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(54) Title: CRYSTAL STRUCTURE OF A BACTERIAL HOMOLOGUE OF NA(+) CL(-)-DEPENDENT NEUROTRANSMITTER TRANSPORTERS

(57) Abstract: The present invention relates to three dimensional structural models of the $LeuT_{Aa}$ transporter, and, in particular, the modeled sites of these proteins. The structural information of the present invention may be used for the rational design of compounds which act as modulators of the $LeuT_{Aa}$ transporter and its eukaryotic counterparts. The present invention further provides for actual or virtual screening assays which may be used to identify compounds having such modulator activities, or to confirm the activity of designed compounds.

CRYSTAL STRUCTURE OF A BACTERIAL HOMOLOGUE OF NA (+) / CL (-) - DEPENDENT NEUROTRANSMITTER TRANSPORTERS

SPECIFICATION

GRANT INFORMATION

Certain subject matter disclosed herein was developed under National Institutes of Health Grant No. RO1MH070039-01A1, so that the United States government has certain rights herein.

1. INTRODUCTION

The present invention relates to three dimensional structural models of the $LeuT_{Aa}$ transporter, and, in particular, the modeled sites of these proteins. It is based, at least in part, on the X-ray crystallographic structures of $LeuT_{Aa}$ transporters. The structural information provides a basis for designing modulators of the activity of the $LeuTA_a$ transporter and its eukaryotic counterparts.

2. BACKGROUND OF THE INVENTION

2.1. NEUROTRANSMITTERS AND NEUROTRANSMITTER RECEPTORS

Communication between cells of the central nervous system (CNS) is controlled by the interactions between neurotransmitters produced by a sending (presynaptic) cell and their receptors in the membrane of a receiving (postsynaptic) cell. This communication is critically dependent on the transmission of nerve impulses through chemical synapses, or junctions. Neurotransmitters such as serotonin, norepinephrine, dopamine, glycine, and GABA (γ-aminobutyric acid) relay electrical signals between neurons at these synapses (Vanhatalo *et al*, 1998). The release of neurotransmitter molecules is triggered by the arrival of an action potential at the cell terminal of the presynaptic cell. Once released, the neurotransmitter can activate receptors in the membrane of the postsynaptic cells. These receptors may be fast acting ligand-gated ion channels, or slower acting G-protein-coupled receptors. After release and receptor activation, the neurotransmitters are actively cleared from the synapse by specific, high-affinity integral membrane transporters located on the presynaptic terminal and surrounding glial cells. This energy-driven re-uptake not only returns synaptic neurotransmitter concentrations to basal levels, but also allows

for the replenishment of presynaptic neurotransmitter stores, making neurotransmitter available for packaging into neurosecretory vesicles (Masson *et al,* 1999).

Na^+ / Cl^- -dependent transporters, also referred to as neurotransmitter sodium symporters (NSS), use sodium and chloride electrochemical gradients to catalyze the thermodynamically uphill movement of a wide array of substrates. These substrates include neurotransmitters such as the biogenic amines (serotonin, dopamine, norepinephrine), amino acids (GABA, glycine, proline, taurine), and osmolytes (betaine, creatine) (Masson *et al,* 1999). NSS members are distinct in terms of amino acid sequence and functional properties from a second major family of plasma membrane neurotransmitter transporters, the high-affinity sodium-dependent glutamate transporters (Masson *et al,* 1999). Prokaryotic organisms possess NSS homologues which have high sequence conservation with eukaryotic, including human, counterparts at functionally important residues, although their overall sequence identity is low. One such homologue from *Aquifex aeolicus* is $LeuTA_a$-

A breakthrough in understanding the structure and function OfNa^+ / Cl^- - dependent transporters occurred when the gene encoding the rat GABA transporter type 1 (GATl), along with other NSS family member genes, was cloned (Guastella *et al,* 1990; Nelson, 1998; Torres *et al,* 2003). Analysis of the predicted amino acid sequences confirmed the existence of 12 transmembrane segments (TMl - TM12), in which the amino and carboxy termini reside in the cytoplasm (Chen *et al,* 1998). Subsequent analysis implicated residues involved in inhibitor recognition, substrate specificity, gating, and ion binding. A number of residues have been identified that are crucial to the function of the transporter. Among these are a strictly conserved tyrosine in TM3 that is indispensable for substrate binding and transport, a negatively charged residue in extracellular loop 5 (EL5) / TMlO that is postulated to comprise part of an external gate, and a position in TMl that is occupied by either an aspartate or glycine. If occupied by aspartate, monoamines are selectively transported, while glycine shifts the transporters selectivity to amino acids (Torres *et al,* 2003; Bismuth *et al,* 1997). Additionally, Sodium:chloride:substrate stoichiometries have also been elaborated and vary from 1:1:1, 2:1:1, to 3:1:1 among different transporters (Rudnick *et al,* 2002; Kavanaugh *et al,* 1992; Roux *et al,* 2000).

Dysfunction of Na^+ / Cl^- - dependent transporters has been associated with multiple disorders including depression, Parkinson's disease, orthostatic intolerance, epilepsy, schizophrenia, Tourette's syndrome, and Lesch-Nyhan

syndrome (Hahn *et al.*, 2002; Richerson *et al.*, 2004). They are also the target of addictive substances such as cocaine and amphetamines, as well as therapeutic agents such as anticonvulsants and the selective serotonergic re-uptake inhibitors (Amara *et al,* 1998; Krogsgaard-Larsen *et al,* 2000; Barker at al., 2000).

2.2. THERAPEUTIC COMPOUNDS FOR MENTAL ILLNESS

Major depression represents one of the most common behavioral or mental illnesses, and is characterized by extreme changes in mood which may also be associated with psychosis. It has generally been found that antidepressant agents with the most significant effect at alleviating symptoms of mental illnesses target the function of Na+/Cl- dependent neurotransmitter transporters.

Na+/Cl- neurotransmitter transporters have been implicated in mental disorders because they act to sequester neurotransmitters, such as serotonin, from the synapse. Many therapeutic compounds developed for the treatment of mental and behavioral disorders are believed to alleviate clinical symptoms by regulating serotonin (5-hydroxytryptamine; 5-HT) function. Monoamine oxidase inhibitors (MAOI) block the enzyme monoamine oxidase (MAO) from metabolizing serotonin, resulting in heightened serotonin levels at synapses. Selective serotonin reuptake inhibitors (SSRIs), such as fluoxetine, and the tricyclic antidepressants (TCAs) block the sequestering of serotonin from the synapse into the surrounding pre-synaptic cells by serotonin transporting Na+/Cl- dependent neurotransmitter transporters. The consequence of each of these typical antidepressants is the prolonged presence of serotonin in the synaptic cleft (Hahn *et al,* 2002).

The Na+/Cl- dependent neurotransmitter transporters are also critical recognition sites for illicit dopaminergic drugs such as cocaine, methamphetamine, and amphetamine. Inhibition of the transporters' function likely mediates the drugs' acute behavioral and reinforcing effects. Both the SSRIs and cocaine operate to enhance the function of neurotransmitter by reducing its removal and reuptake into the surrounding cells from the synaptic cleft (Baldessarini, 1996; Kuhar *et al,* 1991; Ritz *et al,* 1987). By extending the time the transmitter exists in the synapse, the transmitter has a greater opportunity to bind receptors on the post-synaptic target cells and elicit a response.

The current treatments for mental and behavioral illnesses induce side-affects which may dissuade patients from continuing treatment. MAOI use can result in dangerous changes in blood pressure (Keck *et ah,* 1989), while TCAs can cause deadly heart arrhythmias (Bailey *et al.,* 2004) and SSRIs can induce dyspepsia and gastrointestinal disturbances (James *et al.,* 2005). The development of new compounds that bind the Na+/Cl- dependent neurotransmitter transporters more specifically, without causing unwanted side-affects, would be beneficial for treating these mental illnesses.

The success of new antidepressant agents is dependent on their ability to bind the Na+/Cl- dependent neurotransmitter transporter's active site and modulate the movement of neurotransmitter across cell membranes. Knowledge about the structure and identity of residues that comprise the transporter substrate binding sites would help promote the development of compounds that bind the transporter and modulate its activity. These compounds may have therapeutic benefits such as blocking the affects of cocaine by displacing it from transporter binding sites, or alleviating the symptoms of mental disorders such as depression and anxiety. Solving the crystal structure of this transporter would provide insight into the shape, organization, and atomic interactions at the transporter's substrate binding site. This understanding would provide a model on which the structure of new compounds could be designed, allowing for more specific interactions with the transporter and better modulatory function.

Alteration in the function of Na+/Cl- dependent neurotransmitter transporters may play a role in many mental illnesses and neurodegenerative disorders. Perturbation of serotonin function has been implicated in mental disorders such as depression, anxiety disorders, obsessive compulsive disorder, bipolar disorder, and cyclothymia. It has also been shown that changes in serotonin levels can affect many facets of mood, including aggression, sleep, appetite, and pain perception.

Neurodegenerative disorders such as Parkinson's disease, which occurs when dopaminergic cells of the substantia nigra die or become impaired, may also be linked to the function of Na+/Cl- dependent transporter function. Studies show that the expression density of dopamine transporters strongly correlates with the extent of dopaminergic cell loss in Parkinson's disease. Additionally, dopamine transporter gene polymorphisms have been found that are associated with the disease. This

suggests a potential role of the transporter in the pathogenesis of Parkinson's disease (Storch, A., *et ah,* 2004).

Changes in transport of serotonin across cell membranes may also cause the degeneration of synaptic terminals of serotonergic cells. When administered to animals, 3-4 methylenedioxymethamphetamine ("MDMA," also known as "Ecstasy") binds the serotonin transporter, and causes it to function in reverse. This results in a massive dumping of serotonin into the synapse which is believed to be responsible for the drug's neurotoxicity (Green, A. R., *et ah,* 1995).

2.3. X-RAY CRYSTALLOGRAPHY

X-ray crystallography is a powerful technique for determining the atomic structure of compounds, such as biological macromolecules (Hendrickson, 2000), and is a promising tool for drug design. The atomic structures derived from X-ray crystallography not only provide insight into mechanism but may also accelerate the discovery of therapeutic agents (Blundell *et ah,* 2002; Kuhn *et ah,* 2002). For example, the development of anti-human immunodeficiency virus (HIV) drugs for the treatment of AIDS benefited enormously from the atomic resolution structures of the water-soluble proteins HIV protease and HIV reverse transcriptase (Kaldor *et ah, 1997;* Wlodawer and Vondrasek, 1998).

X-ray crystallography involves the bombardment of a crystallized protein or compound with X-rays. Each atom in a crystal scatters X-rays in all directions, but crystalline diffraction is observed only when a crystal is oriented relative to the X-ray beam so that the atomic scattering interferes constructively. The orientations that lead to diffraction may be computed if the wavelength of the X-rays used and the symmetry and dimensions of the crystal's unit cell are known (Blundell *et ah, 191β).* The result is that if a detector is placed behind a crystal that is being irradiated with monochromatic X-rays of an appropriate wavelength, the diffraction pattern recorded will consist of spots, each spot representing one of the orientations that gives rise to constructive interference.

Each spot in such a pattern, however it is recorded, is characterized by (i) an intensity (its blackness); (ii) a location, which encodes the information about diffraction orientation; and (iii) a phase. If these three characteristics are known about each spot in a crystal diffraction pattern, the distribution of electrons in the unit cell of

the crystal may be computed by Fourier transformation (Blundell *et ah,* 1976), and from that distribution or electron density map, atomic positions can be determined

Phase differences between diffracted spots, which cannot be directly measured from the diffraction pattern, may be determined from intensity changes following the introduction of new X-ray scatterers, such as heavy-metals, into the unit cell of the crystal in a process known as multiple isomorphous replacement (MIR). These heavy metals are usually diffused into the channels of the preformed crystal where they can interact with the molecule's exposed side chains. Since such heavy metals contain many more electrons than the light atoms of the protein, the heavy metals scatter X-rays more strongly. AU diffracted beams would therefore increase in intensity after heavy-metal substitution if all interference were positive. However, some interference is negative; consequently, following heavy-metal substitution, some spots increase in intensity, others decrease, and many show no detectable difference. Phase differences between diffracted spots can be determined from intensity changes following heavy-metal substitution.

The amplitudes and the phases of the diffraction data from the protein crystals are used to calculate an electron-density map of the repeating unit of the crystal. This map is then interpreted to accommodate the residues of the molecule of interest. The interpretation is made complex due to differences in phase angles calculation, as well as the quality of the map, which is dependent on the resolution of the diffraction data. The resolution data, in turn, is dependent on how well ordered the crystals are. These limitations directly influence the quality of the map that can be produced. The resolution is measured in angstrom units (A); the smaller this number is, the higher the resolution and, therefore, the greater the amount of detail that can be seen. (For more details see United States Patent Numbers 6,947,845 and 6,952,650; Drenth, J. (1999) Principles of Protein X-ray Crystallography (Springer Advanced Texts in Chemistry), Springer Verlag; Berlin).

2.4. THE LEUT ΛANEUROTRANSMITTER SODIUM SYMPORTER ("LEUTAA" OR"LEUTAA TRANSPORTERS

At the present time there is no structural paradigm for the interpretation of the available data on Na^+ / Cl^- - dependent transporter function. Furthermore, there is no information, at the level of atomic detail, on the molecular principles underlying sodium-ion selectivity, sodium ion - substrate coupling, and

transport mechanism. A better understanding of how transporter structure and function are related would facilitate the development of compounds that can selectively interact with specific transporters. Such knowledge would assist in the development of new drugs and targets for the treatment of mental illness. Thus, there is a need for structural information regarding Na+/Cl- dependent neurotransmitter transporters. Based upon the high sequence conservation of functionally important residues in the NSS homologues found in prokaryotic organisms and eukaryotic organisms, in particular humans, structural information regarding NSS homologues such as $LeuTA_a$ may be useful for the investigation of mental disorders, neurodegenerative diseases, and drug abuse.

3. SUMMARY OF THE INVENTION

The present invention relates to structural models of the $LeuT_{Aa}$ transporter, and in particular, a modeled site of the transporter. It is based, at least in part, on the X-ray crystallographic structure of $LeuT_{Aa}$ when bound to leucine and one or more sodium ions. The X-ray crystallographic structure shows that the protein core consists of the first ten of the twelve transmembrane segments, with segments 1-5 related to 6-10 by a pseudo-two-fold axis in the membrane plane. Leucine and the sodium ions are bound within the protein core, halfway across the membrane bilayer, in an occluded site devoid of water. The leucine and ion binding sites are defined by partially unwound transmembrane helices, with main-chain atoms and helix dipoles having key roles in substrate and ion binding. The structure reveals the architecture of this important class of transporter, illuminates the determinants of substrate binding and ion selectivity, and defines the external and internal gates.

The structural information of the present invention is useful, *inter alia*, for the rational design of compounds which act as modulators of $LeuT_{Aa}$ activity and the activity of its eukaryotic, including human, counterparts. Furthermore, the invention provides for actual as well as virtual screening assays which may be used to identify compounds (for example, members of a combinatorial library) having such modulator activities, or to confirm the activity of designed compounds. In view of the biological importance of eukaryotic, and especially human, counterparts of $LeuT_{Aa}$ in particular, modulators of the activities of these enzymes may be used in the treatment of various diseases and disorders, including, but not limited to mental disorders such

as depression, anxiety disorders, obsessive compulsive disorder, bipolar disorder, cyclothymia, aggression, sleep, appetite, pain perception, neurodegenerative disorders such as Parkinson's disease and Alzheimer's disease, and other diseases such as orthostatic intolerance, epilepsy, schizophrenia, Tourette's syndrome, and Lesch-Nyhan syndrome. The present invention may also be used to design and/or screen metabolic enhancers that may be used to treat the foregoing diseases and disorders.

In one embodiment, the present invention provides the atomic coordinates which define the three-dimensional structure of $LeuT_{Aa}$, or a portion thereof, alone or in complex with a ligand or ligands. In preferred non-limiting embodiments, the atomic coordinates may be derived from X-ray crystallography performed at a resolution of 75 A or less, 50 A or less, 25 A or less, 10 A or less, 5 A or less, 2.5 A or less, or 1.65 A or less.

In further embodiments, the present invention provides for methods of using a computer to identify modulators of $LeuT_{Aa}$ transporter neurotransmitter activity, comprising using a computer-readable three-dimensional model of $LeuT_{Aa}$, or a portion thereof. The three-dimensional model of $LeuT_{Aa}$ may include the binding site(s) of leucine and/or sodium ion or other modeled functional site(s) of the $LeuT_{Aa}$ transporter. Such sites may be modeled individually or in combination.

In still further embodiments the present invention provides for a method of designing or selecting an antagonist or agonist of a $LeuT_{Aa}$ transporter comprising creating a computer model of the negative space present in an unoccupied LeuTAa transporter ligand or substrate binding site or active site, preferably taking into account the electron densities at the boundaries of this space, and using such a model to design or select molecules that modulate the activity of $LeuT_{Aa}$ transporter or another neurotransmitter symporter homologue. Such a negative space, particularly a space presented in the context of electrophilic and electrophobic boundaries, in computer readable, electronic form, stored or storable on a floppy disk or computer hard drive, may provide a simple template for the design and/or selection of enzyme-interactive compounds.

In addition, the present invention provides for a method of evaluating the binding properties of a potential modulator comprising co-crystallizing the potential modulator with a LeuTAa transporter, determining the three-dimensional structure of the modulator bound to the $LeuTA_a$ transporter and analyzing the three-

dimensional structure of the $LeuT_{Aa}$ transporter bound to the modulator to evaluate the structural aspects of binding.

In another embodiment, the present invention provides the atomic coordinates for a $LeuT_{Aa}$ transporter as depicted in FIGURE 1. The present invention also provides for a database in computer readable form containing the atomic coordinates of a $LeuT_{Aa}$ transporter, and a computer displaying the atomic coordinates of a $LeuT_{Aa}$ transporter. In another embodiment, the present invention provides a three dimensional computer model of a $LeuT_{Aa}$ transporter.

In particular non-limiting embodiments, the present invention provides for a three dimensional computer model comprising the coordinates of one or more atom(s) of at least one, at least two, at least three, at least four, at least five, at least six, at least seven, at least eight, at least nine, at least ten, or eleven of the following amino acid residues: G26, L25, Y108, S256, T254, F253, A22, V104, F259, S355, and 1359 (associated with the leucine binding site), preferably having coordinates as set forth in Table 3, or within a root mean square deviation (r.m.s.d.) of the alpha carbon of the residue of at most 8 A, at most 6 A, at most 4 A, or at most 2 A. Alternatively, or in addition, the three dimensional computer model may comprise the coordinates of one or more atom(s) of at least one, at least two, at least three, at least four, at least five, at least six, at least seven, at least eight, or nine of the following amino acid residues: T254, N286, A22, N27, V23, G20, T354, A351, and S355 (associated with the sodium ion binding site), preferably having coordinates as set forth in Table 3, or within a root mean square deviation (r.m.s.d.) of the alpha carbon of the residue of at most 8 A, at most 6 A, at most 4 A, or at most 2 A. Alternatively, or in addition, the three dimensional computer model may comprise the coordinates of one or more atom(s) of at least one, at least two, at least three, at least four, or five of the following amino acid residues: F253, F259, V104, S355, and 1359 (hydrophobic interactions associated with the leucine binding site), preferably having coordinates as set forth in Table 3, or within a root mean square deviation (r.m.s.d.) of the alpha carbon of the residue of at most 8 A, at most 6 A, at most 4 A, or at most 2 A. Alternatively, or in addition, the three dimensional computer model may comprise the coordinates of one or more atom(s) of at least one, at least two, at least three, at least four, or five of the following amino acids: G62, 1262, A261, G260, and G258 (associated with leucine binding, and in particular stabilization of the unwound region of TM6), preferably having coordinates as set forth in Table 3, or within a root mean

square deviation (r.m.s.d.) of the alpha carbon of the residue of at most 8 A, at most 6 A, at most 4 A, or at most 2 A. Alternatively, or in addition, the three dimensional computer model may comprise the coordinates of one or more atom(s) of at least one, at least two, at least three, at least four, at least five, at least six, at least seven, or eight of the following amino acids: F253, T254, E290, Y47, Q250, D404, Y108, and R30 (associated with the extracellular gate), preferably having coordinates as set forth in Table 3, or within a root mean square deviation (r.m.s.d.) of the alpha carbon of the residue of at most 8 A, at most 6 A, at most 4 A, or at most 2 A. Alternatively, or in addition, the three dimensional computer model may comprise the coordinates of one or more atom(s) of at least one, at least two, at least three, at least four, at least five, at least six, at least seven, at least eight, or nine of the following amino acids: R5, Y265, A266, S267, Y268, D369, L14, M16, and A17 (associated with the cytoplasmic gate), preferably having coordinates as set forth in Table 3, or within a root mean square deviation (r.m.s.d.) of the alpha carbon of the residue of at most 8 A, at most 6 A, at most 4 A, or at most 2 A. The three dimensional computer model may also comprise one or more of the twelve transmembrane regions, designated TMl to TMl 2, of the $LeuT_{Aa}$ protein. The transmembrane regions are depicted schematically in FIGURE IB. In particular, the three dimensional computer model may comprise one or more of the following transmembrane regions of the $LeuT_{Aa}$ molecule: TMl or TM6. Alternatively, or in addition, the three dimensional computer model may comprise one or more of the following transmembrane regions of the $LeuT_{Aa}$ molecule: TM2, TM3, TM7, TM8. In each of the foregoing embodiments, it may be desirable to select, as a residue in a modeled site, an amino acid residue which is conserved between LeuTAa and an NSS of a species of interest, such as a human (See Figure 1).

In another embodiment, the present invention provides for a computer-based method for identifying binding affinity of a test molecule to a $LeuT_{Aa}$ transporter or homologues thereof, including eukaryotic, particularly human, homologues, comprising the steps of : a) entering input data characterizing the atomic coordinates of a $LeuT_{Aa}$ transporter, or portions thereof, into a computer program; b) generating a three dimensional computer model of the LeuTAa transporter, or a portion thereof (e.g., a modeled site); c) entering input data characterizing the three dimensional structure of at least one test molecule; d) generating a three dimensional computer model of the test molecule or molecules; e) analyzing the ability of each test molecule to conform to the modeled structure of the modeled site using the computer

program; f) generating a prediction of a relative binding affinity for each test molecule; and g) outputting such prediction.

In yet another embodiment, the present invention provides for a computer-based method of using three-dimensional structure of $LeuTA_a$ or homologues thereof in a drug screening assay comprising: a) performing the above method to identify a test molecule with high binding affinity; b) obtaining the test molecule; c) contacting the test molecule to a $LeuT_{Aa}$ transporter or homologues thereof; and d) detecting the binding of the test molecule with the $LeuT_{Aa}$ transporter; wherein binding of the test molecule to the $LeuT_{Aa}$ transporter indicates that the test molecule is a drug candidate.

In a further embodiment, the present invention provides for a computer-based method for identifying a potential modulator of a $LeuT_{Aa}$ transporter or homologues thereof, comprising the steps of: a) entering input data characterizing the atomic coordinates of a $LeuT_{Aa}$ transporter, or a portion thereof, into a computer program; b) generating a three dimensional computer model of the $LeuT_{Aa}$ transporter, or a portion thereof *(e.g.*, a modeled site); c) entering input data characterizing the three dimensional structure of a potential modulator; d) generating a three dimensional computer model of the potential modulator; e) analyzing the ability of the potential modulator to modulate the modeled structure or modeled site using the computer program; f) generating a prediction of the ability of the potential modulator to modulate the $LeuTA_a$ transporter; and g) outputting such prediction; wherein the ability of the potential modulator, when associated with the modeled structure or modeled site, to alter the conformation of the structure or site, indicates that the potential modulator is an actual modulator, and wherein the nature of the conformational change can be used to predict whether the modulator increases or decreases $LeuT_Aa$ activity. The ability of a potential modulator to increase $LeuT_Aa$ activity indicates that it is an agonist, and the ability of a potential modulator to decrease $LeuT_{Aa}$ activity indicates that it is an antagonist. The method may further comprise an *in vivo* or *in vitro* assay comprising the steps of: a) obtaining the potential modulator; b) contacting the potential modulator to a LeuTAa transporter or a eukaryotic homologue thereof; and c) detecting the ability of the potential modulator to modulate the $LeuT_{Aa}$ transporter homologue; wherein a potential modulator is selected as a drug if the potential modulator modulates the $LeuTA_a$ transporter, wherein the ability of the potential modulator to increase $LeuT_Aa$ activity indicates an

agonist, and the ability of the potential modulator to decrease $LeuT_{Aa}$ activity indicates an antagonist.

In another embodiment, the present invention provides for an isolated, crystalline form of $LeuT_{Aa}$, wherein the crystalline form of LeuTAa is capable of being used for X-ray crystallographic studies, and wherein the crystalline form of the $LeuT_{Aa}$ transporter has a crystal structure with atomic coordinates as set forth in TABLE 3. The crystalline form of $LeuT_{Aa}$ may further comprise leucine and/or sodium ions.

DEFINITIONS

As used herein, the term "modeled site" refers to a representation of a biologically functional region of a NSS, such as $LeuT_{Aa}$, or a human homologue thereof. The representation may be graphic, mathematic, computer-readable, or any otherwise recognizable depiction of atomic coordinates and/or electron distribution. The term "biologically functional site" or "functional site" refers to a region of a NSS which binds to another molecule *(e.g.,* leucine, sodium ion, or water) and/or participates in transport activity).

A "modulator" of transporter activity as used herein refers to a compound which can alter the activity of a target transporter. The alteration may be an increase or a decrease. A compound that increases the activity of the target transporter is considered an agonist and a compound that decreases the activity of the target transporter is considered an inhibitor or an antagonist. For example, a modulator which increases neurotransmitter transport via $LeuT_{Aa}$ would be considered an agonist of $LeuT_{Aa}$- Conversely, a modulator which decreases neurotransmitter transport activity of LeuTAa would be considered an antagonist of $LeuTA_a$-

An agonist according to the invention may increase the intracellular response mediated by a transporter by at least 2-fold, 5-fold, 10-fold, 100-fold, or more, as compared to the intracellular response in the absence of agonist.

An antagonist may competitively bind to the transporter at the same site as a natural ligand in a manner which prevents the binding of natural ligands to the transporter domain, but would not activate an intracellular response initiated by an active form of the transporter, thereby inhibiting the intracellular response induced by

an agonist. Enzyme activity may be decreased by at least 10-15%, 15-25%, 25-50%, or 50-100%, as compared to the intracellular response absence of an antagonist.

As used herein, the term "atomic coordinates" or "structural coordinates" refers to mathematical coordinates (for example, "X," "Y," and "Z" values) that describe the positions of atoms relative to other atoms in a crystal of a Na+/Cl- dependent neurotransmitter transporter. The spatial relationship of the atoms in a crystal may also be referred to as the "three dimensional structure." The atomic coordinates may comprise the Na+/Cl- dependent neurotransmitter transporter alone or in complex with one or more substrates. For example, the atomic coordinates may describe a $LeuT_{Aa}$ molecule or a $LeuT_{Aa}$ ligand complex. Alternatively or in addition, the atomic coordinates may describe a $LeuT_{Aa}$ molecule in complex with one or more of the following: leucine, sodium, and/or water. The atomic coordinates may also describe multiple substrates, for example, $LeuT_{Aa}$ complexed with multiple sodium ions. Structural coordinates may be obtained using x-ray crystallography techniques or NMR techniques, or may be derived using molecular replacement analysis or homology modeling. X-ray crystallography diffraction data obtained from the crystals are used to calculate an electron density map of the repeating unit of the crystal. The electron density maps are used to establish the positions of the individual atoms within a single $LeuT_{A}a$ molecule or a $LeuT_{Aa}$ ligand complex. Various software programs allow for the graphical representation of a set of structural coordinates to obtain a three dimensional representation of a molecule or molecular complex. These graphical representations are often referred to as "three dimensional computer models." The three dimensional computer models are in a computer readable format, and may be displayed visually on an output device such as a computer monitor.

As used herein, a "computer program" refers to the hardware means, software means, and data storage means used to analyze or produce a model from the sequence and/or x-ray diffraction data of the present invention. The minimum hardware means of the computer-based systems of the present invention comprises a central processing unit (CPU), input means, output means, and data storage means. A skilled artisan can readily appreciate which of the currently available computer-based systems are suitable for use in the present invention. A visualization device, such as a monitor is optionally provided to visualize structure data.

4. BRIEF DESCRIPTION OF THE FIGURES

Figure IA- IB. Amino acid sequence alignment and secondary structure of LeuTAa. (A) Amino acid sequence alignment of *A. aeolicus* LeuTAa (NP_214423) with the human transporter homologues for glycine (GIyTIb; 157956), GABA (GATl; P30531), dopamine (DAT; Q01959) and serotonin (SERT; P31645) using Psi-BLAST (http://www.ncbi.nlm.nih.gov/BLAST/) with manual adjustment. Strictly conserved residues are highlighted in dark grey, and α-helices and β-strands in $LeuT_{Aa}$ are depicted as coils and arrows, respectively. The open and filled triangles show residues involved in coordinating sodium ions NaI and Na2, respectively, and the residues whose side-chain atoms interact with the sodium ions are further highlighted in light grey (e.g., N27, T254, N286, T354, S355). The filled black circles indicate the residues involved in L-leucine binding, and the residues whose side chains interact with the leucine are enclosed by boxes. The open and filled stars indicate the charged pairs at the extracellular and cytoplasmic entrances, respectively. The residues in the $LeuT_{Aa}$ dimer interface are shown in light grey letters. For the eukaryotic transporters, residues at the N- and C termini and between TM3 and TM4 are truncated in the alignment, and the numbers of truncated residues are shown in parentheses. (B) The LeuTAa topology. The positions of leucine and the two sodium ions are depicted as a triangle and two circles, respectively.

Figure 2A-2D. $LeuT_{Aa}$ structure. (A) Stereoview in the plane of the membrane. Bound L-leucine, two sodium ions and a chloride ion are shown as CPK models and are labeled accordingly; the chloride ion is not labeled, and appears as a sphere located behind the EL4b portion of the protein. Detergent molecules (β-OG) are shown as stick models. Coloring and numbering of helices (cylinders) and strands (arrows) are the same as in Fig. 1. (B) Stereoview from the extracellular side. (C) Pseudo-symmetry in the $LeuT_{Aa}$ molecule. Shown are transmembrane segments TMl- TMlO, viewed approximately parallel to the pseudo-two-fold axis of symmetry that relates TM1-TM5 (red) and TM6-TM10 (green). The pseudo-two-fold rotation axis is depicted as a black ellipsoid. (D) The $LeuT_{Aa}$ dimer, with the subunits related by the crystallographic two-fold axis of symmetry (black arrow). One protomer is on the right half (light green), the other is on the left half (pink), and TM9 and TM12 are highlighted and numbered. Leucine and the sodium ions are shown in CPK representation as light spheres and dark spheres, respectively.

Figure 3A-3D. Leucine binding site. (A) F_0 - F_c simulated-annealing omit map, contoured at 3.8σ, showing density for leucine and sodium ions, where leucine and the two sodium ions were omitted from the simulated annealing run and subsequent phase calculation. View of $LeuT_{Aa}$ rotated 110° anticlockwise in the membrane plane and 25° towards the reader relative to the view in Fig. 2A. TMlO-TM 12 are omitted from the figure for clarity. A magnified view of the density is shown in the enclosed box. (B) [^{3}FfJLeucine transport by $LeuT_{Aa}$ reconstituted into liposomes. The filled circles, open squares and filled triangles represent uptake from an external solution containing NaCl (sodium and chloride gradients), sodium gluconate (sodium gradient) and KCl (chloride gradient), respectively. The data points were fit to a single exponential (solid line). Error bars for each data point represent the standard deviation for duplicate measurements. (C) Hydrogen bonds and ionic interactions in the leucine binding pocket are depicted as dashed lines. (D) Hydrophobic interactions between the leucine and $LeuT_{Aa}$- Van der Waals surfaces for the leucine side chain and interacting residues are shown as spheres. Tyr 108 and Ser 256 are omitted from the figure for clarity.

Figure 4A-4D. Sodium ion binding sites. (A) NaI and residues from TMIa, TMIb, TM6a and TM7 together with bound leucine are shown. (B) Na2 and residues from TMIa and TM8 are shown. Distances shown are in A.

Figure 5A-5C. Extracellular and cytoplasmic gates. (A) Slice through the surface of $LeuT_{Aa}$, viewed parallel to the membrane, showing the extracellular cavity. Connolly surface of $LeuTA_a$ is shown as thick grey density. L-Leucine, Tyr 108, Phe 253 and the two charged pairs (Arg 30-Asp 404 and Arg 5-Asp 369) are depicted as labeled stick models. (B, C) Key interacting residues at the extracellular (B) and at the cytoplasmic (C) gate.

Figure 6. Speculative transport mechanism. Schematic drawing of a possible conformational change upon substrate/sodium ion transport. The left panel shows the outward-facing state. TMIa and TM6b assume the closed arrangement, whereas TMIb and TM6a adopt the open one. The middle panel shows the substrate-occluded state, which corresponds to the current crystal structure. TMIa and TM6b assume the closed arrangement, whereas TMIb and TM6a adopt a partially open one with some residues blocking the permeation pathway. The right panel shows the inward-facing state. TMIb and TM6a assume the closed arrangement, whereas TMIa and TM6b adopt the closed one, to open the pathway to the cytoplasm.

Figure 7. Stereoview of LeuT$_A$a from the cytoplasm. All settings are the same as in FIG. 2.

Figure 8A-8C. Dimer interface in the LeuTA$_a$ crystal. (A) The LeuTAa dimer, as depicted in FIG. 3C. The black and gray boxes pinpoint those regions shown in panel b and c, respectively. (B,C) Magnification of the dimer intermolecular interaction sites.

Figure 9. Chloride ion binding site. Distances (A) are written in bold letters. The chloride ion is represented as a sphere, with all residues within 4 A appearing as stick models.

Figure 10A-1OB. Preliminary characterization of [^{3}H]-leucine transport by LeuTA$_a$ proteoliposomes. (A) Effect of valinomycin. The closed circles and open squares represent uptake in the presence and absence of 1 mM valinomycin, respectively. The data points were fit to a single exponential (solid line). Error bars for each data point represent the standard deviation for triplicate measurements. (B) Effect of competitors. Error bars for each data set represent the standard deviation for duplicate measurements.

Figure 1IA-I ID. Water and aromatic residue distribution in LeuT$_A$^{a}-Leucine and detergent molecules are shown as stick models; the two sodium and single chloride ions are depicted as blue and magenta spheres, respectively. The approximate boundaries of the membrane bilayer are demarcated with horizontal lines in both a and c. (A) Water molecules in the structure, with water 4 oxygen atoms represented as cyan spheres. (B) Histogram of water molecule distribution as a function of membrane depth, divided into 5-A bins along the crystallographic y-axis. (C) Tryptophan and tyrosine residues in the structure. The 16 tryptophans and 17 tyrosines are shown as black stick models. The Nεl nitrogen atoms in tryptophan and the hydroxyl oxygen atoms in tyrosine are displayed as dark gray and light gray spheres, respectively. (D) Histogram of tryptophan and tyrosine distribution as a function of membrane depth, divided into 5-A bins along the crystallographic y-axis. The dark gray and light gray bars indicate the number of tryptophan and tyrosine residues, respectively.

5. DETAILED DESCRIPTION OF THE INVENTION

5.1. DETERMINATION OF CRYSTAL STRUCTURES

The three dimensional structure of a $LeuTA_a$ transporter may be determined by obtaining its crystal structure directly and/or by comparing the primary and/or secondary structure of the $LeuT_{Aa}$ transporter, and/or an incomplete set of components of its three dimensional structure, with a crystal structure which has already been solved. The atomic coordinates calculated for the $LeuT_{Aa}$ transporter are set forth in Table 3.

Structural information is desirably obtained from a pure preparation of a $LeuT_{Aa}$ transporter or from the purified transporter complexed with a ligand or ligands thereof. Preferably, the $LeuT_A$a transporter is comprised in a protein composition where it constitutes greater than 70 percent, and more preferably greater than 90 percent, of the total protein.

The $LeuT_{Aa}$ transporter may be prepared from a natural source, may be produced by recombinant DNA technology, or may be chemically synthesized (although this last possibility would be extremely cumbersome). For example, a full-length cDNA encoding a $LeuTA_a$ transporter may be amplified from a cDNA preparation by the polymerase chain reaction (PCR), using at least one primer designed based of known, homologous, or obtained protein sequence, and inserted into an expression vector. A large number of suitable vector-host systems are known in the art. *See e.g.* Current Protocols in Molecular Biology, Volume I, Ausubel *et ah,* eds. John Wiley:New York NY, first published in 1989 but with annual updating. Natural, recombinant or synthetic LeuTAa transporter may be purified by methods known in the art, including, but not limited to, selective precipitation, dialysis, chromatography, and/or electrophoresis. In one embodiment, the $LeuT_{Aa}$ DNA is derived from *A. aeoHcus* and the protein is produced via recombinant technology in *E. coli* C41 cells. Purification may be performed and the protein concentrated by any means known in the art. See Ausubel, *supra.*

After purification, preferably such that at least 70 percent, and more preferably at least 90 percent, of total protein is $LeuT_{Aa}$ transporter, or a mixture of the $LeuT_{Aa}$ transporter and one or more ligands/substrates thereof, may be concentrated to greater than 1 mg/ml for crystallization purposes. In one

embodiment, the concentration is about 7 mg/mL. In another embodiment, the concentration is greater than 10 mg/ml, and may be greater than 20 mg/ml. The concentration of purified transporter may include the ligand or ligands complexed with the transporter. For example, the $LeuT_{Aa}$ transporter concentration may include the $LeuT_{Aa}$ transporter in complex with leucine, in the presence of sodium ions.

Any crystallization technique known to those skilled in the art may be employed to obtain the crystals of the present invention, including, but not limited to, batch crystallization, vapor diffusion (either by sitting drop or hanging drop) and micro dialysis. Seeding of the crystals in some instances may be required to obtain X-ray quality crystals. Standard micro and/or macro seeding of crystals may therefore be used. In a preferred embodiment, the crystals are obtained using the hanging-drop vapor diffusion method.

Once crystallized, X-ray crystallography may be used to obtain a diffraction pattern for derivation of the three dimensional structure. X-ray crystallography allows the mapping of electron density, which assists in the prediction of molecular structures. The diffraction pattern of X-rays diffracted off of repeating unit cell of a crystal allows for the mapping of the three dimensional electron density of the unit cell. A density map is then constructed from the diffraction data. A model of the three dimensional structure of the molecule may be constructed based upon the experimentally determined electron density, as well as data generated from different crystals. Utilizing these techniques, an accurate three dimensional structure can be visualized. X-ray crystallography is well known in the art, and usage of the necessary equipment and practice of the necessary methods are within the ability of a person of ordinary skill in the art.

Preferably, the protein crystals and protein-ligand complex co-crystals of the present invention diffract to a resolution of 70 A or less, 50 A or less, 25 A or less, 10 A or less, 5 A or less, 2 A or less, or 1.65 A or less; it should be noted that a greater resolution, represented by smaller A values, is associated with the ability to distinguish atoms placed closer together.

The three-dimensional structural information and the specific atomic coordinates associated with said structural information of $LeuT_{A}a$ transporter may be useful for solving the structure of crystallized forms of other NSS homologues, for example, but not by way of limitation, using molecular replacement *(e.g.*, using a program such as AMORE, see Acta Crystallog., 1994, D50:760-763). The refined

three-dimensional $LeuT_{Aa}$ transporter structures of the present invention are represented by the atomic coordinates set forth in Table 3.

The three-dimensional data for the $LeuT_{Aa}$ transporter is available on-line through the Research Collaboratory for Structural Bioinformatics. This non-profit organization maintains the Protein Data Bank, a repository for structural information on proteins. The three-dimensional structural data for the $LeuT_{Aa}$ transporter, including the atomic coordinates, can be accessed at the Protein Data Bank at http://www.rcsb.org/pdb, under PDB Accession No. 2A65.

5.2. COMPUTER ASSISTED DRUG DESIGN UTILIZING THREE DIMENSIONAL STRUCTURE DATA

Three dimensional structure data may be used to design compounds potentially useful as therapeutic drugs. The three dimensional structure data may be used to predict the conformation of a peptide, polypeptide, protein, or conformational interaction between a peptide or polypeptide, and a compound. Drug design using the three dimensional structure data is sometimes referred to as "structure based drug design" or "rational drug design," and may be performed with the assistance of a computer. Drug design based upon the three dimensional structure of a protein enables a person of ordinary skill in the art to design a compound having a desired conformation, or to select such a compound from available libraries of compounds.

