00           C
ATOM   2988  C   HIS A 702       7.703  32.597  51.199  1.00 27.63           C
ATOM   2989  O   HIS A 702       7.992  33.738  51.571  1.00 27.59           O
ATOM   2990  CB  HIS A 702       6.826  31.217  53.096  1.00 26.88           C
ATOM   2991  CG  HIS A 702       5.516  30.867  52.471  1.00 26.99           C
ATOM   2992  ND1 HIS A 702       4.568  31.816  52.150  1.00 27.26           N
ATOM   2993  CD2 HIS A 702       4.989  29.672  52.115  1.00 27.42           C
ATOM   2994  CE1 HIS A 702       3.514  31.220  51.621  1.00 27.71           C
ATOM   2995  NE2 HIS A 702       3.745  29.919  51.588  1.00 28.48           N
ATOM   2996  N   THR A 703       7.167  32.344  50.010  1.00 28.42           N
ATOM   2997  CA  THR A 703       6.748  33.417  49.111  1.00 29.06           C
ATOM   2998  C   THR A 703       5.617  32.953  48.206  1.00 29.68           C
ATOM   2999  O   THR A 703       5.580  31.793  47.820  1.00 29.84           O
ATOM   3000  CB  THR A 703       7.919  33.952  48.251  1.00 29.01           C
ATOM   3001  OG1 THR A 703       7.453  35.053  47.464  1.00 28.58           O
ATOM   3002  CG2 THR A 703       8.488  32.861  47.332  1.00 28.40           C
ATOM   3003  N   MET A 704       4.708  33.860  47.864  1.00 30.37           N
ATOM   3004  CA  MET A 704       3.579  33.534  46.992  1.00 30.95           C
ATOM   3005  C   MET A 704       3.755  34.177  45.627  1.00 31.65           C
ATOM   3006  O   MET A 704       3.897  35.400  45.525  1.00 32.07           O
ATOM   3007  CB  MET A 704       2.257  33.994  47.614  1.00 30.63           C
ATOM   3008  CG  MET A 704       1.802  33.165  48.805  1.00 30.20           C
ATOM   3009  SD  MET A 704       1.565  31.422  48.419  1.00 29.61           S
ATOM   3010  CE  MET A 704       0.203  31.522  47.265  1.00 29.77           C
ATOM   3011  N   HIS A 705       3.747  33.356  44.581  1.00 32.21           N
ATOM   3012  CA  HIS A 705       3.848  33.863  43.215  1.00 32.81           C
ATOM   3013  C   HIS A 705       2.721  33.373  42.303  1.00 33.17           C
ATOM   3014  O   HIS A 705       2.657  32.196  41.938  1.00 33.18           O
ATOM   3015  CB  HIS A 705       5.219  33.544  42.611  1.00 32.82           C
ATOM   3016  CG  HIS A 705       5.522  34.319  41.368  1.00 32.82           C
ATOM   3017  ND1 HIS A 705       5.440  33.767  40.108  1.00 32.78           N
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ATOM   3018  CD2 HIS A 705       5.893  35.610  41.190  1.00 32.98           C
ATOM   3019  CE1 HIS A 705       5.760  34.680  39.208  1.00 33.05           C
ATOM   3020  NE2 HIS A 705       6.035  35.808  39.838  1.00 33.05           N
ATOM   3021  N   GLU A 706       1.827  34.296  41.964  1.00 33.91           N
ATOM   3022  CA  GLU A 706       0.738  34.069  41.006  1.00 34.54           C
ATOM   3023  C   GLU A 706      -0.084  32.804  41.264  1.00 34.89           C
ATOM   3024  O   GLU A 706      -0.424  32.082  40.322  1.00 34.87           O
ATOM   3025  CB  GLU A 706       1.281  34.041  39.572  1.00 34.62           C
ATOM   3026  CG  GLU A 706       1.994  35.301  39.103  1.00 34.47           C
ATOM   3027  CD  GLU A 706       2.406  35.216  37.637  1.00 34.59           C
ATOM   3028  OE1 GLU A 706       2.314  34.113  37.051  1.00 35.10           O
ATOM   3029  OE2 GLU A 706       2.822  36.247  37.070  1.00 33.50           O
ATOM   3030  N   GLY A 707      -0.402  32.526  42.526  1.00 35.36           N
ATOM   3031  CA  GLY A 707      -1.252  31.376  42.834  1.00 35.89           C
ATOM   3032  C   GLY A 707      -0.817  30.493  43.984  1.00 36.11           C
ATOM   3033  O   GLY A 707      -1.468  30.489  45.027  1.00 36.49           O
ATOM   3034  N   LYS A 708       0.258  29.727  43.781  1.00 36.24           N
ATOM   3035  CA  LYS A 708       0.838  28.809  44.796  1.00 36.25           C
ATOM   3036  C   LYS A 708       2.226  28.390  44.300  1.00 35.76           C
ATOM   3037  O   LYS A 708       2.420  28.335  43.081  1.00 36.02           O
ATOM   3038  CB  LYS A 708      -0.010  27.526  44.968  1.00 36.49           C
ATOM   3039  CG  LYS A 708      -1.448  27.671  45.538  1.00 37.08           C
ATOM   3040  CD  LYS A 708      -1.504  27.832  47.078  1.00 37.89           C
ATOM   3041  CE  LYS A 708      -1.406  26.492  47.814  1.00 37.82           C
ATOM   3042  NZ  LYS A 708      -1.937  26.587  49.203  1.00 37.19           N
ATOM   3043  N   GLU A 709       3.212  28.118  45.171  1.00 35.06           N
ATOM   3044  CA  GLU A 709       3.295  28.503  46.587  1.00 33.89           C
ATOM   3045  C   GLU A 709       4.757  28.870  46.894  1.00 33.44           C
ATOM   3046  O   GLU A 709       5.020  29.968  47.375  1.00 33.62           O
ATOM   3047  CB  GLU A 709       2.810  27.421  47.559  1.00 33.76           C
ATOM   3048  CG  GLU A 709       3.063  27.838  49.015  1.00 33.61           C
ATOM   3049  CD  GLU A 709       2.382  26.986  50.069  1.00 33.57           C
ATOM   3050  OE1 GLU A 709       1.636  26.050  49.717  1.00 33.17           O
ATOM   3051  OE2 GLU A 709       2.597  27.275  51.271  1.00 32.91           O
ATOM   3052  N   TYR A 710       5.690  27.951  46.629  1.00 32.24           N
ATOM   3053  CA  TYR A 710       7.154  28.225  46.653  1.00 31.17           C
ATOM   3054  C   TYR A 710       7.866  28.511  47.992  1.00 30.36           C
ATOM   3055  O   TYR A 710       7.322  29.155  48.891  1.00 30.13           O
ATOM   3056  CB  TYR A 710       7.533  29.332  45.650  1.00 31.34           C
ATOM   3057  CG  TYR A 710       6.977  29.131  44.261  1.00 31.63           C
ATOM   3058  CD1 TYR A 710       7.560  28.218  43.379  1.00 31.60           C
ATOM   3059  CD2 TYR A 710       5.866  29.849  43.829  1.00 31.64           C
ATOM   3060  CE1 TYR A 710       7.044  28.021  42.106  1.00 31.66           C
ATOM   3061  CE2 TYR A 710       5.342  29.664  42.554  1.00 32.03           C
ATOM   3062  CZ  TYR A 710       5.936  28.749  41.700  1.00 31.58           C
ATOM   3063  OH  TYR A 710       5.423  28.565  40.438  1.00 31.67           O
ATOM   3064  N   ILE A 711       9.107  28.029  48.082  1.00 29.40           N
ATOM   3065  CA  ILE A 711      10.072  28.431  49.107  1.00 28.19           C
ATOM   3066  C   ILE A 711      11.390  28.813  48.439  1.00 27.72           C
ATOM   3067  O   ILE A 711      11.834  28.156  47.500  1.00 27.67           O
ATOM   3068  CB  ILE A 711      10.350  27.308  50.137  1.00 28.32           C
ATOM   3069  CG1 ILE A 711       9.127  27.056  51.020  1.00 27.47           C
ATOM   3070  CG2 ILE A 711      11.571  27.654  51.017  1.00 27.99           C
ATOM   3071  CD1 ILE A 711       9.270  25.843  51.886  1.00 27.46           C
ATOM   3072  N   ILE A 712      12.013  29.874  48.938  1.00 27.17           N
ATOM   3073  CA  ILE A 712      13.318  30.310  48.461  1.00 26.48           C
ATOM   3074  C   ILE A 712      14.355  30.076  49.557  1.00 26.17           C
ATOM   3075  O   ILE A 712      14.196  30.543  50.687  1.00 26.14           O
ATOM   3076  CB  ILE A 712      13.298  31.799  48.050  1.00 26.61           C
ATOM   3077  CG1 ILE A 712      12.251  32.041  46.961  1.00 26.21           C
ATOM   3078  CG2 ILE A 712      14.668  32.243  47.572  1.00 26.53           C
ATOM   3079  CD1 ILE A 712      11.979  33.494  46.696  1.00 26.70           C
ATOM   3080  N   LEU A 713      15.407  29.343  49.211  1.00 25.71           N
ATOM   3081  CA  LEU A 713      16.463  28.965  50.147  1.00 25.35           C
ATOM   3082  C   LEU A 713      17.799  29.450  49.591  1.00 25.14           C
ATOM   3083  O   LEU A 713      18.073  29.299  48.403  1.00 25.04           O
ATOM   3084  CB  LEU A 713      16.462  27.440  50.332  1.00 25.27           C
ATOM   3085  CG  LEU A 713      17.357  26.570  51.240  1.00 25.21           C
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ATOM   3086  CD1 LEU A 713      18.864  26.793  51.065  1.00 24.85           C
ATOM   3087  CD2 LEU A 713      16.960  26.638  52.697  1.00 24.30           C
ATOM   3088  N   SER A 714      18.625  30.037  50.448  1.00 25.00           N
ATOM   3089  CA  SER A 714      19.942  30.498  50.029  1.00 24.85           C
ATOM   3090  C   SER A 714      21.084  29.931  50.881  1.00 24.82           C
ATOM   3091  O   SER A 714      21.061  30.021  52.113  1.00 24.66           O
ATOM   3092  CB  SER A 714      19.988  32.026  50.013  1.00 24.72           C
ATOM   3093  OG  SER A 714      21.243  32.478  49.542  1.00 24.67           O
ATOM   3094  N   ASN A 715      22.077  29.352  50.211  1.00 24.85           N
ATOM   3095  CA  ASN A 715      23.307  28.883  50.865  1.00 25.20           C
ATOM   3096  C   ASN A 715      24.463  28.716  49.878  1.00 25.35           C
ATOM   3097  O   ASN A 715      24.283  28.883  48.667  1.00 25.31           O
ATOM   3098  CB  ASN A 715      23.076  27.578  51.653  1.00 24.93           C
ATOM   3099  CG  ASN A 715      22.655  26.425  50.769  1.00 24.64           C
ATOM   3100  OD1 ASN A 715      22.284  26.620  49.612  1.00 24.79           O
ATOM   3101  ND2 ASN A 715      22.707  25.214  51.311  1.00 23.84           N
ATOM   3102  N   ALA A 716      25.642  28.397  50.408  1.00 25.53           N
ATOM   3103  CA  ALA A 716      26.821  28.133  49.586  1.00 25.91           C
ATOM   3104  C   ALA A 716      26.618  26.909  48.701  1.00 26.22           C
ATOM   3105  O   ALA A 716      26.096  25.888  49.149  1.00 26.23           O
ATOM   3106  CB  ALA A 716      28.048  27.961  50.458  1.00 25.73           C
ATOM   3107  N   GLY A 717      27.013  27.034  47.436  1.00 26.72           N
ATOM   3108  CA  GLY A 717      26.961  25.925  46.485  1.00 27.20           C
ATOM   3109  C   GLY A 717      28.117  24.967  46.691  1.00 27.74           C
ATOM   3110  O   GLY A 717      27.986  23.764  46.458  1.00 27.73           O
ATOM   3111  N   GLY A 718      29.247  25.502  47.142  1.00 28.24           N
ATOM   3112  CA  GLY A 718      30.439  24.696  47.375  1.00 29.34           C
ATOM   3113  C   GLY A 718      31.263  24.435  46.120  1.00 30.01           C
ATOM   3114  O   GLY A 718      31.059  25.096  45.095  1.00 29.99           O
ATOM   3115  N   PRO A 719      32.235  23.502  46.206  1.00 30.44           N
ATOM   3116  CA  PRO A 719      32.637  22.833  47.446  1.00 30.70           C
ATOM   3117  C   PRO A 719      33.302  23.868  48.342  1.00 31.04           C
ATOM   3118  O   PRO A 719      33.976  24.767  47.830  1.00 31.59           O
ATOM   3119  CB  PRO A 719      33.673  21.810  46.972  1.00 30.71           C
ATOM   3120  CG  PRO A 719      34.221  22.385  45.709  1.00 30.60           C
ATOM   3121  CD  PRO A 719      33.050  23.060  45.058  1.00 30.55           C
ATOM   3122  N   LYS A 720      33.121  23.759  49.654  1.00 30.77           N
ATOM   3123  CA  LYS A 720      33.574  24.810  50.577  1.00 30.85           C
ATOM   3124  C   LYS A 720      32.602  26.000  50.587  1.00 30.50           C
ATOM   3125  O   LYS A 720      31.617  26.024  49.841  1.00 30.39           O
ATOM   3126  CB  LYS A 720      34.997  25.294  50.241  1.00 30.80           C
ATOM   3127  CG  LYS A 720      36.109  24.270  50.450  1.00 31.45           C
ATOM   3128  CD  LYS A 720      37.471  24.856  50.041  1.00 31.58           C
ATOM   3129  CE  LYS A 720      38.634  24.181  50.774  1.00 32.90           C
ATOM   3130  NZ  LYS A 720      38.837  22.749  50.378  1.00 32.69           N
ATOM   3131  N   ARG A 721      32.889  26.988  51.433  1.00 30.16           N
ATOM   3132  CA  ARG A 721      31.994  28.124  51.619  1.00 29.69           C
ATOM   3133  C   ARG A 721      32.145  29.124  50.479  1.00 29.72           C
ATOM   3134  O   ARG A 721      32.746  30.197  50.628  1.00 29.73           O
ATOM   3135  CB  ARG A 721      32.199  28.761  52.997  1.00 29.60           C
ATOM   3136  CG  ARG A 721      31.831  27.821  54.138  1.00 28.98           C
ATOM   3137  CD  ARG A 721      32.058  28.449  55.498  1.00 28.72           C
ATOM   3138  NE  ARG A 721      31.618  27.565  56.577  1.00 27.93           N
ATOM   3139  CZ  ARG A 721      31.409  27.947  57.833  1.00 27.15           C
ATOM   3140  NH1 ARG A 721      31.599  29.209  58.194  1.00 27.91           N
ATOM   3141  NH2 ARG A 721      31.008  27.062  58.733  1.00 26.44           N
ATOM   3142  N   GLU A 722      31.575  28.747  49.336  1.00 29.54           N
ATOM   3143  CA  GLU A 722      31.720  29.491  48.096  1.00 29.56           C
ATOM   3144  C   GLU A 722      30.567  29.198  47.136  1.00 29.27           C
ATOM   3145  O   GLU A 722      29.791  28.259  47.351  1.00 28.91           O
ATOM   3146  CB  GLU A 722      33.069  29.163  47.437  1.00 29.33           C
ATOM   3147  CG  GLU A 722      33.116  27.813  46.726  1.00 29.98           C
ATOM   3148  CD  GLU A 722      34.514  27.418  46.285  1.00 30.27           C
ATOM   3149  OE1 GLU A 722      35.348  28.313  46.029  1.00 31.99           O
ATOM   3150  OE2 GLU A 722      34.780  26.203  46.188  1.00 30.74           O
ATOM   3151  N   ASN A 723      30.485  30.006  46.077  1.00 29.23           N
ATOM   3152  CA  ASN A 723      29.463  29.899  45.022  1.00 29.42           C
ATOM   3153  C   ASN A 723      28.032  30.004  45.547  1.00 29.03           C
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ATOM   3154  O   ASN A 723      27.261  29.054  45.463  1.00 28.86           O
ATOM   3155  CB  ASN A 723      29.657  28.641  44.149  1.00 29.69           C
ATOM   3156  CG  ASN A 723      29.013  28.778  42.763  1.00 31.10           C
ATOM   3157  OD1 ASN A 723      29.215  29.775  42.064  1.00 32.89           O
ATOM   3158  ND2 ASN A 723      28.244  27.769  42.361  1.00 32.07           N
ATOM   3159  N   GLY A 724      27.695  31.175  46.081  1.00 28.87           N
ATOM   3160  CA  GLY A 724      26.376  31.439  46.642  1.00 28.51           C
ATOM   3161  C   GLY A 724      25.241  31.069  45.717  1.00 28.41           C
ATOM   3162  O   GLY A 724      25.237  31.444  44.548  1.00 28.25           O
ATOM   3163  N   MET A 725      24.280  30.324  46.254  1.00 28.44           N
ATOM   3164  CA  MET A 725      23.150  29.829  45.478  1.00 28.50           C
ATOM   3165  C   MET A 725      21.829  30.275  46.080  1.00 28.23           C
ATOM   3166  O   MET A 725      21.680  30.347  47.301  1.00 28.16           O
ATOM   3167  CB  MET A 725      23.171  28.299  45.410  1.00 28.52           C
ATOM   3168  CG  MET A 725      24.381  27.707  44.723  1.00 29.50           C
ATOM   3169  SD  MET A 725      24.497  28.173  42.991  1.00 31.56           S
ATOM   3170  CE  MET A 725      23.597  26.826  42.225  1.00 32.01           C
ATOM   3171  N   VAL A 726      20.876  30.581  45.209  1.00 27.97           N
ATOM   3172  CA  VAL A 726      19.499  30.767  45.624  1.00 27.67           C
ATOM   3173  C   VAL A 726      18.697  29.662  44.965  1.00 27.70           C
ATOM   3174  O   VAL A 726      18.625  29.594  43.738  1.00 28.03           O
ATOM   3175  CB  VAL A 726      18.953  32.146  45.228  1.00 27.71           C
ATOM   3176  CG1 VAL A 726      17.551  32.317  45.746  1.00 27.74           C
ATOM   3177  CG2 VAL A 726      19.838  33.257  45.793  1.00 27.29           C
ATOM   3178  N   HIS A 727      18.126  28.785  45.788  1.00 27.40           N
ATOM   3179  CA  HIS A 727      17.356  27.640  45.317  1.00 27.30           C
ATOM   3180  C   HIS A 727      15.849  27.899  45.416  1.00 27.52           C
ATOM   3181  O   HIS A 727      15.376  28.462  46.409  1.00 27.44           O
ATOM   3182  CB  HIS A 727      17.707  26.392  46.127  1.00 27.23           C
ATOM   3183  CG  HIS A 727      19.172  26.210  46.370  1.00 26.74           C
ATOM   3184  ND1 HIS A 727      19.992  25.523  45.501  1.00 26.22           N
ATOM   3185  CD2 HIS A 727      19.962  26.613  47.394  1.00 25.82           C
ATOM   3186  CE1 HIS A 727      21.223  25.513  45.977  1.00 26.18           C
ATOM   3187  NE2 HIS A 727      21.232  26.167  47.124  1.00 26.34           N
ATOM   3188  N   LEU A 728      15.103  27.471  44.394  1.00 27.48           N
ATOM   3189  CA  LEU A 728      13.656  27.672  44.345  1.00 27.77           C
ATOM   3190  C   LEU A 728      12.913  26.341  44.351  1.00 28.04           C
ATOM   3191  O   LEU A 728      13.161  25.488  43.507  1.00 27.99           O
ATOM   3192  CB  LEU A 728      13.272  28.496  43.105  1.00 27.85           C
ATOM   3193  CG  LEU A 728      11.793  28.690  42.727  1.00 27.49           C
ATOM   3194  CD1 LEU A 728      11.033  29.499  43.761  1.00 25.66           C
ATOM   3195  CD2 LEU A 728      11.681  29.350  41.358  1.00 27.66           C
ATOM   3196  N   ALA A 729      12.009  26.168  45.310  1.00 28.51           N
ATOM   3197  CA  ALA A 729      11.194  24.953  45.387  1.00 29.38           C
ATOM   3198  C   ALA A 729       9.705  25.259  45.332  1.00 29.81           C
ATOM   3199  O   ALA A 729       9.241  26.206  45.962  1.00 29.89           O
ATOM   3200  CB  ALA A 729      11.509  24.169  46.648  1.00 29.16           C
ATOM   3201  N   ARG A 730       8.960  24.456  44.579  1.00 30.58           N
ATOM   3202  CA  ARG A 730       7.502  24.524  44.611  1.00 31.66           C
ATOM   3203  C   ARG A 730       7.016  23.727  45.806  1.00 32.02           C
ATOM   3204  O   ARG A 730       7.512  22.624  46.067  1.00 32.00           O
ATOM   3205  CB  ARG A 730       6.893  23.966  43.318  1.00 31.51           C
ATOM   3206  CG  ARG A 730       5.363  23.818  43.342  1.00 32.21           C
ATOM   3207  CD  ARG A 730       4.786  23.385  41.986  1.00 32.63           C
ATOM   3208  NE  ARG A 730       5.296  22.085  41.539  1.00 33.64           N
ATOM   3209  CZ  ARG A 730       6.117  21.912  40.506  1.00 33.62           C
ATOM   3210  NH1 ARG A 730       6.522  22.952  39.790  1.00 33.72           N
ATOM   3211  NH2 ARG A 730       6.532  20.693  40.186  1.00 33.88           N
ATOM   3212  N   VAL A 731       6.065  24.292  46.542  1.00 32.68           N
ATOM   3213  CA  VAL A 731       5.385  23.541  47.586  1.00 33.65           C
ATOM   3214  C   VAL A 731       4.257  22.735  46.947  1.00 34.53           C
ATOM   3215  O   VAL A 731       3.318  23.301  46.383  1.00 34.33           O
ATOM   3216  CB  VAL A 731       4.824  24.449  48.689  1.00 33.49           C
ATOM   3217  CG1 VAL A 731       4.184  23.611  49.790  1.00 33.14           C
ATOM   3218  CG2 VAL A 731       5.924  25.334  49.255  1.00 33.41           C
ATOM   3219  N   GLU A 732       4.369  21.414  47.046  1.00 35.74           N
ATOM   3220  CA  GLU A 732       3.415  20.500  46.433  1.00 37.09           C
ATOM   3221  C   GLU A 732       2.117  20.330  47.217  1.00 38.22           C
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ATOM   3222  O   GLU A 732       1.159  21.085  47.032  1.00 38.53           O
ATOM   3223  CB  GLU A 732       4.048  19.115  46.193  1.00 36.90           C
ATOM   3224  CG  GLU A 732       5.187  19.072  45.181  1.00 36.31           C
ATOM   3225  CD  GLU A 732       4.789  19.550  43.791  1.00 35.68           C
ATOM   3226  OE1 GLU A 732       3.578  19.609  43.483  1.00 34.90           O
ATOM   3227  OE2 GLU A 732       5.703  19.865  43.004  1.00 35.40           O
ATOM   3228  N   GLU A 733       2.100  19.330  48.093  1.00 39.63           N
ATOM   3229  CA  GLU A 733       0.854  18.702  48.512  1.00 40.84           C
ATOM   3230  C   GLU A 733       0.825  18.350  49.994  1.00 41.32           C
ATOM   3231  O   GLU A 733      -0.004  18.881  50.734  1.00 41.78           O
ATOM   3232  CB  GLU A 733       0.604  17.447  47.657  1.00 41.08           C
ATOM   3233  CG  GLU A 733       1.665  16.355  47.838  1.00 42.03           C
ATOM   3234  CD  GLU A 733       1.976  15.606  46.564  1.00 43.87           C
ATOM   3235  OE1 GLU A 733       1.126  14.806  46.116  1.00 45.07           O
ATOM   3236  OE2 GLU A 733       3.083  15.802  46.017  1.00 44.28           O
ATOM   3237  N   ASN A 734       1.734  17.473  50.426  1.00 41.94           N
ATOM   3238  CA  ASN A 734       1.642  16.859  51.763  1.00 42.57           C
ATOM   3239  C   ASN A 734       2.939  16.672  52.584  1.00 42.56           C
ATOM   3240  O   ASN A 734       3.195  15.570  53.085  1.00 42.70           O
ATOM   3241  CB  ASN A 734       0.906  15.509  51.670  1.00 42.74           C
ATOM   3242  CG  ASN A 734      -0.504  15.564  52.237  1.00 43.60           C
ATOM   3243  OD1 ASN A 734      -0.730  16.072  53.341  1.00 44.32           O
ATOM   3244  ND2 ASN A 734      -1.460  15.016  51.489  1.00 43.91           N
ATOM   3245  N   GLY A 735       3.761  17.711  52.736  1.00 42.53           N
ATOM   3246  CA  GLY A 735       3.669  18.979  52.012  1.00 42.26           C
ATOM   3247  C   GLY A 735       5.000  19.056  51.303  1.00 42.05           C
ATOM   3248  O   GLY A 735       5.971  19.608  51.830  1.00 42.01           O
ATOM   3249  N   GLU A 736       5.049  18.465  50.116  1.00 41.76           N
ATOM   3250  CA  GLU A 736       6.324  18.130  49.490  1.00 41.38           C
ATOM   3251  C   GLU A 736       6.964  19.291  48.733  1.00 40.68           C
ATOM   3252  O   GLU A 736       6.293  20.260  48.356  1.00 40.59           O
ATOM   3253  CB  GLU A 736       6.172  16.886  48.610  1.00 41.61           C
ATOM   3254  CG  GLU A 736       5.622  15.691  49.387  1.00 42.97           C
ATOM   3255  CD  GLU A 736       5.690  14.386  48.621  1.00 44.95           C
ATOM   3256  OE1 GLU A 736       6.402  14.321  47.592  1.00 45.28           O
ATOM   3257  OE2 GLU A 736       5.024  13.416  49.059  1.00 46.05           O
ATOM   3258  N   LEU A 737       8.275  19.183  48.533  1.00 39.73           N
ATOM   3259  CA  LEU A 737       9.046  20.227  47.882  1.00 38.85           C
ATOM   3260  C   LEU A 737       9.680  19.709  46.599  1.00 38.35           C
ATOM   3261  O   LEU A 737      10.304  18.647  46.589  1.00 38.38           O
ATOM   3262  CB  LEU A 737      10.119  20.766  48.832  1.00 38.82           C
ATOM   3263  CG  LEU A 737       9.661  21.231  50.220  1.00 38.66           C
ATOM   3264  CD1 LEU A 737      10.852  21.421  51.135  1.00 38.55           C
ATOM   3265  CD2 LEU A 737       8.829  22.510  50.138  1.00 38.52           C
ATOM   3266  N   THR A 738       9.504  20.460  45.518  1.00 37.55           N
ATOM   3267  CA  THR A 738      10.124  20.129  44.246  1.00 36.79           C
ATOM   3268  C   THR A 738      11.096  21.234  43.876  1.00 36.40           C
ATOM   3269  O   THR A 738      10.691  22.360  43.583  1.00 36.39           O
ATOM   3270  CB  THR A 738       9.078  19.937  43.131  1.00 36.71           C
ATOM   3271  OG1 THR A 738       8.106  18.974  43.552  1.00 36.46           O
ATOM   3272  CG2 THR A 738       9.734  19.446  41.852  1.00 36.74           C
ATOM   3273  N   TRP A 739      12.380  20.898  43.893  1.00 35.93           N
ATOM   3274  CA  TRP A 739      13.438  21.852  43.585  1.00 35.44           C
ATOM   3275  C   TRP A 739      13.505  22.125  42.098  1.00 35.52           C
ATOM   3276  O   TRP A 739      13.827  21.239  41.310  1.00 35.58           O
ATOM   3277  CB  TRP A 739      14.779  21.371  44.147  1.00 35.01           C
ATOM   3278  CG  TRP A 739      14.752  21.381  45.630  1.00 34.52           C
ATOM   3279  CD1 TRP A 739      14.635  20.304  46.453  1.00 34.23           C
ATOM   3280  CD2 TRP A 739      14.773  22.537  46.477  1.00 34.30           C
ATOM   3281  NE1 TRP A 739      14.608  20.713  47.764  1.00 34.23           N
ATOM   3282  CE2 TRP A 739      14.690  22.079  47.806  1.00 34.00           C
ATOM   3283  CE3 TRP A 739      14.871  23.916  46.241  1.00 34.29           C
ATOM   3284  CZ2 TRP A 739      14.703  22.948  48.897  1.00 34.13           C
ATOM   3285  CZ3 TRP A 739      14.876  24.779  47.326  1.00 34.36           C
ATOM   3286  CH2 TRP A 739      14.797  24.291  48.639  1.00 34.36           C
ATOM   3287  N   LEU A 740      13.194  23.367  41.733  1.00 35.72           N
ATOM   3288  CA  LEU A 740      12.974  23.742  40.340  1.00 35.84           C
ATOM   3289  C   LEU A 740      14.180  24.390  39.683  1.00 36.05           C
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ATOM   3290  O   LEU A 740      14.465  24.130  38.510  1.00 35.95           O
ATOM   3291  CB  LEU A 740      11.747  24.648  40.217  1.00 35.90           C
ATOM   3292  CG  LEU A 740      10.375  24.007  40.461  1.00 36.16           C
ATOM   3293  CD1 LEU A 740       9.303  25.082  40.577  1.00 36.47           C
ATOM   3294  CD2 LEU A 740      10.013  22.989  39.368  1.00 36.32           C
ATOM   3295  N   LYS A 741      14.878  25.247  40.424  1.00 36.22           N
ATOM   3296  CA  LYS A 741      16.068  25.890  39.882  1.00 36.32           C
ATOM   3297  C   LYS A 741      17.078  26.300  40.945  1.00 35.92           C
ATOM   3298  O   LYS A 741      16.724  26.541  42.105  1.00 35.96           O
ATOM   3299  CB  LYS A 741      15.697  27.073  38.981  1.00 36.61           C
ATOM   3300  CG  LYS A 741      16.420  27.018  37.644  1.00 38.19           C
ATOM   3301  CD  LYS A 741      16.146  28.235  36.800  1.00 41.04           C
ATOM   3302  CE  LYS A 741      17.165  28.347  35.679  1.00 42.69           C
ATOM   3303  NZ  LYS A 741      17.545  29.779  35.497  1.00 44.09           N
ATOM   3304  N   HIS A 742      18.340  26.369  40.524  1.00 35.48           N
ATOM   3305  CA  HIS A 742      19.465  26.629  41.411  1.00 34.81           C
ATOM   3306  C   HIS A 742      20.356  27.676  40.759  1.00 34.51           C
ATOM   3307  O   HIS A 742      21.215  27.346  39.941  1.00 34.81           O
ATOM   3308  CB  HIS A 742      20.243  25.332  41.672  1.00 34.72           C
ATOM   3309  CG  HIS A 742      19.367  24.152  41.963  1.00 34.17           C
ATOM   3310  ND1 HIS A 742      18.881  23.878  43.224  1.00 34.17           N
ATOM   3311  CD2 HIS A 742      18.876  23.184  41.153  1.00 33.89           C
ATOM   3312  CE1 HIS A 742      18.135  22.788  43.181  1.00 33.97           C
ATOM   3313  NE2 HIS A 742      18.112  22.348  41.935  1.00 34.13           N
ATOM   3314  N   ASN A 743      20.144  28.939  41.124  1.00 33.99           N
ATOM   3315  CA  ASN A 743      20.777  30.067  40.441  1.00 33.52           C
ATOM   3316  C   ASN A 743      21.896  30.722  41.245  1.00 32.97           C
ATOM   3317  O   ASN A 743      21.674  31.112  42.394  1.00 33.20           O
ATOM   3318  CB  ASN A 743      19.724  31.117  40.075  1.00 33.64           C
ATOM   3319  CG  ASN A 743      18.794  30.655  38.968  1.00 34.30           C
ATOM   3320  OD1 ASN A 743      19.239  30.182  37.916  1.00 34.90           O
ATOM   3321  ND2 ASN A 743      17.491  30.800  39.194  1.00 34.91           N
ATOM   3322  N   PRO A 744      23.098  30.860  40.640  1.00 32.26           N
ATOM   3323  CA  PRO A 744      24.236  31.475  41.326  1.00 31.63           C
ATOM   3324  C   PRO A 744      23.997  32.959  41.570  1.00 31.15           C
ATOM   3325  O   PRO A 744      23.542  33.667  40.676  1.00 31.05           O
ATOM   3326  CB  PRO A 744      25.405  31.278  40.342  1.00 31.83           C
ATOM   3327  CG  PRO A 744      24.931  30.274  39.337  1.00 31.74           C
ATOM   3328  CD  PRO A 744      23.448  30.451  39.266  1.00 32.17           C
ATOM   3329  N   ILE A 745      24.294  33.417  42.782  1.00 30.81           N
ATOM   3330  CA  ILE A 745      24.078  34.811  43.151  1.00 30.35           C
ATOM   3331  C   ILE A 745      25.383  35.532  43.509  1.00 30.17           C
ATOM   3332  O   ILE A 745      25.473  36.757  43.402  1.00 29.97           O
ATOM   3333  CB  ILE A 745      23.007  34.950  44.277  1.00 30.41           C
ATOM   3334  CG1 ILE A 745      22.519  36.396  44.381  1.00 29.88           C
ATOM   3335  CG2 ILE A 745      23.524  34.414  45.624  1.00 30.54           C
ATOM   3336  CD1 ILE A 745      21.113  36.523  44.841  1.00 29.70           C
ATOM   3337  N   GLN A 746      26.387  34.763  43.926  1.00 29.93           N
ATOM   3338  CA  GLN A 746      27.687  35.319  44.273  1.00 29.60           C
ATOM   3339  C   GLN A 746      28.801  34.293  44.111  1.00 29.73           C
ATOM   3340  O   GLN A 746      28.825  33.265  44.799  1.00 29.82           O
ATOM   3341  CB  GLN A 746      27.674  35.882  45.699  1.00 29.39           C
ATOM   3342  CG  GLN A 746      28.993  36.493  46.142  1.00 29.02           C
ATOM   3343  CD  GLN A 746      29.435  37.643  45.252  1.00 28.60           C
ATOM   3344  OE1 GLN A 746      28.836  38.721  45.267  1.00 28.66           O
ATOM   3345  NE2 GLN A 746      30.486  37.419  44.473  1.00 26.94           N
ATOM   3346  N   LYS A 747      29.715  34.584  43.191  1.00 29.76           N
ATOM   3347  CA  LYS A 747      30.919  33.791  42.999  1.00 29.99           C
ATOM   3348  C   LYS A 747      31.947  34.170  44.059  1.00 29.68           C
ATOM   3349  O   LYS A 747      31.830  35.218  44.691  1.00 29.60           O
ATOM   3350  CB  LYS A 747      31.495  34.035  41.604  1.00 30.35           C
ATOM   3351  CG  LYS A 747      30.527  33.715  40.475  1.00 31.96           C
ATOM   3352  CD  LYS A 747      31.024  34.293  39.156  1.00 34.52           C
ATOM   3353  CE  LYS A 747      29.860  34.748  38.273  1.00 35.36           C
ATOM   3354  NZ  LYS A 747      30.345  35.313  36.979  1.00 35.56           N
ATOM   3355  N   GLY A 748      32.956  33.320  44.241  1.00 29.43           N
ATOM   3356  CA  GLY A 748      33.984  33.542  45.259  1.00 28.77           C
ATOM   3357  C   GLY A 748      33.491  33.084  46.618  1.00 28.41           C
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ATOM   3358  O   GLY A 748      32.558  32.286  46.699  1.00 28.29           O
ATOM   3359  N   GLU A 749      34.113  33.590  47.681  1.00 28.06           N
ATOM   3360  CA  GLU A 749      33.739  33.233  49.051  1.00 28.06           C
ATOM   3361  C   GLU A 749      32.268  33.541  49.355  1.00 27.51           C
ATOM   3362  O   GLU A 749      31.776  34.618  49.028  1.00 27.33           O
ATOM   3363  CB  GLU A 749      34.646  33.955  50.055  1.00 28.41           C
ATOM   3364  CG  GLU A 749      36.027  33.322  50.235  1.00 30.01           C
ATOM   3365  CD  GLU A 749      35.970  31.954  50.899  1.00 32.99           C
ATOM   3366  OE1 GLU A 749      35.064  31.726  51.743  1.00 35.42           O
ATOM   3367  OE2 GLU A 749      36.829  31.102  50.580  1.00 33.53           O
ATOM   3368  N   PHE A 750      31.569  32.587  49.967  1.00 26.86           N
ATOM   3369  CA  PHE A 750      30.167  32.787  50.336  1.00 26.31           C
ATOM   3370  C   PHE A 750      29.764  31.968  51.555  1.00 26.04           C
ATOM   3371  O   PHE A 750      29.811  30.740  51.524  1.00 26.24           O
ATOM   3372  CB  PHE A 750      29.244  32.439  49.163  1.00 26.12           C
ATOM   3373  CG  PHE A 750      27.804  32.806  49.394  1.00 25.77           C
ATOM   3374  CD1 PHE A 750      27.311  34.034  48.960  1.00 24.39           C
ATOM   3375  CD2 PHE A 750      26.939  31.926  50.049  1.00 25.14           C
ATOM   3376  CE1 PHE A 750      25.980  34.371  49.163  1.00 24.41           C
ATOM   3377  CE2 PHE A 750      25.606  32.260  50.257  1.00 24.53           C
ATOM   3378  CZ  PHE A 750      25.125  33.484  49.814  1.00 24.30           C
ATOM   3379  N   ALA A 751      29.342  32.645  52.616  1.00 25.60           N
ATOM   3380  CA  ALA A 751      28.938  31.948  53.835  1.00 25.29           C
ATOM   3381  C   ALA A 751      27.509  32.316  54.269  1.00 24.92           C
ATOM   3382  O   ALA A 751      26.566  32.089  53.515  1.00 25.03           O
ATOM   3383  CB  ALA A 751      29.963  32.173  54.951  1.00 25.27           C
ATOM   3384  N   TYR A 752      27.351  32.896  55.456  1.00 24.51           N
ATOM   3385  CA  TYR A 752      26.027  33.181  56.013  1.00 24.29           C
ATOM   3386  C   TYR A 752      25.229  34.163  55.170  1.00 24.28           C
ATOM   3387  O   TYR A 752      25.799  34.934  54.397  1.00 24.50           O
ATOM   3388  CB  TYR A 752      26.143  33.702  57.445  1.00 24.20           C
ATOM   3389  CG  TYR A 752      26.530  32.663  58.476  1.00 23.96           C
ATOM   3390  CD1 TYR A 752      26.060  32.753  59.783  1.00 23.48           C
ATOM   3391  CD2 TYR A 752      27.365  31.588  58.146  1.00 23.60           C
ATOM   3392  CE1 TYR A 752      26.414  31.811  60.738  1.00 24.01           C
ATOM   3393  CE2 TYR A 752      27.725  30.640  59.092  1.00 23.59           C
ATOM   3394  CZ  TYR A 752      27.245  30.757  60.385  1.00 24.10           C
ATOM   3395  OH  TYR A 752      27.591  29.817  61.325  1.00 24.41           O
ATOM   3396  N   ASN A 753      23.908  34.131  55.329  1.00 24.12           N
ATOM   3397  CA  ASN A 753      23.001  34.935  54.509  1.00 23.99           C
ATOM   3398  C   ASN A 753      21.586  34.980  55.073  1.00 23.83           C
ATOM   3399  O   ASN A 753      21.189  34.101  55.844  1.00 23.40           O
ATOM   3400  CB  ASN A 753      22.963  34.406  53.068  1.00 23.96           C
ATOM   3401  CG  ASN A 753      22.316  33.044  52.968  1.00 23.99           C
ATOM   3402  OD1 ASN A 753      21.088  32.928  52.934  1.00 23.59           O
ATOM   3403  ND2 ASN A 753      23.141  31.997  52.920  1.00 23.78           N
ATOM   3404  N   SER A 754      20.830  36.000  54.663  1.00 23.78           N
ATOM   3405  CA  SER A 754      19.449  36.182  55.110  1.00 23.84           C
ATOM   3406  C   SER A 754      18.556  36.746  54.001  1.00 23.94           C
ATOM   3407  O   SER A 754      18.852  37.794  53.415  1.00 23.85           O
ATOM   3408  CB  SER A 754      19.395  37.074  56.351  1.00 23.70           C
ATOM   3409  OG  SER A 754      18.113  37.042  56.951  1.00 23.74           O
ATOM   3410  N   LEU A 755      17.468  36.033  53.722  1.00 24.16           N
ATOM   3411  CA  LEU A 755      16.509  36.426  52.692  1.00 24.50           C
ATOM   3412  C   LEU A 755      15.300  37.159  53.264  1.00 24.79           C
ATOM   3413  O   LEU A 755      14.854  36.875  54.376  1.00 24.62           O
ATOM   3414  CB  LEU A 755      16.011  35.194  51.938  1.00 24.33           C
ATOM   3415  CG  LEU A 755      16.972  34.364  51.094  1.00 24.06           C
ATOM   3416  CD1 LEU A 755      16.331  33.016  50.817  1.00 23.29           C
ATOM   3417  CD2 LEU A 755      17.339  35.076  49.794  1.00 22.82           C
ATOM   3418  N   GLN A 756      14.773  38.098  52.485  1.00 25.28           N
ATOM   3419  CA  GLN A 756      13.483  38.711  52.779  1.00 25.79           C
ATOM   3420  C   GLN A 756      12.692  38.940  51.507  1.00 26.50           C
ATOM   3421  O   GLN A 756      13.257  39.130  50.424  1.00 26.40           O
ATOM   3422  CB  GLN A 756      13.635  40.037  53.533  1.00 25.58           C
ATOM   3423  CG  GLN A 756      13.944  39.899  55.019  1.00 24.84           C
ATOM   3424  CD  GLN A 756      12.816  39.270  55.819  1.00 23.88           C
ATOM   3425  OE1 GLN A 756      11.903  39.963  56.268  1.00 23.82           O
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ATOM   3426  NE2 GLN A 756      12.890  37.954  56.023  1.00 21.62           N
ATOM   3427  N   GLU A 757      11.374  38.895  51.660  1.00 27.24           N
ATOM   3428  CA  GLU A 757      10.438  39.295  50.631  1.00 28.11           C
ATOM   3429  C   GLU A 757      10.424  40.817  50.655  1.00 28.21           C
ATOM   3430  O   GLU A 757      10.441  41.419  51.729  1.00 28.26           O
ATOM   3431  CB  GLU A 757       9.060  38.755  50.991  1.00 28.00           C
ATOM   3432  CG  GLU A 757       8.121  38.508  49.826  1.00 29.19           C
ATOM   3433  CD  GLU A 757       6.898  37.698  50.242  1.00 29.26           C
ATOM   3434  OE1 GLU A 757       6.560  37.703  51.447  1.00 31.25           O
ATOM   3435  OE2 GLU A 757       6.271  37.058  49.370  1.00 31.40           O
ATOM   3436  N   LEU A 758      10.408  41.441  49.482  1.00 28.62           N
ATOM   3437  CA  LEU A 758      10.467  42.899  49.404  1.00 28.96           C
ATOM   3438  C   LEU A 758       9.153  43.552  48.991  1.00 29.28           C
ATOM   3439  O   LEU A 758       8.974  44.757  49.165  1.00 29.40           O
ATOM   3440  CB  LEU A 758      11.602  43.344  48.477  1.00 28.80           C
ATOM   3441  CG  LEU A 758      12.901  43.843  49.120  1.00 29.29           C
ATOM   3442  CD1 LEU A 758      13.366  42.977  50.293  1.00 28.64           C
ATOM   3443  CD2 LEU A 758      13.988  43.953  48.064  1.00 28.93           C
ATOM   3444  N   GLY A 759       8.232  42.751  48.468  1.00 29.68           N
ATOM   3445  CA  GLY A 759       7.006  43.272  47.890  1.00 30.12           C
ATOM   3446  C   GLY A 759       7.180  43.406  46.392  1.00 30.55           C
ATOM   3447  O   GLY A 759       8.305  43.507  45.895  1.00 30.45           O
ATOM   3448  N   ASN A 760       6.062  43.371  45.672  1.00 30.78           N
ATOM   3449  CA  ASN A 760       6.054  43.572  44.224  1.00 30.87           C
ATOM   3450  C   ASN A 760       6.916  42.592  43.426  1.00 30.84           C
ATOM   3451  O   ASN A 760       7.468  42.956  42.387  1.00 31.30           O
ATOM   3452  CB  ASN A 760       6.444  45.016  43.889  1.00 30.82           C
ATOM   3453  CG  ASN A 760       5.573  46.037  44.595  1.00 31.00           C
ATOM   3454  OD1 ASN A 760       4.348  45.901  44.650  1.00 30.22           O
ATOM   3455  ND2 ASN A 760       6.203  47.078  45.131  1.00 31.07           N
ATOM   3456  N   GLY A 761       7.017  41.354  43.903  1.00 30.83           N
ATOM   3457  CA  GLY A 761       7.779  40.307  43.211  1.00 30.33           C
ATOM   3458  C   GLY A 761       9.293  40.464  43.279  1.00 30.11           C
ATOM   3459  O   GLY A 761      10.017  39.864  42.481  1.00 30.25           O
ATOM   3460  N   GLU A 762       9.765  41.273  44.227  1.00 29.67           N
ATOM   3461  CA  GLU A 762      11.194  41.473  44.464  1.00 29.39           C
ATOM   3462  C   GLU A 762      11.620  40.872  45.796  1.00 28.69           C
ATOM   3463  O   GLU A 762      10.803  40.697  46.701  1.00 28.61           O
ATOM   3464  CB  GLU A 762      11.564  42.962  44.425  1.00 29.53           C
ATOM   3465  CG  GLU A 762      11.362  43.622  43.061  1.00 29.98           C
ATOM   3466  CD  GLU A 762      12.089  44.953  42.913  1.00 30.13           C
ATOM   3467  OE1 GLU A 762      12.521  45.544  43.928  1.00 30.44           O
ATOM   3468  OE2 GLU A 762      12.223  45.417  41.759  1.00 31.91           O
ATOM   3469  N   TYR A 763      12.909  40.557  45.901  1.00 28.18           N
ATOM   3470  CA  TYR A 763      13.475  39.930  47.088  1.00 27.55           C
ATOM   3471  C   TYR A 763      14.837  40.519  47.420  1.00 27.34           C
ATOM   3472  O   TYR A 763      15.532  41.029  46.540  1.00 27.23           O
ATOM   3473  CB  TYR A 763      13.603  38.421  46.885  1.00 27.43           C
ATOM   3474  CG  TYR A 763      12.309  37.738  46.505  1.00 27.27           C
ATOM   3475  CD1 TYR A 763      11.959  37.565  45.165  1.00 27.29           C
ATOM   3476  CD2 TYR A 763      11.431  37.269  47.483  1.00 27.11           C
ATOM   3477  CE1 TYR A 763      10.769  36.944  44.810  1.00 27.59           C
ATOM   3478  CE2 TYR A 763      10.242  36.647  47.139  1.00 26.62           C
ATOM   3479  CZ  TYR A 763       9.918  36.483  45.802  1.00 27.17           C
ATOM   3480  OH  TYR A 763       8.745  35.861  45.446  1.00 26.84           O
ATOM   3481  N   GLY A 764      15.211  40.439  48.696  1.00 27.17           N
ATOM   3482  CA  GLY A 764      16.488  40.969  49.174  1.00 26.79           C
ATOM   3483  C   GLY A 764      17.342  39.934  49.884  1.00 26.64           C
ATOM   3484  O   GLY A 764      16.833  38.940  50.413  1.00 26.42           O
ATOM   3485  N   ILE A 765      18.649  40.167  49.895  1.00 26.56           N
ATOM   3486  CA  ILE A 765      19.569  39.246  50.551  1.00 26.59           C
ATOM   3487  C   ILE A 765      20.795  39.936  51.140  1.00 26.78           C
ATOM   3488  O   ILE A 765      21.483  40.694  50.462  1.00 26.90           O
ATOM   3489  CB  ILE A 765      19.979  38.063  49.623  1.00 26.34           C
ATOM   3490  CG1 ILE A 765      20.648  36.949  50.443  1.00 26.04           C
ATOM   3491  CG2 ILE A 765      20.835  38.550  48.443  1.00 26.28           C
ATOM   3492  CD1 ILE A 765      21.025  35.708  49.648  1.00 26.28           C
ATOM   3493  N   LEU A 766      21.032  39.679  52.422  1.00 27.11           N
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ATOM   3494  CA  LEU A 766      22.256  40.092  53.094  1.00 27.30           C
ATOM   3495  C   LEU A 766      23.124  38.850  53.275  1.00 27.85           C
ATOM   3496  O   LEU A 766      22.690  37.870  53.889  1.00 27.85           O
ATOM   3497  CB  LEU A 766      21.928  40.739  54.441  1.00 27.07           C
ATOM   3498  CG  LEU A 766      23.044  41.393  55.261  1.00 26.94           C
ATOM   3499  CD1 LEU A 766      23.665  42.592  54.553  1.00 25.88           C
ATOM   3500  CD2 LEU A 766      22.499  41.799  56.618  1.00 26.80           C
ATOM   3501  N   TYR A 767      24.335  38.880  52.722  1.00 28.47           N
ATOM   3502  CA  TYR A 767      25.208  37.706  52.750  1.00 28.99           C
ATOM   3503  C   TYR A 767      26.667  38.001  53.086  1.00 29.39           C
ATOM   3504  O   TYR A 767      27.159  39.112  52.876  1.00 29.28           O
ATOM   3505  CB  TYR A 767      25.122  36.932  51.430  1.00 28.98           C
ATOM   3506  CG  TYR A 767      25.578  37.709  50.216  1.00 29.26           C
ATOM   3507  CD1 TYR A 767      26.928  37.780  49.875  1.00 28.30           C
ATOM   3508  CD2 TYR A 767      24.656  38.366  49.401  1.00 29.67           C
ATOM   3509  CE1 TYR A 767      27.349  38.491  48.767  1.00 28.66           C
ATOM   3510  CE2 TYR A 767      25.069  39.081  48.282  1.00 29.59           C
ATOM   3511  CZ  TYR A 767      26.418  39.135  47.972  1.00 29.43           C
ATOM   3512  OH  TYR A 767      26.836  39.839  46.868  1.00 29.26           O
ATOM   3513  N   GLU A 768      27.340  36.974  53.604  1.00 29.91           N
ATOM   3514  CA  GLU A 768      28.771  36.998  53.868  1.00 30.18           C
ATOM   3515  C   GLU A 768      29.555  36.679  52.600  1.00 30.96           C
ATOM   3516  O   GLU A 768      29.289  35.674  51.926  1.00 30.73           O
ATOM   3517  CB  GLU A 768      29.124  35.965  54.936  1.00 30.20           C
ATOM   3518  CG  GLU A 768      28.623  36.302  56.330  1.00 29.67           C
ATOM   3519  CD  GLU A 768      29.176  35.366  57.390  1.00 29.40           C
ATOM   3520  OE1 GLU A 768      29.245  34.141  57.159  1.00 27.76           O
ATOM   3521  OE2 GLU A 768      29.543  35.857  58.468  1.00 28.50           O
ATOM   3522  N   HIS A 769      30.522  37.538  52.290  1.00 31.73           N
ATOM   3523  CA  HIS A 769      31.411  37.363  51.142  1.00 32.59           C
ATOM   3524  C   HIS A 769      32.636  38.254  51.311  1.00 32.88           C
ATOM   3525  O   HIS A 769      32.556  39.317  51.937  1.00 32.98           O
ATOM   3526  CB  HIS A 769      30.667  37.686  49.838  1.00 32.74           C
ATOM   3527  CG  HIS A 769      31.554  37.856  48.642  1.00 33.80           C
ATOM   3528  ND1 HIS A 769      31.979  36.795  47.869  1.00 34.57           N
ATOM   3529  CD2 HIS A 769      32.073  38.968  48.069  1.00 34.03           C
ATOM   3530  CE1 HIS A 769      32.729  37.246  46.879  1.00 34.57           C
ATOM   3531  NE2 HIS A 769      32.801  38.561  46.978  1.00 34.49           N
ATOM   3532  N   THR A 770      33.767  37.798  50.772  1.00 33.21           N
ATOM   3533  CA  THR A 770      34.997  38.591  50.726  1.00 33.58           C
ATOM   3534  C   THR A 770      35.560  38.679  49.308  1.00 33.87           C
ATOM   3535  O   THR A 770      35.279  37.841  48.447  1.00 33.69           O
ATOM   3536  CB  THR A 770      36.110  38.032  51.653  1.00 33.45           C
ATOM   3537  OG1 THR A 770      36.483  36.721  51.220  1.00 33.58           O
ATOM   3538  CG2 THR A 770      35.650  37.981  53.096  1.00 33.54           C
ATOM   3539  N   GLU A 771      36.370  39.707  49.098  1.00 34.35           N
ATOM   3540  CA  GLU A 771      37.035  39.968  47.836  1.00 35.04           C
ATOM   3541  C   GLU A 771      38.316  40.703  48.136  1.00 34.92           C
ATOM   3542  O   GLU A 771      38.440  41.336  49.183  1.00 35.22           O
ATOM   3543  CB  GLU A 771      36.176  40.885  46.971  1.00 35.00           C
ATOM   3544  CG  GLU A 771      35.432  40.192  45.847  1.00 36.22           C
ATOM   3545  CD  GLU A 771      34.497  41.133  45.114  1.00 35.95           C
ATOM   3546  OE1 GLU A 771      34.646  42.365  45.264  1.00 37.47           O
ATOM   3547  OE2 GLU A 771      33.612  40.640  44.387  1.00 37.56           O
ATOM   3548  N   LYS A 772      39.273  40.614  47.220  1.00 34.91           N
ATOM   3549  CA  LYS A 772      40.395  41.549  47.190  1.00 34.87           C
ATOM   3550  C   LYS A 772      41.043  41.771  48.571  1.00 34.34           C
ATOM   3551  O   LYS A 772      41.366  42.901  48.947  1.00 34.65           O
ATOM   3552  CB  LYS A 772      39.919  42.873  46.574  1.00 34.83           C
ATOM   3553  CG  LYS A 772      39.081  42.678  45.303  1.00 35.36           C
ATOM   3554  CD  LYS A 772      38.708  43.990  44.634  1.00 35.58           C
ATOM   3555  CE  LYS A 772      37.933  43.744  43.337  1.00 36.38           C
ATOM   3556  NZ  LYS A 772      37.662  45.024  42.612  1.00 36.45           N
ATOM   3557  N   GLY A 773      41.210  40.684  49.321  1.00 33.71           N
ATOM   3558  CA  GLY A 773      41.888  40.715  50.616  1.00 33.19           C
ATOM   3559  C   GLY A 773      41.059  41.200  51.792  1.00 33.01           C
ATOM   3560  O   GLY A 773      41.613  41.633  52.804  1.00 33.00           O
ATOM   3561  N   GLN A 774      39.734  41.126  51.673  1.00 32.68           N
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ATOM   3562  CA  GLN A 774      38.853  41.502  52.779  1.00 32.45           C
ATOM   3563  C   GLN A 774      38.888  40.476  53.915  1.00 32.12           C
ATOM   3564  O   GLN A 774      38.921  39.267  53.674  1.00 32.15           O
ATOM   3565  CB  GLN A 774      37.431  41.741  52.286  1.00 32.72           C
ATOM   3566  CG  GLN A 774      37.219  43.124  51.669  1.00 32.85           C
ATOM   3567  CD  GLN A 774      35.982  43.194  50.789  1.00 33.27           C
ATOM   3568  OE1 GLN A 774      35.259  42.211  50.628  1.00 33.49           O
ATOM   3569  NE2 GLN A 774      35.740  44.359  50.208  1.00 33.85           N
ATOM   3570  N   ASN A 775      38.872  40.978  55.146  1.00 31.63           N
ATOM   3571  CA  ASN A 775      39.194  40.189  56.346  1.00 31.33           C
ATOM   3572  C   ASN A 775      38.369  38.927  56.657  1.00 31.19           C
ATOM   3573  O   ASN A 775      38.946  37.908  57.085  1.00 31.75           O
ATOM   3574  CB  ASN A 775      39.231  41.101  57.573  1.00 31.20           C
ATOM   3575  CG  ASN A 775      40.473  41.976  57.615  1.00 31.07           C
ATOM   3576  OD1 ASN A 775      41.354  41.863  56.772  1.00 31.09           O
ATOM   3577  ND2 ASN A 775      40.547  42.849  58.608  1.00 31.36           N
ATOM   3578  N   ALA A 776      37.050  39.000  56.443  1.00 30.02           N
ATOM   3579  CA  ALA A 776      36.064  37.950  56.809  1.00 29.30           C
ATOM   3580  C   ALA A 776      35.114  38.395  57.935  1.00 28.63           C
ATOM   3581  O   ALA A 776      35.508  38.467  59.095  1.00 28.65           O
ATOM   3582  CB  ALA A 776      36.732  36.618  57.163  1.00 29.10           C
ATOM   3583  N   TYR A 777      33.880  38.748  57.597  1.00 27.88           N
ATOM   3584  CA  TYR A 777      33.427  38.909  56.229  1.00 27.28           C
ATOM   3585  C   TYR A 777      33.036  40.366  55.995  1.00 27.36           C
ATOM   3586  O   TYR A 777      32.959  41.162  56.936  1.00 27.40           O
ATOM   3587  CB  TYR A 777      32.211  38.020  55.981  1.00 26.89           C
ATOM   3588  CG  TYR A 777      32.542  36.563  55.786  1.00 26.62           C
ATOM   3589  CD1 TYR A 777      32.873  36.073  54.523  1.00 26.45           C
ATOM   3590  CD2 TYR A 777      32.524  35.670  56.857  1.00 26.05           C
ATOM   3591  CE1 TYR A 777      33.181  34.736  54.329  1.00 25.38           C
ATOM   3592  CE2 TYR A 777      32.834  34.327  56.672  1.00 25.74           C
ATOM   3593  CZ  TYR A 777      33.158  33.870  55.401  1.00 25.73           C
ATOM   3594  OH  TYR A 777      33.464  32.547  55.193  1.00 26.01           O
ATOM   3595  N   THR A 778      32.800  40.713  54.736  1.00 27.29           N
ATOM   3596  CA  THR A 778      32.065  41.924  54.407  1.00 27.31           C
ATOM   3597  C   THR A 778      30.631  41.479  54.121  1.00 27.40           C
ATOM   3598  O   THR A 778      30.412  40.528  53.375  1.00 27.44           O
ATOM   3599  CB  THR A 778      32.685  42.659  53.189  1.00 27.36           C
ATOM   3600  OG1 THR A 778      33.956  43.208  53.563  1.00 27.09           O
ATOM   3601  CG2 THR A 778      31.774  43.786  52.686  1.00 26.50           C
ATOM   3602  N   LEU A 779      29.667  42.156  54.733  1.00 27.55           N
ATOM   3603  CA  LEU A 779      28.253  41.823  54.558  1.00 27.65           C
ATOM   3604  C   LEU A 779      27.594  42.705  53.502  1.00 27.69           C
ATOM   3605  O   LEU A 779      27.549  43.932  53.640  1.00 27.70           O
ATOM   3606  CB  LEU A 779      27.510  41.924  55.892  1.00 27.50           C
ATOM   3607  CG  LEU A 779      27.514  40.707  56.829  1.00 27.97           C
ATOM   3608  CD1 LEU A 779      28.915  40.214  57.185  1.00 28.23           C
ATOM   3609  CD2 LEU A 779      26.733  41.024  58.097  1.00 27.73           C
ATOM   3610  N   SER A 780      27.071  42.069  52.457  1.00 27.76           N
ATOM   3611  CA  SER A 780      26.578  42.792  51.291  1.00 27.98           C
ATOM   3612  C   SER A 780      25.134  42.475  50.909  1.00 28.05           C
ATOM   3613  O   SER A 780      24.641  41.375  51.141  1.00 27.72           O
ATOM   3614  CB  SER A 780      27.497  42.547  50.099  1.00 28.02           C
ATOM   3615  OG  SER A 780      28.835  42.862  50.436  1.00 28.14           O
ATOM   3616  N   PHE A 781      24.484  43.459  50.295  1.00 28.29           N
ATOM   3617  CA  PHE A 781      23.080  43.374  49.929  1.00 28.59           C
ATOM   3618  C   PHE A 781      22.885  43.289  48.415  1.00 28.89           C
ATOM   3619  O   PHE A 781      23.643  43.885  47.650  1.00 29.11           O
ATOM   3620  CB  PHE A 781      22.345  44.593  50.493  1.00 28.40           C
ATOM   3621  CG  PHE A 781      20.908  44.689  50.086  1.00 28.19           C
ATOM   3622  CD1 PHE A 781      19.946  43.867  50.672  1.00 28.15           C
ATOM   3623  CD2 PHE A 781      20.511  45.612  49.119  1.00 27.88           C
ATOM   3624  CE1 PHE A 781      18.602  43.955  50.297  1.00 27.87           C
ATOM   3625  CE2 PHE A 781      19.178  45.712  48.736  1.00 28.61           C
ATOM   3626  CZ  PHE A 781      18.218  44.878  49.327  1.00 28.60           C
ATOM   3627  N   ARG A 782      21.867  42.540  48.002  1.00 29.36           N
ATOM   3628  CA  ARG A 782      21.430  42.476  46.605  1.00 29.81           C
ATOM   3629  C   ARG A 782      19.920  42.280  46.526  1.00 30.17           C
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ATOM   3630  O   ARG A 782      19.341  41.551  47.334  1.00 30.01           O
ATOM   3631  CB  ARG A 782      22.095  41.311  45.875  1.00 29.58           C
ATOM   3632  CG  ARG A 782      23.501  41.557  45.386  1.00 29.78           C
ATOM   3633  CD  ARG A 782      23.935  40.365  44.565  1.00 30.21           C
ATOM   3634  NE  ARG A 782      25.372  40.294  44.345  1.00 30.12           N
ATOM   3635  CZ  ARG A 782      25.973  40.581  43.195  1.00 31.28           C
ATOM   3636  NH1 ARG A 782      25.264  40.989  42.148  1.00 31.63           N
ATOM   3637  NH2 ARG A 782      27.292  40.466  43.095  1.00 31.52           N
ATOM   3638  N   LYS A 783      19.299  42.942  45.550  1.00 30.71           N
ATOM   3639  CA  LYS A 783      17.909  42.699  45.181  1.00 31.48           C
ATOM   3640  C   LYS A 783      17.902  41.783  43.975  1.00 31.67           C
ATOM   3641  O   LYS A 783      18.860  41.772  43.196  1.00 31.82           O
ATOM   3642  CB  LYS A 783      17.203  43.996  44.767  1.00 31.69           C
ATOM   3643  CG  LYS A 783      16.767  44.921  45.881  1.00 32.91           C
ATOM   3644  CD  LYS A 783      16.670  46.357  45.350  1.00 35.08           C
ATOM   3645  CE  LYS A 783      15.713  47.208  46.176  1.00 35.63           C
ATOM   3646  NZ  LYS A 783      15.889  48.671  45.926  1.00 35.71           N
ATOM   3647  N   PHE A 784      16.814  41.035  43.813  1.00 31.77           N
ATOM   3648  CA  PHE A 784      16.551  40.305  42.574  1.00 31.93           C
ATOM   3649  C   PHE A 784      15.052  40.128  42.354  1.00 32.26           C
ATOM   3650  O   PHE A 784      14.257  40.329  43.278  1.00 32.23           O
ATOM   3651  CB  PHE A 784      17.286  38.956  42.535  1.00 31.64           C
ATOM   3652  CG  PHE A 784      17.066  38.096  43.746  1.00 31.27           C
ATOM   3653  CD1 PHE A 784      16.009  37.187  43.790  1.00 30.95           C
ATOM   3654  CD2 PHE A 784      17.927  38.178  44.837  1.00 30.62           C
ATOM   3655  CE1 PHE A 784      15.808  36.380  44.905  1.00 30.82           C
ATOM   3656  CE2 PHE A 784      17.737  37.374  45.958  1.00 30.61           C
ATOM   3657  CZ  PHE A 784      16.676  36.474  45.995  1.00 30.77           C
ATOM   3658  N   ASN A 785      14.679  39.764  41.128  1.00 32.73           N
ATOM   3659  CA  ASN A 785      13.281  39.519  40.769  1.00 33.29           C
ATOM   3660  C   ASN A 785      12.985  38.038  40.508  1.00 33.79           C
ATOM   3661  O   ASN A 785      13.860  37.184  40.674  1.00 33.86           O
ATOM   3662  CB  ASN A 785      12.870  40.378  39.567  1.00 33.13           C
ATOM   3663  CG  ASN A 785      13.790  40.196  38.366  1.00 32.99           C
ATOM   3664  OD1 ASN A 785      14.340  39.114  38.132  1.00 32.29           O
ATOM   3665  ND2 ASN A 785      13.960  41.266  37.597  1.00 32.58           N
ATOM   3666  N   TRP A 786      11.754  37.749  40.091  1.00 34.51           N
ATOM   3667  CA  TRP A 786      11.307  36.380  39.863  1.00 35.28           C
ATOM   3668  C   TRP A 786      11.993  35.725  38.663  1.00 35.83           C
ATOM   3669  O   TRP A 786      12.202  34.509  38.662  1.00 36.17           O
ATOM   3670  CB  TRP A 786       9.785  36.326  39.703  1.00 35.53           C
ATOM   3671  CG  TRP A 786       9.267  34.923  39.617  1.00 35.98           C
ATOM   3672  CD1 TRP A 786       8.942  34.236  38.480  1.00 36.17           C
ATOM   3673  CD2 TRP A 786       9.054  34.020  40.707  1.00 35.84           C
ATOM   3674  NE1 TRP A 786       8.524  32.967  38.797  1.00 36.52           N
ATOM   3675  CE2 TRP A 786       8.585  32.805  40.157  1.00 36.11           C
ATOM   3676  CE3 TRP A 786       9.207  34.121  42.096  1.00 35.63           C
ATOM   3677  CZ2 TRP A 786       8.265  31.697  40.948  1.00 35.77           C
ATOM   3678  CZ3 TRP A 786       8.885  33.019  42.884  1.00 35.89           C
ATOM   3679  CH2 TRP A 786       8.423  31.823  42.305  1.00 35.85           C
ATOM   3680  N   ASP A 787      12.329  36.529  37.652  1.00 36.19           N
ATOM   3681  CA  ASP A 787      13.050  36.055  36.463  1.00 36.61           C
ATOM   3682  C   ASP A 787      14.412  35.480  36.829  1.00 36.96           C
ATOM   3683  O   ASP A 787      14.829  34.459  36.273  1.00 37.08           O
ATOM   3684  CB  ASP A 787      13.233  37.183  35.434  1.00 36.51           C
ATOM   3685  CG  ASP A 787      11.992  37.417  34.576  1.00 36.46           C
ATOM   3686  OD1 ASP A 787      11.039  36.603  34.640  1.00 36.27           O
ATOM   3687  OD2 ASP A 787      11.977  38.421  33.830  1.00 35.51           O
ATOM   3688  N   PHE A 788      15.097  36.140  37.763  1.00 37.24           N