Molecules used for drug design may include novel molecules designed specifically to interact with the transporter, or may be identified from databases or libraries of known compounds. A person of ordinary skill in the art would understand and appreciate the necessary interactions which would characterize a molecule that will mimic, enhance, disrupt or compete with the transporter and its ligands. Three dimensional modeling of the test molecules also allows for the molecules to be modified and tested without physically synthesizing the molecule. For example, moieties may be added, removed, or substituted in a test compound, or specific structural features may be added. Test compounds may be selected based upon known functions of the compound. Various methods of drug design based upon three dimensional structure data can be found in U.S. Patent No. 6,820,01 1.

The three dimensional structural data, for example, the atomic coordinates, obtained by the methods described above may be used to construct a three dimensional computer model. This three dimensional computer model can be

used for the design of molecules which optimally bind to the $LeuT_{Aa}$ modeled site based on specified criteria or which otherwise alter transporter activity, for example by modulating the cytoplasmic gate function. For example, such molecules may be designed to form the desired interactions with one or more amino acids in the modeled site and/or active site of the $LeuT_{Aa}$ transporter or the cytoplasmic gate, or to create a desired conformational change in the transporter molecule. It is well known that a ligand binding to a transporter will effect a conformational change on the transporter. Thus, binding of an agonist to a transporter will result in a specific conformational change in the transporter; other compounds which effect the same or similar conformational change can be expected to act as an agonist of that transporter as well. Accordingly, the three dimensional computer model may be used to design molecules which effect the same conformational change.

For example, based on the three dimensional structure information of the $LeuT_{Aa}$ transporter bound to leucine and sodium, molecules which cause similar conformational changes to the $LeuT_{Aa}$ transporter may be designed. Without being bound by theory, it is believed that $LeuT_{A}a$ comprises three states. Li the outward facing state, the $LeuT_{Aa}$ transporter is accessible by substrates outside of the cell membrane. In the presence of a substrate, the $LeuT_{Aa}$ transporter may form a complex with the substrate to form an occluded state; conformational changes and ionic interactions may occur to stabilize the complex. When bound by a substrate in the presence of sodium ions, a conformational change is triggered which causes the LeuTAa transporter to shift to the inward facing state, which allows the substrate to enter the cell. Thus, the three dimensional computer model may be used to design molecules which agonize or antagonize the transporter, thereby assisting or hindering the conformational change triggered by the substrate.

Alternatively, the LeuTAa transporter modeled site described herein may be used to develop a modulator for other neurotransmitter symporter homologues, such as eukaryotic symporters and human symporters in particular. A modulator designed to interact with a $LeuT_{Aa}$ transporter modeled site may be reasonably expected to interact not only with $LeuT_{Aa}$ transporter but also with the modeled sites of other eukaryotic or human homologues, or other related neurotransmitter symporter homologues due to the structural homology and high conservation of functionally important residues which are shared by members of this transporter family (even where amino acid homology is not great). As shown by

Figure 1, clusters of high sequence conservation, including functionally important residues, are distributed throughout the primary structure and the functionally important residues are highly conserved, although the overall sequence identity of eukaryotic and prokaryotic homologues is only 20-25%. The ability for such a modulator to modulate the activity of a neurotransmitter symporter homologue is desirably confirmed by further computer analysis, *in vitro*, and/or *in vivo* testing.

In non-limiting embodiments, the present invention provides for an actual or virtual $LeuT_{Aa}$ transporter modeled site that comprises the leucine and/or sodium binding sites. One binding site is capable of binding leucine, the two other binding sites are capable of binding sodium. The modeled site model may be comprised in a virtual or actual structure that is smaller than, larger than, or the same size as a native LeuTAa transporter protein. The protein environment surrounding the modeled site may be homologous or identical to native $LeuT_{A}a$ transporter, or it may be partially or completely non-homologous. The modeled site may include structural data of LeuTAa free from ligand, or it may include structural data of $LeuTA_{a}$ with ligands bound.

The $LeuT_{Aa}$ transporter has a number of functionally relevant sites, schematically depicted in FIGURES 3, 4, and/or 6; according to the invention, models of these sites may be produced, termed "modeled sites." In one non-limiting embodiment, the modeled site comprises one or more atom(s) of at least one, at least two, at least three, at least four, at least five, at least six, at least seven, at least eight, at least nine, or ten of the following amino acid residues: G26, L25, Y108, S256, T254, F253, A22, V104, F253, S256, F259, S355, and I359 (associated with the leucine binding site), preferably having coordinates as set forth in Table 3, or within a root mean square deviation (r.m.s.d.) of the alpha carbon of the residue of at most 8 A, at most 6 A, at most 4 A, or at most 2 A. These residues interact with the leucine molecule via hydrogen bonding or ionic interactions. In addition to interacting with leucine, the residues may concurrently interact with other molecules, such as sodium, water, or other residues. Alternatively, or in addition, the modeled site may comprise one or more atom(s) of at least one, at least two, at least three, at least four, at least five, at least six, at least seven, at least eight, or nine of the following amino acid residues: T254, N286, A22, N27, V23, G20, T354, A351, and S355 (associated with the sodium binding site), preferably having coordinates as set forth in Table 3, or within a root mean square deviation (r.m.s.d.) of the alpha carbon of the residue of at

most 8 A, at most 6 A, at most 4 A, or at most 2 A. These residues interact with the sodium molecules via hydrogen bonding or ionic interactions. In addition to interacting with sodium, the residues may concurrently interact with other molecules, such as leucine, water, or other residues. Alternatively, or in addition, the modeled site may comprise one or more atom(s) of at least one, at least two, at least three, at least four, or five of the following amino acid residues: F253, F259, V104, S355, and 1359 (hydrophobic interactions associated with the leucine binding site), preferably having coordinates as set forth in Table 3, or within a root mean square deviation (r.m.s.d.) of the alpha carbon of the residue of at most 8 A, at most 6 A, at most 4 A, or at most 2 A. These residues may interact with one or more of the leucine, sodium, or water molecules via hydrophobic interactions. Alternatively, or in addition, the $LeuT_{Aa}$ binding site may comprise one or more atom(s) of at least one, at least two, at least three, at least four, or five of the following amino acids: G62, 1262, A261, G260, and G258 (associated with leucine binding, and in particular, stabilization of the unwound region of TM6), preferably having coordinates as set forth in Table 3, or within a root mean square deviation (r.m.s.d.) of the alpha carbon of the residue of at most 8 A, at most 6 A, at most 4 A, or at most 2 A. These residues interact with water molecules via hydrogen bonding or ionic interactions. In addition to interacting with water, the residues may concurrently interact with other molecules, such as sodium, leucine, or other residues. Alternatively, or in addition, the $LeuT_{Aa}$ modeled site may comprise one or more atom(s) of at least one, at least two, at least three, at least four, at least five, at least six, at least seven, or eight of the following amino acids: F253, T254, E290, Y47, Q250, D404, Y108, and R30 (associated with the extra-cellular gate), preferably having coordinates as set forth in Table 3, or within a root mean square deviation (r.m.s.d.) of the alpha carbon of the residue of at most 8 A, at most 6 A, at most 4 A, or at most 2 A. Alternatively, or in addition, the $LeuT_{Aa}$ modeled site may comprise one or more atom(s) of at least one, at least two, at least three, at least four, at least five, at least six, at least seven, at least eight, or nine of the following amino acids: R5, Y265, A266, S267, Y268, D369, L14, M16, and A17 (associated with the cytoplasmic gate), preferably having coordinates as set forth in Table 3, or within a root mean square deviation (r.m.s.d.) of the alpha carbon of the residue of at most 8 A, at most 6 A, at most 4 A, or at most 2 A. These residues interact with one or more of the leucine, sodium, or water molecules via hydrogen bonding or ionic interactions, and may also interact with other residues. The $LeuT_{Aa}$ modeled site may

also include interactions with one or more of the TMl, TM6, TM7, and TM8 regions of the $LeuT_{Aa}$ molecule, as described in FIGURES 1 and 3. Preferably, and not by way of limitation, in each of the foregoing embodiments, the modeled site comprises the coordinates of at least two, at least three, at least four, at least five, or at least six atoms from the recited set of amino acid molecules.

Computer programs may be utilized in the present invention to calculate the three dimensional structure of the transporter molecules, based upon the three dimensional data acquired from the methods discussed above. Based upon physical and chemical considerations, as well as empirical data, the computer programs may predict the three dimensional structure of the transporter molecules alone, or when bound by other molecules. This procedure can include computer fitting of potential modulators to a modeled site to ascertain how well the shape and the chemical structure of the potential modulator will complement the active site or to compare the potential modulators with the binding of a substrate or a known inhibitor in the active site. The computer programs may also predict the molecular interactions which occur within a given molecule or between two or more molecules and/or may predict conformational changes within and between interacting molecules. For example, the computer programs can predict the binding affinity of a given molecule, or its ability to agonize or antagonize the transporter molecule.

Many programs for the determination of three dimensional structure are commercially available and may be used in the present invention. In a preferred embodiment, the programs SOLVE (Terwilliger *et ah*, Acta Crystallogr., 1999, D55.-849-861) and CNS (Brunger *et ah*, Acta Crystallogr., 1998, D54:905-921) are utilized. Other programs which may be utilized in the present invention are well known in the art, and are described in greater detail in U.S. Patent No. 6,947,847.

Molecules designed based upon the three dimensional computer model may be determined based upon the interactions between the molecule and the atoms and/or electron densities within the model. For example, promising compounds which may be useful as drugs may be selected based upon the analysis of predicted binding affinity between the transporter and the compound. Compounds which may be potential drugs may be predicted to mimic, enhance, disrupt or compete with the interactions of the transporter and its ligands. Computer programs may also be employed to estimate or predict the attraction, repulsion and/or steric hindrance associated with a postulated interaction between the modeled site and the potential

modulator compound. The computer program may predict or estimate conformational changes occurring within proteins and other molecules. Generally, characteristics of an interaction that are associated with modulator activity include, but are not limited to, tight fit, low steric hindrance, positive attractive forces, and specificity.

Preferably, a candidate chemical compound comprises a conformation that promotes the formation of covalent or noncovalent crosslinking between the modeled site and the candidate chemical compound. Preferably, a candidate chemical compound binds to a surface within or adjacent to a modeled site to provide an additional site of interaction in a complex. For example, antagonists should be designed to bind with sufficient affinity to substantially prevent other ligands from binding; the antagonist may bind within the modeled site of the transporter, or at a location outside of the modeled site. A person of ordinary skill in the art will understand and appreciate that the compound and the modeled site need not be completely complementary in order for binding to have sufficient affinity.

As noted above, compounds are designed based upon the predicted interaction of the compound with the residues located in the modeled site of the transporter. However, it is not necessary for the compound to interact with all atoms or residues located in the modeled site. Compounds designed to cause different conformational changes in the transporter molecule will be expected to interact with different molecules in the modeled site. Compounds can therefore interact with a subset of residues on the transporter molecule.

Modulator compounds of the present invention may also be designed by visually inspecting the three-dimensional structure of the modeled site, $LeuT_{Aa}$ transporter, a technique known in the art as "manual" drug design. Manual drug design may employ visual inspection and analysis using a graphics visualization program known in the art.

As an alternative or an adjunct to rationally designing modulators, random screening of a small molecule library for compounds that interact with and/or bind to a modeled site of $LeuT_{A}$a transporter may be used to identify useful compounds. Such screening may be virtual; small molecule data bases can be computationally screened for chemical entities or compounds that can bind to or otherwise interact with a virtual model of a $LeuT_{A}$a transporter modeled site. Alternatively, screening can be against actual molecular models of the modeled site.

5.4. ASSAY SYSTEMS

Once tested using a modeled site, compounds may be synthesized for testing *in vitro* or *in vivo.* Methods to synthesize suitable chemical compounds are known to those of skill in the art and depend upon the structure of the chemical being synthesized. Suitable compounds to test using the method of the present invention include proteins, polypeptides, organic molecules, and inorganic molecules. The compounds may be synthesized or produced by means known in the art, or may be purchased from commercial sources. Potential modulators of $LeuT_{Aa}$ transporter activity, identified, for example, by rational drug design or by screening of libraries as described above, may be subjected to one of the following assays to confirm their activity.

A potential modulator may be evaluated for its ability to physically interact with $LeuT_{Aa}$ transporter by co-crystallizing the potential modulator with $LeuT_{Aa}$ transporter and then determining the structure of the resulting co-crystal. For example, the structure of the co-crystal may be determined by molecular replacement to assess the binding characteristics. The ability of the compound to modulate transporter activity may be correlated with its ability to physically interact with the $LeuT_{Aa}$ transporter and/or to assume an orientation that would facilitate or inhibit neurotransmitter transport (as discussed above). In one specific example, a modulator may be determined to interact with a $LeuT_{Aa}$ transporter, in a co-crystal of the modulator and $LeuT_{Aa}$ transporter, where the modulator contains an atom, and preferably a functional group, within 10 A or within 5 A of one or more atom(s) in at least one, at least two, at least three, at least four, at least five, at least six, at least seven, at least eight, at least nine, or ten of the following $LeuT_{Aa}$ transporter amino acid residues: G26, L25, Y108, S256, T254, F253, A22, V104, F259, S355, and 1359 (associated with the leucine binding site), preferably having coordinates as set forth in Table 3. Alternatively, or in addition, a modulator may be determined to interact with a $LeuTA_a$ transporter modeled site if, in a co-crystal of the modulator and $LeuT_{Aa}$ transporter, the modulator contains an atom, and preferably a functional group, within 10 A or within 5 A of one or more atom(s) in at least one, at least two, at least three, at least four, at least five, at least six, at least seven, at least eight, or nine of the following amino acid residues: T254, N286, A22, N27, V23, G20, T354, A351, and S355 (associated with the sodium binding site), preferably having coordinates as set forth in Table 3. Alternatively, or in addition, a modulator may be determined to

interact with a $LeuT_{Aa}$ transporter modeled site if, in a co-crystal of the modulator and $LeuT_{Aa}$ transporter, the modulator contains an atom, and preferably a functional group, within 10 A or within 5 A of one or more atom(s) in at least one, at least two, at least three, at least four, or five of the following amino acid residues: F253, F259, V104, S355, and 1359 (hydrophobic interactions associated with the leucine binding site), preferably having coordinates as set forth in Table 3. Alternatively, or in addition, a modulator may be determined to interact with a $LeuT_{A}$a transporter modeled site if, in a co-crystal of the modulator and $LeuT_{Aa}$ transporter, the modulator contains an atom, and preferably a functional group, within 10 A or within 5 A of one or more atom(s) in at least one, at least two, at least three, at least four, or five of the following amino acids: G62, 1262, A261, G260, and G258 (associated with leucine binding, and in particular, stabilization of the unwound region of TM6), preferably having coordinates as set forth in Table 3. Alternatively, or in addition, a modulator may be determined to interact with a $LeuT_{A}$a transporter modeled site if, in a co-crystal of the modulator and $LeuT_{Aa}$ transporter, the modulator contains an atom, and preferably a functional group, within 10 A or within 5 A of one or more atom(s) in at least one, at least two, at least three, at least four, at least five, at least six, at least seven, or eight of the following amino acids: F253, T254, E290, Y47, Q250, D404, Y108, and R30 (associated with the extra-cellular gate), preferably having coordinates as set forth in Table 3. Alternatively, or in addition, a modulator may be determined to interact with a $LeuT_{Aa}$ transporter modeled site if, in a co-crystal of the modulator and $LeuTA_{a}$ transporter, the modulator contains one or more atom(s), and preferably a functional group, within 10 A or within 5 A of an atom in at least one, at least two, at least three, at least four, at least five, at least six, at least seven, at least eight, or nine of the following amino acids: R5, Y265, A266, S267, Y268, D369, L14, M16, and A17 (associated with the cytoplasmic gate), preferably having coordinates as set forth in Table 3.

Potential modulators identified utilizing the methods of the present invention may also be tested for modulating activity against eukaryotic homologues of $LeuT_{Aa}$ transporters. A modulator found to interact with a $LeuT_{Aa}$ transporter modeled site may be reasonably expected to interact other eukaryotic or human LeuTAa transporter homologues due to the structural homology and high conservation of functionally important residues which are shared by members of this transporter family. See Figure IA. A potential modulator identified utilizing the three

dimensional modeled site of the $LeuT_{Aa}$ transporter may be evaluated for its ability to interact with eukaryotic or human $LeuT_{Aa}$ transporter homologues by co-crystallizing the potential modulator with the eukaryotic or human LeuTAa transporter homologue, and then determining the structure of the resulting co-crystal. The ability of the potential modulator to modulate transporter activity may be correlated with its ability to physically interact with the eukaryotic or human LeuTAa transporter homologue, or to assume an orientation that would facilitate or inhibit neurotransmitter transport. The modulating activity of the potential modulators against eukaryotic, and in particular, human, homologues of $LeuT_{Aa}$ transporters may also be tested via *in vitro* methods, for example, by administering the potential modulators to suitable cells or organisms which express the eukaryotic or human LeuTAa transporter homologue, and testing the cells or organisms for increases or decreases in transporter activity.

The present invention further provides for methods that determine the effect of a potential modulator *in vivo.* Such methods may provide important information, as the effect of the modulator on molecules involved in interrelated pathways may be determined. The *in vitro* assays may be performed in a cell in the context of a cell culture; the *in vivo* assays may be performed in the context of a tissue explant and/or an organism. Equivalent *in vitro* systems that duplicate one or more sodium transporter pathways may also be used to assay the modulator for desired activity.

6. EXAMPLES

6.1 CRYSTALLIZATION

The DNA coding for *A. aeolicus* $LeuT_{Aa}$ was amplified by polymerase chain reaction from genomic DNA and cloned into a pETl ób derivative that included a C-terminal octahistidine tag and a thrombin site. The protein was produced in *Escherichia coli* C41 cells cultured in Terrific broth after induction at an absorbance at 600 nm (A600) of 0.6 with 0.1 mM isopropyl-β-d-thiogalactopyranoside for 20 h at 20 ^{0}C. Cell membranes were isolated from disrupted cells and solubilized with 40 mM dodecylmaltoside (DDM). LeuTAa was eluted from a metal ion affinity chromatography column in buffer composed of 20 mM Tris-HCl (pH 8.0), 190 mM NaCl, 10 mM KCl, 300 mM imidazole and 1 mM DDM. After thrombin digestion,

the protein was loaded onto a size exclusion column equilibrated in 20 niM Tris-HCl (pH 8.0), 190 niM NaCl, 10 mM KCl, and 40 niM n-octyl-β-d-glucopyranoside (β-OG). Purified protein was concentrated and dialysed overnight at 4 °C against 10 mM Tris-HCl (pH 8.0), 45 mM NaCl, 5 mM KCl and 40 mM β-OG before crystallization. Selenomethionine-labelled protein (SeMet-LeuTAa) was expressed in C41 cells as previously reported, using 1 mM -mercaptoethanol in all buffers to minimize oxidation.

$LeuT_{Aa}$ crystals were grown by hanging-drop vapor diffusion at 18 °C by mixing protein solution (~7 mg ml^{-1}) with a reservoir solution composed of 0.1 M HEPES-NaOH (pH 7.0), 18-22% PEG 550 MME, and 0.2 M NaCl. Before freezing in liquid nitrogen, crystals were cryoprotected with a reservoir solution containing 35% PEG 550 MME and 40 mM β-OG. The crystals belong to the space group of C2 with cell dimensions of a = 87.9 A, b = 86.3 A, c = 81.0 A and = 95.7°.

The structure of $LeuTA_a$, together with that of the prokaryotic glutamate transporter homologue GItPh of *Pyrococcus horikoshii,* a representative of the other family of plasma membrane neurotransmitter transporters, reveals important common principles between them, although their overall folds are markedly different. First, both structures have captured an occluded state, therefore suggesting that mechanisms of transport for these transporters must include at least three iconic states: open to outside, occluded, and open to inside. Second, key portions of the substrate and ion binding sites are composed of extended elements of polypeptide insinuated in the middle of disrupted transmembrane -helices, thereby allowing main-chain atoms to participate in hydrogen bonding interactions. Finally, substrate and sodium binding sites (LeuTAa) or residues implicated in sodium binding (GItPh) are located close in three-dimensional space, thereby demonstrating that the long-described thermodynamic coupling of substrate and ion transport in these two families of sodium-dependent transporters is the consequence of direct or nearly direct interactions.

6.2 STRUCTURE DETERMINATION

X-ray diffraction data sets were collected using an ADSC QUANTUM 315 detector at the Advanced Light Source 8.2.2 and processed with HKL2000. Phases were obtained by the multiwavelength anomalous dispersion method using a

three-wavelength data set from a SeMet-LeuT$_{A}$a crystal. The program SOLVE was used to determine selenium sites and initial phases, which were improved by solvent flattening and histogram matching using DM (Collaborative Computational Project). The initial structure was automatically built by Arp/wArp (Perrakis *et al.),* subsequent manual rebuilding was accomplished with TURBO-FRODO, and the model was refined with CNS (Brunger *et al.).*

LeuTAa yielded crystals readily, and initial phases were determined by multiwavelength anomalous dispersion (MAD) (Hendrickson *et al.)* using a single crystal grown from selenomethionine-labelled protein and diffraction data measured to Bragg spacings of 1.9 A (Table 2). The resultant electron density map was unambiguous over almost the entire molecule. An initial model derived from automatic tracing was subjected to rounds of manual rebuilding and crystallographic refinement using a native data set to 1.65 A resolution. The final model contains residues 5-133 and 135-513 of LeuTAa, leucine, two sodium ions, a chloride ion, five detergent molecules and 210 water molecules (Table 1). Additional information regarding the X-ray crystallography materials and methods can be found in Table 4.

6.3 TRANSPORTER ARCHITECTURE

The LeuT$_{Aa}$ protomer resembles a shallow 'shot glass', with the opening facing the extracellular space, the base facing the cytoplasm, and the bottom of the 'glass' located 6 A into the bilayer-spanning portion of the transporter (FIG. 2A, B). In the current structure there are no solvent-accessible channels traversing the membrane-spanning portion of the protein. The protomer is 70 A tall and 48 A in diameter and comprises 12 transmembrane helical regions (TMl to TM12), together with numerous loops and helices on the intracellular and extracellular surfaces. To the best of our knowledge, the fold of LeuT$_{Aa}$ is not similar to that of any previously reported membrane protein structure.

There is an unanticipated internal structural repeat in the first ten transmembrane helices of the LeuTAa protomer, relating TM1-TM5 and TM6-TM10 by a pseudo-two-fold axis located in the plane of the membrane (Figs Ib and 2c). Specifically, the -carbon atoms of the 130 residues comprising helices TM1-TM5 can be superposed onto those from TM6-TM10 by a rotation of 176.5°, yielding a root mean square deviation (r.m.s.d.) of 5.3 A. This approximate symmetry is not

detectable in the amino acid sequence, and it positions the pseudo repeats with opposite orientations in the membrane bilayer. Not surprisingly, there are bacterial homologues that possess only the first 10-11 transmembrane helices, thus reinforcing the concept that the first ten helices form the essential core of Na+/Cl~dependent neurotransmitter transporters. Interestingly, other membrane transport proteins, such as aquaporin and the oxalate transporter, possess pseudo-two-fold axes parallel and perpendicular to the membrane.

TMl and TM6, which harbor the greatest density of conserved residues (FIG. IA), are oriented antiparallel to one another and, most importantly, are not continuous helices. In fact, TMl and TM6 have breaks in helical structure at positions approximately halfway across the membrane bilayer. In TMl, residues VaI 23 and GIy 24 adopt an extended conformation, linking segments Ia and Ib. The interruption of helical structure is greater in TM6, with residues Ser 256 to GIy 260 adopting extended, non-helical conformations. These two breaks in helical structure expose main-chain carbonyl oxygen and nitrogen atoms for hydrogen bonding and ion coordination. TM3 and TM8, long helices tilted by 50° from the membrane normal, are also related by the pseudo-two-fold axis and possess key conserved amino acid residues located near the unwound segments of TMl and TM6. As discussed below, TM3, TM8 and the zone surrounding the TMl and TM6 unwound regions comprise the substrate and sodium ion binding sites.

The remaining transmembrane segments surround TMl, TM3, TM6 and TM8, support the protein core and comprise most of the lipid-exposed LeuTAa surface, with TM2 and TM7 buttressing TM6 and TMl, respectively. A prominent V-shaped structure formed by TM4-TM5 and a pseudo-two-fold related inverted V created by TM9-TM10 hold TM3 and TM8 like pincers. TMlO is followed by TMl 1 and TMl 2, flanking the outer surfaces of TM9 and TMlO. TMl 2 is a helix to the C terminus of the protein and protrudes the deepest into the cytoplasm (FIG. 2A). Conserved amino acid residues are observed throughout TM2, TM4, TM5, TM7 and TM9-TM12 (FIG. IA), reinforcing their importance in structure and function.

There are substantial helical and loop segments on the solvent-exposed surfaces of $LeuT_{Aa}$, some of which are situated in regions that suggest a role in the transport mechanism. The first six residues at the N terminus (Arg 5 to Thr 10) possess an extended structure and are located in the crevices between the ends of TMIa, TM4, TM5, TM6b and TM8 (FIG. 7). Specifically, two strictly conserved

residues, Arg 5 and Trp 8, make numerous interactions in these crevices. Between TM2 and TM3 are a re-entrant segment of polypeptide and a short helix (ILl) that occlude the intracellular face of $LeuTA_a$ (FIG. 7). On the opposite side of the bilayer, between TM3 and TM4, a stretch of 41 residues (EL2) reaches 'up' from TM3 via extended polypeptide and then returns 'down' to TM4 via a helix and a -turn. In eukaryotic transporters the number of residues between TM3 and TM4 is substantially greater (FIG. IA), harboring glycosylation sites and a probable disulphide bond. The helical segment of EL2 is juxtaposed across from EL4, a segment of polypeptide between TM7 and TM8 that is composed of two short helices separated by an acute bend. The EL4a helix, in turn, makes numerous contacts with TMIb. Together, EL2 and EL4 define a portion of the shot-glass rim above the membrane bilayer.

$LeuT_{Aa}$ forms a dimer in the crystal, located on the two-fold axis of crystallographic symmetry, and the two protomers adopt a parallel orientation (FIG. 2D). The dimer interface is formed by EL2, TM9 and TMl 2, and the latter two elements of structure, together with their symmetry partners, form a four-helix bundle (FIG. IA; see also FIG. 8). The relevance of this interface to eukaryotic NSS members, most of which are thought to form oligomers, is supported by experiments on SERT, which indicate that TM 12, together with TMIl, participate in multimerization. TM2, TM4 and TM6 have also been implicated in dimerization of some eukaryotic counterparts, but because TM2 and TM6 are substantially sequestered within the $LeuT_A$a core, it is unlikely that these transmembrane segments participate in extensive protomer-protomer contacts in eukaryotic transporters. However, TM4, which lies on the surface, could partake in multimerization, although it is not part of the $LeuT_A$a dimer interface.

6.4 LEUCINE BINDING SITE

Prominent non-protein electron density located in the core of the $LeuTA_a$ protein, near the middle regions of TM3 and TM8 and adjacent to the unwound regions of TMl and TM6 (FIG. 3A), pin-pointed the location of substrate and sodium ion binding sites. The larger electron density feature indicated that it was 1-leucine, whereas the other two were interpreted as sodium ions (see below). Indeed, LeuTAa reconstituted into liposomes exhibited sodium-dependent uptake of 1-leucine (FIG. 3B). Transport was not chloride dependent, consistent with the absence of a

chloride ion located near the leucine and sodium ions, although a chloride ion is bound on the outer surface of the protein (FIG. 2A, B; see also FIG. 9). Leucine uptake by LeuI A_a proteoliposomes was stimulated 20-30% by valinomycin, suggesting that under the current assay conditions leucine transport is enhanced by vesicles with an internal negative potential, and therefore transport may be electrogenic (FIG. 10A). Further experiments, however, are required to establish the stoichiometries of substrate and ion(s) in the transport cycle of LeuTAa-

The most striking feature of the leucine binding site is that exposed main chain atoms from the unwound regions of TMl and TM6 make most of the contacts with the -amino and -carboxy groups of the bound leucine (FIG. 3C). Unwinding of TMl and TM6 not only affords direct hydrogen-bonding partners but also allows the -amino and -carboxy groups to bind close to the ends of the helical segments and exploit -helix dipole moments. Specifically, the negatively charged ends of the TMIa and TM6a helix dipoles are proximal to the amino group of leucine, whereas the positively charged end of the TMIb helix dipole is near the carboxy group. Notably, no residues that bear a formal charge interact with the substituents of leucine. Furthermore, the leucine binding site is completely dehydrated, and the closest water molecules are >9 A away from the leucine -carbon atom (FIGURE 11). Although the ionization state of the substituents cannot be directly discerned from the electron density maps, the pattern of hydrogen bonding interactions suggests that leucine is bound as a zwitterion.

Copious polar contacts, therefore, satisfy the hydrogen bonding requirements of the charged substituents. The amino group is coordinated by main-chain carbonyl oxygens from Ala 22 in TMl, Phe 253 and Thr 254 in TM6, and by a side-chain hydroxyl from Ser 256 in TM6. The carboxy group interacts with a sodium ion, amide nitrogens from Leu 25 and GIy 26 in TMl, and a hydroxyl from Tyr 108 in TM3 (FIG. 3C). The Tyr 108 hydroxyl also forms a hydrogen bond with the main-chain amide nitrogen of Leu 25, an interaction that may function as a latch to stabilize the irregular structure near the unwound region in TMl (FIG. 3C). This tyrosine is strictly conserved among all NSS family members (FIG. IA) and has been implicated in substrate binding and transport in GATl (Bismuth *et ah,* J. Biol. Chem., 1997, 272:16096-16102), SERT (Chen *et al,* J. Biol. Chem., 1997, 272:16096-16102) and GLYT2a. The structure of the unwound region in TM6 is stabilized by GIu 62, which interacts with the amide nitrogen of GIy 258 directly and with the amide nitrogens of

GIy 260, Ala 261 and lie 262 through a water molecule (FIG. 3C). This glutamate is conserved (FIG. IA) and in GATl its replacement by aspartate renders the transporter inactive.

The aliphatic side chain of leucine, by contrast with the substituents, is cradled within a hydrophobic pocket created by the side-chain atoms of VaI 104 and Tyr 108 in TM3, Phe 253, Ser 256 and Phe 259 in TM6, and Ser 355 and He 359 in TM8. The complementarity of the van der Waals surface formed by these residues to the side chain of 1-leucine (FIG. 3D) is consistent with the specificity of $LeuT_{Aa}$ for its namesake substrate. Indeed, in a competition experiment 0.1 mM cold L-leucine quantitatively blocks uptake, whereas 0.1 mM of either glycine or tryptophan are much less effective competitors, reducing the uptake of [3H]leucine by only 30% (Supplementary FIG. 4B).

The location of the substrate binding site in $LeuT_{Aa}$, together with amino acid sequence information on eukaryotic homologues, allows us to understand why some eukaryotic transporters are specific for glycine and GABA, molecules that possess amino and carboxy groups, whereas other transporters are specific for biogenic amines, including dopamine, serotonin and norepinephrine, molecules that lack a carboxy group. Amino acid sequence analysis illustrates that a key difference between amino acid and biogenic amine transporters is that the former have a glycine and the latter have an aspartate at position 24 in the $LeuT_{Aa}$ sequence (FIG. IA). Upon modeling an aspartate at glycine 24, the -carboxy group of the aspartate can be positioned to within 1 A of the carboxy group of the substrate leucine and within 3 A of a sodium ion. Therefore, it is theorized that in the biogenic amine transporters the aspartate's carboxy group supplants the carboxy group of amino acid substrates and coordinates a sodium ion. In addition, the carboxy group of the aspartate in the biogenic amine transporters may form a hydrogen bond to the amine group of the substrate and the hydroxyl group of Tyr 108.

Identification of residues shaping the leucine binding site in $LeuT_{Aa}$ illuminates determinants of substrate specificity in the eukaryotic homologues. In the glycine transporter GIyTIb, for example, residues at equivalent positions to those surrounding the isopropyl moiety of leucine in $LeuT_{Aa}$ are replaced with amino acids of a larger size or different shape, such as VaI 104 to He, Phe 259 to Tip and He 359 to Leu (FIG. IA). Together, these changes reduce the volume of the binding pocket, thereby rendering it more complementary to glycine. By contrast, residues in SERT

are replaced with smaller amino acids, such as Ser 256 to GIy and He 359 to GIy (FIG. IA), to accommodate the larger serotonin molecule. Phe 259, also a phenylalanine in the biogenic amine transporters (FIG. IA), may participate in π-π stacking interactions with the aromatic rings of serotonin, dopamine or norepinephrine in their respective transporters.

6.5 SODIUM BINDING SITES

In the $LeuTA_a$ structure two sodium ion binding sites have been identified, named NaI and Na2, within 6 A of the -carbon of the bound leucine molecule, located halfway across the membrane bilayer, at the unwound regions of TMl and TM6 (FIG. 3A). Because distinguishing between a sodium ion and a water molecule, even at 1.65 A resolution, is non-trivial, the determination is made based on a number of observations. First, when the two peaks were modeled as oxygen atoms of water molecules there was residual density greater than 3 in electron density maps calculated with F_0 - F_c coefficients, after refinement of atomic positions and temperature factors, even though the temperature factors of the oxygen atoms refined to values that were lower (10.41 and 8.81 A2) than those of surrounding protein atoms. Second, when the two electron density features were modeled as sodium ions, the F_0 - F_0 residual density disappeared, and the temperature factors refined to values (17.28 and 15.78 A^2) comparable to those of neighboring protein atoms. Third, valence calculations yielded a sodium-specific valence (Na+) of 1.32 for NaI and 1.34 for Na2, in agreement with the values expected for bound sodium ions (Na+ 1.0). By contrast, Li+, K+ and Mg2+ yielded valence values far from the expected figures. Fourth, the distances between the sodium ions and coordinating atoms were appropriate for sodium but too short for water or potassium. Valence calculations on all the other water molecules built into the electron density did not suggest the presence of additional cations.

The two sodium ions have key roles in stabilizing the $LeuT_{Aa}$ core, the unwound structures of TMl and TM6, and the bound leucine molecule. Octahedral coordination of NaI is provided by the leucine carboxy oxygen, the carbonyl oxygens of Ala 22 (TMl) and Thr 254 (TM6), the side-chain carbonyl oxygens of Asn 27 (TMl) and Asn 286 (TM7), and the hydroxyl oxygen of Thr 254 (TM6; FIG. 4A). In the biogenic amine transporters, an aspartate residue, located at position 24 in the

$LeuT_{Aa}$ sequence, probably coordinates a sodium ion equivalent to NaI. Na2 is positioned between the TMl unwound region and TM8, about 7.0 A from NaI and 5.9 A from the -carbon of bound leucine (FIG. 3A). Trigonal bi-pyramidal coordination to Na2 is achieved by carbonyl oxygens from GIy 20 and VaI 23 (TMl), Ala 351 (TM8), and the hydroxyl oxygens from Thr 354 and Ser 355 (TM8; FIG. 4B). Notably, coordination for both NaI and Na2 is accomplished by partial charges from the protein, with the carboxy group of the bound leucine being the only ligand bearing a formal charge.

What do the sodium binding sites in the $LeuT_{Aa}$ structure tell us about the mechanism by which Na+/Cl-dependent transporters preferentially bind sodium instead of potassium, ions that differ in ionic radius by only 0.38 A? It is theorized that the primary mechanism is that the sodium binding sites in $LeuT_{Aa}$ are simply too 'small' to accommodate the larger potassium ion. Indeed, the mean sodium ion-ligand distance in $LeuT_{Aa}$ is 2.28 A (σ = 0.15 A), a distance that agrees well with sodium ion-oxygen distances obtained from high-resolution crystal structures. By comparison, the mean potassium-oxygen distances are 2.84 A (Harding *et ah,* Acta Crystallogr., 2002, D58:872-874). The ion binding sites in $LeuT_{Aa}$ are devoid of water (FIG. 11) and in order for the protein to compensate for the unfavorable dehydration of sodium ions, it must form precise binding sites complementary in size and charge. Because the sodium ions are situated within the core of the protein, the binding sites are constrained from expanding or contracting by a large number of hydrogen-bonding and packing interactions, and are unable to accommodate ions of different size or valence. In fact, the residues surrounding the sodium and leucine binding sites are the most well defined in the entire structure, as indicated by low crystallographic temperature factors (data not shown).

The intimate disposition of the sodium and leucine binding sites implies a mechanism for the coupling of sodium and substrate transport. It is theorized that binding of sodium ions is required to organize the substrate binding site, which is partially formed by the potentially flexible and unwound regions of TMl and TM6, for high-affinity substrate binding. The coordination of the two sodium ions by residues in TM7 and TM8 further stabilizes the architecture of the substrate-binding site (FIG. 4).

The $LeuT_{Aa}$ structure, together with functional and amino acid sequence data on eukaryotic homologues, suggest that the NaI site is present in

eukaryotic NSS family members. First, TMl, TM6 and TM7, the helices surrounding NaI, are implicated in sodium binding in GATl (Mager *et al,* J. Neurosci., 1996, 16:5405-5414), SERT (Penado *et al,* J. Biol. Chem., 1998, 273:28098-29106) and DAT (Chen *et al,* Eur. J. Pharmacol., 2003, 479:213-221). Second, coordinating residues are conserved or conservatively substituted in NSS transporters (FIG. IA), and in SERT the residue equivalent to Asn 286 is involved in sodium binding. In an invertebrate NSS homologue that can use either Na+ or K+ to drive uptake of neutral amino acids, the corresponding residue is an aspartate, and mutation of this residue alters ion selectivity, suggesting that this transporter also shares the NaI site. Residues coordinating Na2, by contrast, are less well conserved. For example, Thr 354 is a glycine in GIyTIb and an aspartate in GATl and the biogenic amine transporters (FIG. IA). Whereas the aspartate residue probably participates in sodium coordination, in GIyTIb the loss of the threonine hydroxyl leaves only four coordinating atoms and begs the question of whether this site is present in GIyTIb.

Sodium ion to substrate stoichiometry required for transport varies among eukaryotic transporters and is certainly related to the number of sodium ion binding sites. Although the norepinephrine transporter (NET) and SERT both transport Na+ and their respective substrate in a ratio of 1:1 (Rudnick, Neurotransmitter Transporters: Structure, Function, and Regulation 25-52 (Humana Press, Totowa, NJ 2002), the sodium-to-substrate ratio in GATl (Kavanaugh *et al,* J. Biol. Chem., 1992, 267:22007-22009) and GIyTIb (Roux *et al,* Neuron, 2000, 25:373-383) is 2:1, and in GlyT2a it is 3:1 (Roux *et al,* Neuron, 2000, 25:373-383). The NaI site is most likely a common binding site for the co-transported sodium ion in all NSS members and that those transporters with 2:1 and 3:1 stoichiometries have additional sites that may include the Na2 site. At present, the location of a third sodium site is unknown.

6.6. TRANSPORTASSAY

Proteoliposomes were reconstituted as described previously using LeuTAa as purified for crystallization except with 1 mM DDM as the detergent. 1-Leucine uptake was initiated by diluting liposomes loaded with buffer 1 (20 mM HEPES-Tris, pH 7.4, 100 mM potassium gluconate) supplemented with 1 μM valinomycin into a 200-fold excess of buffer 2 (20 mM HEPES-Tris, pH 7.4, 0.1 μM

l-[3,4,5-^{3}H(N)]leucine) also containing 1 μM valinomycin and either 100 niM NaCl, 100 niM sodium gluconate, or 100 rnM KCl at 20 °C. Reactions were quenched by diluting each assay tenfold with ice-cold buffer 1, followed by filtration through nitrocellulose filters. The filters were washed twice with 1 ml of ice-cold buffer 1, placed in scintillation fluid, and counted on a scintillation counter. Background counts were subtracted from each data point and were estimated by averaging [^{3}H]leucine counts over a 10-min time window using liposomes prepared in the absence of $LeuT_{Aa}$ and reaction conditions as described above. Specific transport activity was estimated from the protein concentration before reconstitution, assuming an incorporation efficiency of 100%.

6.7. PRELIMINARY CHARACTERIZATION OF L-[^{3}Hl-LEUCINE TRANSPORT BY LEUTAA PROTEOLIPOSOMES

To determine the extent to which [^{3}H]-leucine transport depends upon membrane potential, uptake experiments were carried out in the presence and absence of valinomycin. $LeuT_{Aa}$ proteoliposom.es were loaded with Buffer 1 (20 mM HEPES-Tris (pH 7.4), 100 mM potassium gluconate) and then divided into two aliquots. For the "minus valinomycin" condition, liposomes were used as prepared. For the "plus valinomycin" condition, these liposomes were preincubated with 1 μM valinomycin for 2 hours prior to use. Transport was initiated by adding the liposomes to Buffer 2 (20 mM HEPES-Tris, pH 7.4, 0.1 μM [^{3}H]-leucine (11.7 μCi/mL)) containing 100 mM NaCl either without or with 1 μM valinomycin, and the assays were carried out as described in the methods section of the main text. To gauge substrate specificity of LeuTAa, a competition experiment was performed. Proteoliposomes loaded with Buffer 1 supplemented with 1 μM valinomycin were added to Buffer 2 containing 100 mM NaCl, 1 μM valinomycin, and either 100 μM L-leucine, 100 μM glycine, or 100 μM L-trytophan. In each case, reactions were terminated after 4 minutes, and [^{3}H]-leucine uptake was normalized to that measured in the absence of a competitor.

6.8. DISCUSSION: MECHANISTIC IMPLICATIONS

Na+/Cl-dependent transporters are membrane-spanning proteins that catalyze the movement of molecules (substrates) and ions across lipid bilayer membranes. These transporters, like many ion channels, have selective binding sites

for permeant molecules and ions, but unlike most ion channels, transporters are believed to possess two 'gates' that can alternately allow access to the binding sites from either side of the membrane bilayer, as judged by their function. The $LeuT_{Aa}$ crystal structure defines the residues and protein domains that comprise the extracellular and intracellular gates, and it suggests conformational changes that might occur during the transport cycle.

The conformation of the $LeuT_{Aa}$ protein reported here is one in which the leucine and sodium sites are occluded from solution on both the extracellular and cytoplasmic sides of the protein; that is, both the extracellular and intracellular gates are closed. Access to the extracellular solution from the leucine and sodium binding sites is primarily obstructed by Tyr 108 and Phe 253, and layered on top of these aromatic residues is a conserved charged pair composed of Arg 30 and Asp 404, which together define at least part of the extracellular gate (FIG. 5A). Arg 30 and Asp 404 interact via a pair of water molecules but could form a salt bridge upon rearrangement of the guanidium group (FIG. 5B). Arg 30 also forms a cation-π interaction with Phe 253, and is ultimately connected to NaI via a hydrogen-bond network that includes GIn 250. These residues are highly conserved in the NSS family (FIG. IA), with residues equivalent to Arg 30 and Asp 404 being important for eukaryotic transporter function. The charged pair lies at the bottom of the extracellular cavity, lined with small pockets and protrusions, defined by TMIb, TM3, TM6a, TM8, TMlO and the 'V-shaped' tip of EL4 (Figs 3a and 5a). It is proposed that when the extracellular gate is open, Arg 30 and Asp 404 may move apart, disrupting their interaction. When the gate is closed, Arg 30 and Asp 404 form a water-mediated salt link, stabilizing the extracellular gate in a closed conformation.

In contrast to the extracellular gate, where just a few residues obstruct the leucine and sodium ion binding sites, the cytoplasmic gate is far more substantial, being composed of 20 A of ordered protein structure (FIG. 5A). Directly beneath the leucine and sodium binding sites are TMIa, TM6b and TM8, with these main-chain scaffolds themselves blocking cytoplasmic access to the binding sites. Near the cytoplasmic face of the protein, another conserved charged pair, Arg 5 and Asp 369, forms an important and partially buried salt bridge. Arg 5 also forms a hydrogen bond with Ser 267 and a cation-π interaction with Tyr 268 (FIG. 5C). Adjacent to these residues lies Trp 8, the indole ring of which fits snugly in a hydrophobic pocket created by TMIa and TM6b, with its N nitrogen atom hydrogen bonding to the

carbonyl oxygen of Tyr 265 in TM6b (FIG. 5C). The conserved Tip 8 stabilizes the conformation of TMla-TM6b and anchors the amino terminus, including Arg 5. All these residues are strictly conserved among other NSS family members (FIG. IA), and mutation of residues equivalent to either Arg 5 or Trp 8 in GATl (Bennett *et al.,* J. Biol. Chem., 2000, 275:34106-34113) and Asp 369 (Loland *et al,* J. Biol. Chem., 2004, 279:3228-3238) or Tyr 268 (Loland et al., Proc. Natl. Acad. Sci. USA_5 2002, 99:1683-1688) in DAT impairs transport.

How might the extracellular and cytoplasmic gates open? The architecture of $LeuT_{Aa}$ provides tantalizing clues to possible movements of the protein backbone. If the unwound regions are viewed as 'joints', it is proposed that the extracellular and cytoplasmic helical segments, that is TMlb-TM6a and TMla-TM6b, respectively, might move relative to TM3 and TM8, helping to open and close the outward and inward gates (FIG. 6). Binding and unbinding of substrate and ions to the unwound joints may stabilize the helices in different conformational states. In calcium ATPase, for example, binding and release of calcium ions to unwound regions in transmembrane helices effects structural rearrangements. Movement in TMl may be accompanied by a conformational change in the linker between TMl and TM2, which contains the highly conserved motif NGGGAF. In GLYT2a (Lopez-Corcuera *et al*.) and SERT (Sato *et al),* accessibility studies have revealed that this region moves during the transport cycle. The TM3 and TM8 may also shift their positions or rotate slightly. In addition, the extracellular and cytoplasmic entries could expand upon movement of surface-exposed elements, including the N terminus, ILl, EL2 and EL4. Indeed, construction of chimaeras between NET and SERT revealed that both EL2 (Stephan *et al,* Biochemistry, 1997, 36:1322-1328) and EL4 (Smicun *et al.,* J. Biol. Chem., 1999, 274:36058-36064) participate in conformational changes during transport. Finally, the surrounding transmembrane segments, TM2, TM7, TMlO and TMIl, may accommodate movement of TMl, TM3, TM6 and TM8 because they have interruptions in the middle of their helical structures caused by GIy 55 and Pro 57 in TM2, GIy 294 in TM7, GIy 408 in TMlO and Pro 457 in TMl 1, most of which are conserved residues in the NSS family (FIG. IA).

Table 1 | Refinement statistics

Resolution (Å)	50–1.65
R_{work}/R_{free}*	0.199/0.217
Number of atoms	
Protein	4,044
Substrate/ion	12
Detergent	100
Water	210
B-factors	
Protein	27.7
Substrate/ion	19.2
Detergent	58.8
Water	44.2
R.m.s.d.	
Bond lengths (Å)	0.005
Bond angles (°)	1.111

*$R_{work} = \Sigma||F_o| - |F_c||/\Sigma|F_o|$. R_{free} is the *R*-value for a subset of 5% of the reflection data, which were not included in the crystallographic refinement.

Table 1

Table 2 Data collection and phasing statistics.

Data Set	Native	Se-Met peak	Se-Met edge	Se-Met remote
Wavelength (A)	0.9950	0.9793	0.9795	0.9641
Resolution (A)	50-1.65	50-1.90	50-1.90	50-1.90
Observed reflections	281458	301333	295418	289492
Unique reflections	70306	47655	47429	47380
Completeness (%) [a]	97.3 (85.9)	99.5 (97.3)	99.5 (99.8)	99.4 (99.6)
I/σ	30.5(1.81)	34.9(3.62)	38.7(5.36)	37.0(4.95)
R_{sym} (%) [a,b]	8.2 (55.4)	8.8 (44.6)	11.1 (42.9)	11.3 (44.6)
Phasing				
Phasing Power [c] (anomalous)		0.8	0.4	0.4
Phasing Power [c] (dispersive)				
peak vs edge		0.2		
peak vs remote		0.4		
edge vs remote		0.7		
Mean Figure of Merit		0.50		

[a]Values in parentheses refer to data in the highest resolution shell, 1.71-1.65 A for the native and 1.97-1.90 A for the Se-Met data sets.

[b]$R_{sym} = \sum|I - \langle I \rangle| / \sum I$, where I is the observed intensity and $\langle I \rangle$ is the average intensity from multiple observations of the symmetry related reflections.

[c]Phasing power is root mean square of F_H/E, where F_H for anomalous and dispersive are F' and F'' part of F_n, respectively, and E is the lack-of-closure error.