ATOM   3689  CA  PHE A 788      16.381  35.660  38.257  1.00 37.61           C
ATOM   3690  C   PHE A 788      16.238  34.291  38.914  1.00 37.92           C
ATOM   3691  O   PHE A 788      17.173  33.490  38.912  1.00 37.81           O
ATOM   3692  CB  PHE A 788      16.998  36.652  39.246  1.00 37.56           C
ATOM   3693  CG  PHE A 788      18.275  36.156  39.873  1.00 37.90           C
ATOM   3694  CD1 PHE A 788      19.475  36.193  39.164  1.00 37.33           C
ATOM   3695  CD2 PHE A 788      18.275  35.632  41.164  1.00 38.18           C
ATOM   3696  CE1 PHE A 788      20.652  35.723  39.729  1.00 37.41           C
ATOM   3697  CE2 PHE A 788      19.453  35.159  41.740  1.00 38.38           C
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ATOM   3698  CZ  PHE A 788      20.645  35.208  41.019  1.00 37.63           C
ATOM   3699  N   LEU A 789      15.057  34.033  39.468  1.00 38.47           N
ATOM   3700  CA  LEU A 789      14.788  32.797  40.191  1.00 38.74           C
ATOM   3701  C   LEU A 789      14.315  31.661  39.301  1.00 39.06           C
ATOM   3702  O   LEU A 789      14.682  30.507  39.523  1.00 38.92           O
ATOM   3703  CB  LEU A 789      13.744  33.051  41.272  1.00 38.77           C
ATOM   3704  CG  LEU A 789      14.252  33.631  42.587  1.00 38.85           C
ATOM   3705  CD1 LEU A 789      13.138  34.385  43.290  1.00 38.34           C
ATOM   3706  CD2 LEU A 789      14.804  32.512  43.459  1.00 38.53           C
ATOM   3707  N   SER A 790      13.504  31.992  38.298  1.00 39.53           N
ATOM   3708  CA  SER A 790      12.776  30.983  37.528  1.00 40.12           C
ATOM   3709  C   SER A 790      13.377  30.638  36.156  1.00 40.38           C
ATOM   3710  O   SER A 790      13.124  29.555  35.621  1.00 40.61           O
ATOM   3711  CB  SER A 790      11.309  31.393  37.379  1.00 40.10           C
ATOM   3712  OG  SER A 790      11.188  32.567  36.596  1.00 40.62           O
ATOM   3713  N   LYS A 791      14.161  31.555  35.593  1.00 40.67           N
ATOM   3714  CA  LYS A 791      14.769  31.350  34.276  1.00 40.92           C
ATOM   3715  C   LYS A 791      16.163  31.963  34.171  1.00 40.88           C
ATOM   3716  O   LYS A 791      17.053  31.386  33.546  1.00 40.94           O
ATOM   3717  CB  LYS A 791      13.861  31.897  33.166  1.00 41.08           C
ATOM   3718  CG  LYS A 791      13.522  33.386  33.293  1.00 41.13           C
ATOM   3719  CD  LYS A 791      12.691  33.883  32.121  1.00 41.00           C
ATOM   3720  CE  LYS A 791      11.264  33.354  32.177  1.00 41.36           C
ATOM   3721  NZ  LYS A 791      10.317  34.245  31.442  1.00 41.47           N
TER    3722      LYS A 791
ATOM   3723  N   ALA B 322      26.470  -5.993 127.959  1.00 69.14           N
ATOM   3724  CA  ALA B 322      25.819  -7.228 127.433  1.00 69.17           C
ATOM   3725  C   ALA B 322      25.536  -7.095 125.941  1.00 69.25           C
ATOM   3726  O   ALA B 322      25.639  -6.002 125.378  1.00 69.21           O
ATOM   3727  CB  ALA B 322      24.530  -7.523 128.201  1.00 69.07           C
ATOM   3728  N   LEU B 323      25.197  -8.220 125.311  1.00 69.27           N
ATOM   3729  CA  LEU B 323      24.792  -8.265 123.907  1.00 69.18           C
ATOM   3730  C   LEU B 323      23.977  -9.529 123.652  1.00 69.12           C
ATOM   3731  O   LEU B 323      24.427 -10.638 123.960  1.00 69.24           O
ATOM   3732  CB  LEU B 323      26.016  -8.213 122.980  1.00 69.26           C
ATOM   3733  CG  LEU B 323      25.855  -8.541 121.484  1.00 69.38           C
ATOM   3734  CD1 LEU B 323      24.853  -7.622 120.792  1.00 69.30           C
ATOM   3735  CD2 LEU B 323      27.202  -8.491 120.773  1.00 69.28           C
ATOM   3736  N   THR B 324      22.783  -9.355 123.091  1.00 68.91           N
ATOM   3737  CA  THR B 324      21.884 -10.479 122.819  1.00 68.76           C
ATOM   3738  C   THR B 324      22.362 -11.300 121.621  1.00 68.62           C
ATOM   3739  O   THR B 324      23.011 -10.772 120.716  1.00 68.63           O
ATOM   3740  CB  THR B 324      20.429 -10.013 122.577  1.00 68.73           C
ATOM   3741  OG1 THR B 324      20.400  -9.064 121.505  1.00 68.97           O
ATOM   3742  CG2 THR B 324      19.848  -9.374 123.832  1.00 68.60           C
ATOM   3743  N   GLU B 325      22.038 -12.592 121.631  1.00 68.42           N
ATOM   3744  CA  GLU B 325      22.423 -13.503 120.554  1.00 68.30           C
ATOM   3745  C   GLU B 325      21.633 -13.257 119.267  1.00 67.98           C
ATOM   3746  O   GLU B 325      20.596 -12.587 119.275  1.00 67.93           O
ATOM   3747  CB  GLU B 325      22.297 -14.966 121.001  1.00 68.28           C
ATOM   3748  CG  GLU B 325      23.494 -15.471 121.813  1.00 68.73           C
ATOM   3749  CD  GLU B 325      23.454 -16.974 122.089  1.00 68.74           C
ATOM   3750  OE1 GLU B 325      22.463 -17.459 122.682  1.00 69.26           O
ATOM   3751  OE2 GLU B 325      24.428 -17.669 121.726  1.00 69.19           O
ATOM   3752  N   LYS B 326      22.148 -13.809 118.170  1.00 67.58           N
ATOM   3753  CA  LYS B 326      21.582 -13.659 116.830  1.00 67.11           C
ATOM   3754  C   LYS B 326      20.105 -14.065 116.766  1.00 66.67           C
ATOM   3755  O   LYS B 326      19.738 -15.181 117.139  1.00 66.63           O
ATOM   3756  CB  LYS B 326      22.402 -14.500 115.845  1.00 67.22           C
ATOM   3757  CG  LYS B 326      22.231 -14.144 114.382  1.00 67.41           C
ATOM   3758  CD  LYS B 326      22.678 -15.300 113.498  1.00 67.80           C
ATOM   3759  CE  LYS B 326      22.830 -14.869 112.046  1.00 68.19           C
ATOM   3760  NZ  LYS B 326      22.902 -16.032 111.113  1.00 68.21           N
ATOM   3761  N   THR B 327      19.270 -13.143 116.294  1.00 66.14           N
ATOM   3762  CA  THR B 327      17.838 -13.389 116.125  1.00 65.57           C
ATOM   3763  C   THR B 327      17.415 -13.021 114.703  1.00 65.20           C
ATOM   3764  O   THR B 327      17.288 -11.841 114.367  1.00 65.17           O
ATOM   3765  CB  THR B 327      16.997 -12.590 117.150  1.00 65.60           C
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ATOM   3766  OG1 THR B 327      17.517 -12.802 118.466  1.00 65.49           O
ATOM   3767  CG2 THR B 327      15.532 -13.019 117.110  1.00 65.49           C
ATOM   3768  N   ASP B 328      17.200 -14.043 113.878  1.00 64.62           N
ATOM   3769  CA  ASP B 328      16.871 -13.860 112.466  1.00 64.01           C
ATOM   3770  C   ASP B 328      15.414 -13.443 112.265  1.00 63.82           C
ATOM   3771  O   ASP B 328      14.504 -14.048 112.838  1.00 63.73           O
ATOM   3772  CB  ASP B 328      17.165 -15.145 111.681  1.00 63.92           C
ATOM   3773  CG  ASP B 328      18.545 -15.727 111.985  1.00 63.38           C
ATOM   3774  OD1 ASP B 328      19.417 -15.003 112.514  1.00 62.54           O
ATOM   3775  OD2 ASP B 328      18.753 -16.922 111.689  1.00 62.45           O
ATOM   3776  N   ILE B 329      15.204 -12.404 111.455  1.00 63.51           N
ATOM   3777  CA  ILE B 329      13.856 -11.933 111.112  1.00 63.20           C
ATOM   3778  C   ILE B 329      13.478 -12.323 109.678  1.00 62.98           C
ATOM   3779  O   ILE B 329      12.386 -12.845 109.437  1.00 62.95           O
ATOM   3780  CB  ILE B 329      13.683 -10.393 111.322  1.00 63.19           C
ATOM   3781  CG1 ILE B 329      13.882 -10.005 112.789  1.00 63.18           C
ATOM   3782  CG2 ILE B 329      12.300  -9.924 110.878  1.00 63.09           C
ATOM   3783  CD1 ILE B 329      15.287  -9.605 113.132  1.00 62.92           C
ATOM   3784  N   PHE B 330      14.384 -12.069 108.737  1.00 62.72           N
ATOM   3785  CA  PHE B 330      14.147 -12.381 107.329  1.00 62.53           C
ATOM   3786  C   PHE B 330      15.121 -13.451 106.841  1.00 62.57           C
ATOM   3787  O   PHE B 330      16.210 -13.141 106.358  1.00 62.52           O
ATOM   3788  CB  PHE B 330      14.254 -11.119 106.467  1.00 62.36           C
ATOM   3789  CG  PHE B 330      13.293 -10.027 106.853  1.00 61.98           C
ATOM   3790  CD1 PHE B 330      11.946 -10.110 106.514  1.00 61.73           C
ATOM   3791  CD2 PHE B 330      13.740  -8.900 107.541  1.00 61.74           C
ATOM   3792  CE1 PHE B 330      11.056  -9.092 106.864  1.00 61.58           C
ATOM   3793  CE2 PHE B 330      12.859  -7.877 107.892  1.00 61.45           C
ATOM   3794  CZ  PHE B 330      11.515  -7.975 107.554  1.00 61.49           C
ATOM   3795  N   GLU B 331      14.707 -14.709 106.965  1.00 62.71           N
ATOM   3796  CA  GLU B 331      15.574 -15.859 106.707  1.00 62.84           C
ATOM   3797  C   GLU B 331      15.738 -16.136 105.216  1.00 62.73           C
ATOM   3798  O   GLU B 331      14.754 -16.335 104.506  1.00 62.72           O
ATOM   3799  CB  GLU B 331      15.018 -17.106 107.405  1.00 62.98           C
ATOM   3800  CG  GLU B 331      14.803 -16.954 108.913  1.00 63.55           C
ATOM   3801  CD  GLU B 331      13.620 -17.765 109.436  1.00 64.17           C
ATOM   3802  OE1 GLU B 331      12.761 -18.181 108.624  1.00 64.29           O
ATOM   3803  OE2 GLU B 331      13.544 -17.974 110.668  1.00 63.91           O
ATOM   3804  N   SER B 332      16.986 -16.150 104.752  1.00 62.76           N
ATOM   3805  CA  SER B 332      17.296 -16.515 103.368  1.00 62.82           C
ATOM   3806  C   SER B 332      17.361 -18.038 103.197  1.00 62.98           C
ATOM   3807  O   SER B 332      17.080 -18.787 104.133  1.00 62.96           O
ATOM   3808  CB  SER B 332      18.597 -15.846 102.898  1.00 62.80           C
ATOM   3809  OG  SER B 332      19.651 -16.019 103.830  1.00 62.55           O
ATOM   3810  N   GLY B 333      17.715 -18.487 101.995  1.00 63.14           N
ATOM   3811  CA  GLY B 333      17.858 -19.915 101.712  1.00 63.27           C
ATOM   3812  C   GLY B 333      19.275 -20.419 101.920  1.00 63.40           C
ATOM   3813  O   GLY B 333      20.146 -19.683 102.395  1.00 63.31           O
ATOM   3814  N   ARG B 334      19.504 -21.678 101.555  1.00 63.54           N
ATOM   3815  CA  ARG B 334      20.798 -22.324 101.758  1.00 63.80           C
ATOM   3816  C   ARG B 334      21.320 -22.954 100.470  1.00 63.91           C
ATOM   3817  O   ARG B 334      20.581 -23.652  99.774  1.00 63.99           O
ATOM   3818  CB  ARG B 334      20.698 -23.408 102.838  1.00 63.90           C
ATOM   3819  CG  ARG B 334      20.417 -22.916 104.250  1.00 64.03           C
ATOM   3820  CD  ARG B 334      20.156 -24.102 105.161  1.00 64.39           C
ATOM   3821  NE  ARG B 334      19.840 -23.702 106.530  1.00 64.70           N
ATOM   3822  CZ  ARG B 334      19.429 -24.539 107.479  1.00 64.85           C
ATOM   3823  NH1 ARG B 334      19.276 -25.832 107.213  1.00 64.82           N
ATOM   3824  NH2 ARG B 334      19.168 -24.083 108.698  1.00 64.73           N
ATOM   3825  N   ASN B 335      22.593 -22.700 100.166  1.00 64.00           N
ATOM   3826  CA  ASN B 335      23.313 -23.353  99.059  1.00 64.12           C
ATOM   3827  C   ASN B 335      22.664 -23.215  97.673  1.00 64.08           C
ATOM   3828  O   ASN B 335      22.868 -24.061  96.795  1.00 63.98           O
ATOM   3829  CB  ASN B 335      23.579 -24.832  99.391  1.00 64.22           C
ATOM   3830  CG  ASN B 335      24.155 -25.025 100.785  1.00 64.56           C
ATOM   3831  OD1 ASN B 335      23.458 -25.469 101.699  1.00 64.80           O
ATOM   3832  ND2 ASN B 335      25.428 -24.676 100.958  1.00 64.83           N
ATOM   3833  N   GLY B 336      21.895 -22.144  97.483  1.00 64.09           N
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ATOM   3834  CA  GLY B 336      21.187 -21.905  96.225  1.00 64.03           C
ATOM   3835  C   GLY B 336      19.765 -22.441  96.228  1.00 64.02           C
ATOM   3836  O   GLY B 336      19.088 -22.426  95.195  1.00 64.08           O
ATOM   3837  N   LYS B 337      19.318 -22.923  97.388  1.00 63.84           N
ATOM   3838  CA  LYS B 337      17.941 -23.383  97.567  1.00 63.62           C
ATOM   3839  C   LYS B 337      17.048 -22.224  98.003  1.00 63.32           C
ATOM   3840  O   LYS B 337      17.490 -21.348  98.751  1.00 63.29           O
ATOM   3841  CB  LYS B 337      17.859 -24.497  98.619  1.00 63.67           C
ATOM   3842  CG  LYS B 337      18.505 -25.822  98.227  1.00 63.83           C
ATOM   3843  CD  LYS B 337      18.422 -26.824  99.376  1.00 63.70           C
ATOM   3844  CE  LYS B 337      19.151 -28.121  99.051  1.00 64.22           C
ATOM   3845  NZ  LYS B 337      18.449 -28.928  98.013  1.00 64.12           N
ATOM   3846  N   PRO B 338      15.788 -22.211  97.532  1.00 62.95           N
ATOM   3847  CA  PRO B 338      14.811 -21.282  98.090  1.00 62.64           C
ATOM   3848  C   PRO B 338      14.388 -21.756  99.481  1.00 62.30           C
ATOM   3849  O   PRO B 338      14.331 -22.963  99.723  1.00 62.36           O
ATOM   3850  CB  PRO B 338      13.629 -21.380  97.115  1.00 62.69           C
ATOM   3851  CG  PRO B 338      14.117 -22.183  95.946  1.00 62.85           C
ATOM   3852  CD  PRO B 338      15.207 -23.043  96.465  1.00 62.91           C
ATOM   3853  N   ASN B 339      14.099 -20.821 100.385  1.00 61.79           N
ATOM   3854  CA  ASN B 339      13.695 -21.172 101.750  1.00 61.26           C
ATOM   3855  C   ASN B 339      12.277 -21.760 101.808  1.00 61.01           C
ATOM   3856  O   ASN B 339      11.712 -22.120 100.770  1.00 61.00           O
ATOM   3857  CB  ASN B 339      13.857 -19.970 102.696  1.00 61.23           C
ATOM   3858  CG  ASN B 339      12.827 -18.865 102.451  1.00 61.10           C
ATOM   3859  OD1 ASN B 339      12.101 -18.867 101.455  1.00 60.91           O
ATOM   3860  ND2 ASN B 339      12.769 -17.910 103.371  1.00 60.82           N
ATOM   3861  N   LYS B 340      11.713 -21.855 103.015  1.00 60.55           N
ATOM   3862  CA  LYS B 340      10.356 -22.384 103.225  1.00 60.08           C
ATOM   3863  C   LYS B 340       9.328 -21.820 102.242  1.00 59.62           C
ATOM   3864  O   LYS B 340       8.492 -22.556 101.717  1.00 59.58           O
ATOM   3865  CB  LYS B 340       9.881 -22.112 104.657  1.00 60.17           C
ATOM   3866  CG  LYS B 340      10.681 -22.808 105.739  1.00 60.43           C
ATOM   3867  CD  LYS B 340      10.045 -22.605 107.104  1.00 60.72           C
ATOM   3868  CE  LYS B 340      10.822 -23.351 108.176  1.00 61.28           C
ATOM   3869  NZ  LYS B 340      10.024 -23.535 109.418  1.00 61.76           N
ATOM   3870  N   ASP B 341       9.405 -20.513 101.998  1.00 59.05           N
ATOM   3871  CA  ASP B 341       8.408 -19.806 101.196  1.00 58.44           C
ATOM   3872  C   ASP B 341       8.886 -19.510  99.772  1.00 57.87           C
ATOM   3873  O   ASP B 341       8.345 -18.627  99.099  1.00 57.85           O
ATOM   3874  CB  ASP B 341       7.989 -18.518 101.908  1.00 58.48           C
ATOM   3875  CG  ASP B 341       7.479 -18.770 103.312  1.00 58.61           C
ATOM   3876  OD1 ASP B 341       6.377 -19.340 103.457  1.00 59.00           O
ATOM   3877  OD2 ASP B 341       8.180 -18.396 104.274  1.00 58.74           O
ATOM   3878  N   GLY B 342       9.897 -20.251  99.323  1.00 57.12           N
ATOM   3879  CA  GLY B 342      10.416 -20.121  97.962  1.00 56.17           C
ATOM   3880  C   GLY B 342      11.148 -18.818  97.689  1.00 55.49           C
ATOM   3881  O   GLY B 342      11.327 -18.432  96.531  1.00 55.55           O
ATOM   3882  N   ILE B 343      11.567 -18.141  98.758  1.00 54.67           N
ATOM   3883  CA  ILE B 343      12.300 -16.882  98.651  1.00 53.81           C
ATOM   3884  C   ILE B 343      13.782 -17.135  98.910  1.00 53.22           C
ATOM   3885  O   ILE B 343      14.188 -17.402 100.043  1.00 53.13           O
ATOM   3886  CB  ILE B 343      11.741 -15.802  99.620  1.00 53.81           C
ATOM   3887  CG1 ILE B 343      10.280 -15.486  99.277  1.00 53.56           C
ATOM   3888  CG2 ILE B 343      12.590 -14.527  99.560  1.00 53.74           C
ATOM   3889  CD1 ILE B 343       9.454 -14.982 100.438  1.00 53.10           C
ATOM   3890  N   LYS B 344      14.581 -17.058  97.848  1.00 52.41           N
ATOM   3891  CA  LYS B 344      16.008 -17.344  97.939  1.00 51.68           C
ATOM   3892  C   LYS B 344      16.726 -16.341  98.832  1.00 51.21           C
ATOM   3893  O   LYS B 344      17.524 -16.727  99.685  1.00 51.21           O
ATOM   3894  CB  LYS B 344      16.671 -17.356  96.554  1.00 51.70           C
ATOM   3895  CG  LYS B 344      16.393 -18.578  95.688  1.00 51.34           C
ATOM   3896  CD  LYS B 344      17.526 -18.774  94.677  1.00 51.30           C
ATOM   3897  CE  LYS B 344      17.070 -19.489  93.404  1.00 50.83           C
ATOM   3898  NZ  LYS B 344      16.747 -20.928  93.594  1.00 50.19           N
ATOM   3899  N   SER B 345      16.426 -15.059  98.645  1.00 50.60           N
ATOM   3900  CA  SER B 345      17.246 -14.003  99.222  1.00 49.95           C
ATOM   3901  C   SER B 345      16.479 -12.922  99.966  1.00 49.55           C
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ATOM   3902  O   SER B 345      15.364 -12.559  99.592  1.00 49.48           O
ATOM   3903  CB  SER B 345      18.099 -13.356  98.131  1.00 49.98           C
ATOM   3904  OG  SER B 345      18.742 -12.191  98.615  1.00 49.84           O
ATOM   3905  N   TYR B 346      17.106 -12.421 101.026  1.00 49.13           N
ATOM   3906  CA  TYR B 346      16.664 -11.217 101.720  1.00 48.73           C
ATOM   3907  C   TYR B 346      17.832 -10.251 101.803  1.00 48.46           C
ATOM   3908  O   TYR B 346      18.984 -10.668 101.930  1.00 48.46           O
ATOM   3909  CB  TYR B 346      16.111 -11.534 103.109  1.00 48.65           C
ATOM   3910  CG  TYR B 346      14.680 -12.013 103.080  1.00 48.56           C
ATOM   3911  CD1 TYR B 346      13.627 -11.113 102.897  1.00 48.61           C
ATOM   3912  CD2 TYR B 346      14.374 -13.363 103.231  1.00 48.29           C
ATOM   3913  CE1 TYR B 346      12.306 -11.550 102.866  1.00 48.79           C
ATOM   3914  CE2 TYR B 346      13.057 -13.810 103.203  1.00 48.37           C
ATOM   3915  CZ  TYR B 346      12.030 -12.900 103.019  1.00 48.59           C
ATOM   3916  OH  TYR B 346      10.727 -13.336 102.987  1.00 48.67           O
ATOM   3917  N   ARG B 347      17.529  -8.959 101.727  1.00 48.11           N
ATOM   3918  CA  ARG B 347      18.555  -7.952 101.510  1.00 47.78           C
ATOM   3919  C   ARG B 347      18.073  -6.570 101.943  1.00 47.73           C
ATOM   3920  O   ARG B 347      16.872  -6.312 101.995  1.00 47.77           O
ATOM   3921  CB  ARG B 347      18.924  -7.948 100.024  1.00 47.68           C
ATOM   3922  CG  ARG B 347      20.225  -7.270  99.668  1.00 47.49           C
ATOM   3923  CD  ARG B 347      21.421  -8.196  99.701  1.00 46.20           C
ATOM   3924  NE  ARG B 347      22.444  -7.733  98.768  1.00 45.04           N
ATOM   3925  CZ  ARG B 347      23.225  -6.675  98.960  1.00 44.53           C
ATOM   3926  NH1 ARG B 347      23.119  -5.947 100.064  1.00 44.12           N
ATOM   3927  NH2 ARG B 347      24.118  -6.342  98.037  1.00 44.53           N
ATOM   3928  N   ILE B 348      19.023  -5.694 102.264  1.00 47.75           N
ATOM   3929  CA  ILE B 348      18.760  -4.270 102.553  1.00 47.82           C
ATOM   3930  C   ILE B 348      17.856  -4.050 103.785  1.00 47.86           C
ATOM   3931  O   ILE B 348      16.642  -3.868 103.644  1.00 48.00           O
ATOM   3932  CB  ILE B 348      18.204  -3.488 101.302  1.00 47.74           C
ATOM   3933  CG1 ILE B 348      18.846  -3.965  99.984  1.00 47.75           C
ATOM   3934  CG2 ILE B 348      18.355  -1.985 101.488  1.00 47.77           C
ATOM   3935  CD1 ILE B 348      20.356  -3.746  99.858  1.00 47.38           C
ATOM   3936  N   PRO B 349      18.452  -4.070 104.993  1.00 47.78           N
ATOM   3937  CA  PRO B 349      17.737  -3.858 106.248  1.00 47.73           C
ATOM   3938  C   PRO B 349      17.346  -2.403 106.493  1.00 47.80           C
ATOM   3939  O   PRO B 349      18.099  -1.486 106.158  1.00 47.90           O
ATOM   3940  CB  PRO B 349      18.761  -4.284 107.302  1.00 47.74           C
ATOM   3941  CG  PRO B 349      20.067  -4.040 106.680  1.00 47.83           C
ATOM   3942  CD  PRO B 349      19.886  -4.325 105.222  1.00 47.76           C
ATOM   3943  N   ALA B 350      16.173  -2.205 107.083  1.00 47.79           N
ATOM   3944  CA  ALA B 350      15.756  -0.893 107.565  1.00 47.91           C
ATOM   3945  C   ALA B 350      15.011  -1.073 108.882  1.00 48.03           C
ATOM   3946  O   ALA B 350      14.053  -1.846 108.957  1.00 48.06           O
ATOM   3947  CB  ALA B 350      14.883  -0.190 106.535  1.00 47.78           C
ATOM   3948  N   LEU B 351      15.462  -0.367 109.917  1.00 48.17           N
ATOM   3949  CA  LEU B 351      14.898  -0.516 111.257  1.00 48.33           C
ATOM   3950  C   LEU B 351      14.356   0.795 111.816  1.00 48.64           C
ATOM   3951  O   LEU B 351      15.074   1.795 111.877  1.00 48.55           O
ATOM   3952  CB  LEU B 351      15.941  -1.104 112.216  1.00 48.26           C
ATOM   3953  CG  LEU B 351      15.473  -1.448 113.634  1.00 47.83           C
ATOM   3954  CD1 LEU B 351      14.732  -2.776 113.654  1.00 47.56           C
ATOM   3955  CD2 LEU B 351      16.653  -1.476 114.592  1.00 47.33           C
ATOM   3956  N   LEU B 352      13.091   0.776 112.233  1.00 49.13           N
ATOM   3957  CA  LEU B 352      12.450   1.946 112.837  1.00 49.45           C
ATOM   3958  C   LEU B 352      11.702   1.614 114.130  1.00 49.82           C
ATOM   3959  O   LEU B 352      10.928   0.658 114.178  1.00 49.94           O
ATOM   3960  CB  LEU B 352      11.497   2.609 111.836  1.00 49.38           C
ATOM   3961  CG  LEU B 352      10.715   3.858 112.268  1.00 49.32           C
ATOM   3962  CD1 LEU B 352      11.633   5.033 112.599  1.00 48.78           C
ATOM   3963  CD2 LEU B 352       9.713   4.247 111.192  1.00 49.34           C
ATOM   3964  N   LYS B 353      11.949   2.407 115.172  1.00 50.18           N
ATOM   3965  CA  LYS B 353      11.132   2.385 116.379  1.00 50.39           C
ATOM   3966  C   LYS B 353      10.185   3.583 116.339  1.00 50.51           C
ATOM   3967  O   LYS B 353      10.613   4.710 116.071  1.00 50.41           O
ATOM   3968  CB  LYS B 353      12.001   2.406 117.641  1.00 50.56           C
ATOM   3969  CG  LYS B 353      11.236   2.113 118.934  1.00 50.89           C
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ATOM   3970  CD  LYS B 353      12.098   1.369 119.957  1.00 51.58           C
ATOM   3971  CE  LYS B 353      11.347   1.160 121.278  1.00 51.78           C
ATOM   3972  NZ  LYS B 353      11.834  -0.017 122.058  1.00 51.32           N
ATOM   3973  N   THR B 354       8.904   3.328 116.604  1.00 50.68           N
ATOM   3974  CA  THR B 354       7.846   4.329 116.426  1.00 50.85           C
ATOM   3975  C   THR B 354       7.460   5.055 117.724  1.00 51.03           C
ATOM   3976  O   THR B 354       8.191   4.999 118.714  1.00 51.04           O
ATOM   3977  CB  THR B 354       6.593   3.713 115.757  1.00 50.88           C
ATOM   3978  OG1 THR B 354       5.856   2.941 116.712  1.00 50.76           O
ATOM   3979  CG2 THR B 354       6.993   2.828 114.585  1.00 50.77           C
ATOM   3980  N   ASP B 355       6.318   5.745 117.703  1.00 51.24           N
ATOM   3981  CA  ASP B 355       5.854   6.521 118.855  1.00 51.56           C
ATOM   3982  C   ASP B 355       5.273   5.630 119.947  1.00 51.73           C
ATOM   3983  O   ASP B 355       5.427   5.915 121.134  1.00 51.90           O
ATOM   3984  CB  ASP B 355       4.834   7.589 118.431  1.00 51.47           C
ATOM   3985  CG  ASP B 355       3.563   6.993 117.843  1.00 51.63           C
ATOM   3986  OD1 ASP B 355       3.662   6.076 117.000  1.00 51.93           O
ATOM   3987  OD2 ASP B 355       2.462   7.450 118.221  1.00 51.46           O
ATOM   3988  N   LYS B 356       4.615   4.549 119.532  1.00 51.87           N
ATOM   3989  CA  LYS B 356       4.010   3.592 120.454  1.00 51.97           C
ATOM   3990  C   LYS B 356       5.036   2.600 121.012  1.00 51.87           C
ATOM   3991  O   LYS B 356       4.697   1.744 121.839  1.00 51.95           O
ATOM   3992  CB  LYS B 356       2.865   2.844 119.761  1.00 52.13           C
ATOM   3993  CG  LYS B 356       1.680   3.724 119.394  1.00 52.79           C
ATOM   3994  CD  LYS B 356       0.646   2.960 118.585  1.00 53.70           C
ATOM   3995  CE  LYS B 356      -0.595   3.808 118.347  1.00 53.91           C
ATOM   3996  NZ  LYS B 356      -1.516   3.160 117.370  1.00 54.11           N
ATOM   3997  N   GLY B 357       6.283   2.721 120.557  1.00 51.67           N
ATOM   3998  CA  GLY B 357       7.374   1.846 121.000  1.00 51.30           C
ATOM   3999  C   GLY B 357       7.657   0.691 120.053  1.00 51.04           C
ATOM   4000  O   GLY B 357       8.680   0.013 120.181  1.00 51.03           O
ATOM   4001  N   THR B 358       6.747   0.477 119.104  1.00 50.66           N
ATOM   4002  CA  THR B 358       6.838  -0.600 118.115  1.00 50.36           C
ATOM   4003  C   THR B 358       8.142  -0.573 117.311  1.00 50.21           C
ATOM   4004  O   THR B 358       8.666   0.496 116.996  1.00 50.14           O
ATOM   4005  CB  THR B 358       5.661  -0.524 117.117  1.00 50.36           C
ATOM   4006  OG1 THR B 358       4.453  -0.185 117.812  1.00 50.23           O
ATOM   4007  CG2 THR B 358       5.475  -1.845 116.380  1.00 50.43           C
ATOM   4008  N   LEU B 359       8.658  -1.757 116.989  1.00 50.00           N
ATOM   4009  CA  LEU B 359       9.769  -1.881 116.048  1.00 49.71           C
ATOM   4010  C   LEU B 359       9.287  -2.383 114.685  1.00 49.41           C
ATOM   4011  O   LEU B 359       8.510  -3.337 114.596  1.00 49.38           O
ATOM   4012  CB  LEU B 359      10.876  -2.788 116.598  1.00 49.68           C
ATOM   4013  CG  LEU B 359      11.779  -2.226 117.704  1.00 49.93           C
ATOM   4014  CD1 LEU B 359      12.587  -3.342 118.350  1.00 49.79           C
ATOM   4015  CD2 LEU B 359      12.705  -1.136 117.180  1.00 49.93           C
ATOM   4016  N   ILE B 360       9.744  -1.709 113.633  1.00 49.00           N
ATOM   4017  CA  ILE B 360       9.483  -2.116 112.259  1.00 48.46           C
ATOM   4018  C   ILE B 360      10.804  -2.504 111.613  1.00 48.12           C
ATOM   4019  O   ILE B 360      11.776  -1.751 111.670  1.00 47.96           O
ATOM   4020  CB  ILE B 360       8.825  -0.981 111.437  1.00 48.47           C
ATOM   4021  CG1 ILE B 360       7.496  -0.560 112.070  1.00 48.47           C
ATOM   4022  CG2 ILE B 360       8.616  -1.414 109.987  1.00 48.29           C
ATOM   4023  CD1 ILE B 360       6.952   0.755 111.556  1.00 48.37           C
ATOM   4024  N   ALA B 361      10.835  -3.694 111.022  1.00 47.76           N
ATOM   4025  CA  ALA B 361      11.976  -4.133 110.232  1.00 47.42           C
ATOM   4026  C   ALA B 361      11.540  -4.331 108.782  1.00 47.15           C
ATOM   4027  O   ALA B 361      10.560  -5.027 108.512  1.00 47.05           O
ATOM   4028  CB  ALA B 361      12.569  -5.411 110.806  1.00 47.35           C
ATOM   4029  N   GLY B 362      12.265  -3.699 107.861  1.00 46.87           N
ATOM   4030  CA  GLY B 362      11.951  -3.760 106.432  1.00 46.49           C
ATOM   4031  C   GLY B 362      13.077  -4.347 105.604  1.00 46.16           C
ATOM   4032  O   GLY B 362      14.254  -4.185 105.937  1.00 46.11           O
ATOM   4033  N   ALA B 363      12.714  -5.022 104.516  1.00 45.89           N
ATOM   4034  CA  ALA B 363      13.688  -5.739 103.697  1.00 45.72           C
ATOM   4035  C   ALA B 363      13.297  -5.836 102.229  1.00 45.65           C
ATOM   4036  O   ALA B 363      12.127  -5.672 101.871  1.00 45.58           O
ATOM   4037  CB  ALA B 363      13.909  -7.136 104.262  1.00 45.59           C
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ATOM   4038  N   ASP B 364      14.298  -6.099 101.391  1.00 45.71           N
ATOM   4039  CA  ASP B 364      14.088  -6.549 100.018  1.00 45.79           C
ATOM   4040  C   ASP B 364      13.752  -8.041 100.047  1.00 45.76           C
ATOM   4041  O   ASP B 364      14.560  -8.859 100.491  1.00 45.77           O
ATOM   4042  CB  ASP B 364      15.350  -6.334  99.167  1.00 45.73           C
ATOM   4043  CG  ASP B 364      15.442  -4.935  98.567  1.00 46.25           C
ATOM   4044  OD1 ASP B 364      15.251  -3.933  99.295  1.00 46.69           O
ATOM   4045  OD2 ASP B 364      15.736  -4.841  97.355  1.00 46.25           O
ATOM   4046  N   GLU B 365      12.554  -8.388  99.590  1.00 45.69           N
ATOM   4047  CA  GLU B 365      12.169  -9.784  99.426  1.00 45.56           C
ATOM   4048  C   GLU B 365      12.576 -10.256  98.032  1.00 45.46           C
ATOM   4049  O   GLU B 365      11.749 -10.322  97.116  1.00 45.56           O
ATOM   4050  CB  GLU B 365      10.667  -9.942  99.642  1.00 45.66           C
ATOM   4051  CG  GLU B 365      10.188 -11.372  99.806  1.00 45.78           C
ATOM   4052  CD  GLU B 365       8.854 -11.437 100.520  1.00 45.95           C
ATOM   4053  OE1 GLU B 365       8.848 -11.433 101.772  1.00 45.59           O
ATOM   4054  OE2 GLU B 365       7.815 -11.487  99.829  1.00 45.80           O
ATOM   4055  N   ARG B 366      13.861 -10.574  97.885  1.00 45.24           N
ATOM   4056  CA  ARG B 366      14.435 -10.965  96.597  1.00 44.93           C
ATOM   4057  C   ARG B 366      14.233 -12.455  96.330  1.00 45.00           C
ATOM   4058  O   ARG B 366      15.082 -13.282  96.661  1.00 45.01           O
ATOM   4059  CB  ARG B 366      15.919 -10.582  96.532  1.00 44.82           C
ATOM   4060  CG  ARG B 366      16.170  -9.092  96.693  1.00 43.87           C
ATOM   4061  CD  ARG B 366      17.638  -8.746  96.586  1.00 42.36           C
ATOM   4062  NE  ARG B 366      17.862  -7.315  96.781  1.00 40.97           N
ATOM   4063  CZ  ARG B 366      19.019  -6.694  96.571  1.00 40.40           C
ATOM   4064  NH1 ARG B 366      20.085  -7.370  96.162  1.00 40.04           N
ATOM   4065  NH2 ARG B 366      19.113  -5.389  96.779  1.00 40.30           N
ATOM   4066  N   ARG B 367      13.101 -12.772  95.706  1.00 45.12           N
ATOM   4067  CA  ARG B 367      12.622 -14.147  95.558  1.00 45.09           C
ATOM   4068  C   ARG B 367      13.529 -15.083  94.759  1.00 44.98           C
ATOM   4069  O   ARG B 367      13.737 -16.230  95.156  1.00 45.15           O
ATOM   4070  CB  ARG B 367      11.209 -14.157  94.959  1.00 45.16           C
ATOM   4071  CG  ARG B 367      10.533 -15.517  95.025  1.00 45.58           C
ATOM   4072  CD  ARG B 367       9.034 -15.434  94.802  1.00 46.25           C
ATOM   4073  NE  ARG B 367       8.670 -15.472  93.387  1.00 47.11           N
ATOM   4074  CZ  ARG B 367       8.644 -16.571  92.633  1.00 47.46           C
ATOM   4075  NH1 ARG B 367       8.983 -17.753  93.142  1.00 47.77           N
ATOM   4076  NH2 ARG B 367       8.285 -16.486  91.358  1.00 47.42           N
ATOM   4077  N   LEU B 368      14.068 -14.599  93.646  1.00 44.89           N
ATOM   4078  CA  LEU B 368      14.708 -15.486  92.671  1.00 44.77           C
ATOM   4079  C   LEU B 368      16.237 -15.579  92.741  1.00 44.73           C
ATOM   4080  O   LEU B 368      16.812 -16.589  92.334  1.00 44.75           O
ATOM   4081  CB  LEU B 368      14.229 -15.148  91.255  1.00 44.76           C
ATOM   4082  CG  LEU B 368      12.786 -15.579  90.963  1.00 44.78           C
ATOM   4083  CD1 LEU B 368      12.110 -14.628  89.985  1.00 45.16           C
ATOM   4084  CD2 LEU B 368      12.719 -17.024  90.463  1.00 45.06           C
ATOM   4085  N   HIS B 369      16.878 -14.524  93.244  1.00 44.65           N
ATOM   4086  CA  HIS B 369      18.330 -14.482  93.457  1.00 44.62           C
ATOM   4087  C   HIS B 369      18.676 -13.314  94.379  1.00 44.62           C
ATOM   4088  O   HIS B 369      17.784 -12.595  94.830  1.00 44.69           O
ATOM   4089  CB  HIS B 369      19.088 -14.358  92.129  1.00 44.66           C
ATOM   4090  CG  HIS B 369      18.498 -13.355  91.189  1.00 44.74           C
ATOM   4091  ND1 HIS B 369      18.651 -11.995  91.358  1.00 44.68           N
ATOM   4092  CD2 HIS B 369      17.746 -13.513  90.074  1.00 44.34           C
ATOM   4093  CE1 HIS B 369      18.021 -11.360  90.387  1.00 44.02           C
ATOM   4094  NE2 HIS B 369      17.464 -12.258  89.595  1.00 44.13           N
ATOM   4095  N   SER B 370      19.963 -13.130  94.660  1.00 44.71           N
ATOM   4096  CA  SER B 370      20.413 -12.031  95.516  1.00 44.85           C
ATOM   4097  C   SER B 370      21.070 -10.874  94.749  1.00 44.90           C
ATOM   4098  O   SER B 370      21.878 -10.129  95.308  1.00 45.06           O
ATOM   4099  CB  SER B 370      21.339 -12.551  96.626  1.00 44.88           C
ATOM   4100  OG  SER B 370      22.632 -12.845  96.138  1.00 44.99           O
ATOM   4101  N   SER B 371      20.717 -10.716  93.475  1.00 44.98           N
ATOM   4102  CA  SER B 371      21.215  -9.588  92.688  1.00 45.00           C
ATOM   4103  C   SER B 371      20.292  -8.371  92.790  1.00 44.99           C
ATOM   4104  O   SER B 371      19.149  -8.479  93.239  1.00 44.97           O
ATOM   4105  CB  SER B 371      21.434  -9.994  91.232  1.00 45.05           C
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ATOM   4106  OG  SER B 371      22.617 -10.761  91.102  1.00 45.18           O
ATOM   4107  N   ASP B 372      20.797  -7.215  92.369  1.00 44.92           N
ATOM   4108  CA  ASP B 372      20.069  -5.954  92.502  1.00 44.79           C
ATOM   4109  C   ASP B 372      18.957  -5.768  91.451  1.00 44.74           C
ATOM   4110  O   ASP B 372      18.801  -4.683  90.883  1.00 44.57           O
ATOM   4111  CB  ASP B 372      21.055  -4.776  92.495  1.00 44.77           C
ATOM   4112  CG  ASP B 372      22.114  -4.888  93.586  1.00 44.78           C
ATOM   4113  OD1 ASP B 372      21.822  -5.457  94.659  1.00 44.27           O
ATOM   4114  OD2 ASP B 372      23.244  -4.401  93.371  1.00 45.46           O
ATOM   4115  N   TRP B 373      18.189  -6.835  91.213  1.00 44.81           N
ATOM   4116  CA  TRP B 373      17.060  -6.835  90.269  1.00 44.96           C
ATOM   4117  C   TRP B 373      16.212  -8.111  90.397  1.00 45.10           C
ATOM   4118  O   TRP B 373      16.465  -8.946  91.265  1.00 45.06           O
ATOM   4119  CB  TRP B 373      17.554  -6.677  88.826  1.00 44.83           C
ATOM   4120  CG  TRP B 373      18.462  -7.785  88.378  1.00 44.82           C
ATOM   4121  CD1 TRP B 373      18.090  -9.028  87.944  1.00 44.62           C
ATOM   4122  CD2 TRP B 373      19.891  -7.750  88.317  1.00 44.65           C
ATOM   4123  NE1 TRP B 373      19.199  -9.769  87.621  1.00 44.43           N
ATOM   4124  CE2 TRP B 373      20.318  -9.010  87.838  1.00 44.62           C
ATOM   4125  CE3 TRP B 373      20.853  -6.777  88.618  1.00 44.70           C
ATOM   4126  CZ2 TRP B 373      21.667  -9.322  87.652  1.00 44.50           C
ATOM   4127  CZ3 TRP B 373      22.196  -7.091  88.437  1.00 44.79           C
ATOM   4128  CH2 TRP B 373      22.588  -8.354  87.957  1.00 44.65           C
ATOM   4129  N   GLY B 374      15.218  -8.257  89.524  1.00 45.41           N
ATOM   4130  CA  GLY B 374      14.335  -9.429  89.527  1.00 46.01           C
ATOM   4131  C   GLY B 374      12.984  -9.168  90.169  1.00 46.28           C
ATOM   4132  O   GLY B 374      12.479  -8.046  90.126  1.00 46.37           O
ATOM   4133  N   ASP B 375      12.391 -10.211  90.749  1.00 46.67           N
ATOM   4134  CA  ASP B 375      11.153 -10.068  91.510  1.00 46.93           C
ATOM   4135  C   ASP B 375      11.481  -9.769  92.961  1.00 47.23           C
ATOM   4136  O   ASP B 375      11.916 -10.651  93.709  1.00 47.40           O
ATOM   4137  CB  ASP B 375      10.274 -11.319  91.409  1.00 46.99           C
ATOM   4138  CG  ASP B 375       9.056 -11.260  92.329  1.00 46.98           C
ATOM   4139  OD1 ASP B 375       8.441 -10.180  92.468  1.00 47.12           O
ATOM   4140  OD2 ASP B 375       8.713 -12.303  92.916  1.00 46.95           O
ATOM   4141  N   ILE B 376      11.280  -8.510  93.340  1.00 47.52           N
ATOM   4142  CA  ILE B 376      11.541  -8.043  94.695  1.00 47.73           C
ATOM   4143  C   ILE B 376      10.289  -7.381  95.266  1.00 48.20           C
ATOM   4144  O   ILE B 376       9.669  -6.534  94.613  1.00 48.20           O
ATOM   4145  CB  ILE B 376      12.717  -7.037  94.746  1.00 47.53           C
ATOM   4146  CG1 ILE B 376      13.933  -7.575  93.984  1.00 47.62           C
ATOM   4147  CG2 ILE B 376      13.081  -6.710  96.192  1.00 47.41           C
ATOM   4148  CD1 ILE B 376      15.052  -6.559  93.780  1.00 47.57           C
ATOM   4149  N   GLY B 377       9.924  -7.780  96.483  1.00 48.57           N
ATOM   4150  CA  GLY B 377       8.837  -7.141  97.213  1.00 49.24           C
ATOM   4151  C   GLY B 377       9.353  -6.303  98.365  1.00 49.81           C
ATOM   4152  O   GLY B 377      10.409  -6.591  98.932  1.00 49.81           O
ATOM   4153  N   MET B 378       8.621  -5.247  98.697  1.00 50.50           N
ATOM   4154  CA  MET B 378       8.917  -4.466  99.889  1.00 51.26           C
ATOM   4155  C   MET B 378       8.093  -5.069 101.023  1.00 52.00           C
ATOM   4156  O   MET B 378       6.862  -5.055 100.973  1.00 52.07           O
ATOM   4157  CB  MET B 378       8.576  -2.985  99.688  1.00 51.01           C
ATOM   4158  CG  MET B 378       9.220  -2.314  98.468  1.00 50.64           C
ATOM   4159  SD  MET B 378      10.994  -1.972  98.586  1.00 49.65           S
ATOM   4160  CE  MET B 378      11.700  -3.429  97.816  1.00 49.55           C
ATOM   4161  N   VAL B 379       8.773  -5.623 102.024  1.00 52.85           N
ATOM   4162  CA  VAL B 379       8.090  -6.301 103.129  1.00 53.77           C
ATOM   4163  C   VAL B 379       8.565  -5.832 104.500  1.00 54.44           C
ATOM   4164  O   VAL B 379       9.725  -5.448 104.673  1.00 54.47           O
ATOM   4165  CB  VAL B 379       8.210  -7.853 103.047  1.00 53.67           C
ATOM   4166  CG1 VAL B 379       7.345  -8.411 101.917  1.00 53.82           C
ATOM   4167  CG2 VAL B 379       9.668  -8.290 102.899  1.00 53.59           C
ATOM   4168  N   ILE B 380       7.651  -5.863 105.468  1.00 55.29           N
ATOM   4169  CA  ILE B 380       7.976  -5.541 106.855  1.00 56.03           C
ATOM   4170  C   ILE B 380       7.469  -6.591 107.846  1.00 56.52           C
ATOM   4171  O   ILE B 380       6.537  -7.345 107.554  1.00 56.49           O
ATOM   4172  CB  ILE B 380       7.466  -4.127 107.275  1.00 56.02           C
ATOM   4173  CG1 ILE B 380       5.968  -3.957 106.984  1.00 56.35           C
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ATOM   4174  CG2 ILE B 380       8.289  -3.025 106.610  1.00 56.03           C
ATOM   4175  CD1 ILE B 380       5.061  -4.298 108.159  1.00 56.33           C
ATOM   4176  N   ARG B 381       8.109  -6.632 109.011  1.00 57.23           N
ATOM   4177  CA  ARG B 381       7.662  -7.442 110.140  1.00 57.82           C
ATOM   4178  C   ARG B 381       7.702  -6.591 111.408  1.00 58.23           C
ATOM   4179  O   ARG B 381       8.651  -5.832 111.627  1.00 58.21           O
ATOM   4180  CB  ARG B 381       8.520  -8.701 110.288  1.00 57.70           C
ATOM   4181  CG  ARG B 381       8.238  -9.771 109.233  1.00 57.88           C
ATOM   4182  CD  ARG B 381       8.938 -11.087 109.549  1.00 58.00           C
ATOM   4183  NE  ARG B 381       8.420 -11.712 110.766  1.00 57.96           N
ATOM   4184  CZ  ARG B 381       8.975 -12.754 111.382  1.00 57.98           C
ATOM   4185  NH1 ARG B 381      10.083 -13.310 110.907  1.00 57.46           N
ATOM   4186  NH2 ARG B 381       8.418 -13.241 112.483  1.00 58.15           N
ATOM   4187  N   ARG B 382       6.666  -6.725 112.234  1.00 58.83           N
ATOM   4188  CA  ARG B 382       6.459  -5.837 113.379  1.00 59.30           C
ATOM   4189  C   ARG B 382       6.782  -6.474 114.729  1.00 59.69           C
ATOM   4190  O   ARG B 382       6.727  -7.696 114.880  1.00 59.82           O
ATOM   4191  CB  ARG B 382       5.018  -5.326 113.382  1.00 59.28           C
ATOM   4192  CG  ARG B 382       4.686  -4.378 112.237  1.00 59.41           C
ATOM   4193  CD  ARG B 382       3.249  -3.879 112.289  1.00 59.34           C
ATOM   4194  NE  ARG B 382       3.007  -2.992 113.425  1.00 59.66           N
ATOM   4195  CZ  ARG B 382       2.445  -3.370 114.572  1.00 60.05           C
ATOM   4196  NH1 ARG B 382       2.056  -4.629 114.752  1.00 59.80           N
ATOM   4197  NH2 ARG B 382       2.268  -2.486 115.545  1.00 59.89           N
ATOM   4198  N   SER B 383       7.117  -5.634 115.708  1.00 60.20           N
ATOM   4199  CA  SER B 383       7.337  -6.086 117.084  1.00 60.66           C
ATOM   4200  C   SER B 383       6.814  -5.083 118.104  1.00 60.93           C
ATOM   4201  O   SER B 383       7.239  -3.926 118.124  1.00 60.94           O
ATOM   4202  CB  SER B 383       8.816  -6.362 117.347  1.00 60.65           C
ATOM   4203  OG  SER B 383       9.017  -6.788 118.681  1.00 60.84           O
ATOM   4204  N   GLU B 384       5.895  -5.546 118.948  1.00 61.31           N
ATOM   4205  CA  GLU B 384       5.325  -4.737 120.022  1.00 61.55           C
ATOM   4206  C   GLU B 384       6.128  -4.961 121.295  1.00 61.62           C
ATOM   4207  O   GLU B 384       6.102  -4.138 122.209  1.00 61.58           O
ATOM   4208  CB  GLU B 384       3.857  -5.115 120.279  1.00 61.63           C
ATOM   4209  CG  GLU B 384       2.995  -5.340 119.033  1.00 61.92           C
ATOM   4210  CD  GLU B 384       3.219  -6.703 118.384  1.00 62.54           C
ATOM   4211  OE1 GLU B 384       3.764  -7.613 119.049  1.00 62.91           O
ATOM   4212  OE2 GLU B 384       2.852  -6.866 117.201  1.00 62.79           O
ATOM   4213  N   ASP B 385       6.849  -6.079 121.334  1.00 61.85           N
ATOM   4214  CA  ASP B 385       7.555  -6.523 122.535  1.00 62.15           C
ATOM   4215  C   ASP B 385       9.067  -6.260 122.500  1.00 62.19           C
ATOM   4216  O   ASP B 385       9.860  -7.099 122.941  1.00 62.23           O
ATOM   4217  CB  ASP B 385       7.263  -8.012 122.802  1.00 62.24           C
ATOM   4218  CG  ASP B 385       7.516  -8.898 121.582  1.00 62.66           C
ATOM   4219  OD1 ASP B 385       8.534  -8.699 120.881  1.00 63.07           O
ATOM   4220  OD2 ASP B 385       6.696  -9.807 121.329  1.00 62.71           O
ATOM   4221  N   ASN B 386       9.452  -5.092 121.979  1.00 62.23           N
ATOM   4222  CA  ASN B 386      10.861  -4.659 121.909  1.00 62.19           C
ATOM   4223  C   ASN B 386      11.814  -5.638 121.193  1.00 62.10           C
ATOM   4224  O   ASN B 386      13.010  -5.703 121.499  1.00 62.04           O
ATOM   4225  CB  ASN B 386      11.388  -4.289 123.312  1.00 62.17           C
ATOM   4226  CG  ASN B 386      12.706  -3.518 123.267  1.00 62.21           C
ATOM   4227  OD1 ASN B 386      13.022  -2.851 122.278  1.00 62.54           O
ATOM   4228  ND2 ASN B 386      13.480  -3.611 124.343  1.00 61.54           N
ATOM   4229  N   GLY B 387      11.280  -6.391 120.236  1.00 62.02           N
ATOM   4230  CA  GLY B 387      12.087  -7.322 119.454  1.00 62.00           C
ATOM   4231  C   GLY B 387      12.296  -8.676 120.104  1.00 62.01           C
ATOM   4232  O   GLY B 387      13.271  -9.366 119.804  1.00 62.00           O
ATOM   4233  N   LYS B 388      11.382  -9.052 120.996  1.00 62.00           N
ATOM   4234  CA  LYS B 388      11.386 -10.380 121.603  1.00 62.00           C
ATOM   4235  C   LYS B 388      10.924 -11.389 120.549  1.00 61.88           C
ATOM   4236  O   LYS B 388      11.704 -12.239 120.115  1.00 61.91           O
ATOM   4237  CB  LYS B 388      10.486 -10.398 122.848  1.00 62.09           C
ATOM   4238  CG  LYS B 388      10.386 -11.732 123.587  1.00 62.24           C
ATOM   4239  CD  LYS B 388       9.306 -11.670 124.666  1.00 62.14           C
ATOM   4240  CE  LYS B 388       8.913 -13.053 125.166  1.00 62.55           C
ATOM   4241  NZ  LYS B 388       9.897 -13.611 126.137  1.00 62.98           N
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ATOM   4242  N   THR B 389       9.662 -11.274 120.137  1.00 61.73           N
ATOM   4243  CA  THR B 389       9.110 -12.050 119.022  1.00 61.54           C
ATOM   4244  C   THR B 389       8.523 -11.096 117.970  1.00 61.30           C
ATOM   4245  O   THR B 389       8.168  -9.954 118.285  1.00 61.22           O
ATOM   4246  CB  THR B 389       8.021 -13.067 119.484  1.00 61.69           C
ATOM   4247  OG1 THR B 389       6.980 -12.380 120.192  1.00 61.65           O
ATOM   4248  CG2 THR B 389       8.615 -14.162 120.377  1.00 61.60           C
ATOM   4249  N   TRP B 390       8.417 -11.567 116.728  1.00 60.89           N
ATOM   4250  CA  TRP B 390       7.989 -10.716 115.617  1.00 60.51           C
ATOM   4251  C   TRP B 390       6.728 -11.226 114.912  1.00 60.15           C
ATOM   4252  O   TRP B 390       6.528 -12.435 114.774  1.00 60.17           O
ATOM   4253  CB  TRP B 390       9.131 -10.539 114.605  1.00 60.56           C
ATOM   4254  CG  TRP B 390      10.385  -9.913 115.183  1.00 60.76           C
ATOM   4255  CD1 TRP B 390      11.354 -10.545 115.913  1.00 60.87           C
ATOM   4256  CD2 TRP B 390      10.804  -8.543 115.065  1.00 60.96           C
ATOM   4257  NE1 TRP B 390      12.343  -9.656 116.261  1.00 60.96           N
ATOM   4258  CE2 TRP B 390      12.034  -8.421 115.754  1.00 60.90           C
ATOM   4259  CE3 TRP B 390      10.262  -7.407 114.442  1.00 61.10           C
ATOM   4260  CZ2 TRP B 390      12.732  -7.207 115.841  1.00 60.71           C
ATOM   4261  CZ3 TRP B 390      10.957  -6.197 114.531  1.00 60.75           C
ATOM   4262  CH2 TRP B 390      12.178  -6.111 115.227  1.00 60.81           C
ATOM   4263  N   GLY B 391       5.889 -10.293 114.463  1.00 59.61           N
ATOM   4264  CA  GLY B 391       4.686 -10.624 113.700  1.00 59.05           C
ATOM   4265  C   GLY B 391       5.012 -11.118 112.303  1.00 58.74           C
ATOM   4266  O   GLY B 391       6.179 -11.213 111.926  1.00 58.88           O
ATOM   4267  N   ASP B 392       3.979 -11.421 111.524  1.00 58.31           N
ATOM   4268  CA  ASP B 392       4.163 -11.994 110.189  1.00 57.92           C
ATOM   4269  C   ASP B 392       4.589 -10.968 109.134  1.00 57.59           C
ATOM   4270  O   ASP B 392       4.887  -9.817 109.458  1.00 57.63           O
ATOM   4271  CB  ASP B 392       2.895 -12.735 109.747  1.00 57.96           C
ATOM   4272  CG  ASP B 392       2.647 -14.000 110.549  1.00 57.76           C
ATOM   4273  OD1 ASP B 392       3.622 -14.708 110.886  1.00 57.35           O
ATOM   4274  OD2 ASP B 392       1.470 -14.288 110.836  1.00 57.88           O
ATOM   4275  N   ARG B 393       4.621 -11.400 107.874  1.00 57.12           N
ATOM   4276  CA  ARG B 393       5.016 -10.538 106.762  1.00 56.62           C
ATOM   4277  C   ARG B 393       3.837  -9.740 106.223  1.00 55.94           C
ATOM   4278  O   ARG B 393       2.779 -10.301 105.907  1.00 55.95           O
ATOM   4279  CB  ARG B 393       5.626 -11.357 105.619  1.00 56.69           C
ATOM   4280  CG  ARG B 393       6.905 -12.115 105.960  1.00 57.12           C
ATOM   4281  CD  ARG B 393       7.416 -12.880 104.739  1.00 57.27           C
ATOM   4282  NE  ARG B 393       6.453 -13.874 104.257  1.00 58.49           N
ATOM   4283  CZ  ARG B 393       6.726 -15.160 104.048  1.00 58.97           C
ATOM   4284  NH1 ARG B 393       7.949 -15.637 104.256  1.00 59.42           N
ATOM   4285  NH2 ARG B 393       5.773 -15.973 103.612  1.00 59.05           N
ATOM   4286  N   VAL B 394       4.028  -8.429 106.121  1.00 55.02           N
ATOM   4287  CA  VAL B 394       3.068  -7.555 105.459  1.00 54.11           C
ATOM   4288  C   VAL B 394       3.744  -6.927 104.245  1.00 53.41           C
ATOM   4289  O   VAL B 394       4.675  -6.126 104.381  1.00 53.48           O
ATOM   4290  CB  VAL B 394       2.540  -6.454 106.403  1.00 54.16           C
ATOM   4291  CG1 VAL B 394       1.554  -5.543 105.672  1.00 54.33           C
ATOM   4292  CG2 VAL B 394       1.890  -7.071 107.631  1.00 54.23           C
ATOM   4293  N   THR B 395       3.286  -7.309 103.059  1.00 52.35           N
ATOM   4294  CA  THR B 395       3.852  -6.785 101.825  1.00 51.30           C
ATOM   4295  C   THR B 395       3.377  -5.348 101.592  1.00 50.60           C
ATOM   4296  O   THR B 395       2.174  -5.077 101.528  1.00 50.44           O
ATOM   4297  CB  THR B 395       3.513  -7.685 100.615  1.00 51.36           C
ATOM   4298  OG1 THR B 395       3.799  -9.051 100.938  1.00 51.10           O
ATOM   4299  CG2 THR B 395       4.328  -7.279  99.392  1.00 51.41           C
ATOM   4300  N   ILE B 396       4.339  -4.435 101.498  1.00 49.63           N
ATOM   4301  CA  ILE B 396       4.070  -3.032 101.201  1.00 48.62           C
ATOM   4302  C   ILE B 396       3.750  -2.879  99.715  1.00 47.87           C
ATOM   4303  O   ILE B 396       2.710  -2.329  99.348  1.00 47.76           O
ATOM   4304  CB  ILE B 396       5.269  -2.128 101.593  1.00 48.69           C
ATOM   4305  CG1 ILE B 396       5.470  -2.123 103.115  1.00 48.69           C
ATOM   4306  CG2 ILE B 396       5.075  -0.710 101.060  1.00 48.75           C
ATOM   4307  CD1 ILE B 396       6.683  -1.323 103.598  1.00 48.63           C
ATOM   4308  N   THR B 397       4.654  -3.370  98.872  1.00 47.01           N
ATOM   4309  CA  THR B 397       4.486  -3.347  97.423  1.00 46.16           C
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ATOM   4310  C   THR B 397       5.247  -4.513  96.810  1.00 45.64           C
ATOM   4311  O   THR B 397       6.390  -4.787  97.188  1.00 45.47           O
ATOM   4312  CB  THR B 397       5.021  -2.027  96.794  1.00 46.19           C
ATOM   4313  OG1 THR B 397       4.451  -0.895  97.461  1.00 46.02           O
ATOM   4314  CG2 THR B 397       4.683  -1.952  95.310  1.00 45.89           C
ATOM   4315  N   ASN B 398       4.601  -5.208  95.881  1.00 44.97           N
ATOM   4316  CA  ASN B 398       5.290  -6.151  95.013  1.00 44.52           C
ATOM   4317  C   ASN B 398       4.607  -6.196  93.667  1.00 44.22           C
ATOM   4318  O   ASN B 398       3.491  -6.702  93.547  1.00 44.41           O
ATOM   4319  CB  ASN B 398       5.347  -7.553  95.624  1.00 44.55           C
ATOM   4320  CG  ASN B 398       6.351  -8.459  94.921  1.00 44.54           C
ATOM   4321  OD1 ASN B 398       6.687  -8.267  93.746  1.00 44.31           O
ATOM   4322  ND2 ASN B 398       6.839  -9.456  95.648  1.00 44.71           N
ATOM   4323  N   LEU B 399       5.279  -5.659  92.656  1.00 43.79           N
ATOM   4324  CA  LEU B 399       4.722  -5.620  91.311  1.00 43.45           C
ATOM   4325  C   LEU B 399       4.800  -7.002  90.681  1.00 43.31           C
ATOM   4326  O   LEU B 399       5.805  -7.697  90.829  1.00 43.25           O
ATOM   4327  CB  LEU B 399       5.442  -4.577  90.451  1.00 43.32           C
ATOM   4328  CG  LEU B 399       5.396  -3.125  90.948  1.00 43.02           C
ATOM   4329  CD1 LEU B 399       6.385  -2.259  90.187  1.00 42.65           C
ATOM   4330  CD2 LEU B 399       3.994  -2.542  90.863  1.00 42.52           C
ATOM   4331  N   ARG B 400       3.727  -7.402  90.002  1.00 43.23           N
ATOM   4332  CA  ARG B 400       3.667  -8.713  89.365  1.00 43.33           C
ATOM   4333  C   ARG B 400       4.728  -8.845  88.273  1.00 43.68           C
ATOM   4334  O   ARG B 400       5.140  -7.849  87.670  1.00 43.71           O
ATOM   4335  CB  ARG B 400       2.264  -9.007  88.819  1.00 43.24           C
ATOM   4336  CG  ARG B 400       1.805  -8.133  87.651  1.00 43.22           C
ATOM   4337  CD  ARG B 400       0.375  -8.483  87.256  1.00 43.00           C
ATOM   4338  NE  ARG B 400      -0.127  -7.677  86.144  1.00 42.29           N
ATOM   4339  CZ  ARG B 400      -0.216  -8.095  84.883  1.00 42.43           C
ATOM   4340  NH1 ARG B 400       0.172  -9.320  84.547  1.00 42.64           N
ATOM   4341  NH2 ARG B 400      -0.692  -7.284  83.949  1.00 42.17           N
ATOM   4342  N   ASP B 401       5.179 -10.074  88.041  1.00 43.91           N
ATOM   4343  CA  ASP B 401       6.196 -10.344  87.032  1.00 44.05           C
ATOM   4344  C   ASP B 401       5.606 -10.260  85.625  1.00 43.88           C
ATOM   4345  O   ASP B 401       4.388 -10.177  85.458  1.00 43.93           O
ATOM   4346  CB  ASP B 401       6.843 -11.717  87.269  1.00 44.27           C
ATOM   4347  CG  ASP B 401       5.852 -12.873  87.130  1.00 45.42           C
ATOM   4348  OD1 ASP B 401       4.777 -12.830  87.775  1.00 46.37           O
ATOM   4349  OD2 ASP B 401       6.159 -13.835  86.385  1.00 46.40           O
ATOM   4350  N   ASN B 402       6.481 -10.243  84.624  1.00 43.70           N
ATOM   4351  CA  ASN B 402       6.067 -10.419  83.243  1.00 43.53           C
ATOM   4352  C   ASN B 402       6.002 -11.918  82.994  1.00 43.56           C
ATOM   4353  O   ASN B 402       7.033 -12.594  83.033  1.00 43.58           O
ATOM   4354  CB  ASN B 402       7.058  -9.750  82.283  1.00 43.44           C
ATOM   4355  CG  ASN B 402       6.608  -9.803  80.827  1.00 43.21           C
ATOM   4356  OD1 ASN B 402       5.542 -10.331  80.506  1.00 43.76           O
ATOM   4357  ND2 ASN B 402       7.424  -9.248  79.940  1.00 42.61           N
ATOM   4358  N   PRO B 403       4.787 -12.451  82.767  1.00 43.51           N
ATOM   4359  CA  PRO B 403       4.658 -13.883  82.517  1.00 43.41           C
ATOM   4360  C   PRO B 403       5.164 -14.273  81.128  1.00 43.36           C
ATOM   4361  O   PRO B 403       5.332 -15.459  80.851  1.00 43.35           O
ATOM   4362  CB  PRO B 403       3.148 -14.119  82.626  1.00 43.42           C
ATOM   4363  CG  PRO B 403       2.538 -12.818  82.239  1.00 43.40           C
ATOM   4364  CD  PRO B 403       3.482 -11.761  82.737  1.00 43.45           C
ATOM   4365  N   LYS B 404       5.400 -13.281  80.270  1.00 43.25           N
ATOM   4366  CA  LYS B 404       5.856 -13.530  78.898  1.00 43.29           C
ATOM   4367  C   LYS B 404       7.365 -13.346  78.695  1.00 43.18           C
ATOM   4368  O   LYS B 404       7.899 -13.706  77.645  1.00 43.11           O
ATOM   4369  CB  LYS B 404       5.069 -12.674  77.897  1.00 43.20           C
ATOM   4370  CG  LYS B 404       3.594 -13.049  77.776  1.00 43.76           C
ATOM   4371  CD  LYS B 404       3.399 -14.420  77.142  1.00 44.35           C
ATOM   4372  CE  LYS B 404       1.998 -14.960  77.402  1.00 44.96           C
ATOM   4373  NZ  LYS B 404       0.967 -14.304  76.546  1.00 45.38           N
ATOM   4374  N   ALA B 405       8.039 -12.788  79.701  1.00 43.05           N
ATOM   4375  CA  ALA B 405       9.483 -12.562  79.655  1.00 42.95           C
ATOM   4376  C   ALA B 405      10.259 -13.872  79.541  1.00 42.96           C
ATOM   4377  O   ALA B 405      10.077 -14.790  80.351  1.00 43.00           O
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ATOM   4378  CB  ALA B 405       9.936 -11.782  80.881  1.00 42.92           C
ATOM   4379  N   SER B 406      11.133 -13.942  78.539  1.00 42.86           N
ATOM   4380  CA  SER B 406      11.881 -15.164  78.233  1.00 42.69           C
ATOM   4381  C   SER B 406      12.944 -15.521  79.283  1.00 42.54           C
ATOM   4382  O   SER B 406      13.562 -16.584  79.205  1.00 42.55           O
ATOM   4383  CB  SER B 406      12.502 -15.072  76.836  1.00 42.73           C
ATOM   4384  OG  SER B 406      13.423 -14.001  76.763  1.00 42.63           O
ATOM   4385  N   ASP B 407      13.140 -14.638  80.263  1.00 42.43           N
ATOM   4386  CA  ASP B 407      14.057 -14.881  81.383  1.00 42.09           C
ATOM   4387  C   ASP B 407      13.456 -14.316  82.671  1.00 42.12           C
ATOM   4388  O   ASP B 407      13.482 -13.101  82.884  1.00 42.19           O
ATOM   4389  CB  ASP B 407      15.432 -14.254  81.103  1.00 41.88           C
ATOM   4390  CG  ASP B 407      16.457 -14.531  82.205  1.00 41.41           C