Table 3

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HEADER    TRANSPORT PROTEIN                          01-JUL-05   2A65
TITLE     CRYSTAL STRUCTURE OF LEUTAA, A BACTERIAL HOMOLOG OF NA+/CL-
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TITLE    2 DEPENDENT NEUROTRANSMITTER TRANSPORTERS
COMPND    MOL_ID: 1;
COMPND   2 MOLECULE: NA(+) :NEUROTRANSMITTER SYMPORTER (SNF FAMILY);
COMPND   3 CHAIN: A;
COMPND   4 SYNONYM: LEUTAA;
COMPND   5 ENGINEERED: YES
SOURCE    MOL_ID: 1;
SOURCE   2 ORGANISMJSCIENTIFIC: AQUIFEX AEOLICUS VF5;
SOURCE   3 EXPRESS ION_S YSTEM: ESCHERICHIA COLI;
SOURCE   4 EXPRESSION_SYSTEM_COMMON: BACTERIA;
SOURCE   5 EXPRESSION_SYSTEM_STRAIN: C41(DE3);
SOURCE   6 EXPRESSION_SYSTEM_VECTOR_TYPE: PLASMID;
SOURCE   7 EXPRESSION_SYSTEM_PLASMID: PETl6B
KEYWDS    MEMBRANE PROTEIN
EXPDTA    X-RAY DIFFRACTION
AUTHOR    A.YAMASHITA, S.K.SINGH, T.KAWATE, Y.JIN, E.GOUAUX
REVDAT   2   13-SEP-05 2A65    1       JRNL
REVDAT   1   02-AUG-05 2A65    0
JRNL        AUTH   A.YAMASHITA, S.K.SINGH, T.KAWATE, Y.JIN, E.GOUAUX
JRNL        TITL   CRYSTAL STRUCTURE OF A BACTERIAL HOMOLOGUE OF
JRNL        TITL 2 NA(+)/CL(-)-DEPENDENT NEUROTRANSMITTER
JRNL        TITL 3 TRANSPORTERS.
JRNL        REF    NATURE                          V. 437   215 2005
JRNL        REFN   ASTM NATUAS  UK ISSN 1476-4687
REMARK   1
REMARK   2
REMARK   2 RESOLUTION. 1.65 ANGSTROMS.
REMARK   3
REMARK   3 REFINEMENT.
REMARK   3   PROGRAM     : CNS
REMARK   3   AUTHORS     : BRUNGER, ADAMS, CLORE, DELANO, GROS, GROSSE-
REMARK   3               : KUNSTLEVE, JIANG, KUSZEWSKI, NILGES, PANNU,
REMARK   3               : READ, RICE, SIMONSON, WARREN
REMARK   3
REMARK   3  REFINEMENT TARGET : ENGH & HUBER
REMARK   3
REMARK   3  DATA USED IN REFINEMENT.
REMARK   3   RESOLUTION RANGE HIGH (ANGSTROMS) : 1.65
REMARK   3   RESOLUTION RANGE LOW  (ANGSTROMS) : 50.00
REMARK   3   DATA CUTOFF            (SIGMA(F)) : 0.000
REMARK   3   DATA CUTOFF HIGH         (ABS(F)) : 1843610.000
REMARK   3   DATA CUTOFF LOW          (ABS(F)) : 0.0000
REMARK   3   COMPLETENESS (WORKING+TEST)   (%) : 97.2
REMARK   3   NUMBER OF REFLECTIONS             : 70261
REMARK   3
REMARK   3  FIT TO DATA USED IN REFINEMENT.
REMARK   3   CROSS-VALIDATION METHOD          : THROUGHOUT
REMARK   3   FREE R VALUE TEST SET SELECTION  : RANDOM
REMARK   3   R VALUE            (WORKING SET) : 0.199
REMARK   3   FREE R VALUE                     : 0.217
REMARK   3   FREE R VALUE TEST SET SIZE   (%) : 4.900
REMARK   3   FREE R VALUE TEST SET COUNT      : 3563
REMARK   3   ESTIMATED ERROR OF FREE R VALUE  : NULL
REMARK   3
REMARK   3  FIT IN THE HIGHEST RESOLUTION BIN.
REMARK   3   TOTAL NUMBER OF BINS USED          : 10
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REMARK   3  BIN RESOLUTION RANGE HIGH       (A) : 1.65
REMARK   3  BIN RESOLUTION RANGE LOW        (A) : 1.71
REMARK   3  BIN COMPLETENESS (WORKING+TEST) (%) : 84.40
REMARK   3  REFLECTIONS IN BIN    (WORKING SET) : 5786
REMARK   3  BIN R VALUE           (WORKING SET) : 0.2939
REMARK   3  BIN FREE R VALUE                    : 0.3199
REMARK   3  BIN FREE R VALUE TEST SET SIZE  (%) : 4.40
REMARK   3  BIN FREE R VALUE TEST SET COUNT     : 318
REMARK   3  ESTIMATED ERROR OF BIN FREE R VALUE : NULL
REMARK   3
REMARK   3 NUMBER OF NON-HYDROGEN ATOMS USED IN REFINEMENT.
REMARK   3  PROTEIN ATOMS            : 4044
REMARK   3  NUCLEIC ACID ATOMS       : 0
REMARK   3  HETEROGEN ATOMS          : 112
REMARK   3  SOLVENT ATOMS            : 210
REMARK   3
REMARK   3 B VALUES.
REMARK   3  FROM WILSON PLOT           (A**2) : 23.50
REMARK   3  MEAN B VALUE      (OVERALL, A**2) : 29.21
REMARK   3  OVERALL ANISOTROPIC B VALUE.
REMARK   3   BIl (A**2) : -2.56100
REMARK   3   B22 (A**2) : 1.84700
REMARK   3   B33 (A**2) : 0.71400
REMARK   3   B12 (A**2) : 0.00000
REMARK   3   B13 (A**2) : 2.90100
REMARK   3   B23 (A**2) : 0.00000
REMARK   3
REMARK   3 ESTIMATED COORDINATE ERROR.
REMARK   3  ESD FROM LUZZATI PLOT       (A) : 0.20
REMARK   3  ESD FROM SIGMAA             (A) : 0.20
REMARK   3  LOW RESOLUTION CUTOFF       (A) : 5.00
REMARK   3
REMARK   3 CROSS-VALIDATED ESTIMATED COORDINATE ERROR.
REMARK   3  ESD FROM C-V LUZZATI PLOT   (A) : 0.21
REMARK   3  ESD FROM C-V SIGMAA         (A) : 0.22
REMARK   3
REMARK   3 RMS DEVIATIONS FROM IDEAL VALUES.
REMARK   3  BOND LENGTHS                (A) : 0.005
REMARK   3  BOND ANGLES            (DEGREES) : 1.11
REMARK   3  DIHEDRAL ANGLES        (DEGREES) : 17.96
REMARK   3  IMPROPER ANGLES        (DEGREES) : 0.76
REMARK   3
REMARK   3 ISOTROPIC THERMAL MODEL : RESTRAINED
REMARK   3
REMARK   3 ISOTROPIC THERMAL FACTOR RESTRAINTS.     RMS     SIGMA
REMARK   3  MAIN-CHAIN BOND             (A**2) : 1.223 ; 1.500
REMARK   3  MAIN-CHAIN ANGLE            (A**2) : 1.891 ; 2.000
REMARK   3  SIDE-CHAIN BOND             (A**2) : 1.901 ; 2.000
REMARK   3  SIDE-CHAIN ANGLE            (A**2) : 2.902 ; 2.500
REMARK   3
REMARK   3 BULK SOLVENT MODELING.
REMARK   3  METHOD USED : FLAT MODEL
REMARK   3  KSOL        : 0.44
REMARK   3  BSOL        : 89.18
REMARK   3
REMARK   3 NCS MODEL : NULL
REMARK   3
REMARK   3 NCS RESTRAINTS.                         RMS
SIGMA/WEIGHT
REMARK   3  GROUP  1  POSITIONAL            (A) : NULL  ; NULL
REMARK   3  GROUP  1  B-FACTOR          (A**2) : NULL  ; NULL
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REMARK   3
REMARK   3  PARAMETER FILE  1  : PROTEIN_REP .PARAM
REMARK   3  PARAMETER FILE  2  : WATER_REP .PARAM
REMARK   3  PARAMETER FILE  3  : BOG_XPLOR_PAR. TXT
REMARK   3  PARAMETER FILE  4  : ION. PARAM
REMARK   3  PARAMETER FILE  5  : NULL
REMARK   3  TOPOLOGY FILE  1   : PROTEIN. TOP
REMARK   3  TOPOLOGY FILE  2   : WATER. TOP
REMARK   3  TOPOLOGY FILE  3   : BOG_XPLOR_TOP .TXT
REMARK   3  TOPOLOGY FILE  4   : ION. TOP
REMARK   3  TOPOLOGY FILE  5   : NULL
REMARK   3
REMARK   3  OTHER REFINEMENT REMARKS: NULL
REMARK   4
REMARK   4 2A65 COMPLIES WITH FORMAT V. 2.3, 09-JULY-1998
REMARK 100
REMARK 100 THIS ENTRY HAS BEEN PROCESSED BY RCSB ON 12-JUL-2005.
REMARK 100 THE RCSB ID CODE IS RCSB033535.
REMARK 200
REMARK 200 EXPERIMENTAL DETAILS
REMARK 200  EXPERIMENT TYPE                : X-RAY DIFFRACTION
REMARK 200  DATE OF DATA COLLECTION        : 12-DEC-2004; 12-DEC-2004
REMARK 200  TEMPERATURE           (KELVIN) : 100.0
REMARK 200  PH                             : 7.00
REMARK 200  NUMBER OF CRYSTALS USED        : 2
REMARK 200
REMARK 200  SYNCHROTRON              (Y/N) : Y; Y
REMARK 200  RADIATION SOURCE               : ALS; ALS
REMARK 200  BEAMLINE                       : 8.2.2; 8.2.2
REMARK 200  X-RAY GENERATOR MODEL          : NULL
REMARK 200  MONOCHROMATIC OR LAUE    (M/L) : M; M
REMARK 200  WAVELENGTH OR RANGE        (A) : 0.9950; 0.9793, 0.9795,
0.9641
REMARK 200  MONOCHROMATOR                  : DOUBLE CRYSTAL, SI(IIl);
REMARK 200                                   DOUBLE CRYSTAL, SI(IIl)
REMARK 200  OPTICS                         : NULL
REMARK 200
REMARK 200  DETECTOR TYPE                  : CCD; CCD
REMARK 200  DETECTOR MANUFACTURER          : ADSC QUANTUM 315; ADSC
REMARK 200                                   QUANTUM 315
REMARK 200  INTENSITY-INTEGRATION SOFTWARE : HKL-2000
REMARK 200  DATA SCALING SOFTWARE          : SCALEPACK
REMARK 200
REMARK 200  NUMBER OF UNIQUE REFLECTIONS   : 70306
REMARK 200  RESOLUTION RANGE HIGH      (A) : 1.650
REMARK 200  RESOLUTION RANGE LOW       (A) : 50.000
REMARK 200  REJECTION CRITERIA  (SIGMA(I)) : -3.000
REMARK 200
REMARK 200 OVERALL .
REMARK 200  COMPLETENESS FOR RANGE     (%) : 97.3
REMARK 200  DATA REDUNDANCY                : 4.000
REMARK 200  R MERGE                    (I) : NULL
REMARK 200  R SYM                      (I) : 0.08200
REMARK 200  <I/SIGMA(I)> FOR THE DATA SET  : 30.5000
REMARK 200
REMARK 200 IN THE HIGHEST RESOLUTION SHELL.
REMARK 200  HIGHEST RESOLUTION SHELL, RANGE HIGH (A) : 1.65
REMARK 200  HIGHEST RESOLUTION SHELL, RANGE LOW  (A) : 1.71
REMARK 200  COMPLETENESS FOR SHELL     (%) : 85.9
REMARK 200  DATA REDUNDANCY IN SHELL       : NULL
REMARK 200  R MERGE FOR SHELL          (I) : NULL
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REMARK 200  R SYM FOR SHELL             (D  : 0.55400
REMARK 200  <I/SIGMA(I)>  FOR SHELL         : 1.810
REMARK 200
REMARK 200 DIFFRACTION  PROTOCOL: SINGLE WAVELENGTH;  MAD
REMARK 200 METHOD  USED  TO DETERMINE  THE STRUCTURE:  MAD
REMARK 200 SOFTWARE  USED:  SOLVE
REMARK 200 STARTING  MODEL:  NULL
REMARK 200
REMARK 200 REMARK:  NULL
REMARK 280
REMARK 280 CRYSTAL
REMARK 280 SOLVENT  CONTENT,  VS    (%) : 52.90
REMARK 280 MATTHEWS  COEFFICIENT,  VM  (ANGSTROMS**3/DA) : 2.60
REMARK 280
REMARK 280  CRYSTALLIZATION CONDITIONS : PEGMME550, NACL, HEPES, PH
7.0,
REMARK 280  VAPOR  DIFFUSION,  HANGING DROP,  TEMPERATURE 291K
REMARK 290
REMARK 290 CRYSTALLOGRAPHIC  SYMMETRY
REMARK 290 SYMMETRY  OPERATORS  FOR SPACE GROUP:  C 1 2 1
REMARK 290
REMARK 290      SYMOP    SYMMETRY
REMARK 290     NNNMMM    OPERATOR
REMARK 290       1555    X,Y,Z
REMARK 290       2555    -X,Y,-Z
REMARK 290       3555    l/2+X,l/2+Y,Z
REMARK 290       4555    1/2-X, l/2+Y,-Z
REMARK 290
REMARK 290     WHERE  NNN -> OPERATOR NUMBER
REMARK 290            MMM -> TRANSLATION  VECTOR
REMARK 290
REMARK 290 CRYSTALLOGRAPHIC  SYMMETRY TRANSFORMATIONS
REMARK 290 THE FOLLOWING  TRANSFORMATIONS  OPERATE  ON THE ATOM/HETATM
REMARK 290 RECORDS  IN THIS ENTRY  TO PRODUCE  CRYS TALLOGRAPH ICALLY
REMARK 290 RELATED  MOLECULES.
REMARK 290   SMTRYl    1   1,000000   0.000000   0.,000000         0.00000
REMARK 290   SMTRY2    1   0,000000   1.000000   0.,000000         0,00000
REMARK 290   SMTRY3    1   0,000000   0.000000   1.000000         0,00000
REMARK 290   SMTRYl    2  -1.,000000  0.000000   0.,000000         0.00000
REMARK 290   SMTRY2    2   0.000000   1.000000   0..000000        0,00000
REMARK 290   SMTRY3    2   0.000000   0.000000  -1.,000000        0.00000
REMARK 290   SMTRYl    3   1,000000   0.000000   0.,000000       43.93000
REMARK 290   SMTRY2    3   0.000000   1.000000   0.,000000       43,.15500
REMARK 290   SMTRY3    3   0,000000   0.000000   1.,000000        0,00000
REMARK 290   SMTRYl    4  -1.000000  '0.000000   0.,000000       43.93000
REMARK 290   SMTRY2    4   0.000000   1.000000   0.,000000       43.15500
REMARK 290   SMTRY3    4   0.000000   0.000000  -1.,000000        0.00000
REMARK 290
REMARK 290 REMARK:  NULL
REMARK 300
REMARK 300 BIOMOLECULE:  1
REMARK 300 THIS ENTRY  CONTAINS  THE CRYSTALLOGRAPHIC  ASYMMETRIC  UNIT
REMARK 300 WHICH  CONSISTS  OF 1 CHAIN(S).  SEE REMARK  350 FOR
REMARK 300 INFORMATION  ON GENERATING  THE BIOLOGICAL  MOLECULE(S).
REMARK 350
REMARK 350 GENERATING  THE BIOMOLECULE
REMARK 350 COORDINATES  FOR A COMPLETE  MULTIMER  REPRESENTING  THE KNOWN
REMARK 350 BIOLOGICALLY  SIGNIFICANT  OLIGOMERIZATION  STATE  OF THE
REMARK 350 MOLECULE  CAN BE GENERATED  BY APPLYING  BIOMT
TRANSFORMATIONS
REMARK 350 GIVEN  BELOW.  BOTH NON-CRYSTALLOGRAPHIC  AND
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REMARK 350 CRYSTALLOGRAPHIC  OPERATIONS ARE GIVEN.
REMARK 350
REMARK 350 BIOMOLECULE : 1
REMARK 350 APPLY THE FOLLOWING TO CHAINS: A
REMARK 350   BIOMTl    1  1.000000   0.000000   0.000000         0.00000
REMARK 350   BIOMT2    1  0.000000   1.000000   0.000000         0.00000
REMARK 350   BIOMT3    1  0.000000   0.000000   1.000000         0.00000
REMARK 465
REMARK 465 MISSING RESIDUES
REMARK 465 THE FOLLOWING RESIDUES WERE NOT LOCATED IN THE
REMARK 465 EXPERIMENT.  (M=MODEL NUMBER; RES=RESIDUE NAME; C=CHAIN
REMARK 465 IDENTIFIER; SSSEQ=SEQUENCE NUMBER ; I=INSERTION CODE.)
REMARK 465
REMARK 465   M RES C SSSEQI
REMARK 465     MET A      1
REMARK 465     GLU A      2
REMARK 465     VAL A      3
REMARK 465     LYS A      4
REMARK 465     ASN A    133
REMARK 465     ALA A    134
REMARK 465     LEU A    516
REMARK 465     VAL A    517
REMARK 465     PRO A    518
REMARK 465     ARG A    519
REMARK 500
REMARK 500 GEOMETRY AND STEREOCHEMISTRY
REMARK 500 SUBTOPIC: COVALENT BOND LENGTHS
REMARK 500
REMARK 500 THE STEREOCHEMICAL PARAMETERS OF THE FOLLOWING RESIDUES
REMARK 500 HAVE VALUES WHICH DEVIATE FROM EXPECTED VALUES BY MORE
REMARK 500 THAN 6*RMSD (M=MODEL NUMBER; RES=RESIDUE NAME; C=CHAIN
REMARK 500 IDENTIFIER; SSEQ=SEQUENCE NUMBER; I=INSERTION CODE) .
REMARK 500
REMARK 500 STANDARD TABLE:
REMARK 500 FORMAT: (10X, 13, IX, 2(A3, IX, Al, 14,Al, IX, A4, 3X) ,F6.3)
REMARK 500
REMARK 500 EXPECTED VALUES: ENGH AND HUBER, 1991
REMARK 500
REMARK 500  M RES CSSEQI ATMl    RES CSSEQI ATM2    DEVIATION
REMARK 500    MET A 199   SD     MET A 199   CE     -0.052
REMARK 500    MET A 360   SD     MET A 360   CE     -0.053
REMARK 500
REMARK 500 GEOMETRY AND STEREOCHEMISTRY
REMARK 500 SUBTOPIC: COVALENT BOND ANGLES
REMARK 500
REMARK 500 THE STEREOCHEMICAL PARAMETERS OF THE FOLLOWING RESIDUES
REMARK 500 HAVE VALUES WHICH DEVIATE FROM EXPECTED VALUES BY MORE
REMARK 500 THAN 6*RMSD (M=MODEL NUMBER; RES=RESIDUE NAME; C=CHAIN
REMARK 500 IDENTIFIER; SSEQ=SEQUENCE NUMBER; I=INSERTION CODE) .
REMARK 500
REMARK 500 STANDARD TABLE:
REMARK 500 FORMAT: (10X, 13, IX, A3, IX, Al, 14, Al,3(1X,A4,2X), 12X,F5.1)
REMARK 500
REMARK 500 EXPECTED VALUES: ENGH AND HUBER, 1991
REMARK 500
REMARK 500  M RES CSSEQI ATMl   ATM2   ATM3
REMARK 500    PHE A  28   N    -  CA  -  C   ANGL . DEV . =  7.0 DEGREES
REMARK 500    THR A  77   N    -  CA  -  C   ANGL . DEV . =  9.7 DEGREES
REMARK 500    PRO A  78   C    -  N   -  CA  ANGL. DEV. = -8.3 DEGREES
REMARK 500    TRP A 231   N    -  CA  -  C   ANGL . DEV . =  6.7 DEGREES
REMARK 500    GLY A 323   N    -  CA  -  C   ANGL . DEV . =  6.9 DEGREES
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REMARK  500       PRO  A  328      C     —   N     —   CA    ANGL.   DEV.   =  -6.7   DEGREES
REMARK  500       PHE  A  395      N     —   CA    -   C     ANGL.   DEV.   =   7.8   DEGREES
REMARK  500       GLY  A  408      N     —   CA    -   C     ANGL.   DEV.   =   7.1   DEGREES
REMARK  500       ILE  A  442      N     —   CA    -   C     ANGL.   DEV.   =  -7.5   DEGREES
REMARK  500       TYR  A  471      N     —   CA    -   C     ANGL.   DEV.   =   6.6   DEGREES
DBREF   2A65  A       1     513   GB       15607041     NP_214423              1      513
SEQADV  2A65  GLY  A   5[illegible]144  GB   15607041                  CLONING   ARTIFACT
SEQADV  2A65  THR  A   5[illegible]155  GB   15607041                  CLONING   ARTIFACT
SEQADV  2A65  LEU  A   5[illegible]166  GB   15607041                  CLONING   ARTIFACT
SEQADV  2A65  VAL  A   5[illegible]177  GB   15607041                  CLONING   ARTIFACT
SEQADV  2A65  PRO  A   5[illegible]188  GB   155660077004411           CLONING   ARTIFACT
SEQADV  2A65  ARG  A   5[illegible]199  GB   155660077004411           CLONING   ARTIFACT
SEQRES    1  A   519  MET  GLU  VAL  LYS  ARG  GLU  HIS  TRP  ALA  THR  ARG  LEU  GLY
SEQRES    2  A   519  LEU  ILE  LEU  ALA  MET  ALA  GLY  ASN  ALA  VAL  GLY  LEU  GLY
SEQRES    3  A   519  ASN  PHE  LEU  ARG  PHE  PRO  VAL  GLN  ALA  ALA  GLU  ASN  GLY
SEQRES    4  A   519  GLY  GLY  ALA  PHE  MET  ILE  PRO  TYR  ILE  ILE  ALA  PHE  LEU
SEQRES    5  A   519  LEU  VAL  GLY  ILE  PRO  LEU  MET  TRP  ILE  GLU  TRP  ALA  MET
SEQRES    6  A   519  GLY  ARG  TYR  GLY  GLY  ALA  GLN  GLY  HIS  GLY  THR  THR  PRO
SEQRES    7  A   519  ALA  ILE  PHE  TYR  LEU  LEU  TRP  ARG  ASN  ARG  PHE  ALA  LYS
SEQRES    8  A   519  ILE  LEU  GLY  VAL  PHE  GLY  LEU  TRP  ILE  PRO  LEU  VAL  VAL
SEQRES    9  A   519  ALA  ILE  TYR  TYR  VAL  TYR  ILE  GLU  SER  TRP  THR  LEU  GLY
SEQRES   10  A   519  PHE  ALA  ILE  LYS  PHE  LEU  VAL  GLY  LEU  VAL  PRO  GLU  PRO
SEQRES   11  A   519  PRO  PRO  ASN  ALA  THR  ASP  PRO  ASP  SER  ILE  LEU  ARG  PRO
SEQRES   12  A   519  PHE  LYS  GLU  PHE  LEU  TYR  SER  TYR  ILE  GLY  VAL  PRO  LYS
SEQRES   13  A   519  GLY  ASP  GLU  PRO  ILE  LEU  LYS  PRO  SER  LEU  PHE  ALA  TYR
SEQRES   14  A   519  ILE  VAL  PHE  LEU  ILE  THR  MET  PHE  ILE  ASN  VAL  SER  ILE
SEQRES   15  A   519  LEU  ILE  ARG  GLY  ILE  SER  LYS  GLY  ILE  GLU  ARG  PHE  ALA
SEQRES   16  A   519  LYS  ILE  ALA  MET  PRO  THR  LEU  PHE  ILE  LEU  ALA  VAL  PHE
SEQRES   17  A   519  LEU  VAL  ILE  ARG  VAL  PHE  LEU  LEU  GLU  THR  PRO  ASN  GLY
SEQRES   18  A   519  THR  ALA  ALA  ASP  GLY  LEU  ASN  PHE  LEU  TRP  THR  PRO  ASP
SEQRES   19  A   519  PHE  GLU  LYS  LEU  LYS  ASP  PRO  GLY  VAL  TRP  ILE  ALA  ALA
SEQRES   20  A   519  VAL  GLY  GLN  ILE  PHE  PHE  THR  LEU  SER  LEU  GLY  PHE  GLY
SEQRES   21  A   519  ALA  ILE  ILE  THR  TYR  ALA  SER  TYR  VAL  ARG  LYS  ASP  GLN
SEQRES   22  A   519  ASP  ILE  VAL  LEU  SER  GLY  LEU  THR  ALA  ALA  THR  LEU  ASN
SEQRES   23  A   519  GLU  LYS  ALA  GLU  VAL  ILE  LEU  GLY  GLY  SER  ILE  SER  ILE
SEQRES   24  A   519  PRO  ALA  ALA  VAL  ALA  PHE  PHE  GLY  VAL  ALA  ASN  ALA  VAL
SEQRES   25  A   519  ALA  ILE  ALA  LYS  ALA  GLY  ALA  PHE  ASN  LEU  GLY  PHE  ILE
SEQRES   26  A   519  THR  LEU  PRO  ALA  ILE  PHE  SER  GLN  THR  ALA  GLY  GLY  THR
SEQRES   27  A   519  PHE  LEU  GLY  PHE  LEU  TRP  PHE  PHE  LEU  LEU  PHE  PHE  ALA
SEQRES   28  A   519  GLY  LEU  THR  SER  SER  ILE  ALA  ILE  MET  GLN  PRO  MET  ILE
SEQRES   29  A   519  ALA  PHE  LEU  GLU  ASP  GLU  LEU  LYS  LEU  SER  ARG  LYS  HIS
SEQRES   30  A   519  ALA  VAL  LEU  TRP  THR  ALA  ALA  ILE  VAL  PHE  PHE  SER  ALA
SEQRES   31  A   519  HIS  LEU  VAL  MET  PHE  LEU  ASN  LYS  SER  LEU  ASP  GLU  MET
SEQRES   32  A   519  ASP  PHE  TRP  ALA  GLY  THR  ILE  GLY  VAL  VAL  PHE  PHE  GLY
SEQRES   33  A   519  LEU  THR  GLU  LEU  ILE  ILE  PHE  PHE  TRP  ILE  PHE  GLY  ALA
SEQRES   34  A   519  ASP  LYS  ALA  TRP  GLU  GLU  ILE  ASN  ARG  GLY  GLY  ILE  ILE
SEQRES   35  A   519  LYS  VAL  PRO  ARG  ILE  TYR  TYR  TYR  VAL  MET  ARG  TYR  ILE
SEQRES   36  A   519  THR  PRO  ALA  PHE  LEU  ALA  VAL  LEU  LEU  VAL  VAL  TRP  ALA
SEQRES   37  A   519  ARG  GLU  TYR  ILE  PRO  LYS  ILE  MET  GLU  GLU  THR  HIS  TRP
SEQRES   38  A   519  THR  VAL  TRP  ILE  THR  ARG  PHE  TYR  ILE  ILE  GLY  LEU  PHE
SEQRES   39  A   519  LEU  PHE  LEU  THR  PHE  LEU  VAL  PHE  LEU  ALA  GLU  ARG  ARG
SEQRES   40  A   519  ARG  ASN  HIS  GLU  SER  ALA  GLY  THR  LEU  VAL  PRO  ARG
HET     BOG       701        20
HET     BOG       702        20
HET     BOG       703        20
HET     BOG       704        20
HET     BOG       705        20
HET      NA       751         1
HET      NA       752         1
HET      CL       753         1
HET     LEU       601         9
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HETNAM     BOG B-OCTYLGLUCOSIDE ;
HETNAM      NA SODIUM ION
HETNAM      CL CHLORIDE ION
HETNAM     LEU LEUCINE
FORMUL   2  BOG    5(C14 H28 06)
FORMUL   7   NA    2(NAl 1+)
FORMUL   9   CL    CLl 1-
FORMUL  10  LEU    C6 H13 Nl 02
FORMUL  11  HOH   *210(H2 01)
HELIX    1   1 THR A   10  VAL A   23  1                          14
HELIX    2   2 GLY A   24  LEU A   29  1                           6
HELIX    3   3 LEU A   29  ASN A   38  1                          10
HELIX    4   4 GLY A   40  VAL A   54  1                          15
HELIX    5   5 VAL A   54  ALA A   71  1                          18
HELIX    6   6 THR A   76  TRP A   85  1                          10
HELIX    7   7 ASN A   87  VAL A   95  1                           9
HELIX    8   8 VAL A   95  GLY A  125  1                          31
HELIX    9   9 ASP A  136  GLY A  153  1                          18
HELIX   10  10 SER A  165  ILE A  184  1                          20
HELIX   11  11 GLY A  190  PHE A  214  1                          25
HELIX   12  12 ALA A  223  THR A  232  1                          10
HELIX   13  13 ASP A  240  SER A  256  1                          17
HELIX   14  14 GLY A  260  SER A  267  1                           8
HELIX   15  15 ILE A  275  ILE A  292  1                          18
HELIX   16  16 LEU A  293  GLY A  307  1                          15
HELIX   17  17 GLY A  307  GLY A  318  1                          12
HELIX   18  18 PHE A  320  ILE A  325  1                           6
HELIX   19  19 ILE A  325  SER A  332  1                           8
HELIX   20  20 GLY A  336  GLU A  370  1                          35
HELIX   21  21 SER A  374  LEU A  396  1                          23
HELIX   22  22 LYS A  398  ALA A  407  1                          10
HELIX   23  23 THR A  409  TRP A  425  1                          17
HELIX   24  24 GLY A  428  ARG A  438  1                          11
HELIX   25  25 ARG A  446  TYR A  454  1                           9
HELIX   26  26 TYR A  454  TYR A  471  1                          18
HELIX   27  27 TYR A  471  GLU A  478  1                          8'
HELIX   28  28 THR A  482  GLY A  514  1                          33
SHEET    1   A 2 GLU A 217  THR A 218  0
SHEET    2   A 2 GLY A 221  THR A 222 -1  O  GLY A 221   N  THR A 218
CRYSTl   87.860   86.310   81.020  90.00  95.73  90.00 C 1 2 1       4
ORIGXl      1.000000   0.000000   0.000000         0.00000
ORIGX2      0.000000   1.000000   0.000000         0.00000
ORIGX3      0.000000   0.000000   1.000000         0.00000
SCALEl      0.011382   0.000000   0.001142         0.00000
SCALE2      0.000000   0.011586   0.000000         0.00000
SCALE3      0.000000   0.000000   0.012405         0.00000
ATOM      1  N   ARG A   5      31.803  57.476  22.631  1.00 33.98
N
ATOM      2  CA  ARG A   5      31.636  55.994  22.539  1.00 32.05
C
ATOM      3  C   ARG A   5      31.718  55.534  21.088  1.00 31.40
C
ATOM      4  O   ARG A   5      31.312  56.259  20.180  1.00 31.98
O
ATOM      5  CB  ARG A   5      30.277  55.588  23.122  1.00 31.45
C
ATOM      6  CG  ARG A   5      30.059  54.084  23.227  1.00 29.17
C
ATOM      7  CD  ARG A   5      28.709  53.753  23.855  1.00 28.43
C
```

ATOM	8	NE	ARG	A	5	28.622	52.342	24.231	1.00	24.23
N										
ATOM	9	CZ	ARG	A	5	29.322	51.794	25.217	1.00	24.07
C										
ATOM	10	NHl	ARG	A	5	29.190	50.503	25.490	1.00	21.60
N										
ATOM	11	NH2	ARG	A	5	30.144	52.543	25.942	1.00	24.42
N										
ATOM	12	N	GLU	A	6	32.253	54.336	20.865	1.00	29.37
N										
ATOM	13	CA	GLU	A	6	32.333	53.805	19.510	1.00	29.05
C										
ATOM	14	C	GLU	A	6	30.919	53.554	19.003	1.00	27.44
C										
ATOM	15	O	GLU	A	6	29.992	53.358	19.786	1.00	26.22
O										
ATOM	16	CB	GLU	A	6	33.100	52.478	19.467	1.00	30.95
C										
ATOM	17	CG	GLU	A	6	34.616	52.592	19.379	1.00	33.07
C										
ATOM	18	CD	GLU	A	6	35.228	51.452	18.569	1.00	33.44
C										
ATOM	19	OEl	GLU	A	6	35.134	51.485	17.319	1.00	34.80
O										
ATOM	20	OE2	GLU	A	6	35.788	50.517	19.183	1.00	33.05
O										
ATOM	21	N	HIS	A	7	30.760	53.560	17.686	1.00	27.69
N										
ATOM	22	CA	HIS	A	7	29.466	53.307	17.075	1.00	27.01
C										
ATOM	23	C	HIS	A	7	29.665	52.529	15.790	1.00	25.63
C										
ATOM	24	O	HIS	A	7	30.720	52.611	15.168	1.00	26.30
O										
ATOM	25	CB	HIS	A	7	28.744	54.624	16.762	1.00	28.56
C										
ATOM	26	CG	HIS	A	7	28.255	55.346	17.977	1.00	30.10
C										
ATOM	27	NDl	HIS	A	7	28.690	56.610	18.317	1.00	32.22
N										
ATOM	28	CD2	HIS	A	7	27.382	54.976	18.942	1.00	30.49
C										
ATOM	29	CEl	HIS	A	7	28.105	56.985	19.439	1.00	31.72
C										
ATOM	30	NE2	HIS	A	7	27.306	56.011	19.840	1.00	32.57
N										
ATOM	31	N	TRP	A	8	28.659	51.749	15.409	1.00-	24.65
N										
ATOM	32	CA	TRP	A	8	28.733	50.999	14.168	1.00	24.99
C										
ATOM	33	C	TRP	A	8	28.740	52.049	13.068	1.00	27.07
C										
ATOM	34	O	TRP	A	8	27.948	52.990	13.104	1.00	28.45
O										
ATOM	35	CB	TRP	A	8	27.513	50.095	14.015	1.00	24.17
C										
ATOM	36	CG	TRP	A	8	27.390	49.103	15.121	1.00	22.29
C										
ATOM	37	CDl	TRP	A	8	26.573	49.180	16.210	1.00	21.93
C										

ATOM	38	CD2	TRP	A	8	28.143	47.897	15.267	1.00	21.01	C
ATOM	39	NEl	TRP	A	8	26.771	48.092	17.029	1.00	22.08	N
ATOM	40	CE2	TRP	A	8	27.731	47.290	16.472	1.00	20.90	C
ATOM	41	CE3	TRP	A	8	29.131	47.271	14.496	1.00	21.47	C
ATOM	42	CZ2	TRP	A	8	28.272	46.083	16.926	1.00	20.00	C
ATOM	43	CZ3	TRP	A	8	29.670	46.072	14.949	1.00	21.21	C
ATOM	44	CH2	TRP	A	8	29.236	45.491	16.155	1.00	18.88	C
ATOM	45	N	ALA	A	9	29.631	51.887	12.099	1.00	27.68	N
ATOM	46	CA	ALA	A	9	29.754	52.842	11.006	1.00	30.26	C
ATOM	47	C	ALA	A	9	28.583	52.800	10.035	1.00	30.83	C
ATOM	48	O	ALA	A	9	28.024	53.840	9.680	1.00	32.37	O
ATOM	49	CB	ALA	A	9	31.058	52.601	10.255	1.00	29.94	C
ATOM	50	N	THR	A	10	28.209	51.601	9.607	1.00	30.90	N
ATOM	51	CA	THR	A	10	27.122	51.454	8.653	1.00	30.58	C
ATOM	52	C	THR	A	10	25.990	50.556	9.124	1.00	30.55	C
ATOM	53	O	THR	A	10	26.145	49.751	10.045	1.00	28.32	O
ATOM	54	CB	THR	A	10	27.639	50.889	7.319	1.00	32.41	C
ATOM	55	OGl	THR	A	10	28.173	49.577	7.536	1.00	34.46	O
ATOM	56	CG2	THR	A	10	28.726	51.787	6.746	1.00	31.50	C
ATOM	57	N	ARG	A	11	24.851	50.695	8.460	1.00	29.22	N
ATOM	58	CA	ARG	A	11	23.671	49.910	8.768	1.00	28.90	C
ATOM	59	C	ARG	A	11	23.913	48.446	8.419	1.00	27.74	C
ATOM	60	O	ARG	A	11	23.561	47.546	9.185	1.00	26.53	O
ATOM	61	CB	ARG	A	11	22.484	50.429	7.962	1.00	31.75	C
ATOM	62	CG	ARG	A	11	21.179	49.767	8.302	1.00	34.38	C
ATOM	63	CD	ARG	A	11	20.836	50.022	9.746	1.00	36.78	C
ATOM	64	NE	ARG	A	11	19.410	49.877	9.987	1.00	39.27	N
ATOM	65	CZ	ARG	A	11	18.828	50.117	11.156	1.00	39.14	C
ATOM	66	NHl	ARG	A	11	19.552	50.513	12.198	1.00	36.10	N
ATOM	67	NH2	ARG	A	11	17.520	49.957	11.280	1.00	40.88	N

ATOM	68	N	LEU	A	12	24.505	48.218	7.249	1.00	26.89
N										
ATOM	69	CA	LEU	A	12	24.794	46.865	6.794	1.00	26.96
C										
ATOM	70	C	LEU	A	12	25.802	46.224	7.738	1.00	25.13
C										
ATOM	71	O	LEU	A	12	25.674	45.055	8.090	1.00	25.38
O										
ATOM	72	CB	LEU	A	12	25.365	46.883	5.376	1.00	27.71
C										
ATOM	73	CG	LEU	A	12	25.804	45.525	4.821	1.00	27.66
C										
ATOM	74	CDl	LEU	A	12	24.603	44.583	4.743	1.00	28.64
C										
ATOM	75	CD2	LEU	A	12	26.425	45.714	3.442	1.00	29.69
C										
ATOM	76	N	GLY	A	13	26.804	47.002	8.138	1.00	24.09
N										
ATOM	77	CA	GLY	A	13	27.819	46.499	9.046	1.00	23.33
C										
ATOM	78	C	GLY	A	13	27.207	46.054	10.358	1.00	22.79
C										
ATOM	79	O	GLY	A	13	27.568	45.008	10.896	1.00	23.09
O										
ATOM	80	N	LEU	A	14	26.284	46.858	10.880	1.00	22.31
N										
ATOM	81	CA	LEU	A	14	25.603	46.542	12.127	1.00	21.81
C										
ATOM	82	C	LEU	A	14	24.833	45.238	11.993	1.00	22.35
C										
ATOM	83	O	LEU	A	14	24.939	44.355	12.842	1.00	21.05
O										
ATOM	84	CB	LEU	A	14	24.625	47.663	12.503	1.00	22.25
C										
ATOM	85	CG	LEU	A	14	23.554	47.311	13.544	1.00	23.58
C										
ATOM	86	CDl	LEU	A	14	24.217	46.964	14.881	1.00	22.88
C										
ATOM	87	CD2	LEU	A	14	22.596	48.487	13.712	1.00	23.70
C										
ATOM	88	N	ILE	A	15	24.053	45.127	10.922	1.00	20.98
N										
ATOM	89	CA	ILE	A	15	23.254	43.933	10.691	1.00	21.76
C										
ATOM	90	C	ILE	A	15	24.109	42.681	10.540	1.00	20.59
C										
ATOM	91	O	ILE	A	15	23.801	41.645	11.129	1.00	21.24
O										
ATOM	92	CB	ILE	A	15	22.367	44.084	9.441	1.00	23.33
C										
ATOM	93	CGl	ILE	A	15	21.392	45.244	9.645	1.00	27.44
C										
ATOM	94	CG2	ILE	A	15	21.597	42.795	9.184	1.00	24.45
C										
ATOM	95	CDl	ILE	A	15	20.519	45.106	10.868	1.00	29.21
C										
ATOM	96	N	LEU	A	16	25.175	42.775	9.753	1.00	19.08
N										
ATOM	97	CA	LEU	A	16	26.047	41.623	9.554	1.00	19.86
C										

ATOM	98	C	LEU	A	16	26.828	41.264	10.821	1.00	19.25
C										
ATOM	99	O	LEU	A	16	27.109	40.088	11.059	1.00	19.48
O										
ATOM	100	CB	LEU	A	16	27.005	41.869	8.385	1.00	19.74
C										
ATOM	101	CG	LEU	A	16	26.313	42.021	7.021	1.00	21.52
C										
ATOM	102	CDl	LEU	A	16	27.361	42.183	5.929	1.00	22.66
C										
ATOM	103	CD2	LEU	A	16	25.441	40.794	6.745	1.00	21.53
C										
ATOM	104	N	ALA	A	17	27.177	42.264	11.631	1.00	19.02
N										
ATOM	105	CA	ALA	A	17	27.905	41.985	12.875	1.00	18.67
C										
ATOM	106	C	ALA	A	17	26.967	41.279	13.847	1.00	18.30
C										
ATOM	107	O	ALA	A	17	27.358	40.336	14.534	1.00	19.22
O										
ATOM	108	CB	ALA	A	17	28.425	43.273	13.488	1.00	19.19
C										
ATOM	109	N	MET	A	18	25.723	41.742	13.904	1.00	17.97
N										
ATOM	110	CA	MET	A	18	24.728	41.133	14.777	1.00	18.12
C										
ATOM	111	C	MET	A	18	24.384	39.748	14.255	1.00	20.19
C										
ATOM	112	O	MET	A	18	24.174	38.819	15.038	1.00	18.76
O										
ATOM	113	CB	MET	A	18	23.468	42.003	14.831	1.00	20.13
C										
ATOM	114	CG	MET	A	18	23.608	43.204	15.737	1.00	21.10
C										
ATOM	115	SD	MET	A	18	23.455	42.733	17.466	1.00	24.43
S										
ATOM	116	CE	MET	A	18	23.044	44.331	18.224	1.00	22.88
C										
ATOM	117	N	ALA	A	19	24.321	39.613	12.930	1.00	17.96
N										
ATOM	118	CA	ALA	A	19	24.030	38.325	12.313	1.00	20.51
C										
ATOM	119	C	ALA	A	19	25.181	37.362	12.601	1.00	19.41
C										
ATOM	120	O	ALA	A	19	24.956	36.176	12.797	1.00	21.12
O										
ATOM	121	CB	ALA	A	19	23.851	38.483	10.802	1.00	20.96
C										
ATOM	122	N	GLY	A	20	26.406	37.890	12.630	1.00	20.30
N										
ATOM	123	CA	GLY	A	20	27.579	37.067	12.904	1.00	21.03
C										
ATOM	124	C	GLY	A	20	27.628	36.679	14.368	1.00	19.65
C										
ATOM	125	O	GLY	A	20	28.164	35.634	14.739	1.00	20.39
O										
ATOM	126	N	ASN	A	21	27.073	37.546	15.208	1.00	18.86
N										
ATOM	127	CA	ASN	A	21	26.994	37.306	16.644	1.00	18.17
C										

ATOM	128	G	ASN	A	21	26.127	36.052	16.792	1.00	18.09
C										
ATOM	129	O	ASN	A	21	26.499	35.084	17.461	1.00	17.92
O										
ATOM	130	CB	ASN	A	21	26.310	38.516	17.302	1.00	18.75
C										
ATOM	131	CG	ASN	A	21	26.170	38.391	18.810	1.00	22.32
C										
ATOM	132	ODl	ASN	A	21	25.910	37.314	19.340	1.00	23.52
O										
ATOM	133	ND2	ASN	A	21	26.320	39.516	19.508	1.00	23.06
N										
ATOM	134	N	ALA	A	22	24.979	36.066	16.120	1.00	16.41
N										
ATOM	135	CA	ALA	A	22	24.036	34.956	16.185	1.00	15.67
C										
ATOM	136	C	ALA	**A**	22	24.421	33.695	15.415	1.00	16.51
C										
ATOM	137	O	ALA	**A**	22	24.397	32.595	15.974	1.00	15.32
O										
ATOM	138	CB	ALA	**A**	22	22.656	35.432	15.732	1.00	15.58
C										
ATOM	139	N	VAL	**A**	23	24.759	33.841	14.137	1.00	16.67
N										
ATOM	140	CA	VAL	**A**	23	25.106	32.686	13.319	1.00	16.81
C										
ATOM	141	C	VAL	**A**	23	26.466	32.121	13.698	1.00	16.63
C										
ATOM	142	O	VAL	**A**	23	27.505	32.705	13.397	1.00	17.80
O										
ATOM	143	CB	VAL	**A**	23	25.098	33.040	11.818	1.00	18.47
C										
ATOM	144	CGl	VAL	**A**	23	25.463	31.814	10.985	1.00	16.86
C										
ATOM	145	CG2	VAL	**A**	23	23.723	33.562	11.423	1.00	16.44
C										
ATOM	146	N	GLY	A	24	26.452	30.972	14.357	1.00	16.43
N										
ATOM	147	CA	GLY	**A**	24	27.701	30.363	14.771	1.00	16.86
C										
ATOM	148	C	GLY	**A**	24	27.616	28.855	14.849	1.00	15.43
C										
ATOM	149	O	GLY	A	24	26.876	28.217	14.099	1.00	15.53
O										
ATOM	150	N	LEU	**A**	25	28.382	28.279	15.769	1.00	16.20
N										
ATOM	151	CA	LEU	A	25	28.400	26.842	15.961	1.00	16.41
C										
ATOM	152	C	LEU	**A**	25	27.019	26.329	16.367	1.00	18.36
C										
ATOM	153	O	LEU	A	25	26.705	25.155	16.184	1.00	19.36
O										
ATOM	154	CB	LEU	A	25	29.429	26.481	17.034	1.00	15.55
C										
ATOM	155	CG	LEU	A	25	30.870	26.941	16.765	1.00	16.94
C										
ATOM	156	CDl	LEU	A	25	31.740	26.534	17.943	1.00	20.16
C										
ATOM	157	CD2	LEU	A	25	31.398	26.326	15.467	1.00	18.69
C										

ATOM	158	N	GLY	A	26	26.196	27.209	16.925	1.00	18.57	N
ATOM	159	CA	GLY	A	26	24.864	26.796	17.320	1.00	17.32	C
ATOM	160	C	GLY	A	26	24.009	26.391	16.129	1.00	17.73	C
ATOM	161	O	GLY	A	26	23.193	25.479	16.225	1.00	17.63	O
ATOM	162	N	ASN	A	27	24.209	27.064	15.001	1.00	17.62	N
ATOM	163	CA	ASN	A	27	23.443	26.788	13.788	1.00	17.72	C
ATOM	164	C	ASN	A	27	23.849	25.509	13.069	1.00	18.41	C
ATOM	165	O	ASN	A	27	23.000	24.762	12.569	1.00	18.85	O
ATOM	166	CB	ASN	A	27	23.602	27.933	12.783	1.00	17.01	C
ATOM	167	CG	ASN	A	27	23.180	29.265	13.337	1.00	15.81	C
ATOM	168	ODl	ASN	A	27	23.716	29.730	14.345	1.00	17.43	O
ATOM	169	ND2	ASN	A	27	22.221	29.904	12.668	1.00	16.73	N
ATOM	170	N	PHE	A	28	25.155	25.268	13.014	1.00	17.73	N
ATOM	171	CA	PHE	A	28	25.692	24.133	12.282	1.00	17.10	C
ATOM	172	C	PHE	A	28	26.013	22.867	13.055	1.00	18.60	C
ATOM	173	O	PHE	A	28	26.033	21.777	12.474	1.00	18.82	O
ATOM	174	CB	PHE	A	28	26.919	24.618	11.506	1.00	16.69	C
ATOM	175	CG	PHE	A	28	26.595	25.693	10.512	1.00	18.40	C
ATOM	176	CDl	PHE	A	28	25.941	25.377	9.319	1.00	19.18	C
ATOM	177	CD2	PHE	A	28	26.876	27.026	10.788	1.00	19.15	C
ATOM	178	CEl	PHE	A	28	25.568	26.383	8.420	1.00	20.47	C
ATOM	179	CE2	PHE	A	28	26.508	28.034	9.897	1.00	20.22	C
ATOM	180	CZ	PHE	A	28	25.851	27.710	8.710	1.00	20.16	C
ATOM	181	N	LEU	A	29	26.243	23.001	14.358	1.00	17.81	N
ATOM	182	CA	LEU	A	29	26.558	21.850	15.195	1.00	18.68	C
ATOM	183	C	LEU	A	29	25.462	21.529	16.199	1.00	19.36	C
ATOM	184	O	LEU	A	29	25.035	20.380	16.313	1.00	20.47	O
ATOM	185	CB	LEU	A	29	27.861	22.079	15.969	1.00	19.80	C
ATOM	186	CG	LEU	A	29	29.162	22.182	15.171	1.00	21.02	C
ATOM	187	CDl	LEU	A	29	30.318	22.402	16.134	1.00	21.47	C

ATOM	188	CD2	LEU	A	29	29.371	20.904	14.357	1.00	22.54
C										
ATOM	189	N	ARG	A	30	25.006	22.547	16.924	1.00	19.75
N										
ATOM	190	CA	ARG	A	30	23.990	22.346	17.956	1.00	18.72
C										
ATOM	191	C	ARG	A	30	22.597	22.037	17.421	1.00	18.17
C										
ATOM	192	O	ARG	A	30	21.978	21.061	17.840	1.00	19.46
O										
ATOM	193	CB	ARG	A	30	23.931	23.572	18.880	1.00	19.52
C										
ATOM	194	CG	ARG	A	30	23.331	23.295	20.267	1.00	20.46
C										
ATOM	195	CD	ARG	A	30	23.331	24.558	21.132	1.00	19.93
C										
ATOM	196	NE	ARG	A	30	23.019	24.284	22.538	1.00	23.21
N										
ATOM	197	CZ	ARG	A	30	21.812	23.965	23.001	1.00	26.05
C										
ATOM	198	NHl	ARG	A	30	20.772	23.880	22.179	1.00	24.02
N										
ATOM	199	NH2	ARG	A	30	21.645	23.720	24.294	1.00	25.62
N										
ATOM	200	N	PHE	A	31	22.103	22.860	16.500	1.00	16.82
N										
ATOM	201	CA	PHE	A	31	20.766	22.656	15.957	1.00	17.83
C										
ATOM	202	C	PHE	A	31	20.507	21.257	15.393	1.00	18.79
C										
ATOM	203	O	PHE	A	31	19.502	20.632	15.725	1.00	19.82
O										
ATOM	204	CB	PHE	A	31	20.450	23.698	14.879	1.00	18.29
C										
ATOM	205	CG	PHE	A	31	19.117	23.487	14.218	1.00	20.53
C										
ATOM	206	CDl	PHE	A	31	17.934	23.818	14.880	1.00	21.25
C										
ATOM	207	CD2	PHE	A	31	19.040	22.921	12.949	1.00	22.08
C										
ATOM	208	CEl	PHE	A	31	16.695	23.587	14.286	1.00	22.15
C										
ATOM	209	CE2	PHE	A	31	17.805	22.683	12.345	1.00	22.78
C										
ATOM	210	CZ	PHE	A	31	16.630	23.018	13.017	1.00	23.37
C										
ATOM	211	N	PRO	A	32	21.409	20.745	14.534	1.00	19.76
N										
ATOM	212	CA	PRO	A	32	21.199	19.407	13.963	1.00	21.90
C										
ATOM	213	C	PRO	A	32	21.048	18.321	15.025	1.00	21.66
C										
ATOM	214	O	PRO	A	32	20.173	17.460	14.925	1.00	22.88
O										
ATOM	215	CB	PRO	A	32	22.444	19.196	13.098	1.00	21.43
C										
ATOM	216	CG	PRO	A	32	22.815	20.584	12.692	1.00	22.08
C										
ATOM	217	CD	PRO	A	32	22.618	21.371	13.969	1.00	19.29
C										

ATOM	218	N	VAL	A	33	21.906	18.361	16.037	1.00	22.05	N
ATOM	219	CA	VAL	A	33	21.852	17.369	17.103	1.00	23.26	C
ATOM	220	C	VAL	A	33	20.563	17.505	17.908	1.00	24.55	C
ATOM	221	O	VAL	A	33	19.899	16.511	18.193	1.00	24.09	O
ATOM	222	CB	VAL	A	33	23.064	17.497	18.048	1.00	24.00	C
ATOM	223	CGl	VAL	A	33	22.864	16.626	19.279	1.00	23.31	C
ATOM	224	CG2	VAL	A	33	24.337	17.076	17.311	1.00	24.66	C
ATOM	225	N	GLN	A	34	20.210	18.736	18.266	1.00	23.78	N
ATOM	226	CA	GLN	A	34	18.991	18.977	19.034	1.00	24.85	C
ATOM	227	C	GLN	A	34	17.753	18.516	18.272	1.00	25.04	C
ATOM	228	O	GLN	A	34	16.861	17.878	18.840	1.00	25.77	O
ATOM	229	CB	GLN	A	34	18.867	20.465	19.369	1.00	25.47	C
ATOM	230	CG	GLN	A	34	19.978	20.980	20.262	1.00	27.75	C
ATOM	231	CD	GLN	A	34	20.036	20.234	21.574	1.00	30.93	C
ATOM	232	OEl	GLN	A	34	19.031	20.114	22.270	1.00	30.91	O
ATOM	233	NE2	GLN	A	34	21.214	19.723	21.920	1.00	32.53	N
ATOM	234	N	ALA	A	35	17.697	18.841	16.986	1.00	23.72	N
ATOM	235	CA	ALA	A	35	16.561	18.452	16.162	1.00	26.60	C
ATOM	236	C	ALA	A	35	16.503	16.938	15.981	1.00	28.46	C
ATOM	237	O	ALA	A	35	15.434	16.339	16.083	1.00	30.97	O
ATOM	238	CB	ALA	A	35	16.638	19.139	14.803	1.00	24.78	C
ATOM	239	N	ALA	A	36	17.651	16.320	15.723	1.00	29.21	N
ATOM	240	CA	ALA	A	36	17.703	14.870	15.522	1.00	31.87	C
ATOM	241	C	ALA	A	36	17.347	14.071	16.775	1.00	33.69	C
ATOM	242	O	ALA	A	36	16.635	13.068	16.693	1.00	34.79	O
ATOM	243	CB	ALA	A	36	19.085	14.460	15.016	1.00	32.50	C
ATOM	244	N	GLU	A	37	17.844	14.509	17.927	1.00	33.79	N
ATOM	245	CA	GLU	A	37	17.575	13.826	19.191	1.00	36.90	C
ATOM	246	C	GLU	A	37	16.123	13.950	19.625	1.00	37.18	C
ATOM	247	O	GLU	A	37	15.634	13.139	20.411	1.00	38.15	O

ATOM	248	CB	GLU	A	37	18.423	14.405	20.322	1.00	38.78
C										
ATOM	249	CG	GLU	A	37	19.910	14.226	20.210	1.00	42.91
C										
ATOM	250	CD	GLU	A	37	20.606	14.692	21.471	1.00	45.14
C										
ATOM	251	OEl	GLU	A	37	20.322	15.827	21.917	1.00	45.86
O										
ATOM	252	OE2	GLU	A	37	21.430	13.928	22.017	1.00	46.74
O										
ATOM	253	N	ASN	A	38	15.441	14.976	19.130	1.00	36.94
N										
ATOM	254	CA	ASN	A	38	14.059	15.219	19.521	1.00	37.42
C										
ATOM	255	C	ASN	A	38	13.007	14.951	18.450	1.00	38.24
C										
ATOM	256	O	ASN	A	38	12.004	15.659	18.369	1.00	39.23
O										
ATOM	257	CB	ASN	A	38	13.931	16.655	20.042	1.00	34.74
C										
ATOM	258	CG	ASN	A	38	14.677	16.864	21.347	1.00	34.99
C										
ATOM	259	ODl	ASN	A	38	14.266	16.367	22.394	1.00	36.04
O										
ATOM	260	ND2	ASN	A	38	15.787	17.591	21.289	1.00	32.40
N										
ATOM	261	N	GLY	A	39	13.244	13.928	17.634	1.00	38.94
N										
ATOM	262	CA	GLY	A	39	12.294	13.558	16.597	1.00	39.09
C										
ATOM	263	C	GLY	A	39	12.232	14.429	15.359	1.00	39.29
C										
ATOM	264	O	GLY	A	39	11.230	14.413	14.639	1.00	40.89
O										
ATOM	265	N	GLY	A	40	13.293	15.185	15.099	1.00	38.31
N										
ATOM	266	CA	GLY	A	40	13.317	16.043	13.928	1.00	37.55
C										
ATOM	267	C	GLY	A	40	12.109	16.953	13.812	1.00	37.64
C										
ATOM	268	O	GLY	A	40	12.050	18.003	14.451	1.00	37.55
O										
ATOM	269	N	GLY	A	41	11.144	16.548	12.990	1.00	37.45
N										
ATOM	270	CA	GLY	A	41	9.942	17.340	12.798	1.00	36.74
C										
ATOM	271	C	GLY	A	41	9.176	17.648	14.071	1.00	36.01
C										
ATOM	272	O	GLY	A	41	8.525	18.690	14.166	1.00	37.31
O										
ATOM	273	N	ALA	A	42	9.243	16.746	15.046	1.00	34.91
N										
ATOM	274	CA	ALA	A	42	8.549	16.939	16.320	1.00	34.72
C										
ATOM	275	C	ALA	A	42	9.198	18.056	17.132	1.00	34.19
C										
ATOM	276	O	ALA	A	42	8.594	18.609	18.050	1.00	34.48
O										
ATOM	277	CB	ALA	A	42	8.562	15.642	17.125	1.00	35.72
C										

ATOM	278	N	PHE	A	43	10.436	18.380	16.782	1.00	32.21
N										
ATOM	279	CA	PHE	A	43	11.187	19.424	17.469	1.00	30.31
C										
ATOM	280	C	PHE	A	43	10.869	20.790	16.878	1.00	30.08
C										
ATOM	281	O	PHE	A	43	10.845	21.797	17.583	1.00	29.06
O										
ATOM	282	CB	PHE	A	43	12.687	19.149	17.317	1.00	30.09
C										
ATOM	283	CG	PHE	A	43	13.575	20.225	17.885	1.00	27.85
C										
ATOM	284	CDl	PHE	A	43	13.763	20.343	19.258	1.00	27.69
C										
ATOM	285	CD2	PHE	A	43	14.264	21.089	17.039	1.00	27.19
C										
ATOM	286	CEl	PHE	A	43	14.629	21.304	19.782	1.00	28.74
C										
ATOM	287	CE2	PHE	A	43	15.132	22.053	17.549	1.00	26.99
C										
ATOM	288	CZ	PHE	A	43	15.317	22.160	18.925	1.00	26.34
C										
ATOM	289	N	MET	A	44	10.614	20.812	15.576	1.00	29.05
N										
ATOM	290	CA	MET	A	44	10.352	22.054	14.870	1.00	29.96
C										
ATOM	291	C	MET	A	44	9.128	22.858	15.295	1.00	29.90
C										
ATOM	292	O	MET	A	44	9.162	24.086	15.265	1.00	28.55
O										
ATOM	293	CB	MET	A	44	10.313	21.786	13.367	1.00	30.67
C										
ATOM	294	CG	MET	A	44	11.636	21.273	12.824	1.00	30.85
C										
ATOM	295	SD	MET	A	44	13.033	22.325	13.318	1.00	35.15
S										
ATOM	296	CE	MET	A	44	12.734	23.750	12.288	1.00	31.63
C										
ATOM	297	N	ILE	A	45	8.047	22.193	15.690	1.00	30.09
N										
ATOM	298	CA	ILE	A	45	6.867	22.944	16.109	1.00	31.07
C										
ATOM	299	C	ILE	A	45	7.203	23.769	17.350	1.00	28.72
C										
ATOM	300	O	ILE	A	45	7.020	24.987	17.360	1.00	29.82
O										
ATOM	301	CB	ILE	A	45	5.664	22.020	16.409	1.00	33.16
C										
ATOM	302	CGl	ILE	A	45	5.204	21.335	15.121	1.00	35.09
C										
ATOM	303	CG2	ILE	A	45	4.523	22.831	17.013	1.00	33.85
C										
ATOM	304	CDl	ILE	A	45	4.811	22.299	14.021	1.00	36.13
C										
ATOM	305	N	PRO	A	46	7.696	23.118	18.416	1.00	27.28
N										
ATOM	306	CA	PRO	A	46	8.037	23.876	19.621	1.00	26.63
C										
ATOM	307	C	PRO	A	46	9.110	24.924	19.305	1.00	26.13
C										

ATOM 308 O PRO A 46 9.100 26.025 19.853 1.00 24.87 O
ATOM 309 CB PRO A 46 8.540 22.795 20.572 1.00 29.00 C
ATOM 310 CG PRO A 46 7.722 21.606 20.172 1.00 28.97 C
ATOM 311 CD PRO A 46 7.786 21.669 18.668 1.00 28.45 C
ATOM 312 N TYR A 47 10.031 24.566 18.413 1.00 24.09 N
ATOM 313 CA TYR A 47 11.112 25.465 18.015 1.00 23.10 C
ATOM 314 C TYR A 47 10.558 26.749 17.401 1.00 22.69 C
ATOM 315 O TYR A 47 10.964 27.854 17.764 1.00 21.97 O
ATOM 316 CB TYR A 47 12.022 24.764 16.999 1.00 22.58 C
ATOM 317 CG TYR A 47 13.184 25.605 16.520 1.00 22.38 C
ATOM 318 CDl TYR A 47 14.356 25.706 17.268 1.00 23.46 C
ATOM 319 CD2 TYR A 47 13.109 26.298 15.314 1.00 23.26 C
ATOM 320 CEl TYR A 47 15.433 26.483 16.817 1.00 23.18 C
ATOM 321 CE2 TYR A 47 14.167 27.070 14.858 1.00 24.48 C
ATOM 322 CZ TYR A 47 15.326 27.159 15.611 1.00 23.93 C
ATOM 323 OH TYR A 47 16.369 27.926 15.144 1.00 24.84 O
ATOM 324 N ILE A 48 9.633 26.597 16.458 1.00 23.35 N
ATOM 325 CA ILE A 48 9.031 27.746 15.791 1.00 24.97 C
ATOM 326 C ILE A 48 8.223 28.584 16.773 1.00 23.54 C
ATOM 327 O ILE A 48 8.261 29.812 16.723 1.00 23.52 O
ATOM 328 CB ILE A 48 8.124 27.299 14.628 1.00 25.92 C
ATOM 329 CGl ILE A 48 8.984 26.684 13.522 1.00 28.36 C
ATOM 330 CG2 ILE A 48 7.331 28.486 14.088 1.00 28.34 C
ATOM 331 CDl ILE A 48 8.186 26.045 12.405 1.00 29.73 C
ATOM 332 N ILE A 49 7.493 27.921 17.664 1.00 24.23 N
ATOM 333 CA ILE A 49 6.700 28.634 18.659 1.00 24.33 C
ATOM 334 C ILE A 49 7.613 29.398 19.618 1.00 23.72 C
ATOM 335 O ILE A 49 7.319 30.533 19.997 1.00 23.63 O
ATOM 336 CB ILE A 49 5.801 27.666 19.463 1.00 25. 67 C
ATOM 337 CGl ILE A 49 4.741 27.063 18.536 1.00 26.24 C

ATOM	338	CG2	ILE	A	49	5.122	28.405	20.609	1.00	26.36
C										
ATOM	339	CDl	ILE	A	49	3.905	25.976	19.183	1.00	30.06
C										
ATOM	340	N	ALA	A	50	8.722	28.779	20.011	1.00	22.98
N										
ATOM	341	CA	ALA	A	50	9.662	29.431	20.917	1.00	22.03
C										
ATOM	342	C	ALA	A	50	10.271	30.649	20.228	1.00	21.35
C										
ATOM	343	O	ALA	A	50	10.520	31.680	20.860	1.00	21.49
O										
ATOM	344	CB	ALA	A	50	10.761	28.452	21.338	1.00	21.00
C										
ATOM	345	N	PHE	A	51	10.510	30.535	18.927	1.00	20.98
N										
ATOM	346	CA	PHE	A	51	11.076	31.654	18.185	1.00	20.28
C										
ATOM	347	C	PHE	A	51	10.120	32.849	18.239	1.00	21.72
C										
ATOM	348	O	PHE	A	51	10.538	33.983	18.477	1.00	20.62
O										
ATOM	349	CB	PHE	A	51	11.318	31.267	16.725	1.00	21.18
C										
ATOM	350	CG	PHE	A	51	11.843	32.393	15.886	1.00	21.79
C										
ATOM	351	CDl	PHE	A	51	13.090	32.951	16.154	1.00	23.52
C										
ATOM	352	CD2	PHE	A	51	11.082	32.921	14.845	1.00	23.93
C										
ATOM	353	CEl	PHE	A	51	13.574	34.019	15.401	1.00	24.87
C										
ATOM	354	CE2	PHE	A	51	11.557	33.989	14.083	1.00	24.81
C										
ATOM	355	CZ	PHE	A	51	12.803	34.540	14.360	1.00	24.59
C										
ATOM	356	N	LEU	A	52	8.834	32.581	18.029	1.00	22.57
N										
ATOM	357	CA	LEU	A	52	7.814	33.628	18.034	1.00	23.81
C										
ATOM	358	C	LEU	A	52	7.474	34.189	19.413	1.00	24.61
C										
ATOM	359	O	LEU	A	52	7.260	35.392	19.559	1.00	25.22
O										
ATOM	360	CB	LEU	A	52	6.526	33.108	17.386	1.00	25.06
C										
ATOM	361	CG	LEU	A	52	6.614	32.698	15.915	1.00	26.38
C										
ATOM	362	CDl	LEU	A	52	5.297	32.072	15.478	1.00	29.81
C										
ATOM	363	CD2	LEU	A	52	6.945	33.909	15.059	1.00	28.95
C										
ATOM	364	N	LEU	A	53	7.420	33.326	20.421	1.00	24.33
N										
ATOM	365	CA	LEU	A	53	7.059	33.768	21.765	1.00	26.23
C										
ATOM	366	C	LEU	A	53	8.214	34.133	22.688	1.00	26.31
C										
ATOM	367	O	LEU	A	53	8.005	34.782	23.716	1.00	27.41
O										

ATOM	368	CB	LEU	A	53	6.190	32.707	22.444	1.00	27.23
C										
ATOM	369	CG	LEU	A	53	4.858	32.394	21.753	1.00	30.46
C										
ATOM	370	CDl	LEU	A	53	4.153	31.260	22.479	1.00	32.85
C										
ATOM	371	CD2	LEU	A	53	3.983	33.641	21.739	1.00	31.83
C										
ATOM	372	N	VAL	A	54	9.429	33.722	22.335	1.00	25.05
N										
ATOM	373	CA	VAL	A	54	10.587	34.021	23.170	1.00	23.55
C										
ATOM	374	C	VAL	A	54	11.718	34.695	22.409	1.00	22.29
C										
ATOM	375	O	VAL	A	54	12.196	35.754	22.806	1.00	22.51
O										
ATOM	376	CB	VAL	A	54	11.148	32.732	23.826	1.00	25.54
C										
ATOM	377	CGl	VAL	A	54	12.402	33.055	24.625	1.00	27.80
C										
ATOM	378	CG2	VAL	A	54	10.089	32.103	24.721	1.00	27.83
C										
ATOM	379	N	GLY	A	55	12.144	34.070	21.316	1.00	20.45
N										
ATOM	380	CA	GLY	A	55	13.242	34.601	20.527	1.00	21.29
C										
ATOM	381	C	GLY	A	55	13.083	36.030	20.050	1.00	21.67
C										
ATOM	382	O	GLY	A	55	13.892	36.899	20.380	1.00	20.64
O										
ATOM	383	N	ILE	A	56	12.039	36.273	19.267	1.00	21.51
N										
ATOM	384	CA	ILE	A	56	11.787	37.602	18.728	1.00	22.59
C										
ATOM	385	C	ILE	A	56	11.606	38.663	19.816	1.00	21.86
C										
ATOM	386	O	ILE	A	56	12.296	39.681	19.809	1.00	22.56
O										
ATOM	387	CB	ILE	A	56	10.558	37.577	17.783	1.00	23.57
C										
ATOM	388	CGl	ILE	A	56	10.923	36.843	16.493	1.00	26.45
C										
ATOM	389	CG2	ILE	A	56	10.104	38.987	17.461	1.00	25.00
C										
ATOM	390	CDl	ILE	A	56	12.056	37.498	15.724	1.00	31.42
C										
ATOM	391	N	PRO	A	57	10.690	38.438	20.773	1.00	23.04
N										
ATOM	392	CA	PRO	A	57	10.503	39.444	21.825	1.00	23.41
C										
ATOM	393	C	PRO	A	57	11.761	39.758	22.637	1.00	22.78
C										
ATOM	394	O	PRO	A	57	12.062	40.926	22.891	1.00	22.73
O										
ATOM	395	CB	PRO	A	57	9.362	38.863	22.669	1.00	25.16
C										
ATOM	396	CG	PRO	A	57	9.409	37.397	22.382	1.00	26.43
C										
ATOM	397	CD	PRO	A	57	9.717	37.343	20.916	1.00	22.90
C										

ATOM	398	N	LEU	A	58	12.509	38.732	23.033	1.00	21.10
N										
ATOM	399	CA	LEU	A	58	13.727	38.979	23.797	1.00	20.71
C										
ATOM	400	C	LEU	A	58	14.795	39.672	22.961	1.00	19.23
C										
ATOM	401	O	LEU	A	58	15.573	40.459	23.487	1.00	20.89
O										
ATOM	402	CB	LEU	A	58	14.293	37.678	24.378	1.00	22.33
C										
ATOM	403	CG	LEU	A	58	13.644	37.139	25.656	1.00	26.63
C										
ATOM	404	CDl	LEU	A	58	14.462	35.960	26.169	1.00	27.83
C										
ATOM	405	CD2	LEU	A	58	13.591	38.230	26.720	1.00	27.84
C										
ATOM	406	N	MET	A	59	14.848	39.381	21.663	1.00	19.51
N										
ATOM	407	CA	MET	A	59	15.835	40.038	20.811	1.00	19.42
C										
ATOM	408	C	MET	A	59	15.578	41.546	20.838	1.00	19.08
C										
ATOM	409	O	MET	A	59	16.500	42.338	21.036	1.00	18.57
O										
ATOM	410	CB	MET	A	59	15.748	39.515	19.374	1.00	19.77
C										
ATOM	411	CG	MET	A	59	16.734	40.161	18.401	1.00	23.56
C										
ATOM	412	SD	MET	A	59	18.483	39.801	18.768	1.00	27.08
S										
ATOM	413	CE	MET	A	59	18.631	38.142	18.081	1.00	26.55
C										
ATOM	414	N	TRP	A	60	14.322	41.947	20.651	1.00	19.43
N										
ATOM	415	CA	TRP	A	60	14.005	43.371	20.676	1.00	18.38
C										
ATOM	416	C	TRP	A	60	14.323	43.989	22.029	1.00	18.53
C										
ATOM	417	O	TRP	A	60	14.868	45.088	22.105	1.00	18.94
O										
ATOM	418	CB	TRP	A	60	12.531	43.616	20.334	1.00	19.97
C										
ATOM	419	CG	TRP	A	60	12.243	43.560	18.867	1.00	18.00
C										
ATOM	420	CDl	TRP	A	60	13.017	44.064	17.859	1.00	19.52
C										
ATOM	421	CD2	TRP	A	60	11.073	43.022	18.244	1.00	18.17
C										
ATOM	422	NEl	TRP	A	60	12.396	43.875	16.646	1.00	20.10
N										
ATOM	423	CE2	TRP	A	60	11.200	43.241	16.855	1.00	20.23
C										
ATOM	424	CE3	TRP	A	60	9.922	42.383	18.727	1.00	20.51
C										
ATOM	425	CZ2	TRP	A	60	10.220	42.840	15.940	1.00	21.25
C										
ATOM	426	CZ3	TRP	A	60	8.949	41.985	17.820	1.00	22.17
C										
ATOM	427	CH2	TRP	A	60	9.103	42.218	16.441	1.00	21.37
C										

ATOM	428	N	ILE	A	61	13.983	43.282	23.099	1.00	17.88
N										
ATOM	429	CA	ILE	A	61	14.256	43.780	24.437	1.00	18.86
C										
ATOM	430	C	ILE	A	61	15.755	43.979	24.653	1.00	18.83
C										
ATOM	431	O	ILE	A	61	16.175	44.991	25.207	1.00	18.17
O										
ATOM	432	CB	ILE	A	61	13.691	42.814	25.502	1.00	20.73
C										
ATOM	433	CGl	ILE	A	61	12.167	42.965	25.550	1.00	22.81
C										
ATOM	434	CG2	ILE	A	61	14.330	43.078	26.864	1.00	23.94
C										
ATOM	435	CDl	ILE	A	61	11.460	41.914	26.364	1.00	25.41
C										
ATOM	436	N	GLU	A	62	16.573	43.032	24.200	1.00	18.48
N										
ATOM	437	CA	GLU	A	62	18.013	43.180	24.393	1.00	17.96
C										
ATOM	438	C	GLU	A	62	18.599	44.314	23.563	1.00	17.04
C										
ATOM	439	O	GLU	A	62	19.490	45.031	24.024	1.00	17.06
O										
ATOM	440	CB	GLU	A	62	18.737	41.853	24.110	1.00	18.58
C										
ATOM	441	CG	GLU	A	62	18.527	40.864	25.249	1.00	20.45
C										
ATOM	442	CD	GLU	A	62	19.519	39.715	25.253	1.00	24.64
C										
ATOM	443	OEl	GLU	A	62	20.672	39.912	24.815	1.00	27.51
O										
ATOM	444	OE2	GLU	A	62	19.147	38.624	25.725	1.00	25.90
O										
ATOM	445	N	TRP	A	63	18.098	44.488	22.344	1.00	16.37
N										
ATOM	446	CA	TRP	A	63	18.584	45.575	21.503	1.00	17.97
C										
ATOM	447	C	TRP	A	63	18.220	46.899	22.167	1.00	18.05
C										
ATOM	448	O	TRP	A	63	19.016	47.842	22.191	1.00	17.25
O										
ATOM	449	CB	TRP	A	63	17.930	45.542	20.123	1.00	16.71
C										
ATOM	450	CG	TRP	A	63	18.596	44.655	19.114	1.00	18.52
C										
ATOM	451	CDl	TRP	A	63	18.589	43.292	19.082	1.00	19.91
C										
ATOM	452	CD2	TRP	A	63	19.289	45.083	17.936	1.00	19.75
C										
ATOM	453	NEl	TRP	A	63	19.226	42.842	17.944	1.00	20.31
N										
ATOM	454	CE2	TRP	A	63	19.664	43.921	17.225	1.00	18.98
C										
ATOM	455	CE3	TRP	A	63	19.624	46.336	17.409	1.00	19.63
C										
ATOM	456	CZ2	TRP	A	63	20.357	43.975	16.011	1.00	20.29
C										
ATOM	457	CZ3	TRP	A	63	20.316	46.390	16.199	1.00	21.93
C										

ATOM	458	CH2	TRP	A	63	20.672	45.216	15.515	1.00	20.84
C										
ATOM	459	N	ALA	A	64	17.000	46.966	22.693	1.00	18.65
N										
ATOM	460	CA	ALA	A	64	16.521	48.178	23.353	1.00	20.49
C										
ATOM	461	C	ALA	A	64	17.337	48.506	24.598	1.00	20.92
C										
ATOM	462	O	ALA	A	64	17.737	49.653	24.807	1.00	22.58
O										
ATOM	463	CB	ALA	A	64	15.046	48.024	23.723	1.00	19.32
C										
ATOM	464	N	MET	A	65	17.581	47.499	25.426	1.00	20.39
N										
ATOM	465	CA	MET	A	65	18.354	47.709	26.640	1.00	21.01
C										
ATOM	466	C	MET	A	65	19.771	48.165	26.313	1.00	20.28
C										
ATOM	467	O	MET	A	65	20.309	49.051	26.968	1.00	19.97
O										
ATOM	468	CB	MET	A	65	18.387	46. 423	27.470	1.00	20.44
C										
ATOM	469	CG	MET	A	65	17.023	46. 023	28.020	1.00	24.34
C										
ATOM	470	SD	MET	A	65	17.076	44.477	28.944	1.00	29.63
S										
ATOM	471	CE	MET	A	65	17.892	45.012	30.415	1.00	29.39
C										
ATOM	472	N	GLY	A	66	20.371	47.564	25.288	1.00	18.99
N										
ATOM	473	CA	GLY	A	66	21. 720	47.941	24.910	1.00	19. 03
C										
ATOM	474	C	GLY	A	66	21.826	49.359	24.379	1.00	19.40
C										
ATOM	475	O	GLY	A	66	22.718	50.118	24.772	1.00	19.05
O										
ATOM	476	N	ARG	A	67	20.920	49.727	23.482	1.00	18.49
N										
ATOM	477	CA	ARG	A	67	20.948	51.066	22.912	1.00	21.15
C										
ATOM	478	C	ARG	A	67	20.707	52.104	24.007	1.00	20.88
C										
ATOM	479	O	ARG	A	67	21.336	53.163	24.020	1.00	22.22
O										
ATOM	480	CB	ARG	A	67	19.890	51.199	21.819	1.00	20.93
C										
ATOM	481	CG	ARG	A	67	19.911	52.550	21.121	1.00	21.26
C										
ATOM	482	CD	ARG	A	67	18.815	52.652	20.065	1.00	21.73
C										
ATOM	483	NE	ARG	A	67	17.480	52.505	20.638	1.00	21.54
N										
ATOM	484	CZ	ARG	A	67	16. 362	52.870	20.014	1.00	24.34
C										
ATOM	485	NHl	ARG	A	67	16. 425	53.401	18.800	1.00	22.40
N										
ATOM	486	NH2	ARG	A	67	15.185	52.714	20.605	1.00	22.24
N										
ATOM	487	N	TYR	A	68	19.800	51.785	24.924	1.00	22.21
N										

ATOM	488	CA	TYR	A	68	19.470	52.663	26.044	1.00	23.65
C										
ATOM	489	C	TYR	A	68	20.700	52.889	26.928	1.00	24.19
C										
ATOM	490	O	TYR	A	68	21.020	54.021	27.293	1.00	25.39
O										
ATOM	491	CB	TYR	A	68	18.351	52.036	26.876	1.00	24.90
C										
ATOM	492	CG	TYR	A	68	17.907	52.872	28.053	1.00	29.78
C										
ATOM	493	CDl	TYR	A	68	17.091	53.989	27.869	1.00	30.65
C										
ATOM	494	CD2	TYR	A	68	18.294	52.545	29.352	1.00	30.29
C										
ATOM	495	CEl	TYR	A	68	16.667	54.757	28.949	1.00	33.60
C										
ATOM	496	CE2	TYR	A	68	17.875	53.311	30.443	1.00	33.19
C										
ATOM	497	CZ	TYR	A	68	17.062	54.415	30.231	1.00	33.52
C										
ATOM	498	OH	TYR	A	68	16.644	55.181	31.299	1.00	36.47
O										
ATOM	499	N	GLY	A	69	21.387	51.806	27.275	1.00	21.55
N										
ATOM	500	CA	GLY	A	69	22.571	51.931	28.103	1.00	22.07
C										
ATOM	501	C	GLY	A	69	23.703	52.646	27.389	1.00	20.93
C										
ATOM	502	O	GLY	A	69	24.391	53.481	27.978	1.00	21.50
O										
ATOM	503	N	GLY	A	70	23.895	52.321	26.113	1.00	21.54
N										
ATOM	504	CA	GLY	A	70	24.957	52.933	25.333	1.00	22.68
C										
ATOM	505	C	GLY	A	70	24.862	54.443	25.266	1.00	25.35
C										
ATOM	506	O	GLY	A	70	25.877	55.142	25.282	1.00	24.26
O										
ATOM	507	N	ALA	A	71	23.635	54.948	25.187	1.00	26.19
N										
ATOM	508	CA	ALA	A	71	23.404	56.384	25.118	1.00	28.73
C										
ATOM	509	C	ALA	A	71	23.936	57.053	26.386	1.00	30.25
C										
ATOM	510	O	ALA	A	71	24.211	58.254	26.394	1.00	30.61
O										
ATOM	511	CB	ALA	A	71	21.915	56.665	24.950	1.00	28.15
C										
ATOM	512	N	GLN	A	72	24.082	56.273	27.454	1.00	29.57
N										
ATOM	513	CA	GLN	A	72	24.603	56.799	28.710	1.00	30.43
C										
ATOM	514	C	GLN	A	72	26.029	56.331	28.981	1.00	29.84
C										
ATOM	515	O	GLN	A	72	26.552	56.527	30.076	1.00	30.41
O										
ATOM	516	CB	GLN	A	72	23.691	56.405	29.878	1.00	31.27
C										
ATOM	517	CG	GLN	A	72	22.352	57.136	29.871	1.00	36.20
C										

ATOM	518	CD	GLN	A	72	21.461	56.774	31.045	1.00	38.08	C
ATOM	519	OEl	GLN	A	72	21.802	57.022	32.202	1.00	41.29	O
ATOM	520	NE2	GLN	A	72	20.311	56.178	30.750	1.00	40.05	N
ATOM	521	N	GLY	A	73	26.652	55.713	27.982	1.00	28.05	N
ATOM	522	CA	GLY	A	73	28.021	55.243	28.132	1.00	27.87	C
ATOM	523	C	GLY	A	73	28.191	53.892	28.805	1.00	26.66	C
ATOM	524	O	GLY	A	73	29.266	53.588	29.323	1.00	27.57	O
ATOM	525	N	HIS	A	74	27.148	53.069	28.790	1.00	26.10	N
ATOM	526	CA	HIS	A	74	27.214	51.754	29.421	1.00	27.53	C
ATOM	527	C	HIS	A	74	26.732	50.655	28.482	1.00	27.74	C
ATOM	528	O	HIS	A	74	25.635	50.736	27.934	1.00	29.25	O
ATOM	529	CB	HIS	A	74	26.371	51.758	30.696	1.00	28.04	C
ATOM	530	CG	HIS	A	74	26.824	52.765	31.707	1.00	31.82	C
ATOM	531	NDl	HIS	A	74	28.012	52.644	32.397	1.00	32.96	N
ATOM	532	CD2	HIS	A	74	26.264	53.925	32.124	1.00	33.97	C
ATOM	533	CEl	HIS	A	74	28.163	53.685	33.195	1.00	34.10	C
ATOM	534	NE2	HIS	A	74	27.116	54.478	33.049	1.00	35.81	N
ATOM	535	N	GLY	A	75	27.554	49.625	28.302	1.00	25.21	N
ATOM	536	CA	GLY	A	75	27.173	48.543	27.415	1.00	23.25	C
ATOM	537	C	GLY	A	75	26.956	47.190	28.067	1.00	21.38	C
ATOM	538	O	GLY	A	75	26.578	46.237	27.393	1.00	21.35	O
ATOM	539	N	THR	A	76	27.181	47.090	29.373	1.00	20.36	N
ATOM	540	CA	THR	A	76	26.994	45.816	30.050	1.00	20.68	C
ATOM	541	C	THR	A	76	25.935	45.883	31.141	1.00	20.35	C
ATOM	542	O	THR	A	76	25.664	46.949	31.699	1.00	19.84	O
ATOM	543	CB	THR	A	76	28.322	45.294	30.623	1.00	19.80	C
ATOM	544	OGl	THR	A	76	28.871	46.255	31.534	1.00	21.23	O
ATOM	545	CG2	THR	A	76	29.314	45.052	29.490	1.00	21.96	C
ATOM	546	N	THR	A	77	25.353	44.731	31.452	1.00	19.86	N
ATOM	547	CA	THR	A	77	24.269	44.649	32.423	1.00	20.47	C

ATOM	548	C	THR	A	77	24.474	45.110	33.873	1.00	21.10
C										
ATOM	549	O	THR	A	77	23.514	45.554	34.503	1.00	23.23
O										
ATOM	550	CB	THR	A	77	23.645	43.230	32.423	1.00	20.33
C										
ATOM	551	OGl	THR	A	77	24.678	42.242	32.510	1.00	20.82
O										
ATOM	552	CG2	THR	A	77	22.845	43.006	31.142	1.00	22.22
C										
ATOM	553	N	PRO	A	78	25.694	45.009	34.435	1.00	21.43
N										
ATOM	554	CA	PRO	A	78	25.763	45.491	35.823	1.00	22.32
C										
ATOM	555	C	PRO	A	78	25.312	46.955	35.899	1.00	23.90
C										
ATOM	556	O	PRO	A	78	24.591	47.354	36.819	1.00	25.62
O										
ATOM	557	CB	PRO	A	78	27.238	45.320	36.178	1.00	22.41
C										
ATOM	558	CG	PRO	A	78	27.632	44.105	35.378	1.00	20.48
C										
ATOM	559	CD	PRO	A	78	26.968	44.385	34.030	1.00	20.60
C										
ATOM	560	N	ALA	A	79	25.732	47.746	34.920	1.00	22.66
N										
ATOM	561	CA	ALA	A	79	25.365	49.157	34.877	1.00	23.62
C										
ATOM	562	C	ALA	A	79	23.977	49.374	34.275	1.00	24.14
C										
ATOM	563	O	ALA	A	79	23.195	50.188	34.776	1.00	23.56
O										
ATOM	564	CB	ALA	A	79	26.407	49.942	34.084	1.00	22.51
C										
ATOM	565	N	ILE	A	80	23.658	48.647	33.209	1.00	21.70
N										
ATOM	566	CA	ILE	A	80	22.358	48.819	32.572	1.00	22.49
C										
ATOM	567	C	ILE	A	80	21.188	48.412	33.470	1.00	22.10
C										
ATOM	568	O	ILE	A	80	20.163	49.097	33.500	1.00	22.60
O										
ATOM	569	CB	ILE	A	80	22.298	48.061	31.228	1.00	21.87
C										
ATOM	570	CGl	ILE	A	80	23.278	48.717	30.245	1.00	19.70
C										
ATOM	571	CG2	ILE	A	80	20.873	48.077	30.677	1.00	22.51
C										
ATOM	572	CDl	ILE	A	80	23.422	47.994	28.912	1.00	20.78
C										
ATOM	573	N	PHE	A	81	21.331	47.313	34.207	1.00	21.92
N										
ATOM	574	CA	PHE	A	81	20.262	46.886	35.102	1.00	22.66
C										
ATOM	575	C	PHE	A	81	20.049	47.961	36.167	1.00	25.26
C										
ATOM	576	O	PHE	A	81	18.919	48.226	36.579	1.00	25.98
O										
ATOM	577	CB	PHE	A	81	20.616	45.561	35.785	1.00	23.78
C										

ATOM 578 CG PHE A 81 20.330 44.342 34.949 1.00 23.73 C
ATOM 579 CDl PHE A 81 19.970 44.458 33.607 1.00 23.23 C
ATOM 580 CD2 PHE A 81 20.417 43.072 35.510 1.00 24.01 C
ATOM 581 CEl PHE A 81 19.701 43.328 32.837 1.00 25.43 C
ATOM 582 CE2 PHE A 81 20.149 41.935 34.750 1.00 25.04 C
ATOM 583 CZ PHE A 81 19.790 42.065 33.410 1.00 24.58 C
ATOM 584 N TYR A 82 21.143 48.580 36.599 1.00 24.64 N
ATOM 585 CA TYR A 82 21.078 49.618 37.620 1.00 27.33 C
ATOM 586 C TYR A 82 20.381 50.869 37.094 1.00 28.25 C
ATOM 587 O TYR A 82 19.702 51.572 37.847 1.00 29.67 O
ATOM 588 CB TYR A 82 22.482 49.985 38.103 1.00 27.69 C
ATOM 589 CG TYR A 82 22.477 50.867 39.333 1.00 30.27 C
ATOM 590 CDl TYR A 82 21.916 50.420 40.529 1.00 31.02 C
ATOM 591 CD2 TYR A 82 23.025 52.149 39.300 1.00 32.71 C
ATOM 592 CEl TYR A 82 21.901 51.229 41.665 1.00 32.88 C
ATOM 593 CE2 TYR A 82 23.014 52.967 40.433 1.00 34.85 C
ATOM 594 CZ TYR A 82 22.451 52.499 41.608 1.00 34.53 C
ATOM 595 OH TYR A 82 22.442 53.301 42.728 1.00 39.14 O
ATOM 596 N LEU A 83 20.560 51.153 35.807 1.00 27.11 N
ATOM 597 CA LEU A 83 19.930 52.316 35.192 1.00 28.63 C
ATOM 598 C LEU A 83 18.426 52.085 35.112 1.00 29.11 C
ATOM 599 O LEU A 83 17.631 53.021 35.235 1.00 30.70 O
ATOM 600 CB LED A 83 20.488 52.548 33.783 1.00 29.03 C
ATOM 601 CG LEU A 83 21.968 52.915 33.646 1.00 30.12 C
ATOM 602 CDl LEU A 83 22.325 53.077 32.172 1.00 31.07 C
ATOM 603 CD2 LEU A 83 22.247 54.204 34.408 1.00 33.95 C
ATOM 604 N LEU A 84 18.043 50.828 34.911 1.00 27.93 N
ATOM 605 CA LED A 84 16.639 50.447 34.798 1.00 28.71 C
ATOM 606 C LEU A 84 15.986 50.254 36.158 1.00 30.31 C
ATOM 607 O LEU A 84 14.779 50.447 36.313 1.00 31.45 O

ATOM	608	CB	LEU	A	84	16.516	49. 153	33.993	1.00	27.95
C										
ATOM	609	CG	LEU	A	84	17.088	49.196	32.574	1.00	27.96
C										
ATOM	610	CDl	LEU	A	84	16. 979	47.817	31.948	1.00	27.03
C										
ATOM	611	CD2	LEU	A	84	16.338	50.229	31.736	1.00	27.08
C										
ATOM	612	N	TRP	A	85	16. 793	49.872	37.140	1.00	30.60
N										
ATOM	613	CA	TRP	A	85	16.306	49.633	38.490	1.00	31.74
C										
ATOM	614	C	TRP	A	85	17.386	50.043	39. 485	1.00	33.69
C										
ATOM	615	O	TRP	A	85	18.335	49. 297	39.742	1.00	31.42
O										
ATOM	616	CB	TRP	A	85	15.941	48.152	38.637	1.00	31.49
C										
ATOM	617	CG	TRP	A	85	15.485	47.732	40.001	1.00	33.07
C										
ATOM	618	CDl	TRP	A	85	14.770	48.475	40.899	1.00	34.20
C										
ATOM	619	CD2	TRP	A	85	15.656	46.441	40.594	1.00	33.96
C										
ATOM	620	NEl	TRP	A	85	14.486	47.724	42.013	1.00	32.93
N										
ATOM	621	CE2	TRP	A	85	15.018	46.472	41.853	1.00	34.10
C										
ATOM	622	CE3	TRP	A	85	16. 287	45.259	40.183	1.00	34.66
C										
ATOM	623	CZ2	TRP	A	85	14.991	45.365	42.707	1.00	34.31
C										
ATOM	624	CZ3	TRP	A	85	16. 260	44.157	41. 030	1.00	35. 86
C										
ATOM	625	CH2	TRP	A	85	15.615	44.220	42.280	1.00	36.28
C										
ATOM	626	N	ARG	A	86	17.231	51.248	40.029	1.00	34.91
N										
ATOM	627	CA	ARG	A	86	18.179	51.816	40.981	1.00	37.72
C										
ATOM	628	C	ARG	A	86	18.179	51.076	42.309	1.00	38.47
C										
ATOM	629	O	ARG	A	86	17.735	51.605	43.329	1.00	38.89
O										
ATOM	630	CB	ARG	A	86	17.854	53.291	41.221	1.00	40.18
C										
ATOM	631	CG	ARG	A	86	17.883	54.148	39.968	1.00	43.66
C										
ATOM	632	CD	ARG	A	86	19. 298	54.352	39. 455	1.00	46. 08
C										
ATOM	633	NE	ARG	A	86	19.318	55.227	38.286	1.00	49. 50
N										
ATOM	634	CZ	ARG	A	86	20.425	55.710	37.731	1.00	50.61
C										
ATOM	635	NHl	ARG	A	86	21.612	55.406	38.241	1.00	51.47
N										
ATOM	636	NH2	ARG	A	86	20.345	56. 499	36. 668	1.00	51.32
N										
ATOM	637	N	ASN	A	87	18.685	49.851	42.284	1.00	37.03
N										

ATOM	638	CA	ASN	A	87	18.760	49.017	43.472	1.00	36.54	C
ATOM	639	C	ASN	A	87	20.073	48.250	43.392	1.00	37.00	C
ATOM	640	O	ASN	A	87	20.429	47.730	42.338	1.00	34.64	O
ATOM	641	CB	ASN	A	87	17.576	48.049	43.503	1.00	36.87	C
ATOM	642	CG	ASN	A	87	17.475	47.288	44.810	1.00	38.72	C
ATOM	643	ODl	ASN	A	87	18.327	46.458	45.132	1.00	38.72	O
ATOM	644	ND2	ASN	A	87	16.427	47.573	45.576	1.00	39.63	N
ATOM	645	N	ARG	A	88	20.797	48.192	44.503	1.00	37.46	N
ATOM	646	CA	ARG	A	88	22.078	47.498	44.535	1.00	37.40	C
ATOM	647	C	ARG	A	88	21.953	46.060	44.036	1.00	36.62	C
ATOM	648	O	ARG	A	88	22.901	45.502	43.477	1.00	35.54	O
ATOM	649	CB	ARG	A	88	22.643	47.508	45.957	1.00	40.58	C