ATOM   4391  OD1 ASP B 407      16.109 -15.118  83.253  1.00 40.91           O
ATOM   4392  OD2 ASP B 407      17.632 -14.154  82.013  1.00 40.70           O
ATOM   4393  N   PRO B 408      12.909 -15.196  83.534  1.00 42.01           N
ATOM   4394  CA  PRO B 408      12.267 -14.760  84.779  1.00 41.78           C
ATOM   4395  C   PRO B 408      13.180 -13.985  85.740  1.00 41.65           C
ATOM   4396  O   PRO B 408      12.686 -13.145  86.497  1.00 41.65           O
ATOM   4397  CB  PRO B 408      11.807 -16.077  85.417  1.00 41.81           C
ATOM   4398  CG  PRO B 408      11.694 -17.034  84.270  1.00 41.90           C
ATOM   4399  CD  PRO B 408      12.839 -16.660  83.375  1.00 42.12           C
ATOM   4400  N   SER B 409      14.486 -14.254  85.704  1.00 41.25           N
ATOM   4401  CA  SER B 409      15.439 -13.614  86.621  1.00 40.98           C
ATOM   4402  C   SER B 409      15.524 -12.099  86.433  1.00 40.65           C
ATOM   4403  O   SER B 409      15.719 -11.360  87.398  1.00 40.63           O
ATOM   4404  CB  SER B 409      16.832 -14.240  86.494  1.00 41.07           C
ATOM   4405  OG  SER B 409      17.441 -13.892  85.261  1.00 41.54           O
ATOM   4406  N   ILE B 410      15.382 -11.651  85.189  1.00 40.26           N
ATOM   4407  CA  ILE B 410      15.348 -10.223  84.867  1.00 39.83           C
ATOM   4408  C   ILE B 410      13.993  -9.813  84.277  1.00 39.58           C
ATOM   4409  O   ILE B 410      13.875  -8.776  83.626  1.00 39.49           O
ATOM   4410  CB  ILE B 410      16.492  -9.826  83.889  1.00 40.07           C
ATOM   4411  CG1 ILE B 410      16.392 -10.604  82.565  1.00 39.81           C
ATOM   4412  CG2 ILE B 410      17.859 -10.019  84.551  1.00 39.82           C
ATOM   4413  CD1 ILE B 410      17.123  -9.948  81.396  1.00 39.65           C
ATOM   4414  N   GLY B 411      12.972 -10.628  84.522  1.00 39.32           N
ATOM   4415  CA  GLY B 411      11.692 -10.475  83.838  1.00 39.13           C
ATOM   4416  C   GLY B 411      10.577  -9.865  84.659  1.00 38.89           C
ATOM   4417  O   GLY B 411       9.408 -10.222  84.488  1.00 38.80           O
ATOM   4418  N   SER B 412      10.934  -8.934  85.539  1.00 38.61           N
ATOM   4419  CA  SER B 412       9.958  -8.315  86.425  1.00 38.45           C
ATOM   4420  C   SER B 412      10.272  -6.847  86.663  1.00 38.34           C
ATOM   4421  O   SER B 412      11.442  -6.474  86.737  1.00 38.44           O
ATOM   4422  CB  SER B 412       9.906  -9.062  87.762  1.00 38.54           C
ATOM   4423  OG  SER B 412       9.226  -8.312  88.752  1.00 38.11           O
ATOM   4424  N   PRO B 413       9.224  -6.006  86.766  1.00 38.25           N
ATOM   4425  CA  PRO B 413       9.381  -4.645  87.269  1.00 38.04           C
ATOM   4426  C   PRO B 413       9.919  -4.707  88.689  1.00 38.02           C
ATOM   4427  O   PRO B 413       9.565  -5.616  89.441  1.00 38.02           O
ATOM   4428  CB  PRO B 413       7.952  -4.100  87.267  1.00 38.05           C
ATOM   4429  CG  PRO B 413       7.217  -4.945  86.295  1.00 38.13           C
ATOM   4430  CD  PRO B 413       7.829  -6.296  86.387  1.00 38.17           C
ATOM   4431  N   VAL B 414      10.756  -3.739  89.047  1.00 38.00           N
ATOM   4432  CA  VAL B 414      11.584  -3.829  90.241  1.00 38.01           C
ATOM   4433  C   VAL B 414      11.307  -2.723  91.265  1.00 38.24           C
ATOM   4434  O   VAL B 414      11.176  -1.548  90.916  1.00 38.31           O
ATOM   4435  CB  VAL B 414      13.100  -3.816  89.854  1.00 37.97           C
ATOM   4436  CG1 VAL B 414      14.000  -3.888  91.087  1.00 38.00           C
ATOM   4437  CG2 VAL B 414      13.429  -4.959  88.896  1.00 37.76           C
ATOM   4438  N   ASN B 415      11.204  -3.121  92.531  1.00 38.37           N
ATOM   4439  CA  ASN B 415      11.379  -2.204  93.650  1.00 38.54           C
ATOM   4440  C   ASN B 415      12.604  -2.646  94.428  1.00 38.73           C
ATOM   4441  O   ASN B 415      12.893  -3.839  94.499  1.00 38.71           O
ATOM   4442  CB  ASN B 415      10.143  -2.170  94.540  1.00 38.44           C
ATOM   4443  CG  ASN B 415       8.976  -1.478  93.879  1.00 38.66           C
ATOM   4444  OD1 ASN B 415       9.075  -0.319  93.468  1.00 38.26           O
ATOM   4445  ND2 ASN B 415       7.859  -2.186  93.765  1.00 39.63           N
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ATOM   4446  N   ILE B 416      13.332  -1.691  94.999  1.00 39.03           N
ATOM   4447  CA  ILE B 416      14.634  -1.985  95.601  1.00 39.28           C
ATOM   4448  C   ILE B 416      15.098  -0.855  96.521  1.00 39.52           C
ATOM   4449  O   ILE B 416      14.970   0.316  96.171  1.00 39.66           O
ATOM   4450  CB  ILE B 416      15.690  -2.306  94.495  1.00 39.29           C
ATOM   4451  CG1 ILE B 416      17.053  -2.656  95.096  1.00 39.12           C
ATOM   4452  CG2 ILE B 416      15.783  -1.174  93.458  1.00 39.35           C
ATOM   4453  CD1 ILE B 416      17.960  -3.371  94.122  1.00 38.77           C
ATOM   4454  N   ASP B 417      15.620  -1.221  97.696  1.00 39.86           N
ATOM   4455  CA  ASP B 417      16.148  -0.273  98.703  1.00 40.28           C
ATOM   4456  C   ASP B 417      15.056   0.593  99.325  1.00 40.68           C
ATOM   4457  O   ASP B 417      14.347   1.301  98.616  1.00 40.89           O
ATOM   4458  CB  ASP B 417      17.246   0.642  98.126  1.00 39.98           C
ATOM   4459  CG  ASP B 417      18.463  -0.121  97.620  1.00 39.77           C
ATOM   4460  OD1 ASP B 417      18.707  -1.270  98.055  1.00 39.27           O
ATOM   4461  OD2 ASP B 417      19.192   0.450  96.782  1.00 39.23           O
ATOM   4462  N   MET B 418      14.930   0.557 100.647  1.00 41.03           N
ATOM   4463  CA  MET B 418      13.948   1.406 101.315  1.00 41.62           C
ATOM   4464  C   MET B 418      14.532   2.235 102.456  1.00 41.60           C
ATOM   4465  O   MET B 418      15.510   1.841 103.101  1.00 41.31           O
ATOM   4466  CB  MET B 418      12.749   0.585 101.804  1.00 41.57           C
ATOM   4467  CG  MET B 418      13.014  -0.253 103.051  1.00 42.12           C
ATOM   4468  SD  MET B 418      11.604  -1.265 103.541  1.00 42.95           S
ATOM   4469  CE  MET B 418      10.501  -0.042 104.219  1.00 42.03           C
ATOM   4470  N   VAL B 419      13.923   3.398 102.672  1.00 41.88           N
ATOM   4471  CA  VAL B 419      14.166   4.214 103.855  1.00 42.05           C
ATOM   4472  C   VAL B 419      12.874   4.245 104.669  1.00 42.21           C
ATOM   4473  O   VAL B 419      11.789   4.432 104.113  1.00 41.92           O
ATOM   4474  CB  VAL B 419      14.605   5.658 103.488  1.00 42.04           C
ATOM   4475  CG1 VAL B 419      14.719   6.534 104.731  1.00 42.00           C
ATOM   4476  CG2 VAL B 419      15.925   5.648 102.746  1.00 42.11           C
ATOM   4477  N   LEU B 420      12.994   4.038 105.979  1.00 42.57           N
ATOM   4478  CA  LEU B 420      11.866   4.209 106.893  1.00 42.93           C
ATOM   4479  C   LEU B 420      12.037   5.482 107.707  1.00 43.21           C
ATOM   4480  O   LEU B 420      13.161   5.883 108.000  1.00 43.35           O
ATOM   4481  CB  LEU B 420      11.729   3.002 107.823  1.00 42.97           C
ATOM   4482  CG  LEU B 420      11.101   1.734 107.246  1.00 42.73           C
ATOM   4483  CD1 LEU B 420      11.460   0.525 108.092  1.00 42.83           C
ATOM   4484  CD2 LEU B 420       9.585   1.874 107.124  1.00 43.15           C
ATOM   4485  N   VAL B 421      10.923   6.118 108.057  1.00 43.75           N
ATOM   4486  CA  VAL B 421      10.935   7.322 108.898  1.00 44.40           C
ATOM   4487  C   VAL B 421       9.526   7.629 109.425  1.00 44.99           C
ATOM   4488  O   VAL B 421       8.532   7.289 108.776  1.00 45.16           O
ATOM   4489  CB  VAL B 421      11.540   8.549 108.140  1.00 44.28           C
ATOM   4490  CG1 VAL B 421      10.610   9.035 107.028  1.00 44.12           C
ATOM   4491  CG2 VAL B 421      11.903   9.678 109.105  1.00 44.04           C
ATOM   4492  N   GLN B 422       9.442   8.260 110.598  1.00 45.55           N
ATOM   4493  CA  GLN B 422       8.150   8.670 111.151  1.00 46.17           C
ATOM   4494  C   GLN B 422       8.069  10.164 111.475  1.00 46.61           C
ATOM   4495  O   GLN B 422       8.987  10.731 112.075  1.00 46.70           O
ATOM   4496  CB  GLN B 422       7.795   7.851 112.394  1.00 46.05           C
ATOM   4497  CG  GLN B 422       6.360   8.076 112.866  1.00 46.24           C
ATOM   4498  CD  GLN B 422       6.026   7.353 114.152  1.00 46.24           C
ATOM   4499  OE1 GLN B 422       6.860   7.225 115.052  1.00 45.64           O
ATOM   4500  NE2 GLN B 422       4.789   6.882 114.249  1.00 46.60           N
ATOM   4501  N   ASP B 423       6.960  10.786 111.074  1.00 47.04           N
ATOM   4502  CA  ASP B 423       6.656  12.161 111.462  1.00 47.59           C
ATOM   4503  C   ASP B 423       6.200  12.179 112.923  1.00 47.71           C
ATOM   4504  O   ASP B 423       5.211  11.530 113.265  1.00 47.74           O
ATOM   4505  CB  ASP B 423       5.575  12.756 110.549  1.00 47.68           C
ATOM   4506  CG  ASP B 423       5.374  14.250 110.769  1.00 48.46           C
ATOM   4507  OD1 ASP B 423       5.604  15.027 109.815  1.00 48.91           O
ATOM   4508  OD2 ASP B 423       4.994  14.654 111.892  1.00 49.14           O
ATOM   4509  N   PRO B 424       6.921  12.922 113.788  1.00 47.92           N
ATOM   4510  CA  PRO B 424       6.616  12.940 115.227  1.00 47.97           C
ATOM   4511  C   PRO B 424       5.249  13.547 115.574  1.00 47.86           C
ATOM   4512  O   PRO B 424       4.643  13.157 116.574  1.00 48.17           O
ATOM   4513  CB  PRO B 424       7.753  13.784 115.824  1.00 48.04           C
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ATOM   4514  CG  PRO B 424       8.254  14.619 114.694  1.00 48.06           C
ATOM   4515  CD  PRO B 424       8.073  13.783 113.458  1.00 48.02           C
ATOM   4516  N   GLU B 425       4.770  14.475 114.750  1.00 47.46           N
ATOM   4517  CA  GLU B 425       3.507  15.159 115.007  1.00 47.16           C
ATOM   4518  C   GLU B 425       2.303  14.416 114.429  1.00 46.87           C
ATOM   4519  O   GLU B 425       1.236  14.394 115.042  1.00 46.97           O
ATOM   4520  CB  GLU B 425       3.556  16.598 114.482  1.00 47.12           C
ATOM   4521  CG  GLU B 425       4.616  17.468 115.160  1.00 47.30           C
ATOM   4522  CD  GLU B 425       4.710  18.877 114.584  1.00 47.67           C
ATOM   4523  OE1 GLU B 425       4.028  19.176 113.576  1.00 47.76           O
ATOM   4524  OE2 GLU B 425       5.476  19.692 115.148  1.00 48.52           O
ATOM   4525  N   THR B 426       2.480  13.805 113.260  1.00 46.52           N
ATOM   4526  CA  THR B 426       1.393  13.105 112.561  1.00 46.07           C
ATOM   4527  C   THR B 426       1.399  11.595 112.822  1.00 45.59           C
ATOM   4528  O   THR B 426       0.370  10.932 112.680  1.00 45.48           O
ATOM   4529  CB  THR B 426       1.450  13.372 111.036  1.00 46.07           C
ATOM   4530  OG1 THR B 426       1.455  14.781 110.799  1.00 46.12           O
ATOM   4531  CG2 THR B 426       0.252  12.760 110.318  1.00 46.59           C
ATOM   4532  N   LYS B 427       2.560  11.064 113.204  1.00 45.07           N
ATOM   4533  CA  LYS B 427       2.752   9.626 113.465  1.00 44.76           C
ATOM   4534  C   LYS B 427       2.705   8.766 112.197  1.00 44.21           C
ATOM   4535  O   LYS B 427       2.760   7.535 112.267  1.00 44.22           O
ATOM   4536  CB  LYS B 427       1.764   9.093 114.522  1.00 44.77           C
ATOM   4537  CG  LYS B 427       1.578   9.976 115.749  1.00 45.36           C
ATOM   4538  CD  LYS B 427       2.877  10.242 116.482  1.00 46.44           C
ATOM   4539  CE  LYS B 427       2.604  10.927 117.811  1.00 47.45           C
ATOM   4540  NZ  LYS B 427       3.866  11.357 118.470  1.00 48.00           N
ATOM   4541  N   ARG B 428       2.608   9.421 111.044  1.00 43.60           N
ATOM   4542  CA  ARG B 428       2.651   8.738 109.761  1.00 42.88           C
ATOM   4543  C   ARG B 428       4.050   8.182 109.526  1.00 42.34           C
ATOM   4544  O   ARG B 428       5.051   8.883 109.697  1.00 42.25           O
ATOM   4545  CB  ARG B 428       2.239   9.686 108.630  1.00 42.98           C
ATOM   4546  CG  ARG B 428       2.139   9.026 107.259  1.00 42.73           C
ATOM   4547  CD  ARG B 428       1.397   9.904 106.269  1.00 42.52           C
ATOM   4548  NE  ARG B 428      -0.052   9.784 106.413  1.00 43.12           N
ATOM   4549  CZ  ARG B 428      -0.949  10.454 105.690  1.00 42.82           C
ATOM   4550  NH1 ARG B 428      -0.562  11.312 104.752  1.00 42.35           N
ATOM   4551  NH2 ARG B 428      -2.244  10.263 105.907  1.00 42.41           N
ATOM   4552  N   ILE B 429       4.100   6.907 109.161  1.00 41.66           N
ATOM   4553  CA  ILE B 429       5.351   6.219 108.882  1.00 41.07           C
ATOM   4554  C   ILE B 429       5.529   6.139 107.369  1.00 40.60           C
ATOM   4555  O   ILE B 429       4.619   5.719 106.647  1.00 40.85           O
ATOM   4556  CB  ILE B 429       5.371   4.807 109.528  1.00 41.23           C
ATOM   4557  CG1 ILE B 429       5.381   4.924 111.058  1.00 41.42           C
ATOM   4558  CG2 ILE B 429       6.577   3.994 109.054  1.00 41.11           C
ATOM   4559  CD1 ILE B 429       4.714   3.766 111.779  1.00 41.39           C
ATOM   4560  N   PHE B 430       6.698   6.560 106.897  1.00 39.78           N
ATOM   4561  CA  PHE B 430       6.987   6.591 105.468  1.00 38.90           C
ATOM   4562  C   PHE B 430       7.968   5.508 105.040  1.00 38.31           C
ATOM   4563  O   PHE B 430       8.939   5.212 105.736  1.00 38.19           O
ATOM   4564  CB  PHE B 430       7.525   7.965 105.057  1.00 39.03           C
ATOM   4565  CG  PHE B 430       6.533   9.079 105.224  1.00 38.86           C
ATOM   4566  CD1 PHE B 430       6.572   9.899 106.347  1.00 38.81           C
ATOM   4567  CD2 PHE B 430       5.552   9.304 104.263  1.00 38.79           C
ATOM   4568  CE1 PHE B 430       5.648  10.930 106.509  1.00 39.24           C
ATOM   4569  CE2 PHE B 430       4.626  10.334 104.410  1.00 38.59           C
ATOM   4570  CZ  PHE B 430       4.671  11.147 105.533  1.00 39.08           C
ATOM   4571  N   SER B 431       7.690   4.920 103.884  1.00 37.66           N
ATOM   4572  CA  SER B 431       8.615   4.017 103.226  1.00 36.94           C
ATOM   4573  C   SER B 431       8.901   4.574 101.834  1.00 36.48           C
ATOM   4574  O   SER B 431       8.025   4.575 100.965  1.00 36.50           O
ATOM   4575  CB  SER B 431       8.037   2.602 103.142  1.00 36.87           C
ATOM   4576  OG  SER B 431       8.873   1.759 102.363  1.00 36.72           O
ATOM   4577  N   ILE B 432      10.119   5.069 101.639  1.00 35.72           N
ATOM   4578  CA  ILE B 432      10.533   5.616 100.350  1.00 35.08           C
ATOM   4579  C   ILE B 432      11.556   4.689  99.691  1.00 34.61           C
ATOM   4580  O   ILE B 432      12.570   4.339 100.298  1.00 34.57           O
ATOM   4581  CB  ILE B 432      11.056   7.064 100.489  1.00 35.06           C
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ATOM   4582  CG1 ILE B 432       9.946   7.953 101.067  1.00 35.15           C
ATOM   4583  CG2 ILE B 432      11.542   7.596  99.141  1.00 34.85           C
ATOM   4584  CD1 ILE B 432      10.315   9.400 101.276  1.00 35.09           C
ATOM   4585  N   TYR B 433      11.272   4.291  98.453  1.00 33.98           N
ATOM   4586  CA  TYR B 433      12.040   3.247  97.779  1.00 33.66           C
ATOM   4587  C   TYR B 433      12.103   3.430  96.259  1.00 33.46           C
ATOM   4588  O   TYR B 433      11.307   4.170  95.687  1.00 33.49           O
ATOM   4589  CB  TYR B 433      11.480   1.862  98.143  1.00 33.40           C
ATOM   4590  CG  TYR B 433       9.983   1.751  98.008  1.00 33.48           C
ATOM   4591  CD1 TYR B 433       9.133   2.149  99.049  1.00 32.92           C
ATOM   4592  CD2 TYR B 433       9.408   1.250  96.840  1.00 33.35           C
ATOM   4593  CE1 TYR B 433       7.750   2.055  98.923  1.00 32.30           C
ATOM   4594  CE2 TYR B 433       8.024   1.149  96.707  1.00 33.17           C
ATOM   4595  CZ  TYR B 433       7.205   1.552  97.752  1.00 32.81           C
ATOM   4596  OH  TYR B 433       5.842   1.452  97.615  1.00 33.26           O
ATOM   4597  N   ASP B 434      13.057   2.746  95.625  1.00 33.34           N
ATOM   4598  CA  ASP B 434      13.297   2.837  94.181  1.00 33.25           C
ATOM   4599  C   ASP B 434      12.318   2.000  93.366  1.00 33.38           C
ATOM   4600  O   ASP B 434      11.755   1.024  93.863  1.00 33.52           O
ATOM   4601  CB  ASP B 434      14.714   2.364  93.832  1.00 33.11           C
ATOM   4602  CG  ASP B 434      15.801   3.189  94.495  1.00 32.44           C
ATOM   4603  OD1 ASP B 434      15.482   4.133  95.247  1.00 32.26           O
ATOM   4604  OD2 ASP B 434      16.985   2.887  94.252  1.00 31.33           O
ATOM   4605  N   MET B 435      12.140   2.390  92.106  1.00 33.36           N
ATOM   4606  CA  MET B 435      11.384   1.608  91.135  1.00 33.42           C
ATOM   4607  C   MET B 435      12.000   1.701  89.738  1.00 33.41           C
ATOM   4608  O   MET B 435      12.449   2.772  89.309  1.00 33.36           O
ATOM   4609  CB  MET B 435       9.894   1.991  91.156  1.00 33.47           C
ATOM   4610  CG  MET B 435       9.305   2.506  89.848  1.00 33.80           C
ATOM   4611  SD  MET B 435       8.874   1.282  88.608  1.00 34.05           S
ATOM   4612  CE  MET B 435       7.995   2.306  87.453  1.00 34.26           C
ATOM   4613  N   PHE B 436      12.040   0.557  89.059  1.00 33.36           N
ATOM   4614  CA  PHE B 436      12.452   0.459  87.664  1.00 33.44           C
ATOM   4615  C   PHE B 436      11.429  -0.431  86.964  1.00 33.66           C
ATOM   4616  O   PHE B 436      10.896  -1.350  87.586  1.00 33.75           O
ATOM   4617  CB  PHE B 436      13.815  -0.233  87.536  1.00 33.45           C
ATOM   4618  CG  PHE B 436      14.945   0.463  88.245  1.00 33.20           C
ATOM   4619  CD1 PHE B 436      15.785   1.330  87.553  1.00 32.88           C
ATOM   4620  CD2 PHE B 436      15.203   0.210  89.592  1.00 33.08           C
ATOM   4621  CE1 PHE B 436      16.849   1.961  88.197  1.00 32.90           C
ATOM   4622  CE2 PHE B 436      16.263   0.839  90.250  1.00 33.05           C
ATOM   4623  CZ  PHE B 436      17.086   1.717  89.552  1.00 33.19           C
ATOM   4624  N   PRO B 437      11.147  -0.173  85.672  1.00 33.93           N
ATOM   4625  CA  PRO B 437      10.384  -1.171  84.915  1.00 34.23           C
ATOM   4626  C   PRO B 437      11.194  -2.466  84.749  1.00 34.66           C
ATOM   4627  O   PRO B 437      12.294  -2.576  85.298  1.00 34.72           O
ATOM   4628  CB  PRO B 437      10.141  -0.486  83.560  1.00 34.19           C
ATOM   4629  CG  PRO B 437      11.177   0.575  83.458  1.00 33.99           C
ATOM   4630  CD  PRO B 437      11.485   1.011  84.857  1.00 33.99           C
ATOM   4631  N   GLU B 438      10.648  -3.432  84.012  1.00 35.09           N
ATOM   4632  CA  GLU B 438      11.306  -4.721  83.772  1.00 35.54           C
ATOM   4633  C   GLU B 438      12.744  -4.561  83.286  1.00 35.91           C
ATOM   4634  O   GLU B 438      13.003  -3.798  82.352  1.00 35.98           O
ATOM   4635  CB  GLU B 438      10.504  -5.532  82.749  1.00 35.53           C
ATOM   4636  CG  GLU B 438      11.076  -6.907  82.438  1.00 35.32           C
ATOM   4637  CD  GLU B 438      10.459  -7.543  81.207  1.00 35.70           C
ATOM   4638  OE1 GLU B 438       9.307  -7.205  80.846  1.00 35.92           O
ATOM   4639  OE2 GLU B 438      11.133  -8.393  80.596  1.00 36.39           O
ATOM   4640  N   GLY B 439      13.669  -5.282  83.918  1.00 36.29           N
ATOM   4641  CA  GLY B 439      15.078  -5.247  83.522  1.00 36.74           C
ATOM   4642  C   GLY B 439      16.054  -5.413  84.671  1.00 37.05           C
ATOM   4643  O   GLY B 439      15.713  -5.991  85.701  1.00 37.39           O
ATOM   4644  N   LYS B 440      17.270  -4.897  84.491  1.00 37.23           N
ATOM   4645  CA  LYS B 440      18.347  -5.063  85.467  1.00 37.34           C
ATOM   4646  C   LYS B 440      18.514  -3.858  86.396  1.00 37.39           C
ATOM   4647  O   LYS B 440      19.603  -3.632  86.932  1.00 37.44           O
ATOM   4648  CB  LYS B 440      19.673  -5.353  84.758  1.00 37.60           C
ATOM   4649  CG  LYS B 440      19.750  -6.708  84.066  1.00 38.31           C
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ATOM   4650  CD  LYS B 440      21.197  -7.103  83.820  1.00 39.59           C
ATOM   4651  CE  LYS B 440      21.304  -8.437  83.095  1.00 40.85           C
ATOM   4652  NZ  LYS B 440      22.727  -8.871  82.959  1.00 41.75           N
ATOM   4653  N   GLY B 441      17.432  -3.103  86.584  1.00 37.36           N
ATOM   4654  CA  GLY B 441      17.397  -1.902  87.428  1.00 37.38           C
ATOM   4655  C   GLY B 441      18.701  -1.399  88.019  1.00 37.43           C
ATOM   4656  O   GLY B 441      19.137  -1.893  89.059  1.00 37.93           O
ATOM   4657  N   ILE B 442      19.292  -0.397  87.365  1.00 37.12           N
ATOM   4658  CA  ILE B 442      20.606   0.217  87.695  1.00 36.85           C
ATOM   4659  C   ILE B 442      21.714  -0.322  86.799  1.00 36.60           C
ATOM   4660  O   ILE B 442      22.546   0.445  86.314  1.00 36.66           O
ATOM   4661  CB  ILE B 442      21.033   0.176  89.216  1.00 36.85           C
ATOM   4662  CG1 ILE B 442      22.172   1.158  89.495  1.00 36.91           C
ATOM   4663  CG2 ILE B 442      21.530  -1.196  89.648  1.00 37.08           C
ATOM   4664  CD1 ILE B 442      21.737   2.522  89.916  1.00 36.32           C
ATOM   4665  N   PHE B 443      21.714  -1.636  86.581  1.00 36.28           N
ATOM   4666  CA  PHE B 443      22.712  -2.274  85.729  1.00 35.92           C
ATOM   4667  C   PHE B 443      22.150  -2.517  84.332  1.00 35.65           C
ATOM   4668  O   PHE B 443      22.766  -3.209  83.512  1.00 35.62           O
ATOM   4669  CB  PHE B 443      23.218  -3.580  86.361  1.00 35.91           C
ATOM   4670  CG  PHE B 443      23.990  -3.380  87.641  1.00 35.91           C
ATOM   4671  CD1 PHE B 443      25.203  -2.692  87.642  1.00 35.97           C
ATOM   4672  CD2 PHE B 443      23.511  -3.886  88.844  1.00 35.84           C
ATOM   4673  CE1 PHE B 443      25.918  -2.503  88.824  1.00 36.17           C
ATOM   4674  CE2 PHE B 443      24.218  -3.702  90.034  1.00 36.48           C
ATOM   4675  CZ  PHE B 443      25.423  -3.008  90.024  1.00 36.25           C
ATOM   4676  N   GLY B 444      20.982  -1.935  84.066  1.00 35.22           N
ATOM   4677  CA  GLY B 444      20.315  -2.098  82.780  1.00 34.80           C
ATOM   4678  C   GLY B 444      19.541  -0.875  82.338  1.00 34.37           C
ATOM   4679  O   GLY B 444      18.461  -1.001  81.763  1.00 34.54           O
ATOM   4680  N   MET B 445      20.087   0.308  82.608  1.00 34.03           N
ATOM   4681  CA  MET B 445      19.431   1.564  82.233  1.00 33.52           C
ATOM   4682  C   MET B 445      19.783   1.952  80.799  1.00 33.70           C
ATOM   4683  O   MET B 445      20.933   1.797  80.372  1.00 33.63           O
ATOM   4684  CB  MET B 445      19.811   2.692  83.194  1.00 33.54           C
ATOM   4685  CG  MET B 445      19.372   2.472  84.640  1.00 32.48           C
ATOM   4686  SD  MET B 445      19.571   3.957  85.644  1.00 32.50           S
ATOM   4687  CE  MET B 445      18.191   4.946  85.068  1.00 30.52           C
ATOM   4688  N   SER B 446      18.787   2.455  80.066  1.00 33.53           N
ATOM   4689  CA  SER B 446      18.972   2.849  78.669  1.00 33.44           C
ATOM   4690  C   SER B 446      20.060   3.900  78.536  1.00 33.20           C
ATOM   4691  O   SER B 446      20.272   4.708  79.442  1.00 33.38           O
ATOM   4692  CB  SER B 446      17.663   3.358  78.058  1.00 33.62           C
ATOM   4693  OG  SER B 446      17.243   4.574  78.662  1.00 34.60           O
ATOM   4694  N   SER B 447      20.756   3.874  77.406  1.00 32.93           N
ATOM   4695  CA  SER B 447      21.834   4.819  77.136  1.00 32.43           C
ATOM   4696  C   SER B 447      21.303   6.232  76.860  1.00 31.90           C
ATOM   4697  O   SER B 447      21.964   7.228  77.166  1.00 31.98           O
ATOM   4698  CB  SER B 447      22.663   4.328  75.950  1.00 32.43           C
ATOM   4699  OG  SER B 447      23.616   5.300  75.560  1.00 32.99           O
ATOM   4700  N   GLN B 448      20.114   6.306  76.275  1.00 31.04           N
ATOM   4701  CA  GLN B 448      19.528   7.580  75.882  1.00 30.44           C
ATOM   4702  C   GLN B 448      18.304   7.935  76.734  1.00 30.21           C
ATOM   4703  O   GLN B 448      17.587   7.051  77.222  1.00 29.99           O
ATOM   4704  CB  GLN B 448      19.171   7.557  74.390  1.00 30.25           C
ATOM   4705  CG  GLN B 448      20.369   7.357  73.452  1.00 29.72           C
ATOM   4706  CD  GLN B 448      21.385   8.485  73.523  1.00 29.84           C
ATOM   4707  OE1 GLN B 448      21.045   9.664  73.376  1.00 29.89           O
ATOM   4708  NE2 GLN B 448      22.640   8.127  73.749  1.00 28.51           N
ATOM   4709  N   LYS B 449      18.073   9.230  76.916  1.00 29.98           N
ATOM   4710  CA  LYS B 449      16.954   9.686  77.738  1.00 29.95           C
ATOM   4711  C   LYS B 449      15.608   9.537  77.038  1.00 29.80           C
ATOM   4712  O   LYS B 449      15.438   9.939  75.890  1.00 29.38           O
ATOM   4713  CB  LYS B 449      17.138  11.137  78.197  1.00 29.83           C
ATOM   4714  CG  LYS B 449      16.032  11.607  79.130  1.00 30.25           C
ATOM   4715  CD  LYS B 449      16.163  13.067  79.497  1.00 31.70           C
ATOM   4716  CE  LYS B 449      15.244  13.416  80.672  1.00 32.38           C
ATOM   4717  NZ  LYS B 449      15.728  12.839  81.963  1.00 32.40           N
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ATOM   4718  N   GLU B 450      14.672   8.929  77.754  1.00 29.99           N
ATOM   4719  CA  GLU B 450      13.263   8.988  77.420  1.00 30.50           C
ATOM   4720  C   GLU B 450      12.602   9.872  78.465  1.00 30.16           C
ATOM   4721  O   GLU B 450      12.758   9.638  79.658  1.00 29.76           O
ATOM   4722  CB  GLU B 450      12.656   7.584  77.438  1.00 30.48           C
ATOM   4723  CG  GLU B 450      13.186   6.663  76.336  1.00 31.38           C
ATOM   4724  CD  GLU B 450      12.707   5.221  76.468  1.00 31.45           C
ATOM   4725  OE1 GLU B 450      11.728   4.967  77.200  1.00 33.27           O
ATOM   4726  OE2 GLU B 450      13.313   4.332  75.836  1.00 32.81           O
ATOM   4727  N   GLU B 451      11.897  10.910  78.025  1.00 30.50           N
ATOM   4728  CA  GLU B 451      11.148  11.755  78.960  1.00 30.86           C
ATOM   4729  C   GLU B 451      10.071  10.917  79.639  1.00 30.54           C
ATOM   4730  O   GLU B 451       9.367  10.155  78.984  1.00 30.46           O
ATOM   4731  CB  GLU B 451      10.532  12.953  78.245  1.00 31.09           C
ATOM   4732  CG  GLU B 451      11.487  14.124  78.062  1.00 33.25           C
ATOM   4733  CD  GLU B 451      11.411  14.725  76.671  1.00 35.64           C
ATOM   4734  OE1 GLU B 451      10.370  14.561  75.997  1.00 37.37           O
ATOM   4735  OE2 GLU B 451      12.397  15.359  76.242  1.00 36.47           O
ATOM   4736  N   ALA B 452       9.972  11.040  80.956  1.00 30.40           N
ATOM   4737  CA  ALA B 452       9.052  10.217  81.733  1.00 30.30           C
ATOM   4738  C   ALA B 452       7.769  10.960  82.095  1.00 30.37           C
ATOM   4739  O   ALA B 452       6.736  10.336  82.351  1.00 30.33           O
ATOM   4740  CB  ALA B 452       9.744   9.691  82.984  1.00 30.05           C
ATOM   4741  N   TYR B 453       7.846  12.287  82.128  1.00 30.43           N
ATOM   4742  CA  TYR B 453       6.715  13.119  82.525  1.00 30.99           C
ATOM   4743  C   TYR B 453       6.550  14.320  81.614  1.00 31.27           C
ATOM   4744  O   TYR B 453       7.487  14.729  80.932  1.00 31.25           O
ATOM   4745  CB  TYR B 453       6.864  13.592  83.976  1.00 30.93           C
ATOM   4746  CG  TYR B 453       7.074  12.472  84.957  1.00 31.11           C
ATOM   4747  CD1 TYR B 453       8.361  12.067  85.309  1.00 30.25           C
ATOM   4748  CD2 TYR B 453       5.987  11.803  85.527  1.00 30.70           C
ATOM   4749  CE1 TYR B 453       8.563  11.030  86.198  1.00 30.30           C
ATOM   4750  CE2 TYR B 453       6.182  10.764  86.431  1.00 30.41           C
ATOM   4751  CZ  TYR B 453       7.474  10.386  86.758  1.00 30.49           C
ATOM   4752  OH  TYR B 453       7.690   9.363  87.646  1.00 31.20           O
ATOM   4753  N   LYS B 454       5.354  14.892  81.626  1.00 31.89           N
ATOM   4754  CA  LYS B 454       5.025  16.001  80.750  1.00 32.58           C
ATOM   4755  C   LYS B 454       3.950  16.879  81.394  1.00 33.26           C
ATOM   4756  O   LYS B 454       2.910  16.379  81.823  1.00 33.15           O
ATOM   4757  CB  LYS B 454       4.561  15.438  79.402  1.00 32.49           C
ATOM   4758  CG  LYS B 454       4.107  16.452  78.384  1.00 32.56           C
ATOM   4759  CD  LYS B 454       3.977  15.807  77.022  1.00 31.87           C
ATOM   4760  CE  LYS B 454       3.069  16.622  76.116  1.00 32.11           C
ATOM   4761  NZ  LYS B 454       3.465  18.049  76.012  1.00 31.33           N
ATOM   4762  N   LYS B 455       4.211  18.185  81.456  1.00 34.32           N
ATOM   4763  CA  LYS B 455       3.249  19.160  81.990  1.00 35.28           C
ATOM   4764  C   LYS B 455       2.273  19.646  80.927  1.00 35.80           C
ATOM   4765  O   LYS B 455       2.685  20.083  79.852  1.00 35.93           O
ATOM   4766  CB  LYS B 455       3.965  20.362  82.605  1.00 35.33           C
ATOM   4767  CG  LYS B 455       4.766  20.042  83.850  1.00 36.66           C
ATOM   4768  CD  LYS B 455       5.255  21.301  84.557  1.00 38.54           C
ATOM   4769  CE  LYS B 455       4.135  21.974  85.340  1.00 39.34           C
ATOM   4770  NZ  LYS B 455       4.666  22.850  86.426  1.00 40.66           N
ATOM   4771  N   ILE B 456       0.980  19.559  81.238  1.00 36.57           N
ATOM   4772  CA  ILE B 456      -0.091  20.028  80.348  1.00 37.07           C
ATOM   4773  C   ILE B 456      -1.124  20.807  81.170  1.00 37.88           C
ATOM   4774  O   ILE B 456      -1.849  20.221  81.986  1.00 37.96           O
ATOM   4775  CB  ILE B 456      -0.770  18.857  79.598  1.00 36.98           C
ATOM   4776  CG1 ILE B 456       0.270  18.072  78.779  1.00 36.71           C
ATOM   4777  CG2 ILE B 456      -1.910  19.384  78.711  1.00 36.71           C
ATOM   4778  CD1 ILE B 456      -0.165  16.689  78.328  1.00 36.48           C
ATOM   4779  N   ASP B 457      -1.186  22.123  80.944  1.00 38.64           N
ATOM   4780  CA  ASP B 457      -1.851  23.062  81.867  1.00 39.37           C
ATOM   4781  C   ASP B 457      -1.327  22.769  83.265  1.00 39.46           C
ATOM   4782  O   ASP B 457      -2.039  22.916  84.257  1.00 39.56           O
ATOM   4783  CB  ASP B 457      -3.376  22.923  81.813  1.00 39.57           C
ATOM   4784  CG  ASP B 457      -3.917  22.972  80.398  1.00 40.79           C
ATOM   4785  OD1 ASP B 457      -3.128  23.241  79.461  1.00 42.03           O
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ATOM   4786  OD2 ASP B 457      -5.133  22.740  80.219  1.00 42.20           O
ATOM   4787  N   GLY B 458      -0.052  22.381  83.298  1.00 39.55           N
ATOM   4788  CA  GLY B 458       0.573  21.615  84.374  1.00 39.46           C
ATOM   4789  C   GLY B 458       0.073  21.788  85.789  1.00 39.17           C
ATOM   4790  O   GLY B 458       0.055  22.911  86.279  1.00 39.56           O
ATOM   4791  N   LYS B 459      -0.352  20.714  86.466  1.00 38.81           N
ATOM   4792  CA  LYS B 459      -0.598  19.340  85.944  1.00 38.18           C
ATOM   4793  C   LYS B 459       0.530  18.567  85.236  1.00 37.41           C
ATOM   4794  O   LYS B 459       0.747  18.697  84.029  1.00 37.24           O
ATOM   4795  CB  LYS B 459      -1.910  19.260  85.149  1.00 38.40           C
ATOM   4796  CG  LYS B 459      -3.164  19.382  86.004  1.00 39.14           C
ATOM   4797  CD  LYS B 459      -4.378  19.701  85.140  1.00 40.66           C
ATOM   4798  CE  LYS B 459      -5.593  20.074  85.979  1.00 41.66           C
ATOM   4799  NZ  LYS B 459      -6.784  20.335  85.109  1.00 42.45           N
ATOM   4800  N   THR B 460       1.213  17.734  86.013  1.00 36.61           N
ATOM   4801  CA  THR B 460       2.243  16.843  85.505  1.00 35.78           C
ATOM   4802  C   THR B 460       1.669  15.437  85.356  1.00 35.31           C
ATOM   4803  O   THR B 460       1.131  14.884  86.315  1.00 35.25           O
ATOM   4804  CB  THR B 460       3.460  16.799  86.466  1.00 35.88           C
ATOM   4805  OG1 THR B 460       3.802  18.131  86.874  1.00 35.23           O
ATOM   4806  CG2 THR B 460       4.663  16.134  85.799  1.00 35.20           C
ATOM   4807  N   TYR B 461       1.779  14.869  84.155  1.00 34.57           N
ATOM   4808  CA  TYR B 461       1.353  13.491  83.898  1.00 34.01           C
ATOM   4809  C   TYR B 461       2.537  12.599  83.527  1.00 33.40           C
ATOM   4810  O   TYR B 461       3.538  13.083  82.997  1.00 33.22           O
ATOM   4811  CB  TYR B 461       0.335  13.432  82.754  1.00 34.36           C
ATOM   4812  CG  TYR B 461      -0.893  14.290  82.919  1.00 34.82           C
ATOM   4813  CD1 TYR B 461      -1.894  13.947  83.829  1.00 35.48           C
ATOM   4814  CD2 TYR B 461      -1.071  15.433  82.144  1.00 35.18           C
ATOM   4815  CE1 TYR B 461      -3.039  14.730  83.975  1.00 35.41           C
ATOM   4816  CE2 TYR B 461      -2.209  16.226  82.285  1.00 35.95           C
ATOM   4817  CZ  TYR B 461      -3.190  15.865  83.199  1.00 35.55           C
ATOM   4818  OH  TYR B 461      -4.318  16.641  83.335  1.00 35.74           O
ATOM   4819  N   GLN B 462       2.405  11.296  83.779  1.00 32.74           N
ATOM   4820  CA  GLN B 462       3.404  10.323  83.332  1.00 32.07           C
ATOM   4821  C   GLN B 462       3.195   9.932  81.869  1.00 31.52           C
ATOM   4822  O   GLN B 462       2.067   9.696  81.436  1.00 31.54           O
ATOM   4823  CB  GLN B 462       3.430   9.076  84.227  1.00 32.05           C
ATOM   4824  CG  GLN B 462       4.485   8.047  83.783  1.00 32.29           C
ATOM   4825  CD  GLN B 462       4.782   6.975  84.816  1.00 32.12           C
ATOM   4826  OE1 GLN B 462       3.886   6.469  85.496  1.00 32.22           O
ATOM   4827  NE2 GLN B 462       6.050   6.609  84.921  1.00 31.17           N
ATOM   4828  N   ILE B 463       4.298   9.864  81.126  1.00 30.80           N
ATOM   4829  CA  ILE B 463       4.284   9.542  79.702  1.00 29.98           C
ATOM   4830  C   ILE B 463       4.232   8.031  79.448  1.00 29.91           C
ATOM   4831  O   ILE B 463       4.788   7.234  80.210  1.00 29.63           O
ATOM   4832  CB  ILE B 463       5.517  10.159  78.973  1.00 29.94           C
ATOM   4833  CG1 ILE B 463       5.475  11.694  79.047  1.00 29.77           C
ATOM   4834  CG2 ILE B 463       5.604   9.676  77.521  1.00 28.94           C
ATOM   4835  CD1 ILE B 463       6.773  12.383  78.647  1.00 29.46           C
ATOM   4836  N   LEU B 464       3.539   7.659  78.375  1.00 29.71           N
ATOM   4837  CA  LEU B 464       3.570   6.309  77.838  1.00 29.69           C
ATOM   4838  C   LEU B 464       4.056   6.368  76.404  1.00 29.90           C
ATOM   4839  O   LEU B 464       3.686   7.268  75.663  1.00 29.74           O
ATOM   4840  CB  LEU B 464       2.180   5.683  77.849  1.00 29.33           C
ATOM   4841  CG  LEU B 464       1.568   5.259  79.176  1.00 29.13           C
ATOM   4842  CD1 LEU B 464       0.138   4.790  78.935  1.00 27.98           C
ATOM   4843  CD2 LEU B 464       2.397   4.170  79.842  1.00 27.91           C
ATOM   4844  N   TYR B 465       4.882   5.411  76.009  1.00 30.23           N
ATOM   4845  CA  TYR B 465       5.259   5.291  74.607  1.00 30.74           C
ATOM   4846  C   TYR B 465       4.544   4.100  73.985  1.00 31.47           C
ATOM   4847  O   TYR B 465       4.414   3.043  74.614  1.00 31.49           O
ATOM   4848  CB  TYR B 465       6.777   5.181  74.455  1.00 30.18           C
ATOM   4849  CG  TYR B 465       7.498   6.366  75.037  1.00 29.58           C
ATOM   4850  CD1 TYR B 465       7.651   7.541  74.301  1.00 29.46           C
ATOM   4851  CD2 TYR B 465       7.996   6.332  76.336  1.00 28.89           C
ATOM   4852  CE1 TYR B 465       8.301   8.644  74.839  1.00 28.84           C
ATOM   4853  CE2 TYR B 465       8.647   7.429  76.881  1.00 28.47           C
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ATOM   4854  CZ  TYR B 465       8.797   8.580  76.128  1.00 28.72           C
ATOM   4855  OH  TYR B 465       9.437   9.675  76.662  1.00 29.00           O
ATOM   4856  N   ARG B 466       4.056   4.294  72.763  1.00 32.45           N
ATOM   4857  CA  ARG B 466       3.381   3.237  72.030  1.00 33.40           C
ATOM   4858  C   ARG B 466       4.256   2.657  70.927  1.00 34.15           C
ATOM   4859  O   ARG B 466       4.791   3.395  70.095  1.00 34.29           O
ATOM   4860  CB  ARG B 466       2.059   3.717  71.440  1.00 33.33           C
ATOM   4861  CG  ARG B 466       1.193   2.557  71.021  1.00 34.23           C
ATOM   4862  CD  ARG B 466       0.012   2.942  70.177  1.00 35.97           C
ATOM   4863  NE  ARG B 466      -0.633   1.724  69.697  1.00 36.79           N
ATOM   4864  CZ  ARG B 466      -1.940   1.570  69.514  1.00 37.11           C
ATOM   4865  NH1 ARG B 466      -2.783   2.567  69.767  1.00 37.21           N
ATOM   4866  NH2 ARG B 466      -2.402   0.402  69.085  1.00 37.38           N
ATOM   4867  N   GLU B 467       4.381   1.330  70.936  1.00 34.93           N
ATOM   4868  CA  GLU B 467       5.103   0.581  69.915  1.00 35.83           C
ATOM   4869  C   GLU B 467       4.826   1.103  68.503  1.00 35.98           C
ATOM   4870  O   GLU B 467       3.688   1.067  68.036  1.00 36.09           O
ATOM   4871  CB  GLU B 467       4.726  -0.903  70.014  1.00 36.19           C
ATOM   4872  CG  GLU B 467       5.314  -1.802  68.918  1.00 38.01           C
ATOM   4873  CD  GLU B 467       6.831  -1.939  68.997  1.00 40.27           C
ATOM   4874  OE1 GLU B 467       7.423  -1.590  70.047  1.00 41.05           O
ATOM   4875  OE2 GLU B 467       7.432  -2.402  68.001  1.00 41.08           O
ATOM   4876  N   GLY B 468       5.873   1.591  67.840  1.00 36.19           N
ATOM   4877  CA  GLY B 468       5.777   2.054  66.455  1.00 36.30           C
ATOM   4878  C   GLY B 468       5.671   3.558  66.287  1.00 36.54           C
ATOM   4879  O   GLY B 468       5.831   4.078  65.180  1.00 36.46           O
ATOM   4880  N   GLU B 469       5.414   4.262  67.386  1.00 36.66           N
ATOM   4881  CA  GLU B 469       5.095   5.686  67.327  1.00 36.87           C
ATOM   4882  C   GLU B 469       6.022   6.539  68.173  1.00 36.60           C
ATOM   4883  O   GLU B 469       6.403   6.164  69.281  1.00 36.69           O
ATOM   4884  CB  GLU B 469       3.651   5.941  67.782  1.00 36.79           C
ATOM   4885  CG  GLU B 469       2.573   5.369  66.871  1.00 37.40           C
ATOM   4886  CD  GLU B 469       1.192   5.345  67.525  1.00 37.81           C
ATOM   4887  OE1 GLU B 469       0.831   6.325  68.231  1.00 37.58           O
ATOM   4888  OE2 GLU B 469       0.465   4.340  67.320  1.00 38.70           O
ATOM   4889  N   LYS B 470       6.373   7.696  67.633  1.00 36.48           N
ATOM   4890  CA  LYS B 470       6.975   8.757  68.413  1.00 36.30           C
ATOM   4891  C   LYS B 470       5.826   9.631  68.916  1.00 36.13           C
ATOM   4892  O   LYS B 470       4.807   9.782  68.238  1.00 36.19           O
ATOM   4893  CB  LYS B 470       7.926   9.566  67.534  1.00 36.19           C
ATOM   4894  CG  LYS B 470       8.718  10.625  68.260  1.00 36.27           C
ATOM   4895  CD  LYS B 470       9.273  11.640  67.279  1.00 36.32           C
ATOM   4896  CE  LYS B 470       9.785  12.870  68.006  1.00 36.29           C
ATOM   4897  NZ  LYS B 470      10.563  13.752  67.100  1.00 36.45           N
ATOM   4898  N   GLY B 471       5.975  10.198  70.104  1.00 35.90           N
ATOM   4899  CA  GLY B 471       4.942  11.075  70.634  1.00 35.64           C
ATOM   4900  C   GLY B 471       4.578  10.719  72.055  1.00 35.48           C
ATOM   4901  O   GLY B 471       4.726   9.566  72.466  1.00 35.30           O
ATOM   4902  N   ALA B 472       4.094  11.720  72.790  1.00 35.40           N
ATOM   4903  CA  ALA B 472       3.771  11.595  74.211  1.00 35.25           C
ATOM   4904  C   ALA B 472       2.863  10.412  74.543  1.00 35.06           C
ATOM   4905  O   ALA B 472       3.354   9.306  74.740  1.00 35.26           O
ATOM   4906  CB  ALA B 472       3.173  12.898  74.744  1.00 35.50           C
ATOM   4907  N   TYR B 473       1.550  10.636  74.570  1.00 34.61           N
ATOM   4908  CA  TYR B 473       0.609   9.740  75.264  1.00 34.04           C
ATOM   4909  C   TYR B 473       0.791   9.975  76.752  1.00 33.49           C
ATOM   4910  O   TYR B 473       1.896   9.818  77.281  1.00 33.38           O
ATOM   4911  CB  TYR B 473       0.835   8.252  74.956  1.00 34.06           C
ATOM   4912  CG  TYR B 473       0.309   7.770  73.626  1.00 34.41           C
ATOM   4913  CD1 TYR B 473      -1.061   7.588  73.417  1.00 34.80           C
ATOM   4914  CD2 TYR B 473       1.181   7.460  72.584  1.00 34.04           C
ATOM   4915  CE1 TYR B 473      -1.547   7.136  72.190  1.00 34.66           C
ATOM   4916  CE2 TYR B 473       0.709   7.011  71.363  1.00 34.05           C
ATOM   4917  CZ  TYR B 473      -0.654   6.849  71.169  1.00 34.50           C
ATOM   4918  OH  TYR B 473      -1.123   6.398  69.955  1.00 34.72           O
ATOM   4919  N   THR B 474      -0.289  10.359  77.423  1.00 32.90           N
ATOM   4920  CA  THR B 474      -0.226  10.685  78.847  1.00 32.46           C
ATOM   4921  C   THR B 474      -1.267   9.925  79.664  1.00 32.34           C
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ATOM   4922  O   THR B 474      -2.323   9.541  79.149  1.00 32.27           O
ATOM   4923  CB  THR B 474      -0.366  12.208  79.095  1.00 32.36           C
ATOM   4924  OG1 THR B 474      -1.451  12.732  78.317  1.00 32.38           O
ATOM   4925  CG2 THR B 474       0.921  12.935  78.716  1.00 31.91           C
ATOM   4926  N   ILE B 475      -0.945   9.690  80.932  1.00 32.13           N
ATOM   4927  CA  ILE B 475      -1.875   9.071  81.865  1.00 32.23           C
ATOM   4928  C   ILE B 475      -2.573  10.182  82.643  1.00 32.32           C
ATOM   4929  O   ILE B 475      -1.971  10.785  83.531  1.00 32.34           O
ATOM   4930  CB  ILE B 475      -1.155   8.112  82.850  1.00 32.18           C
ATOM   4931  CG1 ILE B 475      -0.360   7.047  82.086  1.00 32.06           C
ATOM   4932  CG2 ILE B 475      -2.159   7.476  83.805  1.00 32.01           C
ATOM   4933  CD1 ILE B 475       0.395   6.082  82.966  1.00 32.32           C
ATOM   4934  N   ARG B 476      -3.835  10.455  82.307  1.00 32.44           N
ATOM   4935  CA  ARG B 476      -4.577  11.541  82.961  1.00 32.75           C
ATOM   4936  C   ARG B 476      -5.585  11.033  84.000  1.00 32.95           C
ATOM   4937  O   ARG B 476      -5.357   9.984  84.607  1.00 32.95           O
ATOM   4938  CB  ARG B 476      -5.200  12.485  81.926  1.00 32.71           C
ATOM   4939  CG  ARG B 476      -4.186  12.954  80.884  1.00 32.71           C
ATOM   4940  CD  ARG B 476      -4.686  14.131  80.074  1.00 33.01           C
ATOM   4941  NE  ARG B 476      -3.853  14.372  78.894  1.00 31.63           N
ATOM   4942  CZ  ARG B 476      -4.011  15.403  78.070  1.00 31.97           C
ATOM   4943  NH1 ARG B 476      -4.971  16.297  78.299  1.00 32.00           N
ATOM   4944  NH2 ARG B 476      -3.211  15.548  77.020  1.00 31.07           N
ATOM   4945  N   GLU B 477      -6.677  11.767  84.217  1.00 33.20           N
ATOM   4946  CA  GLU B 477      -7.625  11.447  85.300  1.00 33.56           C
ATOM   4947  C   GLU B 477      -8.135  10.007  85.247  1.00 33.45           C
ATOM   4948  O   GLU B 477      -8.388   9.468  84.168  1.00 33.34           O
ATOM   4949  CB  GLU B 477      -8.800  12.440  85.337  1.00 33.50           C
ATOM   4950  CG  GLU B 477      -9.832  12.286  84.207  1.00 34.47           C
ATOM   4951  CD  GLU B 477      -9.298  12.687  82.836  1.00 35.65           C
ATOM   4952  OE1 GLU B 477      -8.414  13.579  82.761  1.00 36.24           O
ATOM   4953  OE2 GLU B 477      -9.767  12.108  81.831  1.00 35.33           O
ATOM   4954  N   ASN B 478      -8.262   9.396  86.425  1.00 33.66           N
ATOM   4955  CA  ASN B 478      -8.732   8.008  86.587  1.00 33.93           C
ATOM   4956  C   ASN B 478      -7.885   6.971  85.847  1.00 34.03           C
ATOM   4957  O   ASN B 478      -8.287   5.816  85.706  1.00 33.98           O
ATOM   4958  CB  ASN B 478     -10.211   7.874  86.190  1.00 33.86           C
ATOM   4959  CG  ASN B 478     -11.044   9.049  86.648  1.00 34.09           C
ATOM   4960  OD1 ASN B 478     -11.688   9.716  85.838  1.00 34.86           O
ATOM   4961  ND2 ASN B 478     -11.020   9.325  87.948  1.00 33.98           N
ATOM   4962  N   GLY B 479      -6.713   7.399  85.384  1.00 34.33           N
ATOM   4963  CA  GLY B 479      -5.787   6.540  84.655  1.00 34.50           C
ATOM   4964  C   GLY B 479      -6.074   6.444  83.170  1.00 34.69           C
ATOM   4965  O   GLY B 479      -5.643   5.495  82.522  1.00 34.83           O
ATOM   4966  N   THR B 480      -6.787   7.428  82.627  1.00 34.83           N
ATOM   4967  CA  THR B 480      -7.160   7.425  81.210  1.00 35.00           C
ATOM   4968  C   THR B 480      -5.990   7.825  80.325  1.00 35.11           C
ATOM   4969  O   THR B 480      -5.391   8.889  80.509  1.00 35.27           O
ATOM   4970  CB  THR B 480      -8.376   8.343  80.923  1.00 35.01           C
ATOM   4971  OG1 THR B 480      -9.484   7.936  81.731  1.00 35.17           O
ATOM   4972  CG2 THR B 480      -8.785   8.274  79.450  1.00 34.87           C
ATOM   4973  N   VAL B 481      -5.676   6.968  79.363  1.00 35.21           N
ATOM   4974  CA  VAL B 481      -4.599   7.241  78.431  1.00 35.47           C
ATOM   4975  C   VAL B 481      -5.064   8.246  77.390  1.00 36.09           C
ATOM   4976  O   VAL B 481      -6.089   8.052  76.730  1.00 36.25           O
ATOM   4977  CB  VAL B 481      -4.075   5.960  77.747  1.00 35.23           C
ATOM   4978  CG1 VAL B 481      -2.929   6.289  76.803  1.00 34.55           C
ATOM   4979  CG2 VAL B 481      -3.635   4.939  78.792  1.00 34.62           C
ATOM   4980  N   TYR B 482      -4.303   9.326  77.267  1.00 36.59           N
ATOM   4981  CA  TYR B 482      -4.553  10.342  76.265  1.00 37.10           C
ATOM   4982  C   TYR B 482      -3.512  10.260  75.165  1.00 37.54           C
ATOM   4983  O   TYR B 482      -2.351   9.952  75.415  1.00 37.60           O
ATOM   4984  CB  TYR B 482      -4.548  11.731  76.905  1.00 37.08           C
ATOM   4985  CG  TYR B 482      -5.889  12.163  77.461  1.00 36.99           C
ATOM   4986  CD1 TYR B 482      -6.545  13.282  76.946  1.00 36.98           C
ATOM   4987  CD2 TYR B 482      -6.504  11.457  78.496  1.00 36.85           C
ATOM   4988  CE1 TYR B 482      -7.777  13.692  77.444  1.00 36.44           C
ATOM   4989  CE2 TYR B 482      -7.734  11.855  79.001  1.00 37.41           C
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ATOM   4990  CZ  TYR B 482      -8.366  12.975  78.467  1.00 37.38           C
ATOM   4991  OH  TYR B 482      -9.586  13.378  78.962  1.00 37.33           O
ATOM   4992  N   THR B 483      -3.953  10.538  73.946  1.00 38.19           N
ATOM   4993  CA  THR B 483      -3.114  10.537  72.758  1.00 38.71           C
ATOM   4994  C   THR B 483      -2.107  11.707  72.848  1.00 39.18           C
ATOM   4995  O   THR B 483      -2.321  12.634  73.637  1.00 39.19           O
ATOM   4996  CB  THR B 483      -4.034  10.626  71.500  1.00 38.72           C
ATOM   4997  OG1 THR B 483      -3.432   9.973  70.377  1.00 39.19           O
ATOM   4998  CG2 THR B 483      -4.348  12.051  71.144  1.00 38.78           C
ATOM   4999  N   PRO B 484      -0.986  11.650  72.090  1.00 39.66           N
ATOM   5000  CA  PRO B 484      -0.061  12.794  72.031  1.00 40.06           C
ATOM   5001  C   PRO B 484      -0.734  14.132  71.686  1.00 40.75           C
ATOM   5002  O   PRO B 484      -0.290  15.175  72.165  1.00 40.76           O
ATOM   5003  CB  PRO B 484       0.926  12.394  70.925  1.00 39.87           C
ATOM   5004  CG  PRO B 484       0.928  10.927  70.934  1.00 39.54           C
ATOM   5005  CD  PRO B 484      -0.480  10.511  71.296  1.00 39.65           C
ATOM   5006  N   ASP B 485      -1.790  14.090  70.870  1.00 41.57           N
ATOM   5007  CA  ASP B 485      -2.595  15.273  70.520  1.00 42.20           C
ATOM   5008  C   ASP B 485      -3.411  15.852  71.671  1.00 42.48           C
ATOM   5009  O   ASP B 485      -3.785  17.022  71.638  1.00 42.57           O
ATOM   5010  CB  ASP B 485      -3.560  14.937  69.381  1.00 42.35           C
ATOM   5011  CG  ASP B 485      -2.941  15.112  68.021  1.00 43.06           C
ATOM   5012  OD1 ASP B 485      -1.752  15.487  67.950  1.00 44.40           O
ATOM   5013  OD2 ASP B 485      -3.651  14.882  67.019  1.00 44.07           O
ATOM   5014  N   GLY B 486      -3.708  15.027  72.668  1.00 43.00           N
ATOM   5015  CA  GLY B 486      -4.550  15.437  73.787  1.00 43.79           C
ATOM   5016  C   GLY B 486      -5.975  14.921  73.680  1.00 44.40           C
ATOM   5017  O   GLY B 486      -6.887  15.449  74.321  1.00 44.60           O
ATOM   5018  N   LYS B 487      -6.168  13.890  72.866  1.00 44.94           N
ATOM   5019  CA  LYS B 487      -7.469  13.246  72.723  1.00 45.58           C
ATOM   5020  C   LYS B 487      -7.536  11.987  73.576  1.00 45.76           C
ATOM   5021  O   LYS B 487      -6.605  11.177  73.581  1.00 45.79           O
ATOM   5022  CB  LYS B 487      -7.766  12.916  71.251  1.00 45.55           C
ATOM   5023  CG  LYS B 487      -8.121  14.131  70.373  1.00 46.34           C
ATOM   5024  CD  LYS B 487      -9.510  14.703  70.706  1.00 47.61           C
ATOM   5025  CE  LYS B 487     -10.064  15.580  69.580  1.00 48.62           C
ATOM   5026  NZ  LYS B 487      -9.302  16.854  69.396  1.00 48.99           N
ATOM   5027  N   ALA B 488      -8.638  11.839  74.304  1.00 46.09           N
ATOM   5028  CA  ALA B 488      -8.883  10.652  75.115  1.00 46.50           C
ATOM   5029  C   ALA B 488      -9.003   9.401  74.244  1.00 46.82           C
ATOM   5030  O   ALA B 488      -9.837   9.347  73.338  1.00 46.85           O
ATOM   5031  CB  ALA B 488     -10.143  10.841  75.956  1.00 46.32           C
ATOM   5032  N   THR B 489      -8.151   8.409  74.504  1.00 47.40           N
ATOM   5033  CA  THR B 489      -8.300   7.093  73.876  1.00 47.81           C
ATOM   5034  C   THR B 489      -9.437   6.372  74.575  1.00 48.27           C
ATOM   5035  O   THR B 489      -9.983   5.402  74.042  1.00 48.37           O
ATOM   5036  CB  THR B 489      -7.020   6.214  73.948  1.00 47.75           C
ATOM   5037  OG1 THR B 489      -6.508   6.198  75.287  1.00 47.54           O
ATOM   5038  CG2 THR B 489      -5.951   6.720  72.990  1.00 47.59           C
ATOM   5039  N   ASP B 490      -9.767   6.866  75.776  1.00 48.73           N
ATOM   5040  CA  ASP B 490     -10.922   6.442  76.585  1.00 49.20           C
ATOM   5041  C   ASP B 490     -10.882   4.945  76.883  1.00 49.13           C
ATOM   5042  O   ASP B 490     -10.995   4.518  78.046  1.00 49.38           O
ATOM   5043  CB  ASP B 490     -12.252   6.844  75.905  1.00 49.54           C
ATOM   5044  CG  ASP B 490     -13.424   6.953  76.887  1.00 50.32           C
ATOM   5045  OD1 ASP B 490     -13.214   6.819  78.115  1.00 51.06           O
ATOM   5046  OD2 ASP B 490     -14.566   7.183  76.422  1.00 51.02           O
ATOM   5047  N   TYR B 491     -10.715   4.168  75.813  1.00 48.63           N
ATOM   5048  CA  TYR B 491     -10.610   2.723  75.871  1.00 48.08           C
ATOM   5049  C   TYR B 491      -9.418   2.354  76.738  1.00 47.37           C
ATOM   5050  O   TYR B 491      -9.563   1.624  77.724  1.00 47.37           O
ATOM   5051  CB  TYR B 491     -10.479   2.162  74.450  1.00 48.26           C
ATOM   5052  CG  TYR B 491     -11.749   2.271  73.620  1.00 48.60           C
ATOM   5053  CD1 TYR B 491     -12.742   3.212  73.925  1.00 48.60           C
ATOM   5054  CD2 TYR B 491     -11.949   1.444  72.513  1.00 49.51           C
ATOM   5055  CE1 TYR B 491     -13.908   3.310  73.163  1.00 49.14           C
ATOM   5056  CE2 TYR B 491     -13.112   1.535  71.739  1.00 49.53           C
ATOM   5057  CZ  TYR B 491     -14.085   2.469  72.070  1.00 49.17           C
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ATOM   5058  OH  TYR B 491     -15.229   2.556  71.309  1.00 48.98           O
ATOM   5059  N   ARG B 492      -8.255   2.905  76.397  1.00 46.47           N
ATOM   5060  CA  ARG B 492      -7.036   2.648  77.153  1.00 45.52           C
ATOM   5061  C   ARG B 492      -6.982   3.389  78.485  1.00 45.00           C
ATOM   5062  O   ARG B 492      -7.197   4.599  78.550  1.00 44.71           O
ATOM   5063  CB  ARG B 492      -5.797   2.927  76.309  1.00 45.40           C
ATOM   5064  CG  ARG B 492      -5.265   1.692  75.632  1.00 44.99           C
ATOM   5065  CD  ARG B 492      -5.715   1.564  74.197  1.00 44.28           C
ATOM   5066  NE  ARG B 492      -5.606   0.171  73.782  1.00 45.00           N
ATOM   5067  CZ  ARG B 492      -5.443  -0.246  72.530  1.00 45.37           C
ATOM   5068  NH1 ARG B 492      -5.345   0.620  71.531  1.00 45.41           N
ATOM   5069  NH2 ARG B 492      -5.362  -1.545  72.280  1.00 45.76           N
ATOM   5070  N   VAL B 493      -6.703   2.627  79.538  1.00 44.56           N
ATOM   5071  CA  VAL B 493      -6.642   3.117  80.916  1.00 44.28           C
ATOM   5072  C   VAL B 493      -5.642   2.287  81.723  1.00 43.90           C
ATOM   5073  O   VAL B 493      -5.492   1.089  81.477  1.00 43.82           O
ATOM   5074  CB  VAL B 493      -8.026   3.042  81.620  1.00 44.24           C
ATOM   5075  CG1 VAL B 493      -8.808   4.328  81.429  1.00 44.52           C
ATOM   5076  CG2 VAL B 493      -8.829   1.844  81.124  1.00 44.55           C
ATOM   5077  N   VAL B 494      -4.957   2.918  82.678  1.00 43.67           N
ATOM   5078  CA  VAL B 494      -4.056   2.185  83.578  1.00 43.57           C
ATOM   5079  C   VAL B 494      -4.565   2.189  85.022  1.00 43.68           C
ATOM   5080  O   VAL B 494      -5.230   3.133  85.455  1.00 43.48           O
ATOM   5081  CB  VAL B 494      -2.558   2.655  83.498  1.00 43.53           C
ATOM   5082  CG1 VAL B 494      -2.168   3.049  82.077  1.00 43.20           C
ATOM   5083  CG2 VAL B 494      -2.273   3.794  84.452  1.00 43.38           C
ATOM   5084  N   VAL B 495      -4.254   1.122  85.753  1.00 44.03           N
ATOM   5085  CA  VAL B 495      -4.661   1.001  87.150  1.00 44.48           C
ATOM   5086  C   VAL B 495      -3.804   1.910  88.032  1.00 44.90           C
ATOM   5087  O   VAL B 495      -2.607   1.680  88.185  1.00 44.78           O
ATOM   5088  CB  VAL B 495      -4.597  -0.472  87.646  1.00 44.37           C
ATOM   5089  CG1 VAL B 495      -5.027  -0.574  89.095  1.00 44.07           C
ATOM   5090  CG2 VAL B 495      -5.472  -1.362  86.785  1.00 44.22           C
ATOM   5091  N   ASP B 496      -4.434   2.941  88.596  1.00 45.73           N
ATOM   5092  CA  ASP B 496      -3.768   3.910  89.481  1.00 46.53           C