ATOM	650	CG	ARG	A	88	24.079	47.029	46.057	1.00	44.90	C
ATOM	651	CD	ARG	A	88	25.045	47.941	45.306	1.00	48.60	C
ATOM	652	NE	ARG	A	88	25.137	49.280	45.887	1.00	52.08	N
ATOM	653	CZ	ARG	A	88	24.327	50.294	45.590	1.00	53.40	C
ATOM	654	NHl	ARG	A	88	23.350	50.136	44.708	1.00	54.09	N
ATOM	655	NH2	ARG	A	88	24.496	51.470	46.179	1.00	55.03	N
ATOM	656	N	PHE	A	89	20.781	45.466	44.232	1.00	33.67	N
ATOM	657	CA	PHE	A	89	20.552	44.096	43.801	1.00	34.11	C
ATOM	658	C	PHE	A	89	20.582	44.006	42.276	1.00	32.02	C
ATOM	659	O	PHE	A	89	20.873	42.950	41.713	1.00	30.58	O
ATOM	660	CB	PHE	A	89	19.208	43.594	44.334	1.00	36.51	C
ATOM	661	CG	PHE	A	89	19.040	42.103	44.247	1.00	40.50	C
ATOM	662	CDl	PHE	A	89	19.947	41.252	44.872	1.00	42.36	C
ATOM	663	CD2	PHE	A	89	17.973	41.548	43.547	1.00	41.75	C
ATOM	664	CEl	PHE	A	89	19.794	39.868	44.802	1.00	42.90	C
ATOM	665	CE2	PHE	A	89	17.811	40.166	43.471	1.00	42.79	C
ATOM	666	CZ	PHE	A	89	18.724	39.325	44.100	1.00	43.72	C
ATOM	667	N	ALA	A	90	20.287	45.117	41.608	1.00	29.54	N

ATOM 668 CA ALA A 90 20.294 45.141 40.149 1.00 29.03 C
ATOM 669 C ALA A 90 21.715 44.933 39.633 1.00 28.32 C
ATOM 670 O ALA A 90 21.926 44.247 38.631 1.00 26.72 O
ATOM 671 CB ALA A 90 19.744 46.468 39.642 1.00 28.27 C
ATOM 672 N LYS A 91 22.685 45.525 40.324 1.00 27.70 N
ATOM 673 CA LYS A 91 24.084 45.406 39.932 1.00 29.11 C
ATOM 674 C LYS A 91 24.568 43.971 40.067 1.00 28.25 C
ATOM 675 O LYS A 91 25.323 43.485 39.227 1.00 27.53 O
ATOM 676 CB LYS A 91 24.963 46.321 40.789 1.00 30.61 C
ATOM 677 CG LYS A 91 24.677 47.801 40.619 1.00 33.79 C
ATOM 678 CD LYS A 91 25.528 48.634 41.568 1.00 35.88 C
ATOM 679 CE LYS A 91 25.196 50.112 41.454 1.00 38.08 C
ATOM 680 NZ LYS A 91 25.963 50.941 42.429 1.00 39.50 N
ATOM 681 N ILE A 92 24.132 43.295 41.126 1.00 27.47 N
ATOM 682 CA ILE A 92 24.535 41.913 41.354 1.00 27.53 C
ATOM 683 C ILE A 92 23.925 40.994 40.302 1.00 26.00 C
ATOM 684 O ILE A 92 24.617 40.146 39.741 1.00 24.98 O
ATOM 685 CB ILE A 92 24.123 41.435 42.759 1.00 29.67 C
ATOM 686 CGl ILE A 92 24.793 42.317 43.815 1.00 31.48 C
ATOM 687 CG2 ILE A 92 24.535 39.981 42.957 1.00 31.78 C
ATOM 688 CDl ILE A 92 24.324 42.049 45.235 1.00 33.19 C
ATOM 689 N LEU A 93 22.632 41.156 40.032 1.00 24.44 N
ATOM 690 CA LEU A 93 21.980 40.332 39.017 1.00 23.98 C
ATOM 691 C LEU A 93 22.652 40.621 37.684 1.00 22.80 C
ATOM 692 O LEU A 93 22.786 39.737 36.835 1.00 21.90 O
ATOM 693 CB LEU A 93 20.489 40.665 38.916 1.00 25.76 C
ATOM 694 CG LEU A 93 19.596 40.236 40.082 1.00 26.71 C
ATOM 695 CDl LEU A 93 18.183 40.749 39.855 1.00 27.43 C
ATOM 696 CD2 LEU A 93 19.605 38.722 40.208 1.00 28.90 C
ATOM 697 N GLY A 94 23.075 41.872 37.517 1.00 21.41 N

ATOM	698	CA	GLY	A	94	23.733	42.289	36.293	1.00	21.33
C										
ATOM	699	C	GLY	A	94	25.043	41.569	36.035	1.00	20.60
C										
ATOM	700	O	GLY	A	94	25.485	41.481	34.893	1.00	19.93
O										
ATOM	701	N	VAL	A	95	25.674	41.065	37.092	1.00	20.60
N										
ATOM	702	CA	VAL	A	95	26.942	40.349	36.947	1.00	20.40
C										
ATOM	703	C	VAL	A	95	26.809	39.138	36.022	1.00	20.26
C										
ATOM	704	O	VAL	A	95	27.770	38.738	35.364	1.00	19.90
O										
ATOM	705	CB	VAL	A	95	27.482	39.890	38.327	1.00	20.89
C										
ATOM	706	CGl	VAL	A	95	28.733	39.027	38.147	1.00	20.73
C										
ATOM	707	CG2	VAL	A	95	27.815	41.110	39.178	1.00	22.18
C										
ATOM	708	N	PHE	A	96	25.619	38.553	35.963	1.00	21.62
N										
ATOM	709	CA	PHE	A	96	25.404	37.402	35.096	1.00	22.50
C										
ATOM	710	C	PHE	A	96	25.606	37.771	33.628	1.00	22.55
C										
ATOM	711	O	PHE	A	96	25.913	36.912	32.803	1.00	21.20
O										
ATOM	712	CB	PHE	A	96	24.004	36.832	35.325	1.00	23.15
C										
ATOM	713	CG	PHE	A	96	23.897	35.984	36.560	1.00	22.89
C										
ATOM	714	CDl	PHE	A	96	24.418	34.693	36.574	1.00	24.21
C										
ATOM	715	CD2	PHE	A	96	23.298	36.477	37.714	1.00	24.26
C										
ATOM	716	CEl	PHE	A	96	24.345	33.900	37.722	1.00	24.88
C										
ATOM	717	CE2	PHE	A	96	23.219	35.694	38.870	1.00	26.71
C										
ATOM	718	CZ	PHE	A	96	23.744	34.402	38.872	1.00	26.36
C										
ATOM	719	N	GLY	A	97	25.454	39.058	33.321	1.00	21.51
N										
ATOM	720	CA	GLY	A	97	25.629	39.542	31.962	1.00	21.86
C										
ATOM	721	C	GLY	A	97	27.088	39.621	31.560	1.00	20.68
C										
ATOM	722	O	GLY	A	97	27.414	39.933	30.411	1.00	22.21
O										
ATOM	723	N	LEU	A	98	27.968	39.371	32.525	1.00	19.68
N										
ATOM	724	CA	LEU	A	98	29.405	39.349	32.286	1.00	20.46
C										
ATOM	725	C	LEU	A	98	29.868	37.910	32.487	1.00	18.90
C										
ATOM	726	O	LEU	A	98	30.708	37.404	31.744	1.00	18.98
O										
ATOM	727	CB	LEU	A	98	30.155	40.239	33.281	1.00	20.39
C										

ATOM	728	CG	LEU	A	98	29.921	41.750	33.255	1.00	23.20
C										
ATOM	729	CDl	LEU	A	98	30.854	42.411	34.262	1.00	22.08
C										
ATOM	730	CD2	LEU	A	98	30.166	42.290	31.852	1.00	23.77
C										
ATOM	731	N	TRP	A	99	29.301	37.257	33.498	1.00	17.84
N										
ATOM	732	CA	TRP	A	99	29.660	35.881	33.836	1.00	16.90
C										
ATOM	733	C	TRP	A	99	29.257	34.872	32.763	1.00	16.74
C										
ATOM	734	O	TRP	A	99	30.069	34.042	32.350	1.00	16.00
O										
ATOM	735	CB	TRP	A	99	29.018	35.497	35.173	1.00	16.88
C										
ATOM	736	CG	TRP	A	99	29.369	34.122	35.676	1.00	16.17
C										
ATOM	737	CDl	TRP	A	99	30.519	33.740	36.308	1.00	18.30
C										
ATOM	738	CD2	TRP	A	99	28.542	32.959	35.606	1.00	15.49
C										
ATOM	739	NEl	TRP	A	99	30.456	32.405	36.642	1.00	15.90
N										
ATOM	740	CE2	TRP	A	99	29.252	31.902	36.222	1.00	17.90
C										
ATOM	741	CE3	TRP	A	99	27.265	32.705	35.083	1.00	17.85
C										
ATOM	742	CZ2	TRP	A	99	28.726	30.609	36.330	1.00	17.45
C										
ATOM	743	CZ3	TRP	A	99	26.739	31.418	35.192	1.00	18.53
C										
ATOM	744	CH2	TRP	A	99	27.472	30.385	35.812	1.00	18.24
C										
ATOM	745	N	ILE	A	100	28.013	34.941	32.301	1.00	16.38
N										
ATOM	746	CA	ILE	A	100	27.562	33.999	31.283	1.00	16.90
C										
ATOM	747	C	ILE	A	100	28.420	34.064	30.019	1.00	15.91
C										
ATOM	748	O	ILE	A	100	28.942	33.042	29.579	1.00	15.79
O										
ATOM	749	CB	ILE	A	100	26.072	34.214	30.933	1.00	17.35
C										
ATOM	750	CGl	ILE	A	100	25.211	33.823	32.139	1.00	18.17
C										
ATOM	751	CG2	ILE	A	100	25.685	33.370	29.715	1.00	17.11
C										
ATOM	752	CDl	ILE	A	100	23.717	34.090	31.965	1.00	18.97
C										
ATOM	753	N	PRO	A	101	28.592	35.260	29.422	1.00	16.76
N										
ATOM	754	CA	PRO	A	101	29.421	35.308	28.212	1.00	17.48
C										
ATOM	755	C	PRO	A	101	30.871	34.876	28.443	1.00	17.52
C										
ATOM	756	O	PRO	A	101	31.466	34.235	27.582	1.00	18.45
O										
ATOM	757	CB	PRO	A	101	29.292	36.765	27.747	1.00	17.43
C										

ATOM 758 CG PRO A 101 28.975 37.514 29.017 1.00 17.63 C
ATOM 759 CD PRO A 101 28.007 36.582 29.713 1.00 14.48 C
ATOM 760 N LEU A 102 31.432 35.208 29.604 1.00 18.22 N
ATOM 761 CA LEU A 102 32.806 34.816 29.904 1.00 19.81 C
ATOM 762 C LEU A 102 32.917 33.296 30.006 1.00 18.42 C
ATOM 763 O LEU A 102 33.815 32.691 29.419 1.00 17.26 O
ATOM 764 CB LEU A 102 33.273 35.457 31.215 1.00 20.82 C
ATOM 765 CG LEU A 102 34.691 35.107 31.680 1.00 26.32 C
ATOM 766 CDl LEU A 102 35.709 35.704 30.710 1.00 27.02 C
ATOM 767 CD2 LEU A 102 34.929 35.652 33.090 1.00 27.86 C
ATOM 768 N VAL A 103 32.009 32.672 30.755 1.00 16.47 N
ATOM 769 CA VAL A 103 32.047 31.222 30.904 1.00 16.17 C
ATOM 770 C VAL A 103 31.811 30.531 29.565 1.00 15.74 C
ATOM 771 O VAL A 103 32.482 29.552 29.235 1.00 15.96 O
ATOM 772 CB VAL A 103 31.009 30.729 31.935 1.00 13.68 C
ATOM 773 CGl VAL A 103 30.932 29.201 31.926 1.00 16.58 C
ATOM 774 CG2 VAL A 103 31.414 31.201 33.329 1.00 15.44 C
ATOM 775 N VAL A 104 30.867 31.036 28.783 1.00 14.91 N
ATOM 776 CA VAL A 104 30.616 30.413 27.496 1.00 14.60 C
ATOM 777 C VAL A 104 31.827 30.605 26.593 1.00 14.56 C
ATOM 778 O VAL A 104 32.212 29.686 25.870 1.00 15.08 O
ATOM 779 CB VAL A 104 29.349 30.987 26.846 1.00 15.43 C
ATOM 780 CGl VAL A 104 29.173 30.431 25.428 1.00 15.87 C
ATOM 781 CG2 VAL A 104 28.147 30.612 27.703 1.00 16.09 C
ATOM 782 N ALA A 105 32.452 31.778 26.651 1.00 15.50 N
ATOM 783 CA ALA A 105 33.627 32.022 25.820 1.00 16.88 C
ATOM 784 C ALA A 105 34.725 31.005 26.125 1.00 17.84 C
ATOM 785 O ALA A 105 35.419 30.524 25.222 1.00 18.57 O
ATOM 786 CB ALA A 105 34.152 33.432 26.054 1.00 17.72 C
ATOM 787 N ILE A 106 34.875 30.675 27.403 1.00 16.03 N

ATOM	788	CA	ILE	A	106	35.908	29. 739	27. 830	1 .00	18. 74
C										
ATOM	789	C	ILE	A	106	35.870	28. 386	27. 114	1 .00	21. 50
C										
ATOM	790	O	ILE	A	106	36.926	27. 818	26. 817	1 .00	26. 35
O										
ATOM	791	CB	ILE	A	106	35.869	29. 566	29. 372	1 .00	20. 20
C										
ATOM	792	CGl	ILE	A	106	36.338	30. 871	30. 027	1 .00	21. 78
C										
ATOM	793	CG2	ILE	A	106	36.768	28. 405	29. 806	1 .00	22. 05
C										
ATOM	794	CDl	ILE	A	106	36.069	30. 973	31. 525	1 .00	23. 45
C										
ATOM	795	N	TYR	A	107	34.683	27. 859	26. 824	1 .00	17. 42
N										
ATOM	796	CA	TYR	A	107	34.624	26. 587	26. 118	1 .00	16. 78
C										
ATOM	797	C	TYR	A	107	34.308	26. 768	24. 641	1 .00	15. 95
C										
ATOM	798	O	TYR	A	107	34.732	25. 966	23. 818	1 .00	17. 34
O										
ATOM	799	CB	TYR	A	107	33.613	25. 623	26. 772	1 .00	17. 37
C										
ATOM	800	CG	TYR	A	107	32.151	26. 012	26. 706	1 .00	17. 28
C										
ATOM	801	CDl	TYR	A	107	31.359	25. 668	25. 604	1 .00	18. 09
C										
ATOM	802	CD2	TYR	A	107	31.544	26. 675	27. 771	1 .00	16. 24
C										
ATOM	803	CEl	TYR	A	107	29.991	25. 971	25. 573	1 .00	18. 34
C										
ATOM	804	CE2	TYR	A	107	30.179	26. 986	27. 749	1 .00	17. 03
C										
ATOM	805	CZ	TYR	A	107	29.412	26. 629	26. 651	1 .00	19. 08
C										
ATOM	806	OH	TYR	A	107	28.065	26. 916	26. 641	1 .00	22. 22
O										
ATOM	807	N	TYR	A	108	33.579	27. 832	24. 302	1 .00	15. 41
N										
ATOM	808	CA	TYR	A	108	33.213	28. 079	22. 910	1 .00	14. 29
C										
ATOM	809	C	TYR	A	108	34.452	28. 369	22. 055	1 .00	14. 82
C										
ATOM	810	O	TYR	A	108	34.565	27. 884	20. 926	1 .00	15. 01
O										
ATOM	811	CB	TYR	A	108	32.229	29. 256	22. 838	1 .00	14. 02
C										
ATOM	812	CG	TYR	A	108	31.486	29. 400	21. 522	1 .00	14. 51
C										
ATOM	813	CDl	TYR	A	108	30.185	28. 916	21. 381	1 .00	16. 49
C										
ATOM	814	CD2	TYR	A	108	32.069	30. 056	20. 437	1 .00	14. 90
C										
ATOM	815	CEl	TYR	A	108	29.473	29. 091	20. 194	1 .00	16. 85
C										
ATOM	816	CE2	TYR	A	108	31.370	30. 235	19. 243	1 .00	15. 39
C										
ATOM	817	CZ	TYR	A	108	30.070	29. 754	Jt9. 132	1 .00	16. 50
C										

ATOM	818	OH	TYR	A	108	29.358	29.964	17.974	1.00	17.07
O										
ATOM	819	N	VAL	A	109	35.386	29.153	22.583	1.00	14.32
N										
ATOM	820	CA	VAL	A	109	36.589	29.446	21.812	1.00	15.49
C										
ATOM	821	C	VAL	A	109	37.415	28.176	21.631	1.00	14.78
C										
ATOM	822	O	VAL	A	109	38.062	27.996	20.598	1.00	14.31
O										
ATOM	823	CB	VAL	A	109	37.464	30.524	22.470	1.00	16.81
C										
ATOM	824	CGl	VAL	A	109	38.693	30.792	21.598	1.00	20.10
C										
ATOM	825	CG2	VAL	A	109	36.663	31.810	22.624	1.00	18.67
C										
ATOM	826	N	TYR	A	110	37.406	27.290	22.621	1.00	14.48
N										
ATOM	827	CA	TYR	A	110	38.170	26.051	22.462	1.00	12.38
C										
ATOM	828	C	TYR	A	110	37.546	25.189	21.362	1.00	14.40
C										
ATOM	829	O	TYR	A	110	38.260	24.653	20.512	1.00	14.70
O										
ATOM	830	CB	TYR	A	110	38.248	25.274	23.787	1.00	14.31
C										
ATOM	831	CG	TYR	A	110	39.143	24.036	23.731	1.00	14.78
C										
ATOM	832	CDl	TYR	A	110	40.371	24.067	23.063	1.00	16.26
C										
ATOM	833	CD2	TYR	A	110	38.770	22.853	24.365	1.00	15.07
C										
ATOM	834	CEl	TYR	A	110	41.209	22.937	23.030	1.00	16.87
C										
ATOM	835	CE2	TYR	A	110	39.598	21.720	24.346	1.00	14.63
C										
ATOM	836	CZ	TYR	A	110	40.812	21.774	23.677	1.00	18.39
C										
ATOM	837	OH	TYR	A	110	41.638	20.672	23.672	1.00	19.13
O										
ATOM	838	N	ILE	A	111	36.221	25.051	21.356	1.00	12.27
N										
ATOM	839	CA	ILE	A	111	35.587	24.255	20.310	1.00	13.62
C										
ATOM	840	C	ILE	A	111	35.856	24.927	18.959	1.00	15.22
C										
ATOM	841	O	ILE	A	111	36.123	24.257	17.965	1.00	15.11
O										
ATOM	842	CB	ILE	A	111	34.067	24.104	20.540	1.00	14.16
C										
ATOM	843	CGl	ILE	A	111	33.812	23.356	21.853	1.00	15.89
C										
ATOM	844	CG2	ILE	A	111	33.459	23.303	19.404	1.00	13.93
C										
ATOM	845	CDl	ILE	A	111	32.353	23.402	22.310	1.00	18.48
C										
ATOM	846	N	GLU	A	112	35.803	26.256	18.931	1.00	13.74
N										
ATOM	847	CA	GLU	A	112	36.094	26.992	17.705	1.00	15.01
C										

ATOM 848 C GLU A 112 37.517 26.644 17.234 1.00 16.07 C
ATOM 849 O GLU A 112 37.756 26.455 16.031 1.00 16.84 O
ATOM 850 CB GLU A 112 35.980 28.492 17.973 1.00 16.08 C
ATOM 851 CG GLU A 112 36.495 29.387 16.864 1.00 18.81 C
ATOM 852 CD GLU A 112 36.402 30.845 17.257 1.00 21.07 C
ATOM 853 OEl GLU A 112 35.337 31.239 17.774 1.00 23.81 O
ATOM 854 OE2 GLU A 112 37.377 31.594 17.057 1.00 19.85 O
ATOM 855 N SER A 113 38.461 26.548 18.170 1.00 15.18 N
ATOM 856 CA SER A 113 39.833 26.215 17.781 1.00 16.04 C
ATOM 857 C SER A 113 39.903 24.827 17.141 1.00 15.42 C
ATOM 858 O SER A 113 40.719 24.611 16.249 1.00 16.31 O
ATOM 859 CB SER A 113 40.813 26.320 18.968 1.00 14.62 C
ATOM 860 OG SER A 113 40.672 25.262 19.894 1.00 16.58 O
ATOM 861 N TRP A 114 39.044 23.895 17.559 1.00 13.91 N
ATOM 862 CA TRP A 114 39.059 22.563 16.949 1.00 14.10 C
ATOM 863 C TRP A 114 38.711 22.674 15.466 1.00 14.44 C
ATOM 864 O TRP A 114 39.286 21.973 14.632 1.00 14.77 O
ATOM 865 CB TRP A 114 38.026 21.612 17.570 1.00 14.51 C
ATOM 866 CG TRP A 114 38.072 21.412 19.060 1.00 14.22 C
ATOM 867 CDl TRP A 114 39.009 21.868 19.937 1.00 15.37 C
ATOM 868 CD2 TRP A 114 37.088 20.723 19.841 1.00 16.20 C
ATOM 869 NEl TRP A 114 38.662 21.511 21.227 1.00 14.22 N
ATOM 870 CE2 TRP A 114 37.488 20.809 21.192 1.00 16.65 C
ATOM 871 CE3 TRP A 114 35.902 20.044 19.525 1.00 16.70 C
ATOM 872 CZ2 TRP A 114 36.744 20.239 22.232 1.00 17.79 C
ATOM 873 CZ3 TRP A 114 35.158 19.478 20.559 1.00 19.32 C
ATOM 874 CH2 TRP A 114 35.587 19.582 21.900 1.00 18.89 C
ATOM 875 N THR A 115 37.750 23.533 15.132 1.00 13.52 N
ATOM 876 CA THR A 115 37.362 23.668 13.733 1.00 15.57 C
ATOM 877 C THR A 115 38.516 24.230 12.909 1.00 14.65 C

ATOM 878 O THR A 115 38.682 23.859 11.747 1.00 16.50 O
ATOM 879 CB THR A 115 36.099 24.550 13.557 1.00 15.69 C
ATOM 880 OGl THR A 115 36.386 25.906 13.915 1.00 15.27 O
ATOM 881 CG2 THR A 115 34.966 24.018 14.440 1.00 16.26 C
ATOM 882 N LEU A 116 39.325 25.105 13.502 1.00 14.99 N
ATOM 883 CA LEU A 116 40.469 25.646 12.770 1.00 15.68 C
ATOM 884 C LEU A 116 41.507 24.538 12.605 1.00 15.62 C
ATOM 885 O LEU A 116 42.081 24.367 11.528 1.00 15.97 O
ATOM 886 CB LEU A 116 41.098 26.827 13.515 1.00 15.71 C
ATOM 887 CG LEU A 116 42.349 27.423 12.856 1.00 16.57 C
ATOM 888 CDl LEU A 116 42.028 27.908 11.441 1.00 19.28 C
ATOM 889 CD2 LEU A 116 42.877 28.561 13.720 1.00 17.63 C
ATOM 890 N GLY A 117 41.739 23.781 13.675 1.00 15.09 N
ATOM 891 CA GLY A 117 42.701 22.692 13.612 1.00 15.76 C
ATOM 892 C GLY A 117 42.307 21.659 12.569 1.00 17.40 C
ATOM 893 O GLY A 117 43.148 21.187 11.791 1.00 17.34 O
ATOM 894 N PHE A 118 41.029 21.293 12.553 1.00 14.18 N
ATOM 895 CA PHE A 118 40.536 20.329 11.575 1.00 14.95 C
ATOM 896 C PHE A 118 40.619 20.907 10.162 1.00 14.65 C
ATOM 897 O PHE A 118 40.989 20.205 9.219 1.00 15.01 O
ATOM 898 CB PHE A 118 39.087 19.935 11.883 1.00 15.47 C
ATOM 899 CG PHE A 118 38.954 18.787 12.848 1.00 17.73 C
ATOM 900 CDl PHE A 118 39.539 18.842 14.109 1.00 16.72 C
ATOM 901 CD2 PHE A 118 38.227 17.654 12.495 1.00 16.89 C
ATOM 902 CEl PHE A 118 39.401 17.784 15.011 1.00 19.17 C
ATOM 903 CE2 PHE A 118 38.079 16.588 13.384 1.00 18.29 C
ATOM 904 CZ PHE A 118 38.668 16.652 14.648 1.00 19.45 C
ATOM 905 N ALA A 119 40.266 22.180 10.009 1.00 15.90 N
ATOM 906 CA ALA A 119 40.322 22.810 8.696 1.00 17.29 C
ATOM 907 C ALA A 119 41.753 22.704 8.166 1.00 18.68 C

ATOM 908 O ALA A 119 41.972 22.325 7.011 1.00 18.07 O
ATOM 909 CB ALA A 119 39.891 24.273 8.786 1.00 17.28 C
ATOM 910 N ILE A 120 42.725 23.036 9.011 1.00 18.27 N
ATOM 911 CA ILE A 120 44.127 22.960 8.607 1.00 17.99 C
ATOM 912 C ILE A 120 44.519 21.537 8.202 1.00 18.42 C
ATOM 913 O ILE A 120 45.068 21.324 7.123 1.00 19.07 O
ATOM 914 CB ILE A 120 45.074 23.438 9.742 1.00 19.27 C
ATOM 915 CGl ILE A 120 44.872 24.936 9.988 1.00 18.42 C
ATOM 916 CG2 ILE A 120 46.536 23.163 9.360 1.00 20.36 C
ATOM 917 CDl ILE A 120 45.608 25.470 11.216 1.00 21.03 C
ATOM 918 N LYS A 121 44.231 20.557 9.056 1.00 16.79 N
ATOM 919 CA LYS A 121 44.591 19.179 8.736 1.00 18.77 C
ATOM 920 C LYS A 121 43.889 18.653 7.489 1.00 18.19 C
ATOM 921 O LYS A 121 44.489 17.917 6.700 1.00 18.09 O
ATOM 922 CB LYS A 121 44.301 18.263 9.923 1.00 19.45 C
ATOM 923 CG LYS A 121 45.085 18.663 11.155 1.00 25.80 C
ATOM 924 CD LYS A 121 44.904 17.669 12.285 1.00 30.24 C
ATOM 925 CE LYS A 121 45.853 16.498 12.120 1.00 32.87 C
ATOM 926 NZ LYS A 121 47.259 16.944 12.334 1.00 37.95 N
ATOM 927 N PHE A 122 42.624 19.021 7.298 1.00 17.32 N
ATOM 928 CA PHE A 122 41.912 18.544 6.117 1.00 19.01 C
ATOM 929 C PHE A 122 42.429 19.216 4.856 1.00 19.10 C
ATOM 930 O PHE A 122 42.517 18.583 3.803 1.00 20.58 O
ATOM 931 CB PHE A 122 40.402 18.759 6.254 1.00 18.51 C
ATOM 932 CG PHE A 122 39.704 17.642 6.981 1.00 18.56 C
ATOM 933 CDl PHE A 122 39.871 17.470 8.356 1.00 19.69 C
ATOM 934 CD2 PHE A 122 38.923 16.730 6.283 1.00 18.95 C
ATOM 935 CEl PHE A 122 39.271 16.400 9.024 1.00 18.80 C
ATOM 936 CE2 PHE A 122 38.319 15.656 6.938 1.00 19.41 C
ATOM 937 CZ PHE A 122 38.495 15.491 8.317 1.00 19.51 C

ATOM	938	N	LEU	A	123	42.774	20.493	4.965	1.00	19.27
N										
ATOM	939	CA	LEU	A	123	43.303	21.226	3.823	1.00	20.08
C										
ATOM	940	C	LEU	A	123	44.587	20.564	3.327	1.00	21.53
C										
ATOM	941	O	LEU	A	123	44.763	20.347	2.124	1.00	21.81
O										
ATOM	942	CB	LEU	A	123	43.603	22.677	4.210	1.00	21.31
C										
ATOM	943	CG	LEU	A	123	44.244	23.542	3.113	1.00	24.47
C										
ATOM	944	CDl	LEU	A	123	43.315	23.630	1.907	1.00	24.24
C										
ATOM	945	CD2	LEU	A	123	44.542	24.926	3.662	1.00	25.26
C										
ATOM	946	N	VAL	A	124	45.473	20.237	4.262	1.00	21.33
N										
ATOM	947	CA	VAL	A	124	46.760	19.627	3.936	1.00	23.01
C										
ATOM	948	C	VAL	A	124	46.702	18.115	3.730	1.00	23.99
C										
ATOM	949	O	VAL	A	124	47.709	17.484	3.390	1.00	24.50
O										
ATOM	950	CB	VAL	A	124	47.804	19.985	5.026	1.00	23.88
C										
ATOM	951	CGl	VAL	A	124	49.160	19.383	4.693	1.00	27.48
C										
ATOM	952	CG2	VAL	A	124	47.917	21.497	5.134	1.00	22.99
C										
ATOM	953	N	GLY	A	125	45.526	17.529	3.939	1.00	22.35
N										
ATOM	954	CA	GLY	A	125	45.366	16. 101	3.732	1.00	23.87
C										
ATOM	955	C	GLY	A	125	45.907	15.190	4.818	1.00	24.84
C										
ATOM	956	O	GLY	A	125	46.141	14.004	4.576	1.00	25.54
O										
ATOM	957	N	LEU	A	126	46.112	15.734	6.012	1.00	24.73
N										
ATOM	958	CA	LEU	A	126	46.606	14.941	7.128	1.00	25.36
C										
ATOM	959	C	LEU	A	126	45.370	14.417	7.849	1.00	27.49
C										
ATOM	960	O	LEU	A	126	45.081	14.798	8.984	1.00	29.12
O										
ATOM	961	CB	LEU	A	126	47.446	15.811	8.062	1.00	24.20
C										
ATOM	962	CG	LEU	A	126	48.719	16. 388	7.433	1.00	25.07
C										
ATOM	963	CDl	LEU	A	126	49.396	17.350	8.403	1.00	25.83
C										
ATOM	964	CD2	LEU	A	126	49. 653	15.247	7.059	1.00	24.04
C										
ATOM	965	N	VAL	A	127	44.640	13.549	7.162	1.00	28.86
N										
ATOM	966	CA	VAL	A	127	43.413	12.983	7.696	1.00	32.84
C										
ATOM	967	C	VAL	A	127	43.431	11.464	7.630	1.00	35.57
C										

ATOM	968	O	VAL	A	127	44.218	10.874	6.888	1.00	33.76
O										
ATOM	969	CB	VAL	A	127	42.190	13.508	6.911	1.00	33.20
C										
ATOM	970	CGl	VAL	A	127	42.122	15.018	7.018	1.00	34.67
C										
ATOM	971	CG2	VAL	A	127	42.285	13.090	5.454	1.00	34.31
C										
ATOM	972	N	PRO	A	128	42.553	10.809	8.404	1.00	39.14
N										
ATOM	973	CA	PRO	A	128	42.495	9.347	8.411	1.00	42.80
C										
ATOM	974	C	PRO	A	128	42.202	8.764	7.037	1.00	46.38
C										
ATOM	975	O	PRO	A	128	41.522	9.382	6.215	1.00	46.00
O										
ATOM	976	CB	PRO	A	128	41.395	9.051	9.430	1.00	42.48
C										
ATOM	977	CG	PRO	A	128	40.507	10.245	9.329	1.00	40.63
C										
ATOM	978	CD	PRO	A	128	41.496	11.379	9.258	1.00	40.00
C										
ATOM	979	N	GLU	A	129	42.734	7.573	6.793	1.00	50.90
N										
ATOM	980	CA	GLU	A	129	42.540	6.895	5.524	1.00	55.55
C										
ATOM	981	C	GLU	A	129	41.690	5.651	5.746	1.00	57.80
C										
ATOM	982	O	GLU	A	129	42.214	4.567	6.002	1.00	58.82
O										
ATOM	983	CB	GLU	A	129	43.894	6.502	4.929	1.00	57.40
C										
ATOM	984	CG	GLU	A	129	44.905	7.637	4.895	1.00	60.23
C										
ATOM	985	CD	GLU	A	129	46.202	7.242	4.219	1.00	62.00
C										
ATOM	986	OEl	GLU	A	129	46.793	6.213	4.614	1.00	62.87
O										
ATOM	987	OE2	GLU	A	129	46.633	7.964	3.294	1.00	63.29
O										
ATOM	988	N	PRO	A	130	40.359	5.796	5.669	1.00	59.91
N										
ATOM	989	CA	PRO	A	130	39.448	4.666	5.864	1.00	61.74
C										
ATOM	990	C	PRO	A	130	39.671	3.591	4.806	1.00	63.46
C										
ATOM	991	O	PRO	A	130	39.883	3.899	3.634	1.00	63.72
O										
ATOM	992	CB	PRO	A	130	38.070	5.312	5.740	1.00	61.38
C										
ATOM	993	CG	PRO	A	130	38.308	6.702	6.223	1.00	61.36
C										
ATOM	994	CD	PRO	A	130	39.606	7.056	5.550	1.00	60.23
C										
ATOM	995	N	PRO	A	131	39.634	2.312	5.208	1.00	65.15
N										
ATOM	996	CA	PRO	A	131	39.836	1.217	4.256	1.00	66.46
C										
ATOM	997	C	PRO	A	131	38.673	1.131	3.271	1.00	67.41
C										

ATOM 998 O PRO A 131 37.553 0.790 3.648 1.00 67.97 O
ATOM 999 CB PRO A 131 39.932 -0.007 5.161 1.00 66.17 C
ATOM 1000 CG PRO A 131 39.024 0.352 6.295 1.00 66.03 C
ATOM 1001 CD PRO A 131 39.400 1.791 6.566 1.00 65.69 C
ATOM 1002 N PRO A 132 38.927 1.458 1.993 1.00 68.41 N
ATOM 1003 CA PRO A 132 37.914 1.426 0.932 1.00 69.10 C
ATOM 1004 C PRO A 132 37.289 0.047 0.727 1.00 69.35 C
ATOM 1005 O PRO A 132 37.017 -0.677 1.683 1.00 69.72 O
ATOM 1006 CB PRO A 132 38.692 1.892 -0.297 1.00 69.18 C
ATOM 1007 CG PRO A 132 39.725 2.806 0.288 1.00 69.28 C
ATOM 1008 CD PRO A 132 40.192 2.014 1.483 1.00 68.80 C
ATOM 1009 N THR A 135 33.540 -1.470 2.986 1.00 62.04 N
ATOM 1010 CA THR A 135 32.161 -1.005 3.056 1.00 62.37 C
ATOM 1011 C THR A 135 31.654 -1.000 4.494 1.00 61.62 C
ATOM 1012 O THR A 135 30.639 -0.375 4.801 1.00 62.14 O
ATOM 1013 CB THR A 135 31.228 -1.895 2.211 1.00 63.11 C
ATOM 1014 OGl THR A 135 31.289 -3.245 2.691 1.00 64.37 O
ATOM 1015 CG2 THR A 135 31.643 -1.863 0.747 1.00 63.79 C
ATOM 1016 N ASP A 136 32.367 -1.702 5.370 1.00 60.97 N
ATOM 1017 CA ASP A 136 32.002 -1.778 6.781 1.00 59.66 C
ATOM 1018 C ASP A 136 31.886 -0.370 7.360 1.00 58.47 C
ATOM 1019 O ASP A 136 32.862 0.377 7.394 1.00 58.28 O
ATOM 1020 CB ASP A 136 33.061 -2.574 7.551 1.00 60.55 C
ATOM 1021 CG ASP A 136 32.711 -2.752 9.017 1.00 61.11 C
ATOM 1022 ODl ASP A 136 33.523 -3.358 9.749 1.00 61.37 O
ATOM 1023 OD2 ASP A 136 31.630 -2.291 9.439 1.00 61.94 O
ATOM 1024 N PRO A 137 30.682 0.008 7.824 1.00 56.89 N
ATOM 1025 CA PRO A 137 30.436 1.333 8.402 1.00 55.40 C
ATOM 1026 C PRO A 137 31.366 1.716 9.553 1.00 54.12 C
ATOM 1027 O PRO A 137 31.699 2.890 9.723 1.00 54.11 O

ATOM	1028	CB	PRO	A	137	28.969	1.256	8.831	1.00	55.87
C										
ATOM	1029	CG	PRO	A	137	28.766	-0.206	9.098	1.00	56.60
C										
ATOM	1030.	CD	PRO	A	137	29.482	-0.837	7.935	1.00	56.52
C										
ATOM	1031	N	ASP	A	138	31. 783	0.731	10.342	1.00	52.25
N										
ATOM	1032	CA	ASP	A	138	32.677	0.995	11.464	1.00	50.27
C										
ATOM	1033	C	ASP	A	138	34.128	1.174	11.027	1.00	48.08
C										
ATOM	1034	O	ASP	A	138	34.885	1.908	11.662	1.00	46. 29
O										
ATOM	1035	CB	ASP	A	138	32.585	-0.131	12.498	1.00	52.70
C										
ATOM	1036	CG	ASP	A	138	31. 498	0.113	13. 527	1.00	55. 54
C										
ATOM	1037	ODl	ASP	A	138	31.580	1.135	14.241	1.00	57.07
O										
ATOM	1038	OD2	ASP	A	138	30.564	-0.712	13.624	1.00	57.98
O										
ATOM	1039	N	SER	A	139	34.513	0.505	9.945	1.00	45.35
N										
ATOM	1040	CA	SER	A	139	35.877	0.607	9.437	1.00	43.95
C										
ATOM	1041	C	SER	A	139	36.120	1.995	8.854	1.00	41.43
C										
ATOM	1042	O	SER	A	139	37.264	2.434	8.721	1.00	40.86
O										
ATOM	1043	CB	SER	A	139	36. 128	-0.453	8.361	1.00	44.88
C										
ATOM	1044	OG	SER	A	139	35.310	-0.232	7.226	1.00	47.83
O										
ATOM	1045	N	ILE	A	140	35.034	2.682	8.512	1.00	38.89
N										
ATOM	1046	CA	ILE	A	140	35.120	4.023	7.944	1.00	37.27
C										
ATOM	1047	C	ILE	A	140	34.994	5.100	9.019	1.00	34.92
C										
ATOM	1048	O	ILE	A	140	35.725	6.088	9.004	1.00	34.97
O										
ATOM	1049	CB	ILE	A	140	34.016	4.250	6.888	1.00	37.69
C										
ATOM	1050	CGl	ILE	A	140	34.142	3.206	5.777	1.00	38.47
C										
ATOM	1051	CG2	ILE	A	140	34.129	5.657	6.312	1.00	37.51
C										
ATOM	1052	CDl	ILE	A	140	33.073	3.304	4.708	1.00	38.14
C										
ATOM	1053	N	LEU	A	141	34.065	4.899	9.949	1.00	31.99
N										
ATOM	1054	CA	LEU	A	141	33.835	5.852	11.032	1.00	31.65
C										
ATOM	1055	C	LEU	A	141	34.907	5.816	12.113	1.00	29.40
C										
ATOM	1056	O	LEU	A	141	35.293	6.856	12.645	1.00	26.97
O										
ATOM	1057	CB	LEU	A	141	32.473	5.598	11.684	1.00	31.54
C										

ATOM 1058 CG LEU A 141 31.217 6.028 10.920 1.00 34.28 C
ATOM 1059 CDl LEU A 141 29.973 5.506 11.633 1.00 34.09 C
ATOM 1060 CD2 LEU A 141 31.178 7.545 10.823 1.00 32.63 C
ATOM 1061 N ARG A 142 35.387 4.620 12.436 1.00 28.34 N
ATOM 1062 CA ARG A 142 36.392 4.473 13.482 1.00 28.60 C
ATOM 1063 C ARG A 142 37.612 5.371 13.306 1.00 26.01 C
ATOM 1064 O ARG A 142 38.051 6.005 14.261 1.00 23.47 O
ATOM 1065 CB ARG A 142 36.847 3.011 13.610 1.00 30.52 C
ATOM 1066 CG ARG A 142 37.732 2.776 14.835 1.00 35.78 C
ATOM 1067 CD ARG A 142 38.211 1.332 14.972 1.00 39.08 C
ATOM 1068 NE ARG A 142 37.109 0.378 15.023 1.00 43.50 N
ATOM 1069 CZ ARG A 142 36.665 -0.308 13.974 1.00 45.64 C
ATOM 1070 NHl ARG A 142 37.236 -0.153 12.787 1.00 47.40 N
ATOM 1071 NH2 ARG A 142 35.644 -1.142 14.109 1.00 46.88 N
ATOM 1072 N PRO A 143 38.183 5.434 12.088 1.00 26.06 N
ATOM 1073 CA PRO A 143 39.357 6.287 11.875 1.00 25.31 C
ATOM 1074 C PRO A 143 39.082 7.757 12.193 1.00 22.52 C
ATOM 1075 O PRO A 143 39.956 8.471 12.678 1.00 22.07 O
ATOM 1076 CB PRO A 143 39.679 6.070 10.395 1.00 26.73 C
ATOM 1077 CG PRO A 143 39.208 4.672 10.152 1.00 28.27 C
ATOM 1078 CD PRO A 143 37.883 4.651 10.874 1.00 27.63 C
ATOM 1079 N PHE A 144 37.867 8.209 11.905 1.00 21.87 N
ATOM 1080 CA PHE A 144 37.511 9.594 12.173 1.00 20.56 C
ATOM 1081 C PHE A 144 37.242 9.821 13.651 1.00 19.57 C
ATOM 1082 O PHE A 144 37.521 10.895 14.182 1.00 18.68 O
ATOM 1083 CB PHE A 144 36.318 9.999 11.307 1.00 20.91 C
ATOM 1084 CG PHE A 144 36.685 10.202 9.866 1.00 22.17 C
ATOM 1085 CDl PHE A 144 37.200 11.420 9.435 1.00 22.72 C
ATOM 1086 CD2 PHE A 144 36.601 9.150 8.960 1.00 22.13 C
ATOM 1087 CEl PHE A 144 37.634 11.590 8.118 1.00 24.07 C

ATOM	1088	CE2	PHE	A	144	37.034	9.312	7.638	1.00	22.34
C										
ATOM	1089	CZ	PHE	A	144	37.550	10.529	7.222	1.00	23.49
C										
ATOM	1090	N	LYS	A	145	36.712	8.807	14.324	1.00	19.90
N										
ATOM	1091	CA	LYS	A	145	36.477	8.941	15.753	1.00	21.41
C										
ATOM	1092	C	LYS	A	145	37.842	9.022	16.432	1.00	21.32
C										
ATOM	1093	O	LYS	A	145	38.064	9.857	17.305	1.00	19.97
O										
ATOM	1094	CB	LYS	A	145	35.692	7.746	16.294	1.00	23.81
C										
ATOM	1095	CG	LYS	A	145	35.546	7.766	17.812	1.00	28.66
C										
ATOM	1096	CD	LYS	A	145	34.554	6.723	18.299	1.00	33.76
C										
ATOM	1097	CE	LYS	A	145	33.131	7.089	17.895	1.00	37.82
C										
ATOM	1098	NZ	LYS	A	145	32.686	8.374	18.501	1.00	41.22
N										
ATOM	1099	N	GLU	A	146	38.768	8.161	16.016	1.00	20.96
N										
ATOM	1100	CA	GLU	A	146	40.105	8.169	16.605	1.00	22.40
C										
ATOM	1101	C	GLU	A	146	40.789	9.509	16.351	1.00	19.52
C										
ATOM	1102	O	GLU	A	146	41.528	10.012	17.198	1.00	19.43
O										
ATOM	1103	CB	GLU	A	146	40.960	7.047	16.016	1.00	24.81
C										
ATOM	1104	CG	GLU	A	146	40.363	5.663	16.167	1.00	30.22
C										
ATOM	1105	CD	GLU	A	146	41.262	4.590	15.584	1.00	32.39
C										
ATOM	1106	OEl	GLU	A	146	41.871	4.841	14.525	1.00	36.48
O										
ATOM	1107	OE2	GLU	A	146	41.350	3.496	16.175	1.00	34.05
O										
ATOM	1108	N	PHE	A	147	40.534	10.084	15.180	1.00	18.52
N										
ATOM	1109	CA	PHE	A	147	41.118	11.368	14.802	1.00	18.22
C										
ATOM	1110	C	PHE	A	147	40.680	12.451	15.794	1.00	17.78
C										
ATOM	1111	O	PHE	A	147	41.503	13.207	16.315	1.00	16.70
O										
ATOM	1112	CB	PHE	A	147	40.663	11.738	13.388	1.00	20.40
C										
ATOM	1113	CG	PHE	A	147	41.312	12.979	12.840	1.00	22.99
C										
ATOM	1114	CDl	PHE	A	147	42.581	12.927	12.271	1.00	26.40
C										
ATOM	1115	CD2	PHE	A	147	40.644	14.199	12.874	1.00	24.15
C										
ATOM	1116	CEl	PHE	A	147	43.172	14.072	11.738	1.00	28.00
C										
ATOM	1117	CE2	PHE	A	147	41.224	15.350	12.346	1.00	27.28
C										

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ATOM   1118  CZ  PHE A 147      42.492  15.287  11.774  1.00 29.06
C
ATOM   1119  N   LEU A 148      39.378  12.533  16.045  1.00 16.64
N
ATOM   1120  CA  LEU A 148      38.869  13.526  16.989  1.00 18.91
C
ATOM   1121  C   LEU A 148      39.380  13.245  18.403  1.00 18.33
C
ATOM   1122  O   LEU A 148      39.843  14.155  19.099  1.00 18.08
O
ATOM   1123  CB  LEU A 148      37.336  13.521  17.007  1.00 18.41
C
ATOM   1124  CG  LEU A 148      36.751  14.394  18.126  1.00 20.89
C
ATOM   1125  CDl LEU A 148      37.134  15.851  17.899  1.00 18.83
C
ATOM   1126  CD2 LEU A 148      35.242  14.229  18.165  1.00 20.99
C
ATOM   1127  N   TYR A 149      39.294  11.986  18.823  1.00 18.70
N
ATOM   1128  CA  TYR A 149      39.722  11.598  20.167  1.00 19.98
C
ATOM   1129  C   TYR A 149      41.194  11.883  20.450  1.00 21.14
C
ATOM   1130  O   TYR A 149      41.552  12.236  21.575  1.00 21.06
O
ATOM   1131  CB  TYR A 149      39.402  10.118  20.411  1.00 21.10
C
ATOM   1132  CG  TYR A 149      37.938   9.850  20.713  1.00 23.87
C
ATOM   1133  CDl TYR A 149      36.933  10.665  20.190  1.00 25.13
C
ATOM   1134  CD2 TYR A 149      37.558   8.773  21.513  1.00 28.15
C
ATOM   1135  CEl TYR A 149      35.582  10.414  20.457  1.00 26.09
C
ATOM   1136  CE2 TYR A 149      36.211   8.513  21.786  1.00 28.59
C
ATOM   1137  CZ  TYR A 149      35.232   9.339  21.254  1.00 28.95
C
ATOM   1138  OH  TYR A 149      33.902   9.093  21.529  1.00 30.31
O
ATOM   1139  N   SER A 150      42.046  11.735  19.438  1.00 20.99
N
ATOM   1140  CA  SER A 150      43.471  12.007  19.614  1.00 21.65
C
ATOM   1141  C   SER A 150      43.731  13.508  19.621  1.00 21.29
C
ATOM   1142  O   SER A 150      44.684  13.980  20.243  1.00 21.02
O
ATOM   1143  CB  SER A 150      44.286  11.367  18.484  1.00 24.11
C
ATOM   1144  OG  SER A 150      44.108   9.964  18.476  1.00 30.32
O
ATOM   1145  N   TYR A 151      42.881  14.260  18.930  1.00 17.53
N
ATOM   1146  CA  TYR A 151      43.044  15.704  18.859  1.00 17.31
C
ATOM   1147  C   TYR A 151      42.771  16.338  20.218  1.00 17.08
C