ATOM   5093  C   ASP B 496      -4.178   3.782  90.951  1.00 46.88           C
ATOM   5094  O   ASP B 496      -3.304   3.632  91.809  1.00 47.07           O
ATOM   5095  CB  ASP B 496      -3.970   5.346  88.983  1.00 46.64           C
ATOM   5096  CG  ASP B 496      -3.167   5.644  87.744  1.00 47.45           C
ATOM   5097  OD1 ASP B 496      -2.327   4.798  87.374  1.00 48.23           O
ATOM   5098  OD2 ASP B 496      -3.366   6.722  87.143  1.00 49.08           O
ATOM   5099  N   PRO B 497      -5.493   3.893  91.260  1.00 47.23           N
ATOM   5100  CA  PRO B 497      -5.940   3.378  92.550  1.00 47.34           C
ATOM   5101  C   PRO B 497      -5.970   1.847  92.491  1.00 47.47           C
ATOM   5102  O   PRO B 497      -6.923   1.244  91.990  1.00 47.57           O
ATOM   5103  CB  PRO B 497      -7.350   3.969  92.706  1.00 47.34           C
ATOM   5104  CG  PRO B 497      -7.475   5.021  91.634  1.00 47.36           C
ATOM   5105  CD  PRO B 497      -6.606   4.524  90.527  1.00 47.35           C
ATOM   5106  N   VAL B 498      -4.905   1.241  92.998  1.00 47.54           N
ATOM   5107  CA  VAL B 498      -4.650  -0.187  92.852  1.00 47.57           C
ATOM   5108  C   VAL B 498      -5.088  -0.965  94.114  1.00 47.58           C
ATOM   5109  O   VAL B 498      -5.123  -0.389  95.204  1.00 47.55           O
ATOM   5110  CB  VAL B 498      -3.155  -0.399  92.454  1.00 47.54           C
ATOM   5111  CG1 VAL B 498      -2.248   0.603  93.163  1.00 47.53           C
ATOM   5112  CG2 VAL B 498      -2.700  -1.797  92.708  1.00 47.71           C
ATOM   5113  N   LYS B 499      -5.420  -2.257  93.964  1.00 47.62           N
ATOM   5114  CA  LYS B 499      -6.095  -3.032  95.038  1.00 47.52           C
ATOM   5115  C   LYS B 499      -5.316  -4.166  95.779  1.00 47.55           C
ATOM   5116  O   LYS B 499      -4.892  -3.944  96.920  1.00 47.69           O
ATOM   5117  CB  LYS B 499      -7.483  -3.501  94.573  1.00 47.66           C
ATOM   5118  CG  LYS B 499      -8.482  -2.372  94.355  1.00 47.83           C
ATOM   5119  CD  LYS B 499      -9.471  -2.721  93.249  1.00 48.58           C
ATOM   5120  CE  LYS B 499     -10.754  -1.884  93.342  1.00 49.19           C
ATOM   5121  NZ  LYS B 499     -11.735  -2.426  94.339  1.00 48.55           N
ATOM   5122  N   PRO B 500      -5.153  -5.372  95.161  1.00 47.27           N
ATOM   5123  CA  PRO B 500      -4.558  -6.596  95.774  1.00 47.10           C
ATOM   5124  C   PRO B 500      -3.345  -6.420  96.718  1.00 46.77           C
ATOM   5125  O   PRO B 500      -3.506  -5.952  97.844  1.00 46.86           O
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ATOM   5126  CB  PRO B 500      -4.168  -7.433  94.553  1.00 47.07           C
ATOM   5127  CG  PRO B 500      -5.173  -7.076  93.525  1.00 46.97           C
ATOM   5128  CD  PRO B 500      -5.583  -5.642  93.773  1.00 47.31           C
ATOM   5129  N   ALA B 501      -2.159  -6.845  96.279  1.00 46.39           N
ATOM   5130  CA  ALA B 501      -0.905  -6.513  96.962  1.00 45.85           C
ATOM   5131  C   ALA B 501      -0.286  -5.293  96.265  1.00 45.58           C
ATOM   5132  O   ALA B 501       0.920  -5.022  96.370  1.00 45.52           O
ATOM   5133  CB  ALA B 501       0.041  -7.689  96.929  1.00 45.82           C
ATOM   5134  N   TYR B 502      -1.153  -4.557  95.569  1.00 44.97           N
ATOM   5135  CA  TYR B 502      -0.776  -3.530  94.600  1.00 44.29           C
ATOM   5136  C   TYR B 502      -0.061  -4.138  93.394  1.00 43.76           C
ATOM   5137  O   TYR B 502       0.512  -3.422  92.570  1.00 43.85           O
ATOM   5138  CB  TYR B 502       0.013  -2.385  95.254  1.00 44.45           C
ATOM   5139  CG  TYR B 502      -0.705  -1.786  96.444  1.00 44.56           C
ATOM   5140  CD1 TYR B 502      -2.002  -1.287  96.319  1.00 44.68           C
ATOM   5141  CD2 TYR B 502      -0.096  -1.729  97.695  1.00 44.75           C
ATOM   5142  CE1 TYR B 502      -2.673  -0.751  97.403  1.00 44.48           C
ATOM   5143  CE2 TYR B 502      -0.761  -1.188  98.789  1.00 44.98           C
ATOM   5144  CZ  TYR B 502      -2.049  -0.704  98.632  1.00 44.49           C
ATOM   5145  OH  TYR B 502      -2.716  -0.159  99.701  1.00 44.77           O
ATOM   5146  N   SER B 503      -0.144  -5.463  93.286  1.00 42.89           N
ATOM   5147  CA  SER B 503       0.466  -6.222  92.198  1.00 42.11           C
ATOM   5148  C   SER B 503      -0.153  -5.900  90.841  1.00 41.49           C
ATOM   5149  O   SER B 503       0.395  -6.271  89.804  1.00 41.54           O
ATOM   5150  CB  SER B 503       0.338  -7.724  92.467  1.00 42.22           C
ATOM   5151  OG  SER B 503      -1.015  -8.144  92.366  1.00 42.13           O
ATOM   5152  N   ASP B 504      -1.298  -5.224  90.857  1.00 40.60           N
ATOM   5153  CA  ASP B 504      -2.017  -4.868  89.635  1.00 39.83           C
ATOM   5154  C   ASP B 504      -1.732  -3.430  89.195  1.00 39.14           C
ATOM   5155  O   ASP B 504      -2.245  -2.976  88.174  1.00 38.99           O
ATOM   5156  CB  ASP B 504      -3.526  -5.079  89.820  1.00 39.83           C
ATOM   5157  CG  ASP B 504      -4.075  -4.319  91.009  1.00 40.22           C
ATOM   5158  OD1 ASP B 504      -3.477  -4.418  92.103  1.00 39.93           O
ATOM   5159  OD2 ASP B 504      -5.095  -3.613  90.856  1.00 41.05           O
ATOM   5160  N   LYS B 505      -0.917  -2.714  89.966  1.00 38.46           N
ATOM   5161  CA  LYS B 505      -0.542  -1.352  89.603  1.00 37.83           C
ATOM   5162  C   LYS B 505       0.139  -1.349  88.244  1.00 37.57           C
ATOM   5163  O   LYS B 505       1.052  -2.132  87.997  1.00 37.74           O
ATOM   5164  CB  LYS B 505       0.372  -0.722  90.657  1.00 37.67           C
ATOM   5165  CG  LYS B 505       0.691   0.737  90.377  1.00 36.47           C
ATOM   5166  CD  LYS B 505       1.435   1.410  91.509  1.00 34.02           C
ATOM   5167  CE  LYS B 505       1.928   2.783  91.073  1.00 33.33           C
ATOM   5168  NZ  LYS B 505       0.834   3.696  90.620  1.00 31.67           N
ATOM   5169  N   GLY B 506      -0.330  -0.477  87.363  1.00 37.32           N
ATOM   5170  CA  GLY B 506       0.247  -0.348  86.033  1.00 36.98           C
ATOM   5171  C   GLY B 506      -0.454  -1.153  84.957  1.00 36.68           C
ATOM   5172  O   GLY B 506      -0.210  -0.935  83.771  1.00 36.72           O
ATOM   5173  N   ASP B 507      -1.315  -2.085  85.367  1.00 36.40           N
ATOM   5174  CA  ASP B 507      -2.087  -2.897  84.426  1.00 36.06           C
ATOM   5175  C   ASP B 507      -2.811  -2.019  83.418  1.00 35.94           C
ATOM   5176  O   ASP B 507      -3.419  -1.006  83.782  1.00 35.70           O
ATOM   5177  CB  ASP B 507      -3.103  -3.772  85.163  1.00 36.09           C
ATOM   5178  CG  ASP B 507      -2.469  -4.961  85.849  1.00 35.83           C
ATOM   5179  OD1 ASP B 507      -1.249  -5.170  85.690  1.00 36.28           O
ATOM   5180  OD2 ASP B 507      -3.197  -5.691  86.553  1.00 35.77           O
ATOM   5181  N   LEU B 508      -2.729  -2.408  82.152  1.00 35.89           N
ATOM   5182  CA  LEU B 508      -3.341  -1.637  81.081  1.00 36.05           C
ATOM   5183  C   LEU B 508      -4.572  -2.342  80.537  1.00 35.98           C
ATOM   5184  O   LEU B 508      -4.528  -3.526  80.205  1.00 35.84           O
ATOM   5185  CB  LEU B 508      -2.349  -1.370  79.944  1.00 35.91           C
ATOM   5186  CG  LEU B 508      -2.902  -0.335  78.961  1.00 36.35           C
ATOM   5187  CD1 LEU B 508      -2.059   0.936  78.962  1.00 36.19           C
ATOM   5188  CD2 LEU B 508      -3.013  -0.916  77.563  1.00 36.59           C
ATOM   5189  N   TYR B 509      -5.662  -1.590  80.437  1.00 36.29           N
ATOM   5190  CA  TYR B 509      -6.930  -2.112  79.953  1.00 36.64           C
ATOM   5191  C   TYR B 509      -7.396  -1.409  78.682  1.00 37.03           C
ATOM   5192  O   TYR B 509      -7.085  -0.238  78.451  1.00 37.00           O
ATOM   5193  CB  TYR B 509      -8.008  -1.964  81.035  1.00 36.59           C
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ATOM   5194  CG  TYR B 509      -7.907  -2.957  82.175  1.00 36.39           C
ATOM   5195  CD1 TYR B 509      -6.904  -2.843  83.139  1.00 36.59           C
ATOM   5196  CD2 TYR B 509      -8.825  -4.000  82.299  1.00 36.16           C
ATOM   5197  CE1 TYR B 509      -6.804  -3.748  84.189  1.00 36.89           C
ATOM   5198  CE2 TYR B 509      -8.739  -4.916  83.349  1.00 36.25           C
ATOM   5199  CZ  TYR B 509      -7.724  -4.783  84.290  1.00 36.97           C
ATOM   5200  OH  TYR B 509      -7.618  -5.677  85.336  1.00 36.84           O
ATOM   5201  N   LYS B 510      -8.137  -2.143  77.858  1.00 37.53           N
ATOM   5202  CA  LYS B 510      -8.964  -1.538  76.822  1.00 37.99           C
ATOM   5203  C   LYS B 510     -10.426  -1.799  77.205  1.00 38.18           C
ATOM   5204  O   LYS B 510     -11.029  -2.784  76.771  1.00 38.33           O
ATOM   5205  CB  LYS B 510      -8.638  -2.116  75.445  1.00 37.95           C
ATOM   5206  CG  LYS B 510      -8.669  -1.072  74.351  1.00 38.45           C
ATOM   5207  CD  LYS B 510      -9.262  -1.598  73.064  1.00 38.67           C
ATOM   5208  CE  LYS B 510      -9.167  -0.543  71.979  1.00 39.11           C
ATOM   5209  NZ  LYS B 510     -10.094  -0.802  70.847  1.00 39.27           N
ATOM   5210  N   GLY B 511     -10.978  -0.917  78.037  1.00 38.46           N
ATOM   5211  CA  GLY B 511     -12.291  -1.130  78.650  1.00 38.62           C
ATOM   5212  C   GLY B 511     -12.153  -2.042  79.858  1.00 38.90           C
ATOM   5213  O   GLY B 511     -11.447  -1.711  80.815  1.00 39.14           O
ATOM   5214  N   ASN B 512     -12.827  -3.190  79.821  1.00 38.83           N
ATOM   5215  CA  ASN B 512     -12.661  -4.215  80.859  1.00 38.75           C
ATOM   5216  C   ASN B 512     -11.716  -5.337  80.423  1.00 38.24           C
ATOM   5217  O   ASN B 512     -11.568  -6.348  81.118  1.00 38.28           O
ATOM   5218  CB  ASN B 512     -14.017  -4.781  81.310  1.00 38.92           C
ATOM   5219  CG  ASN B 512     -14.533  -4.122  82.585  1.00 39.96           C
ATOM   5220  OD1 ASN B 512     -13.947  -4.269  83.664  1.00 41.02           O
ATOM   5221  ND2 ASN B 512     -15.638  -3.397  82.465  1.00 40.62           N
ATOM   5222  N   GLN B 513     -11.078  -5.132  79.272  1.00 37.51           N
ATOM   5223  CA  GLN B 513     -10.123  -6.075  78.705  1.00 36.86           C
ATOM   5224  C   GLN B 513      -8.694  -5.773  79.183  1.00 36.53           C
ATOM   5225  O   GLN B 513      -8.072  -4.810  78.734  1.00 36.53           O
ATOM   5226  CB  GLN B 513     -10.209  -6.028  77.170  1.00 36.66           C
ATOM   5227  CG  GLN B 513      -9.279  -6.984  76.436  1.00 36.53           C
ATOM   5228  CD  GLN B 513      -9.660  -8.435  76.634  1.00 36.49           C
ATOM   5229  OE1 GLN B 513     -10.741  -8.867  76.229  1.00 37.23           O
ATOM   5230  NE2 GLN B 513      -8.773  -9.198  77.260  1.00 35.70           N
ATOM   5231  N   LEU B 514      -8.188  -6.602  80.094  1.00 36.17           N
ATOM   5232  CA  LEU B 514      -6.810  -6.510  80.578  1.00 35.94           C
ATOM   5233  C   LEU B 514      -5.837  -6.947  79.486  1.00 35.78           C
ATOM   5234  O   LEU B 514      -5.864  -8.098  79.059  1.00 35.97           O
ATOM   5235  CB  LEU B 514      -6.627  -7.381  81.830  1.00 35.98           C
ATOM   5236  CG  LEU B 514      -5.207  -7.757  82.282  1.00 36.05           C
ATOM   5237  CD1 LEU B 514      -4.488  -6.576  82.930  1.00 36.24           C
ATOM   5238  CD2 LEU B 514      -5.251  -8.940  83.234  1.00 35.94           C
ATOM   5239  N   LEU B 515      -4.977  -6.032  79.046  1.00 35.51           N
ATOM   5240  CA  LEU B 515      -4.056  -6.305  77.934  1.00 34.98           C
ATOM   5241  C   LEU B 515      -2.632  -6.640  78.370  1.00 34.55           C
ATOM   5242  O   LEU B 515      -1.983  -7.501  77.777  1.00 34.62           O
ATOM   5243  CB  LEU B 515      -4.028  -5.131  76.952  1.00 35.04           C
ATOM   5244  CG  LEU B 515      -5.260  -4.831  76.093  1.00 34.97           C
ATOM   5245  CD1 LEU B 515      -5.085  -3.481  75.415  1.00 34.61           C
ATOM   5246  CD2 LEU B 515      -5.527  -5.925  75.059  1.00 34.62           C
ATOM   5247  N   GLY B 516      -2.150  -5.952  79.397  1.00 34.10           N
ATOM   5248  CA  GLY B 516      -0.780  -6.125  79.859  1.00 33.42           C
ATOM   5249  C   GLY B 516      -0.480  -5.220  81.030  1.00 32.95           C
ATOM   5250  O   GLY B 516      -1.309  -5.059  81.924  1.00 33.30           O
ATOM   5251  N   ASN B 517       0.709  -4.626  81.020  1.00 32.38           N
ATOM   5252  CA  ASN B 517       1.170  -3.769  82.110  1.00 31.66           C
ATOM   5253  C   ASN B 517       2.218  -2.781  81.612  1.00 31.45           C
ATOM   5254  O   ASN B 517       3.134  -3.151  80.870  1.00 31.50           O
ATOM   5255  CB  ASN B 517       1.730  -4.620  83.254  1.00 31.45           C
ATOM   5256  CG  ASN B 517       2.042  -3.811  84.503  1.00 30.97           C
ATOM   5257  OD1 ASN B 517       2.955  -2.989  84.510  1.00 29.64           O
ATOM   5258  ND2 ASN B 517       1.296  -4.064  85.576  1.00 29.73           N
ATOM   5259  N   ILE B 518       2.084  -1.530  82.042  1.00 31.00           N
ATOM   5260  CA  ILE B 518       2.932  -0.437  81.563  1.00 30.58           C
ATOM   5261  C   ILE B 518       4.389  -0.534  82.032  1.00 30.81           C
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ATOM   5262  O   ILE B 518       5.247   0.234  81.576  1.00 31.17           O
ATOM   5263  CB  ILE B 518       2.336   0.951  81.923  1.00 30.31           C
ATOM   5264  CG1 ILE B 518       2.345   1.171  83.439  1.00 30.10           C
ATOM   5265  CG2 ILE B 518       0.936   1.092  81.339  1.00 29.38           C
ATOM   5266  CD1 ILE B 518       1.942   2.569  83.884  1.00 30.42           C
ATOM   5267  N   TYR B 519       4.659  -1.475  82.933  1.00 30.69           N
ATOM   5268  CA  TYR B 519       5.994  -1.672  83.488  1.00 30.74           C
ATOM   5269  C   TYR B 519       6.738  -2.835  82.815  1.00 30.92           C
ATOM   5270  O   TYR B 519       7.910  -3.082  83.109  1.00 30.80           O
ATOM   5271  CB  TYR B 519       5.930  -1.882  85.013  1.00 30.69           C
ATOM   5272  CG  TYR B 519       5.191  -0.803  85.797  1.00 30.58           C
ATOM   5273  CD1 TYR B 519       5.364   0.552  85.505  1.00 30.66           C
ATOM   5274  CD2 TYR B 519       4.342  -1.141  86.853  1.00 30.48           C
ATOM   5275  CE1 TYR B 519       4.699   1.542  86.226  1.00 30.10           C
ATOM   5276  CE2 TYR B 519       3.668  -0.157  87.581  1.00 30.91           C
ATOM   5277  CZ  TYR B 519       3.855   1.184  87.259  1.00 30.90           C
ATOM   5278  OH  TYR B 519       3.201   2.169  87.969  1.00 30.70           O
ATOM   5279  N   PHE B 520       6.057  -3.551  81.920  1.00 31.18           N
ATOM   5280  CA  PHE B 520       6.697  -4.623  81.155  1.00 31.43           C
ATOM   5281  C   PHE B 520       7.464  -4.030  79.981  1.00 31.82           C
ATOM   5282  O   PHE B 520       7.004  -3.071  79.358  1.00 31.76           O
ATOM   5283  CB  PHE B 520       5.673  -5.643  80.641  1.00 31.31           C
ATOM   5284  CG  PHE B 520       4.875  -6.332  81.727  1.00 31.23           C
ATOM   5285  CD1 PHE B 520       5.234  -6.227  83.073  1.00 31.44           C
ATOM   5286  CD2 PHE B 520       3.773  -7.110  81.393  1.00 30.66           C
ATOM   5287  CE1 PHE B 520       4.493  -6.869  84.063  1.00 31.16           C
ATOM   5288  CE2 PHE B 520       3.031  -7.760  82.373  1.00 30.76           C
ATOM   5289  CZ  PHE B 520       3.390  -7.640  83.711  1.00 31.21           C
ATOM   5290  N   THR B 521       8.631  -4.599  79.682  1.00 32.41           N
ATOM   5291  CA  THR B 521       9.486  -4.084  78.600  1.00 32.95           C
ATOM   5292  C   THR B 521       9.806  -5.122  77.519  1.00 33.22           C
ATOM   5293  O   THR B 521      10.343  -4.778  76.465  1.00 33.38           O
ATOM   5294  CB  THR B 521      10.816  -3.473  79.137  1.00 32.94           C
ATOM   5295  OG1 THR B 521      11.597  -4.488  79.783  1.00 33.39           O
ATOM   5296  CG2 THR B 521      10.548  -2.334  80.116  1.00 32.28           C
ATOM   5297  N   THR B 522       9.452  -6.378  77.778  1.00 33.59           N
ATOM   5298  CA  THR B 522       9.831  -7.511  76.928  1.00 33.90           C
ATOM   5299  C   THR B 522       8.606  -8.294  76.478  1.00 34.03           C
ATOM   5300  O   THR B 522       7.668  -8.489  77.259  1.00 34.18           O
ATOM   5301  CB  THR B 522      10.793  -8.452  77.699  1.00 33.89           C
ATOM   5302  OG1 THR B 522      12.080  -7.832  77.799  1.00 34.50           O
ATOM   5303  CG2 THR B 522      10.949  -9.807  77.021  1.00 34.51           C
ATOM   5304  N   ASN B 523       8.617  -8.744  75.223  1.00 34.27           N
ATOM   5305  CA  ASN B 523       7.541  -9.584  74.685  1.00 34.42           C
ATOM   5306  C   ASN B 523       6.167  -9.084  75.136  1.00 34.38           C
ATOM   5307  O   ASN B 523       5.356  -9.850  75.665  1.00 34.43           O
ATOM   5308  CB  ASN B 523       7.734 -11.051  75.109  1.00 34.57           C
ATOM   5309  CG  ASN B 523       9.085 -11.617  74.694  1.00 34.98           C
ATOM   5310  OD1 ASN B 523       9.706 -11.152  73.734  1.00 36.33           O
ATOM   5311  ND2 ASN B 523       9.545 -12.632  75.419  1.00 35.18           N
ATOM   5312  N   LYS B 524       5.926  -7.790  74.924  1.00 34.16           N
ATOM   5313  CA  LYS B 524       4.756  -7.105  75.468  1.00 33.85           C
ATOM   5314  C   LYS B 524       3.437  -7.592  74.884  1.00 34.02           C
ATOM   5315  O   LYS B 524       3.383  -8.039  73.740  1.00 33.94           O
ATOM   5316  CB  LYS B 524       4.888  -5.592  75.290  1.00 33.53           C
ATOM   5317  CG  LYS B 524       5.763  -4.921  76.339  1.00 32.35           C
ATOM   5318  CD  LYS B 524       5.818  -3.414  76.139  1.00 30.50           C
ATOM   5319  CE  LYS B 524       4.507  -2.738  76.525  1.00 29.53           C
ATOM   5320  NZ  LYS B 524       4.206  -2.814  77.981  1.00 28.19           N
ATOM   5321  N   THR B 525       2.385  -7.511  75.695  1.00 34.18           N
ATOM   5322  CA  THR B 525       1.036  -7.871  75.270  1.00 34.34           C
ATOM   5323  C   THR B 525       0.130  -6.638  75.133  1.00 34.07           C
ATOM   5324  O   THR B 525      -0.929  -6.708  74.518  1.00 34.00           O
ATOM   5325  CB  THR B 525       0.391  -8.884  76.236  1.00 34.44           C
ATOM   5326  OG1 THR B 525       1.351  -9.875  76.617  1.00 34.78           O
ATOM   5327  CG2 THR B 525      -0.767  -9.572  75.558  1.00 34.99           C
ATOM   5328  N   SER B 526       0.551  -5.521  75.724  1.00 33.94           N
ATOM   5329  CA  SER B 526      -0.145  -4.245  75.579  1.00 33.71           C
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ATOM   5330  C   SER B 526       0.706  -3.301  74.719  1.00 33.18           C
ATOM   5331  O   SER B 526       1.911  -3.515  74.598  1.00 33.43           O
ATOM   5332  CB  SER B 526      -0.426  -3.637  76.956  1.00 33.82           C
ATOM   5333  OG  SER B 526       0.769  -3.191  77.578  1.00 34.67           O
ATOM   5334  N   PRO B 527       0.091  -2.267  74.105  1.00 32.71           N
ATOM   5335  CA  PRO B 527       0.869  -1.364  73.246  1.00 32.23           C
ATOM   5336  C   PRO B 527       1.687  -0.287  73.969  1.00 31.62           C
ATOM   5337  O   PRO B 527       2.502   0.380  73.332  1.00 31.78           O
ATOM   5338  CB  PRO B 527      -0.202  -0.699  72.359  1.00 32.21           C
ATOM   5339  CG  PRO B 527      -1.524  -1.294  72.773  1.00 32.48           C
ATOM   5340  CD  PRO B 527      -1.329  -1.880  74.130  1.00 32.67           C
ATOM   5341  N   PHE B 528       1.491  -0.123  75.275  1.00 30.93           N
ATOM   5342  CA  PHE B 528       2.091   1.004  76.001  1.00 30.29           C
ATOM   5343  C   PHE B 528       3.104   0.619  77.074  1.00 29.88           C
ATOM   5344  O   PHE B 528       2.906  -0.342  77.817  1.00 29.74           O
ATOM   5345  CB  PHE B 528       1.003   1.867  76.646  1.00 30.08           C
ATOM   5346  CG  PHE B 528       0.037   2.458  75.669  1.00 30.04           C
ATOM   5347  CD1 PHE B 528       0.362   3.613  74.963  1.00 29.60           C
ATOM   5348  CD2 PHE B 528      -1.208   1.868  75.461  1.00 29.91           C
ATOM   5349  CE1 PHE B 528      -0.533   4.170  74.056  1.00 29.89           C
ATOM   5350  CE2 PHE B 528      -2.111   2.417  74.557  1.00 29.62           C
ATOM   5351  CZ  PHE B 528      -1.773   3.574  73.852  1.00 30.24           C
ATOM   5352  N   ARG B 529       4.180   1.394  77.156  1.00 29.42           N
ATOM   5353  CA  ARG B 529       5.128   1.284  78.262  1.00 29.03           C
ATOM   5354  C   ARG B 529       5.547   2.670  78.745  1.00 28.74           C
ATOM   5355  O   ARG B 529       5.469   3.650  77.999  1.00 28.80           O
ATOM   5356  CB  ARG B 529       6.355   0.456  77.863  1.00 28.90           C
ATOM   5357  CG  ARG B 529       7.106   0.993  76.654  1.00 29.06           C
ATOM   5358  CD  ARG B 529       8.522   0.435  76.568  1.00 28.30           C
ATOM   5359  NE  ARG B 529       9.268   1.086  75.494  1.00 28.03           N
ATOM   5360  CZ  ARG B 529       9.974   2.212  75.626  1.00 27.68           C
ATOM   5361  NH1 ARG B 529      10.053   2.835  76.799  1.00 25.14           N
ATOM   5362  NH2 ARG B 529      10.606   2.718  74.573  1.00 27.73           N
ATOM   5363  N   ILE B 530       5.976   2.753  79.997  1.00 28.32           N
ATOM   5364  CA  ILE B 530       6.555   3.983  80.503  1.00 28.05           C
ATOM   5365  C   ILE B 530       8.009   4.068  80.078  1.00 27.85           C
ATOM   5366  O   ILE B 530       8.602   3.078  79.649  1.00 27.94           O
ATOM   5367  CB  ILE B 530       6.484   4.084  82.047  1.00 28.18           C
ATOM   5368  CG1 ILE B 530       7.318   2.976  82.705  1.00 28.30           C
ATOM   5369  CG2 ILE B 530       5.028   4.101  82.526  1.00 28.04           C
ATOM   5370  CD1 ILE B 530       7.708   3.275  84.131  1.00 28.07           C
ATOM   5371  N   ALA B 531       8.572   5.262  80.214  1.00 27.61           N
ATOM   5372  CA  ALA B 531       9.984   5.503  79.986  1.00 27.33           C
ATOM   5373  C   ALA B 531      10.866   4.522  80.761  1.00 27.22           C
ATOM   5374  O   ALA B 531      10.607   4.241  81.936  1.00 27.10           O
ATOM   5375  CB  ALA B 531      10.325   6.940  80.373  1.00 27.17           C
ATOM   5376  N   LYS B 532      11.898   4.002  80.095  1.00 27.23           N
ATOM   5377  CA  LYS B 532      12.960   3.256  80.771  1.00 27.52           C
ATOM   5378  C   LYS B 532      13.844   4.233  81.539  1.00 27.37           C
ATOM   5379  O   LYS B 532      14.741   4.858  80.967  1.00 27.57           O
ATOM   5380  CB  LYS B 532      13.799   2.450  79.776  1.00 27.74           C
ATOM   5381  CG  LYS B 532      13.186   1.122  79.369  1.00 29.16           C
ATOM   5382  CD  LYS B 532      13.978   0.471  78.245  1.00 31.09           C
ATOM   5383  CE  LYS B 532      13.184  -0.656  77.592  1.00 31.74           C
ATOM   5384  NZ  LYS B 532      13.701  -0.934  76.222  1.00 32.70           N
ATOM   5385  N   ASP B 533      13.567   4.364  82.834  1.00 27.13           N
ATOM   5386  CA  ASP B 533      14.265   5.297  83.706  1.00 26.92           C
ATOM   5387  C   ASP B 533      14.228   4.762  85.139  1.00 26.88           C
ATOM   5388  O   ASP B 533      13.670   3.695  85.394  1.00 26.77           O
ATOM   5389  CB  ASP B 533      13.592   6.673  83.630  1.00 27.05           C
ATOM   5390  CG  ASP B 533      14.475   7.800  84.160  1.00 27.62           C
ATOM   5391  OD1 ASP B 533      15.694   7.592  84.344  1.00 28.37           O
ATOM   5392  OD2 ASP B 533      13.943   8.907  84.388  1.00 28.31           O
ATOM   5393  N   SER B 534      14.837   5.496  86.065  1.00 26.89           N
ATOM   5394  CA  SER B 534      14.733   5.184  87.480  1.00 26.99           C
ATOM   5395  C   SER B 534      13.672   6.073  88.115  1.00 27.04           C
ATOM   5396  O   SER B 534      13.558   7.262  87.803  1.00 26.95           O
ATOM   5397  CB  SER B 534      16.079   5.355  88.192  1.00 27.02           C
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ATOM   5398  OG  SER B 534      16.207   6.634  88.797  1.00 27.52           O
ATOM   5399  N   TYR B 535      12.895   5.485  89.012  1.00 27.30           N
ATOM   5400  CA  TYR B 535      11.815   6.202  89.656  1.00 27.55           C
ATOM   5401  C   TYR B 535      11.922   6.074  91.166  1.00 28.22           C
ATOM   5402  O   TYR B 535      12.625   5.198  91.676  1.00 28.48           O
ATOM   5403  CB  TYR B 535      10.465   5.680  89.171  1.00 26.88           C
ATOM   5404  CG  TYR B 535      10.210   5.862  87.697  1.00 26.03           C
ATOM   5405  CD1 TYR B 535      10.622   4.900  86.767  1.00 25.26           C
ATOM   5406  CD2 TYR B 535       9.538   6.984  87.229  1.00 25.95           C
ATOM   5407  CE1 TYR B 535      10.380   5.066  85.412  1.00 25.04           C
ATOM   5408  CE2 TYR B 535       9.283   7.159  85.868  1.00 25.76           C
ATOM   5409  CZ  TYR B 535       9.704   6.199  84.968  1.00 25.57           C
ATOM   5410  OH  TYR B 535       9.446   6.378  83.628  1.00 25.40           O
ATOM   5411  N   LEU B 536      11.216   6.954  91.870  1.00 28.94           N
ATOM   5412  CA  LEU B 536      11.231   6.992  93.321  1.00 29.85           C
ATOM   5413  C   LEU B 536       9.800   6.982  93.850  1.00 30.61           C
ATOM   5414  O   LEU B 536       9.044   7.935  93.647  1.00 30.76           O
ATOM   5415  CB  LEU B 536      11.980   8.238  93.801  1.00 29.68           C
ATOM   5416  CG  LEU B 536      12.635   8.193  95.179  1.00 29.83           C
ATOM   5417  CD1 LEU B 536      13.870   7.304  95.168  1.00 30.44           C
ATOM   5418  CD2 LEU B 536      12.997   9.594  95.625  1.00 29.58           C
ATOM   5419  N   TRP B 537       9.441   5.896  94.526  1.00 31.50           N
ATOM   5420  CA  TRP B 537       8.086   5.687  95.033  1.00 32.36           C
ATOM   5421  C   TRP B 537       7.993   5.828  96.554  1.00 33.62           C
ATOM   5422  O   TRP B 537       8.997   5.701  97.265  1.00 33.77           O
ATOM   5423  CB  TRP B 537       7.588   4.304  94.604  1.00 31.66           C
ATOM   5424  CG  TRP B 537       7.194   4.221  93.159  1.00 30.85           C
ATOM   5425  CD1 TRP B 537       7.418   5.159  92.190  1.00 30.22           C
ATOM   5426  CD2 TRP B 537       6.535   3.131  92.514  1.00 29.72           C
ATOM   5427  NE1 TRP B 537       6.924   4.728  90.990  1.00 29.84           N
ATOM   5428  CE2 TRP B 537       6.372   3.485  91.158  1.00 30.25           C
ATOM   5429  CE3 TRP B 537       6.055   1.890  92.950  1.00 29.73           C
ATOM   5430  CZ2 TRP B 537       5.750   2.640  90.231  1.00 30.26           C
ATOM   5431  CZ3 TRP B 537       5.437   1.053  92.033  1.00 29.76           C
ATOM   5432  CH2 TRP B 537       5.293   1.432  90.688  1.00 30.54           C
ATOM   5433  N   MET B 538       6.781   6.092  97.042  1.00 35.08           N
ATOM   5434  CA  MET B 538       6.518   6.198  98.476  1.00 36.64           C
ATOM   5435  C   MET B 538       5.208   5.531  98.888  1.00 37.14           C
ATOM   5436  O   MET B 538       4.179   5.689  98.228  1.00 37.36           O
ATOM   5437  CB  MET B 538       6.495   7.662  98.919  1.00 36.53           C
ATOM   5438  CG  MET B 538       6.274   7.844 100.419  1.00 37.08           C
ATOM   5439  SD  MET B 538       5.515   9.420 100.833  1.00 38.25           S
ATOM   5440  CE  MET B 538       3.800   9.065 100.473  1.00 37.85           C
ATOM   5441  N   SER B 539       5.265   4.789  99.990  1.00 37.92           N
ATOM   5442  CA  SER B 539       4.074   4.265 100.641  1.00 38.71           C
ATOM   5443  C   SER B 539       4.060   4.702 102.101  1.00 39.46           C
ATOM   5444  O   SER B 539       5.120   4.926 102.701  1.00 39.28           O
ATOM   5445  CB  SER B 539       4.044   2.746 100.547  1.00 38.62           C
ATOM   5446  OG  SER B 539       4.047   2.329  99.196  1.00 38.35           O
ATOM   5447  N   TYR B 540       2.863   4.833 102.669  1.00 40.46           N
ATOM   5448  CA  TYR B 540       2.727   5.210 104.079  1.00 41.43           C
ATOM   5449  C   TYR B 540       1.664   4.404 104.820  1.00 42.03           C
ATOM   5450  O   TYR B 540       0.700   3.916 104.213  1.00 42.09           O
ATOM   5451  CB  TYR B 540       2.463   6.713 104.228  1.00 41.37           C
ATOM   5452  CG  TYR B 540       1.190   7.206 103.573  1.00 41.80           C
ATOM   5453  CD1 TYR B 540      -0.030   7.194 104.261  1.00 42.26           C
ATOM   5454  CD2 TYR B 540       1.205   7.704 102.271  1.00 41.46           C
ATOM   5455  CE1 TYR B 540      -1.201   7.657 103.658  1.00 41.96           C
ATOM   5456  CE2 TYR B 540       0.048   8.167 101.662  1.00 41.23           C
ATOM   5457  CZ  TYR B 540      -1.148   8.142 102.357  1.00 41.85           C
ATOM   5458  OH  TYR B 540      -2.290   8.601 101.747  1.00 42.44           O
ATOM   5459  N   SER B 541       1.865   4.262 106.131  1.00 42.62           N
ATOM   5460  CA  SER B 541       0.894   3.620 107.011  1.00 43.30           C
ATOM   5461  C   SER B 541       0.613   4.511 108.212  1.00 43.76           C
ATOM   5462  O   SER B 541       1.536   5.081 108.801  1.00 43.77           O
ATOM   5463  CB  SER B 541       1.406   2.263 107.486  1.00 43.31           C
ATOM   5464  OG  SER B 541       2.179   2.396 108.665  1.00 43.97           O
ATOM   5465  N   ASP B 542      -0.664   4.624 108.565  1.00 44.48           N
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ATOM   5466  CA  ASP B 542      -1.095   5.412 109.719  1.00 44.93           C
ATOM   5467  C   ASP B 542      -1.414   4.525 110.922  1.00 45.32           C
ATOM   5468  O   ASP B 542      -1.502   5.008 112.050  1.00 45.64           O
ATOM   5469  CB  ASP B 542      -2.310   6.266 109.354  1.00 45.00           C
ATOM   5470  CG  ASP B 542      -1.972   7.380 108.372  1.00 45.18           C
ATOM   5471  OD1 ASP B 542      -1.051   8.177 108.658  1.00 45.15           O
ATOM   5472  OD2 ASP B 542      -2.639   7.468 107.318  1.00 45.10           O
ATOM   5473  N   ASP B 543      -1.583   3.228 110.674  1.00 45.65           N
ATOM   5474  CA  ASP B 543      -1.896   2.265 111.726  1.00 45.81           C
ATOM   5475  C   ASP B 543      -0.652   1.551 112.248  1.00 45.92           C
ATOM   5476  O   ASP B 543      -0.669   0.338 112.469  1.00 46.04           O
ATOM   5477  CB  ASP B 543      -2.933   1.245 111.236  1.00 45.94           C
ATOM   5478  CG  ASP B 543      -2.579   0.634 109.878  1.00 46.38           C
ATOM   5479  OD1 ASP B 543      -1.377   0.501 109.544  1.00 46.82           O
ATOM   5480  OD2 ASP B 543      -3.522   0.279 109.139  1.00 46.36           O
ATOM   5481  N   ASP B 544       0.428   2.310 112.427  1.00 46.12           N
ATOM   5482  CA  ASP B 544       1.678   1.808 113.016  1.00 46.28           C
ATOM   5483  C   ASP B 544       2.313   0.639 112.231  1.00 46.26           C
ATOM   5484  O   ASP B 544       3.132  -0.117 112.768  1.00 46.14           O
ATOM   5485  CB  ASP B 544       1.464   1.461 114.504  1.00 46.44           C
ATOM   5486  CG  ASP B 544       2.764   1.202 115.249  1.00 46.85           C
ATOM   5487  OD1 ASP B 544       3.626   2.109 115.331  1.00 46.65           O
ATOM   5488  OD2 ASP B 544       2.911   0.076 115.763  1.00 47.47           O
ATOM   5489  N   GLY B 545       1.930   0.502 110.959  1.00 46.26           N
ATOM   5490  CA  GLY B 545       2.591  -0.427 110.037  1.00 45.98           C
ATOM   5491  C   GLY B 545       1.849  -1.696 109.662  1.00 45.95           C
ATOM   5492  O   GLY B 545       2.439  -2.599 109.074  1.00 45.95           O
ATOM   5493  N   LYS B 546       0.558  -1.770 109.983  1.00 45.80           N
ATOM   5494  CA  LYS B 546      -0.235  -2.968 109.686  1.00 45.64           C
ATOM   5495  C   LYS B 546      -0.792  -2.989 108.255  1.00 45.23           C
ATOM   5496  O   LYS B 546      -0.761  -4.028 107.593  1.00 45.25           O
ATOM   5497  CB  LYS B 546      -1.341  -3.160 110.728  1.00 45.92           C
ATOM   5498  CG  LYS B 546      -0.808  -3.514 112.117  1.00 46.58           C
ATOM   5499  CD  LYS B 546      -1.780  -3.109 113.212  1.00 47.97           C
ATOM   5500  CE  LYS B 546      -1.141  -3.240 114.590  1.00 49.01           C
ATOM   5501  NZ  LYS B 546      -1.980  -2.623 115.657  1.00 49.63           N
ATOM   5502  N   THR B 547      -1.312  -1.856 107.789  1.00 44.66           N
ATOM   5503  CA  THR B 547      -1.633  -1.689 106.366  1.00 44.11           C
ATOM   5504  C   THR B 547      -0.885  -0.491 105.792  1.00 43.51           C
ATOM   5505  O   THR B 547      -0.496   0.418 106.530  1.00 43.51           O
ATOM   5506  CB  THR B 547      -3.149  -1.522 106.086  1.00 44.17           C
ATOM   5507  OG1 THR B 547      -3.645  -0.356 106.758  1.00 44.21           O
ATOM   5508  CG2 THR B 547      -3.930  -2.757 106.524  1.00 44.45           C
ATOM   5509  N   TRP B 548      -0.695  -0.502 104.474  1.00 42.60           N
ATOM   5510  CA  TRP B 548       0.045   0.538 103.766  1.00 41.61           C
ATOM   5511  C   TRP B 548      -0.754   1.025 102.566  1.00 40.94           C
ATOM   5512  O   TRP B 548      -1.451   0.237 101.923  1.00 40.89           O
ATOM   5513  CB  TRP B 548       1.391  -0.011 103.286  1.00 41.66           C
ATOM   5514  CG  TRP B 548       2.340  -0.333 104.398  1.00 41.64           C
ATOM   5515  CD1 TRP B 548       2.408  -1.496 105.101  1.00 41.83           C
ATOM   5516  CD2 TRP B 548       3.359   0.522 104.933  1.00 41.66           C
ATOM   5517  NE1 TRP B 548       3.403  -1.422 106.045  1.00 42.15           N
ATOM   5518  CE2 TRP B 548       4.005  -0.195 105.962  1.00 41.76           C
ATOM   5519  CE3 TRP B 548       3.790   1.822 104.640  1.00 42.02           C
ATOM   5520  CZ2 TRP B 548       5.057   0.345 106.708  1.00 41.69           C
ATOM   5521  CZ3 TRP B 548       4.838   2.360 105.379  1.00 41.99           C
ATOM   5522  CH2 TRP B 548       5.458   1.620 106.403  1.00 42.00           C
ATOM   5523  N   SER B 549      -0.642   2.316 102.256  1.00 39.99           N
ATOM   5524  CA  SER B 549      -1.311   2.886 101.084  1.00 39.18           C
ATOM   5525  C   SER B 549      -0.731   2.333  99.778  1.00 38.67           C
ATOM   5526  O   SER B 549       0.294   1.642  99.779  1.00 38.54           O
ATOM   5527  CB  SER B 549      -1.206   4.414 101.090  1.00 39.21           C
ATOM   5528  OG  SER B 549       0.113   4.834 100.786  1.00 38.87           O
ATOM   5529  N   ALA B 550      -1.401   2.634  98.670  1.00 37.88           N
ATOM   5530  CA  ALA B 550      -0.861   2.353  97.346  1.00 37.19           C
ATOM   5531  C   ALA B 550       0.369   3.229  97.128  1.00 36.69           C
ATOM   5532  O   ALA B 550       0.452   4.323  97.694  1.00 36.53           O
ATOM   5533  CB  ALA B 550      -1.902   2.621  96.285  1.00 37.15           C
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ATOM   5534  N   PRO B 551       1.336   2.749  96.322  1.00 36.11           N
ATOM   5535  CA  PRO B 551       2.538   3.532  96.068  1.00 35.70           C
ATOM   5536  C   PRO B 551       2.190   4.884  95.470  1.00 35.24           C
ATOM   5537  O   PRO B 551       1.366   4.964  94.560  1.00 35.35           O
ATOM   5538  CB  PRO B 551       3.291   2.698  95.031  1.00 35.64           C
ATOM   5539  CG  PRO B 551       2.786   1.330  95.197  1.00 36.01           C
ATOM   5540  CD  PRO B 551       1.355   1.469  95.594  1.00 36.10           C
ATOM   5541  N   GLN B 552       2.792   5.935  96.010  1.00 34.81           N
ATOM   5542  CA  GLN B 552       2.703   7.262  95.424  1.00 34.41           C
ATOM   5543  C   GLN B 552       4.005   7.478  94.659  1.00 34.06           C
ATOM   5544  O   GLN B 552       5.078   7.071  95.121  1.00 33.95           O
ATOM   5545  CB  GLN B 552       2.530   8.340  96.505  1.00 34.46           C
ATOM   5546  CG  GLN B 552       1.624   7.956  97.689  1.00 34.73           C
ATOM   5547  CD  GLN B 552       0.135   7.981  97.358  1.00 34.94           C
ATOM   5548  OE1 GLN B 552      -0.472   9.046  97.258  1.00 34.95           O
ATOM   5549  NE2 GLN B 552      -0.461   6.800  97.213  1.00 34.68           N
ATOM   5550  N   ASP B 553       3.914   8.089  93.482  1.00 33.43           N
ATOM   5551  CA  ASP B 553       5.103   8.367  92.689  1.00 32.67           C
ATOM   5552  C   ASP B 553       5.588   9.777  92.997  1.00 32.23           C
ATOM   5553  O   ASP B 553       4.921  10.765  92.654  1.00 32.31           O
ATOM   5554  CB  ASP B 553       4.813   8.192  91.198  1.00 32.69           C
ATOM   5555  CG  ASP B 553       6.019   8.506  90.315  1.00 32.97           C
ATOM   5556  OD1 ASP B 553       7.174   8.515  90.805  1.00 33.10           O
ATOM   5557  OD2 ASP B 553       5.798   8.740  89.113  1.00 32.29           O
ATOM   5558  N   ILE B 554       6.742   9.867  93.654  1.00 31.24           N
ATOM   5559  CA  ILE B 554       7.288  11.167  94.039  1.00 30.38           C
ATOM   5560  C   ILE B 554       8.381  11.675  93.087  1.00 29.89           C
ATOM   5561  O   ILE B 554       8.835  12.815  93.206  1.00 29.62           O
ATOM   5562  CB  ILE B 554       7.731  11.213  95.539  1.00 30.30           C
ATOM   5563  CG1 ILE B 554       8.881  10.241  95.827  1.00 30.21           C
ATOM   5564  CG2 ILE B 554       6.530  10.943  96.457  1.00 30.40           C
ATOM   5565  CD1 ILE B 554       9.570  10.458  97.176  1.00 29.97           C
ATOM   5566  N   THR B 555       8.766  10.832  92.127  1.00 29.44           N
ATOM   5567  CA  THR B 555       9.842  11.136  91.171  1.00 28.88           C
ATOM   5568  C   THR B 555       9.834  12.583  90.639  1.00 28.68           C
ATOM   5569  O   THR B 555      10.850  13.263  90.767  1.00 28.71           O
ATOM   5570  CB  THR B 555       9.884  10.119  89.991  1.00 28.94           C
ATOM   5571  OG1 THR B 555       9.828   8.785  90.503  1.00 28.85           O
ATOM   5572  CG2 THR B 555      11.152  10.276  89.167  1.00 28.42           C
ATOM   5573  N   PRO B 556       8.695  13.059  90.066  1.00 28.47           N
ATOM   5574  CA  PRO B 556       8.679  14.373  89.401  1.00 28.29           C
ATOM   5575  C   PRO B 556       8.890  15.578  90.311  1.00 28.20           C
ATOM   5576  O   PRO B 556       9.163  16.676  89.825  1.00 28.22           O
ATOM   5577  CB  PRO B 556       7.281  14.432  88.776  1.00 28.42           C
ATOM   5578  CG  PRO B 556       6.456  13.526  89.614  1.00 28.24           C
ATOM   5579  CD  PRO B 556       7.370  12.409  89.987  1.00 28.41           C
ATOM   5580  N   MET B 557       8.761  15.384  91.616  1.00 28.23           N
ATOM   5581  CA  MET B 557       8.965  16.482  92.556  1.00 28.15           C
ATOM   5582  C   MET B 557      10.453  16.718  92.815  1.00 27.52           C
ATOM   5583  O   MET B 557      10.858  17.830  93.161  1.00 27.07           O
ATOM   5584  CB  MET B 557       8.231  16.208  93.869  1.00 28.24           C
ATOM   5585  CG  MET B 557       6.729  16.481  93.832  1.00 28.62           C
ATOM   5586  SD  MET B 557       5.909  16.064  95.396  1.00 29.66           S
ATOM   5587  CE  MET B 557       5.738  14.294  95.238  1.00 28.01           C
ATOM   5588  N   VAL B 558      11.258  15.673  92.614  1.00 27.07           N
ATOM   5589  CA  VAL B 558      12.662  15.668  93.038  1.00 26.68           C
ATOM   5590  C   VAL B 558      13.706  15.391  91.940  1.00 26.51           C
ATOM   5591  O   VAL B 558      14.840  15.872  92.036  1.00 26.47           O
ATOM   5592  CB  VAL B 558      12.890  14.673  94.217  1.00 26.64           C
ATOM   5593  CG1 VAL B 558      12.206  15.173  95.479  1.00 26.38           C
ATOM   5594  CG2 VAL B 558      12.405  13.265  93.855  1.00 25.98           C
ATOM   5595  N   LYS B 559      13.333  14.609  90.925  1.00 26.17           N
ATOM   5596  CA  LYS B 559      14.262  14.191  89.864  1.00 25.91           C
ATOM   5597  C   LYS B 559      14.408  15.243  88.764  1.00 25.71           C
ATOM   5598  O   LYS B 559      13.491  15.450  87.972  1.00 25.69           O
ATOM   5599  CB  LYS B 559      13.813  12.857  89.250  1.00 26.06           C
ATOM   5600  CG  LYS B 559      14.867  12.153  88.406  1.00 25.24           C
ATOM   5601  CD  LYS B 559      14.416  10.760  88.044  1.00 25.30           C
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ATOM   5602  CE  LYS B 559      15.511   9.971  87.350  1.00 26.33           C
ATOM   5603  NZ  LYS B 559      15.695  10.363  85.920  1.00 26.55           N
ATOM   5604  N   ALA B 560      15.571  15.890  88.720  1.00 25.47           N
ATOM   5605  CA  ALA B 560      15.885  16.895  87.695  1.00 25.16           C
ATOM   5606  C   ALA B 560      16.142  16.232  86.338  1.00 24.97           C
ATOM   5607  O   ALA B 560      16.381  15.024  86.266  1.00 24.80           O
ATOM   5608  CB  ALA B 560      17.090  17.741  88.122  1.00 24.79           C
ATOM   5609  N   ASP B 561      16.101  17.029  85.272  1.00 24.81           N
ATOM   5610  CA  ASP B 561      16.168  16.505  83.905  1.00 24.95           C
ATOM   5611  C   ASP B 561      17.455  15.750  83.572  1.00 24.74           C
ATOM   5612  O   ASP B 561      17.416  14.750  82.850  1.00 24.57           O
ATOM   5613  CB  ASP B 561      15.919  17.620  82.889  1.00 25.00           C
ATOM   5614  CG  ASP B 561      14.494  18.114  82.919  1.00 26.57           C
ATOM   5615  OD1 ASP B 561      13.606  17.343  83.353  1.00 29.21           O
ATOM   5616  OD2 ASP B 561      14.252  19.272  82.520  1.00 28.90           O
ATOM   5617  N   TRP B 562      18.575  16.230  84.113  1.00 24.45           N
ATOM   5618  CA  TRP B 562      19.895  15.664  83.838  1.00 24.21           C
ATOM   5619  C   TRP B 562      20.142  14.347  84.569  1.00 24.31           C
ATOM   5620  O   TRP B 562      21.037  13.590  84.199  1.00 24.61           O
ATOM   5621  CB  TRP B 562      20.998  16.673  84.187  1.00 24.00           C
ATOM   5622  CG  TRP B 562      21.061  17.071  85.653  1.00 23.80           C
ATOM   5623  CD1 TRP B 562      20.578  18.223  86.207  1.00 23.71           C
ATOM   5624  CD2 TRP B 562      21.635  16.317  86.737  1.00 23.72           C
ATOM   5625  NE1 TRP B 562      20.821  18.241  87.563  1.00 24.04           N
ATOM   5626  CE2 TRP B 562      21.470  17.086  87.914  1.00 24.19           C
ATOM   5627  CE3 TRP B 562      22.281  15.074  86.827  1.00 23.67           C
ATOM   5628  CZ2 TRP B 562      21.922  16.650  89.165  1.00 23.74           C
ATOM   5629  CZ3 TRP B 562      22.727  14.640  88.073  1.00 23.73           C
ATOM   5630  CH2 TRP B 562      22.548  15.430  89.224  1.00 23.92           C
ATOM   5631  N   MET B 563      19.361  14.082  85.613  1.00 24.22           N
ATOM   5632  CA  MET B 563      19.567  12.896  86.440  1.00 24.09           C
ATOM   5633  C   MET B 563      19.247  11.612  85.684  1.00 24.61           C
ATOM   5634  O   MET B 563      18.193  11.495  85.045  1.00 24.33           O
ATOM   5635  CB  MET B 563      18.750  12.973  87.734  1.00 23.82           C
ATOM   5636  CG  MET B 563      19.249  13.997  88.739  1.00 23.06           C
ATOM   5637  SD  MET B 563      18.109  14.161  90.125  1.00 23.74           S
ATOM   5638  CE  MET B 563      18.794  15.557  91.017  1.00 23.20           C
ATOM   5639  N   LYS B 564      20.181  10.662  85.754  1.00 25.02           N
ATOM   5640  CA  LYS B 564      19.978   9.321  85.222  1.00 25.42           C
ATOM   5641  C   LYS B 564      19.348   8.465  86.323  1.00 25.72           C
ATOM   5642  O   LYS B 564      18.154   8.166  86.275  1.00 25.84           O
ATOM   5643  CB  LYS B 564      21.311   8.737  84.744  1.00 25.48           C
ATOM   5644  CG  LYS B 564      21.201   7.532  83.815  1.00 25.63           C
ATOM   5645  CD  LYS B 564      22.565   7.161  83.231  1.00 25.47           C
ATOM   5646  CE  LYS B 564      22.575   5.754  82.640  1.00 25.59           C
ATOM   5647  NZ  LYS B 564      21.694   5.626  81.451  1.00 26.26           N
ATOM   5648  N   PHE B 565      20.147   8.102  87.323  1.00 25.97           N
ATOM   5649  CA  PHE B 565      19.662   7.372  88.488  1.00 25.98           C
ATOM   5650  C   PHE B 565      19.298   8.312  89.627  1.00 26.45           C
ATOM   5651  O   PHE B 565      20.030   9.253  89.931  1.00 26.44           O
ATOM   5652  CB  PHE B 565      20.722   6.368  88.955  1.00 25.91           C
ATOM   5653  CG  PHE B 565      20.435   5.729  90.294  1.00 25.22           C
ATOM   5654  CD1 PHE B 565      19.303   4.932  90.484  1.00 24.74           C
ATOM   5655  CD2 PHE B 565      21.319   5.899  91.355  1.00 24.38           C
ATOM   5656  CE1 PHE B 565      19.052   4.329  91.725  1.00 24.75           C
ATOM   5657  CE2 PHE B 565      21.077   5.304  92.592  1.00 24.26           C
ATOM   5658  CZ  PHE B 565      19.943   4.514  92.776  1.00 24.74           C
ATOM   5659  N   LEU B 566      18.147   8.055  90.241  1.00 27.14           N
ATOM   5660  CA  LEU B 566      17.809   8.649  91.529  1.00 27.66           C
ATOM   5661  C   LEU B 566      17.271   7.565  92.452  1.00 28.17           C
ATOM   5662  O   LEU B 566      16.233   6.950  92.177  1.00 28.23           O
ATOM   5663  CB  LEU B 566      16.792   9.772  91.374  1.00 27.63           C
ATOM   5664  CG  LEU B 566      16.215  10.342  92.669  1.00 27.70           C
ATOM   5665  CD1 LEU B 566      17.205  11.273  93.360  1.00 27.78           C
ATOM   5666  CD2 LEU B 566      14.918  11.061  92.365  1.00 28.28           C
ATOM   5667  N   GLY B 567      17.990   7.334  93.544  1.00 28.66           N
ATOM   5668  CA  GLY B 567      17.614   6.304  94.505  1.00 29.25           C
ATOM   5669  C   GLY B 567      18.082   6.608  95.911  1.00 29.57           C
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ATOM   5670  O   GLY B 567      18.999   7.402  96.116  1.00 29.64           O
ATOM   5671  N   VAL B 568      17.454   5.950  96.876  1.00 29.97           N
ATOM   5672  CA  VAL B 568      17.665   6.243  98.291  1.00 30.48           C
ATOM   5673  C   VAL B 568      18.974   5.681  98.837  1.00 30.86           C
ATOM   5674  O   VAL B 568      19.497   4.687  98.329  1.00 30.82           O
ATOM   5675  CB  VAL B 568      16.493   5.717  99.159  1.00 30.46           C
ATOM   5676  CG1 VAL B 568      15.225   6.531  98.917  1.00 30.37           C
ATOM   5677  CG2 VAL B 568      16.238   4.235  98.901  1.00 30.44           C
ATOM   5678  N   GLY B 569      19.508   6.344  99.857  1.00 31.30           N
ATOM   5679  CA  GLY B 569      20.507   5.729 100.723  1.00 32.08           C
ATOM   5680  C   GLY B 569      19.716   4.937 101.750  1.00 32.52           C
ATOM   5681  O   GLY B 569      19.173   5.527 102.682  1.00 32.58           O
ATOM   5682  N   PRO B 570      19.627   3.602 101.578  1.00 32.83           N
ATOM   5683  CA  PRO B 570      18.696   2.799 102.373  1.00 33.33           C
ATOM   5684  C   PRO B 570      19.030   2.728 103.866  1.00 33.89           C
ATOM   5685  O   PRO B 570      20.175   2.963 104.271  1.00 34.15           O
ATOM   5686  CB  PRO B 570      18.798   1.413 101.741  1.00 33.23           C
ATOM   5687  CG  PRO B 570      20.145   1.377 101.129  1.00 33.35           C
ATOM   5688  CD  PRO B 570      20.405   2.768 100.645  1.00 32.95           C
ATOM   5689  N   GLY B 571      18.017   2.409 104.665  1.00 34.24           N
ATOM   5690  CA  GLY B 571      18.140   2.380 106.110  1.00 34.46           C
ATOM   5691  C   GLY B 571      17.005   3.167 106.721  1.00 34.66           C
ATOM   5692  O   GLY B 571      15.837   2.938 106.396  1.00 34.67           O
ATOM   5693  N   THR B 572      17.349   4.110 107.591  1.00 34.85           N
ATOM   5694  CA  THR B 572      16.346   4.870 108.330  1.00 35.16           C
ATOM   5695  C   THR B 572      16.631   6.369 108.291  1.00 35.38           C
ATOM   5696  O   THR B 572      17.777   6.801 108.461  1.00 35.30           O
ATOM   5697  CB  THR B 572      16.231   4.363 109.791  1.00 35.21           C
ATOM   5698  OG1 THR B 572      15.976   2.950 109.780  1.00 34.70           O
ATOM   5699  CG2 THR B 572      15.106   5.077 110.543  1.00 35.28           C
ATOM   5700  N   GLY B 573      15.579   7.150 108.054  1.00 35.58           N
ATOM   5701  CA  GLY B 573      15.686   8.604 107.998  1.00 36.05           C
ATOM   5702  C   GLY B 573      15.529   9.269 109.352  1.00 36.35           C
ATOM   5703  O   GLY B 573      15.309   8.602 110.367  1.00 36.43           O
ATOM   5704  N   ILE B 574      15.647  10.592 109.364  1.00 36.61           N
ATOM   5705  CA  ILE B 574      15.446  11.366 110.580  1.00 36.94           C
ATOM   5706  C   ILE B 574      14.426  12.472 110.368  1.00 37.18           C
ATOM   5707  O   ILE B 574      14.027  12.760 109.241  1.00 37.34           O
ATOM   5708  CB  ILE B 574      16.763  11.993 111.105  1.00 36.90           C
ATOM   5709  CG1 ILE B 574      17.313  13.025 110.111  1.00 37.13           C
ATOM   5710  CG2 ILE B 574      17.780  10.909 111.422  1.00 36.49           C
ATOM   5711  CD1 ILE B 574      18.160  14.118 110.751  1.00 37.46           C
ATOM   5712  N   VAL B 575      14.002  13.076 111.472  1.00 37.49           N
ATOM   5713  CA  VAL B 575      13.242  14.314 111.435  1.00 37.61           C
ATOM   5714  C   VAL B 575      14.035  15.339 112.232  1.00 37.86           C
ATOM   5715  O   VAL B 575      14.579  15.024 113.289  1.00 37.86           O
ATOM   5716  CB  VAL B 575      11.823  14.147 112.020  1.00 37.43           C
ATOM   5717  CG1 VAL B 575      11.047  15.451 111.935  1.00 37.47           C
ATOM   5718  CG2 VAL B 575      11.076  13.050 111.291  1.00 37.45           C
ATOM   5719  N   LEU B 576      14.116  16.555 111.706  1.00 38.30           N
ATOM   5720  CA  LEU B 576      14.815  17.644 112.380  1.00 38.85           C
ATOM   5721  C   LEU B 576      14.064  18.095 113.636  1.00 39.16           C
ATOM   5722  O   LEU B 576      12.860  18.374 113.590  1.00 39.28           O
ATOM   5723  CB  LEU B 576      15.035  18.817 111.413  1.00 38.80           C
ATOM   5724  CG  LEU B 576      16.334  18.856 110.591  1.00 38.97           C
ATOM   5725  CD1 LEU B 576      16.779  17.485 110.064  1.00 38.94           C
ATOM   5726  CD2 LEU B 576      16.219  19.866 109.451  1.00 38.87           C
ATOM   5727  N   ARG B 577      14.791  18.156 114.751  1.00 39.47           N
ATOM   5728  CA  ARG B 577      14.214  18.464 116.067  1.00 39.57           C
ATOM   5729  C   ARG B 577      14.683  19.818 116.616  1.00 39.85           C
ATOM   5730  O   ARG B 577      14.152  20.300 117.613  1.00 40.02           O
ATOM   5731  CB  ARG B 577      14.559  17.347 117.062  1.00 39.61           C
ATOM   5732  CG  ARG B 577      16.057  17.160 117.235  1.00 39.34           C
ATOM   5733  CD  ARG B 577      16.445  16.001 118.139  1.00 38.90           C
ATOM   5734  NE  ARG B 577      17.856  16.123 118.501  1.00 37.10           N
ATOM   5735  CZ  ARG B 577      18.877  15.747 117.732  1.00 36.86           C
ATOM   5736  NH1 ARG B 577      18.673  15.194 116.543  1.00 36.37           N
ATOM   5737  NH2 ARG B 577      20.117  15.928 118.158  1.00 37.21           N
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ATOM   5738  N   ASN B 578      15.684  20.410 115.965  1.00 40.06           N
ATOM   5739  CA  ASN B 578      16.254  21.694 116.374  1.00 40.32           C
ATOM   5740  C   ASN B 578      16.091  22.747 115.289  1.00 40.25           C
ATOM   5741  O   ASN B 578      15.466  22.500 114.260  1.00 40.30           O
ATOM   5742  CB  ASN B 578      17.752  21.553 116.676  1.00 40.38           C
ATOM   5743  CG  ASN B 578      18.060  20.411 117.614  1.00 41.54           C
ATOM   5744  OD1 ASN B 578      18.634  19.400 117.204  1.00 42.10           O
ATOM   5745  ND2 ASN B 578      17.684  20.561 118.885  1.00 42.88           N
ATOM   5746  N   GLY B 579      16.657  23.925 115.544  1.00 40.26           N
ATOM   5747  CA  GLY B 579      16.872  24.945 114.526  1.00 40.10           C
ATOM   5748  C   GLY B 579      15.645  25.481 113.817  1.00 40.14           C
ATOM   5749  O   GLY B 579      14.511  25.128 114.164  1.00 40.10           O
ATOM   5750  N   PRO B 580      15.867  26.339 112.803  1.00 40.07           N
ATOM   5751  CA  PRO B 580      14.798  27.013 112.069  1.00 39.90           C
ATOM   5752  C   PRO B 580      14.064  26.101 111.080  1.00 39.80           C
ATOM   5753  O   PRO B 580      13.168  26.567 110.364  1.00 39.73           O
ATOM   5754  CB  PRO B 580      15.534  28.135 111.317  1.00 39.81           C
ATOM   5755  CG  PRO B 580      16.966  28.099 111.802  1.00 40.10           C
ATOM   5756  CD  PRO B 580      17.195  26.719 112.293  1.00 40.07           C
ATOM   5757  N   HIS B 581      14.442  24.822 111.043  1.00 39.64           N
ATOM   5758  CA  HIS B 581      13.836  23.853 110.125  1.00 39.49           C
ATOM   5759  C   HIS B 581      13.340  22.605 110.847  1.00 39.40           C
ATOM   5760  O   HIS B 581      13.239  21.530 110.246  1.00 39.44           O
ATOM   5761  CB  HIS B 581      14.815  23.476 109.004  1.00 39.61           C
ATOM   5762  CG  HIS B 581      15.251  24.639 108.170  1.00 39.48           C
ATOM   5763  ND1 HIS B 581      14.450  25.196 107.197  1.00 39.59           N
ATOM   5764  CD2 HIS B 581      16.398  25.359 108.174  1.00 39.57           C
ATOM   5765  CE1 HIS B 581      15.084  26.210 106.635  1.00 39.71           C
ATOM   5766  NE2 HIS B 581      16.270  26.328 107.207  1.00 40.00           N
ATOM   5767  N   LYS B 582      13.027  22.755 112.134  1.00 39.25           N
ATOM   5768  CA  LYS B 582      12.456  21.669 112.927  1.00 39.08           C
ATOM   5769  C   LYS B 582      11.193  21.146 112.248  1.00 38.75           C
ATOM   5770  O   LYS B 582      10.345  21.929 111.818  1.00 38.80           O
ATOM   5771  CB  LYS B 582      12.142  22.146 114.348  1.00 39.21           C
ATOM   5772  CG  LYS B 582      11.474  21.093 115.223  1.00 39.76           C
ATOM   5773  CD  LYS B 582      11.073  21.658 116.569  1.00 40.91           C
ATOM   5774  CE  LYS B 582      10.199  20.677 117.345  1.00 40.90           C
ATOM   5775  NZ  LYS B 582       9.701  21.292 118.608  1.00 41.14           N
ATOM   5776  N   GLY B 583      11.089  19.825 112.141  1.00 38.32           N
ATOM   5777  CA  GLY B 583       9.947  19.190 111.491  1.00 38.00           C
ATOM   5778  C   GLY B 583      10.252  18.663 110.099  1.00 37.82           C
ATOM   5779  O   GLY B 583       9.493  17.853 109.559  1.00 37.66           O
ATOM   5780  N   ARG B 584      11.362  19.123 109.520  1.00 37.58           N
ATOM   5781  CA  ARG B 584      11.797  18.685 108.194  1.00 37.34           C
ATOM   5782  C   ARG B 584      12.222  17.218 108.219  1.00 37.32           C
ATOM   5783  O   ARG B 584      13.001  16.802 109.080  1.00 37.48           O
ATOM   5784  CB  ARG B 584      12.946  19.562 107.690  1.00 37.55           C
ATOM   5785  CG  ARG B 584      13.509  19.178 106.320  1.00 37.16           C
ATOM   5786  CD  ARG B 584      14.540  20.196 105.853  1.00 37.20           C
ATOM   5787  NE  ARG B 584      13.916  21.424 105.358  1.00 36.40           N
ATOM   5788  CZ  ARG B 584      14.566  22.557 105.099  1.00 35.56           C
ATOM   5789  NH1 ARG B 584      15.877  22.646 105.292  1.00 34.74           N
ATOM   5790  NH2 ARG B 584      13.897  23.609 104.645  1.00 34.98           N
ATOM   5791  N   ILE B 585      11.698  16.448 107.269  1.00 36.94           N
ATOM   5792  CA  ILE B 585      11.998  15.027 107.154  1.00 36.55           C
ATOM   5793  C   ILE B 585      13.111  14.814 106.132  1.00 36.36           C