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ATOM	1148	O	TYR	A	151	43.600	17.084	20.738	1.00	17.24
ATOM	1149	CB	TYR	A	151	42.088	16.298	17.823	1.00	16.69
ATOM	1150	CG	TYR	A	151	42.287	17.777	17.563	1.00	16.92
ATOM	1151	CDl	TYR	A	151	43.163	18.219	16.572	1.00	18.15
ATOM	1152	CD2	TYR	A	151	41.591	18.734	18.301	1.00	17.01
ATOM	1153	CEl	TYR	A	151	43.342	19.574	16.317	1.00	17.15
ATOM	1154	CE2	TYR	A	151	41.761	20.093	18.053	1.00	17.60
ATOM	1155	CZ	TYR	A	151	42.639	20.505	17.060	1.00	17.22
ATOM	1156	OH	TYR	A	151	42.823	21.842	16.813	1.00	16.18
ATOM	1157	N	ILE	A	152	41.605	16.044	20.788	1.00	17.83
ATOM-	1158	CA	ILE	A	152	41.247	16.621	22.080	1.00	18.85
ATOM	1159	C	ILE	A	152	41.772	15.801	23.252	1.00	19.58
ATOM	1160	O	ILE	A	152	41.809	16.278	24.388	1.00	19.64
ATOM	1161	CB	ILE	A	152	39.715	16.809	22.207	1.00	21.17
ATOM	1162	CGl	ILE	A	152	39.003	15.457	22.179	1.00	21.03
ATOM	1163	CG2	ILE	A	152	39.207	17.704	21.069	1.00	21.04
ATOM	1164	CDl	ILE	A	152	37.489	15.557	22.302	1.00	26.54
ATOM	1165	N	GLY	A	153	42.191	14.570	22.975	1.00	19.38
ATOM	1166	CA	GLY	A	153	42.731	13.721	24.024	1.00	20.06
ATOM	1167	C	GLY	A	153	41.731	13.074	24.966	1.00	20.55
ATOM	1168	O	GLY	A	153	41.907	13.115	26.184	1.00	21.34
ATOM	1169	N	VAL	A	154	40.686	12.470	24.413	1.00	18.98
ATOM	1170	CA	VAL	A	154	39.673	11.788	25.218	1.00	19.96
ATOM	1171	C	VAL	A	154	40.340	10.734	26.112	1.00	21.84
ATOM	1172	O	VAL	A	154	41.261	10.034	25.680	1.00	20.92
ATOM	1173	CB	VAL	A	154	38.626	11.108	24.299	1.00	20.42
ATOM	1174	CGl	VAL	A	154	37.630	10.301	25.124	1.00	22.23
ATOM	1175	CG2	VAL	A	154	37.899	12.175	23.477	1.00	21.97
ATOM	1176	N	PRO	A	155	39.881	10.608	27.370	1.00	22.63
ATOM	1177	CA	PRO	A	155	40.446	9.636	28.314	1.00	24.38

ATOM	1178	C	PRO	A	155	40.376	8.198	27.822	1.00	26.69
C										
ATOM	1179	O	PRO	A	155	39.330	7.734	27.366	1.00	24.79
O										
ATOM	1180	CB	PRO	A	155	39.600	9.834	29.570	1.00	24.80
C										
ATOM	1181	CG	PRO	A	155	39.155	11.247	29.469	1.00	24.19
C										
ATOM	1182	CD	PRO	A	155	38.814	11.393	28.017	1.00	23.48
C										
ATOM	1183	N	LYS	A	156	41.495	7.492	27.933	1.00	28.73
N										
ATOM	1184	CA	LYS	A	156	41.557	6.101	27.512	1.00	32.89
C										
ATOM	1185	C	LYS	A	156	41.424	5.186	28.728	1.00	34.81
C										
ATOM	1186	O	LYS	A	156	41.244	3.976	28.588	1.00	35.15
O										
ATOM	1187	CB	LYS	A	156	42.876	5.831	26.783	1.00	32.96
C										
ATOM	1188	CG	LYS	A	156	43.023	6.609	25.478	1.00	35.09
C										
ATOM	1189	CD	LYS	A	156	44.348	6.321	24.777	1.00	37.69
C										
ATOM	1190	CE	LYS	A	156	45.540	6.844	25.569	1.00	40.00
C										
ATOM	1191	NZ	LYS	A	156	45.565	8.333	25.674	1.00	40.53
N										
ATOM	1192	N	GLY	A	157	41.496	5.776	29.919	1.00	36.47
N										
ATOM	1193	CA	GLY	A	157	41.388	4.998	31.142	1.00	39.17
C										
ATOM	1194	C	GLY	A	157	40.251	5.411	32.063	1.00	40.87
C										
ATOM	1195	O	GLY	A	157	39.156	5.744	31.607	1.00	42.30
O										
ATOM	1196	N	ASP	A	158	40.516	5.392	33.367	1.00	41.87
N										
ATOM	1197	CA	ASP	A	158	39.513	5.750	34.366	1.00	42.90
C										
ATOM	1198	C	ASP	A	158	39.611	7.199	34.825	1.00	41.36
C										
ATOM	1199	O	ASP	A	158	38.618	7.784	35.264	1.00	43.05
O										
ATOM	1200	CB	ASP	A	158	39.640	4.834	35.582	1.00	46.01
C										
ATOM	1201	CG	ASP	A	158	39.431	3.381	35.235	1.00	49.48
C										
ATOM	1202	ODl	ASP	A	158	38.316	3.031	34.791	1.00	51.32
O										
ATOM	1203	OD2	ASP	A	158	40.384	2.589	35.405	1.00	52.95
O										
ATOM	1204	N	GLU	A	159	40.808	7.770	34.738	1.00	38.24
N										
ATOM	1205	CA	GLU	A	159	41.021	9.151	35.151	1.00	35.51
C										
ATOM	1206	C	GLU	A	159	40.258	10.095	34.221	1.00	32.14
C										
ATOM	1207	O	GLU	A	159	40.268	9.928	33.002	1.00	30.67
O										

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ATOM   1208  CB  GLU A 159      42.515   9.481  35.133  1.00 37.86
C
ATOM   1209  CG  GLU A 159      43.351   8.546  35.999  1.00 42.79
C
ATOM   1210  CD  GLU A 159      44.826   8.890  35.978  1.00 45.54
C
ATOM   1211  OEl GLU A 159      45.397   8.998  34.870  1.00 48.15
O
ATOM   1212  OE2 GLU A 159      45.419   9.043  37.068  1.00 47.35
O
ATOM   1213  N   PRO A 160      39.579  11.097  34.793  1.00 28.89
N
ATOM   1214  CA  PRO A 160      38.802  12.071  34.018  1.00 26.34
C
ATOM   1215  C   PRO A 160      39.689  13.173  33.457  1.00 25.23
C
ATOM   1216  O   PRO A 160      39.352  14.353  33.539  1.00 26.23
O
ATOM   1217  CB  PRO A 160      37.817  12.601  35.048  1.00 27.07
C
ATOM   1218  CG  PRO A 160      38.674  12.659  36.285  1.00 27.10
C
ATOM   1219  CD  PRO A 160      39.437  11.342  36.242  1.00 28.54
C
ATOM   1220  N   ILE A 161      40.818  12.779  32.881  1.00 23.43
N
ATOM   1221  CA  ILE A 161      41.778  13.728  32.342  1.00 25.02
C
ATOM   1222  C   ILE A 161      41.921  13.689  30.827  1.00 24.68
C
ATOM   1223  O   ILE A 161      42.016  12.619  30.232  1.00 25.86
O
ATOM   1224  CB  ILE A 161      43.166  13.484  32.964  1.00 27.61
C
ATOM   1225  CGl ILE A 161      43.062  13.588  34.484  1.00 31.01
C
ATOM   1226  CG2 ILE A 161      44.177  14.471  32.409  1.00 31.69
C
ATOM   1227  CDl ILE A 161      42.407  14.864  34.959  1.00 30.00
C
ATOM   1228  N   LEU A 162      41.951  14.871  30.218  1.00 22.19
N
ATOM   1229  CA  LEU A 162      42.110  14.996  28.775  1.00 22.19
C
ATOM   1230  C   LEU A 162      43.576  15.274  28.463  1.00 22.85
C
ATOM   1231  O   LEU A 162      44.279  15.916  29.247  1.00 20.86
O
ATOM   1232  CB  LEU A 162      41.246  16.141  28.246  1.00 20.19
C
ATOM   1233  CG  LEU A 162      39.733  15.963  28.395  1.00 20.70
C
ATOM   1234  CDl LEU A 162      39.030  17.303  28.232  1.00 21.48
C
ATOM   1235  CD2 LEU A 162      39.245  14.954  27.362  1.00 23.07
C
ATOM   1236  N   LYS A 163      44.034  14.786  27.315  1.00 25.62
N
ATOM   1237  CA  LYS A 163      45.417  14.975  26.896  1.00 27.13
C
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ATOM   1238  C   LYS A 163      45.411  15.499  25.461  1.00 27.29
C
ATOM   1239  O   LYS A 163      45.694  14.757  24.524  1.00 26.92
O
ATOM   1240  CB  LYS A 163      46.158  13.637  26.959  1.00 32.09
C
ATOM   1241  CG  LYS A 163      47.666  13.726  27.142  1.00 37.40
C
ATOM   1242  CD  LYS A 163      48.352  14.471  26.020  1.00 40.69
C
ATOM   1243  CE  LYS A 163      49.850  14.223  26.073  1.00 43.41
C
ATOM   1244  NZ  LYS A 163      50.390  14.383  27.450  1.00 46.78
N
ATOM   1245  N   PRO A 164      45.080  16.787  25.276  1.00 27.67
N
ATOM   1246  CA  PRO A 164      45.035  17.408  23.948  1.00 26.92
C
ATOM   1247  C   PRO A 164      46.379  17.302  23.241  1.00 24.77
C
ATOM   1248  O   PRO A 164      47.432  17.378  23.879  1.00 22.75
O
ATOM   1249  CB  PRO A 164      44.690  18.863  24.249  1.00 28.06
C
ATOM   1250  CG  PRO A 164      44.011  18.803  25.584  1.00 31.39
C
ATOM   1251  CD  PRO A 164      44.806  17.781  26.326  1.00 29.01
C
ATOM   1252  N   SER A 165      46.340  17.141  21.924  1.00 22.61
N
ATOM   1253  CA  SER A 165      47.567  17.051  21.149  1.00 21.72
C
ATOM   1254  C   SER A 165      48.264  18.407  21.175  1.00 20.88
C
ATOM   1255  O   SER A 165      47.636  19.441  21.439  1.00 18.33
O
ATOM   1256  CB  SER A 165      47.262  16.660  19.700  1.00 22.05
C
ATOM   1257  OG  SER A 165      46.601  17.706  19.007  1.00 21.50
O
ATOM   1258  N   LEU A 166      49.565  18.404  20.908  1.00 20.53
N
ATOM   1259  CA  LEU A 166      50.327  19.644  20.885  1.00 20.17
C
ATOM   1260  C   LEU A 166      49.752  20.556  19.805  1.00 18.92
C
ATOM   1261  O   LEU A 166      49.644  21.767  19.989  1.00 18.93
O
ATOM   1262  CB  LEU A 166      51.803  19.359  20.584  1.00 21.06
C
ATOM   1263  CG  LEU A 166      52.690  20.602  20.459  1.00 25.01
C
ATOM   1264  CDl LEU A 166      52.576  21.457  21.719  1.00 23.59
C
ATOM   1265  CD2 LEU A 166      54.138  20.173  20.235  1.00 26.67
C
ATOM   1266  N   PHE A 167      49.388  19.962  18.675  1.00 18.90
N
ATOM   1267  CA  PHE A 167      48.812  20.721  17.580  1.00 19.10
C
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ATOM 1268 C PHE A 167 47.536 21.428 18.056 1.00 18.36 C
ATOM 1269 O PHE A 167 47.347 22.610 17.795 1.00 19.80 O
ATOM 1270 CB PHE A 167 48.488 19.797 16.406 1.00 20.27 C
ATOM 1271 CG PHE A 167 47.872 20.505 15.237 1.00 22.38 C
ATOM 1272 CDl PHE A 167 48.571 21.501 14.562 1.00 22.64 C
ATOM 1273 CD2 PHE A 167 46.591 20.178 14.808 1.00 22.75 C
ATOM 1274 CEl PHE A 167 48.002 22.163 13.472 1.00 25.18 C
ATOM 1275 CE2 PHE A 167 46.015 20.832 13.721 1.00 21.69 C
ATOM 1276 CZ PHE A 167 46.722 21.824 13.053 1.00 22.29 C
ATOM 1277 N ALA A 168 46.667 20.701 18.751 1.00 17.51 N
ATOM 1278 CA ALA A 168 45.422 21.290 19.256 1.00 17.26 C
ATOM 1279 C ALA A 168 45.693 22.478 20.173 1.00 18.21 C
ATOM 1280 O ALA A 168 45.002 23.497 20.110 1.00 15.93 O
ATOM 1281 CB ALA A 168 44.612 20.243 20.005 1.00 16.69 C
ATOM 1282 N TYR A 169 46.700 22.343 21.031 1.00 17.16 N
ATOM 1283 CA TYR A 169 47.043 23.407 21.967 1.00 18.31 C
ATOM 1284 C TYR A 169 47.542 24.644 21.233 1.00 19.10 C
ATOM 1285 O TYR A 169 47.124 25.764 21.527 1.00 19.62 O
ATOM 1286 CB TYR A 169 48.110 22.920 22.946 1.00 19.96 C
ATOM 1287 CG TYR A 169 48.322 23.864 24.105 1.00 20.95 C
ATOM 1288 CDl TYR A 169 47.413 23.912 25.162 1.00 21.57 C
ATOM 1289 CD2 TYR A 169 49.419 24.723 24.135 1.00 23.49 C
ATOM 1290 CEl TYR A 169 47.592 24.794 26.224 1.00 21.03 C
ATOM 1291 CE2 TYR A 169 49.607 25.611 25.190 1.00 24.29 C
ATOM 1292 CZ TYR A 169 48.691 25.639 26.230 1.00 23.13 C
ATOM 1293 OH TYR A 169 48.883 26.503 27.277 1.00 24.24 O
ATOM 1294 N ILE A 170 48.440 24.437 20.277 1.00 18.14 N
ATOM 1295 CA ILE A 170 48.977 25.537 19.489 1.00 19.87 C
ATOM 1296 C ILE A 170 47.855 26.207 18.690 1.00 18.89 C
ATOM 1297 O ILE A 170 47.810 27.429 18.582 1.00 19.69 O

ATOM	1298	CB	ILE	A	170	50.075	25.032	18.525	1.00	22.23
C										
ATOM	1299	CGl	ILE	A	170	51.289	24.572	19.339	1.00	24.30
C										
ATOM	1300	CG2	ILE	A	170	50.461	26.128	17.535	1.00	24.13
C										
ATOM	1301	CDl	ILE	A	170	52.394	23.939	18.509	1.00	28.78
C										
ATOM	1302	N	VAL	A	171	46.943	25.408	18.139	1.00	17.21
N										
ATOM	1303	CA	VAL	A	171	45.841	25.974	17.372	1.00	17.52
C										
ATOM	1304	C	VAL	A	171	44.916	26.811	18.265	1.00	16.60
C										
ATOM	1305	O	VAL	A	171	44.326	27.790	17.809	1.00	16.38
O										
ATOM	1306	CB	VAL	A	171	45.045	24.867	16.645	1.00	17.07
C										
ATOM	1307	CGl	VAL	A	171	43.800	25.448	16.002	1.00	16.37
C										
ATOM	1308	CG2	VAL	A	171	45.928	24.237	15.565	1.00	18.46
C										
ATOM	1309	N	PHE	A	172	44.794	26.440	19.534	1.00	17.15
N										
ATOM	1310	CA	PHE	A	172	43.960	27.225	20.448	1.00	17.10
C										
ATOM	1311	C	PHE	A	172	44.630	28.587	20.636	1.00	18.72
C										
ATOM	1312	O	PHE	A	172	43.963	29.625	20.646	1.00	16.50
O										
ATOM	1313	CB	PHE	A	172	43.804	26.524	21.798	1.00	17.30
C										
ATOM	1314	CG	PHE	A	172	42.991	27.313	22.794	1.00	16.54
C										
ATOM	1315	CDl	PHE	A	172	41.667	27.648	22.522	1.00	17.98
C										
ATOM	1316	CD2	PHE	A	172	43.554	27.736	23.989	1.00	19.28
C										
ATOM	1317	CEl	PHE	A	172	40.916	28.397	23.429	1.00	19.80
C										
ATOM	1318	CE2	PHE	A	172	42.811	28.488	24.905	1.00	19.50
C										
ATOM	1319	CZ	PHE	A	172	41.493	28.817	24.623	1.00	17.37
C										
ATOM	1320	N	LEU	A	173	45.954	28.579	20.776	1.00	19.07
N										
ATOM	1321	CA	LEU	A	173	46.715	29.818	20.917	1.00	20.82
C										
ATOM	1322	C	LEU	A	173	46.483	30.695	19.685	1.00	19.75
C										
ATOM	1323	O	LEU	A	173	46.200	31.886	19.799	1.00	18.95
O										
ATOM	1324	CB	LEU	A	173	48.209	29.512	21.046	1.00	24.10
C										
ATOM	1325	CG	LEU	A	173	48.698	28.981	22.388	1.00	29.07
C										
ATOM	1326	CDl	LEU	A	173	50.123	28.451	22.250	1.00	31.81
C										
ATOM	1327	CD2	LEU	A	173	48.643	30.103	23.411	1.00	31.98
C										

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ATOM   1328  N   ILE A 174      46.605  30.100  18.503  1.00 18.27
N
ATOM   1329  CA  ILE A 174      46.389  30.846  17.268  1.00 18.15
C
ATOM   1330  C   ILE A 174      44.964  31.398  17.221  1.00 17.66
C
ATOM   1331  O   ILE A 174      44.744  32.535  16.822  1.00 17.06
O
ATOM   1332  CB  ILE A 174      46.628  29.949  16.035  1.00 19.14
C
ATOM   1333  CGl ILE A 174      48.110  29.569  15.969  1.00 21.88
C
ATOM   1334  CG2 ILE A 174      46.174  30.657  14.763  1.00 20.17
C
ATOM   1335  CDl ILE A 174      48.427  28.487  14.956  1.00 22.91
C
ATOM   1336  N   THR A 175      43.998  30.588  17.638  1.00 17.69
N
ATOM   1337  CA  THR A 175      42.606  31.012  17.637  1.00 16.82
C
ATOM   1338  C   THR A 175      42.405  32.216  18.555  1.00 16.48
C
ATOM   1339  O   THR A 175      41.696  33.161  18.203  1.00 16.28
O
ATOM   1340  CB  THR A 175      41.689  29.849  18.069  1.00 17.25
C
ATOM   1341  OGl THR A 175      41.815  28.783  17.120  1.00 16.31
O
ATOM   1342  CG2 THR A 175      40.233  30.296  18.124  1.00 17.72
C
ATOM   1343  N   MET A 176      43.021  32.190  19.732  1.00 16.91
N
ATOM   1344  CA  MET A 176      42.895  33.320  20.647  1.00 18.50
C
ATOM   1345  C   MET A 176      43.527  34.556  20.003  1.00 18.53
C
ATOM   1346  O   MET A 176      42.986  35.659  20.088  1.00 19.45
O
ATOM   1347  CB  MET A 176      43.586  33.020  21.981  1.00 18.70
C
ATOM   1348  CG  MET A 176      42.839  32.041  22.887  1.00 24.02
C
ATOM   1349  SD  MET A 176      41.180  32.589  23.363  1.00 28.69
S
ATOM   1350  CE  MET A 176      41.483  34.293  23.843  1.00 26.27
C
ATOM   1351  N   PHE A 177      44.666  34.368  19.346  1.00 17.72
N
ATOM   1352  CA  PHE A 177      45.338  35.481  18.686  1.00 19.76
C
ATOM   1353  C   PHE A 177      44.458  36.106  17.602  1.00 18.48
C
ATOM   1354  O   PHE A 177      44.416  37.330  17.451  1.00 18.75
O
ATOM   1355  CB  PHE A 177      46.650  35.022  18.054  1.00 21.50
C
ATOM   1356  CG  PHE A 177      47.330  36.091  17.251  1.00 27.70
C
ATOM   1357  CDl PHE A 177      47.978  37.148  17.882  1.00 30.28
C
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ATOM	1358	CD2	PHE	A	177	47.288	36.065	15.860	1.00	28.66
C										
ATOM	1359	CEl	PHE	A	177	48.575	38.166	17.136	1.00	32.85
C										
ATOM	1360	CE2	PHE	A	177	47.879	37.076	15.108	1.00	31.87
C										
ATOM	1361	CZ	PHE	A	177	48.523	38.127	15.746	1.00	31.13
C										
ATOM	1362	N	ILE	A	178	43.765	35.267	16.837	1.00	17.03
N										
ATOM	1363	CA	ILE	A	178	42.895	35.767	15.779	1.00	17.16
C										
ATOM	1364	C	ILE	A	178	41.733	36.550	16.385	1.00	17.82
C										
ATOM	1365	O	ILE	A	178	41.380	37.622	15.892	1.00	17.65
O										
ATOM	1366	CB	ILE	A	178	42.369	34.615	14.899	1.00	18.09
C										
ATOM	1367	CGl	ILE	A	178	43.545	33.986	14.138	1.00	19.37
C										
ATOM	1368	CG2	ILE	A	178	41.307	35.129	13.934	1.00	19.73
C										
ATOM	1369	CDl	ILE	A	178	43.188	32.733	13.348	1.00	19.31
C										
ATOM	1370	N	ASN	A	179	41.140	36.023	17.455	1.00	16.75
N										
ATOM	1371	CA	ASN	A	179	40.042	36.731	18.114	1.00	16.27
C										
ATOM	1372	C	ASN	A	179	40.549	38.090	18.608	1.00	17.36
C										
ATOM	1373	O	ASN	A	179	39.886	39.117	18.443	1.00	16.00
O										
ATOM	1374	CB	ASN	A	179	39.505	35.907	19.296	1.00	16.83
C										
ATOM	1375	CG	ASN	A	179	38.447	34.888	18.874	1.00	19.25
C										
ATOM	1376	ODl	ASN	A	179	37.244	35.149	18.962	1.00	19.77
O										
ATOM	1377	ND2	ASN	A	179	38.893	33.731	18.404	1.00	18.95
N										
ATOM	1378	N	VAL	A	180	41.734	38.095	19.209	1.00	16.17
N										
ATOM	1379	CA	VAL	A	180	42.312	39.331	19.712	1.00	18.63
C										
ATOM	1380	C	VAL	A	180	42.577	40.329	18.583	1.00	19.71
C										
ATOM	1381	O	VAL	A	180	42.276	41.516	18.716	1.00	20.44
O										
ATOM	1382	CB	VAL	A	180	43.636	39.053	20.477	1.00	19.65
C										
ATOM	1383	CGl	VAL	A	180	44.380	40.354	20.746	1.00	20.14
C										
ATOM	1384	CG2	VAL	A	180	43.328	38.357	21.794	1.00	21.62
C										
ATOM	1385	N	SER	A	181	43.116	39.841	17.469	1.00	20.50
N										
ATOM	1386	CA	SER	A	181	43.442	40.711	16.342	1.00	21.13
C										
ATOM	1387	C	SER	A	181	42.227	41.485	15.834	1.00	20.99
C										

ATOM 1388 O SER A 181 42.352 42.624 15.384 1.00 21.47 O
ATOM 1389 CB SER A 181 44.068 39.898 15.201 1.00 21.98 C
ATOM 1390 OG SER A 181 43.108 39.085 14.547 1.00 30.27 O
ATOM 1391 N ILE A 182 41.053 40.869 15.905 1.00 19.05 N
ATOM 1392 CA ILE A 182 39.832 41.533 15.464 1.00 18.54 C
ATOM 1393 C ILE A 182 39.324 42.485 16.547 1.00 19.73 C
ATOM 1394 O ILE A 182 39.058 43.655 16.288 1.00 19.64 O
ATOM 1395 CB ILE A 182 38.722 40.505 15.152 1.00 18.59 C
ATOM 1396 CGl ILE A 182 39.141 39.636 13.961 1.00 20.09 C
ATOM 1397 CG2 ILE A 182 37.404 41.230 14.860 1.00 17.88 C
ATOM 1398 CDl ILE A 182 38.308 38.385 13.794 1.00 19.91 C
ATOM 1399 N LEU A 183 39.209 41.980 17.771 1.00 17.70 N
ATOM 1400 CA LEU A 183 38.708 42.783 18.881 1.00 17.54 C
ATOM 1401 C LEU A 183 39.532 44.019 19.223 1.00 18.44 C
ATOM 1402 O LEU A 183 38.983 45.060 19.596 1.00 17.94 O
ATOM 1403 CB LEU A 183 38.583 41.904 20.132 1.00 17.07 C
ATOM 1404 CG LEU A 183 37.470 40.852 20.054 1.00 18.09 C
ATOM 1405 CDl LEU A 183 37.644 39.825 21.159 1.00 18.61 C
ATOM 1406 CD2 LEU A 183 36.110 41.541 20.157 1.00 17.89 C
ATOM 1407 N ILE A 184 40.845 43.903 19.103 1.00 19.31 N
ATOM 1408 CA ILE A 184 41.730 45.006 19.443 1.00 21.26 C
ATOM 1409 C ILE A 184 41.567 46.192 18.490 1.00 23.72 C
ATOM 1410 O ILE A 184 41.966 47.315 18.812 1.00 23.46 O
ATOM 1411 CB ILE A 184 43.201 44.529 19.481 1.00 23.37 C
ATOM 1412 CGl ILE A 184 44.022 45.472 20.361 1.00 27.60 C
ATOM 1413 CG2 ILE A 184 43.777 44.472 18.071 1.00 25.10 C
ATOM 1414 CDl ILE A 184 45.342 44.880 20.827 1.00 30.28 C
ATOM 1415 N ARG A 185 40.969 45.947 17.326 1.00 22.96 N
ATOM 1416 CA ARG A 185 40.738 47.014 16.354 1.00 24.11 C
ATOM 1417 C ARG A 185 39.426 47.735 16.666 1.00 22.94 C

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ATOM   1418  O   ARG A 185      39.109  48.756  16.054  1.00 24.31
O
ATOM   1419  CB  ARG A 185      40.689  46.459  14.925  1.00 26.78
C
ATOM   1420  CG  ARG A 185      42.005  45.892  14.405  1.00 31.46
C
ATOM   1421  CD  ARG A 185      41.920  45.647  12.902  1.00 38.47
C
ATOM   1422  NE  ARG A 185      43.030  44.854  12.378  1.00 43.51
N
ATOM   1423  CZ  ARG A 185      44.311  45.199  12.461  1.00 45.76
C
ATOM   1424  NHl ARG A 185      45.244  44.407  11.954  1.00 46.78
N
ATOM   1425  NH2 ARG A 185      44.663  46.330  13.055  1.00 48.11
N
ATOM   1426  N   GLY A 186      38.654  47.190  17.603  1.00 21.10
N
ATOM   1427  CA  GLY A 186      37.409  47.830  17.989  1.00 20.78
C
ATOM   1428  C   GLY A 186      36.152  47.440  17.237  1.00 21.29
C
ATOM   1429  O   GLY A 186      36.152  46.532  16.411  1.00 22.29
O
ATOM   1430  N   ILE A 187      35.075  48.160  17.523  1.00 21.91
N
ATOM   1431  CA  ILE A 187      33.776  47.905  16.917  1.00 23.17
C
ATOM   1432  C   ILE A 187      33.689  48.113  15.403  1.00 24.95
C
ATOM   1433  O   ILE A 187      33.426  47.164  14.663  1.00 25.62
O
ATOM   1434  CB  ILE A 187      32.681  48.766  17.610  1.00 24.28
C
ATOM   1435  CGl ILE A 187      32.626  48.425  19.102  1.00 23.48
C
ATOM   1436  CG2 ILE A 187      31.323  48.547  16.944  1.00 24.17
C
ATOM   1437  CDl ILE A 187      32.371  46.949  19.406  1.00 25.00
C
ATOM   1438  N   SER A 188      33.909  49.339  14.937  1.00 27.08
N
ATOM   1439  CA  SER A 188      33.796  49.620  13.506  1.00 29.17
C
ATOM   1440  C   SER A 188      34.919  49.070  12.638  1.00 29.05
C
ATOM   1441  O   SER A 188      34.657  48.447  11.611  1.00 30.82
O
ATOM   1442  CB  SER A 188      33.658  51.131  13.260  1.00 31.00
C
ATOM   1443  OG  SER A 188      34.831  51.834  13.633  1.00 34.43
O
ATOM   1444  N   LYS A 189      36.166  49.290  13.043  1.00 28.64
N
ATOM   1445  CA  LYS A 189      37.304  48.815  12.261  1.00 27.91
C
ATOM   1446  C   LYS A 189      37.677  47.363  12.538  1.00 26.37
C
ATOM   1447  O   LYS A 189      38.485  46.773  11.817  1.00 26.88
O
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ATOM	1448	CB	LYS	A	189	38.518	49.711	12.511	1.00	30.57
ATOM	1449	CG	LYS	A	189	38.297	51.158	12.105	1.00	34.47
ATOM	1450	CD	LYS	A	189	39.548	51.991	12.322	1.00	37.78
ATOM	1451	CE	LYS	A	189	39.358	53.407	11.801	1.00	41.65
ATOM	1452	NZ	LYS	A	189	40.601	54.219	11.933	1.00	44.29
ATOM	1453	N	GLY	A	190	37.086	46.786	13.578	1.00	24.04
ATOM	1454	CA	GLY	A	190	37.393	45.408	13.913	1.00	22.24
ATOM	1455	C	GLY	A	190	36.248	44.457	13.628	1.00	20.55
ATOM	1456	O	GLY	A	190	36.221	43.796	12.589	1.00	21.17
ATOM	1457	N	ILE	A	191	35.292	44.403	14.551	1.00	20.55
ATOM	1458	CA	ILE	A	191	34.139	43.518	14.421	1.00	19.26
ATOM	1459	C	ILE	A	191	33.319	43.775	13.157	1.00	20.79
ATOM	1460	O	ILE	A	191	33.014	42.846	12.404	1.00	19.64
ATOM	1461	CB	ILE	A	191	33.214	43.643	15.651	1.00	20.38
ATOM	1462	CGl	ILE	A	191	33.989	43.268	16.920	1.00	21.46
ATOM	1463	CG2	ILE	A	191	31.995	42.730	15.490	1.00	19.81
ATOM	1464	CDl	ILE	A	191	33.171	43.403	18.206	1.00	21.32
ATOM	1465	N	GLU	A	192	32.967	45.033	12.922	1.00	20.47
ATOM	1466	CA	GLU	A	192	32.160	45.382	11.755	1.00	22.35
ATOM	1467	C	GLU	A	192	32.863	45.043	10.441	1.00	21.97
ATOM	1468	O	GLU	A	192	32.294	44.372	9.579	1.00	22.41
ATOM	1469	CB	GLU	A	192	31.805	46.870	11.790	1.00	23.38
ATOM	1470	CG	GLU	A	192	30.690	47.261	10.836	1.00	25.36
ATOM	1471	CD	GLU	A	192	30.329	48.738	10.924	1.00	29.15
ATOM	1472	OEl	GLU	A	192	30.727	49.394	11.911	1.00	28.41
ATOM	1473	OE2	GLU	A	192	29.637	49.240	10.009	1.00	29.01
ATOM	1474	N	ARG	A	193	34.097	45.505	10.285	1.00	24.05
ATOM	1475	CA	ARG	A	193	34.849	45.229	9.069	1.00	25.40
ATOM	1476	C	ARG	A	193	34.980	43.732	8.817	1.00	24.48
ATOM	1477	O	ARG	A	193	34.836	43.273	7.686	1.00	23.98

ATOM	1478	CB	ARG	A	193	36.237	45.869	9.138	1.00	29.40
C										
ATOM	1479	CG	ARG	A	193	36.212	47.387	9.067	1.00	36.91
C										
ATOM	1480	CD	ARG	A	193	37.578	47.945	8.688	1.00	41.58
C										
ATOM	1481	NE	ARG	A	193	37.595	49.406	8.707	1.00	46.79
N										
ATOM	1482	CZ	ARG	A	193	36.824	50.175	7.946	1.00	49.13
C										
ATOM	1483	NHl	ARG	A	193	35.966	49.628	7.097	1.00	50.85
N										
ATOM	1484	NH2	ARG	A	193	36.908	51.496	8.039	1.00	51.31
N										
ATOM	1485	N	PHE	A	194	35.245	42.966	9.870	1.00	22.96
N										
ATOM	1486	CA	PHE	A	194	35.381	41.527	9.709	1.00	22.17
C										
ATOM	1487	C	PHE	A	194	34.059	40.873	9.316	1.00	20.78
C										
ATOM	1488	O	PHE	A	194	34.036	39.977	8.477	1.00	20.42
O										
ATOM	1489	CB	PHE	A	194	35.892	40.871	10.994	1.00	22.79
C										
ATOM	1490	CG	PHE	A	194	36.116	39.394	10.856	1.00	23.27
C										
ATOM	1491	CDl	PHE	A	194	37.145	38.908	10.057	1.00	25.82
C										
ATOM	1492	CD2	PHE	A	194	35.273	38.486	11.486	1.00	23.14
C										
ATOM	1493	CEl	PHE	A	194	37.332	37.536	9.883	1.00	26.49
C										
ATOM	1494	CE2	PHE	A	194	35.452	37.114	11.319	1.00	23.69
C										
ATOM	1495	CZ	PHE	A	194	36.482	36.639	10.517	1.00	27.22
C										
ATOM	1496	N	ALA	A	195	32.959	41.317	9.922	1.00	20.94
N										
ATOM	1497	CA	ALA	A	195	31.649	40.748	9.616	1.00	21.96
C										
ATOM	1498	C	ALA	A	195	31.273	40.930	8.144	1.00	23.06
C										
ATOM	1499	O	ALA	A	195	30.627	40.068	7.552	1.00	21.56
O										
ATOM	1500	CB	ALA	A	195	30.574	41.377	10.515	1.00	23.50
C										
ATOM	1501	N	LYS	A	196	31.675	42.049	7.552	1.00	25.44
N										
ATOM	1502	CA	LYS	A	196	31.354	42.302	6.153	1.00	27.99
C										
ATOM	1503	C	LYS	A	196	32.081	41.333	5.229	1.00	29.01
C										
ATOM	1504	O	LYS	A	196	31.694	41.150	4.074	1.00	30.68
O										
ATOM	1505	CB	LYS	A	196	31.699	43.747	5.783	1.00	29.88
C										
ATOM	1506	CG	LYS	A	196	30.752	44.771	6.382	1.00	30.83
C										
ATOM	1507	CD	LYS	A	196	31.042	46.160	5.846	1.00	34.88
C										

ATOM 1508 CE LYS A 196 29.988 47.155 6.299 1.00 36.48 C
ATOM 1509 NZ LYS A 196 30.228 48.499 5.706 1.00 38.91 N
ATOM 1510 N ILE A 197 33.130 40.706 5.748 1.00 28.90 N
ATOM 1511 CA ILE A 197 33.914 39.748 4.979 1.00 29.55 C
ATOM 1512 C ILE A 197 33.501 38.314 5.307 1.00 28.10 C
ATOM 1513 O ILE A 197 33.291 37.487 4.416 1.00 26.87 O
ATOM 1514 CB ILE A 197 35.418 39.885 5.298 1.00 31.85 C
ATOM 1515 CG1 ILE A 197 35.902 41.296 4.966 1.00 34.26 C
ATOM 1516 CG2 ILE A 197 36.211 38.849 4.515 1.00 33.64 C
ATOM 1517 CD1 ILE A 197 37.316 41.578 5.438 1.00 37.40 C
ATOM 1518 N ALA A 198 33.379 38.030 6.598 1.00 25.20 N
ATOM 1519 CA ALA A 198 33.033 36.694 7.061 1.00 25.24 C
ATOM 1520 C ALA A 198 31.627 36.210 6.736 1.00 24.10 C
ATOM 1521 O ALA A 198 31.446 35.052 6.364 1.00 24.96 O
ATOM 1522 CB ALA A 198 33.271 36.595 8.565 1.00 23.69 C
ATOM 1523 N MET A 199 30.628 37.073 6.874 1.00 24.61 N
ATOM 1524 CA MET A 199 29.263 36.636 6.614 1.00 24.74 C
ATOM 1525 C MET A 199 29.008 36.220 5.170 1.00 24.79 C
ATOM 1526 O MET A 199 28.379 35.194 4.927 1.00 24.43 O
ATOM 1527 CB MET A 199 28.267 37.703 7.070 1.00 25.64 C
ATOM 1528 CG MET A 199 28.362 37.988 8.567 1.00 26.57 C
ATOM 1529 SD MET A 199 28.523 36.476 9.565 1.00 33.09 S
ATOM 1530 CE MET A 199 26.918 35.827 9.406 1.00 27.07 C
ATOM 1531 N PRO A 200 29.479 37.012 4.191 1.00 25.08 N
ATOM 1532 CA PRO A 200 29.253 36.616 2.796 1.00 26.75 C
ATOM 1533 C PRO A 200 29.994 35.311 2.513 1.00 26.79 C
ATOM 1534 O PRO A 200 29.503 34.442 1.794 1.00 26.20 O
ATOM 1535 CB PRO A 200 29.832 37.791 2.006 1.00 27.52 C
ATOM 1536 CG PRO A 200 29.575 38.958 2.921 1.00 27.19 C
ATOM 1537 CD PRO A 200 29.978 38.396 4.268 1.00 25.11 C

ATOM 1538 N THR A 201 31.183 35.180 3.094 1.00 26.02 N
ATOM 1539 CA THR A 201 31.994 33.976 2.923 1.00 26.79 C
ATOM 1540 C THR A 201 31.254 32.769 3.496 1.00 26.67 C
ATOM 1541 O THR A 201 31.137 31.729 2.846 1.00 26.05 O
ATOM 1542 CB THR A 201 33.355 34.111 3.645 1.00 26.20 C
ATOM 1543 OGl THR A 201 34.113 35.171 3.047 1.00 28.07 O
ATOM 1544 CG2 THR A 201 34.144 32.817 3.546 1.00 27.22 C
ATOM 1545 N LEU A 202 30.755 32.923 4.718 1.00 25.74 N
ATOM 1546 CA LEU A 202 30.022 31.864 5.403 1.00 25.44 C
ATOM 1547 C LEU A 202 28.797 31.441 4.588 1.00 25.11 C
ATOM 1548 O LEU A 202 28.524 30.251 4.431 1.00 23.12 O
ATOM 1549 CB LEU A 202 29.600 32.361 6.797 1.00 28.61 C
ATOM 1550 CG LEU A 202 28.940 31.422 7.813 1.00 30.54 C
ATOM 1551 CDl LEU A 202 28.920 32.104 9.183 1.00 31.71 C
ATOM 1552 CD2 LEU A 202 27.529 31.063 7.375 1.00 31.61 C
ATOM 1553 N PHE A 203 28.063 32.420 4.067 1.00 23.10 N
ATOM 1554 CA PHE A 203 26.873 32.137 3.271 1.00 25.48 C
ATOM 1555 C PHE A 203 27.225 31.297 2.044 1.00 25.60 C
ATOM 1556 O PHE A 203 26.590 30.275 1.773 1.00 23.78 O
ATOM 1557 CB PHE A 203 26.216 33.448 2.830 1.00 28.61 C
ATOM 1558 CG PHE A 203 25.029 33.260 1.924 1.00 33.50 C
ATOM 1559 CDl PHE A 203 23.878 32.629 2.384 1.00 35.91 C
ATOM 1560 CD2 PHE A 203 25.065 33.713 0.610 1.00 35.84 C
ATOM 1561 CEl PHE A 203 22.777 32.453 1.546 1.00 37.27 C
ATOM 1562 CE2 PHE A 203 23.969 33.541 -0.236 1.00 37.00 C
ATOM 1563 CZ PHE A 203 22.825 32.910 0.235 1.00 37.07 C
ATOM 1564 N ILE A 204 28.245 31.728 1.311 1.00 24.44 N
ATOM 1565 CA ILE A 204 28.675 31.021 0.108 1.00 26.52 C
ATOM 1566 C ILE A 204 29.143 29.600 0.398 1.00 25.93 C
ATOM 1567 O ILE A 204 28.800 28.665 -0.332 1.00 25.86 O

ATOM	1568	CB	ILE	A	204	29.803	31.791	-0.606	1.00	27.64
C										
ATOM	1569	CGl	ILE	A	204	29.268	33.139	-1.092	1.00	29.08
C										
ATOM	1570	CG2	ILE	A	204	30.338	30.973	-1.777	1.00	29.51
C										
ATOM	1571	CDl	ILE	A	204	30.330	34.055	-1.665	1.00	29.97
C										
ATOM	1572	N	LEU	A	205	29.928	29.435	1.457	1.00	23.81
N										
ATOM	1573	CA	LEU	A	205	30.418	28.113	1.831	1.00	23.40
C										
ATOM	1574	C	LEU	A	205	29.246	27.212	2.215	1.00	21.35
C										
ATOM	1575	O	LEU	A	205	29.178	26.055	1.801	1.00	20.81
O										
ATOM	1576	CB	LEU	A	205	31.395	28.214	3.013	1.00	24.46
C										
ATOM	1577	CG	LEU	A	205	32.776	28.821	2.747	1.00	25.93
C										
ATOM	1578	CDl	LEU	A	205	33.518	29.001	4.065	1.00	26. 64
C										
ATOM	1579	CD2	LEU	A	205	33.563	27.922	1.806	1.00	29. 27
C										
ATOM	1580	N	ALA	A	206	28.320	27.752	3.002	1.00	19.56
N										
ATOM	1581	CA	ALA	A	206	27.159	26.987	3.443	1.00	19.85
C										
ATOM	1582	C	ALA	A	206	26.277	26.561	2.271	1.00	19.55
C										
ATOM	1583	O	ALA	A	206	25.828	25.419	2.207	1.00	20.37
O										
ATOM	1584	CB	ALA	A	206	26.344	27.802	4.447	1.00	19. 21
C										
ATOM	1585	N	VAL	A	207	26.023	27.478	1.346	1.00	20.64
N										
ATOM	1586	CA	VAL	A	207	25.188	27.147	0.196	1.00	21.65
C										
ATOM	1587	C	VAL	A	207	25.858	26.050	-0.631	1.00	21.59
C										
ATOM	1588	O	VAL	A	207	25.215	25.076	-1.022	1.00	21.96
O										
ATOM	1589	CB	VAL	A	207	24.926	28.396	-0.678	1.00	21.93
C										
ATOM	1590	CGl	VAL	A	207	24.229	27.996	-1.972	1.00	23.38
C										
ATOM	1591	CG2	VAL	A	207	24.060	29.389	0.089	1.00	24.16
C										
ATOM	1592	N	PHE	A	208	27.155	26.196	-0.874	1.00	21.26
N										
ATOM	1593	CA	PHE	A	208	27.894	25.199	-1.640	1.00	22.72
C										
ATOM	1594	C	PHE	A	208	27.796	23.820	-0.988	1.00	21.52
C										
ATOM	1595	O	PHE	A	208	27.577	22.814	-1.662	1.00	21.14
O										
ATOM	1596	CB	PHE	A	208	29.366	25.595	-1.759	1.00	23.83
C										
ATOM	1597	CG	PHE	A	208	30.186	24.620	-2.557	1.00	27.26
C										

ATOM	1598	CDl	PHE	A	208	30.028	24.526	--3.938	1.00	29.39
C										
ATOM	1599	CD2	PHE	A	208	31.093	23.777	--1.929	1.00	27.83
C										
ATOM	1600	CEl	PHE	A	208	30.765	23.601	--4.683	1.00	29. 52
C										
ATOM	1601	CE2	PHE	A	208	31.834	22.850	--2.661	1.00	29.01
C										
ATOM	1602	CZ	PHE	A	208	31.669	22.763	--4.042	1.00	30.17
C										
ATOM	1603	N	LEU	A	209	27.964	23.775	0.330	1.00	21.34
N										
ATOM	1604	CA	LEU	A	209	27.889	22.511	1.047	1.00	20.56
C										
ATOM	1605	C	LEU	A	209	26. 499	21.895	0.964	1.00	20.43
C										
ATOM	1606	O	LEU	A	209	26.362	20.685	0.823	1.00	20.75
O										
ATOM	1607	CB	LEU	A	209	28.304	22.712	2.506	1.00	20.92
C										
ATOM	1608	CG	LEU	A	209	29.816	22.920	2.655	1.00	24.06
C										
ATOM	1609	CDl	LEU	A	209	30.159	23.403	4.058	1.00	25.05
C										
ATOM	1610	CD2	LEU	A	209	30.524	21.618	2.350	1.00	25.75
C										
ATOM	1611	N	VAL	A	210	25. 463	22.721	1.059	1.00	20.90
N										
ATOM	1612	CA	VAL	A	210	24.106	22.199	0.964	1.00	21.34
C										
ATOM	1613	C	VAL	A	210	23.910	21.550	-0.404	1.00	22.74
C										
ATOM	1614	O	VAL	A	210	23.348	20.461	-0.509	1.00	23.40
O										
ATOM	1615	CB	VAL	A	210	23.053	23.313	1.149	1.00	22.45
C										
ATOM	1616	CGl	VAL	A	210	21.666	22.787	0.792	1.00	22.52
C										
ATOM	1617	CG2	VAL	A	210	23.061	23.790	2.592	1.00	22.12
C										
ATOM	1618	N	ILE	A	211	24.389	22.220	-1.444	1.00	22.81
N										
ATOM	1619	CA	ILE	A	211	24.270	21.709	-2.809	1.00	25.10
C										
ATOM	1620	C	ILE	A	211	24.987	20.365	-2.953	1.00	24.52
C										
ATOM	1621	O	ILE	A	211	24.434	19. 413	-3.509	1.00	24.95
O										
ATOM	1622	CB	ILE	A	211	24.851	22.714	-3.830	1.00	26.79
C										
ATOM	1623	CGl	ILE	A	211	24.013	23.995	-3.830	1.00	28.48
C										
ATOM	1624	CG2	ILE	A	211	24.862	22.098	-5.229	1.00	30.90
C										
ATOM	1625	CDl	ILE	A	211	24.607	25.113	-4.662	1.00	30.31
C										
ATOM	1626	N	ARG	A	212	26.208	20.278	-2.439	1.00	23.07
N										