ATOM   5794  O   ILE B 585      12.997  15.242 104.986  1.00 36.43           O
ATOM   5795  CB  ILE B 585      10.746  14.220 106.755  1.00 36.45           C
ATOM   5796  CG1 ILE B 585       9.583  14.554 107.694  1.00 36.12           C
ATOM   5797  CG2 ILE B 585      11.052  12.731 106.769  1.00 36.33           C
ATOM   5798  CD1 ILE B 585       8.226  14.168 107.161  1.00 36.54           C
ATOM   5799  N   LEU B 586      14.180  14.149 106.560  1.00 36.05           N
ATOM   5800  CA  LEU B 586      15.366  13.948 105.728  1.00 35.62           C
ATOM   5801  C   LEU B 586      15.514  12.509 105.230  1.00 35.08           C
ATOM   5802  O   LEU B 586      15.666  11.579 106.024  1.00 34.98           O
ATOM   5803  CB  LEU B 586      16.630  14.392 106.482  1.00 35.81           C
ATOM   5804  CG  LEU B 586      17.278  15.743 106.137  1.00 36.16           C
ATOM   5805  CD1 LEU B 586      16.293  16.904 106.136  1.00 36.88           C
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ATOM   5806  CD2 LEU B 586      18.431  16.039 107.073  1.00 35.80           C
ATOM   5807  N   ILE B 587      15.459  12.351 103.907  1.00 34.31           N
ATOM   5808  CA  ILE B 587      15.686  11.074 103.237  1.00 33.55           C
ATOM   5809  C   ILE B 587      16.980  11.154 102.422  1.00 33.01           C
ATOM   5810  O   ILE B 587      17.060  11.920 101.458  1.00 33.09           O
ATOM   5811  CB  ILE B 587      14.506  10.698 102.294  1.00 33.56           C
ATOM   5812  CG1 ILE B 587      13.152  10.863 103.002  1.00 33.79           C
ATOM   5813  CG2 ILE B 587      14.684   9.289 101.715  1.00 33.31           C
ATOM   5814  CD1 ILE B 587      12.878   9.860 104.120  1.00 33.62           C
ATOM   5815  N   PRO B 588      18.001  10.373 102.814  1.00 32.39           N
ATOM   5816  CA  PRO B 588      19.259  10.302 102.071  1.00 31.76           C
ATOM   5817  C   PRO B 588      19.070   9.642 100.712  1.00 31.10           C
ATOM   5818  O   PRO B 588      18.436   8.589 100.619  1.00 31.22           O
ATOM   5819  CB  PRO B 588      20.137   9.413 102.956  1.00 31.68           C
ATOM   5820  CG  PRO B 588      19.491   9.452 104.306  1.00 31.90           C
ATOM   5821  CD  PRO B 588      18.038   9.515 104.009  1.00 32.36           C
ATOM   5822  N   VAL B 589      19.609  10.268  99.670  1.00 30.21           N
ATOM   5823  CA  VAL B 589      19.554   9.719  98.313  1.00 29.28           C
ATOM   5824  C   VAL B 589      20.881   9.947  97.587  1.00 28.85           C
ATOM   5825  O   VAL B 589      21.765  10.654  98.085  1.00 28.63           O
ATOM   5826  CB  VAL B 589      18.374  10.311  97.456  1.00 29.24           C
ATOM   5827  CG1 VAL B 589      17.014   9.908  98.009  1.00 29.04           C
ATOM   5828  CG2 VAL B 589      18.472  11.830  97.323  1.00 29.02           C
ATOM   5829  N   TYR B 590      21.014   9.340  96.413  1.00 28.16           N
ATOM   5830  CA  TYR B 590      22.165   9.592  95.559  1.00 27.74           C
ATOM   5831  C   TYR B 590      21.829   9.522  94.070  1.00 27.39           C
ATOM   5832  O   TYR B 590      20.942   8.770  93.653  1.00 27.57           O
ATOM   5833  CB  TYR B 590      23.359   8.705  95.937  1.00 27.74           C
ATOM   5834  CG  TYR B 590      23.156   7.221  95.777  1.00 27.61           C
ATOM   5835  CD1 TYR B 590      22.175   6.543  96.500  1.00 27.56           C
ATOM   5836  CD2 TYR B 590      23.974   6.484  94.927  1.00 27.72           C
ATOM   5837  CE1 TYR B 590      21.998   5.167  96.356  1.00 27.93           C
ATOM   5838  CE2 TYR B 590      23.811   5.108  94.783  1.00 28.39           C
ATOM   5839  CZ  TYR B 590      22.820   4.457  95.500  1.00 27.82           C
ATOM   5840  OH  TYR B 590      22.655   3.098  95.354  1.00 28.09           O
ATOM   5841  N   THR B 591      22.538  10.324  93.282  1.00 26.90           N
ATOM   5842  CA  THR B 591      22.256  10.461  91.857  1.00 26.48           C
ATOM   5843  C   THR B 591      23.436  10.024  91.007  1.00 26.34           C
ATOM   5844  O   THR B 591      24.580  10.046  91.467  1.00 26.34           O
ATOM   5845  CB  THR B 591      21.961  11.923  91.491  1.00 26.30           C
ATOM   5846  OG1 THR B 591      23.095  12.728  91.836  1.00 26.15           O
ATOM   5847  CG2 THR B 591      20.720  12.433  92.225  1.00 26.33           C
ATOM   5848  N   THR B 592      23.146   9.626  89.770  1.00 26.01           N
ATOM   5849  CA  THR B 592      24.163   9.540  88.730  1.00 26.13           C
ATOM   5850  C   THR B 592      23.840  10.551  87.621  1.00 26.25           C
ATOM   5851  O   THR B 592      22.731  11.100  87.579  1.00 26.39           O
ATOM   5852  CB  THR B 592      24.276   8.127  88.105  1.00 26.07           C
ATOM   5853  OG1 THR B 592      23.108   7.849  87.327  1.00 25.95           O
ATOM   5854  CG2 THR B 592      24.467   7.047  89.173  1.00 26.68           C
ATOM   5855  N   ASN B 593      24.813  10.797  86.743  1.00 26.05           N
ATOM   5856  CA  ASN B 593      24.621  11.643  85.575  1.00 25.99           C
ATOM   5857  C   ASN B 593      24.926  10.865  84.309  1.00 26.11           C
ATOM   5858  O   ASN B 593      25.407   9.738  84.376  1.00 26.40           O
ATOM   5859  CB  ASN B 593      25.457  12.934  85.664  1.00 26.00           C
ATOM   5860  CG  ASN B 593      26.961  12.702  85.496  1.00 25.94           C
ATOM   5861  OD1 ASN B 593      27.408  11.822  84.752  1.00 25.81           O
ATOM   5862  ND2 ASN B 593      27.749  13.521  86.177  1.00 26.36           N
ATOM   5863  N   ASN B 594      24.651  11.471  83.162  1.00 26.38           N
ATOM   5864  CA  ASN B 594      24.794  10.800  81.871  1.00 26.51           C
ATOM   5865  C   ASN B 594      26.202  10.864  81.306  1.00 26.61           C
ATOM   5866  O   ASN B 594      26.502  10.207  80.305  1.00 26.57           O
ATOM   5867  CB  ASN B 594      23.792  11.370  80.865  1.00 26.64           C
ATOM   5868  CG  ASN B 594      22.373  10.941  81.161  1.00 26.66           C
ATOM   5869  OD1 ASN B 594      22.070   9.746  81.177  1.00 28.18           O
ATOM   5870  ND2 ASN B 594      21.492  11.908  81.388  1.00 25.44           N
ATOM   5871  N   VAL B 595      27.061  11.656  81.948  1.00 26.75           N
ATOM   5872  CA  VAL B 595      28.459  11.766  81.536  1.00 26.87           C
ATOM   5873  C   VAL B 595      29.241  10.506  81.914  1.00 26.95           C
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ATOM   5874  O   VAL B 595      29.977   9.973  81.085  1.00 27.11           O
ATOM   5875  CB  VAL B 595      29.153  13.036  82.115  1.00 26.95           C
ATOM   5876  CG1 VAL B 595      30.642  13.078  81.743  1.00 26.70           C
ATOM   5877  CG2 VAL B 595      28.452  14.298  81.632  1.00 26.93           C
ATOM   5878  N   SER B 596      29.077  10.032  83.151  1.00 26.91           N
ATOM   5879  CA  SER B 596      29.875   8.895  83.647  1.00 26.87           C
ATOM   5880  C   SER B 596      29.094   7.830  84.424  1.00 26.76           C
ATOM   5881  O   SER B 596      29.647   6.769  84.747  1.00 26.56           O
ATOM   5882  CB  SER B 596      31.067   9.386  84.477  1.00 26.82           C
ATOM   5883  OG  SER B 596      30.652  10.117  85.619  1.00 27.17           O
ATOM   5884  N   HIS B 597      27.823   8.116  84.714  1.00 26.59           N
ATOM   5885  CA  HIS B 597      26.920   7.166  85.378  1.00 26.64           C
ATOM   5886  C   HIS B 597      27.582   6.478  86.591  1.00 26.73           C
ATOM   5887  O   HIS B 597      28.069   7.162  87.490  1.00 26.88           O
ATOM   5888  CB  HIS B 597      26.340   6.173  84.354  1.00 26.55           C
ATOM   5889  CG  HIS B 597      25.268   5.280  84.899  1.00 26.12           C
ATOM   5890  ND1 HIS B 597      24.331   5.709  85.816  1.00 26.34           N
ATOM   5891  CD2 HIS B 597      24.977   3.983  84.643  1.00 26.46           C
ATOM   5892  CE1 HIS B 597      23.519   4.709  86.114  1.00 26.28           C
ATOM   5893  NE2 HIS B 597      23.886   3.651  85.413  1.00 26.62           N
ATOM   5894  N   LEU B 598      27.633   5.150  86.605  1.00 26.92           N
ATOM   5895  CA  LEU B 598      28.153   4.419  87.764  1.00 27.20           C
ATOM   5896  C   LEU B 598      29.659   4.562  87.977  1.00 27.30           C
ATOM   5897  O   LEU B 598      30.142   4.434  89.100  1.00 27.52           O
ATOM   5898  CB  LEU B 598      27.760   2.936  87.702  1.00 27.08           C
ATOM   5899  CG  LEU B 598      26.335   2.580  88.153  1.00 27.37           C
ATOM   5900  CD1 LEU B 598      26.156   1.068  88.243  1.00 26.86           C
ATOM   5901  CD2 LEU B 598      25.973   3.235  89.495  1.00 27.20           C
ATOM   5902  N   ASN B 599      30.382   4.853  86.900  1.00 27.41           N
ATOM   5903  CA  ASN B 599      31.841   4.907  86.916  1.00 27.26           C
ATOM   5904  C   ASN B 599      32.458   6.139  87.572  1.00 27.24           C
ATOM   5905  O   ASN B 599      33.580   6.057  88.072  1.00 27.48           O
ATOM   5906  CB  ASN B 599      32.387   4.755  85.493  1.00 27.40           C
ATOM   5907  CG  ASN B 599      31.937   3.461  84.834  1.00 27.46           C
ATOM   5908  OD1 ASN B 599      31.794   2.429  85.492  1.00 28.03           O
ATOM   5909  ND2 ASN B 599      31.716   3.511  83.530  1.00 27.49           N
ATOM   5910  N   GLY B 600      31.748   7.271  87.567  1.00 26.96           N
ATOM   5911  CA  GLY B 600      32.295   8.508  88.137  1.00 26.57           C
ATOM   5912  C   GLY B 600      31.358   9.616  88.609  1.00 26.50           C
ATOM   5913  O   GLY B 600      31.808  10.744  88.832  1.00 26.38           O
ATOM   5914  N   SER B 601      30.071   9.314  88.792  1.00 26.34           N
ATOM   5915  CA  SER B 601      29.101  10.375  89.106  1.00 26.22           C
ATOM   5916  C   SER B 601      28.231  10.209  90.363  1.00 25.97           C
ATOM   5917  O   SER B 601      27.520  11.139  90.741  1.00 25.72           O
ATOM   5918  CB  SER B 601      28.205  10.652  87.896  1.00 26.05           C
ATOM   5919  OG  SER B 601      27.281   9.604  87.718  1.00 25.94           O
ATOM   5920  N   GLN B 602      28.275   9.042  90.997  1.00 25.94           N
ATOM   5921  CA  GLN B 602      27.492   8.810  92.215  1.00 26.00           C
ATOM   5922  C   GLN B 602      27.681   9.944  93.229  1.00 25.96           C
ATOM   5923  O   GLN B 602      28.796  10.187  93.710  1.00 25.50           O
ATOM   5924  CB  GLN B 602      27.811   7.443  92.816  1.00 25.87           C
ATOM   5925  CG  GLN B 602      27.200   6.294  92.034  1.00 26.76           C
ATOM   5926  CD  GLN B 602      27.801   4.941  92.378  1.00 28.33           C
ATOM   5927  OE1 GLN B 602      27.131   4.082  92.944  1.00 28.47           O
ATOM   5928  NE2 GLN B 602      29.069   4.743  92.023  1.00 28.92           N
ATOM   5929  N   SER B 603      26.581  10.651  93.507  1.00 25.99           N
ATOM   5930  CA  SER B 603      26.598  11.867  94.317  1.00 26.03           C
ATOM   5931  C   SER B 603      25.506  11.870  95.395  1.00 26.61           C
ATOM   5932  O   SER B 603      24.310  11.798  95.089  1.00 26.42           O
ATOM   5933  CB  SER B 603      26.452  13.095  93.424  1.00 25.94           C
ATOM   5934  OG  SER B 603      27.558  13.236  92.550  1.00 25.81           O
ATOM   5935  N   SER B 604      25.936  11.963  96.654  1.00 26.84           N
ATOM   5936  CA  SER B 604      25.036  11.939  97.799  1.00 27.26           C
ATOM   5937  C   SER B 604      24.345  13.280  97.980  1.00 27.43           C
ATOM   5938  O   SER B 604      24.959  14.336  97.822  1.00 27.52           O
ATOM   5939  CB  SER B 604      25.798  11.597  99.082  1.00 27.31           C
ATOM   5940  OG  SER B 604      26.301  10.270  99.062  1.00 27.63           O
ATOM   5941  N   ARG B 605      23.057  13.216  98.297  1.00 27.67           N
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ATOM   5942  CA  ARG B 605      22.272  14.380  98.709  1.00 27.87           C
ATOM   5943  C   ARG B 605      21.086  13.879  99.536  1.00 27.96           C
ATOM   5944  O   ARG B 605      20.961  12.683  99.791  1.00 27.61           O
ATOM   5945  CB  ARG B 605      21.805  15.205  97.497  1.00 27.65           C
ATOM   5946  CG  ARG B 605      20.676  14.572  96.681  1.00 28.18           C
ATOM   5947  CD  ARG B 605      20.193  15.484  95.559  1.00 27.65           C
ATOM   5948  NE  ARG B 605      21.177  15.604  94.486  1.00 27.34           N
ATOM   5949  CZ  ARG B 605      21.264  16.639  93.651  1.00 27.57           C
ATOM   5950  NH1 ARG B 605      20.425  17.666  93.747  1.00 26.48           N
ATOM   5951  NH2 ARG B 605      22.196  16.643  92.708  1.00 27.95           N
ATOM   5952  N   ILE B 606      20.229  14.792  99.971  1.00 28.51           N
ATOM   5953  CA  ILE B 606      18.978  14.388 100.601  1.00 29.16           C
ATOM   5954  C   ILE B 606      17.782  14.954  99.853  1.00 29.61           C
ATOM   5955  O   ILE B 606      17.911  15.918  99.093  1.00 29.76           O
ATOM   5956  CB  ILE B 606      18.902  14.769 102.112  1.00 29.06           C
ATOM   5957  CG1 ILE B 606      19.113  16.273 102.334  1.00 29.14           C
ATOM   5958  CG2 ILE B 606      19.900  13.949 102.928  1.00 29.31           C
ATOM   5959  CD1 ILE B 606      17.850  17.113 102.226  1.00 28.96           C
ATOM   5960  N   ILE B 607      16.630  14.323 100.052  1.00 30.18           N
ATOM   5961  CA  ILE B 607      15.349  14.933  99.723  1.00 30.64           C
ATOM   5962  C   ILE B 607      14.627  15.161 101.043  1.00 30.96           C
ATOM   5963  O   ILE B 607      14.878  14.451 102.020  1.00 30.90           O
ATOM   5964  CB  ILE B 607      14.514  14.080  98.737  1.00 30.78           C
ATOM   5965  CG1 ILE B 607      14.104  12.739  99.371  1.00 30.89           C
ATOM   5966  CG2 ILE B 607      15.294  13.884  97.419  1.00 30.69           C
ATOM   5967  CD1 ILE B 607      13.109  11.912  98.558  1.00 30.47           C
ATOM   5968  N   TYR B 608      13.752  16.159 101.080  1.00 31.45           N
ATOM   5969  CA  TYR B 608      13.149  16.587 102.335  1.00 31.80           C
ATOM   5970  C   TYR B 608      11.688  16.996 102.201  1.00 32.17           C
ATOM   5971  O   TYR B 608      11.207  17.271 101.101  1.00 32.22           O
ATOM   5972  CB  TYR B 608      13.964  17.728 102.949  1.00 31.85           C
ATOM   5973  CG  TYR B 608      14.000  18.994 102.123  1.00 31.75           C
ATOM   5974  CD1 TYR B 608      14.921  19.145 101.090  1.00 32.30           C
ATOM   5975  CD2 TYR B 608      13.122  20.047 102.383  1.00 31.80           C
ATOM   5976  CE1 TYR B 608      14.964  20.305 100.324  1.00 32.00           C
ATOM   5977  CE2 TYR B 608      13.154  21.217 101.624  1.00 31.68           C
ATOM   5978  CZ  TYR B 608      14.084  21.338 100.599  1.00 32.12           C
ATOM   5979  OH  TYR B 608      14.138  22.484  99.838  1.00 32.33           O
ATOM   5980  N   SER B 609      10.990  17.023 103.333  1.00 32.54           N
ATOM   5981  CA  SER B 609       9.601  17.467 103.380  1.00 32.95           C
ATOM   5982  C   SER B 609       9.363  18.375 104.574  1.00 33.27           C
ATOM   5983  O   SER B 609       9.672  18.016 105.716  1.00 33.38           O
ATOM   5984  CB  SER B 609       8.642  16.282 103.432  1.00 32.84           C
ATOM   5985  OG  SER B 609       7.305  16.743 103.396  1.00 33.16           O
ATOM   5986  N   ASP B 610       8.820  19.555 104.291  1.00 33.58           N
ATOM   5987  CA  ASP B 610       8.516  20.548 105.309  1.00 33.99           C
ATOM   5988  C   ASP B 610       7.012  20.598 105.614  1.00 34.18           C
ATOM   5989  O   ASP B 610       6.564  21.409 106.426  1.00 34.26           O
ATOM   5990  CB  ASP B 610       9.019  21.926 104.862  1.00 34.02           C
ATOM   5991  CG  ASP B 610      10.538  22.052 104.918  1.00 34.47           C
ATOM   5992  OD1 ASP B 610      11.165  21.470 105.826  1.00 34.96           O
ATOM   5993  OD2 ASP B 610      11.108  22.760 104.060  1.00 34.58           O
ATOM   5994  N   ASP B 611       6.235  19.735 104.964  1.00 34.49           N
ATOM   5995  CA  ASP B 611       4.785  19.700 105.187  1.00 34.78           C
ATOM   5996  C   ASP B 611       4.257  18.304 105.546  1.00 35.01           C
ATOM   5997  O   ASP B 611       3.155  17.915 105.147  1.00 35.21           O
ATOM   5998  CB  ASP B 611       4.018  20.329 104.008  1.00 34.62           C
ATOM   5999  CG  ASP B 611       4.292  19.644 102.671  1.00 34.72           C
ATOM   6000  OD1 ASP B 611       5.063  18.656 102.615  1.00 34.47           O
ATOM   6001  OD2 ASP B 611       3.714  20.106 101.661  1.00 34.96           O
ATOM   6002  N   HIS B 612       5.055  17.570 106.320  1.00 35.40           N
ATOM   6003  CA  HIS B 612       4.690  16.247 106.841  1.00 35.62           C
ATOM   6004  C   HIS B 612       4.533  15.207 105.736  1.00 35.75           C
ATOM   6005  O   HIS B 612       3.606  14.393 105.760  1.00 35.77           O
ATOM   6006  CB  HIS B 612       3.432  16.323 107.731  1.00 35.71           C
ATOM   6007  CG  HIS B 612       3.451  17.462 108.705  1.00 35.47           C
ATOM   6008  ND1 HIS B 612       4.215  17.448 109.853  1.00 35.22           N
ATOM   6009  CD2 HIS B 612       2.821  18.662 108.687  1.00 35.10           C
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ATOM   6010  CE1 HIS B 612       4.047  18.586 110.504  1.00 34.91           C
ATOM   6011  NE2 HIS B 612       3.206  19.339 109.818  1.00 34.78           N
ATOM   6012  N   GLY B 613       5.445  15.249 104.765  1.00 35.94           N
ATOM   6013  CA  GLY B 613       5.538  14.207 103.739  1.00 36.05           C
ATOM   6014  C   GLY B 613       4.575  14.338 102.574  1.00 36.36           C
ATOM   6015  O   GLY B 613       4.450  13.416 101.767  1.00 36.22           O
ATOM   6016  N   LYS B 614       3.890  15.475 102.481  1.00 36.65           N
ATOM   6017  CA  LYS B 614       3.011  15.724 101.346  1.00 36.99           C
ATOM   6018  C   LYS B 614       3.830  16.029 100.092  1.00 36.76           C
ATOM   6019  O   LYS B 614       3.769  15.287  99.119  1.00 36.98           O
ATOM   6020  CB  LYS B 614       2.022  16.857 101.638  1.00 37.22           C
ATOM   6021  CG  LYS B 614       0.857  16.887 100.663  1.00 37.79           C
ATOM   6022  CD  LYS B 614       0.258  18.271 100.555  1.00 39.70           C
ATOM   6023  CE  LYS B 614      -0.439  18.449  99.213  1.00 40.53           C
ATOM   6024  NZ  LYS B 614      -1.048  19.803  99.106  1.00 41.84           N
ATOM   6025  N   THR B 615       4.589  17.121 100.124  1.00 36.69           N
ATOM   6026  CA  THR B 615       5.458  17.499  99.008  1.00 36.38           C
ATOM   6027  C   THR B 615       6.920  17.272  99.377  1.00 36.22           C
ATOM   6028  O   THR B 615       7.290  17.322 100.552  1.00 36.21           O
ATOM   6029  CB  THR B 615       5.265  18.975  98.580  1.00 36.40           C
ATOM   6030  OG1 THR B 615       5.552  19.844  99.682  1.00 36.52           O
ATOM   6031  CG2 THR B 615       3.843  19.231  98.090  1.00 36.66           C
ATOM   6032  N   TRP B 616       7.740  17.014  98.363  1.00 35.93           N
ATOM   6033  CA  TRP B 616       9.162  16.776  98.553  1.00 35.60           C
ATOM   6034  C   TRP B 616       9.999  17.710  97.682  1.00 35.51           C
ATOM   6035  O   TRP B 616       9.561  18.135  96.607  1.00 35.66           O
ATOM   6036  CB  TRP B 616       9.504  15.313  98.251  1.00 35.56           C
ATOM   6037  CG  TRP B 616       8.823  14.360  99.178  1.00 35.55           C
ATOM   6038  CD1 TRP B 616       7.589  13.799  99.013  1.00 35.50           C
ATOM   6039  CD2 TRP B 616       9.325  13.869 100.427  1.00 35.18           C
ATOM   6040  NE1 TRP B 616       7.294  12.984 100.079  1.00 35.41           N
ATOM   6041  CE2 TRP B 616       8.340  13.007 100.962  1.00 35.03           C
ATOM   6042  CE3 TRP B 616      10.511  14.068 101.143  1.00 35.17           C
ATOM   6043  CZ2 TRP B 616       8.503  12.346 102.183  1.00 34.96           C
ATOM   6044  CZ3 TRP B 616      10.672  13.412 102.364  1.00 35.76           C
ATOM   6045  CH2 TRP B 616       9.671  12.560 102.869  1.00 35.47           C
ATOM   6046  N   HIS B 617      11.198  18.031  98.159  1.00 35.00           N
ATOM   6047  CA  HIS B 617      12.153  18.823  97.396  1.00 34.53           C
ATOM   6048  C   HIS B 617      13.523  18.172  97.464  1.00 34.18           C
ATOM   6049  O   HIS B 617      13.822  17.431  98.403  1.00 34.32           O
ATOM   6050  CB  HIS B 617      12.221  20.253  97.927  1.00 34.45           C
ATOM   6051  CG  HIS B 617      10.891  20.932  97.996  1.00 34.78           C
ATOM   6052  ND1 HIS B 617      10.339  21.601  96.923  1.00 34.89           N
ATOM   6053  CD2 HIS B 617       9.995  21.035  99.006  1.00 34.79           C
ATOM   6054  CE1 HIS B 617       9.164  22.093  97.273  1.00 35.00           C
ATOM   6055  NE2 HIS B 617       8.932  21.763  98.532  1.00 35.11           N
ATOM   6056  N   ALA B 618      14.343  18.438  96.455  1.00 33.67           N
ATOM   6057  CA  ALA B 618      15.707  17.928  96.415  1.00 33.24           C
ATOM   6058  C   ALA B 618      16.671  18.941  97.008  1.00 32.94           C
ATOM   6059  O   ALA B 618      16.612  20.134  96.693  1.00 32.87           O
ATOM   6060  CB  ALA B 618      16.108  17.593  94.983  1.00 33.16           C
ATOM   6061  N   GLY B 619      17.555  18.466  97.876  1.00 32.58           N
ATOM   6062  CA  GLY B 619      18.667  19.285  98.339  1.00 32.27           C
ATOM   6063  C   GLY B 619      19.746  19.300  97.275  1.00 31.96           C
ATOM   6064  O   GLY B 619      19.709  18.499  96.347  1.00 31.84           O
ATOM   6065  N   GLU B 620      20.694  20.226  97.393  1.00 31.89           N
ATOM   6066  CA  GLU B 620      21.864  20.240  96.520  1.00 31.82           C
ATOM   6067  C   GLU B 620      22.785  19.098  96.913  1.00 31.67           C
ATOM   6068  O   GLU B 620      22.819  18.694  98.073  1.00 31.28           O
ATOM   6069  CB  GLU B 620      22.629  21.550  96.652  1.00 31.88           C
ATOM   6070  CG  GLU B 620      21.887  22.776  96.183  1.00 32.68           C
ATOM   6071  CD  GLU B 620      22.734  24.032  96.277  1.00 33.77           C
ATOM   6072  OE1 GLU B 620      23.886  23.955  96.764  1.00 34.06           O
ATOM   6073  OE2 GLU B 620      22.246  25.104  95.861  1.00 35.05           O
ATOM   6074  N   ALA B 621      23.531  18.583  95.941  1.00 31.77           N
ATOM   6075  CA  ALA B 621      24.474  17.501  96.194  1.00 31.76           C
ATOM   6076  C   ALA B 621      25.675  17.989  97.000  1.00 31.80           C
ATOM   6077  O   ALA B 621      26.023  19.170  96.966  1.00 31.73           O
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ATOM   6078  CB  ALA B 621      24.924  16.870  94.884  1.00 31.51           C
ATOM   6079  N   VAL B 622      26.301  17.069  97.728  1.00 32.03           N
ATOM   6080  CA  VAL B 622      27.564  17.351  98.408  1.00 32.21           C
ATOM   6081  C   VAL B 622      28.626  17.706  97.368  1.00 32.39           C
ATOM   6082  O   VAL B 622      29.471  18.580  97.603  1.00 32.51           O
ATOM   6083  CB  VAL B 622      28.029  16.148  99.266  1.00 32.18           C
ATOM   6084  CG1 VAL B 622      29.389  16.420  99.885  1.00 31.98           C
ATOM   6085  CG2 VAL B 622      27.001  15.831 100.348  1.00 31.89           C
ATOM   6086  N   ASN B 623      28.554  17.034  96.217  1.00 32.49           N
ATOM   6087  CA  ASN B 623      29.464  17.268  95.093  1.00 32.84           C
ATOM   6088  C   ASN B 623      29.177  18.504  94.229  1.00 33.29           C
ATOM   6089  O   ASN B 623      29.893  18.747  93.259  1.00 33.57           O
ATOM   6090  CB  ASN B 623      29.531  16.026  94.196  1.00 32.75           C
ATOM   6091  CG  ASN B 623      30.187  14.846  94.879  1.00 31.84           C
ATOM   6092  OD1 ASN B 623      31.038  15.010  95.747  1.00 31.67           O
ATOM   6093  ND2 ASN B 623      29.790  13.649  94.489  1.00 30.91           N
ATOM   6094  N   ASP B 624      28.146  19.279  94.562  1.00 33.92           N
ATOM   6095  CA  ASP B 624      27.834  20.490  93.793  1.00 34.82           C
ATOM   6096  C   ASP B 624      28.737  21.660  94.169  1.00 35.79           C
ATOM   6097  O   ASP B 624      28.775  22.079  95.332  1.00 35.82           O
ATOM   6098  CB  ASP B 624      26.360  20.881  93.933  1.00 34.49           C
ATOM   6099  CG  ASP B 624      25.428  19.947  93.172  1.00 34.02           C
ATOM   6100  OD1 ASP B 624      25.914  19.122  92.368  1.00 33.13           O
ATOM   6101  OD2 ASP B 624      24.200  20.038  93.387  1.00 33.13           O
ATOM   6102  N   ASN B 625      29.450  22.181  93.166  1.00 36.95           N
ATOM   6103  CA  ASN B 625      30.427  23.269  93.328  1.00 38.11           C
ATOM   6104  C   ASN B 625      31.481  22.944  94.391  1.00 38.93           C
ATOM   6105  O   ASN B 625      31.882  23.799  95.187  1.00 39.20           O
ATOM   6106  CB  ASN B 625      29.734  24.617  93.593  1.00 38.18           C
ATOM   6107  CG  ASN B 625      30.598  25.813  93.195  1.00 38.89           C
ATOM   6108  OD1 ASN B 625      31.236  25.818  92.135  1.00 39.62           O
ATOM   6109  ND2 ASN B 625      30.620  26.831  94.048  1.00 38.89           N
ATOM   6110  N   ARG B 626      31.920  21.688  94.384  1.00 39.83           N
ATOM   6111  CA  ARG B 626      32.857  21.182  95.368  1.00 40.63           C
ATOM   6112  C   ARG B 626      34.268  21.167  94.793  1.00 41.43           C
ATOM   6113  O   ARG B 626      34.540  20.498  93.793  1.00 41.60           O
ATOM   6114  CB  ARG B 626      32.446  19.776  95.805  1.00 40.47           C
ATOM   6115  CG  ARG B 626      33.412  19.116  96.767  1.00 40.21           C
ATOM   6116  CD  ARG B 626      33.204  17.621  96.769  1.00 40.05           C
ATOM   6117  NE  ARG B 626      34.335  16.903  97.349  1.00 39.64           N
ATOM   6118  CZ  ARG B 626      34.540  15.596  97.216  1.00 39.83           C
ATOM   6119  NH1 ARG B 626      33.693  14.850  96.518  1.00 39.11           N
ATOM   6120  NH2 ARG B 626      35.597  15.030  97.787  1.00 40.07           N
ATOM   6121  N   GLN B 627      35.156  21.918  95.435  1.00 42.26           N
ATOM   6122  CA  GLN B 627      36.563  21.948  95.062  1.00 42.98           C
ATOM   6123  C   GLN B 627      37.224  20.604  95.379  1.00 43.14           C
ATOM   6124  O   GLN B 627      37.285  20.187  96.537  1.00 43.14           O
ATOM   6125  CB  GLN B 627      37.269  23.096  95.790  1.00 43.22           C
ATOM   6126  CG  GLN B 627      38.794  23.020  95.799  1.00 44.30           C
ATOM   6127  CD  GLN B 627      39.440  23.667  94.590  1.00 45.55           C
ATOM   6128  OE1 GLN B 627      38.766  24.256  93.738  1.00 46.26           O
ATOM   6129  NE2 GLN B 627      40.763  23.570  94.517  1.00 46.09           N
ATOM   6130  N   VAL B 628      37.686  19.923  94.333  1.00 43.46           N
ATOM   6131  CA  VAL B 628      38.444  18.680  94.475  1.00 43.59           C
ATOM   6132  C   VAL B 628      39.519  18.583  93.383  1.00 43.77           C
ATOM   6133  O   VAL B 628      39.233  18.759  92.196  1.00 43.71           O
ATOM   6134  CB  VAL B 628      37.521  17.421  94.517  1.00 43.63           C
ATOM   6135  CG1 VAL B 628      36.739  17.247  93.215  1.00 43.52           C
ATOM   6136  CG2 VAL B 628      38.321  16.160  94.861  1.00 43.72           C
ATOM   6137  N   ASP B 629      40.759  18.337  93.810  1.00 44.06           N
ATOM   6138  CA  ASP B 629      41.914  18.215  92.911  1.00 44.20           C
ATOM   6139  C   ASP B 629      42.149  19.495  92.099  1.00 44.03           C
ATOM   6140  O   ASP B 629      42.469  19.447  90.906  1.00 43.89           O
ATOM   6141  CB  ASP B 629      41.768  16.982  91.999  1.00 44.39           C
ATOM   6142  CG  ASP B 629      41.463  15.702  92.779  1.00 45.17           C
ATOM   6143  OD1 ASP B 629      41.671  15.674  94.018  1.00 45.33           O
ATOM   6144  OD2 ASP B 629      41.013  14.721  92.147  1.00 45.84           O
ATOM   6145  N   GLY B 630      41.980  20.639  92.762  1.00 43.84           N
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ATOM   6146  CA  GLY B 630      42.144  21.947  92.120  1.00 43.49           C
ATOM   6147  C   GLY B 630      40.889  22.476  91.445  1.00 43.15           C
ATOM   6148  O   GLY B 630      40.653  23.689  91.419  1.00 43.21           O
ATOM   6149  N   GLN B 631      40.080  21.560  90.910  1.00 42.72           N
ATOM   6150  CA  GLN B 631      38.909  21.908  90.101  1.00 42.08           C
ATOM   6151  C   GLN B 631      37.596  21.871  90.888  1.00 41.27           C
ATOM   6152  O   GLN B 631      37.486  21.179  91.902  1.00 41.26           O
ATOM   6153  CB  GLN B 631      38.813  20.980  88.880  1.00 42.45           C
ATOM   6154  CG  GLN B 631      40.034  20.985  87.945  1.00 43.30           C
ATOM   6155  CD  GLN B 631      40.276  22.334  87.281  1.00 44.74           C
ATOM   6156  OE1 GLN B 631      40.769  23.272  87.914  1.00 45.85           O
ATOM   6157  NE2 GLN B 631      39.942  22.433  85.995  1.00 44.75           N
ATOM   6158  N   LYS B 632      36.610  22.628  90.413  1.00 40.17           N
ATOM   6159  CA  LYS B 632      35.259  22.591  90.962  1.00 39.08           C
ATOM   6160  C   LYS B 632      34.406  21.650  90.117  1.00 38.05           C
ATOM   6161  O   LYS B 632      34.397  21.758  88.892  1.00 38.10           O
ATOM   6162  CB  LYS B 632      34.641  23.991  90.980  1.00 39.12           C
ATOM   6163  CG  LYS B 632      35.232  24.931  92.025  1.00 39.55           C
ATOM   6164  CD  LYS B 632      34.617  26.323  91.930  1.00 39.56           C
ATOM   6165  CE  LYS B 632      35.340  27.329  92.827  1.00 40.31           C
ATOM   6166  NZ  LYS B 632      35.048  27.142  94.281  1.00 39.87           N
ATOM   6167  N   ILE B 633      33.709  20.723  90.771  1.00 36.62           N
ATOM   6168  CA  ILE B 633      32.791  19.802  90.085  1.00 35.21           C
ATOM   6169  C   ILE B 633      31.311  20.083  90.407  1.00 34.11           C
ATOM   6170  O   ILE B 633      30.989  20.865  91.304  1.00 33.95           O
ATOM   6171  CB  ILE B 633      33.114  18.305  90.386  1.00 35.23           C
ATOM   6172  CG1 ILE B 633      33.095  18.029  91.897  1.00 35.46           C
ATOM   6173  CG2 ILE B 633      34.442  17.899  89.753  1.00 35.13           C
ATOM   6174  CD1 ILE B 633      33.029  16.548  92.276  1.00 35.24           C
ATOM   6175  N   HIS B 634      30.427  19.443  89.649  1.00 32.61           N
ATOM   6176  CA  HIS B 634      28.997  19.432  89.926  1.00 31.14           C
ATOM   6177  C   HIS B 634      28.545  17.987  89.768  1.00 30.28           C
ATOM   6178  O   HIS B 634      29.146  17.241  88.999  1.00 30.19           O
ATOM   6179  CB  HIS B 634      28.269  20.333  88.929  1.00 31.15           C
ATOM   6180  CG  HIS B 634      26.860  20.660  89.314  1.00 30.24           C
ATOM   6181  ND1 HIS B 634      25.796  19.833  89.026  1.00 29.34           N
ATOM   6182  CD2 HIS B 634      26.338  21.735  89.951  1.00 30.00           C
ATOM   6183  CE1 HIS B 634      24.680  20.380  89.472  1.00 29.34           C
ATOM   6184  NE2 HIS B 634      24.982  21.535  90.038  1.00 30.20           N
ATOM   6185  N   SER B 635      27.506  17.583  90.495  1.00 29.11           N
ATOM   6186  CA  SER B 635      26.977  16.221  90.373  1.00 28.04           C
ATOM   6187  C   SER B 635      26.431  15.915  88.969  1.00 27.70           C
ATOM   6188  O   SER B 635      26.425  14.756  88.541  1.00 27.05           O
ATOM   6189  CB  SER B 635      25.908  15.942  91.436  1.00 27.88           C
ATOM   6190  OG  SER B 635      24.818  16.840  91.338  1.00 26.71           O
ATOM   6191  N   SER B 636      25.989  16.958  88.262  1.00 27.32           N
ATOM   6192  CA  SER B 636      25.428  16.807  86.911  1.00 27.42           C
ATOM   6193  C   SER B 636      26.478  16.561  85.823  1.00 27.66           C
ATOM   6194  O   SER B 636      26.159  16.009  84.772  1.00 27.51           O
ATOM   6195  CB  SER B 636      24.521  17.997  86.532  1.00 27.18           C
ATOM   6196  OG  SER B 636      25.254  19.163  86.216  1.00 26.00           O
ATOM   6197  N   THR B 637      27.724  16.960  86.082  1.00 27.97           N
ATOM   6198  CA  THR B 637      28.763  16.932  85.052  1.00 28.33           C
ATOM   6199  C   THR B 637      30.034  16.143  85.402  1.00 28.89           C
ATOM   6200  O   THR B 637      30.873  15.914  84.538  1.00 29.27           O
ATOM   6201  CB  THR B 637      29.141  18.364  84.603  1.00 28.37           C
ATOM   6202  OG1 THR B 637      29.527  19.145  85.737  1.00 27.92           O
ATOM   6203  CG2 THR B 637      27.964  19.040  83.908  1.00 27.92           C
ATOM   6204  N   MET B 638      30.167  15.711  86.652  1.00 29.49           N
ATOM   6205  CA  MET B 638      31.403  15.080  87.127  1.00 29.95           C
ATOM   6206  C   MET B 638      31.715  13.724  86.486  1.00 30.08           C
ATOM   6207  O   MET B 638      30.809  12.946  86.167  1.00 30.00           O
ATOM   6208  CB  MET B 638      31.378  14.927  88.653  1.00 29.81           C
ATOM   6209  CG  MET B 638      30.412  13.855  89.154  1.00 30.05           C
ATOM   6210  SD  MET B 638      30.300  13.721  90.945  1.00 30.64           S
ATOM   6211  CE  MET B 638      31.896  13.016  91.361  1.00 29.91           C
ATOM   6212  N   ASN B 639      33.011  13.471  86.299  1.00 30.42           N
ATOM   6213  CA  ASN B 639      33.542  12.150  85.977  1.00 30.51           C
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ATOM   6214  C   ASN B 639      34.784  11.921  86.841  1.00 30.90           C
ATOM   6215  O   ASN B 639      35.918  12.150  86.408  1.00 30.95           O
ATOM   6216  CB  ASN B 639      33.863  12.037  84.480  1.00 30.39           C
ATOM   6217  CG  ASN B 639      34.277  10.615  84.055  1.00 30.13           C
ATOM   6218  OD1 ASN B 639      34.191   9.662  84.826  1.00 30.23           O
ATOM   6219  ND2 ASN B 639      34.713  10.481  82.813  1.00 29.51           N
ATOM   6220  N   ASN B 640      34.554  11.502  88.083  1.00 31.45           N
ATOM   6221  CA  ASN B 640      35.633  11.296  89.053  1.00 31.97           C
ATOM   6222  C   ASN B 640      35.288  10.186  90.044  1.00 32.21           C
ATOM   6223  O   ASN B 640      34.527  10.400  90.990  1.00 32.49           O
ATOM   6224  CB  ASN B 640      35.971  12.609  89.782  1.00 31.92           C
ATOM   6225  CG  ASN B 640      37.235  12.510  90.643  1.00 31.97           C
ATOM   6226  OD1 ASN B 640      37.501  11.490  91.281  1.00 31.32           O
ATOM   6227  ND2 ASN B 640      38.003  13.592  90.680  1.00 31.96           N
ATOM   6228  N   ARG B 641      35.863   9.008  89.812  1.00 32.49           N
ATOM   6229  CA  ARG B 641      35.540   7.791  90.557  1.00 32.86           C
ATOM   6230  C   ARG B 641      35.703   7.959  92.064  1.00 32.87           C
ATOM   6231  O   ARG B 641      34.816   7.588  92.840  1.00 32.81           O
ATOM   6232  CB  ARG B 641      36.406   6.628  90.062  1.00 32.80           C
ATOM   6233  CG  ARG B 641      35.973   5.269  90.580  1.00 33.41           C
ATOM   6234  CD  ARG B 641      36.905   4.161  90.105  1.00 33.67           C
ATOM   6235  NE  ARG B 641      36.912   3.051  91.056  1.00 35.87           N
ATOM   6236  CZ  ARG B 641      37.665   3.004  92.157  1.00 36.27           C
ATOM   6237  NH1 ARG B 641      38.495   4.002  92.455  1.00 36.05           N
ATOM   6238  NH2 ARG B 641      37.585   1.955  92.964  1.00 36.68           N
ATOM   6239  N   ARG B 642      36.831   8.537  92.463  1.00 32.85           N
ATOM   6240  CA  ARG B 642      37.184   8.666  93.872  1.00 33.07           C
ATOM   6241  C   ARG B 642      36.357   9.723  94.595  1.00 32.61           C
ATOM   6242  O   ARG B 642      36.105   9.604  95.798  1.00 32.71           O
ATOM   6243  CB  ARG B 642      38.681   8.953  94.025  1.00 33.04           C
ATOM   6244  CG  ARG B 642      39.574   7.756  93.697  1.00 33.88           C
ATOM   6245  CD  ARG B 642      41.050   8.017  94.027  1.00 34.29           C
ATOM   6246  NE  ARG B 642      41.268   8.245  95.460  1.00 37.31           N
ATOM   6247  CZ  ARG B 642      41.457   7.282  96.361  1.00 37.98           C
ATOM   6248  NH1 ARG B 642      41.463   6.005  95.990  1.00 38.69           N
ATOM   6249  NH2 ARG B 642      41.641   7.598  97.638  1.00 37.84           N
ATOM   6250  N   ALA B 643      35.932  10.747  93.857  1.00 32.16           N
ATOM   6251  CA  ALA B 643      35.142  11.849  94.414  1.00 31.41           C
ATOM   6252  C   ALA B 643      33.667  11.488  94.622  1.00 31.11           C
ATOM   6253  O   ALA B 643      32.887  12.299  95.132  1.00 30.94           O
ATOM   6254  CB  ALA B 643      35.264  13.074  93.532  1.00 31.43           C
ATOM   6255  N   GLN B 644      33.286  10.277  94.222  1.00 30.62           N
ATOM   6256  CA  GLN B 644      31.919   9.816  94.408  1.00 30.47           C
ATOM   6257  C   GLN B 644      31.524   9.710  95.876  1.00 30.49           C
ATOM   6258  O   GLN B 644      32.357   9.480  96.751  1.00 30.49           O
ATOM   6259  CB  GLN B 644      31.696   8.471  93.720  1.00 30.52           C
ATOM   6260  CG  GLN B 644      31.484   8.568  92.220  1.00 29.92           C
ATOM   6261  CD  GLN B 644      31.467   7.215  91.541  1.00 29.58           C
ATOM   6262  OE1 GLN B 644      30.637   6.959  90.673  1.00 30.06           O
ATOM   6263  NE2 GLN B 644      32.389   6.341  91.931  1.00 29.22           N
ATOM   6264  N   ASN B 645      30.240   9.919  96.127  1.00 30.46           N
ATOM   6265  CA  ASN B 645      29.640   9.644  97.415  1.00 30.49           C
ATOM   6266  C   ASN B 645      28.243   9.125  97.164  1.00 30.53           C
ATOM   6267  O   ASN B 645      27.442   9.769  96.500  1.00 30.67           O
ATOM   6268  CB  ASN B 645      29.648  10.877  98.326  1.00 30.58           C
ATOM   6269  CG  ASN B 645      29.560  12.182  97.561  1.00 30.20           C
ATOM   6270  OD1 ASN B 645      28.510  12.539  97.028  1.00 30.62           O
ATOM   6271  ND2 ASN B 645      30.666  12.913  97.524  1.00 30.23           N
ATOM   6272  N   THR B 646      27.961   7.939  97.678  1.00 30.74           N
ATOM   6273  CA  THR B 646      26.791   7.190  97.249  1.00 30.73           C
ATOM   6274  C   THR B 646      25.737   7.151  98.353  1.00 31.05           C
ATOM   6275  O   THR B 646      25.209   8.194  98.739  1.00 30.70           O
ATOM   6276  CB  THR B 646      27.192   5.774  96.829  1.00 30.69           C
ATOM   6277  OG1 THR B 646      27.561   5.028  97.992  1.00 30.51           O
ATOM   6278  CG2 THR B 646      28.384   5.818  95.876  1.00 30.41           C
ATOM   6279  N   GLU B 647      25.435   5.950  98.848  1.00 31.56           N
ATOM   6280  CA  GLU B 647      24.525   5.768  99.975  1.00 32.18           C
ATOM   6281  C   GLU B 647      25.054   6.515 101.186  1.00 32.43           C
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ATOM   6282  O   GLU B 647      26.270   6.637 101.374  1.00 32.48           O
ATOM   6283  CB  GLU B 647      24.369   4.291 100.321  1.00 32.27           C
ATOM   6284  CG  GLU B 647      23.775   3.457  99.201  1.00 32.91           C
ATOM   6285  CD  GLU B 647      24.100   1.988  99.335  1.00 33.55           C
ATOM   6286  OE1 GLU B 647      25.078   1.656 100.039  1.00 33.54           O
ATOM   6287  OE2 GLU B 647      23.382   1.163  98.730  1.00 34.03           O
ATOM   6288  N   SER B 648      24.136   7.024 101.996  1.00 32.58           N
ATOM   6289  CA  SER B 648      24.510   7.835 103.134  1.00 32.94           C
ATOM   6290  C   SER B 648      23.516   7.691 104.273  1.00 33.01           C
ATOM   6291  O   SER B 648      22.379   7.262 104.075  1.00 32.79           O
ATOM   6292  CB  SER B 648      24.652   9.311 102.724  1.00 33.13           C
ATOM   6293  OG  SER B 648      23.469   9.802 102.113  1.00 33.64           O
ATOM   6294  N   THR B 649      23.971   8.033 105.471  1.00 33.15           N
ATOM   6295  CA  THR B 649      23.102   8.109 106.627  1.00 33.32           C
ATOM   6296  C   THR B 649      23.231   9.493 107.251  1.00 33.56           C
ATOM   6297  O   THR B 649      24.300  10.108 107.209  1.00 33.69           O
ATOM   6298  CB  THR B 649      23.379   6.985 107.650  1.00 33.37           C
ATOM   6299  OG1 THR B 649      22.621   7.229 108.844  1.00 33.36           O
ATOM   6300  CG2 THR B 649      24.868   6.883 107.993  1.00 33.03           C
ATOM   6301  N   VAL B 650      22.136   9.982 107.820  1.00 33.77           N
ATOM   6302  CA  VAL B 650      22.065  11.368 108.249  1.00 34.11           C
ATOM   6303  C   VAL B 650      21.682  11.501 109.727  1.00 34.60           C
ATOM   6304  O   VAL B 650      20.816  10.776 110.222  1.00 34.57           O
ATOM   6305  CB  VAL B 650      21.100  12.182 107.326  1.00 34.04           C
ATOM   6306  CG1 VAL B 650      19.651  11.696 107.458  1.00 33.59           C
ATOM   6307  CG2 VAL B 650      21.206  13.673 107.599  1.00 33.79           C
ATOM   6308  N   VAL B 651      22.355  12.415 110.423  1.00 35.13           N
ATOM   6309  CA  VAL B 651      22.017  12.759 111.805  1.00 35.93           C
ATOM   6310  C   VAL B 651      22.063  14.267 112.028  1.00 36.31           C
ATOM   6311  O   VAL B 651      22.900  14.967 111.453  1.00 36.43           O
ATOM   6312  CB  VAL B 651      22.952  12.074 112.845  1.00 36.03           C
ATOM   6313  CG1 VAL B 651      22.773  10.571 112.836  1.00 36.31           C
ATOM   6314  CG2 VAL B 651      24.408  12.436 112.604  1.00 36.27           C
ATOM   6315  N   GLN B 652      21.160  14.769 112.861  1.00 36.82           N
ATOM   6316  CA  GLN B 652      21.233  16.161 113.264  1.00 37.41           C
ATOM   6317  C   GLN B 652      21.910  16.273 114.623  1.00 37.78           C
ATOM   6318  O   GLN B 652      21.678  15.451 115.512  1.00 37.95           O
ATOM   6319  CB  GLN B 652      19.850  16.810 113.302  1.00 37.43           C
ATOM   6320  CG  GLN B 652      19.899  18.313 113.047  1.00 37.72           C
ATOM   6321  CD  GLN B 652      18.720  19.077 113.632  1.00 38.16           C
ATOM   6322  OE1 GLN B 652      17.766  18.491 114.150  1.00 38.47           O
ATOM   6323  NE2 GLN B 652      18.786  20.402 113.548  1.00 37.82           N
ATOM   6324  N   LEU B 653      22.753  17.290 114.761  1.00 38.25           N
ATOM   6325  CA  LEU B 653      23.405  17.630 116.023  1.00 38.70           C
ATOM   6326  C   LEU B 653      22.532  18.598 116.816  1.00 39.15           C
ATOM   6327  O   LEU B 653      21.577  19.162 116.273  1.00 39.25           O
ATOM   6328  CB  LEU B 653      24.769  18.263 115.746  1.00 38.70           C
ATOM   6329  CG  LEU B 653      25.999  17.360 115.592  1.00 38.71           C
ATOM   6330  CD1 LEU B 653      25.699  16.004 114.947  1.00 38.44           C
ATOM   6331  CD2 LEU B 653      27.103  18.091 114.842  1.00 38.52           C
ATOM   6332  N   ASN B 654      22.858  18.790 118.095  1.00 39.62           N
ATOM   6333  CA  ASN B 654      22.079  19.676 118.967  1.00 40.08           C
ATOM   6334  C   ASN B 654      22.290  21.168 118.691  1.00 40.13           C
ATOM   6335  O   ASN B 654      21.469  21.997 119.087  1.00 40.19           O
ATOM   6336  CB  ASN B 654      22.346  19.368 120.443  1.00 40.32           C
ATOM   6337  CG  ASN B 654      21.733  18.053 120.892  1.00 40.87           C
ATOM   6338  OD1 ASN B 654      20.739  17.583 120.335  1.00 41.05           O
ATOM   6339  ND2 ASN B 654      22.325  17.456 121.918  1.00 41.61           N
ATOM   6340  N   ASN B 655      23.388  21.504 118.017  1.00 40.19           N
ATOM   6341  CA  ASN B 655      23.628  22.881 117.588  1.00 40.29           C
ATOM   6342  C   ASN B 655      22.899  23.218 116.281  1.00 40.45           C
ATOM   6343  O   ASN B 655      22.902  24.368 115.837  1.00 40.61           O
ATOM   6344  CB  ASN B 655      25.130  23.177 117.478  1.00 40.22           C
ATOM   6345  CG  ASN B 655      25.822  22.350 116.412  1.00 40.34           C
ATOM   6346  OD1 ASN B 655      25.177  21.668 115.611  1.00 39.94           O
ATOM   6347  ND2 ASN B 655      27.150  22.408 116.396  1.00 40.27           N
ATOM   6348  N   GLY B 656      22.278  22.208 115.674  1.00 40.28           N
ATOM   6349  CA  GLY B 656      21.464  22.410 114.481  1.00 40.20           C
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ATOM   6350  C   GLY B 656      22.104  21.954 113.182  1.00 40.06           C
ATOM   6351  O   GLY B 656      21.459  21.995 112.133  1.00 40.16           O
ATOM   6352  N   ASP B 657      23.366  21.524 113.253  1.00 39.76           N
ATOM   6353  CA  ASP B 657      24.093  21.012 112.093  1.00 39.45           C
ATOM   6354  C   ASP B 657      23.578  19.650 111.651  1.00 39.31           C
ATOM   6355  O   ASP B 657      23.130  18.844 112.469  1.00 39.23           O
ATOM   6356  CB  ASP B 657      25.595  20.909 112.381  1.00 39.57           C
ATOM   6357  CG  ASP B 657      26.311  22.243 112.277  1.00 39.98           C
ATOM   6358  OD1 ASP B 657      25.646  23.267 112.021  1.00 40.62           O
ATOM   6359  OD2 ASP B 657      27.547  22.268 112.455  1.00 40.78           O
ATOM   6360  N   VAL B 658      23.656  19.410 110.344  1.00 38.99           N
ATOM   6361  CA  VAL B 658      23.281  18.136 109.755  1.00 38.53           C
ATOM   6362  C   VAL B 658      24.554  17.447 109.277  1.00 38.26           C
ATOM   6363  O   VAL B 658      25.348  18.037 108.537  1.00 38.28           O
ATOM   6364  CB  VAL B 658      22.286  18.325 108.577  1.00 38.55           C
ATOM   6365  CG1 VAL B 658      22.095  17.029 107.815  1.00 38.48           C
ATOM   6366  CG2 VAL B 658      20.941  18.850 109.075  1.00 38.16           C
ATOM   6367  N   LYS B 659      24.746  16.206 109.714  1.00 37.76           N
ATOM   6368  CA  LYS B 659      25.906  15.418 109.315  1.00 37.33           C
ATOM   6369  C   LYS B 659      25.483  14.301 108.375  1.00 37.13           C
ATOM   6370  O   LYS B 659      24.463  13.647 108.593  1.00 36.88           O
ATOM   6371  CB  LYS B 659      26.632  14.839 110.537  1.00 37.31           C
ATOM   6372  CG  LYS B 659      27.303  15.875 111.445  1.00 37.18           C
ATOM   6373  CD  LYS B 659      28.607  16.418 110.863  1.00 36.75           C
ATOM   6374  CE  LYS B 659      29.096  17.630 111.648  1.00 36.02           C
ATOM   6375  NZ  LYS B 659      30.472  18.040 111.259  1.00 35.60           N
ATOM   6376  N   LEU B 660      26.276  14.092 107.329  1.00 37.06           N
ATOM   6377  CA  LEU B 660      25.977  13.079 106.322  1.00 36.95           C
ATOM   6378  C   LEU B 660      27.154  12.126 106.145  1.00 36.91           C
ATOM   6379  O   LEU B 660      28.214  12.511 105.631  1.00 37.04           O
ATOM   6380  CB  LEU B 660      25.607  13.745 104.991  1.00 36.86           C
ATOM   6381  CG  LEU B 660      24.945  12.895 103.905  1.00 36.91           C
ATOM   6382  CD1 LEU B 660      23.559  12.412 104.334  1.00 37.17           C
ATOM   6383  CD2 LEU B 660      24.861  13.682 102.601  1.00 36.71           C
ATOM   6384  N   PHE B 661      26.958  10.885 106.583  1.00 36.70           N
ATOM   6385  CA  PHE B 661      27.981   9.850 106.478  1.00 36.49           C
ATOM   6386  C   PHE B 661      27.794   9.100 105.172  1.00 36.20           C
ATOM   6387  O   PHE B 661      26.821   8.355 105.015  1.00 36.27           O
ATOM   6388  CB  PHE B 661      27.903   8.883 107.665  1.00 36.74           C
ATOM   6389  CG  PHE B 661      28.026   9.553 109.001  1.00 36.81           C
ATOM   6390  CD1 PHE B 661      26.896   9.970 109.689  1.00 37.20           C
ATOM   6391  CD2 PHE B 661      29.274   9.773 109.567  1.00 37.20           C
ATOM   6392  CE1 PHE B 661      27.008  10.598 110.922  1.00 37.74           C
ATOM   6393  CE2 PHE B 661      29.398  10.399 110.798  1.00 37.22           C
ATOM   6394  CZ  PHE B 661      28.262  10.811 111.480  1.00 37.41           C
ATOM   6395  N   MET B 662      28.737   9.290 104.250  1.00 35.65           N
ATOM   6396  CA  MET B 662      28.597   8.803 102.878  1.00 35.13           C
ATOM   6397  C   MET B 662      29.526   7.640 102.549  1.00 35.17           C
ATOM   6398  O   MET B 662      30.739   7.713 102.770  1.00 35.24           O
ATOM   6399  CB  MET B 662      28.846   9.938 101.882  1.00 35.15           C
ATOM   6400  CG  MET B 662      28.151  11.245 102.221  1.00 34.88           C
ATOM   6401  SD  MET B 662      28.756  12.609 101.223  1.00 34.36           S
ATOM   6402  CE  MET B 662      30.406  12.865 101.881  1.00 34.45           C
ATOM   6403  N   ARG B 663      28.943   6.577 102.003  1.00 34.95           N
ATOM   6404  CA  ARG B 663      29.704   5.456 101.472  1.00 34.97           C
ATOM   6405  C   ARG B 663      30.557   5.937 100.295  1.00 35.40           C
ATOM   6406  O   ARG B 663      30.040   6.526  99.336  1.00 35.40           O
ATOM   6407  CB  ARG B 663      28.754   4.333 101.046  1.00 34.72           C
ATOM   6408  CG  ARG B 663      29.364   3.270 100.151  1.00 33.52           C
ATOM   6409  CD  ARG B 663      28.285   2.352  99.644  1.00 31.63           C
ATOM   6410  NE  ARG B 663      28.770   1.410  98.641  1.00 30.82           N
ATOM   6411  CZ  ARG B 663      28.104   0.323  98.268  1.00 29.94           C
ATOM   6412  NH1 ARG B 663      26.934   0.046  98.819  1.00 29.40           N
ATOM   6413  NH2 ARG B 663      28.603  -0.487  97.345  1.00 29.21           N
ATOM   6414  N   GLY B 664      31.863   5.694 100.385  1.00 35.71           N
ATOM   6415  CA  GLY B 664      32.810   6.214  99.405  1.00 36.17           C
ATOM   6416  C   GLY B 664      33.890   5.226  99.029  1.00 36.59           C
ATOM   6417  O   GLY B 664      33.860   4.062  99.439  1.00 36.76           O
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ATOM   6418  N   LEU B 665      34.853   5.699  98.249  1.00 36.89           N
ATOM   6419  CA  LEU B 665      35.900   4.844  97.718  1.00 37.23           C
ATOM   6420  C   LEU B 665      37.297   5.274  98.168  1.00 37.62           C
ATOM   6421  O   LEU B 665      38.290   4.966  97.506  1.00 37.57           O
ATOM   6422  CB  LEU B 665      35.801   4.779  96.190  1.00 37.18           C
ATOM   6423  CG  LEU B 665      34.682   3.890  95.638  1.00 36.93           C
ATOM   6424  CD1 LEU B 665      34.257   4.329  94.249  1.00 36.63           C
ATOM   6425  CD2 LEU B 665      35.092   2.412  95.644  1.00 36.88           C
ATOM   6426  N   THR B 666      37.364   5.974  99.301  1.00 38.06           N
ATOM   6427  CA  THR B 666      38.646   6.360  99.897  1.00 38.66           C
ATOM   6428  C   THR B 666      39.148   5.333 100.914  1.00 38.88           C
ATOM   6429  O   THR B 666      40.321   5.349 101.287  1.00 38.87           O
ATOM   6430  CB  THR B 666      38.592   7.753 100.584  1.00 38.75           C
ATOM   6431  OG1 THR B 666      37.646   7.730 101.662  1.00 39.11           O
ATOM   6432  CG2 THR B 666      38.211   8.844  99.590  1.00 38.80           C
ATOM   6433  N   GLY B 667      38.260   4.442 101.351  1.00 39.30           N
ATOM   6434  CA  GLY B 667      38.576   3.491 102.416  1.00 39.73           C
ATOM   6435  C   GLY B 667      38.369   4.111 103.785  1.00 40.20           C
ATOM   6436  O   GLY B 667      38.405   3.419 104.804  1.00 40.13           O
ATOM   6437  N   ASP B 668      38.158   5.428 103.787  1.00 40.78           N
ATOM   6438  CA  ASP B 668      37.900   6.227 104.982  1.00 41.31           C
ATOM   6439  C   ASP B 668      36.405   6.427 105.177  1.00 41.36           C
ATOM   6440  O   ASP B 668      35.604   6.106 104.300  1.00 41.66           O
ATOM   6441  CB  ASP B 668      38.546   7.614 104.834  1.00 41.62           C
ATOM   6442  CG  ASP B 668      39.972   7.664 105.350  1.00 42.29           C
ATOM   6443  OD1 ASP B 668      40.392   6.725 106.056  1.00 43.63           O
ATOM   6444  OD2 ASP B 668      40.672   8.658 105.061  1.00 42.93           O
ATOM   6445  N   LEU B 669      36.038   6.969 106.332  1.00 41.26           N
ATOM   6446  CA  LEU B 669      34.698   7.487 106.538  1.00 41.04           C
ATOM   6447  C   LEU B 669      34.659   8.909 105.994  1.00 41.03           C
ATOM   6448  O   LEU B 669      35.568   9.707 106.254  1.00 41.00           O
ATOM   6449  CB  LEU B 669      34.345   7.479 108.025  1.00 40.95           C
ATOM   6450  CG  LEU B 669      33.055   8.178 108.455  1.00 40.63           C
ATOM   6451  CD1 LEU B 669      31.834   7.316 108.176  1.00 40.02           C
ATOM   6452  CD2 LEU B 669      33.136   8.530 109.921  1.00 40.31           C
ATOM   6453  N   GLN B 670      33.613   9.220 105.233  1.00 40.89           N
ATOM   6454  CA  GLN B 670      33.448  10.557 104.672  1.00 40.53           C
ATOM   6455  C   GLN B 670      32.218  11.249 105.254  1.00 40.66           C
ATOM   6456  O   GLN B 670      31.122  10.676 105.289  1.00 40.71           O
ATOM   6457  CB  GLN B 670      33.380  10.494 103.148  1.00 40.55           C
ATOM   6458  CG  GLN B 670      34.729  10.279 102.483  1.00 39.86           C
ATOM   6459  CD  GLN B 670      34.626  10.223 100.975  1.00 39.49           C
ATOM   6460  OE1 GLN B 670      34.779  11.374 100.325  1.00 39.01           O
ATOM   6461  NE2 GLN B 670      34.419   9.158 100.398  1.00 39.28           N
ATOM   6462  N   VAL B 671      32.412  12.480 105.721  1.00 40.61           N
ATOM   6463  CA  VAL B 671      31.358  13.223 106.408  1.00 40.53           C
ATOM   6464  C   VAL B 671      31.248  14.638 105.860  1.00 40.54           C
ATOM   6465  O   VAL B 671      32.255  15.328 105.701  1.00 40.65           O
ATOM   6466  CB  VAL B 671      31.602  13.284 107.941  1.00 40.73           C
ATOM   6467  CG1 VAL B 671      30.418  13.933 108.659  1.00 40.16           C
ATOM   6468  CG2 VAL B 671      31.865  11.891 108.503  1.00 40.42           C
ATOM   6469  N   ALA B 672      30.014  15.054 105.576  1.00 40.45           N
ATOM   6470  CA  ALA B 672      29.715  16.402 105.098  1.00 40.37           C
ATOM   6471  C   ALA B 672      28.747  17.121 106.045  1.00 40.34           C
ATOM   6472  O   ALA B 672      27.950  16.477 106.734  1.00 40.25           O
ATOM   6473  CB  ALA B 672      29.150  16.347 103.685  1.00 40.35           C
ATOM   6474  N   THR B 673      28.819  18.453 106.064  1.00 40.29           N
ATOM   6475  CA  THR B 673      28.036  19.271 106.990  1.00 40.34           C
ATOM   6476  C   THR B 673      27.122  20.264 106.264  1.00 40.43           C
ATOM   6477  O   THR B 673      27.548  20.954 105.329  1.00 40.35           O
ATOM   6478  CB  THR B 673      28.955  20.048 107.968  1.00 40.25           C
ATOM   6479  OG1 THR B 673      29.985  19.182 108.453  1.00 40.57           O
ATOM   6480  CG2 THR B 673      28.168  20.587 109.152  1.00 40.04           C
ATOM   6481  N   SER B 674      25.867  20.320 106.707  1.00 40.49           N
ATOM   6482  CA  SER B 674      24.899  21.311 106.239  1.00 40.62           C
ATOM   6483  C   SER B 674      24.460  22.223 107.378  1.00 40.70           C
ATOM   6484  O   SER B 674      24.114  21.749 108.462  1.00 40.73           O
ATOM   6485  CB  SER B 674      23.670  20.629 105.643  1.00 40.64           C
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ATOM   6486  OG  SER B 674      22.635  21.571 105.414  1.00 40.66           O
ATOM   6487  N   LYS B 675      24.462  23.528 107.117  1.00 40.88           N
ATOM   6488  CA  LYS B 675      24.060  24.526 108.116  1.00 41.07           C
ATOM   6489  C   LYS B 675      22.715  25.192 107.821  1.00 41.02           C
ATOM   6490  O   LYS B 675      22.285  26.090 108.552  1.00 41.19           O
ATOM   6491  CB  LYS B 675      25.173  25.560 108.334  1.00 40.96           C
ATOM   6492  CG  LYS B 675      25.978  25.270 109.592  1.00 41.67           C
ATOM   6493  CD  LYS B 675      27.452  25.608 109.472  1.00 42.34           C
ATOM   6494  CE  LYS B 675      28.180  25.176 110.739  1.00 42.70           C
ATOM   6495  NZ  LYS B 675      29.664  25.223 110.620  1.00 43.32           N
ATOM   6496  N   ASP B 676      22.052  24.729 106.762  1.00 40.93           N
ATOM   6497  CA  ASP B 676      20.725  25.218 106.384  1.00 40.81           C
ATOM   6498  C   ASP B 676      19.693  24.089 106.330  1.00 40.64           C
ATOM   6499  O   ASP B 676      18.710  24.164 105.588  1.00 40.61           O
ATOM   6500  CB  ASP B 676      20.782  25.977 105.050  1.00 40.92           C
ATOM   6501  CG  ASP B 676      21.579  25.238 103.978  1.00 41.34           C
ATOM   6502  OD1 ASP B 676      21.555  23.986 103.936  1.00 41.19           O
ATOM   6503  OD2 ASP B 676      22.236  25.924 103.170  1.00 41.38           O
ATOM   6504  N   GLY B 677      19.934  23.046 107.120  1.00 40.51           N
ATOM   6505  CA  GLY B 677      18.985  21.950 107.290  1.00 40.38           C
ATOM   6506  C   GLY B 677      18.970  20.909 106.187  1.00 40.40           C
ATOM   6507  O   GLY B 677      17.936  20.282 105.943  1.00 40.23           O
ATOM   6508  N   GLY B 678      20.108  20.729 105.518  1.00 40.47           N
ATOM   6509  CA  GLY B 678      20.259  19.682 104.501  1.00 40.44           C
ATOM   6510  C   GLY B 678      20.237  20.119 103.044  1.00 40.42           C
ATOM   6511  O   GLY B 678      20.337  19.284 102.149  1.00 40.42           O
ATOM   6512  N   VAL B 679      20.110  21.419 102.794  1.00 40.44           N
ATOM   6513  CA  VAL B 679      20.050  21.927 101.422  1.00 40.53           C
ATOM   6514  C   VAL B 679      21.461  22.135 100.851  1.00 40.77           C
ATOM   6515  O   VAL B 679      21.855  21.465  99.899  1.00 40.75           O
ATOM   6516  CB  VAL B 679      19.193  23.222 101.311  1.00 40.40           C
ATOM   6517  CG1 VAL B 679      18.906  23.553  99.857  1.00 40.37           C
ATOM   6518  CG2 VAL B 679      17.887  23.071 102.068  1.00 40.05           C
ATOM   6519  N   THR B 680      22.210  23.058 101.447  1.00 41.17           N
ATOM   6520  CA  THR B 680      23.593  23.343 101.060  1.00 41.65           C
ATOM   6521  C   THR B 680      24.555  22.554 101.942  1.00 41.93           C
ATOM   6522  O   THR B 680      24.216  22.202 103.069  1.00 42.06           O
ATOM   6523  CB  THR B 680      23.878  24.864 101.155  1.00 41.61           C
ATOM   6524  OG1 THR B 680      23.286  25.526 100.030  1.00 42.10           O
ATOM   6525  CG2 THR B 680      25.373  25.182 101.205  1.00 41.77           C
ATOM   6526  N   TRP B 681      25.743  22.268 101.416  1.00 42.27           N
ATOM   6527  CA  TRP B 681      26.790  21.572 102.159  1.00 42.70           C
ATOM   6528  C   TRP B 681      28.060  22.410 102.169  1.00 43.18           C
ATOM   6529  O   TRP B 681      28.294  23.197 101.251  1.00 43.39           O
ATOM   6530  CB  TRP B 681      27.062  20.193 101.547  1.00 42.52           C
ATOM   6531  CG  TRP B 681      25.836  19.343 101.476  1.00 42.57           C
ATOM   6532  CD1 TRP B 681      25.009  19.189 100.404  1.00 42.40           C
ATOM   6533  CD2 TRP B 681      25.277  18.550 102.533  1.00 42.69           C
ATOM   6534  NE1 TRP B 681      23.975  18.339 100.720  1.00 42.45           N
ATOM   6535  CE2 TRP B 681      24.114  17.934 102.022  1.00 42.23           C
ATOM   6536  CE3 TRP B 681      25.651  18.292 103.859  1.00 42.48           C
ATOM   6537  CZ2 TRP B 681      23.320  17.079 102.788  1.00 42.01           C
ATOM   6538  CZ3 TRP B 681      24.859  17.442 104.622  1.00 42.47           C
ATOM   6539  CH2 TRP B 681      23.708  16.846 104.081  1.00 42.35           C
ATOM   6540  N   GLU B 682      28.872  22.247 103.210  1.00 43.77           N
ATOM   6541  CA  GLU B 682      30.123  22.993 103.338  1.00 44.40           C
ATOM   6542  C   GLU B 682      31.169  22.536 102.329  1.00 44.64           C
ATOM   6543  O   GLU B 682      31.127  21.401 101.850  1.00 44.38           O
ATOM   6544  CB  GLU B 682      30.694  22.862 104.750  1.00 44.45           C
ATOM   6545  CG  GLU B 682      30.150  23.866 105.754  1.00 44.71           C
ATOM   6546  CD  GLU B 682      30.851  23.779 107.108  1.00 44.68           C
ATOM   6547  OE1 GLU B 682      31.979  23.236 107.179  1.00 44.39           O
ATOM   6548  OE2 GLU B 682      30.270  24.257 108.106  1.00 45.64           O
ATOM   6549  N   LYS B 683      32.103  23.440 102.029  1.00 45.23           N
ATOM   6550  CA  LYS B 683      33.246  23.177 101.151  1.00 45.90           C
ATOM   6551  C   LYS B 683      33.833  21.785 101.327  1.00 46.24           C
ATOM   6552  O   LYS B 683      34.064  21.072 100.350  1.00 46.31           O
ATOM   6553  CB  LYS B 683      34.370  24.182 101.433  1.00 45.93           C
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ATOM   6554  CG  LYS B 683      34.285  25.494 100.692  1.00 46.09           C
ATOM   6555  CD  LYS B 683      35.606  26.237 100.819  1.00 46.33           C
ATOM   6556  CE  LYS B 683      35.524  27.630 100.231  1.00 46.73           C
ATOM   6557  NZ  LYS B 683      35.371  27.610  98.744  1.00 46.64           N
ATOM   6558  N   ASP B 684      34.064  21.414 102.583  1.00 46.70           N
ATOM   6559  CA  ASP B 684      34.958  20.316 102.915  1.00 47.23           C
ATOM   6560  C   ASP B 684      34.266  19.041 103.350  1.00 47.32           C
ATOM   6561  O   ASP B 684      33.252  19.068 104.048  1.00 47.24           O
ATOM   6562  CB  ASP B 684      35.958  20.760 103.987  1.00 47.36           C
ATOM   6563  CG  ASP B 684      36.894  21.846 103.493  1.00 47.92           C
ATOM   6564  OD1 ASP B 684      37.594  21.614 102.483  1.00 48.11           O
ATOM   6565  OD2 ASP B 684      36.931  22.930 104.114  1.00 49.22           O
ATOM   6566  N   ILE B 685      34.844  17.929 102.909  1.00 47.68           N
ATOM   6567  CA  ILE B 685      34.452  16.598 103.338  1.00 48.00           C
ATOM   6568  C   ILE B 685      35.488  16.120 104.349  1.00 48.37           C
ATOM   6569  O   ILE B 685      36.681  16.011 104.029  1.00 48.48           O
ATOM   6570  CB  ILE B 685      34.367  15.621 102.135  1.00 47.90           C
ATOM   6571  CG1 ILE B 685      33.134  15.941 101.282  1.00 47.90           C
ATOM   6572  CG2 ILE B 685      34.353  14.155 102.602  1.00 47.95           C
ATOM   6573  CD1 ILE B 685      32.951  15.033 100.078  1.00 48.05           C
ATOM   6574  N   LYS B 686      35.034  15.864 105.574  1.00 48.57           N
ATOM   6575  CA  LYS B 686      35.904  15.329 106.614  1.00 48.86           C
ATOM   6576  C   LYS B 686      36.127  13.844 106.384  1.00 48.77           C
ATOM   6577  O   LYS B 686      35.176  13.079 106.216  1.00 48.63           O
ATOM   6578  CB  LYS B 686      35.321  15.567 108.012  1.00 48.99           C
ATOM   6579  CG  LYS B 686      35.474  16.991 108.526  1.00 49.78           C
ATOM   6580  CD  LYS B 686      34.584  17.240 109.741  1.00 50.51           C
ATOM   6581  CE  LYS B 686      34.607  18.707 110.157  1.00 50.94           C
ATOM   6582  NZ  LYS B 686      33.600  19.007 111.219  1.00 51.37           N
ATOM   6583  N   ARG B 687      37.397  13.457 106.362  1.00 48.98           N
ATOM   6584  CA  ARG B 687      37.787  12.057 106.300  1.00 49.08           C
ATOM   6585  C   ARG B 687      38.231  11.603 107.686  1.00 49.30           C
ATOM   6586  O   ARG B 687      39.055  12.267 108.323  1.00 49.42           O
ATOM   6587  CB  ARG B 687      38.915  11.862 105.289  1.00 49.01           C
ATOM   6588  CG  ARG B 687      38.480  11.999 103.836  1.00 48.44           C
ATOM   6589  CD  ARG B 687      39.643  11.767 102.891  1.00 47.59           C
ATOM   6590  NE  ARG B 687      40.095  10.378 102.916  1.00 47.31           N
ATOM   6591  CZ  ARG B 687      41.181   9.928 102.293  1.00 47.30           C
ATOM   6592  NH1 ARG B 687      41.941  10.758 101.588  1.00 47.38           N
ATOM   6593  NH2 ARG B 687      41.509   8.644 102.376  1.00 46.54           N
ATOM   6594  N   TYR B 688      37.667  10.491 108.157  1.00 49.37           N
ATOM   6595  CA  TYR B 688      38.048   9.913 109.447  1.00 49.52           C
ATOM   6596  C   TYR B 688      38.725   8.552 109.275  1.00 49.68           C
ATOM   6597  O   TYR B 688      38.041   7.530 109.190  1.00 49.78           O
ATOM   6598  CB  TYR B 688      36.835   9.805 110.379  1.00 49.56           C
ATOM   6599  CG  TYR B 688      36.301  11.142 110.830  1.00 49.61           C
ATOM   6600  CD1 TYR B 688      35.131  11.669 110.281  1.00 49.34           C
ATOM   6601  CD2 TYR B 688      36.973  11.892 111.797  1.00 49.74           C
ATOM   6602  CE1 TYR B 688      34.640  12.907 110.688  1.00 49.34           C
ATOM   6603  CE2 TYR B 688      36.492  13.129 112.211  1.00 49.56           C
ATOM   6604  CZ  TYR B 688      35.327  13.630 111.653  1.00 49.62           C
ATOM   6605  OH  TYR B 688      34.849  14.852 112.066  1.00 49.63           O
ATOM   6606  N   PRO B 689      40.075   8.537 109.221  1.00 49.86           N
ATOM   6607  CA  PRO B 689      40.873   7.312 109.052  1.00 49.87           C
ATOM   6608  C   PRO B 689      40.729   6.298 110.189  1.00 49.96           C
ATOM   6609  O   PRO B 689      40.927   5.097 109.964  1.00 49.84           O
ATOM   6610  CB  PRO B 689      42.314   7.833 108.985  1.00 49.78           C
ATOM   6611  CG  PRO B 689      42.272   9.155 109.643  1.00 49.94           C
ATOM   6612  CD  PRO B 689      40.935   9.731 109.312  1.00 49.88           C
ATOM   6613  N   GLN B 690      40.386   6.781 111.386  1.00 50.02           N
ATOM   6614  CA  GLN B 690      40.162   5.918 112.551  1.00 50.19           C
ATOM   6615  C   GLN B 690      38.971   4.979 112.341  1.00 50.18           C
ATOM   6616  O   GLN B 690      38.780   4.035 113.110  1.00 50.24           O
ATOM   6617  CB  GLN B 690      39.946   6.741 113.831  1.00 50.32           C
ATOM   6618  CG  GLN B 690      41.043   7.753 114.170  1.00 50.65           C
ATOM   6619  CD  GLN B 690      40.742   9.157 113.645  1.00 51.51           C
ATOM   6620  OE1 GLN B 690      39.580   9.535 113.463  1.00 51.72           O
ATOM   6621  NE2 GLN B 690      41.792   9.937 113.407  1.00 51.29           N
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ATOM   6622  N   VAL B 691      38.173   5.256 111.308  1.00 50.12           N
ATOM   6623  CA  VAL B 691      37.027   4.422 110.930  1.00 49.96           C
ATOM   6624  C   VAL B 691      37.199   3.911 109.494  1.00 49.82           C
ATOM   6625  O   VAL B 691      37.492   4.688 108.578  1.00 49.87           O
ATOM   6626  CB  VAL B 691      35.682   5.197 111.075  1.00 50.20           C
ATOM   6627  CG1 VAL B 691      34.504   4.400 110.495  1.00 49.82           C
ATOM   6628  CG2 VAL B 691      35.421   5.566 112.543  1.00 49.91           C
ATOM   6629  N   LYS B 692      37.024   2.604 109.308  1.00 49.51           N
ATOM   6630  CA  LYS B 692      37.158   1.988 107.988  1.00 49.15           C
ATOM   6631  C   LYS B 692      35.842   1.973 107.217  1.00 48.80           C
ATOM   6632  O   LYS B 692      34.763   1.921 107.812  1.00 48.51           O
ATOM   6633  CB  LYS B 692      37.719   0.562 108.099  1.00 49.19           C
ATOM   6634  CG  LYS B 692      39.212   0.485 108.425  1.00 49.43           C
ATOM   6635  CD  LYS B 692      40.085   0.769 107.203  1.00 49.70           C
ATOM   6636  CE  LYS B 692      41.567   0.776 107.557  1.00 50.10           C
ATOM   6637  NZ  LYS B 692      41.951   1.968 108.372  1.00 50.65           N
ATOM   6638  N   ASP B 693      35.958   2.025 105.890  1.00 48.52           N
ATOM   6639  CA  ASP B 693      34.830   1.869 104.968  1.00 48.19           C
ATOM   6640  C   ASP B 693      35.309   1.042 103.782  1.00 47.97           C
ATOM   6641  O   ASP B 693      36.155   1.486 103.001  1.00 48.09           O
ATOM   6642  CB  ASP B 693      34.306   3.243 104.509  1.00 48.18           C
ATOM   6643  CG  ASP B 693      33.185   3.151 103.461  1.00 48.23           C
ATOM   6644  OD1 ASP B 693      32.438   2.146 103.428  1.00 48.53           O
ATOM   6645  OD2 ASP B 693      33.044   4.110 102.670  1.00 47.72           O
ATOM   6646  N   VAL B 694      34.772  -0.166 103.658  1.00 47.60           N
ATOM   6647  CA  VAL B 694      35.160  -1.076 102.577  1.00 47.20           C
ATOM   6648  C   VAL B 694      34.241  -0.942 101.359  1.00 47.03           C
ATOM   6649  O   VAL B 694      34.066  -1.896 100.593  1.00 46.86           O
ATOM   6650  CB  VAL B 694      35.221  -2.547 103.061  1.00 47.17           C
ATOM   6651  CG1 VAL B 694      36.454  -2.772 103.926  1.00 47.07           C
ATOM   6652  CG2 VAL B 694      33.949  -2.928 103.810  1.00 46.92           C
ATOM   6653  N   TYR B 695      33.680   0.258 101.190  1.00 46.94           N
ATOM   6654  CA  TYR B 695      32.687   0.574 100.150  1.00 46.79           C
ATOM   6655  C   TYR B 695      31.403  -0.251 100.317  1.00 46.59           C
ATOM   6656  O   TYR B 695      31.110  -1.165  99.539  1.00 46.43           O
ATOM   6657  CB  TYR B 695      33.288   0.468  98.736  1.00 46.61           C
ATOM   6658  CG  TYR B 695      32.411   1.024  97.632  1.00 46.85           C
ATOM   6659  CD1 TYR B 695      32.036   2.372  97.614  1.00 46.66           C
ATOM   6660  CD2 TYR B 695      31.969   0.205  96.591  1.00 46.80           C
ATOM   6661  CE1 TYR B 695      31.239   2.883  96.594  1.00 46.55           C
ATOM   6662  CE2 TYR B 695      31.174   0.708  95.565  1.00 46.44           C
ATOM   6663  CZ  TYR B 695      30.811   2.043  95.573  1.00 46.56           C
ATOM   6664  OH  TYR B 695      30.021   2.534  94.556  1.00 46.37           O
ATOM   6665  N   VAL B 696      30.654   0.094 101.359  1.00 46.56           N
ATOM   6666  CA  VAL B 696      29.424  -0.600 101.739  1.00 46.60           C
ATOM   6667  C   VAL B 696      28.543   0.382 102.527  1.00 46.71           C
ATOM   6668  O   VAL B 696      29.032   1.412 103.002  1.00 46.77           O
ATOM   6669  CB  VAL B 696      29.740  -1.882 102.567  1.00 46.48           C
ATOM   6670  CG1 VAL B 696      30.425  -1.532 103.894  1.00 46.68           C
ATOM   6671  CG2 VAL B 696      28.487  -2.728 102.791  1.00 46.48           C
ATOM   6672  N   GLN B 697      27.253   0.079 102.648  1.00 46.86           N
ATOM   6673  CA  GLN B 697      26.334   0.933 103.402  1.00 47.10           C
ATOM   6674  C   GLN B 697      26.653   0.947 104.902  1.00 47.33           C
ATOM   6675  O   GLN B 697      27.111  -0.050 105.467  1.00 47.16           O
ATOM   6676  CB  GLN B 697      24.883   0.509 103.149  1.00 47.03           C
ATOM   6677  CG  GLN B 697      23.803   1.352 103.830  1.00 46.80           C
ATOM   6678  CD  GLN B 697      23.380   0.792 105.181  1.00 46.92           C
ATOM   6679  OE1 GLN B 697      23.952  -0.184 105.671  1.00 47.39           O
ATOM   6680  NE2 GLN B 697      22.376   1.410 105.789  1.00 46.50           N
ATOM   6681  N   MET B 698      26.400   2.094 105.525  1.00 47.73           N
ATOM   6682  CA  MET B 698      26.601   2.290 106.957  1.00 48.22           C
ATOM   6683  C   MET B 698      25.335   2.856 107.610  1.00 48.47           C
ATOM   6684  O   MET B 698      24.393   3.229 106.914  1.00 48.55           O
ATOM   6685  CB  MET B 698      27.797   3.215 107.196  1.00 48.21           C
ATOM   6686  CG  MET B 698      27.680   4.581 106.536  1.00 48.18           C
ATOM   6687  SD  MET B 698      29.260   5.427 106.401  1.00 48.35           S
ATOM   6688  CE  MET B 698      30.082   4.435 105.156  1.00 48.55           C
ATOM   6689  N   SER B 699      25.320   2.916 108.941  1.00 48.82           N
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ATOM   6690  CA  SER B 699      24.168   3.426 109.686  1.00 49.15           C
ATOM   6691  C   SER B 699      24.617   4.254 110.883  1.00 49.42           C
ATOM   6692  O   SER B 699      25.491   3.832 111.633  1.00 49.46           O
ATOM   6693  CB  SER B 699      23.287   2.265 110.145  1.00 49.06           C
ATOM   6694  OG  SER B 699      22.249   2.701 110.999  1.00 49.17           O
ATOM   6695  N   ALA B 700      24.015   5.428 111.058  1.00 49.81           N
ATOM   6696  CA  ALA B 700      24.365   6.318 112.167  1.00 50.38           C
ATOM   6697  C   ALA B 700      23.153   6.959 112.839  1.00 50.88           C
ATOM   6698  O   ALA B 700      22.199   7.353 112.169  1.00 50.91           O
ATOM   6699  CB  ALA B 700      25.327   7.389 111.705  1.00 50.29           C
ATOM   6700  N   ILE B 701      23.208   7.069 114.166  1.00 51.54           N
ATOM   6701  CA  ILE B 701      22.137   7.698 114.943  1.00 52.16           C
ATOM   6702  C   ILE B 701      22.662   8.664 116.003  1.00 52.73           C
ATOM   6703  O   ILE B 701      23.728   8.444 116.589  1.00 52.70           O
ATOM   6704  CB  ILE B 701      21.206   6.661 115.624  1.00 52.19           C
ATOM   6705  CG1 ILE B 701      22.023   5.538 116.278  1.00 52.01           C
ATOM   6706  CG2 ILE B 701      20.175   6.122 114.624  1.00 52.08           C
ATOM   6707  CD1 ILE B 701      21.279   4.785 117.361  1.00 52.16           C
ATOM   6708  N   HIS B 702      21.904   9.736 116.231  1.00 53.42           N
ATOM   6709  CA  HIS B 702      22.162  10.658 117.334  1.00 54.11           C
ATOM   6710  C   HIS B 702      21.631  10.068 118.641  1.00 54.67           C
ATOM   6711  O   HIS B 702      20.560   9.451 118.664  1.00 54.71           O
ATOM   6712  CB  HIS B 702      21.509  12.017 117.071  1.00 54.06           C
ATOM   6713  CG  HIS B 702      21.893  13.069 118.064  1.00 54.05           C
ATOM   6714  ND1 HIS B 702      21.279  13.194 119.292  1.00 53.95           N
ATOM   6715  CD2 HIS B 702      22.840  14.036 118.017  1.00 54.05           C
ATOM   6716  CE1 HIS B 702      21.829  14.194 119.957  1.00 54.15           C
ATOM   6717  NE2 HIS B 702      22.775  14.725 119.203  1.00 54.50           N
ATOM   6718  N   THR B 703      22.383  10.268 119.724  1.00 55.41           N
ATOM   6719  CA  THR B 703      22.007   9.746 121.042  1.00 56.13           C
ATOM   6720  C   THR B 703      22.635  10.517 122.213  1.00 56.76           C
ATOM   6721  O   THR B 703      23.855  10.642 122.311  1.00 56.73           O
ATOM   6722  CB  THR B 703      22.319   8.221 121.171  1.00 56.04           C
ATOM   6723  OG1 THR B 703      21.857   7.737 122.437  1.00 55.79           O
ATOM   6724  CG2 THR B 703      23.818   7.933 121.025  1.00 55.96           C
ATOM   6725  N   MET B 704      21.787  11.035 123.096  1.00 57.51           N
ATOM   6726  CA  MET B 704      22.254  11.661 124.326  1.00 58.37           C
ATOM   6727  C   MET B 704      22.429  10.590 125.394  1.00 58.99           C
ATOM   6728  O   MET B 704      21.593   9.685 125.516  1.00 59.21           O
ATOM   6729  CB  MET B 704      21.250  12.706 124.818  1.00 58.36           C
ATOM   6730  CG  MET B 704      20.936  13.808 123.825  1.00 58.63           C
ATOM   6731  SD  MET B 704      22.359  14.854 123.507  1.00 59.47           S
ATOM   6732  CE  MET B 704      22.411  15.839 125.008  1.00 59.89           C
ATOM   6733  N   HIS B 705      23.516  10.685 126.156  1.00 59.62           N
ATOM   6734  CA  HIS B 705      23.681   9.861 127.355  1.00 60.26           C
ATOM   6735  C   HIS B 705      24.406  10.597 128.479  1.00 60.65           C
ATOM   6736  O   HIS B 705      25.639  10.690 128.485  1.00 60.55           O
ATOM   6737  CB  HIS B 705      24.378   8.534 127.051  1.00 60.24           C
ATOM   6738  CG  HIS B 705      24.394   7.594 128.215  1.00 60.57           C
ATOM   6739  ND1 HIS B 705      25.383   7.617 129.175  1.00 60.95           N
ATOM   6740  CD2 HIS B 705      23.529   6.622 128.587  1.00 60.91           C
ATOM   6741  CE1 HIS B 705      25.133   6.690 130.083  1.00 61.08           C
ATOM   6742  NE2 HIS B 705      24.013   6.073 129.750  1.00 61.23           N
ATOM   6743  N   GLU B 706      23.614  11.120 129.417  1.00 61.19           N
ATOM   6744  CA  GLU B 706      24.100  11.853 130.597  1.00 61.71           C
ATOM   6745  C   GLU B 706      24.848  13.154 130.291  1.00 61.98           C
ATOM   6746  O   GLU B 706      24.784  14.099 131.079  1.00 62.09           O
ATOM   6747  CB  GLU B 706      24.942  10.946 131.507  1.00 61.68           C
ATOM   6748  CG  GLU B 706      24.125   9.945 132.321  1.00 61.83           C
ATOM   6749  CD  GLU B 706      24.974   8.842 132.935  1.00 61.83           C
ATOM   6750  OE1 GLU B 706      26.216   8.990 132.982  1.00 61.80           O
ATOM   6751  OE2 GLU B 706      24.397   7.821 133.370  1.00 61.73           O
ATOM   6752  N   GLY B 707      25.549  13.202 129.158  1.00 62.30           N
ATOM   6753  CA  GLY B 707      26.339  14.372 128.774  1.00 62.54           C
ATOM   6754  C   GLY B 707      26.142  14.778 127.328  1.00 62.70           C
ATOM   6755  O   GLY B 707      25.012  14.825 126.838  1.00 62.82           O
ATOM   6756  N   LYS B 708      27.250  15.068 126.649  1.00 62.79           N
ATOM   6757  CA  LYS B 708      27.236  15.510 125.249  1.00 62.81           C
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ATOM   6758  C   LYS B 708      28.391  14.902 124.437  1.00 62.61           C
ATOM   6759  O   LYS B 708      29.539  14.899 124.896  1.00 62.60           O
ATOM   6760  CB  LYS B 708      27.285  17.044 125.160  1.00 62.85           C
ATOM   6761  CG  LYS B 708      25.924  17.724 125.198  1.00 63.02           C
ATOM   6762  CD  LYS B 708      26.020  19.185 124.770  1.00 63.09           C
ATOM   6763  CE  LYS B 708      24.637  19.814 124.639  1.00 63.33           C
ATOM   6764  NZ  LYS B 708      24.703  21.300 124.602  1.00 63.21           N
ATOM   6765  N   GLU B 709      28.104  14.399 123.231  1.00 62.27           N
ATOM   6766  CA  GLU B 709      26.768  14.425 122.622  1.00 61.76           C
ATOM   6767  C   GLU B 709      26.448  13.080 121.965  1.00 61.33           C
ATOM   6768  O   GLU B 709      25.286  12.692 121.880  1.00 61.32           O
ATOM   6769  CB  GLU B 709      26.670  15.577 121.613  1.00 61.85           C
ATOM   6770  CG  GLU B 709      25.275  15.878 121.068  1.00 61.87           C
ATOM   6771  CD  GLU B 709      25.243  17.133 120.202  1.00 61.81           C
ATOM   6772  OE1 GLU B 709      25.532  18.232 120.724  1.00 62.07           O
ATOM   6773  OE2 GLU B 709      24.925  17.022 119.000  1.00 61.61           O
ATOM   6774  N   TYR B 710      27.492  12.399 121.490  1.00 60.80           N
ATOM   6775  CA  TYR B 710      27.452  10.983 121.057  1.00 60.34           C
ATOM   6776  C   TYR B 710      26.693  10.627 119.764  1.00 59.96           C
ATOM   6777  O   TYR B 710      25.506  10.937 119.603  1.00 59.88           O
ATOM   6778  CB  TYR B 710      27.041  10.052 122.214  1.00 60.39           C
ATOM   6779  CG  TYR B 710      27.845  10.271 123.478  1.00 60.52           C
ATOM   6780  CD1 TYR B 710      29.191   9.910 123.539  1.00 60.55           C
ATOM   6781  CD2 TYR B 710      27.264  10.848 124.610  1.00 60.28           C
ATOM   6782  CE1 TYR B 710      29.939  10.117 124.691  1.00 60.71           C
ATOM   6783  CE2 TYR B 710      28.004  11.058 125.770  1.00 60.42           C
ATOM   6784  CZ  TYR B 710      29.341  10.690 125.802  1.00 60.69           C
ATOM   6785  OH  TYR B 710      30.090  10.887 126.939  1.00 60.73           O
ATOM   6786  N   ILE B 711      27.414   9.965 118.857  1.00 59.38           N
ATOM   6787  CA  ILE B 711      26.844   9.346 117.657  1.00 58.85           C
ATOM   6788  C   ILE B 711      27.340   7.905 117.548  1.00 58.59           C
ATOM   6789  O   ILE B 711      28.527   7.632 117.742  1.00 58.36           O
ATOM   6790  CB  ILE B 711      27.211  10.121 116.356  1.00 58.88           C
ATOM   6791  CG1 ILE B 711      26.386  11.408 116.239  1.00 58.70           C
ATOM   6792  CG2 ILE B 711      27.004   9.241 115.114  1.00 58.41           C
ATOM   6793  CD1 ILE B 711      26.898  12.380 115.190  1.00 58.71           C
ATOM   6794  N   ILE B 712      26.421   6.993 117.244  1.00 58.32           N
ATOM   6795  CA  ILE B 712      26.765   5.600 116.983  1.00 58.12           C
ATOM   6796  C   ILE B 712      26.770   5.344 115.476  1.00 57.91           C
ATOM   6797  O   ILE B 712      25.771   5.576 114.798  1.00 57.71           O
ATOM   6798  CB  ILE B 712      25.779   4.624 117.677  1.00 58.19           C
ATOM   6799  CG1 ILE B 712      25.626   4.970 119.165  1.00 58.34           C
ATOM   6800  CG2 ILE B 712      26.238   3.176 117.495  1.00 57.99           C
ATOM   6801  CD1 ILE B 712      24.405   4.354 119.835  1.00 58.23           C
ATOM   6802  N   LEU B 713      27.905   4.872 114.966  1.00 57.78           N
ATOM   6803  CA  LEU B 713      28.052   4.523 113.554  1.00 57.79           C
ATOM   6804  C   LEU B 713      28.383   3.039 113.428  1.00 57.75           C
ATOM   6805  O   LEU B 713      29.301   2.548 114.085  1.00 57.73           O
ATOM   6806  CB  LEU B 713      29.141   5.391 112.896  1.00 57.79           C
ATOM   6807  CG  LEU B 713      29.387   5.480 111.375  1.00 57.69           C
ATOM   6808  CD1 LEU B 713      30.290   4.371 110.844  1.00 57.58           C
ATOM   6809  CD2 LEU B 713      28.097   5.543 110.568  1.00 57.11           C
ATOM   6810  N   SER B 714      27.634   2.330 112.588  1.00 57.80           N
ATOM   6811  CA  SER B 714      27.839   0.895 112.409  1.00 57.91           C
ATOM   6812  C   SER B 714      27.999   0.491 110.945  1.00 58.00           C
ATOM   6813  O   SER B 714      27.213   0.898 110.087  1.00 58.03           O
ATOM   6814  CB  SER B 714      26.699   0.108 113.058  1.00 57.92           C
ATOM   6815  OG  SER B 714      26.924  -1.287 112.953  1.00 57.82           O
ATOM   6816  N   ASN B 715      29.024  -0.317 110.681  1.00 58.16           N
ATOM   6817  CA  ASN B 715      29.313  -0.846 109.341  1.00 58.35           C
ATOM   6818  C   ASN B 715      30.270  -2.043 109.395  1.00 58.46           C
ATOM   6819  O   ASN B 715      30.509  -2.602 110.469  1.00 58.48           O
ATOM   6820  CB  ASN B 715      29.873   0.255 108.425  1.00 58.29           C
ATOM   6821  CG  ASN B 715      31.113   0.925 108.997  1.00 58.20           C
ATOM   6822  OD1 ASN B 715      31.373   0.872 110.200  1.00 58.26           O
ATOM   6823  ND2 ASN B 715      31.883   1.568 108.130  1.00 58.20           N
ATOM   6824  N   ALA B 716      30.808  -2.433 108.241  1.00 58.59           N
ATOM   6825  CA  ALA B 716      31.773  -3.532 108.164  1.00 58.75           C
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ATOM   6826  C   ALA B 716      33.139  -3.132 108.720  1.00 58.91           C
ATOM   6827  O   ALA B 716      33.450  -1.946 108.836  1.00 58.89           O
ATOM   6828  CB  ALA B 716      31.908  -4.023 106.733  1.00 58.73           C
ATOM   6829  N   GLY B 717      33.947  -4.133 109.064  1.00 59.14           N
ATOM   6830  CA  GLY B 717      35.292  -3.910 109.591  1.00 59.31           C
ATOM   6831  C   GLY B 717      36.376  -4.089 108.548  1.00 59.45           C
ATOM   6832  O   GLY B 717      37.346  -3.327 108.516  1.00 59.35           O
ATOM   6833  N   GLY B 718      36.212  -5.099 107.698  1.00 59.62           N
ATOM   6834  CA  GLY B 718      37.176  -5.382 106.643  1.00 60.03           C
ATOM   6835  C   GLY B 718      38.308  -6.287 107.095  1.00 60.40           C
ATOM   6836  O   GLY B 718      38.376  -6.646 108.275  1.00 60.33           O
ATOM   6837  N   PRO B 719      39.202  -6.675 106.158  1.00 60.70           N
ATOM   6838  CA  PRO B 719      39.130  -6.334 104.731  1.00 60.93           C
ATOM   6839  C   PRO B 719      38.054  -7.156 104.016  1.00 61.10           C
ATOM   6840  O   PRO B 719      37.949  -8.363 104.248  1.00 61.35           O
ATOM   6841  CB  PRO B 719      40.526  -6.696 104.213  1.00 60.96           C
ATOM   6842  CG  PRO B 719      40.992  -7.788 105.118  1.00 60.96           C
ATOM   6843  CD  PRO B 719      40.387  -7.501 106.469  1.00 60.75           C
ATOM   6844  N   LYS B 720      37.281  -6.497 103.151  1.00 61.04           N
ATOM   6845  CA  LYS B 720      36.070  -7.065 102.524  1.00 60.92           C
ATOM   6846  C   LYS B 720      34.853  -6.882 103.435  1.00 60.78           C
ATOM   6847  O   LYS B 720      34.971  -6.344 104.539  1.00 60.76           O
ATOM   6848  CB  LYS B 720      36.240  -8.540 102.126  1.00 60.94           C
ATOM   6849  CG  LYS B 720      37.156  -8.776 100.937  1.00 61.13           C
ATOM   6850  CD  LYS B 720      37.226 -10.253 100.600  1.00 61.22           C
ATOM   6851  CE  LYS B 720      38.261 -10.527  99.527  1.00 61.31           C
ATOM   6852  NZ  LYS B 720      38.410 -11.986  99.282  1.00 61.29           N
ATOM   6853  N   ARG B 721      33.687  -7.321 102.967  1.00 60.62           N
ATOM   6854  CA  ARG B 721      32.445  -7.133 103.716  1.00 60.51           C
ATOM   6855  C   ARG B 721      32.330  -8.107 104.881  1.00 60.46           C
ATOM   6856  O   ARG B 721      31.655  -9.132 104.790  1.00 60.48           O
ATOM   6857  CB  ARG B 721      31.226  -7.186 102.788  1.00 60.41           C
ATOM   6858  CG  ARG B 721      30.940  -5.838 102.154  1.00 60.07           C
ATOM   6859  CD  ARG B 721      30.137  -5.935 100.879  1.00 59.58           C
ATOM   6860  NE  ARG B 721      30.076  -4.631 100.224  1.00 59.13           N
ATOM   6861  CZ  ARG B 721      29.298  -4.333  99.189  1.00 58.61           C
ATOM   6862  NH1 ARG B 721      28.492  -5.245  98.664  1.00 58.43           N
ATOM   6863  NH2 ARG B 721      29.328  -3.110  98.682  1.00 58.56           N
ATOM   6864  N   GLU B 722      32.999  -7.756 105.976  1.00 60.42           N
ATOM   6865  CA  GLU B 722      33.148  -8.635 107.129  1.00 60.43           C
ATOM   6866  C   GLU B 722      33.359  -7.852 108.422  1.00 60.46           C
ATOM   6867  O   GLU B 722      33.761  -6.687 108.393  1.00 60.26           O
ATOM   6868  CB  GLU B 722      34.322  -9.594 106.910  1.00 60.38           C
ATOM   6869  CG  GLU B 722      35.670  -8.895 106.746  1.00 60.46           C
ATOM   6870  CD  GLU B 722      36.766  -9.826 106.282  1.00 60.44           C
ATOM   6871  OE1 GLU B 722      36.515 -10.651 105.378  1.00 60.64           O
ATOM   6872  OE2 GLU B 722      37.890  -9.719 106.811  1.00 60.27           O
ATOM   6873  N   ASN B 723      33.091  -8.523 109.545  1.00 60.59           N
ATOM   6874  CA  ASN B 723      33.310  -7.996 110.899  1.00 60.69           C
ATOM   6875  C   ASN B 723      32.506  -6.755 111.246  1.00 60.74           C
ATOM   6876  O   ASN B 723      33.003  -5.632 111.155  1.00 60.70           O
ATOM   6877  CB  ASN B 723      34.802  -7.785 111.189  1.00 60.73           C
ATOM   6878  CG  ASN B 723      35.481  -9.044 111.689  1.00 61.05           C
ATOM   6879  OD1 ASN B 723      35.288 -10.133 111.141  1.00 61.50           O
ATOM   6880  ND2 ASN B 723      36.284  -8.901 112.739  1.00 61.14           N
ATOM   6881  N   GLY B 724      31.260  -6.972 111.652  1.00 60.89           N
ATOM   6882  CA  GLY B 724      30.391  -5.890 112.090  1.00 61.13           C
ATOM   6883  C   GLY B 724      31.039  -5.090 113.196  1.00 61.34           C
ATOM   6884  O   GLY B 724      31.373  -5.630 114.249  1.00 61.27           O
ATOM   6885  N   MET B 725      31.239  -3.803 112.938  1.00 61.57           N
ATOM   6886  CA  MET B 725      31.824  -2.905 113.922  1.00 61.81           C
ATOM   6887  C   MET B 725      30.804  -1.873 114.366  1.00 61.78           C
ATOM   6888  O   MET B 725      29.976  -1.425 113.573  1.00 61.89           O
ATOM   6889  CB  MET B 725      33.062  -2.201 113.359  1.00 61.93           C
ATOM   6890  CG  MET B 725      34.235  -3.121 113.023  1.00 62.55           C
ATOM   6891  SD  MET B 725      34.854  -4.102 114.409  1.00 64.24           S
ATOM   6892  CE  MET B 725      35.431  -2.822 115.522  1.00 63.96           C
ATOM   6893  N   VAL B 726      30.862  -1.515 115.643  1.00 61.79           N
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ATOM   6894  CA  VAL B 726      30.067  -0.417 116.173  1.00 61.79           C
ATOM   6895  C   VAL B 726      31.008   0.626 116.775  1.00 61.78           C
ATOM   6896  O   VAL B 726      31.727   0.353 117.741  1.00 61.78           O
ATOM   6897  CB  VAL B 726      29.010  -0.904 117.194  1.00 61.81           C
ATOM   6898  CG1 VAL B 726      28.343   0.270 117.888  1.00 61.82           C
ATOM   6899  CG2 VAL B 726      27.961  -1.759 116.500  1.00 61.82           C
ATOM   6900  N   HIS B 727      31.001   1.814 116.176  1.00 61.75           N
ATOM   6901  CA  HIS B 727      31.914   2.892 116.543  1.00 61.70           C
ATOM   6902  C   HIS B 727      31.177   3.966 117.335  1.00 61.65           C
ATOM   6903  O   HIS B 727      30.006   4.241 117.069  1.00 61.62           O
ATOM   6904  CB  HIS B 727      32.529   3.525 115.286  1.00 61.70           C
ATOM   6905  CG  HIS B 727      33.017   2.536 114.269  1.00 61.83           C
ATOM   6906  ND1 HIS B 727      34.345   2.186 114.147  1.00 61.83           N
ATOM   6907  CD2 HIS B 727      32.358   1.844 113.309  1.00 61.77           C
ATOM   6908  CE1 HIS B 727      34.481   1.311 113.167  1.00 61.62           C
ATOM   6909  NE2 HIS B 727      33.290   1.087 112.641  1.00 61.74           N
ATOM   6910  N   LEU B 728      31.861   4.572 118.303  1.00 61.63           N
ATOM   6911  CA  LEU B 728      31.282   5.683 119.063  1.00 61.70           C
ATOM   6912  C   LEU B 728      32.142   6.944 118.971  1.00 61.77           C
ATOM   6913  O   LEU B 728      33.371   6.875 119.052  1.00 61.76           O
ATOM   6914  CB  LEU B 728      31.039   5.294 120.529  1.00 61.71           C
ATOM   6915  CG  LEU B 728      30.180   6.240 121.390  1.00 61.73           C
ATOM   6916  CD1 LEU B 728      28.694   6.136 121.053  1.00 61.40           C
ATOM   6917  CD2 LEU B 728      30.400   5.989 122.875  1.00 61.68           C
ATOM   6918  N   ALA B 729      31.477   8.087 118.799  1.00 61.78           N
ATOM   6919  CA  ALA B 729      32.139   9.385 118.687  1.00 61.82           C
ATOM   6920  C   ALA B 729      31.570  10.401 119.673  1.00 61.88           C
ATOM   6921  O   ALA B 729      30.369  10.407 119.949  1.00 61.81           O
ATOM   6922  CB  ALA B 729      32.017   9.917 117.269  1.00 61.81           C
ATOM   6923  N   ARG B 730      32.439  11.261 120.195  1.00 61.94           N
ATOM   6924  CA  ARG B 730      32.012  12.344 121.076  1.00 62.07           C
ATOM   6925  C   ARG B 730      31.808  13.614 120.258  1.00 61.97           C
ATOM   6926  O   ARG B 730      32.750  14.154 119.670  1.00 61.81           O
ATOM   6927  CB  ARG B 730      33.028  12.570 122.202  1.00 62.10           C
ATOM   6928  CG  ARG B 730      32.488  13.346 123.404  1.00 62.57           C
ATOM   6929  CD  ARG B 730      33.254  12.995 124.684  1.00 63.51           C
ATOM   6930  NE  ARG B 730      34.665  13.388 124.623  1.00 64.43           N
ATOM   6931  CZ  ARG B 730      35.649  12.793 125.296  1.00 64.75           C
ATOM   6932  NH1 ARG B 730      35.399  11.756 126.092  1.00 64.77           N
ATOM   6933  NH2 ARG B 730      36.893  13.233 125.166  1.00 64.62           N
ATOM   6934  N   VAL B 731      30.564  14.075 120.219  1.00 61.92           N
ATOM   6935  CA  VAL B 731      30.217  15.258 119.451  1.00 61.94           C
ATOM   6936  C   VAL B 731      30.621  16.521 120.205  1.00 62.04           C
ATOM   6937  O   VAL B 731      30.004  16.904 121.202  1.00 61.96           O
ATOM   6938  CB  VAL B 731      28.716  15.286 119.076  1.00 61.93           C
ATOM   6939  CG1 VAL B 731      28.384  16.526 118.253  1.00 61.80           C
ATOM   6940  CG2 VAL B 731      28.326  14.019 118.322  1.00 61.65           C
ATOM   6941  N   GLU B 732      31.677  17.154 119.711  1.00 62.29           N
ATOM   6942  CA  GLU B 732      32.150  18.421 120.246  1.00 62.59           C
ATOM   6943  C   GLU B 732      31.208  19.561 119.868  1.00 62.59           C
ATOM   6944  O   GLU B 732      30.276  19.376 119.087  1.00 62.58           O
ATOM   6945  CB  GLU B 732      33.572  18.697 119.764  1.00 62.67           C
ATOM   6946  CG  GLU B 732      34.572  17.648 120.217  1.00 63.34           C
ATOM   6947  CD  GLU B 732      35.929  18.239 120.519  1.00 64.65           C
ATOM   6948  OE1 GLU B 732      36.452  18.999 119.671  1.00 65.52           O
ATOM   6949  OE2 GLU B 732      36.469  17.946 121.608  1.00 64.38           O
ATOM   6950  N   GLU B 733      31.459  20.740 120.420  1.00 62.71           N
ATOM   6951  CA  GLU B 733      30.505  21.846 120.330  1.00 62.97           C
ATOM   6952  C   GLU B 733      30.586  22.656 119.028  1.00 62.90           C
ATOM   6953  O   GLU B 733      29.692  23.456 118.735  1.00 62.88           O
ATOM   6954  CB  GLU B 733      30.653  22.762 121.554  1.00 62.94           C
ATOM   6955  CG  GLU B 733      30.468  22.032 122.892  1.00 63.26           C
ATOM   6956  CD  GLU B 733      30.498  22.957 124.103  1.00 63.31           C
ATOM   6957  OE1 GLU B 733      31.237  23.968 124.086  1.00 63.48           O
ATOM   6958  OE2 GLU B 733      29.781  22.659 125.083  1.00 63.64           O
ATOM   6959  N   ASN B 734      31.631  22.415 118.237  1.00 62.89           N
ATOM   6960  CA  ASN B 734      31.982  23.297 117.112  1.00 62.75           C
ATOM   6961  C   ASN B 734      31.400  23.072 115.694  1.00 62.72           C
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ATOM   6962  O   ASN B 734      31.341  24.030 114.922  1.00 62.86           O
ATOM   6963  CB  ASN B 734      33.504  23.494 117.033  1.00 62.76           C
ATOM   6964  CG  ASN B 734      34.255  22.197 116.808  1.00 62.54           C
ATOM   6965  OD1 ASN B 734      33.923  21.157 117.381  1.00 62.40           O
ATOM   6966  ND2 ASN B 734      35.289  22.258 115.980  1.00 62.05           N
ATOM   6967  N   GLY B 735      30.983  21.857 115.319  1.00 62.55           N
ATOM   6968  CA  GLY B 735      31.012  20.654 116.142  1.00 62.34           C
ATOM   6969  C   GLY B 735      31.604  19.458 115.420  1.00 62.23           C
ATOM   6970  O   GLY B 735      30.898  18.728 114.718  1.00 62.11           O
ATOM   6971  N   GLU B 736      32.909  19.262 115.596  1.00 62.12           N
ATOM   6972  CA  GLU B 736      33.599  18.085 115.078  1.00 62.02           C
ATOM   6973  C   GLU B 736      33.209  16.866 115.913  1.00 61.88           C
ATOM   6974  O   GLU B 736      32.333  16.951 116.775  1.00 61.83           O
ATOM   6975  CB  GLU B 736      35.117  18.294 115.117  1.00 62.03           C
ATOM   6976  CG  GLU B 736      35.884  17.493 114.066  1.00 62.32           C
ATOM   6977  CD  GLU B 736      37.321  17.197 114.468  1.00 62.41           C
ATOM   6978  OE1 GLU B 736      37.556  16.771 115.621  1.00 62.40           O
ATOM   6979  OE2 GLU B 736      38.218  17.378 113.618  1.00 62.24           O
ATOM   6980  N   LEU B 737      33.852  15.734 115.651  1.00 61.85           N
ATOM   6981  CA  LEU B 737      33.625  14.527 116.437  1.00 61.91           C
ATOM   6982  C   LEU B 737      34.904  13.711 116.605  1.00 61.98           C
ATOM   6983  O   LEU B 737      35.623  13.453 115.639  1.00 61.98           O
ATOM   6984  CB  LEU B 737      32.485  13.686 115.846  1.00 61.91           C
ATOM   6985  CG  LEU B 737      32.399  13.475 114.333  1.00 61.99           C
ATOM   6986  CD1 LEU B 737      33.036  12.155 113.935  1.00 62.32           C
ATOM   6987  CD2 LEU B 737      30.953  13.500 113.891  1.00 62.27           C
ATOM   6988  N   THR B 738      35.187  13.334 117.850  1.00 62.13           N
ATOM   6989  CA  THR B 738      36.357  12.519 118.184  1.00 62.11           C
ATOM   6990  C   THR B 738      35.913  11.110 118.577  1.00 62.06           C
ATOM   6991  O   THR B 738      35.059  10.932 119.452  1.00 62.02           O
ATOM   6992  CB  THR B 738      37.211  13.163 119.312  1.00 62.12           C
ATOM   6993  OG1 THR B 738      36.377  13.481 120.433  1.00 61.84           O
ATOM   6994  CG2 THR B 738      37.893  14.441 118.814  1.00 62.01           C
ATOM   6995  N   TRP B 739      36.486  10.114 117.910  1.00 62.02           N
ATOM   6996  CA  TRP B 739      36.080   8.726 118.102  1.00 62.02           C
ATOM   6997  C   TRP B 739      36.667   8.142 119.381  1.00 62.17           C
ATOM   6998  O   TRP B 739      37.818   8.416 119.731  1.00 62.10           O
ATOM   6999  CB  TRP B 739      36.452   7.885 116.877  1.00 61.95           C
ATOM   7000  CG  TRP B 739      35.720   8.340 115.649  1.00 61.87           C
ATOM   7001  CD1 TRP B 739      36.168   9.218 114.707  1.00 61.77           C
ATOM   7002  CD2 TRP B 739      34.392   7.968 115.252  1.00 61.81           C
ATOM   7003  NE1 TRP B 739      35.210   9.408 113.739  1.00 61.71           N
ATOM   7004  CE2 TRP B 739      34.109   8.653 114.049  1.00 61.69           C
ATOM   7005  CE3 TRP B 739      33.417   7.115 115.790  1.00 61.61           C
ATOM   7006  CZ2 TRP B 739      32.891   8.514 113.375  1.00 61.61           C
ATOM   7007  CZ3 TRP B 739      32.202   6.982 115.120  1.00 61.71           C
ATOM   7008  CH2 TRP B 739      31.954   7.675 113.923  1.00 61.74           C
ATOM   7009  N   LEU B 740      35.859   7.348 120.081  1.00 62.27           N
ATOM   7010  CA  LEU B 740      36.251   6.793 121.371  1.00 62.32           C
ATOM   7011  C   LEU B 740      36.641   5.323 121.262  1.00 62.45           C
ATOM   7012  O   LEU B 740      37.805   4.970 121.456  1.00 62.46           O
ATOM   7013  CB  LEU B 740      35.142   6.997 122.414  1.00 62.29           C
ATOM   7014  CG  LEU B 740      34.636   8.421 122.703  1.00 62.17           C
ATOM   7015  CD1 LEU B 740      33.593   8.395 123.814  1.00 61.97           C
ATOM   7016  CD2 LEU B 740      35.762   9.391 123.057  1.00 61.76           C
ATOM   7017  N   LYS B 741      35.672   4.472 120.942  1.00 62.65           N
ATOM   7018  CA  LYS B 741      35.924   3.040 120.824  1.00 62.95           C
ATOM   7019  C   LYS B 741      35.221   2.420 119.616  1.00 63.04           C
ATOM   7020  O   LYS B 741      34.161   2.891 119.188  1.00 63.11           O
ATOM   7021  CB  LYS B 741      35.535   2.310 122.117  1.00 63.00           C
ATOM   7022  CG  LYS B 741      36.479   2.580 123.290  1.00 63.30           C
ATOM   7023  CD  LYS B 741      36.304   1.575 124.417  1.00 63.71           C
ATOM   7024  CE  LYS B 741      37.329   1.805 125.520  1.00 63.90           C
ATOM   7025  NZ  LYS B 741      37.254   0.762 126.586  1.00 64.23           N
ATOM   7026  N   HIS B 742      35.834   1.371 119.071  1.00 63.10           N
ATOM   7027  CA  HIS B 742      35.277   0.615 117.950  1.00 63.14           C
ATOM   7028  C   HIS B 742      35.162  -0.852 118.360  1.00 63.04           C
ATOM   7029  O   HIS B 742      36.174  -1.539 118.518  1.00 63.14           O
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ATOM   7030  CB  HIS B 742      36.162   0.750 116.701  1.00 63.17           C
ATOM   7031  CG  HIS B 742      36.831   2.085 116.566  1.00 63.59           C
ATOM   7032  ND1 HIS B 742      38.203   2.231 116.549  1.00 63.88           N
ATOM   7033  CD2 HIS B 742      36.320   3.334 116.447  1.00 63.85           C
ATOM   7034  CE1 HIS B 742      38.507   3.511 116.422  1.00 64.00           C
ATOM   7035  NE2 HIS B 742      37.382   4.202 116.358  1.00 64.10           N
ATOM   7036  N   ASN B 743      33.931  -1.327 118.531  1.00 62.92           N
ATOM   7037  CA  ASN B 743      33.696  -2.658 119.089  1.00 62.87           C
ATOM   7038  C   ASN B 743      32.994  -3.609 118.125  1.00 62.73           C
ATOM   7039  O   ASN B 743      31.950  -3.266 117.568  1.00 62.71           O
ATOM   7040  CB  ASN B 743      32.888  -2.567 120.387  1.00 62.94           C
ATOM   7041  CG  ASN B 743      33.136  -1.278 121.144  1.00 63.17           C
ATOM   7042  OD1 ASN B 743      32.253  -0.425 121.238  1.00 63.68           O
ATOM   7043  ND2 ASN B 743      34.341  -1.125 121.682  1.00 63.37           N
ATOM   7044  N   PRO B 744      33.568  -4.811 117.930  1.00 62.64           N
ATOM   7045  CA  PRO B 744      32.964  -5.838 117.080  1.00 62.52           C
ATOM   7046  C   PRO B 744      31.626  -6.329 117.627  1.00 62.40           C
ATOM   7047  O   PRO B 744      31.530  -6.730 118.786  1.00 62.46           O
ATOM   7048  CB  PRO B 744      34.003  -6.969 117.094  1.00 62.56           C
ATOM   7049  CG  PRO B 744      35.280  -6.320 117.532  1.00 62.53           C
ATOM   7050  CD  PRO B 744      34.854  -5.260 118.492  1.00 62.62           C
ATOM   7051  N   ILE B 745      30.605  -6.284 116.780  1.00 62.27           N
ATOM   7052  CA  ILE B 745      29.253  -6.694 117.146  1.00 62.14           C
ATOM   7053  C   ILE B 745      28.898  -8.057 116.525  1.00 61.99           C
ATOM   7054  O   ILE B 745      28.021  -8.771 117.020  1.00 62.01           O
ATOM   7055  CB  ILE B 745      28.213  -5.590 116.761  1.00 62.12           C
ATOM   7056  CG1 ILE B 745      26.813  -5.933 117.283  1.00 62.17           C
ATOM   7057  CG2 ILE B 745      28.213  -5.315 115.249  1.00 62.19           C
ATOM   7058  CD1 ILE B 745      25.782  -4.863 117.018  1.00 62.19           C
ATOM   7059  N   GLN B 746      29.601  -8.407 115.450  1.00 61.84           N
ATOM   7060  CA  GLN B 746      29.360  -9.639 114.709  1.00 61.70           C
ATOM   7061  C   GLN B 746      30.625 -10.030 113.952  1.00 61.63           C
ATOM   7062  O   GLN B 746      31.306  -9.173 113.385  1.00 61.63           O
ATOM   7063  CB  GLN B 746      28.185  -9.452 113.737  1.00 61.70           C
ATOM   7064  CG  GLN B 746      27.910 -10.621 112.793  1.00 61.73           C
ATOM   7065  CD  GLN B 746      27.292 -11.822 113.487  1.00 62.13           C
ATOM   7066  OE1 GLN B 746      26.141 -11.781 113.924  1.00 62.00           O
ATOM   7067  NE2 GLN B 746      28.053 -12.907 113.577  1.00 62.17           N
ATOM   7068  N   LYS B 747      30.939 -11.323 113.969  1.00 61.51           N
ATOM   7069  CA  LYS B 747      32.035 -11.877 113.179  1.00 61.33           C
ATOM   7070  C   LYS B 747      31.463 -12.577 111.951  1.00 61.06           C
ATOM   7071  O   LYS B 747      30.262 -12.841 111.887  1.00 60.90           O
ATOM   7072  CB  LYS B 747      32.875 -12.851 114.011  1.00 61.46           C
ATOM   7073  CG  LYS B 747      33.632 -12.196 115.156  1.00 61.81           C
ATOM   7074  CD  LYS B 747      34.425 -13.215 115.951  1.00 62.37           C
ATOM   7075  CE  LYS B 747      35.035 -12.588 117.192  1.00 62.40           C
ATOM   7076  NZ  LYS B 747      35.907 -13.551 117.918  1.00 62.72           N
ATOM   7077  N   GLY B 748      32.327 -12.871 110.982  1.00 60.85           N
ATOM   7078  CA  GLY B 748      31.896 -13.425 109.699  1.00 60.66           C
ATOM   7079  C   GLY B 748      31.683 -12.320 108.682  1.00 60.43           C
ATOM   7080  O   GLY B 748      32.087 -11.176 108.912  1.00 60.36           O
ATOM   7081  N   GLU B 749      31.050 -12.649 107.557  1.00 60.16           N
ATOM   7082  CA  GLU B 749      30.782 -11.631 106.544  1.00 59.97           C
ATOM   7083  C   GLU B 749      29.573 -10.755 106.906  1.00 59.50           C
ATOM   7084  O   GLU B 749      28.508 -11.259 107.261  1.00 59.47           O
ATOM   7085  CB  GLU B 749      30.726 -12.211 105.116  1.00 59.97           C
ATOM   7086  CG  GLU B 749      29.544 -13.110 104.763  1.00 60.25           C
ATOM   7087  CD  GLU B 749      29.384 -13.292 103.247  1.00 60.47           C
ATOM   7088  OE1 GLU B 749      30.031 -12.550 102.472  1.00 60.77           O
ATOM   7089  OE2 GLU B 749      28.606 -14.175 102.822  1.00 61.35           O
ATOM   7090  N   PHE B 750      29.775  -9.441 106.820  1.00 59.03           N
ATOM   7091  CA  PHE B 750      28.840  -8.435 107.332  1.00 58.65           C
ATOM   7092  C   PHE B 750      28.756  -7.238 106.372  1.00 58.34           C
ATOM   7093  O   PHE B 750      29.787  -6.752 105.893  1.00 58.32           O
ATOM   7094  CB  PHE B 750      29.314  -7.979 108.717  1.00 58.60           C
ATOM   7095  CG  PHE B 750      28.491  -6.876 109.324  1.00 58.78           C
ATOM   7096  CD1 PHE B 750      27.502  -7.167 110.257  1.00 59.05           C
ATOM   7097  CD2 PHE B 750      28.722  -5.542 108.988  1.00 58.81           C
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ATOM   7098  CE1 PHE B 750      26.748  -6.151 110.837  1.00 58.91           C
ATOM   7099  CE2 PHE B 750      27.968  -4.523 109.556  1.00 58.72           C
ATOM   7100  CZ  PHE B 750      26.980  -4.828 110.483  1.00 58.75           C
ATOM   7101  N   ALA B 751      27.541  -6.751 106.112  1.00 57.83           N
ATOM   7102  CA  ALA B 751      27.334  -5.688 105.114  1.00 57.47           C
ATOM   7103  C   ALA B 751      26.444  -4.510 105.560  1.00 57.17           C
ATOM   7104  O   ALA B 751      26.910  -3.601 106.255  1.00 57.03           O
ATOM   7105  CB  ALA B 751      26.834  -6.287 103.793  1.00 57.36           C
ATOM   7106  N   TYR B 752      25.179  -4.529 105.139  1.00 56.95           N
ATOM   7107  CA  TYR B 752      24.235  -3.437 105.401  1.00 56.77           C
ATOM   7108  C   TYR B 752      23.599  -3.571 106.782  1.00 56.62           C
ATOM   7109  O   TYR B 752      23.334  -4.686 107.245  1.00 56.38           O
ATOM   7110  CB  TYR B 752      23.127  -3.408 104.338  1.00 56.74           C
ATOM   7111  CG  TYR B 752      23.494  -2.810 102.992  1.00 56.84           C
ATOM   7112  CD1 TYR B 752      22.607  -1.957 102.329  1.00 56.71           C
ATOM   7113  CD2 TYR B 752      24.712  -3.106 102.369  1.00 57.10           C
ATOM   7114  CE1 TYR B 752      22.924  -1.408 101.088  1.00 56.47           C
ATOM   7115  CE2 TYR B 752      25.041  -2.556 101.129  1.00 57.01           C
ATOM   7116  CZ  TYR B 752      24.141  -1.711 100.496  1.00 56.86           C
ATOM   7117  OH  TYR B 752      24.462  -1.170  99.273  1.00 56.72           O
ATOM   7118  N   ASN B 753      23.336  -2.430 107.419  1.00 56.39           N
ATOM   7119  CA  ASN B 753      22.765  -2.396 108.768  1.00 56.22           C
ATOM   7120  C   ASN B 753      21.921  -1.150 109.040  1.00 56.26           C
ATOM   7121  O   ASN B 753      22.049  -0.142 108.344  1.00 56.10           O
ATOM   7122  CB  ASN B 753      23.871  -2.519 109.821  1.00 56.00           C
ATOM   7123  CG  ASN B 753      24.824  -1.343 109.805  1.00 55.60           C
ATOM   7124  OD1 ASN B 753      24.660  -0.398 110.572  1.00 54.87           O
ATOM   7125  ND2 ASN B 753      25.822  -1.391 108.918  1.00 55.35           N
ATOM   7126  N   SER B 754      21.069  -1.231 110.063  1.00 56.41           N
ATOM   7127  CA  SER B 754      20.231  -0.106 110.479  1.00 56.53           C
ATOM   7128  C   SER B 754      20.116  -0.019 112.007  1.00 56.77           C
ATOM   7129  O   SER B 754      19.758  -0.996 112.664  1.00 56.83           O
ATOM   7130  CB  SER B 754      18.847  -0.210 109.836  1.00 56.40           C
ATOM   7131  OG  SER B 754      18.108   0.984 110.018  1.00 56.22           O
ATOM   7132  N   LEU B 755      20.421   1.156 112.558  1.00 57.02           N
ATOM   7133  CA  LEU B 755      20.419   1.379 114.008  1.00 57.23           C
ATOM   7134  C   LEU B 755      19.213   2.184 114.490  1.00 57.55           C
ATOM   7135  O   LEU B 755      18.723   3.068 113.788  1.00 57.64           O
ATOM   7136  CB  LEU B 755      21.689   2.120 114.435  1.00 57.13           C
ATOM   7137  CG  LEU B 755      23.074   1.488 114.304  1.00 56.88           C
ATOM   7138  CD1 LEU B 755      24.131   2.574 114.389  1.00 56.42           C
ATOM   7139  CD2 LEU B 755      23.306   0.440 115.377  1.00 56.80           C
ATOM   7140  N   GLN B 756      18.754   1.883 115.701  1.00 57.92           N
ATOM   7141  CA  GLN B 756      17.712   2.669 116.361  1.00 58.32           C
ATOM   7142  C   GLN B 756      18.018   2.870 117.847  1.00 58.83           C
ATOM   7143  O   GLN B 756      18.878   2.189 118.411  1.00 58.95           O
ATOM   7144  CB  GLN B 756      16.335   2.016 116.186  1.00 58.21           C
ATOM   7145  CG  GLN B 756      15.635   2.357 114.876  1.00 57.48           C
ATOM   7146  CD  GLN B 756      15.135   3.794 114.818  1.00 56.35           C
ATOM   7147  OE1 GLN B 756      14.191   4.168 115.511  1.00 55.68           O
ATOM   7148  NE2 GLN B 756      15.765   4.603 113.976  1.00 55.89           N
ATOM   7149  N   GLU B 757      17.313   3.812 118.468  1.00 59.34           N
ATOM   7150  CA  GLU B 757      17.431   4.056 119.900  1.00 59.81           C
ATOM   7151  C   GLU B 757      16.196   3.488 120.593  1.00 60.24           C
ATOM   7152  O   GLU B 757      15.075   3.942 120.346  1.00 60.28           O
ATOM   7153  CB  GLU B 757      17.575   5.555 120.168  1.00 59.77           C
ATOM   7154  CG  GLU B 757      18.000   5.912 121.582  1.00 59.87           C
ATOM   7155  CD  GLU B 757      18.594   7.310 121.691  1.00 59.84           C
ATOM   7156  OE1 GLU B 757      18.462   8.112 120.741  1.00 59.98           O
ATOM   7157  OE2 GLU B 757      19.202   7.607 122.737  1.00 59.50           O
ATOM   7158  N   LEU B 758      16.406   2.490 121.452  1.00 60.77           N
ATOM   7159  CA  LEU B 758      15.301   1.778 122.104  1.00 61.20           C
ATOM   7160  C   LEU B 758      14.868   2.397 123.433  1.00 61.45           C
ATOM   7161  O   LEU B 758      13.864   1.984 124.014  1.00 61.53           O
ATOM   7162  CB  LEU B 758      15.644   0.292 122.301  1.00 61.21           C
ATOM   7163  CG  LEU B 758      16.190  -0.545 121.134  1.00 61.35           C
ATOM   7164  CD1 LEU B 758      16.378  -1.988 121.573  1.00 61.47           C
ATOM   7165  CD2 LEU B 758      15.306  -0.481 119.893  1.00 61.11           C
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ATOM   7166  N   GLY B 759      15.617   3.394 123.902  1.00 61.82           N
ATOM   7167  CA  GLY B 759      15.363   4.007 125.203  1.00 62.18           C
ATOM   7168  C   GLY B 759      16.062   3.233 126.304  1.00 62.50           C
ATOM   7169  O   GLY B 759      16.580   2.140 126.063  1.00 62.53           O
ATOM   7170  N   ASN B 760      16.070   3.798 127.513  1.00 62.82           N
ATOM   7171  CA  ASN B 760      16.780   3.221 128.671  1.00 63.15           C
ATOM   7172  C   ASN B 760      18.275   3.006 128.413  1.00 63.30           C
ATOM   7173  O   ASN B 760      18.907   2.147 129.034  1.00 63.37           O
ATOM   7174  CB  ASN B 760      16.128   1.905 129.134  1.00 63.15           C
ATOM   7175  CG  ASN B 760      14.796   2.120 129.831  1.00 63.39           C
ATOM   7176  OD1 ASN B 760      14.666   1.870 131.031  1.00 63.45           O
ATOM   7177  ND2 ASN B 760      13.796   2.580 129.082  1.00 63.36           N
ATOM   7178  N   GLY B 761      18.830   3.795 127.494  1.00 63.48           N
ATOM   7179  CA  GLY B 761      20.204   3.612 127.043  1.00 63.69           C
ATOM   7180  C   GLY B 761      20.404   2.296 126.310  1.00 63.83           C
ATOM   7181  O   GLY B 761      21.493   1.726 126.347  1.00 63.79           O
ATOM   7182  N   GLU B 762      19.347   1.813 125.655  1.00 63.98           N
ATOM   7183  CA  GLU B 762      19.411   0.591 124.846  1.00 64.12           C
ATOM   7184  C   GLU B 762      19.232   0.880 123.362  1.00 64.15           C
ATOM   7185  O   GLU B 762      18.469   1.770 122.984  1.00 64.19           O
ATOM   7186  CB  GLU B 762      18.365  -0.427 125.298  1.00 64.14           C
ATOM   7187  CG  GLU B 762      18.866  -1.419 126.331  1.00 64.25           C
ATOM   7188  CD  GLU B 762      17.976  -2.644 126.447  1.00 64.53           C
ATOM   7189  OE1 GLU B 762      17.154  -2.886 125.536  1.00 64.62           O
ATOM   7190  OE2 GLU B 762      18.103  -3.371 127.452  1.00 64.48           O
ATOM   7191  N   TYR B 763      19.938   0.115 122.531  1.00 64.22           N
ATOM   7192  CA  TYR B 763      19.920   0.301 121.081  1.00 64.20           C
ATOM   7193  C   TYR B 763      19.697  -1.020 120.348  1.00 64.27           C
ATOM   7194  O   TYR B 763      20.063  -2.085 120.848  1.00 64.30           O
ATOM   7195  CB  TYR B 763      21.218   0.968 120.608  1.00 64.12           C
ATOM   7196  CG  TYR B 763      21.621   2.170 121.437  1.00 64.09           C
ATOM   7197  CD1 TYR B 763      22.707   2.108 122.307  1.00 64.05           C
ATOM   7198  CD2 TYR B 763      20.900   3.362 121.367  1.00 64.28           C
ATOM   7199  CE1 TYR B 763      23.074   3.206 123.080  1.00 64.06           C
ATOM   7200  CE2 TYR B 763      21.258   4.465 122.136  1.00 64.42           C
ATOM   7201  CZ  TYR B 763      22.343   4.381 122.988  1.00 64.12           C
ATOM   7202  OH  TYR B 763      22.693   5.472 123.746  1.00 63.98           O
ATOM   7203  N   GLY B 764      19.085  -0.937 119.169  1.00 64.33           N
ATOM   7204  CA  GLY B 764      18.817  -2.112 118.338  1.00 64.42           C
ATOM   7205  C   GLY B 764      19.419  -1.999 116.949  1.00 64.48           C
ATOM   7206  O   GLY B 764      19.555  -0.899 116.408  1.00 64.51           O
ATOM   7207  N   ILE B 765      19.777  -3.141 116.367  1.00 64.53           N
ATOM   7208  CA  ILE B 765      20.397  -3.167 115.041  1.00 64.59           C
ATOM   7209  C   ILE B 765      20.001  -4.384 114.203  1.00 64.79           C
ATOM   7210  O   ILE B 765      20.290  -5.527 114.568  1.00 64.78           O
ATOM   7211  CB  ILE B 765      21.950  -3.038 115.121  1.00 64.56           C
ATOM   7212  CG1 ILE B 765      22.589  -3.210 113.734  1.00 64.43           C
ATOM   7213  CG2 ILE B 765      22.524  -4.023 116.133  1.00 64.50           C
ATOM   7214  CD1 ILE B 765      24.053  -2.817 113.654  1.00 64.40           C
ATOM   7215  N   LEU B 766      19.328  -4.122 113.084  1.00 65.03           N
ATOM   7216  CA  LEU B 766      19.101  -5.138 112.059  1.00 65.20           C
ATOM   7217  C   LEU B 766      20.224  -5.047 111.031  1.00 65.40           C
ATOM   7218  O   LEU B 766      20.543  -3.957 110.547  1.00 65.47           O
ATOM   7219  CB  LEU B 766      17.737  -4.946 111.390  1.00 65.16           C
ATOM   7220  CG  LEU B 766      17.366  -5.866 110.218  1.00 65.21           C
ATOM   7221  CD1 LEU B 766      17.208  -7.322 110.651  1.00 65.18           C
ATOM   7222  CD2 LEU B 766      16.102  -5.368 109.524  1.00 65.21           C
ATOM   7223  N   TYR B 767      20.820  -6.192 110.706  1.00 65.60           N
ATOM   7224  CA  TYR B 767      21.995  -6.227 109.833  1.00 65.85           C
ATOM   7225  C   TYR B 767      22.017  -7.403 108.851  1.00 65.87           C
ATOM   7226  O   TYR B 767      21.142  -8.264 108.883  1.00 65.88           O
ATOM   7227  CB  TYR B 767      23.289  -6.176 110.660  1.00 65.95           C
ATOM   7228  CG  TYR B 767      23.463  -7.297 111.672  1.00 66.30           C
ATOM   7229  CD1 TYR B 767      24.076  -8.501 111.313  1.00 66.37           C
ATOM   7230  CD2 TYR B 767      23.041  -7.142 112.996  1.00 66.34           C
ATOM   7231  CE1 TYR B 767      24.248  -9.528 112.238  1.00 66.42           C
ATOM   7232  CE2 TYR B 767      23.209  -8.163 113.929  1.00 66.35           C
ATOM   7233  CZ  TYR B 767      23.813  -9.353 113.543  1.00 66.49           C
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ATOM   7234  OH  TYR B 767      23.981 -10.369 114.458  1.00 66.48           O
ATOM   7235  N   GLU B 768      23.026  -7.419 107.984  1.00 65.95           N
ATOM   7236  CA  GLU B 768      23.182  -8.449 106.959  1.00 66.09           C
ATOM   7237  C   GLU B 768      24.312  -9.413 107.318  1.00 66.34           C
ATOM   7238  O   GLU B 768      25.435  -8.981 107.596  1.00 66.30           O
ATOM   7239  CB  GLU B 768      23.470  -7.800 105.602  1.00 66.09           C
ATOM   7240  CG  GLU B 768      22.288  -7.077 104.978  1.00 65.78           C
ATOM   7241  CD  GLU B 768      22.523  -6.708 103.524  1.00 65.81           C
ATOM   7242  OE1 GLU B 768      23.671  -6.378 103.162  1.00 65.19           O
ATOM   7243  OE2 GLU B 768      21.555  -6.745 102.738  1.00 65.61           O
ATOM   7244  N   HIS B 769      24.016 -10.714 107.303  1.00 66.63           N
ATOM   7245  CA  HIS B 769      24.998 -11.737 107.685  1.00 66.92           C
ATOM   7246  C   HIS B 769      24.750 -13.100 107.033  1.00 66.98           C
ATOM   7247  O   HIS B 769      23.617 -13.430 106.672  1.00 67.03           O
ATOM   7248  CB  HIS B 769      25.047 -11.885 109.212  1.00 67.04           C
ATOM   7249  CG  HIS B 769      26.175 -12.739 109.698  1.00 67.46           C
ATOM   7250  ND1 HIS B 769      25.996 -14.039 110.120  1.00 68.01           N
ATOM   7251  CD2 HIS B 769      27.501 -12.486 109.811  1.00 67.70           C
ATOM   7252  CE1 HIS B 769      27.161 -14.546 110.483  1.00 68.23           C
ATOM   7253  NE2 HIS B 769      28.091 -13.624 110.303  1.00 67.93           N
ATOM   7254  N   THR B 770      25.823 -13.881 106.898  1.00 67.09           N
ATOM   7255  CA  THR B 770      25.770 -15.231 106.336  1.00 67.24           C
ATOM   7256  C   THR B 770      26.564 -16.236 107.171  1.00 67.28           C
ATOM   7257  O   THR B 770      27.663 -15.937 107.643  1.00 67.17           O
ATOM   7258  CB  THR B 770      26.268 -15.248 104.868  1.00 67.31           C
ATOM   7259  OG1 THR B 770      25.190 -14.885 104.000  1.00 67.62           O
ATOM   7260  CG2 THR B 770      26.796 -16.630 104.451  1.00 67.37           C
ATOM   7261  N   GLU B 771      25.981 -17.421 107.342  1.00 67.36           N
ATOM   7262  CA  GLU B 771      26.638 -18.565 107.977  1.00 67.43           C
ATOM   7263  C   GLU B 771      25.866 -19.844 107.660  1.00 67.44           C
ATOM   7264  O   GLU B 771      24.675 -19.791 107.368  1.00 67.40           O
ATOM   7265  CB  GLU B 771      26.758 -18.370 109.494  1.00 67.47           C
ATOM   7266  CG  GLU B 771      25.434 -18.155 110.227  1.00 67.46           C
ATOM   7267  CD  GLU B 771      25.610 -17.981 111.727  1.00 67.54           C
ATOM   7268  OE1 GLU B 771      26.764 -18.018 112.209  1.00 67.34           O
ATOM   7269  OE2 GLU B 771      24.588 -17.806 112.426  1.00 67.81           O
ATOM   7270  N   LYS B 772      26.547 -20.987 107.727  1.00 67.52           N
ATOM   7271  CA  LYS B 772      25.954 -22.294 107.402  1.00 67.55           C
ATOM   7272  C   LYS B 772      25.457 -22.367 105.949  1.00 67.57           C
ATOM   7273  O   LYS B 772      24.386 -22.923 105.670  1.00 67.62           O
ATOM   7274  CB  LYS B 772      24.831 -22.662 108.388  1.00 67.52           C
ATOM   7275  CG  LYS B 772      25.280 -22.836 109.840  1.00 67.61           C
ATOM   7276  CD  LYS B 772      24.091 -23.050 110.779  1.00 67.59           C
ATOM   7277  CE  LYS B 772      23.268 -21.771 110.957  1.00 67.57           C
ATOM   7278  NZ  LYS B 772      22.052 -21.991 111.784  1.00 67.45           N
ATOM   7279  N   GLY B 773      26.246 -21.798 105.036  1.00 67.52           N
ATOM   7280  CA  GLY B 773      25.943 -21.804 103.602  1.00 67.49           C
ATOM   7281  C   GLY B 773      24.698 -21.030 103.205  1.00 67.49           C
ATOM   7282  O   GLY B 773      24.028 -21.380 102.231  1.00 67.37           O
ATOM   7283  N   GLN B 774      24.393 -19.974 103.957  1.00 67.58           N
ATOM   7284  CA  GLN B 774      23.202 -19.159 103.709  1.00 67.69           C
ATOM   7285  C   GLN B 774      23.357 -18.253 102.483  1.00 67.72           C
ATOM   7286  O   GLN B 774      24.428 -17.686 102.242  1.00 67.66           O
ATOM   7287  CB  GLN B 774      22.824 -18.351 104.956  1.00 67.67           C
ATOM   7288  CG  GLN B 774      22.092 -19.168 106.027  1.00 67.65           C
ATOM   7289  CD  GLN B 774      21.957 -18.439 107.361  1.00 67.65           C
ATOM   7290  OE1 GLN B 774      22.808 -17.629 107.738  1.00 67.84           O
ATOM   7291  NE2 GLN B 774      20.884 -18.735 108.085  1.00 67.41           N
ATOM   7292  N   ASN B 775      22.266 -18.123 101.728  1.00 67.77           N
ATOM   7293  CA  ASN B 775      22.247 -17.447 100.424  1.00 67.84           C
ATOM   7294  C   ASN B 775      22.668 -15.976 100.392  1.00 67.98           C
ATOM   7295  O   ASN B 775      23.041 -15.467  99.330  1.00 68.04           O
ATOM   7296  CB  ASN B 775      20.868 -17.600  99.773  1.00 67.75           C
ATOM   7297  CG  ASN B 775      20.659 -18.969  99.152  1.00 67.52           C
ATOM   7298  OD1 ASN B 775      21.604 -19.733  98.957  1.00 67.27           O
ATOM   7299  ND2 ASN B 775      19.412 -19.280  98.828  1.00 67.59           N
ATOM   7300  N   ALA B 776      22.599 -15.307 101.545  1.00 68.12           N
ATOM   7301  CA  ALA B 776      22.960 -13.885 101.698  1.00 68.25           C
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ATOM   7302  C   ALA B 776      21.870 -12.925 101.214  1.00 68.37           C
ATOM   7303  O   ALA B 776      21.588 -12.843 100.017  1.00 68.27           O
ATOM   7304  CB  ALA B 776      24.313 -13.562 101.038  1.00 68.21           C
ATOM   7305  N   TYR B 777      21.258 -12.198 102.147  1.00 68.60           N
ATOM   7306  CA  TYR B 777      21.594 -12.283 103.568  1.00 68.89           C
ATOM   7307  C   TYR B 777      20.402 -12.754 104.404  1.00 69.29           C
ATOM   7308  O   TYR B 777      19.283 -12.857 103.900  1.00 69.23           O
ATOM   7309  CB  TYR B 777      22.112 -10.934 104.075  1.00 68.75           C
ATOM   7310  CG  TYR B 777      23.424 -10.492 103.458  1.00 68.51           C
ATOM   7311  CD1 TYR B 777      23.450  -9.741 102.282  1.00 68.46           C
ATOM   7312  CD2 TYR B 777      24.640 -10.813 104.056  1.00 68.55           C
ATOM   7313  CE1 TYR B 777      24.655  -9.327 101.715  1.00 68.12           C
ATOM   7314  CE2 TYR B 777      25.850 -10.404 103.498  1.00 68.30           C
ATOM   7315  CZ  TYR B 777      25.849  -9.664 102.330  1.00 68.22           C
ATOM   7316  OH  TYR B 777      27.044  -9.261 101.779  1.00 68.23           O
ATOM   7317  N   THR B 778      20.650 -13.030 105.684  1.00 69.86           N
ATOM   7318  CA  THR B 778      19.631 -13.603 106.568  1.00 70.46           C
ATOM   7319  C   THR B 778      19.027 -12.579 107.535  1.00 70.88           C
ATOM   7320  O   THR B 778      18.070 -12.881 108.246  1.00 70.93           O
ATOM   7321  CB  THR B 778      20.187 -14.835 107.324  1.00 70.40           C
ATOM   7322  OG1 THR B 778      20.727 -15.759 106.374  1.00 70.46           O
ATOM   7323  CG2 THR B 778      19.096 -15.542 108.120  1.00 70.51           C
ATOM   7324  N   LEU B 779      19.590 -11.373 107.547  1.00 71.48           N
ATOM   7325  CA  LEU B 779      19.028 -10.227 108.278  1.00 72.14           C
ATOM   7326  C   LEU B 779      18.638 -10.502 109.732  1.00 72.57           C
ATOM   7327  O   LEU B 779      17.527 -10.954 110.015  1.00 72.58           O
ATOM   7328  CB  LEU B 779      17.848  -9.615 107.510  1.00 72.14           C
ATOM   7329  CG  LEU B 779      18.168  -8.974 106.157  1.00 72.40           C
ATOM   7330  CD1 LEU B 779      16.893  -8.644 105.418  1.00 72.76           C
ATOM   7331  CD2 LEU B 779      19.016  -7.729 106.324  1.00 72.44           C
ATOM   7332  N   SER B 780      19.553 -10.194 110.647  1.00 73.16           N
ATOM   7333  CA  SER B 780      19.392 -10.562 112.053  1.00 73.76           C
ATOM   7334  C   SER B 780      19.389  -9.364 113.002  1.00 74.13           C
ATOM   7335  O   SER B 780      19.986  -8.327 112.708  1.00 74.17           O
ATOM   7336  CB  SER B 780      20.484 -11.555 112.456  1.00 73.75           C
ATOM   7337  OG  SER B 780      20.560 -12.623 111.528  1.00 73.95           O
ATOM   7338  N   PHE B 781      18.720  -9.528 114.143  1.00 74.63           N
ATOM   7339  CA  PHE B 781      18.579  -8.467 115.141  1.00 75.11           C
ATOM   7340  C   PHE B 781      19.447  -8.691 116.380  1.00 75.47           C
ATOM   7341  O   PHE B 781      19.689  -9.832 116.787  1.00 75.51           O
ATOM   7342  CB  PHE B 781      17.109  -8.323 115.550  1.00 75.07           C
ATOM   7343  CG  PHE B 781      16.844  -7.203 116.521  1.00 75.18           C
ATOM   7344  CD1 PHE B 781      16.981  -5.873 116.131  1.00 75.09           C
ATOM   7345  CD2 PHE B 781      16.441  -7.480 117.823  1.00 75.12           C
ATOM   7346  CE1 PHE B 781      16.731  -4.838 117.027  1.00 74.98           C
ATOM   7347  CE2 PHE B 781      16.188  -6.450 118.726  1.00 75.14           C
ATOM   7348  CZ  PHE B 781      16.334  -5.127 118.327  1.00 75.06           C
ATOM   7349  N   ARG B 782      19.916  -7.585 116.958  1.00 75.96           N
ATOM   7350  CA  ARG B 782      20.612  -7.576 118.245  1.00 76.35           C
ATOM   7351  C   ARG B 782      20.209  -6.333 119.043  1.00 76.87           C
ATOM   7352  O   ARG B 782      20.234  -5.211 118.529  1.00 76.91           O
ATOM   7353  CB  ARG B 782      22.134  -7.624 118.060  1.00 76.27           C
ATOM   7354  CG  ARG B 782      22.706  -9.000 117.713  1.00 76.13           C
ATOM   7355  CD  ARG B 782      24.225  -8.948 117.587  1.00 76.05           C
ATOM   7356  NE  ARG B 782      24.795 -10.193 117.073  1.00 75.70           N
ATOM   7357  CZ  ARG B 782      25.310 -11.164 117.824  1.00 75.36           C
ATOM   7358  NH1 ARG B 782      25.338 -11.059 119.147  1.00 74.93           N
ATOM   7359  NH2 ARG B 782      25.800 -12.250 117.244  1.00 75.23           N
ATOM   7360  N   LYS B 783      19.821  -6.553 120.296  1.00 77.48           N
ATOM   7361  CA  LYS B 783      19.429  -5.489 121.216  1.00 78.13           C
ATOM   7362  C   LYS B 783      20.542  -5.332 122.244  1.00 78.59           C
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ATOM   7364  CB  LYS B 783      18.112  -5.873 121.905  1.00 78.09           C
ATOM   7365  CG  LYS B 783      17.927  -5.328 123.317  1.00 78.21           C
ATOM   7366  CD  LYS B 783      17.330  -6.386 124.237  1.00 78.51           C
ATOM   7367  CE  LYS B 783      17.769  -6.171 125.681  1.00 78.49           C
ATOM   7368  NZ  LYS B 783      17.341  -7.280 126.579  1.00 78.50           N
ATOM   7369  N   PHE B 784      20.829  -4.091 122.659  1.00 79.16           N
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ATOM   7370  CA  PHE B 784      21.813  -3.843 123.734  1.00 79.71           C
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ATOM   7372  O   PHE B 784      22.481  -1.667 122.901  1.00 79.92           O
ATOM   7373  CB  PHE B 784      22.992  -4.832 123.617  1.00 79.88           C
ATOM   7374  CG  PHE B 784      23.909  -4.557 122.451  1.00 80.24           C
ATOM   7375  CD1 PHE B 784      25.285  -4.515 122.638  1.00 80.69           C
ATOM   7376  CD2 PHE B 784      23.402  -4.330 121.170  1.00 80.52           C
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ATOM   7383  O   ASN B 785      25.134  -2.797 125.109  1.00 80.55           O
ATOM   7384  CB  ASN B 785      23.290  -0.539 126.910  1.00 80.34           C
ATOM   7385  CG  ASN B 785      23.560  -1.606 127.958  1.00 80.46           C
ATOM   7386  OD1 ASN B 785      24.623  -1.623 128.582  1.00 80.55           O
ATOM   7387  ND2 ASN B 785      22.603  -2.511 128.145  1.00 80.30           N
ATOM   7388  N   TRP B 786      26.152  -0.942 125.768  1.00 80.73           N
ATOM   7389  CA  TRP B 786      26.437   0.479 126.073  1.00 80.95           C
ATOM   7390  C   TRP B 786      27.685   0.383 126.949  1.00 81.12           C
ATOM   7391  O   TRP B 786      28.591   1.215 126.860  1.00 81.16           O
ATOM   7392  CB  TRP B 786      25.349   1.265 126.812  1.00 80.97           C
ATOM   7393  CG  TRP B 786      25.895   2.541 127.417  1.00 81.10           C
ATOM   7394  CD1 TRP B 786      26.165   2.768 128.736  1.00 81.20           C
ATOM   7395  CD2 TRP B 786      26.286   3.737 126.719  1.00 81.33           C
ATOM   7396  NE1 TRP B 786      26.679   4.033 128.907  1.00 81.36           N
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ATOM   7398  CE3 TRP B 786      26.266   4.131 125.372  1.00 81.40           C
ATOM   7399  CZ2 TRP B 786      27.224   5.931 127.351  1.00 81.21           C
ATOM   7400  CZ3 TRP B 786      26.723   5.410 125.039  1.00 81.24           C
ATOM   7401  CH2 TRP B 786      27.192   6.292 126.028  1.00 81.17           C
ATOM   7402  N   ASP B 787      27.702  -0.640 127.808  1.00 81.30           N
ATOM   7403  CA  ASP B 787      28.926  -1.127 128.444  1.00 81.43           C
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ATOM   7405  O   ASP B 787      30.983  -1.862 127.432  1.00 81.48           O
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ATOM   7409  OD2 ASP B 787      26.827  -2.277 131.138  1.00 81.40           O
ATOM   7410  N   PHE B 788      29.048  -2.326 126.357  1.00 81.57           N
ATOM   7411  CA  PHE B 788      29.632  -2.813 125.114  1.00 81.65           C
ATOM   7412  C   PHE B 788      30.368  -1.677 124.400  1.00 81.63           C
ATOM   7413  O   PHE B 788      31.387  -1.902 123.746  1.00 81.61           O
ATOM   7414  CB  PHE B 788      28.516  -3.370 124.226  1.00 81.72           C
ATOM   7415  CG  PHE B 788      28.975  -3.840 122.874  1.00 81.81           C
ATOM   7416  CD1 PHE B 788      29.337  -5.170 122.672  1.00 82.00           C
ATOM   7417  CD2 PHE B 788      29.012  -2.960 121.791  1.00 81.93           C
ATOM   7418  CE1 PHE B 788      29.749  -5.611 121.417  1.00 82.21           C
ATOM   7419  CE2 PHE B 788      29.419  -3.391 120.535  1.00 81.98           C
ATOM   7420  CZ  PHE B 788      29.789  -4.717 120.346  1.00 82.17           C
ATOM   7421  N   LEU B 789      29.839  -0.463 124.539  1.00 81.65           N
ATOM   7422  CA  LEU B 789      30.429   0.731 123.935  1.00 81.66           C
ATOM   7423  C   LEU B 789      31.477   1.392 124.831  1.00 81.65           C
ATOM   7424  O   LEU B 789      32.517   1.842 124.344  1.00 81.63           O
ATOM   7425  CB  LEU B 789      29.334   1.741 123.574  1.00 81.66           C
ATOM   7426  CG  LEU B 789      28.525   1.482 122.300  1.00 81.71           C
ATOM   7427  CD1 LEU B 789      27.137   2.094 122.404  1.00 81.70           C
ATOM   7428  CD2 LEU B 789      29.261   2.006 121.070  1.00 81.72           C
ATOM   7429  N   SER B 790      31.194   1.449 126.132  1.00 81.65           N
ATOM   7430  CA  SER B 790      32.065   2.118 127.101  1.00 81.64           C
ATOM   7431  C   SER B 790      33.285   1.271 127.465  1.00 81.63           C
ATOM   7432  O   SER B 790      34.426   1.713 127.310  1.00 81.66           O
ATOM   7433  CB  SER B 790      31.286   2.483 128.374  1.00 81.67           C
ATOM   7434  OG  SER B 790      30.077   3.162 128.076  1.00 81.64           O
ATOM   7435  N   LYS B 791      33.029   0.053 127.940  1.00 81.59           N
ATOM   7436  CA  LYS B 791      34.065  -0.814 128.497  1.00 81.50           C
ATOM   7437  C   LYS B 791      34.594  -1.792 127.452  1.00 81.41           C
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ATOM   7438  O   LYS B 791      35.550  -1.494 126.738  1.00 81.27           O
ATOM   7439  CB  LYS B 791      33.503  -1.574 129.701  1.00 81.48           C
ATOM   7440  CG  LYS B 791      34.512  -1.890 130.790  1.00 81.53           C
ATOM   7441  CD  LYS B 791      33.801  -2.426 132.019  1.00 81.58           C
ATOM   7442  CE  LYS B 791      34.737  -2.553 133.201  1.00 81.41           C
ATOM   7443  NZ  LYS B 791      33.990  -2.994 134.409  1.00 81.35           N
```

[00230] Such a search can be carried out commericially, for example, by Schrödinger (Schrödinger LLC, Portland, OR, USA) to yield candidate neuraminidase inhibitors that are predicted to bind the neuraminidase active site. Visualization, structural refinement, and docking can be performed using Maestro 7.0, MacroModel 9.0, Prime 1.2, Glide 3.5, and IFD script from Schrödinger, LLC (New York).

EXAMPLE 3 - *The NanA neuraminidase of Streptococcus pneumoniae is involved in biofilm formation*

[00231] **ABSTRACT**

[00232] *Streptococcus pneumoniae* remains a major cause of bacteremia, pneumonia and otitis media despite vaccines and effective antibiotics. The neuraminidase of *S. pneumoniae*, which catalyzes the release of terminal sialic acid residues from glycoconjugates, is involved in host colonization in animal models of infection and can provide a new target to prevent pneumococcal infection. We demonstrate that the *S. pneumoniae* neuraminidase (NanA) cleaves sialic acid and show that it is involved in biofilm formation, indicating an additional role in pathogenesis, and sharing this property with the neuraminidase of *Pseudomonas aeruginosa* even though we show the two enzymes are phylogenetically divergent. Using an *in vitro* model of biofilm formation incorporating human airway epithelial cells, we demonstrate that small molecule inhibitors of NanA block biofilm formation and can provide a new target for preventative therapy. This work highlights the role played by the neuraminidase in pathogenesis and represents an important step in drug development to prevent colonization of the respiratory tract by this important pathogen.

[00233] **INTRODUCTION**

[00234] Neuraminidases are widespread among animals and microorganisms, catalyzing the release of terminal sialic acid residues from glycoconjugates (B51). The best characterized is the influenza neuraminidase, required to facilitate spread of the virus. The influenza neuraminidase is not only a key antigen for the highly successful influenza vaccine,

it is also the target for the drugs zanamivir and oseltamivir, which have been useful to prevent and ameliorate influenza infection (B57). *S. pneumoniae* produces at least three distinct neuraminidases (B41); NanA being the most active and most highly expressed at the transcriptional level (B5, B31) that is conserved in all strains (B21, B24, B41). Production of NanA can be detected *in vivo*, and its expression is upregulated upon interaction with host cells (B27, B39, B46, B59). The pneumococcal neuraminidase modifies host glycoconjugates, including immune defense proteins (B22, B23) and exposes potential binding receptors (B3, B26, B28, B54, B55). Pneumococcal neuraminidase activity also provides a source of carbohydrates for bacterial metabolism, cleaving sugars from the mucosal surface (B8, B23, B61), but whether this significantly contributes to bacterial growth *in vivo* is not clearly established. Several studies have indicated that *nanA* mutants colonize the rodent respiratory tract less efficiently than wild type strains (B31, B40, B52) and vaccination with purified NanA affords some protection against nasopharyngeal colonization and otitis media (B29, B30, B53). However, these differences can be mouse strain and animal model dependent (B6, B13, B22, B23).

[00235] In addition to targeting host glycoconjugates some bacterial neuraminidases have a role in biofilm formation; presumably by targeting sialylated bacterial exopolysaccharides (B47). *S. pneumoniae* biofilms have been characterized (B1, B34, B36) and have been observed directly in the middle ear mucosa from children with chronic otitis media (B15), contributing to the colonization process (36). Of note, expression of *nanA* is upregulated when *S. pneumoniae* is grown under biofilm conditions (39). There is a need for new therapeutic strategies as serotypes not covered by available vaccines are rising in prevalence by genetic recombination and strain replacement, and are increasingly associated with invasive disease (B7, B20, B45, B58). Without being bound by theory, the neuraminidase of *S. pneumoniae* is similarly involved in biofilm formation and sought to identify compounds to inhibit its activity *in vitro*.

[00236] **MATERIALS AND METHODS**

[00237] **Bacterial strains and media**. *S. pneumoniae* strains D39 (B4), D39 *nanA* (B22) and R6 (B18) and R6 *nanA* (B23) were grown on trypticase-soy (TS) agar or broth supplemented with 200U/ml catalase (Worthington) and 1μg/ml of chloramphenicol for *nanA* strains. Plate cultures were grown at 37°C in the presence of carbon dioxide (5%). All chemicals were purchased from Sigma unless otherwise stated.

[00238] **Epithelial cell culture**. Human bronchial epithelial cells, 16HBE14o$^-$ and human airway cells, 1HAEo$^-$ (Originally from D. Gruenert California Pacific Medical Center Research Institute, San Francisco, California, USA), were grown in minimum essential medium with Earle's salts (Cellgro and Gibco respectively) supplemented with 10% fetal bovine serum (Cambrex and Gibco respectively), 100U/ml penicillin and 100ug/ml streptomycin. 16HBE14o$^-$ cells were additionally supplemented with 2 mM glutamine (Invitrogen). Cells were grown at 37°C with 5% CO_2 in a humidified incubator.

[00239] **Neuraminidase assay**. NanA was purified as previously described (B19). Neuraminidase activity of NanA was detected using the fluorogenic substrate 2'-(4-methylumbelliferyl)-α-D-*N*-acetylneuraminic acid (MNN, Sigma). Reactions contained 1.5 mM MNN, 1 nM of NanA in 2.5 mM sodium phosphate buffer (pH 5). Reactions were allowed to incubate for 2 h at 37°C before fluorescence intensity was measured at excitation and emission wavelengths of 360 nm and 465 nm in a Tecan microplate reader (Männedorf, Switzerland). Compounds were obtained from a variety of sources (Otava, Kiev, Ukraine; Interbioscreen, Moscow, Russia; Chembridge San Diego, USA; Maybridge, Cornwell, UK; Sigma, St Louis, USA; Princeton, Princeton, USA; Lifechem, Burlington, Canada; Enamine, Kiev, Ukraine). Neuraminidase assays with oseltamivir were performed using the hydrolyzed version of the compound. Briefly, a mixture of oseltamivir (300 mg) in methanol (10 ml) was added to 5N NaOH (3 ml). The mixture was stirred overnight and evaporated under reduced pressure. The residue was dissolved in 10 ml H_2O and the washed with 5 ml of ethyl acetate. The aqueous solution was acidified with 5N HCl to pH=2-3. Evaporation of water under reduced pressure gave the hydrolyzed product. The structure of the product was confirmed by NMR and MS. Divalent cations were supplied in the form of calcium, magnesium, ferric and copper chloride. All neuraminidase assays were performed at least in triplicate.

[00240] **Quantification of asialoGM1 exposure by flow cytometry**. 16HBE14o$^-$ cells were grown in 24-well plates to confluence and exposed to bacterial supernatants for 3 h followed by three PBS washes. Supernatants were concentrated approximately 30-fold (Amicon Ultra, Millipore) and adjusted for protein quantity. As a control, media alone was also concentrated. Cells were stained with rabbit polyclonal anti aGM1 antibody (Wako) followed by Alexa Fluor 488 donkey anti-rabbit IgG (Molecular Probes). Cells were detached from the plates using 0.02% EGTA in HBSS (Hanks buffered saline solution), fixed with 1%

paraformaldehyde and analyzed on a FACSCalibur using CellQuest software (version 3.3; BD). Data were analyzed using WinMDI (version 2.8, Joseph Trotter).

[00241] **Adherence assay**. Adherence assays were performed using 16HBE14o$^-$ cells. Bacterial strains were grown to mid-log phase, washed with PBS and 0.7-2x10^7 cfu of bacterial cells were added to confluent monolayers in 24-well plates (MOI=30). Bacterial cells were allowed to adhere for 1 h at 37°C before three washes with PBS. Bacteria were dissociated from epithelial cells using TrypLE Express (Gibco) and were serially diluted before plating to determine adherent numbers. The assay was performed with three biological replicates with duplicate technical replicates over two separate experiments.

[00242] **Biofilm assay**. Bacterial strains were grown to mid-log phase before being diluted 1:100 in TS broth and catalase. 100 µl of diluted culture was added in triplicate to 96-well flat bottom tissue culture treated plates (Falcon) and left for 18-24 h at 37°C with 5% CO_2. Plates were read at 600 nm to determine levels of growth before being washed in water. Adherent biofilm-forming cells were then stained with 125 µL of 1% crystal violet for 15 min before two further washes in water and allowed to dry. Bound crystal violet was then suspended in 200 µL of ethanol, shaken for 15 min and read at 540 nm.

[00243] **Biofilm formation after epithelial cell interaction**. Bacterial strains were grown and inoculated onto 1HAEo$^-$ cells as per adherence assay. After the initial PBS washes fresh MEM media was applied before a further 1h incubation. This removal and addition of fresh media was repeated a further four times before detachment of adherent bacteria using TrypLE Express (Gibco). The detached bacteria were then diluted 1:100 in TS broth and catalase and assayed as per the biofilm assay. Samples were repeated four times, each time in sextuplicate using epithelial cells without bacteria as a negative control. When using inhibitors, inhibitors were present during epithelial cell interaction and in microtitre trays for biofilm formation. Inhibition with NANA was performed using 0.2% w/v NANA (Sigma) (B56). Images of crystal violet stained microtitre wells were taken with a standard digital camera. Fluorescence microscopy was performed using a Zeiss Observer Z1 inverted fluorescence microscope with ApoTome (Zeiss) for optical sectioning and AxioVision software (v 4.6.2.0, Zeiss). Microtitre wells were stained using the live/dead BacLight stain from Invitrogen (Carlsbad, CA, USA).

[00244] **Phylogenetic analysis**. Our sampling strategy was aimed at maximizing phylogenetic breadth in order to understand the overall pattern of evolution in the neuraminidase/sialidase gene family. We began with a list of well-known neuraminidases including those from *V. cholerae*, *S. typhimurium*, *C. perfringens*, *S. pneumoniae*, *T. cruzi*, and *P. aeruginosa*. For each sequence we did a standard BLAST search and collected one sequence from each genus in the list of hits that had an e-value score of $1x10^{-5}$ or lower. Duplicates were deleted. We also included sequences that have been included in other prior publications on the evolution of sialidases (B43). A list of sequences and gene identification numbers is included as supplemental information. Sequences were aligned using the ClustalW algorithm as implemented in the program BioEdit using default settings. Sequences were aligned as amino acids and then transposed back to the original nucleotide sequences maintaining the gaps determined by the initial alignment (5394 characters total, 4124 parsimony informative characters with gaps as a fifth state, 3766 parsimony informative characters with gaps as treated as missing).

[00245] A rigorous phylogenetic analysis was undertaken using maximum parsimony (MP) algorithm implemented in PAUP* (B50). 1000 replicates of random addition (RA) was performed followed by the tree branch reconnection (TBR) algorithm using the "multrees" option to save more than one optimal tree if discovered in the search. All characters and state transformations were given equal weight. Terminal gaps were scored as missing data in all analyses. We performed two analyses designating internal gaps as a fifth character state in one and as missing data in the other. Although the trees had many nodes in agreement there were major differences between the structures of the 2 trees. Since gaps can be informative characters (B14, B42) we favor the analysis in which internal gaps are counted as character states. We performed nonparametric bootstrap analyses with 100 iterations consisting of 100 RA replicates followed by TBR to gauge the robustness of the tree.

[00246] **Statistics**. Data significance was determined with a students *t*-test and for multivariant data with ANOVA followed with a post Dunnetti test using GraphPad Prism software.

[00247] **RESULTS**

[00248] ***Biochemical properties of NanA***. To better understand the biochemical properties of NanA and to later facilitiate screening of candidate inhibitory compounds we

established an assay to measure its neuraminidase activity. The biochemical activity of NanA was assayed using the fluorogenic sialic acid derivative 2'-(4-methylumbelliferyl)-α-D-*N*-acetylneuraminic acid (MNN). NanA cleaved the fluorogenic substrate significantly at low nanomolar and even at picomolar concentrations (**FIG. 5A**). The Km of NanA for this substrate is about 1.4 mM, which is generally comparable to the Km values reported for other neuraminidases. The neuraminidase from *Vibrio cholerae* requires divalent cations, specifically calcium to be active (B10, B17). We investigated the effect of adding calcium ions to the reaction and observed that calcium was not essential for NanA activity, but did increase activity of NanA by 70% at a concentration of 1 mM (**FIG. 5B**), a 50% activity increase in the presence of magnesium ions (**FIG. 5B**) and decreased activity in the presence of iron and copper, presumably due to their larger molecular masses (**FIG. 5B**). The presence of either copper or ferric ions decreased activity by 90% or greater at millimolar levels.

[00249] The ability of sialic acids to competitively inhibit NanA activity was also tested. The two sialic acids used, *N*-acetylneuraminic acid (NANA) and 2,3-dehydro-2-deoxy-*N*-acetylneuraminic acid (DANA) were both utilized to obtain co-crystals of NanA (B19). NANA caused 50% inhibition at 600 μM (**FIG. 6**). We observed higher inhibition with the transition state analog DANA compared to NANA. DANA reduced activity by 50% at 200 μM.

[00250] ***Phylogeny of the neuraminidases***. The neuraminidase superfamily is known to be highly divergent (B43, B51). Without being bound by theory, neuraminidases from organisms that infect a common site can have similar functions and hence can be evolutionarily related; which can be useful in the identification of common inhibitors. To better ascertain the evolutionary relatedness of NanA, a phylogenetic analysis of a number bacterial, eukaryotic and viral neuraminidases was conducted (**FIG. 4**). NanA clustered closely to the large neuraminidase of *C. perfringens* (B38) and was more closely related to well characterized bacterial neuraminidases. NanA did not cluster with the neuraminidase from *Pseudomonas aeruginosa*, which is also involved in respiratory tract colonization.

[00251] ***Biological activity of pneumococcal NanA***. Many lung pathogens, including *S. pneumoniae* and *P. aeruginosa*, bind to the asialylated ganglioside receptor GM1 (aGM1, Galβ1-3GalNAcβ1-4Galβ1-4Glcβ1-1Cer) (B26). Either purified NanA or concentrated supernatant from wild-type *S. pneumoniae* strain D39 but not its isogenic *nanA* mutant exposed aGM1 on the surface of 16HBE14o$^-$ epithelial cells (**FIG. 7**). However, no effect

was observed on bacterial adherence nor was there a growth advantage in the presence of airway epithelial cells.

[00252] ***NanA is involved in biofilm formation***. As *S. pneumoniae nanA* expression is upregulated in lung tissue and in biofilm-growing cells (B39) the contribution of *nanA* to the formation of biofilms was examined (**FIG. 12**). This increase in expression was exploited by initially growing the bacteria on airway epithelial cells over the course of the day (see Materials and Methods). Adherent bacterial cells were then recovered before setting up the standard microtitre biofilm assay. Exposure of *S. pneumoniae* to airway epithelial cells prior to setting up the biofilm assay not only caused a significant increase in biofilm formation, but showed the *nanA* mutant to have significantly reduced capacity to form biofilms. When *S. pneumoniae* did not have previous airway epithelial cell exposure, no difference in biofilm formation was observed between the WT and *nanA* strains, nor was much biofilm formation observed. In an *S. pneumoniae* R6, unencapsulated background, significantly more biofilm was produced and the *nanA* strain was also significantly reduced in its ability to form biofilms (**FIG. 12A**). Consistent with NANA acting as an inhibitor in the neuraminidase assay (**FIG. 6**) adding exogenous NANA to the biofilm assay also resulted in decreased biofilm formation of the wild-type strain (**FIG. 12B**).

[00253] The biofilms produced by R6 were present as even layers of cells on the microtitre plate and the reduction in biofilm observed with the *nanA* mutant was evident as reduced intensity of crystal violet staining (**FIG. 13A**). In the D39 background, after exposure to epithelial cells, the WT strain was seen as more intense crystal violet (CV) staining overall compared to the *nanA* strain (**FIG. 13A**). Macroscopically, the WT strain had regions of intense CV staining seen as clumps. When the D39 biofilms were examined under the microscope (**FIG. 13B**) a lattice arrangement of cells was observed in both WT and *nanA* strains. Regions of concentrated cells were observed with *nanA* but no macro-structures were observed. However in the WT background structures were observed that had significant height (**FIG. 13B-C**). These structures were approximately 70 μm in height, as seen on the 3D reconstruction (**FIG. 13C**). In the *nanA* background only cells on the initial sections were observed attached to the microtitre well (**FIGS. 13B, D**).

[00254] ***Identification of small molecule inhibitors to the neuraminidases***. A virtual library screen was performed (Schrödinger LLC, Portland, OR, USA) (B25, B44) that identified small molecules that were predicted to interact with the active site of the enzyme.

As a control we tested the ability of the influenza neuraminidase inhibitor oseltamivir to inhibit NanA (**FIG. 10**). Oseltamivir had an IC_{50} of 2 mM. A number of compounds identified from this screen showed high degrees of inhibition *in vitro* (**FIG. 14A**). A lead compound, designated XX1 (**FIG. 14D**), with a pyrrolidine-2,3-dione chemical scaffold was found to inhibit NanA over a range of concentrations and in a dose-dependent manner (**FIG. 14B**). An IC_{50} of 28 μM was determined. The inhibition afforded by XX1 to NanA was greater than 7, 20 and 70 times more effective than DANA, NANA and oseltamivir, respectively. At a concentration of 100 μM we observed a significant reduction in biofilm formation with XX1 and at 400 μM the levels of biofilm formation were comparative to the *nanA* strain (**FIG. 14C**). XX1 did not affect growth of planktonic cells.

[00255] DISCUSSION

[00256] For *S. pneumoniae*, the biofilm phenotype is most evident *in vivo* (B15), or as we show, under *in vitro* conditions that favor neuraminidase expression. We were able to demonstrate a difference in biofilm production after growth on human airway cells, which has been shown to induce *nanA* expression (B27, B39, B46) and reduce capsule production (B16). By selecting for organisms on human airway cells, we apparently mimic a *in vivo* process in which encapsulated organisms that are able to avoid mucus entrapment and clearance gradually produce less capsule to facilitate epithelial attachment (B20). This association between capsule expression and biofilm formation was evident with the R6 strain. R6 does not produce capsule and we observed it to produce significant biofilms, with its *nanA* mutant displaying reduced propensity for biofilm formation. This reduced capsule is important in initial airway colonization both from facilitating initial adherence and promoting cell-to-cell interaction for biofilm formation (B20). This is also consistent with other studies that showed cells induced to a biofilm state had greater propensity to cause pneumonia compared to planktonic cells (B39).

[00257] Without being bound by theory, the role of the neuraminidase lies somewhere between the two processes of cluster formation and biofilm maturation (B1). This is based on the fact that the biofilms observed with the wild-type strain resembled those seen in mature biofilms grown under flow conditions (B2) and while the *nanA* strain still had regions of clustered cells it had no large cellular structures. It should be noted that some differences are also to be expected when comparing static and continuous flow systems. Even though the development and composition of biofilms is complex and numerous genes and proteins are

differentially expressed (B1, B34, B39), the high expression of *nanA* in biofilms and subsequent data presented here, indicate a crucial role for this enzyme in biofilm production. A recent study by Trappetti *et al* (B56) demonstrated the role of sialic acid in pneumococcal biofilm formation. Addition of sialic acid and not other sugars resulted in increased biofilm formation as well as increased organisms present in the nasopharynx in a murine model of colonization (B56). NANA at high concentrations inhibits biofilm formation by *S. pneumoniae* by occupying the binding site of NanA. Based on this study and our own work, the liberation of sialic acid residues from the airway epithelium by the action of NanA appears to contribute to biofilm formation by *S. pneumoniae*, and hence would be a desirable target for therapeutic intervention.

[00258] Even though *nanA* is the most highly expressed neuraminidase gene the other neuraminidases of *S. pneumoniae* can contribute to biofilm formation. In the serotype 4 background (TIGR4) *nanB* is involved to a small extent in biofilm formation (B36). It should be noted that a mutation exists in *nanA* in this strain affecting its cell wall attachment. These studies highlighted the important role biofilms play in pathogenesis, establishing a link between biofilm formation and colonization of the murine nasopharynx. Our data are consistent with these observations indicating a reduced capacity to form biofilms is behind the reduced pathogenesis of the neuraminidase (*nanA*) mutant in animal models (B31, B40). Based on this work and others a model for the establishment of infection in the respiratory tract by *S. pneumoniae* can be established. Encapsulated cells reach the mucus layer where the capsule is required to avoid mucous entrapment. NanA is also able to utilize the mucin as a carbon source (B61). Upon reaching the respiratory epithelium capsule expression is down regulated to facilitate intimate attachment. It is at this point that neuraminidase expression is increased and cells begin to establish a biofilm state.

[00259] Another respiratory pathogen, *P. aeruginosa* also produces a neuraminidase (NanPs), important for biofilm formation and pathogenesis in animal models (B47), indicating a conserved role in pathogenesis for the two neuraminidases. Desialylated glyco-lipids provide receptors for many of the common bacterial pulmonary pathogens including both *S. pneumoniae* and *P. aeruginosa* (B26), which bind to the exposed GalNAcβ1-4Gal residues when terminal sialic acid is cleaved. We demonstrated that NanA like *P. aeruginosa* (B47) was capable of exposing this receptor on human airway cells. The neuraminidase activity associated with intact organisms, either *S. pneumoniae* or *P. aeruginosa* (B47) was

not associated with increased bacterial attachment, which is an interesting observation given that the desialylation of airway mucosal cells by the influenza neuraminidase increases susceptibility to secondary infection often caused by *S. pneumoniae* (B33).

[00260] The crystal structures of both NanA and NanPs were recently solved (B19, B60). Structural analysis indicated that while both enzymes had similar overall structure their active sites were remarkably different, indicating differences in substrate specificity and biochemical function (B9, B47). We also observed that both enzymes are phylogenetically distinct, with NanA clustering closer to other well characterized canonical neuraminidases and NanPs located in a phylogenetically diverse branch of the tree. Yet despite their differences in structure, and different substrates, both neuraminidases possess similar functions in pathogenesis.

[00261] The neuraminidase from *Vibrio cholerae* requires divalent cations, specifically calcium, to be active (B10, B17), while we observed an increase in activity in the presence of calcium ions it was not an absolute requirement for activity. This is an analogous observation with the neuraminidase of *P. aeruginosa* (B9). The inhibition we did observe with iron and copper ions is consistent with metal ions inhibiting such enzymes (B17). The increase of activity with calcium can indicat the presence of a calcium binding site as in *V. cholerae* (B10) and *C. perfringens* (B38) although this is not a categorical feature of neuraminidases nor was one identified from the crystal structure (B9, B11, B19, B48, B60). However, the presence of a calcium binding site would not be incongruous given the close phylogenetic relationship between NanA and the other well characterized bacterial neuraminidases.

[00262] New therapeutic strategies needed against *S. pneumoniae* as serotypes not covered by available vaccines are rising in prevalence by genetic recombination and are increasingly associated with invasive disease (B7, B20, B45, B58); in addition, antibiotic resistance amongst *S. pneumoniae* is a growing problem (B32). We identified a number of compounds based on *in silico* docking studies that were significantly more inhibitory than the sialic acids NANA and DANA, and the influenza inhibitor oseltamivir. Many neuraminidases have been crystallized in the presence of the sialic acid DANA (B11, B19, B35, B38) and we subsequently observed it to inhibit the neuraminidase activity of NanA better than NANA. Although the inhibition observed by DANA was not as great as some neuraminidases tested to-date, it is within the observed ranges of inhibition (B12, B48). Our lead compound XX1 was found to inhibit the neuraminidase activity of NanA in the low micromolar range and

also inhibit the organisms ability to form biofilms. Some work has been done looking into inhibition of other bacterial neuraminidases but the most work to date has been with the trypanosome trans-sialidases (B37, B48, B49). Studies to-date have identified trypanosome inhibitors with IC_{50}'s in the range of 100-300 μM, indicating that the studies presented here are already progressing well comparative to the scientific community. We are actively involved in synthesizing XX1 in an attempt to examine its ability to prevent infection *in vivo*.

[00263] Based on structural data, inhibitors developed to the pneumococcal neuraminidase will be organism specific. The NanPs neuraminidase of *P. aeruginosa* has a significantly different active site. The binding pocket of NanA is tight while NanPs has an open conformation that can require different inhibitor structures for effective inhibition (B19). Thus, neuraminidase inhibitor delivery to the lung can be used as a prophylaxis to circumvent bacterial pneumonia post influenza infection and also to at-risk populations.

[00264] Despite biochemical, structural and phylogenetic differences we demonstrate a common role for the neuraminidases of *S. pneumoniae* and *P. aeruginosa* in biofilm formation and the pathogenesis of respiratory tract infection. Due to the importance of biofilms in colonization of *S. pneumoniae* we have begun to identify inhibitors targeting the pneumococcal neuraminidase to prevent infection. This study represents a starting point in the development of a new drug against pneumococcal pneumonia.

[00265] **SUPPORTING INFORMATION**

[00266] ***Accession numbers***. The GenBank (http://www.ncbi.nlm.nih.gov/Entrez/) accession numbers utilized for phylogenetic analysis are: *Verrucomicrobium spinosum* gi|164421336:353068-354225, *Blastopirellula marina* gi|87311313:89394-90503, *Lentisphaera araneosa* gi|149198907:89577-90743, *Propionibacterium acnes* gi|50841496:752060-754375, *Ruminococcus lactaris* gi|197302028:32228-35857, *Erysipelothrix rhusiopathiae* gi|13516389:295-3807, *Pasteurella multocida* gi|15601865:1176085-1179327, *Actinomyces odontolyticus* gi|145845834:308755-310992, *Mannheimia haemolytica* gi|125433996:1-2376, *Haemophilus parasuis* gi|167854877:54475-56886, *Bacteroides fragilis* gi|53711291:4836372-4838006, *Akkermansia muciniphila* gi|187734516:2229943-2231967, *Capnocytophaga canimorsus* gi|194454827:2197-3765, *Parabacteroides distasonis* gi|150006674:3525685-3527310, *Shewanella pealeana* gi|157959830:1838982-1841831, *Flavobacteriales bacterium* gi|88710837:680637-681797,

Rhodopirellula baltica gi|32470666:1724290-1725519, *Opitutaceae bacterium* gi|153892517:3249-4847, *Sassharopolyspora erythraea* gi|134096620:5769332-5771182, *Pseudoalteromonas haloplanktis* gi|77361923:196316-197458, *Chthoniobacter flavus* gi|196231426:66519-67730, *Janibacter sp.* gi|84494251:767782-770736, *Monosiga brevicollis* gi|167534964:1-984, *Strongylocentrotus purpuratus* gi|115616575:1-719, *Planctomyces maris* gi|149177549:10030-11205, *Acinetobacter baumannii* gi|169632029:647539-649371, *Opitutaceae bacterium* gi|153890920:5481-6641, *Danio rerio* gi|148539964:69-1220, *Corynebacterium diptheriae* gi|38232642:512872-515037, *Gemmata obscuriglobus* gi|163804184:63331-64515, *Streptomyces coelicolor* gi|32141095:7255596-7257542, *Takifugu rubripes* gi|148372013:1-87, *V. cholerae* gi|12057212:1933231-1935654, *C. perfringens nanI* gi|18308982:900997-903081, *C. perfringens nanH* gi|18308982:904693-905499, *P. aeruginosa* gi|110227054:3150886-3152202, *C. septicum* gi|40662, *C. sordellii* gi|1710442, *A. viscosus* gi|39254, *Trypanosoma rangeli* gi|2894809, *T. cruzi* gi|162265, *T. cruzi* SAPA (shed-acute-phase-antigen) gi|10943, *Micromonosporta viridifaciens* gi|216782:816-2759, *Arthrobacter ureafaciens* gi|60544840, *Influenzae* A H5N1 gi|108671038, *Macrobdella decora* gi|1353880, *Salmonella typhimurium* gi|16763390:1002088-1003326, *S. pneumoniae* gi|116515308:1522475-1525468, *Arcanobacterium pyogenes* gi|18146340:1026-6239, *Xenopus laevis* gi|148228846:180-1376, *Trichomonas vaginalis* gi|123473002:1-1050, *Rattus norvegicus* gi|71896601:59-1288, *Bos taurus* gi|149676185:61-219, 650-842, 1541-1803, 2490-2672, 2849-3071, 3185-3411, and *Monodelphis domestica* gi|126309689:1-1404.

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B55. **Tong, H. H., M. A. McIver, L. M. Fisher, and T. F. DeMaria.** 1999. Effect of lacto-N-neotetraose, asialoganglioside-GM1 and neuraminidase on adherence of otitis media-associated serotypes of *Streptococcus pneumoniae* to chinchilla tracheal epithelium. Microb Pathog **26:**111-119.

B56. **Trappetti, C., A. Kadioglu, C. Carter, J. Hayre, F. Iannelli, G. Pozzi, P. W. Andrew, and M. R. Oggioni.** 2009. Sialic Acid: A Preventable Signal for Pneumococcal Biofilm Formation, Colonization, and Invasion of the Host. J Infect Dis **199:**1497-1505.

B57. **von Itzstein, M.** 2007. The war against influenza: discovery and development of sialidase inhibitors. Nat Rev Drug Discov **6:**967-974.

B58. **World Health Organisation (WHO).** 2007. Pneumococcal conjugate vaccine for childhood immunization - WHO position paper. Weekly epidemiological record. World Health Organisation.

B59. **Williamson, Y. M., R. Gowrisankar, D. L. Longo, R. Facklam, I. K. Gipson, E. P. Ades, G. M. Carlone, and J. S. Sampson.** 2008. Adherence of nontypeable *Streptococcus pneumoniae* to human conjunctival epithelial cells. Microb Pathog **44:**175-185.

B60. **Xu, G., X. Li, P. W. Andrew, and G. L. Taylor.** 2008. Structure of the catalytic domain of *Streptococcus pneumoniae* sialidase NanA. Acta Cryst. **F64:**772-775.

B61. **Yesilkaya, H., S. Manco, A. Kadioglu, V. S. Terra, and P. W. Andrew.** 2008. The ability to utilize mucin affects the regulation of virulence gene expression in *Streptococcus pneumoniae*. FEMS Microbiol Lett **278:**231-235.

EQUIVALENTS

[00267] Those skilled in the art will recognize, or be able to ascertain, using no more than routine experimentation, numerous equivalents to the specific substances and procedures described herein. Such equivalents are considered to be within the scope of this invention, and are covered by the following claims.

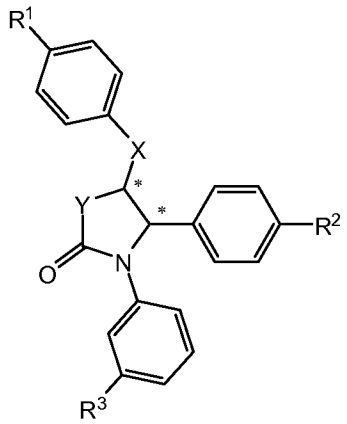
WHAT IS CLAIMED:

1. A method for reducing or inhibiting bacterial biofilm formation, the method comprising contacting a surface with a bacterial neuraminidase inhibitor for a sufficient time so as to modulate bacterial neuraminidase activity, thereby reducing or inhibiting formation of the biofilm.

2. The method of claim 1, wherein the surface comprises a biofilm.

3. The method of claim 1, wherein the biofilm is produced by a bacterium.

4. The method of claim 1, wherein the neuraminidase inhibitor is a compound comprising Formula (I):



(I)

wherein,

R^1 is H, halogen, cyano, azido, nitro, C_1-C_6 alkyl, or C_1-C_6 alkoxy;

R^2 is H, halogen, cyano, azido, nitro, C_1-C_6 alkyl, or C_1-C_6 alkoxy;

R^3 is H, $-CO_2R^4$ or $-CON(R^4)_2$;

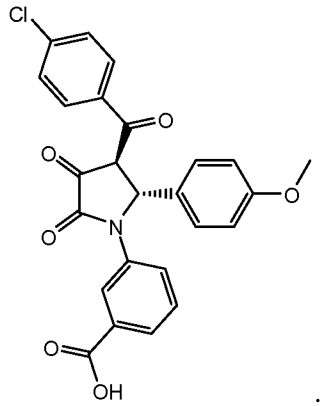
each R^4 is, independently, H or C_1-C_6 alkyl;

X is $-CH_2-$, –(C=O)-, -(C=NH)-, -(C=N-O-C_1-C_6-alkyl)-, or –(C=S)-; and

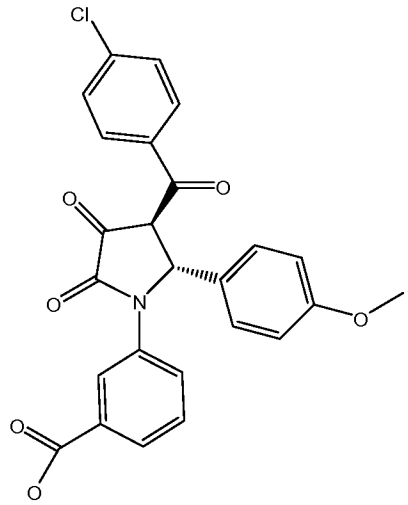
Y is –(C=O)-, -(C=NH)-, -(C=N-O-C_1-C_6-alkyl)-, or –(C=S)-,

or a pharmaceutically acceptable salt or hydrate thereof.

5. The method of claim 1, wherein the neuraminidase inhibitor is a compound comprising Formula (A),



6. The method of claim 1, wherein the neuraminidase inhibitor is a compound comprising Formula (X),



7. The method of claim 1, wherein the neuraminidase inhibitor comprises oseltamivir, peramivir, zanamivir, or a variant thereof.

8. The method of claim 1, wherein the neuraminidase inhibitor is an antibody that specifically binds to the NanA protein of *S. pneumoniae* or a fragment thereof; an antisense RNA or antisense DNA that inhibits expression of a NanA polypeptide; a siRNA that specifically targets a NanA gene, a peptide comprising at least 10 amino acids of SEQ ID NO: 2 wherein the peptide competes with endogenous NanA for ligand binding; or a combination thereof.

9. The method of claim 3, wherein the bacterium is a Gram-negative or Gram-positive bacterium.

10. The method of claim 3, wherein the bacterium is *Pseudomonas*, *Streptococcus, Haemophilus*, *Vibrio*, *Streptococcus pneumoniae*, *Haemophilus influenzae*, or *Vibrio cholerae*.

11. The method of claim 1, wherein the surface comprises a cellular surface of a subject, an oral surface of a subject,or an *in vitro* surface.

12. The method of claim 1, wherein the contacting comprises administering the neuraminidase inhibitor to a subject via subcutaneous, intra-muscular, intra-peritoneal, or intravenous injection; infusion; oral, nasal, or topical delivery; or a combination thereof.

13. The method of claim 11 or 12, wherein the subject is a human, mouse, rat, bird, dog, cat, cow, horse, or pig.

14. The method of claim 1, wherein the surface comprises a prosthetic graft, a catheter, a wound dressing, a wound site, a medical device, a contact lens, an implanted device, an oral device, a pipe, or industrial equipment.

15. The method of claim 1, wherein the contacting comprises applying the neuraminidase inhibitor to a surface of a prosthetic graft, a catheter, a wound dressing, a wound site, or a medical device, and further comprises administering the neuraminidase inhibitor to the subject prior to or during or after the implantation of the prosthetic graft, the implantation of the catheter, the application to the wound site, the application of the wound dressing, or the implantation or insertion of the medical device.

16. The method of claim 14, wherein industrial equipment is found in a GMP facility.

17. The method of claim 14, wherein industrial equipment comprises a plumbing system.

18. The method of claim 1, further comprising administering an effective amount of a therapeutic composition to the subject, the therapeutic composition being different than the neuraminidase inhibitor.

19. The method of claim 18, wherein administering occurs sequentially or simultaneously.

20. The method of claim 18, wherein the therapeutic composition comprises an antibiotic.

21. The method of claim 20, wherein the antibiotic comprises a cephalosporin, a macrolide, a penicillin, a quinolone, a sulfonamide, a tetracycline, or any combination thereof.

22. The method of claim 1, wherein the neuraminidase inhibitor is in a formulation of a paste, a liquid, a powder, a gel, or a tablet.

23. The method of claim 22, wherein the paste formulation further comprises an abrasive.

24. The method of claim 23, wherein the paste formulation is toothpaste.

25. The method of claim 22, wherein the liquid formulation is a mouthwash.

26. A method for treating a biofilm production-related disorder in a subject in need thereof, the method comprising administering to the subject an effective amount of a bacterial neuraminidase inhibitor, thereby treating the biofilm production-related disorder.

27. The method of claim 26, wherein the subject is a human, mouse, rat, bird, dog, cat, cow, horse, or pig.

28. The method of claim 26, wherein the disorder affects an epithelial surface, a mucosal surface, or a combination thereof.

29. The method of claim 28, wherein the surface is a lung surface.

30. The method of claim 26, wherein the biofilm production-related disorder is caused by a bacterium.

31. The method of claim 26, wherein the disorder is pneumonia, cystic fibrosis (CF), otitis media, or chronic obstructive pulmonary disease (COPD).

32. The method of claim 26, wherein the disorder is a medical device-related bacterial infection, the device being implanted or inserted into the subject.

33. The method of claim 30, wherein the bacterium comprises a Gram-negative or Gram-positive bacterium.

34. The method of claim 30, wherein the bacterium comprises *Pseudomonas*, *Streptococcus, Haemophilus*, *Vibrio*, *Streptococcus pneumoniae*, *Haemophilus influenzae*, *Vibrio cholerae*, or a combination thereof.

35. The method of claim 26, wherein the neuraminidase inhibitor is a compound comprising Formula (X), Formula (I), or Formula (A).

36. The method of claim 26, wherein the neuraminidase inhibitor is an antibody that specifically binds to the NanA protein of *S. pneumoniae* or a fragment thereof; an antisense RNA or antisense DNA that inhibits expression of a NanA polypeptide; a siRNA that specifically targets a NanA gene, a peptide comprising at least 10 amino acids of SEQ ID NO: 2 wherein the peptide competes with endogenous NanA for ligand binding; or a combination thereof.

37. A method for identifying a compound that modulates neuraminidase activity, the method comprising:

a) providing an electronic library of test compounds;

b) providing atomic coordinates for at least twenty amino acid residues for the active site of *Streptococcus* neuraminidase listed in Table 2, wherein the coordinates have a root mean square deviation therefrom, with respect to at least 50% of the Cα atoms, of not greater than about 2Å, in a computer readable format;

c) converting the atomic coordinates into electrical signals readable by a computer processor to generate a three dimensional model of the neuraminidase;

d) performing a data processing method, wherein electronic test compounds from the library are superimposed upon the three dimensional model of the neuraminidase; and

e) determining which test compound fits into the binding pocket of the three dimensional model of the neuraminidase,

thereby identifying which compound would modulate the activity of the neuraminidase.

38. A method for identifying a compound that modulates neuraminidase activity, the method comprising:

a) providing an electronic library of test compounds;

b) providing atomic coordinates listed in Table 2 in a computer readable format for at least 5, 6, 7, 8, 9, 10, 11, or 12 amino acid residues located within about 10 Å of the neuraminidase active site, wherein the residues comprise 5 or more of the following residues: Arg347, Arg366, Asp372, Asp417, Ile442, Phe443, Phe565, Tyr590, Gln602, Glu647, Arg663, Tyr695, Tyr752, or Arg 721;

c) converting the atomic coordinates into electrical signals readable by a computer processor to generate a three dimensional model of the neuraminidase active site;

d) performing a data processing method, wherein electronic test compounds from the library are superimposed upon the three dimensional model of the neuraminidase active site; and

e) determining which test compound fits into the binding pocket of the three dimensional model of the neuraminidase active site,

thereby identifying which compound would modulate the activity of the neuraminidase.

39. The method of claim 37 or 38, further comprising:

f) obtaining or synthesizing the compound determined to bind to NanA or modulate the neuraminidase activity;

g) contacting a bacterium with the compound *in vitro*; and

h) determining whether the compound modulates neuraminidase activity using a biological assay.

40. The method of claim 39, wherein the bacterium is a Gram-negative or Gram-positive bacterium.

41. The method of claim 39, wherein the bacterium is *Pseudomonas*, *Streptococcus, Haemophilus*, *Vibrio*, *Streptococcus pneumoniae*, *Haemophilus influenzae*, or *Vibrio cholerae*.

42. The method of claim 39, wherein the biological assay comprises a biofilm assay, an adherence assay, or a combination thereof.

43. A compound identified by the method of claim 37 or 39, wherein the compound binds to the neuraminidase active site, and comes within 10Å of amino acid residues listed in Table 3.

44. The compound of claim 43, wherein the compound inhibits or reduces biofilm formation.

45. The compound of claim 43, wherein the compound is a peptide that binds to a neuraminidase.

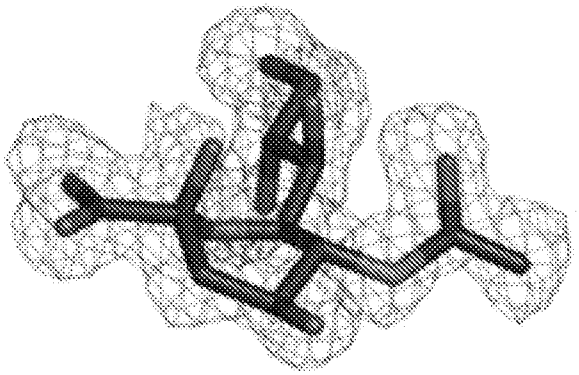
46. The compound of claim 45, wherein the peptide is an anti-neuraminidase antibody or a binding fragment thereof.

47. The compound of claim 45, wherein the peptide interacts with a protein having the amino acid sequence of SEQ ID NO: 2.

48. The compound of claim 45, wherein the compound interacts with a protein having the amino acid sequence of SEQ ID NO: 2.

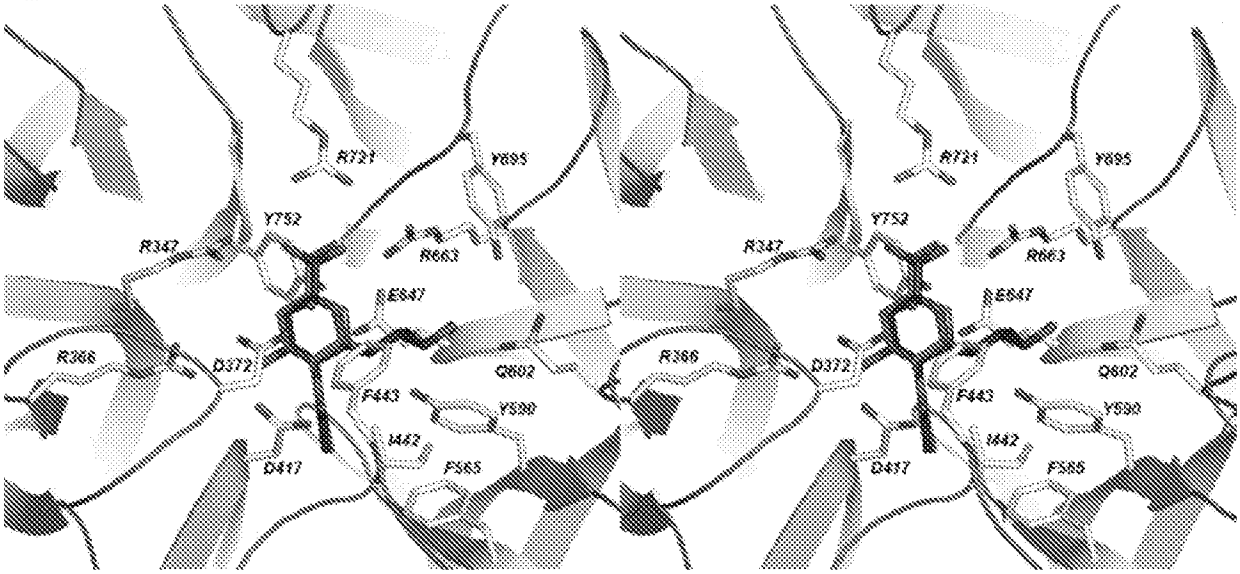
A

B

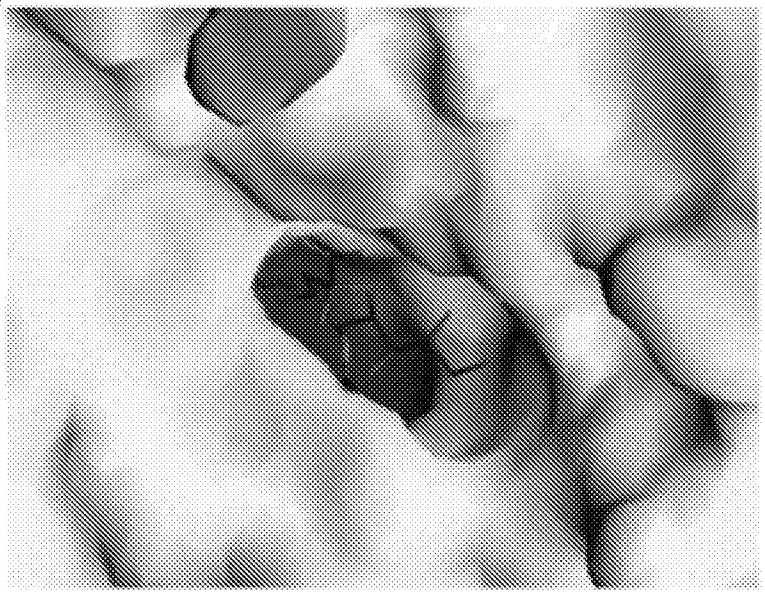


FIGS. 1A-B

C

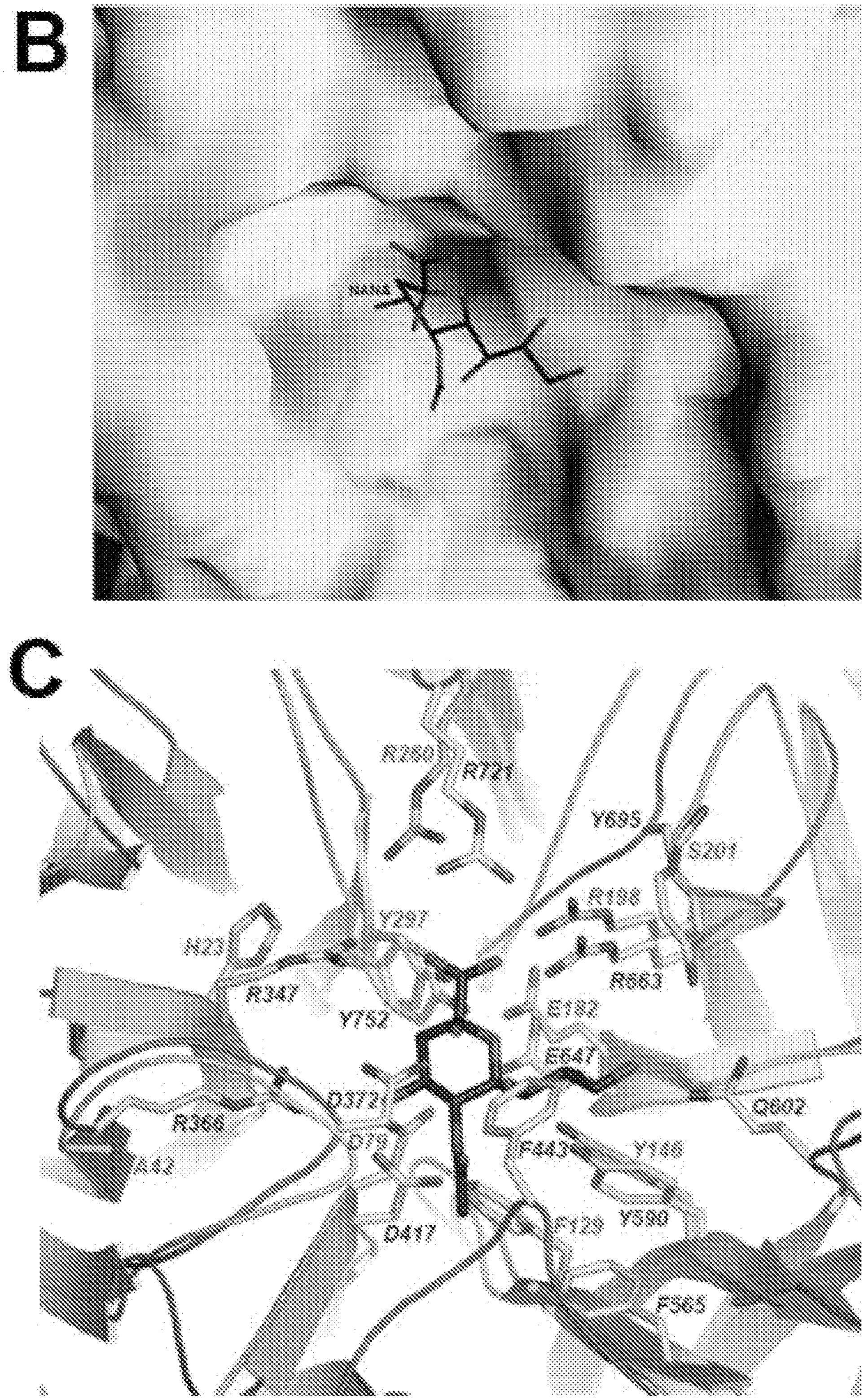

R721
Y895
Y752
R347
R663
E647
R366
D372
Q602
F443
Y530
I442
D417
F565
R721
Y895
Y752
R347
R663
E647
R366
D372
Q602
F443
Y530
I442
D417
F565

D



FIGS. 1C-D

FIG. 2A


B
C
R280
R721
Y695
S201
R198
Y297
H23
R663
R347
Y752
E182
E647
D372
Q802
R368
D79
F443
Y146
A42
D417
F129
Y590
F565

FIGS. 2B-C

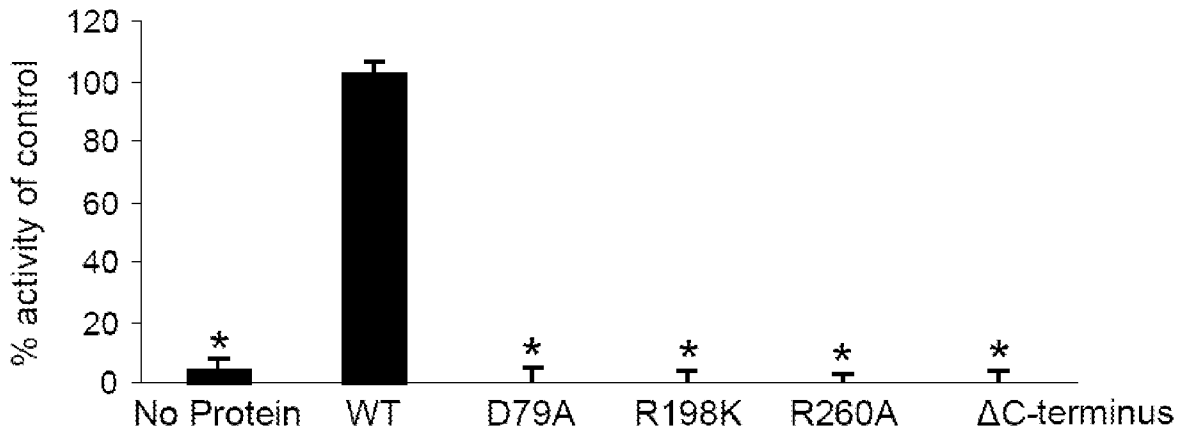

120
100
80
60
40
20
0
% activity of control
*
*
*
*
*
No Protein
WT
D79A
R198K
R260A
ΔC-terminus

FIG. 3

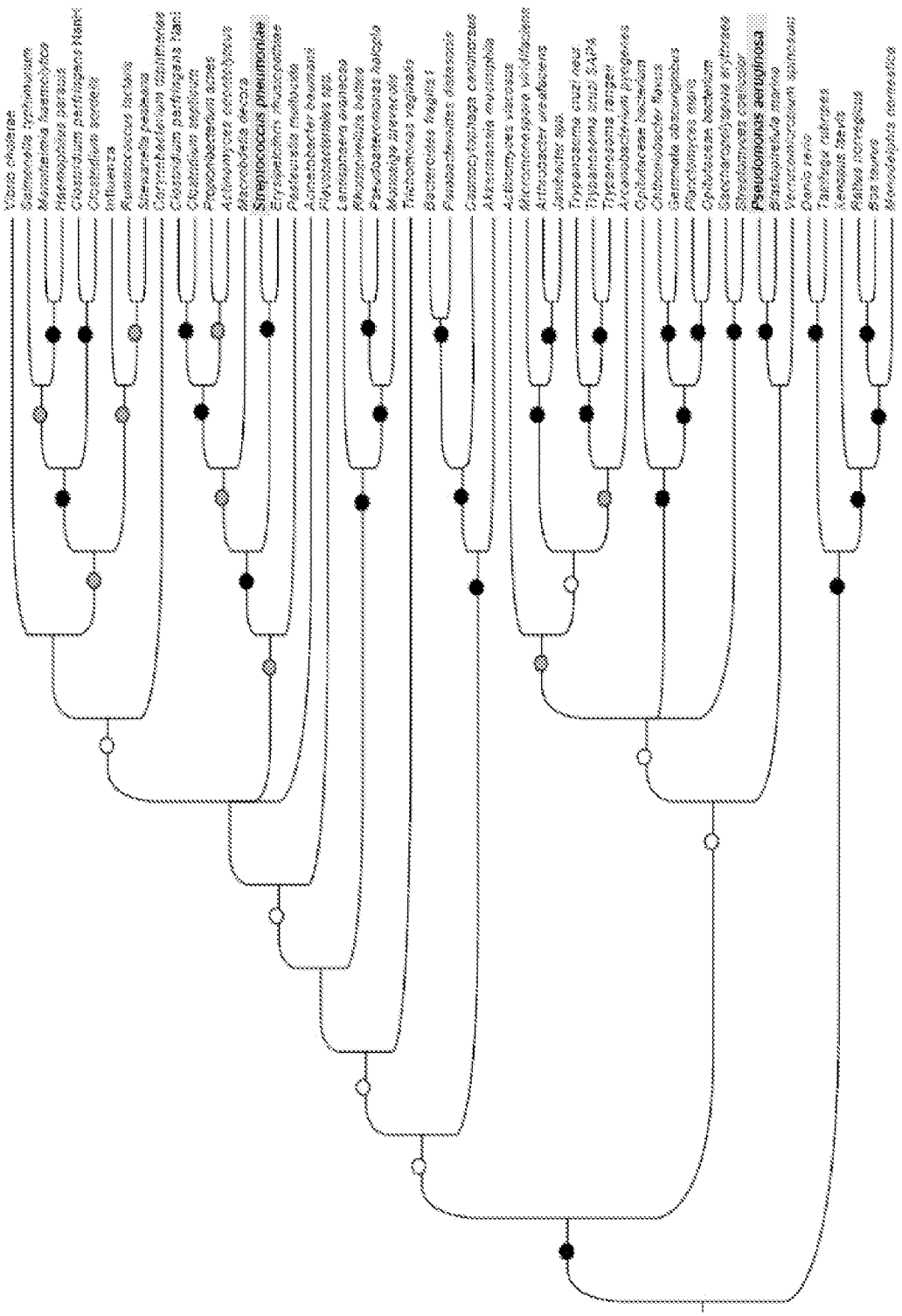

Vibrio cholerae
Salmonella typhimurium
Mannheimia haemolytica
Haemophilus parasuis
Clostridium perfringens Hall
Clostridium tetanii
Influenza
Klebsiella pneumoniae
Shewanella pealeana
Corynebacterium diphtheriae
Clostridium perfringens Yael
Clostridium botulinum
Propionibacterium acnes
Actinomyces odontolyticus
Mycobacteria decora
Streptococcus pneumoniae
Erysipelothrix rhusiopathiae
Pediococcus pentosaceus
Acetobacter aceti
Rhizobiaceae spp.
Leptospirera interrogans
Rickettsiella bellii
Pseudoterconomas halopla
Moraxella atlantae
Trichomonas vaginalis
Bacteroides fragilis
Porphyromonas gingivalis
Cytophaga fermentans
Mycoplasma pneumoniae
Actinomyces viscosus
Micromonospora viridifaciens
Arthrobacter aurescens
Janibacter spp.
Trypanosoma cruzi marinkellei
Trypanosoma cruzi SARA
Trypanosoma brucei
Acanthamoeba polyphaga
Cytophaga bacterium
Orthomobacter flavus
Serratia odorifera biotype
Mycobacteria spp.
Cytophaga bacterium
Saccharopolyspora erythraea
Streptomyces coelicolor
Pseudomonas aeruginosa
Rhodopseudo marina
Verrucomicrobium spinosum
Danio rerio
Takifugu rubripes
Xenopus laevis
Rattus norvegicus
Bos taurus
Monodelphis domestica

FIG. 4

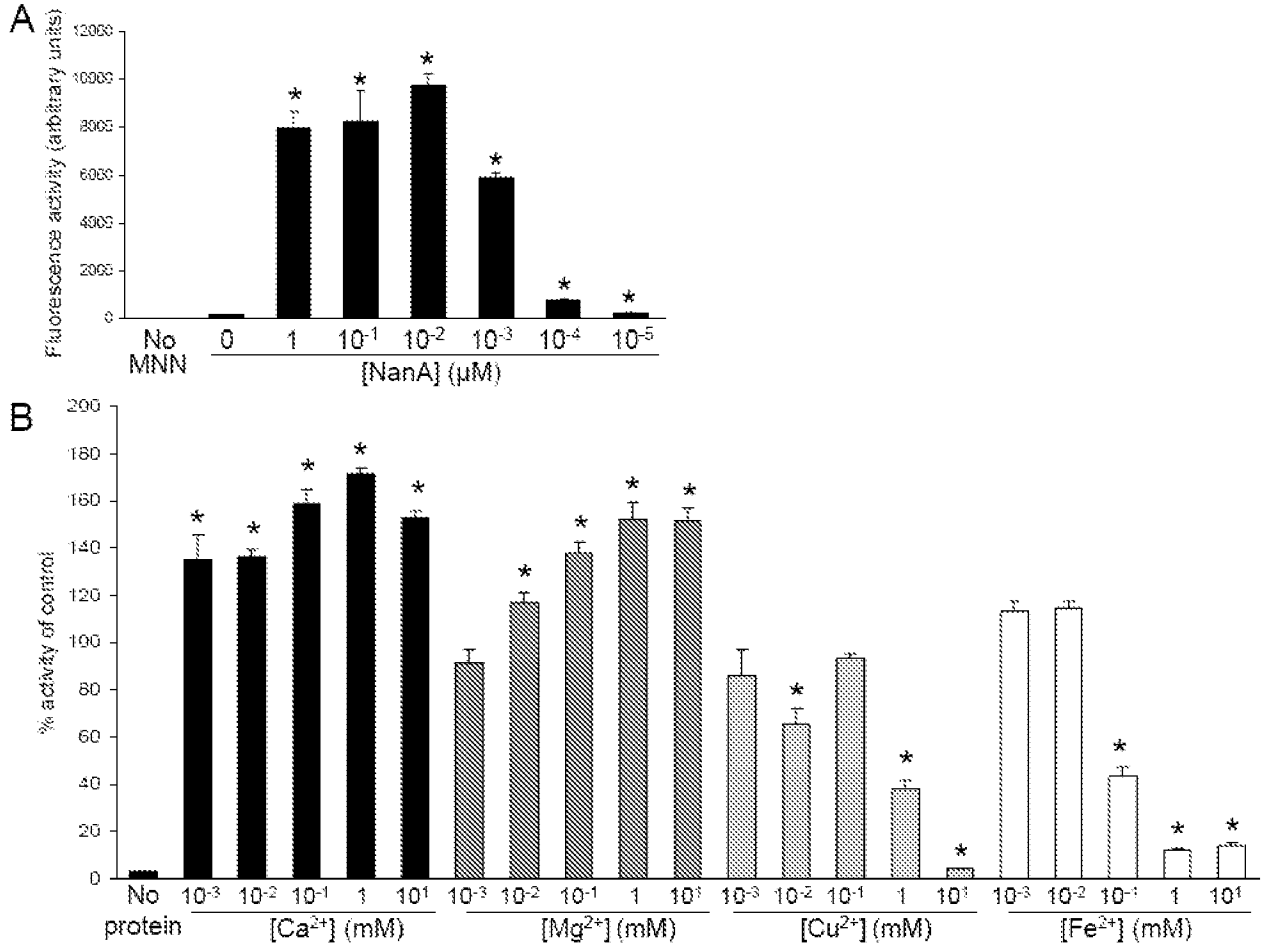

A
Fluorescence activity (arbitrary units)
No MNN
0
1
10-1
10-2
10-3
10-4
10-5
[NanA] (μM)
B
% activity of control
No protein
[Ca2+] (mM)
[Mg2+] (mM)
[Cu2+] (mM)
[Fe2+] (mM)

FIG. 5

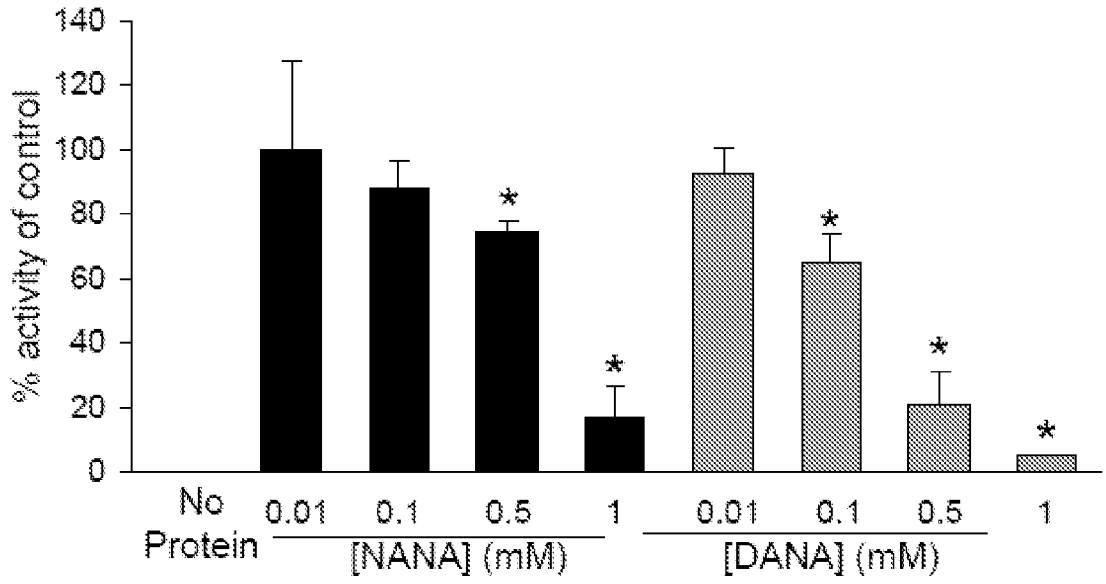

% activity of control
No Protein
0.01
0.1
0.5
1
[NANA] (mM)
[DANA] (mM)

FIG. 6

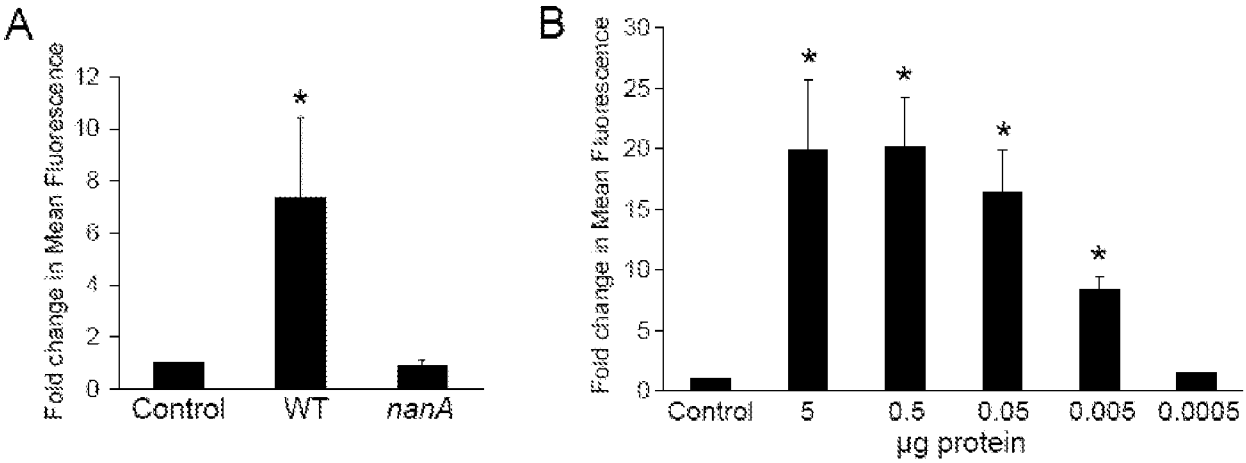

A
Fold change in Mean Fluorescence
12
10
8
6
4
2
0
*
Control
WT
nanA
B
Fold change in Mean Fluorescence
30
25
20
15
10
5
0
*
*
*
*
Control
5
0.5
0.05
0.005
0.0005
µg protein

FIG. 7

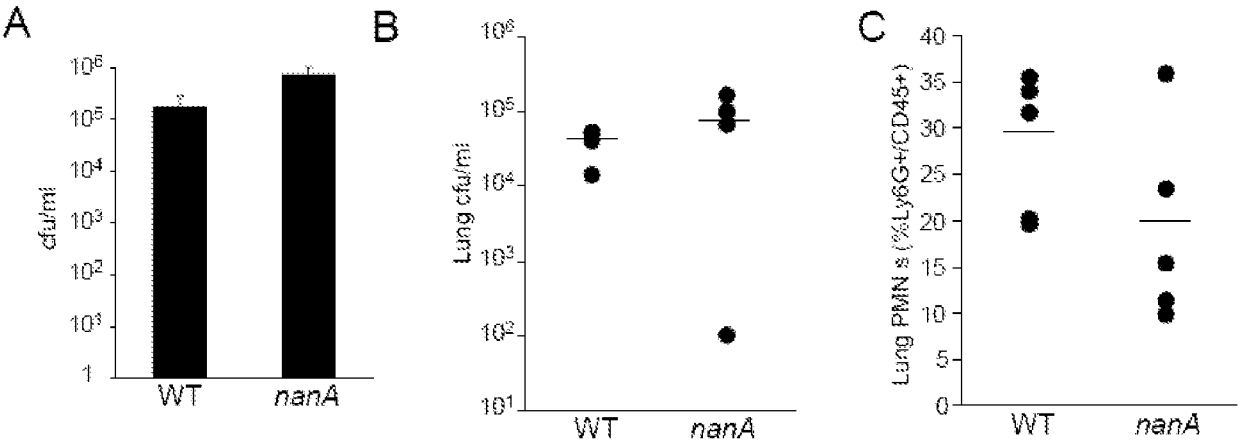

A
cfu/ml
10⁶
10⁵
10⁴
10³
10²
10¹
1
WT
nanA
B
Lung cfu/ml
10⁶
10⁵
10⁴
10³
10²
10¹
WT
nanA
C
Lung PMN s (%Ly6G+/CD45+)
40
35
30
25
20
15
10
5
0
WT
nanA

FIG. 8

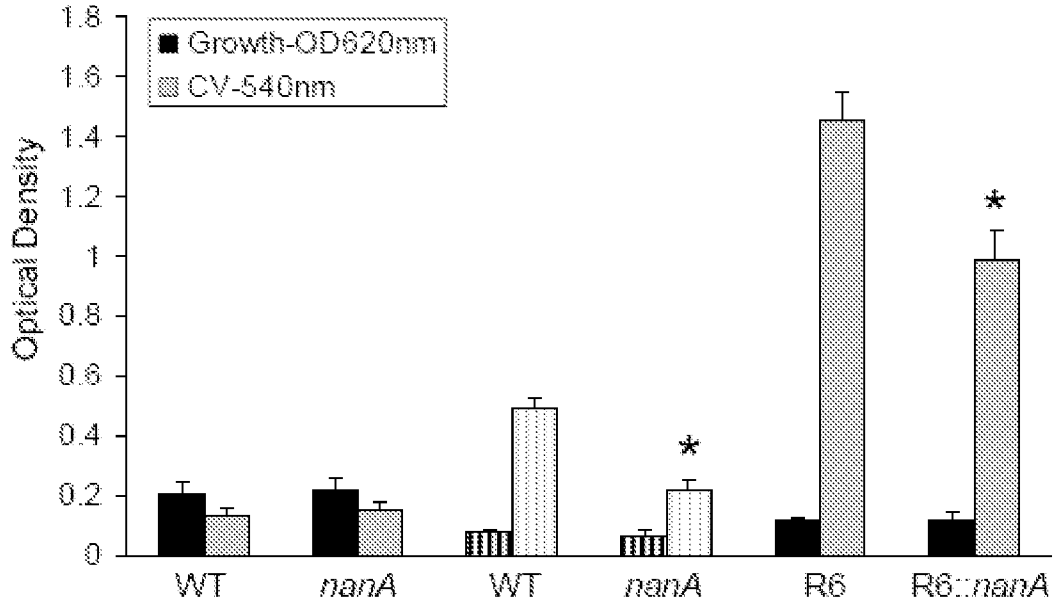

Growth-OD620nm
CV-540nm
Optical Density
1.8
1.6
1.4
1.2
1
0.8
0.6
0.4
0.2
0
WT
nanA
WT
nanA
R6
R6::nanA
*
*

FIG. 9

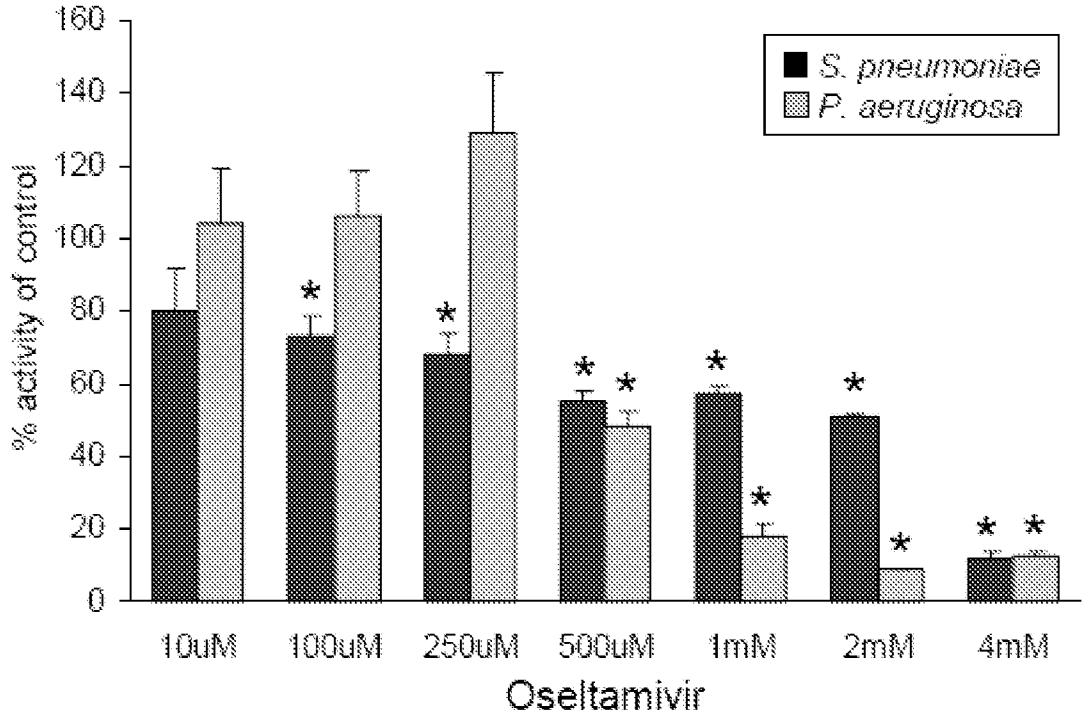

S. pneumoniae
P. aeruginosa
% activity of control
160
140
120
100
80
60
40
20
0
10uM
100uM
250uM
500uM
1mM
2mM
4mM
Oseltamivir
*

FIG. 10

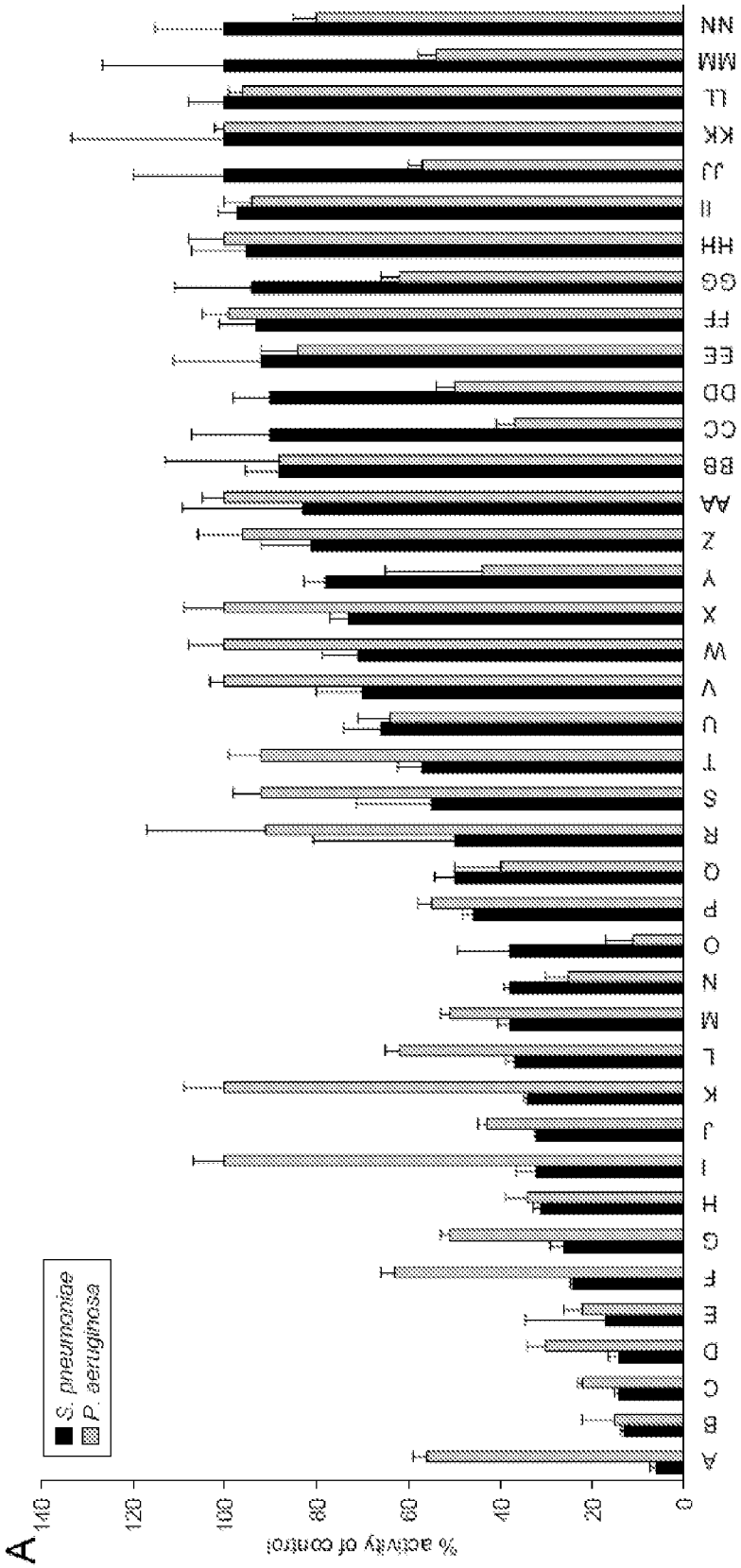
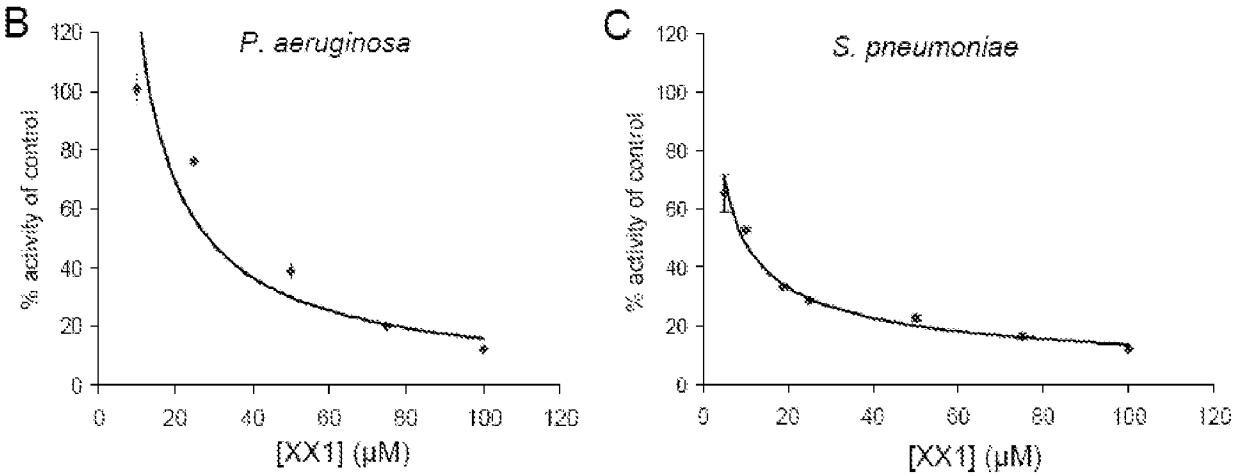

A
% activity of control
0
20
40
60
80
100
120
140
S. pneumoniae
P. aeruginosa
A
B
C
D
E
F
G
H
I
J
K
L
M
N
O
P
Q
R
S
T
U
V
W
X
Y
Z
AA
BB
CC
DD
EE
FF
GG
HH
II
JJ
KK
LL
MM
NN

FIG. 11A



FIGS. 11B-C

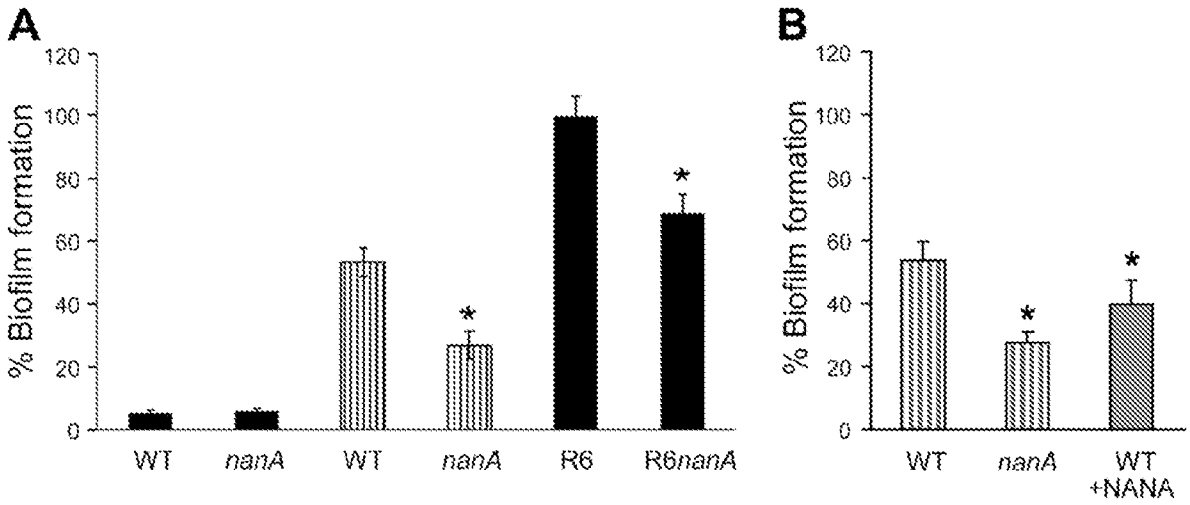
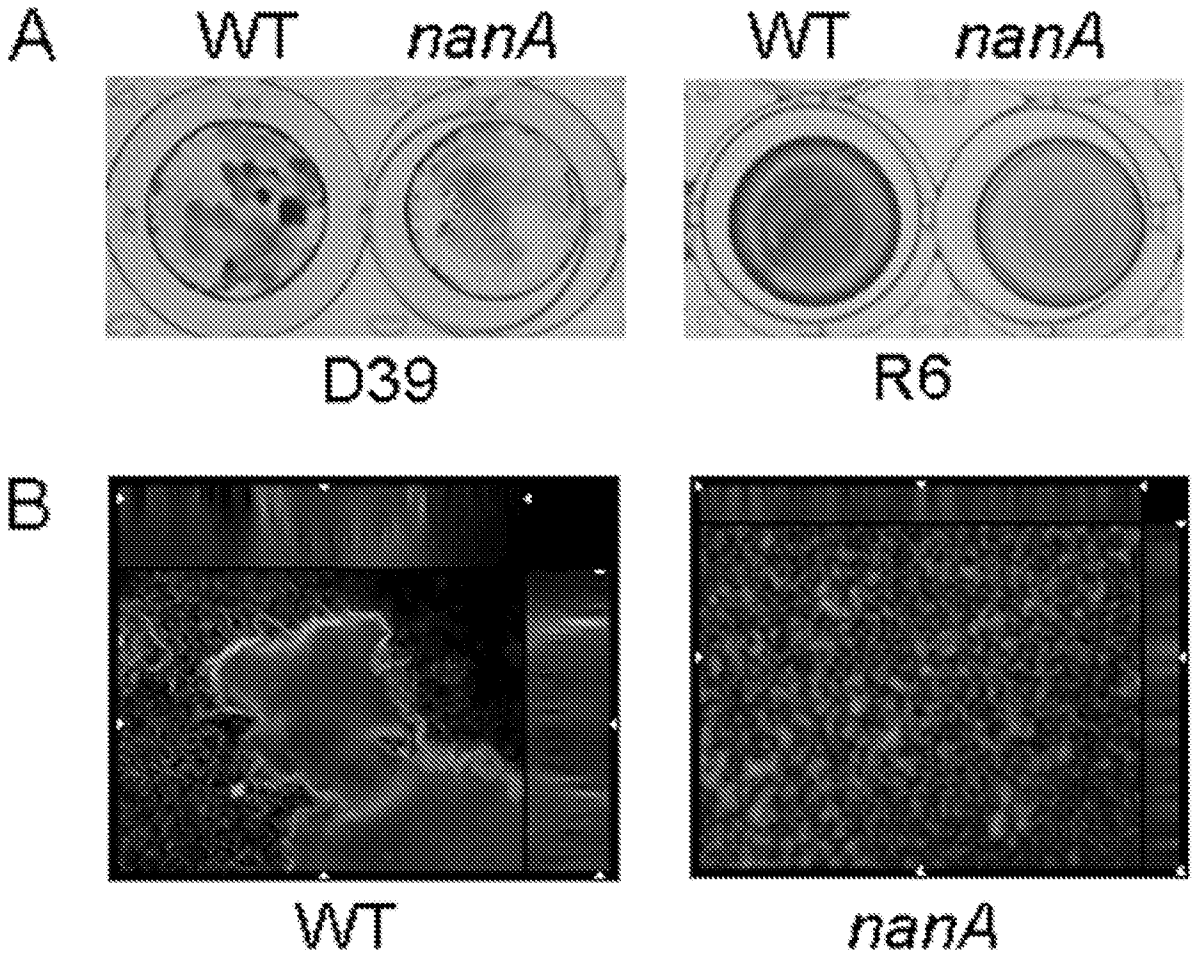
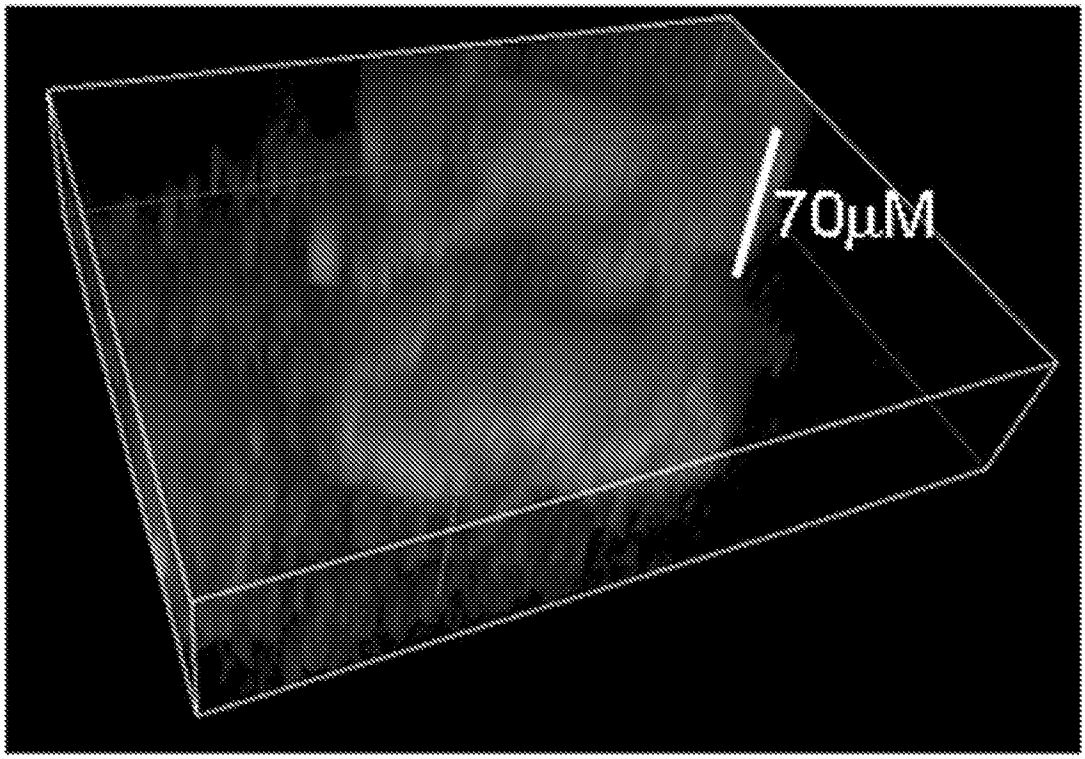


FIG. 12

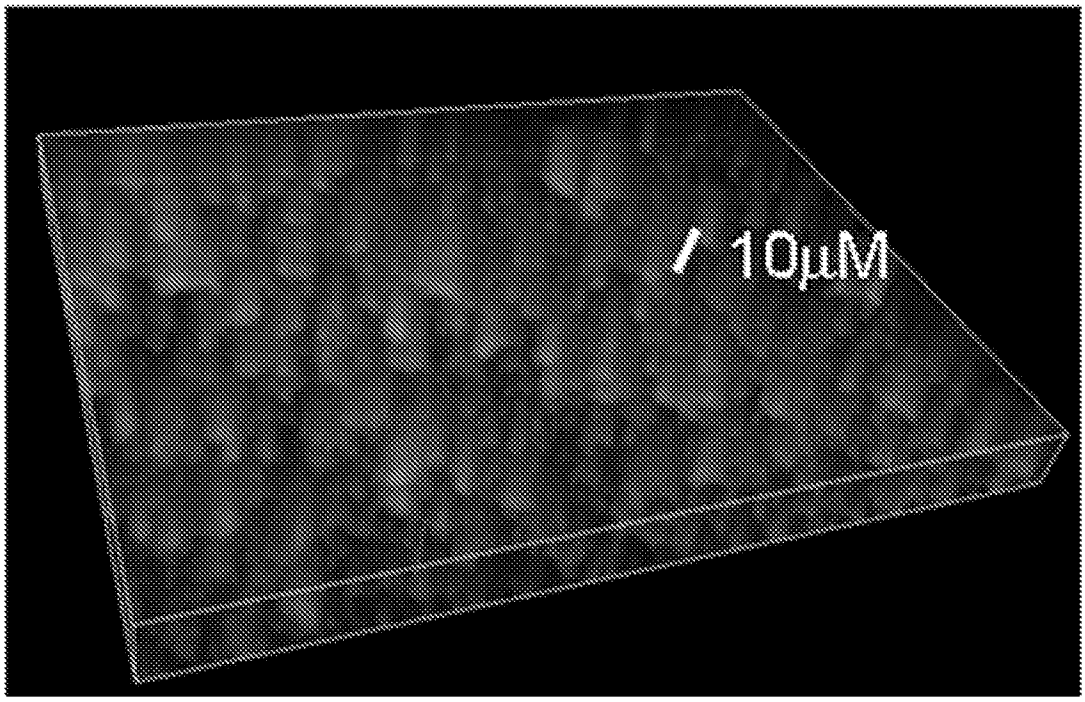


FIGS. 13A-B

C



D



FIGS. 13C-D

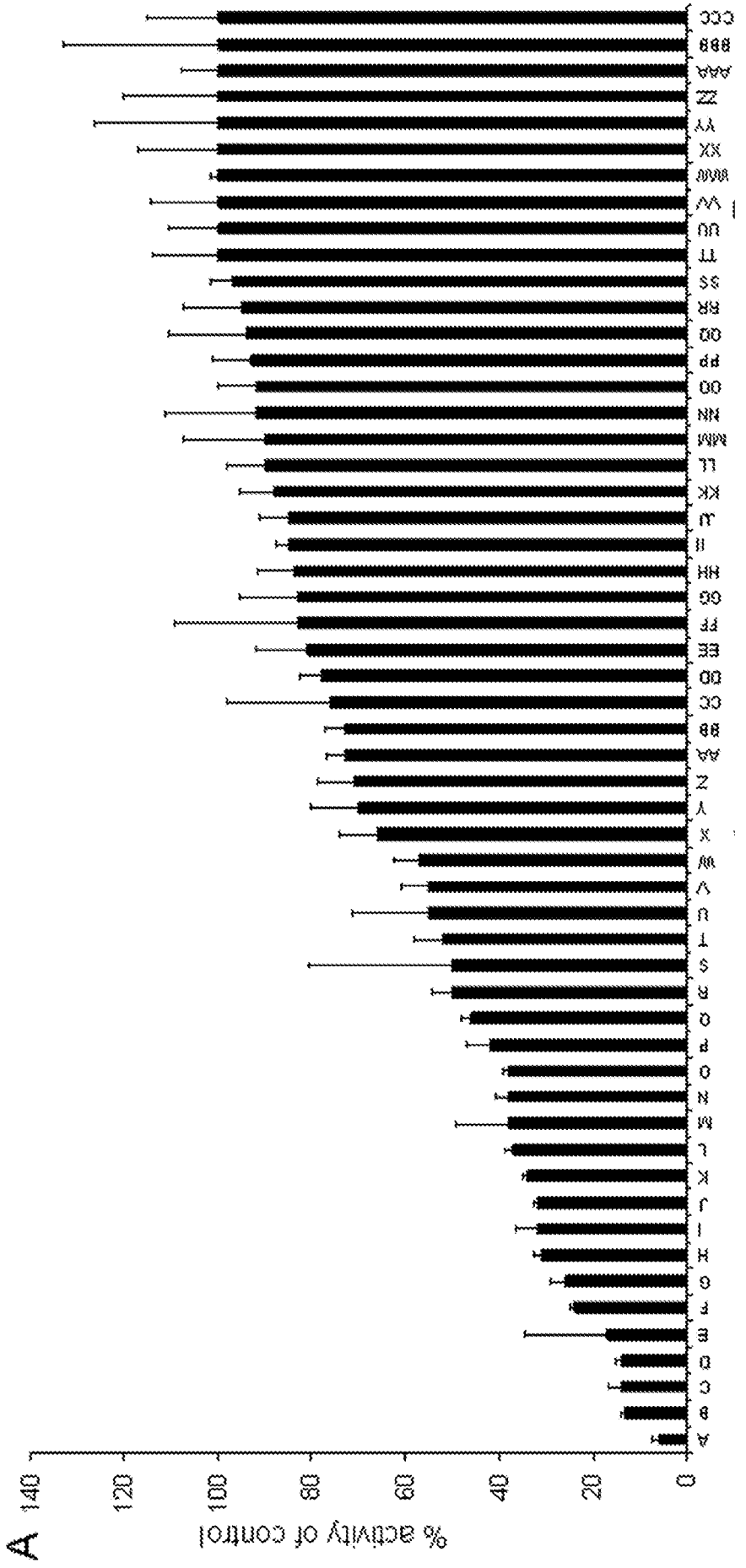
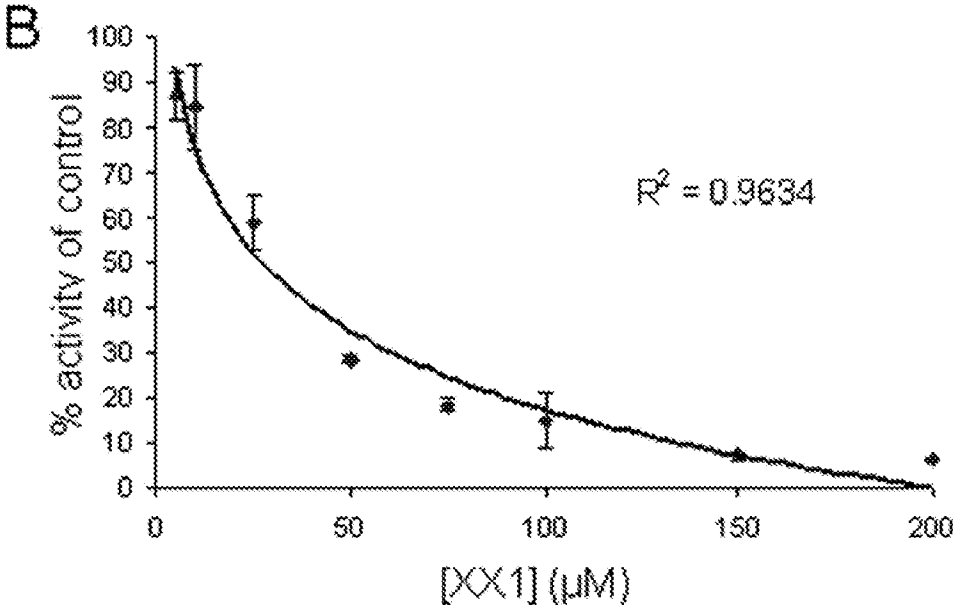
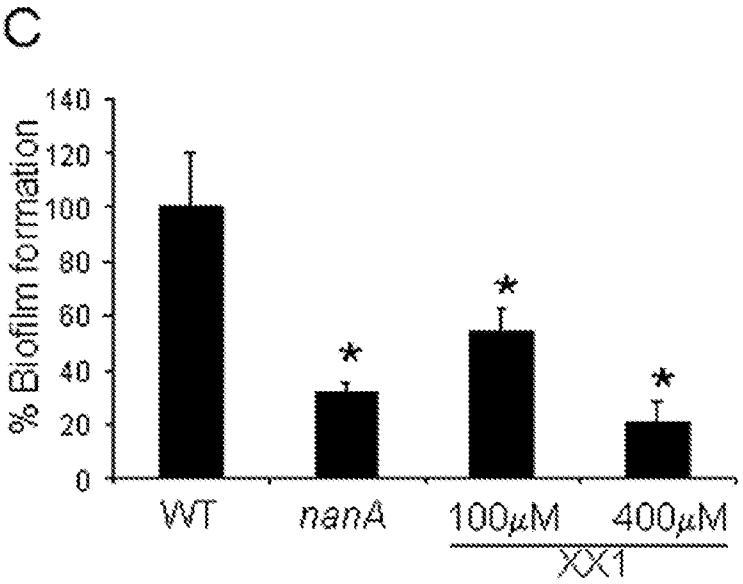
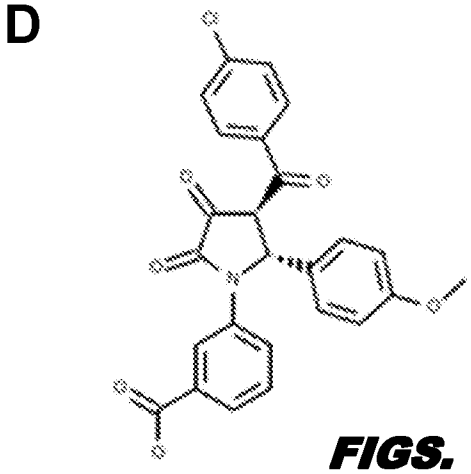

A
% activity of control
0
20
40
60
80
100
120
140
A
B
C
D
E
F
G
H
I
J
K
L
M
N
O
P
Q
R
S
T
U
V
W
X
Y
Z
AA
BB
CC
DD
EE
FF
GG
HH
II
JJ
KK
LL
MM
NN
OO
PP
QQ
RR
SS
TT
UU
VV
WW
XX
YY
ZZ
AAA
BBB
CCC

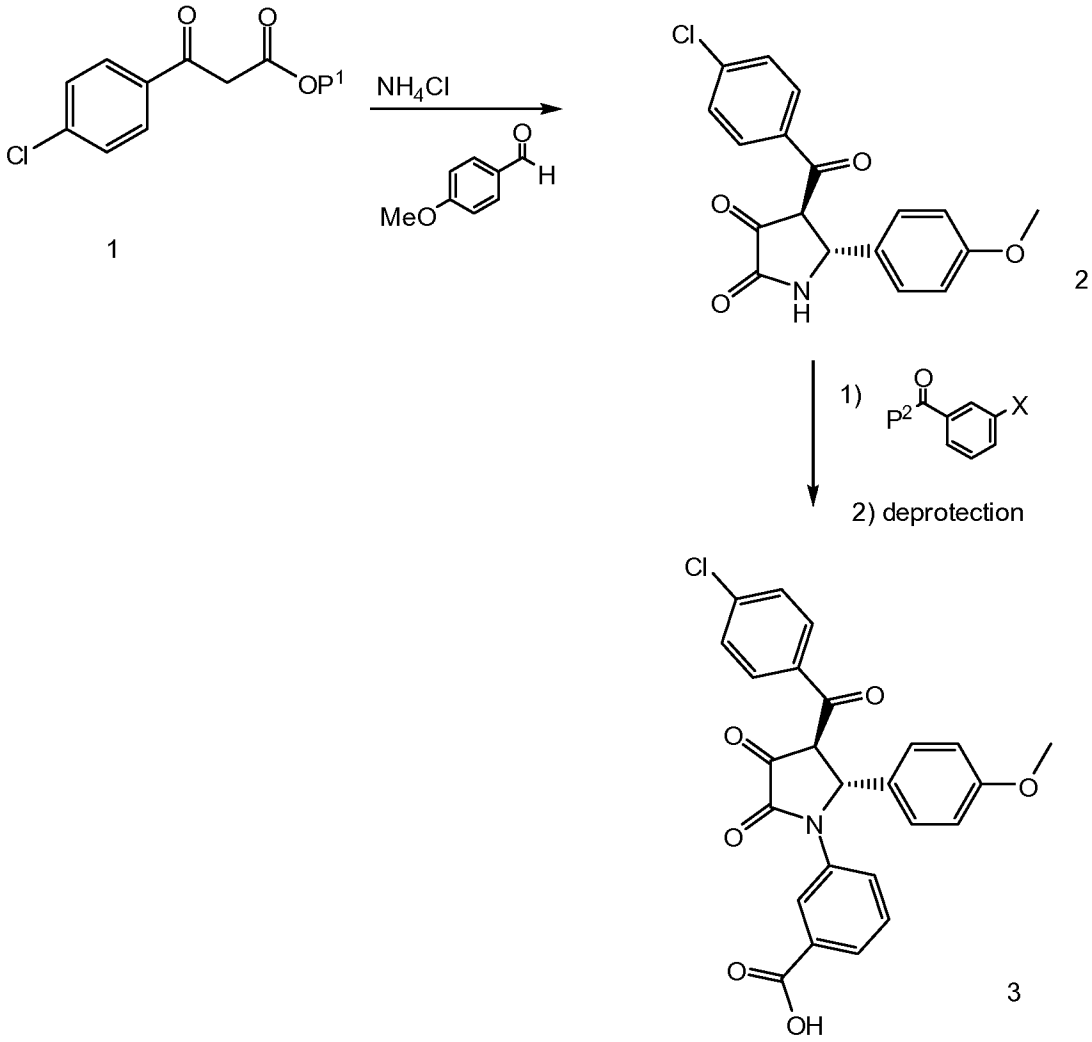
FIG. 14A


B
% activity of control
100
90
80
70
60
50
40
30
20
10
0
0
50
100
150
200
[XX1] (μM)
R^2 = 0.9634


C
% Biofilm formation
140
120
100
80
60
40
20
0
WT
nanA
100μM
400μM
XX1
*
*
*

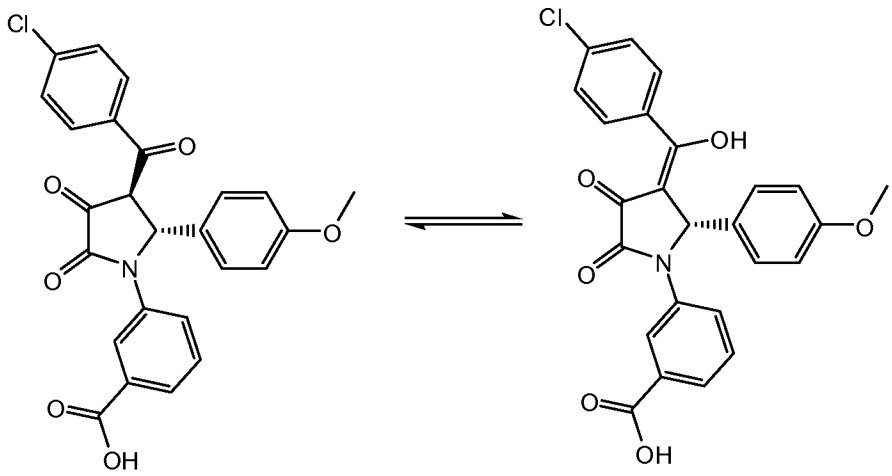

D

FIGS. 14B-D



Scheme 1

FIG. 15



Scheme 2

FIG. 16