ATOM	1627	CA	ARG	A	212	26. 954	19.029	-2.528	1.00	23.29
C										

ATOM	1628	C	ARG	A	212	26.236	17.917	-1.768	1.00	22.36
C										
ATOM	1629	O	ARG	A	212	26.139	16.789	-2.247	1.00	23.47
O										
ATOM	1630	CB	ARG	A	212	28.368	19.200	-1.972	1.00	23.72
C										
ATOM	1631	CG	ARG	A	212	29.207	17.931	-2.066	1.00	29.44
C										
ATOM	1632	CD	ARG	A	212	29.559	17.609	-3.518	1.00	33.77
C										
ATOM	1633	NE	ARG	A	212	30.109	16.265	-3.688	1.00	33.95
N										
ATOM	1634	CZ	ARG	A	212	29.388	15.148	-3.640	1.00	37.70
C										
ATOM	1635	NHl	ARG	A	212	28.081	15.208	-3.422	1.00	37.72
N										
ATOM	1636	NH2	ARG	A	212	29.967	13.966	-3.831	1.00	37.45
N										
ATOM	1637	N	VAL	A	213	25.736	18.234	-0.578	1.00	21.46
N										
ATOM	1638	CA	VAL	A	213	25.031	17.245	0.232	1.00	20.65
C										
ATOM	1639	C	VAL	A	213	23.772	16.743	-0.469	1.00	23.08
C										
ATOM	1640	O	VAL	A	213	23.441	15.557	-0.397	1.00	23.53
O										
ATOM	1641	CB	VAL	A	213	24.649	17.830	1.619	1.00	21.77
C										
ATOM	1642	CGl	VAL	A	213	23.629	16.931	2.318	1.00	20.90
C										
ATOM	1643	CG2	VAL	A	213	25.905	17.949	2.481	1.00	20.55
C										
ATOM	1644	N	PHE	A	214	23.077	17.649	-1.146	1.00	23.36
N										
ATOM	1645	CA	PHE	A	214	21.848	17.302	-1.853	1.00	27.95
C										
ATOM	1646	C	PHE	A	214	22.074	16.343	-3.017	1.00	28.70
C										
ATOM	1647	O	PHE	A	214	21.119	15.801	-3.571	1.00	30.00
O										
ATOM	1648	CB	PHE	A	214	21.150	18.576	-2.341	1.00	30.35
C										
ATOM	1649	CG	PHE	A	214	20.358	19.285	-1.270	1.00	35.14
C										
ATOM	1650	CDl	PHE	A	214	20.535	18.970	0.078	1.00	36.05
C										
ATOM	1651	CD2	PHE	A	214	19.437	20.274	-1.609	1.00	36.48
C										
ATOM	1652	CEl	PHE	A	214	19.808	19.624	1.068	1.00	37.59
C										
ATOM	1653	CE2	PHE	A	214	18.703	20.937	-0.623	1.00	37.90
C										
ATOM	1654	CZ	PHE	A	214	18.889	20.612	0.717	1.00	38.29
C										
ATOM	1655	N	LEU	A	215	23.334	16.129	-3.384	1.00	28.78
N										
ATOM	1656	CA	LEU	A	215	23.662	15.214	-4.474	1.00	29.85
C										
ATOM	1657	C	LEU	A	215	23.898	13.801	-3.951	1.00	30.56
C										

ATOM	1658	O	LEU	A	215	24.049	12.858	-4.729	1.00	30.94
ATOM	1659	CB	LEU	A	215	24.917	15.688	-5.212	1.00	30.63
ATOM	1660	CG	LEU	A	215	24.821	16.996	-5.997	1.00	31.84
ATOM	1661	CD1	LEU	A	215	26.183	17.332	-6.582	1.00	33.16
ATOM	1662	CD2	LEU	A	215	23.779	16.862	-7.095	1.00	33.82
ATOM	1663	N	LEU	A	216	23.925	13.657	-2.629	1.00	30.05
ATOM	1664	CA	LEU	A	216	24.162	12.364	-2.001	1.00	29.76
ATOM	1665	C	LEU	A	216	23.012	11.371	-2.111	1.00	30.24
ATOM	1666	O	LEU	A	216	21.874	11.663	-1.750	1.00	30.10
ATOM	1667	CB	LEU	A	216	24.520	12.554	-0.524	1.00	29.71
ATOM	1668	CG	LEU	A	216	25.824	13.306	-0.239	1.00	30.66
ATOM	1669	CD1	LEU	A	216	25.982	13.498	1.267	1.00	29.33
ATOM	1670	CD2	LEU	A	216	27.006	12.532	-0.814	1.00	30.92
ATOM	1671	N	GLU	A	217	23.334	10.186	-2.616	1.00	30.50
ATOM	1672	CA	GLU	A	217	22.367	9.107	-2.766	1.00	31.79
ATOM	1673	C	GLU	A	217	23.111	7.800	-2.548	1.00	31.51
ATOM	1674	O	GLU	A	217	24.137	7.547	-3.175	1.00	31.53
ATOM	1675	CB	GLU	A	217	21.724	9.131	-4.159	1.00	32.90
ATOM	1676	CG	GLU	A	217	21.030	7.827	-4.544	1.00	38.84
ATOM	1677	CD	GLU	A	217	19.768	8.039	-5.364	1.00	40.90
ATOM	1678	OE1	GLU	A	217	19.724	9.001	-6.168	1.00	41.74
ATOM	1679	OE2	GLU	A	217	18.823	7.232	-5.208	1.00	38.73
ATOM	1680	N	THR	A	218	22.596	6.981	-1.640	1.00	30.49
ATOM	1681	CA	THR	A	218	23.216	5.704	-1.326	1.00	30.53
ATOM	1682	C	THR	A	218	22.122	4.650	-1.243	1.00	29.93
ATOM	1683	O	THR	A	218	20.938	4.960	-1.388	1.00	29.23
ATOM	1684	CB	THR	A	218	23.933	5.747	0.038	1.00	30.53
ATOM	1685	OG1	THR	A	218	22.971	5.577	1.085	1.00	29.20
ATOM	1686	CG2	THR	A	218	24.642	7.080	0.230	1.00	31.15
ATOM	1687	N	PRO	A	219	22.504	3.385	-1.013	1.00	30.87

ATOM	1688	CA	PRO	A	219	21.497	2.325	-0.914	1.00	31.30
C										
ATOM	1689	C	PRO	A	219	20.578	2.532	0.289	1.00	31.98
C										
ATOM	1690	O	PRO	A	219	19.502	1.941	0.366	1.00	32.85
O										
ATOM	1691	CB	PRO	A	219	22.341	1.062	-0.777	1.00	31.89
C										
ATOM	1692	CG	PRO	A	219	23.580	1.401	-1.551	1.00	31.70
C										
ATOM	1693	CD	PRO	A	219	23.860	2.810	-1.095	1.00	31.14
C										
ATOM	1694	N	ASN	A	220	21.007	3.373	1.226	1.00	31.01
N										
ATOM	1695	CA	ASN	A	220	20.227	3.633	2.431	1.00	31.99
C										
ATOM	1696	C	ASN	A	220	19.330	4.859	2.348	1.00	30.05
C										
ATOM	1697	O	ASN	A	220	18.487	5.068	3.217	1.00	31.57
O										
ATOM	1698	CB	ASN	A	220	21.151	3.768	3.646	1.00	33.14
C										
ATOM	1699	CG	ASN	A	220	21.913	2.494	3.939	1.00	36.14
C										
ATOM	1700	ODl	ASN	A	220	21.330	1.412	3.993	1.00	37.73
O										
ATOM	1701	ND2	ASN	A	220	23.220	2.615	4.134	1.00	35.70
N										
ATOM	1702	N	GLY	A	221	19.509	5.674	1.317	1.00	29. 48
N										
ATOM	1703	CA	GLY	A	221	18.672	6.851	1.194	1.00	29. 15
C										
ATOM	1704	C	GLY	A	221	19.277	8.004	0.422	1.00	27.78
C										
ATOM	1705	O	GLY	A	221	20.340	7.885	-0.183	1.00	27.11
O										
ATOM	1706	N	THR	A	222	18.573	9.130	0.444	1.00	26.94
N										
ATOM	1707	CA	THR	A	222	19.007	10.334	-0.244	1.00	27.35
C										
ATOM	1708	C	THR	A	222	18.925	11.485	0.743	1.00	26. 56
C										
ATOM	1709	O	THR	A	222	18.349	11.345	1.819	1.00	25.86
O										
ATOM	1710	CB	THR	A	222	18.087	10.665	-1.430	1.00	28.73
C										
ATOM	1711	OGl	THR	A	222	16. 795	11.044	-0.935	1.00	30.72
O										
ATOM	1712	CG2	THR	A	222	17.934	9.454	-2.344	1.00	29.63
C										
ATOM	1713	N	ALA	A	223	19.498	12.623	0.372	1.00	26.93
N										
ATOM	1714	CA	ALA	A	223	19.465	13.796	1.230	1.00	27.57
C										
ATOM	1715	C	ALA	A	223	18.013	14.209	1.470	1.00	28.79
C										
ATOM	1716	O	ALA	A	223	17.678	14.752	2.522	1.00	27.30
O										
ATOM	1717	CB	ALA	A	223	20.241	14.938	0.584	1.00	28.99
C										

ATOM	1718	N	ALA	A	224	17.151	13.938	0.493	1.00	30.21
N										
ATOM	1719	CA	ALA	A	224	15.737	14.286	0.608	1.00	31.30
C										
ATOM	1720	C	ALA	A	224	15.084	13. 604	1.805	1.00	31.10
C										
ATOM	1721	O	ALA	A	224	14.235	14.195	2.471	1.00	32.43
O										
ATOM	1722	CB	ALA	A	224	14.995	13. 917	-0.680	1.00	33. 03
C										
ATOM	1723	N	ASP	A	225	15.471	12.359	2.076	1.00	30.95
N										
ATOM	1724	CA	ASP	A	225	14.916	11. 630	3.212	1.00	30.89
C										
ATOM	1725	C	ASP	A	225	15.245	12.367	4.505	1.00	30. 73
C										
ATOM	1726	O	ASP	A	225	14.501	12.287	5.486	1.00	29. 90
O										
ATOM	1727	CB	ASP	A	225	15.483	10.209	3.279	1.00	32.89
C										
ATOM	1728	CG	ASP	A	225	15.087	9.366	2.083	1.00	35.72
C										
ATOM	1729	ODl	ASP	A	225	13.891	9.366	1.728	1.00	37.92
O										
ATOM	1730	OD2	ASP	A	225	15.968	8.698	1.503	1.00	37.14
O										
ATOM	1731	N	GLY	A	226	16.372	13.076	4.501	1.00	29. 49
N										
ATOM	1732	CA	GLY	A	226	16.779	13.833	5.671	1.00	28.38
C										
ATOM	1733	C	GLY	A	226	15.875	15.032	5.886	1.00	28.95
C										
ATOM	1734	O	GLY	A	226	15.467	15.319	7.013	1.00	28.91
O										
ATOM	1735	N	LEU	A	227	15.560	15.736	4.805	1.00	30.61
N										
ATOM	1736	CA	LEU	A	227	14.688	16.902	4.886	1.00	33.04
C										
ATOM	1737	C	LEU	A	227	13.290	16. 496	5.339	1.00	34.16
C										
ATOM	1738	O	LEU	A	227	12.658	17.200	6.123	1.00	34.65
O										
ATOM	1739	CB	LEU	A	227	14.599	17.605	3.530	1.00	34.41
C										
ATOM	1740	CG	LEU	A	227	15.871	18.262	2.993	1.00	36. 65
C										
ATOM	1741	CDl	LEU	A	227	15.581	18.895	1.641	1.00	36.94
C										
ATOM	1742	CD2	LEU	A	227	16.365	19.315	3.978	1.00	35.93
C										
ATOM	1743	N '	ASN	A	228	12.804	15.361	4.846	1.00	35.13
N										
ATOM	1744	CA	ASN	A	228	11.477	14.898	5.238	1.00	35.76
C										
ATOM	1745	C	ASN	A	228	11.453	14.589	6.728	1.00	34.92
C										
ATOM	1746	O	ASN	A	228	10.473	14.871	7.415	1.00	34.37
O										
ATOM	1747	CB	ASN	A	228	11.080	13.654	4.439	1.00	38.63
C										

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ATOM   1748  CG  ASN A 228      10.937  13.938   2.959  1.00 41.69
C
ATOM   1749  ODl ASN A 228      10.395  14.972   2.564  1.00 45.03
O
ATOM   1750  ND2 ASN A 228      11.412  13.017   2.130  1.00 44.14
N
ATOM   1751  N   PHE A 229      12.540  14.011   7.227  1.00 33.22
N
ATOM   1752  CA  PHE A 229      12.639  13.679   8.642  1.00 32.88
C
ATOM   1753  C   PHE A 229      12.588  14.944   9.496  1.00 33.07
C
ATOM   1754  O   PHE A 229      11.934  14.978  10.536  1.00 32.68
O
ATOM   1755  CB  PHE A 229      13.949  12.935   8.923  1.00 33.68
C
ATOM   1756  CG  PHE A 229      14.306  12.867  10.382  1.00 34.29
C
ATOM   1757  CDl PHE A 229      13.537  12.121  11.270  1.00 35.34
C
ATOM   1758  CD2 PHE A 229      15.396  13.577  10.875  1.00 34.91
C
ATOM   1759  CEl PHE A 229      13.848  12.085  12.629  1.00 35.77
C
ATOM   1760  CE2 PHE A 229      15.714  13.548  12.230  1.00 35.53
C
ATOM   1761  CZ  PHE A 229      14.937  12.800  13.110  1.00 35.28
C
ATOM   1762  N   LEU A 230      13.276  15.985   9.044  1.00 32.83
N
ATOM   1763  CA  LEU A 230      13.338  17.240   9.781  1.00 33.62
C
ATOM   1764  C   LEU A 230      12.093  18.115   9.676  1.00 34.78
C
ATOM   1765  O   LEU A 230      11.749  18.823  10.623  1.00 33.61
O
ATOM   1766  CB  LEU A 230      14.553  18.053   9.321  1.00 32.82
C
ATOM   1767  CG  LEU A 230      14.757  19.425   9.973  1.00 33.82
C
ATOM   1768  CDl LEU A 230      15.089  19.250  11.445  1.00 34.22
C
ATOM   1769  CD2 LEU A 230      15.879  20.170   9.263  1.00 32.43
C
ATOM   1770  N   TRP A 231      11.410  18.064   8.536  1.00 36.42
N
ATOM   1771  CA  TRP A 231      10.240  18.909   8.342  1.00 37.84
C
ATOM   1772  C   TRP A 231       8.870  18.244   8.364  1.00 39.11
C
ATOM   1773  O   TRP A 231       7.902  18.814   7.864  1.00 39.71
O
ATOM   1774  CB  TRP A 231      10.394  19.708   7.048  1.00 37.91
C
ATOM   1775  CG  TRP A 231      11.580  20.624   7.064  1.00 38.67
C
ATOM   1776  CDl TRP A 231      12.817  20.381   6.537  1.00 37.79
C
ATOM   1777  CD2 TRP A 231      11.645  21.924   7.659  1.00 38.59
C
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ATOM	1778	NEl	TRP	A	231	13.648	21.454	6.763	1.00	37.96	N
ATOM	1779	CE2	TRP	A	231	12.953	22.415	7.450	1.00	38.62	C
ATOM	1780	CE3	TRP	A	231	10.722	22.725	8.348	1.00	39.23	C
ATOM	1781	CZ2	TRP	A	231	13.364	23.672	7.907	1.00	38.40	C
ATOM	1782	CZ3	TRP	A	231	11.131	23.975	8.802	1.00	39.19	C
ATOM	1783	CH2	TRP	A	231	12.441	24.435	8.578	1.00	38.82	C
ATOM	1784	N	THR	A	232	8.781	17.050	8.939	1.00	40.76	N
ATOM	1785	CA	THR	A	232	7.501	16.353	9.027	1.00	42.58	C
ATOM	1786	C	THR	A	232	6.994	16.424	10.465	1.00	44.52	C
ATOM	1787	O	THR	A	232	7.603	15.867	11.377	1.00	44.74	O
ATOM	1788	CB	THR	A	232	7.626	14.876	8.597	1.00	42.75	C
ATOM	1789	OGl	THR	A	232	7.963	14.814	7.205	1.00	40.68	O
ATOM	1790	CG2	THR	A	232	6.310	14.138	8.826	1.00	42.36	C
ATOM	1791	N	PRO	A	233	5.869	17.122	10.682	1.00	46.98	N
ATOM	1792	CA	PRO	A	233	5.247	17.295	12.000	1.00	49.11	C
ATOM	1793	C	PRO	A	233	4.936	16.000	12.751	1.00	51.28	C
ATOM	1794	O	PRO	A	233	4.624	14.975	12.147	1.00	51.57	O
ATOM	1795	CB	PRO	A	233	3.980	18.087	11.680	1.00	48.66	C
ATOM	1796	CG	PRO	A	233	4.384	18.896	10.488	1.00	48.83	C
ATOM	1797	CD	PRO	A	233	5.130	17.880	9.656	1.00	47.47	C
ATOM	1798	N	ASP	A	234	5.026	16.068	14.076	1.00	53.92	N
ATOM	1799	CA	ASP	A	234	4.740	14.933	14.950	1.00	56.55	C
ATOM	1800	C	ASP	A	234	4.057	15.507	16.189	1.00	57.89	C
ATOM	1801	O	ASP	A	234	4.678	15.683	17.237	1.00	58.77	O
ATOM	1802	CB	ASP	A	234	6.034	14.220	15.345	1.00	57.85	C
ATOM	1803	CG	ASP	A	234	5.781	12.913	16.076	1.00	59.00	C
ATOM	1804	ODl	ASP	A	234	5.079	12.931	17.110	1.00	59.79	O
ATOM	1805	OD2	ASP	A	234	6.285	11.867	15.616	1.00	60.13	O
ATOM	1806	N	PHE	A	235	2.768	15.796	16.050	1.00	59.06	N
ATOM	1807	CA	PHE	A	235	1.971	16.387	17.117	1.00	60.35	C

ATOM 1808 C PHE A 235 1.843 15.562 18.394 1.00 61.22 C
ATOM 1809 O PHE A 235 1.273 16.032 19.379 1.00 61.31 O
ATOM 1810 CB PHE A 235 0.579 16.716 16.577 1.00 60.51 C
ATOM 1811 CG PHE A 235 0.600 17.598 15.362 1.00 60.58 C
ATOM 1812 CDl PHE A 235 1.080 18.901 15.441 1.00 60.34 C
ATOM 1813 CD2 PHE A 235 0.158 17.121 14.133 1.00 60.62 C
ATOM 1814 CEl PHE A 235 1.121 19.717 14.313 1.00 60.41 C
ATOM 1815 CE2 PHE A 235 0.195 17.929 12.998 1.00 60.95 C
ATOM 1816 CZ PHE A 235 0.678 19.230 13.090 1.00 60.50 C
ATOM 1817 N GLU A 236 2.374 14.343 18.390 1.00 61.90 N
ATOM 1818 CA GLU A 236 2.287 13.490 19.570 1.00 62.38 C
ATOM 1819 C GLU A 236 3.420 13.735 20.563 1.00 62.34 C
ATOM 1820 O GLU A 236 3.561 13.011 21.548 1.00 62.38 O
ATOM 1821 CB GLU A 236 2.261 12.015 19.156 1.00 63.34 C
ATOM 1822 CG GLU A 236 1.031 11.631 18.340 1.00 64.36 C
ATOM 1823 CD GLU A 236 0.914 10.134 18.117 1.00 65.26 C
ATOM 1824 OEl GLU A 236 1.848 9.539 17.537 1.00 66.03 O
ATOM 1825 OE2 GLU A 236 -0.115 9.552 18.520 1.00 65.24 O
ATOM 1826 N LYS A 237 4.223 14.763 20.304 1.00 61.94 N
ATOM 1827 CA LYS A 237 5.335 15.100 21.185 1.00 61.39 C
ATOM 1828 C LYS A 237 5.157 16.492 21.782 1.00 60.50 C
ATOM 1829 O LYS A 237 5.906 16.897 22.670 1.00 60.06 O
ATOM 1830 CB LYS A 237 6.660 15.032 20.421 1.00 62.62 C
ATOM 1831 CG LYS A 237 7.022 13.640 19.920 1.00 63.81 C
ATOM 1832 CD LYS A 237 7.152 12.645 21.067 1.00 64.53 C
ATOM 1833 CE LYS A 237 8.258 13.044 22.034 1.00 64.95 C
ATOM 1834 NZ LYS A 237 8.388 12.077 23.161 1.00 64.98 N
ATOM 1835 N LEU A 238 4.156 17.218 21.293 1.00 59.89 N
ATOM 1836 CA LEU A 238 3.875 18.566 21.774 1.00 59.52 C
ATOM 1837 C LEU A 238 3.574 18.587 23.269 1.00 59.03 C

ATOM	1838	O	LEU	A	238	3.649	19.636	23.910	1.00	58.66
O										
ATOM	1839	CB	LEU	A	238	2.691	19.161	21.010	1.00	59.69
C										
ATOM	1840	CG	LEU	A	238	2.881	19.357	19.505	1.00	60.11
C										
ATOM	1841	CDl	LEU	A	238	1.586	19.854	18.886	1.00	60.44
C										
ATOM	1842	CD2	LEU	A	238	4.008	20.346	19.256	1.00	60.61
C										
ATOM	1843	N	LYS	A	239	3.232	17.428	23.820	1.00	58.41
N										
ATOM	1844	CA	LYS	A	239	2.919	17.324	25.240	1.00	58.03
C										
ATOM	1845	C	LYS	A	239	4.131	16.896	26.058	1.00	56.89
C										
ATOM	1846	O	LYS	A	239	4.025	16.675	27.263	1.00	57.45
O										
ATOM	1847	CB	LYS	A	239	1.777	16.326	25.463	1.00	59.26
C										
ATOM	1848	CG	LYS	A	239	0.416	16.788	24.953	1.00	59.87
C										
ATOM	1849	CD	LYS	A	239	0.386	16.921	23.439	1.00	61.15
C										
ATOM	1850	CE	LYS	A	239	-0.976	17.399	22.955	1.00	61.74
C										
ATOM	1851	NZ	LYS	A	239	-1.022	17.539	21.473	1.00	62.28
N										
ATOM	1852	N	ASP	A	240	5.282	16.786	25.402	1.00	55.23
N										
ATOM	1853	CA	ASP	A	240	6.510	16.377	26.077	1.00	53.14
C										
ATOM	1854	C	ASP	A	240	7.336	17.589	26.499	1.00	51.17
C										
ATOM	1855	O	ASP	A	240	7.824	18.343	25.658	1.00	50.71
O										
ATOM	1856	CB	ASP	A	240	7.343	15.484	25.154	1.00	54.56
C										
ATOM	1857	CG	ASP	A	240	8.514	14.836	25.870	1.00	55.41
C										
ATOM	1858	ODl	ASP	A	240	9.318	15.565	26.488	1.00	56.45
O										
ATOM	1859	OD2	ASP	A	240	8.632	13.594	25.811	1.00	57.22
O										
ATOM	1860	N	PRO	A	241	7.503	17.789	27.816	1.00	49.07
N										
ATOM	1861	CA	PRO	A	241	8.274	18.912	28.360	1.00	46.33
C										
ATOM	1862	C	PRO	A	241	9.713	18.938	27.849	1.00	44.21
C										
ATOM	1863	O	PRO	A	241	10.268	20.005	27.584	1.00	43.10
O										
ATOM	1864	CB	PRO	A	241	8.205	18.677	29.867	1.00	47.23
C										
ATOM	1865	CG	PRO	A	241	6.875	18.008	30.038	1.00	47.52
C										
ATOM	1866	CD	PRO	A	241	6.877	17.014	28.902	1.00	48.48
C										
ATOM	1867	N	GLY	A	242	10.307	17.755	27.718	1.00	41.27
N										

ATOM 1868 CA GLY A 242 11.677 17.650 27.249 1.00 39.61 C
ATOM 1869 C GLY A 242 11.917 18.315 25.909 1.00 37.53 C
ATOM 1870 O GLY A 242 12.930 18.991 25.717 1.00 36.92 O
ATOM 1871 N VAL A 243 10.992 18.125 24.973 1.00 36.59 N
ATOM 1872 CA VAL A 243 11.131 18.723 23.653 1.00 35.09 C
ATOM 1873 C VAL A 243 11.040 20.244 23.755 1.00 34.28 C
ATOM 1874 O VAL A 243 11.778 20.965 23.080 1.00 32.03 O
ATOM 1875 CB VAL A 243 10.044 18.213 22.685 1.00 36.09 C
ATOM 1876 CGl VAL A 243 10.232 18.844 21.310 1.00 36.68 C
ATOM 1877 CG2 VAL A 243 10.116 16.698 22.582 1.00 37.38 C
ATOM 1878 N TRP A 244 10.135 20.730 24.600 1.00 32.90 N
ATOM 1879 CA TRP A 244 9.973 22.166 24.786 1.00 31.49 C
ATOM 1880 C TRP A 244 11.200 22.787 25.427 1.00 29.90 C
ATOM 1881 O TRP A 244 11.606 23.889 25.067 1.00 29.16 O
ATOM 1882 CB TRP A 244 8.738 22.469 25.640 1.00 33.40 C
ATOM 1883 CG TRP A 244 7.468 22.314 24.879 1.00 35.53 C
ATOM 1884 CDl TRP A 244 6.686 21.199 24.801 1.00 35.48 C
ATOM 1885 CD2 TRP A 244 6.865 23.291 24.022 1.00 36.42 C
ATOM 1886 NEl TRP A 244 5.633 21.420 23.944 1.00 36.12 N
ATOM 1887 CE2 TRP A 244 5.719 22.695 23.452 1.00 36.34 C
ATOM 1888 CE3 TRP A 244 7.184 24.611 23.676 1.00 37.21 C
ATOM 1889 CZ2 TRP A 244 4.887 23.375 22.556 1.00 37.23 C
ATOM 1890 CZ3 TRP A 244 6.357 25.288 22.782 1.00 37.27 C
ATOM 1891 CH2 TRP A 244 5.222 24.666 22.234 1.00 37.92 C
ATOM 1892 N ILE A 245 11.788 22.082 26.385 1.00 28.95 N
ATOM 1893 CA ILE A 245 12.978 22.580 27.053 1.00 29.17 C
ATOM 1894 C ILE A 245 14.122 22.645 26.042 1.00 27.99 C
ATOM 1895 O ILE A 245 14.897 23.601 26.027 1.00 26.30 O
ATOM 1896 CB ILE A 245 13.367 21.671 28.239 1.00 31.33 C
ATOM 1897 CGl ILE A 245 12.340 21.844 29.364 1.00 33.77 C

ATOM	1898	CG2	ILE	A	245	14.773	22.000	28.721	1.00	33.67
C										
ATOM	1899	CDl	ILE	A	245	12.650	21.059	30.623	1.00	36.66
C										
ATOM	1900	N	ALA	A	246	14.211	21.627	25.190	1.00	26.95
N										
ATOM	1901	CA	ALA	A	246	15.253	21.574	24.170	1.00	26.36
C										
ATOM	1902	C	ALA	A	246	15.071	22.692	23.144	1.00	24.97
C										
ATOM	1903	O	ALA	A	246	16.032	23.371	22.773	1.00	24.03
O										
ATOM	1904	CB	ALA	A	246	15.232	20.215	23.471	1.00	27.51
C										
ATOM	1905	N	ALA	A	247	13.836	22.877	22.692	1.00	24.52
N										
ATOM	1906	CA	ALA	A	247	13.514	23.905	21.704	1.00	24.74
C										
ATOM	1907	C	ALA	A	247	13.832	25.308	22.216	1.00	24.44
C										
ATOM	1908	O	ALA	A	247	14.486	26.095	21.531	1.00	22.05
O										
ATOM	1909	CB	ALA	A	247	12.037	23.812	21.317	1.00	26.31
C										
ATOM	1910	N	VAL	A	248	13.369	25.620	23.422	1.00	23.99
N										
ATOM	1911	CA	VAL	A	248	13.621	26.931	24.006	1.00	23.29
C										
ATOM	1912	C	VAL	A	248	15.115	27.135	24.236	1.00	22.46
C										
ATOM	1913	O	VAL	A	248	15.651	28.215	23.981	1.00	21.15
O										
ATOM	1914	CB	VAL	A	248	12.868	27.099	25.346	1.00	24.86
C										
ATOM	1915	CGl	VAL	A	248	13.213	28.438	25.974	1.00	24.49
C										
ATOM	1916	CG2	VAL	A	248	11.364	26.994	25.107	1.00	25.21
C										
ATOM	1917	N	GLY	A	249	15.788	26.092	24.714	1.00	21.59
N										
ATOM	1918	CA	GLY	A	249	17.214	26.193	24.955	1.00	20.30
C										
ATOM	1919	C	GLY	A	249	17.965	26.516	23.678	1.00	18.76
C										
ATOM	1920	O	GLY	A	249	18.890	27.330	23.684	1.00	18.10
O										
ATOM	1921	N	GLN	A	250	17.566	25.882	22.581	1.00	18.57
N										
ATOM	1922	CA	GLN	A	250	18.216	26.114	21.295	1.00	18.10
C										
ATOM	1923	C	GLN	A	250	17.952	27.531	20.805	1.00	17.73
C										
ATOM	1924	O	GLN	A	250	18.851	28.185	20.276	1.00	16.41
O										
ATOM	1925	CB	GLN	A	250	17.726	25.098	20.264	1.00	18.04
C										
ATOM	1926	CG	GLN	A	250	18.279	25.299	18.847	1.00	18.42
C										
ATOM	1927	CD	GLN	A	250	19.794	25.166	18.760	1.00	18.73
C										

ATOM 1928 OEl GLN A 250 20.415 24.442 19.537 1.00 20.00
ATOM 1929 NE2 GLN A 250 20.391 25.852 17.788 1.00 18.72
ATOM 1930 N ILE A 251 16.724 28.012 20.983 1.00 16.57
ATOM 1931 CA ILE A 251 16.391 29.368 20.561 1.00 18.22
ATOM 1932 C ILE A 251 17.260 30.391 21.296 1.00 16.25
ATOM 1933 O ILE A 251 17.769 31.329 20.689 1.00 16.46
ATOM 1934 CB ILE A 251 14.881 29.662 20.787 1.00 18.92
ATOM 1935 CGl ILE A 251 14.056 28.955 19.708 1.00 19.50
ATOM 1936 CG2 ILE A 251 14.622 31.162 20.784 1.00 20.61
ATOM 1937 CDl ILE A 251 14.339 29.437 18.278 1.00 22.49
ATOM 1938 N PHE A 252 17.444 30.214 22.603 1.00 15.65
ATOM 1939 CA PHE A 252 18.287 31.132 23.362 1.00 17.48
ATOM 1940 C PHE A 252 19.717 31.082 22.838 1.00 16.37
ATOM 1941 O PHE A 252 20.329 32.105 22.518 1.00 16.19
ATOM 1942 CB PHE A 252 18.302 30.744 24.842 1.00 17.64
ATOM 1943 CG PHE A 252 17.264 31.442 25.669 1.00 19.74
ATOM 1944 CDl PHE A 252 17.551 32.653 26.289 1.00 20.39
ATOM 1945 CD2 PHE A 252 16.003 30.881 25.840 1.00 22.10
ATOM 1946 CEl PHE A 252 16.587 33.302 27.077 1.00 22.53
ATOM 1947 CE2 PHE A 252 15.032 31.521 26.624 1.00 21.87
ATOM 1948 CZ PHE A 252 15.329 32.729 27.240 1.00 21.03
ATOM 1949 N PHE A 253 20.248 29.871 22.748 1.00 17.32
ATOM 1950 CA PHE A 253 21.618 29.701 22.303 1.00 17.45
ATOM 1951 C PHE A 253 21.874 30.247 20.908 1.00 15.03
ATOM 1952 O PHE A 253 22.805 31.017 20.700 1.00 15.99
ATOM 1953 CB PHE A 253 22.008 28.224 22.334 1.00 17.99
ATOM 1954 CG PHE A 253 23.488 27.992 22.208 1.00 19.44
ATOM 1955 CDl PHE A 253 24.283 27.880 23.345 1.00 20.66
ATOM 1956 CD2 PHE A 253 24.091 27.923 20.956 1.00 20.42
ATOM 1957 CEl PHE A 253 25.666 27.702 23.239 1.00 22.90

ATOM	1958	CE2	PHE	A	253	25.474	27.746	20,.836	1.00	21..12 C
ATOM	1959	CZ	PHE	A	253	26.260	27.635	21.983	1.00	21.00 C
ATOM	1960	N	THR	A	254	21.039	29.858	19.953	1.00	16.18 N
ATOM	1961	CA	THR	A	254	21.263	30.288	18.580	1.00	17.20 C
ATOM	1962	C	THR	A	254	21.086	31.781	18.330	1.00	17.18 C
ATOM	1963	O	THR	A	254	21.751	32.344	17.460	1.00	14.60 O
ATOM	1964	CB	THR	A	254	20.385	29.492	17.592	1.00	17.65 C
ATOM	1965	OGl	THR	A	254	20.909	29.663	16.268	1.00	17.46 O
ATOM	1966	CG2	THR	A	254	18.929	29.979	17.626	1.00	17.65 C
ATOM	1967	N	LEU	A	255	20.212	32.434	19.089	1.00	15.46 N
ATOM	1968	CA	LEU	A	255	20.014	33.870	18.899	1.00	16.74 C
ATOM	1969	C	LEU	A	255	20.910	34.715	19.807	1.00	15.16 C
ATOM	1970	O	LEU	A	255	20.,852	35.946	19.775	1.00	16.97 O
ATOM	1971	CB	LEU	A	255	18..543	34.245	19.123	1.00	16.60 C
ATOM	1972	CG	LEU	A	255	17..578	33.816	18.019	1.00	18.68 C
ATOM	1973	CDl	LEU	A	255	16..148	34.186	18.419	1.00	20.17 C
ATOM	1974	CD2	LEU	A	255	17,.966	34.496	16.715	1.00	18.66 C
ATOM	1975	N	SER	A	256	21..748	34.047	20.601	1.00	17.12 N
ATOM	1976	CA	SER	A	256	22.664	34.714	21.526	1.00	17.60 C
ATOM	1977	C	SER	A	256	21.892	35.485	22.590	1.00	18.47 C
ATOM	1978	O	SER	A	256	22.350	36.523	23.061	1.00	21.39 O
ATOM	1979	CB	SER	A	256	23.583	35.690	20.786	1.00	19.41 C
ATOM	1980	OG	SER	A	256	24.351	35.043	19.792	1.00	20.16 O
ATOM	1981	N	LEU	A	257	20.731	34.968	22.970	1.00	19.01 N
ATOM	1982	CA	LEU	A	257	19.898	35.625	23.971	1.00	20.22 C
ATOM	1983	C	LEU	A	257	20.264	35.181	25.377	1.00	20.72 C
ATOM	1984	O	LEU	A	257	20.505	33.995	25.625	1.00	19.58 O
ATOM	1985	CB	LEU	A	257	18.424	35.316	23.708	1.00	21.94 C
ATOM	1986	CG	LEU	A	257	17.912	35.750	22.332	1.00	25.00 C
ATOM	1987	CDl	LEU	A	257	16.502	35.235	22.135	1.00	27.08 C

ATOM	1988	CD2	LEU	A	257	17.967	37.264	22.211	1.00	27.93
C										
ATOM	1989	N	GLY	A	258	20.302	36.143	26.294	1.00	20.61
N										
ATOM	1990	CA	GLY	A	258	20.636	35.839	27.674	1.00	22.51
C										
ATOM	1991	C	GLY	A	258	22.127	35.710	27.927	1.00	23.09
C										
ATOM	1992	O	GLY	A	258	22.532	35.269	29.001	1.00	22.48
O										
ATOM	1993	N	PHE	A	259	22.936	36.096	26.940	1.00	22.01
N										
ATOM	1994	CA	PHE	A	259	24.398	36.028	27.030	1.00	24.18
C										
ATOM	1995	C	PHE	A	259	25.004	37.417	27.217	1.00	26.84
C										
ATOM	1996	O	PHE	A	259	26.222	37.556	27.348	1.00	27.70
O										
ATOM	1997	CB	PHE	A	259	24.989	35.435	25.746	1.00	23.04
C										
ATOM	1998	CG	PHE	A	259	24.677	33.985	25.529	1.00	21.42
C										
ATOM	1999	CDl	PHE	A	259	25.552	32.994	25.973	1.00	21.26
C										
ATOM	2000	CD2	PHE	A	259	23.529	33.606	24.843	1.00	22.63
C										
ATOM	2001	CEl	PHE	A	259	25.287	31.648	25.733	1.00	20.94
C										
ATOM	2002	CE2	PHE	A	259	23.251	32.263	24.596	1.00	22.58
C										
ATOM	2003	CZ	PHE	A	259	24.135	31.276	25.042	1.00	24.04
C										
ATOM	2004	N	GLY	A	260	24.155	38.442	27.203	1.00	26.08
N										
ATOM	2005	CA	GLY	A	260	24.630	39.807	27.351	1.00	26.17
C										
ATOM	2006	C	GLY	A	260	25.346	40.313	26.106	1.00	24.96
C										
ATOM	2007	O	GLY	A	260	25.748	41.472	26.046	1.00	24.10
O										
ATOM	2008	N	ALA	A	261	25.492	39.448	25.106	1.00	23.41
N										
ATOM	2009	CA	ALA	A	261	26.186	39.796	23.872	1.00	21.74
C										
ATOM	2010	C	ALA	A	261	25.393	40.719	22.950	1.00	19.86
C										
ATOM	2011	O	ALA	A	261	25.955	41.647	22.370	1.00	18.77
O										
ATOM	2012	CB	ALA	A	261	26.579	38.527	23.121	1.00	23.68
C										
ATOM	2013	N	ILE	A	262	24.100	40.456	22.799	1.00	19.02
N										
ATOM	2014	CA	ILE	A	262	23.268	41.300	21.944	1.00	18.45
C										
ATOM	2015	C	ILE	A	262	23.185	42.681	22.578	1.00	18.98
C										
ATOM	2016	O	ILE	A	262	23.261	43.703	21.890	1.00	18.25
O										
ATOM	2017	CB	ILE	A	262	21.843	40.722	21.788	1.00	20.14
C										

ATOM	2018	CGl	ILE	A	262	21.897	39.397	21.025	1.00	19.76
ATOM	2019	CG2	ILE	A	262	20.941	41.732	21.064	1.00	18.80
ATOM	2020	CDl	ILE	A	262	22.429	39.513	19.607	1.00	22.42
ATOM	2021	N	ILE	A	263	23.042	42.703	23.900	1.00	17.35
ATOM	2022	CA	ILE	A	263	22.961	43.954	24.637	1.00	18.16
ATOM	2023	C	ILE	A	263	24.218	44.784	24.410	1.00	17.35
ATOM	2024	O	ILE	A	263	24.135	45.960	24.067	1.00	17.71
ATOM	2025	CB	ILE	A	263	22.773	43.697	26.152	1.00	18.78
ATOM	2026	CGl	ILE	A	263	21.392	43.086	26.396	1.00	20.63
ATOM	2027	CG2	ILE	A	263	22.954	44.995	26.940	1.00	21.30
ATOM	2028	CDl	ILE	A	263	21.106	42.769	27.846	1.00	22.65
ATOM	2029	N	THR	A	264	25.390	44.179	24.573	1.00	15.58
ATOM	2030	CA	THR	A	264	26.618	44.945	24.379	1.00	16.23
ATOM	2031	C	THR	A	264	26.775	45.461	22.950	1.00	16.73
ATOM	2032	O	THR	A	264	27.156	46.613	22.740	1.00	17.50
ATOM	2033	CB	THR	A	264	27.861	44.125	24.776	1.00	18.33
ATOM	2034	OGl	THR	A	264	27.796	43.838	26.178	1.00	20.01
ATOM	2035	CG2	THR	A	264	29.135	44.909	24.483	1.00	18.68
ATOM	2036	N	TYR	A	265	26.491	44.619	21.961	1.00	16.28
ATOM	2037	CA	TYR	A	265	26.604	45.063	20.578	1.00	15.76
ATOM	2038	C	TYR	A	265	25.649	46.229	20.328	1.00	15.78
ATOM	2039	O	TYR	A	265	25.997	47.198	19.659	1.00	16.91
ATOM	2040	CB	TYR	A	265	26.266	43.928	19.616	1.00	16.64
ATOM	2041	CG	TYR	A	265	27.458	43.140	19.121	1.00	16.81
ATOM	2042	CDl	TYR	A	265	28.590	42.970	19.913	1.00	18.53
ATOM	2043	CD2	TYR	A	265	27.433	42.532	17.865	1.00	16.81
ATOM	2044	CEl	TYR	A	265	29.674	42.208	19.465	1.00	19.26
ATOM	2045	CE2	TYR	A	265	28.508	41.768	17.409	1.00	17.72
ATOM	2046	CZ	TYR	A	265	29.622	41.612	18.216	1.00	18.07
ATOM	2047	OH	TYR	A	265	30.679	40.847	17.775	1.00	17.97

ATOM 2048 N ALA A 266 24.446 46.128 20.875 1.00 16.19 N
ATOM 2049 CA ALA A 266 23.443 47.175 20.689 1.00 16.16 C
ATOM 2050 C ALA A 266 23.829 48.477 21.380 1.00 17.94 C
ATOM 2051 O ALA A 266 23.298 49.546 21.048 1.00 18.73 O
ATOM 2052 CB ALA A 266 22.088 46.692 21.200 1.00 16.70 C
ATOM 2053 N SER A 267 24.747 48.401 22.344 1.00 17.57 N
ATOM 2054 CA SER A 267 25.165 49.603 23.061 1.00 18.76 C
ATOM 2055 C SER A 267 25.988 50.524 22.162 1.00 19.40 C
ATOM 2056 O SER A 267 26.293 51.657 22.542 1.00 20.56 O
ATOM 2057 CB SER A 267 25.974 49.238 24.312 1.00 17.99 C
ATOM 2058 OG SER A 267 27.323 48.925 23.993 1.00 20.15 O
ATOM 2059 N TYR A 268 26.339 50.037 20.972 1.00 18.26 N
ATOM 2060 CA TYR A 268 27.115 50.821 20.017 1.00 18.08 C
ATOM 2061 C TYR A 268 26.243 51.380 18.906 1.00 19.75 C
ATOM 2062 O TYR A 268 26.738 52.005 17.971 1.00 21.11 G
ATOM 2063 CB TYR A 268 28.241 49.976 19.432 1.00 19.50 C
ATOM 2064 CG TYR A 268 29.169 49.487 20.511 1.00 19.59 C
ATOM 2065 CDl TYR A 268 29.935 50.389 21.254 1.00 19.35 C
ATOM 2066 CD2 TYR A 268 29.239 48.135 20.837 1.00 19.83 C
ATOM 2067 CEl TYR A 268 30.746 49.953 22.301 1.00 19.47 C
ATOM 2068 CE2 TYR A 268 30.043 47.689 21.883 1.00 19.18 C
ATOM 2069 CZ TYR A 268 30.792 48.603 22.610 1.00 19.63 C
ATOM 2070 OH TYR A 268 31.578 48.166 23.650 1.00 20.52 O
ATOM 2071 N VAL A 269 24.942 51.140 19.017 1.00 20.09 N
ATOM 2072 CA VAL A 269 23.987 51.649 18.042 1.00 22.08 C
ATOM 2073 C VAL A 269 23.649 53.065 18.497 1.00 24.02 C
ATOM 2074 O VAL A 269 23.388 53.286 19.675 1.00 23.86 O
ATOM 2075 CB VAL A 269 22.693 50.812 18.036 1.00 21.24 C
ATOM 2076 CGl VAL A 269 21.686 51.415 17.061 1.00 23.86 C
ATOM 2077 CG2 VAL A 269 23.,004 49.371 17.647 1.00 21.54 C

ATOM	2078	N	ARG	A	270	23.657	54.025	17.578	1.00	26.82	N
ATOM	2079	CA	ARG	A	270	23.341	55.401	17.951	1.00	29.38	C
ATOM	2080	C	ARG	A	270	21.952	55.502	18.574	1.00	29.47	C
ATOM	2081	O	ARG	A	270	21.023	54.800	18.178	1.00	28.49	O
ATOM	2082	CB	ARG	A	270	23.467	56.324	16.737	1.00	31.89	C
ATOM	2083	CG	ARG	A	270	24.909	56.494	16.276	1.00	34.97	C
ATOM	2084	CD	ARG	A	270	25.025	57.388	15.053	1.00	38.21	C
ATOM	2085	NE	ARG	A	270	26.404	57.475	14.579	1.00	41.50	N
ATOM	2086	CZ	ARG	A	270	27.385	58.109	15.216	1.00	42.23	C
ATOM	2087	NHl	ARG	A	270	27.148	58.729	16.365	1.00	44.14	N
ATOM	2088	NH2	ARG	A	270	28.610	58.118	14.706	1.00	43.44	N
ATOM	2089	N	LYS	A	271	21.827	56.382	19.561	1.00	30.57	N
ATOM	2090	CA	LYS	A	271	20.580	56.574	20.291	1.00	32.77	C
ATOM	2091	C	LYS	A	271	19.333	56.706	19.422	1.00	33.41	C
ATOM	2092	O	LYS	A	271	18.261	56.241	19.798	1.00	34.04	O
ATOM	2093	CB	LYS	A	271	20.707	57.804	21.195	1.00	35.14	C
ATOM	2094	CG	LYS	A	271	19.484	58.087	22.052	1.00	39.23	C
ATOM	2095	CD	LYS	A	271	19.710	59.286	22.966	1.00	42.65	C
ATOM	2096	CE	LYS	A	271	19.998	60.552	22.171	1.00	44.46	C
ATOM	2097	NZ	LYS	A	271	18.871	60.913	21.265	1.00	46.25	N
ATOM	2098	N	ASP	A	272	19.488	57.330	18.260	1.00	34.66	N
ATOM	2099	CA	ASP	A	272	18.384	57.568	17.331	1.00	35.96	C
ATOM	2100	C	ASP	A	272	18.119	56.450	16.326	1.00	34.82	C
ATOM	2101	O	ASP	A	272	17.053	56.401	15.707	1.00	33.74	O
ATOM	2102	CB	ASP	A	272	18.665	58.855	16.558	1.00	40.14	C
ATOM	2103	CG	ASP	A	272	20.078	58.889	15.992	1.00	44.19	C
ATOM	2104	ODl	ASP	A	272	21.034	59.008	16.790	1.00	46.07	O
ATOM	2105	OD2	ASP	A	272	20.235	58.784	14.755	1.00	46.74	O
ATOM	2106	N	GLN	A	273	19.087	55.555	16.174	1.00	31.63	N
ATOM	2107	CA	GLN	A	273	19.003	54.464	15.210	1.00	30.48	C

ATOM	2108	C	GLN	A	273	17.965	53.380	15.485	1.00	28.16
ATOM	2109	O	GLN	A	273	17.782	52.944	16.620	1.00	28.40
ATOM	2110	CB	GLN	A	273	20.376	53.810	15.078	1.00	32.18
ATOM	2111	CG	GLN	A	273	20.in	53.479	13.665	1.00	36.46
ATOM	2112	CD	GLN	A	273	22.107	52.762	13.604	1.00	38.87
ATOM	2113	OEl	GLN	A	273	23.070	53.154	14.271	1.00	40.84
ATOM	2114	NE2	GLN	A	273	22.174	51.711	12.795	1.00	37.10
ATOM	2115	N	ASP	A	274	17.309	52.934	14.419	1.00	24.89
ATOM	2116	CA	ASP	A	274	16.297	51.886	14.508	1.00	24.90
ATOM	2117	C	ASP	A	274	16.878	50.591	15.054	1.00	23.57
ATOM	2118	O	ASP	A	274	18.011	50.230	14.736	1.00	22.86
ATOM	2119	CB	ASP	A	274	15.717	51.584	13.125	1.00	23.58
ATOM	2120	CG	ASP	A	274	15.063	50.204	13.051	1.00	24.33
ATOM	2121	ODl	ASP	A	274	13.852	50.086	13.339	1.00	23.60
ATOM	2122	OD2	ASP	A	274	15.771	49.225	12.722	1.00	24.21
ATOM	2123	N	ILE	A	275	16.091	49.897	15.869	1.00	22.74
ATOM	2124	CA	ILE	A	275	16.496	48.606	16.398	1.00	21.46
ATOM	2125	C	ILE	A	275	15.380	47.588	16.153	1.00	20.90
ATOM	2126	O	ILE	A	275	15.591	46.388	16.295	1.00	21.89
ATOM	2127	CB	ILE	A	275	16.820	48.657	17.912	1.00	21.65
ATOM	2128	CGl	ILE	A	275	15.595	49.109	18.707	1.00	23.65
ATOM	2129	CG2	ILE	A	275	18.007	49.577	18.154	1.00	22.58
ATOM	2130	CDl	ILE	A	275	15.811	49.117	20.202	1.00	24.55
ATOM	2131	N	VAL	A	276	14.193	48.059	15.773	1.00	20.40
ATOM	2132	CA	VAL	A	276	13.085	47.140	15.520	1.00	20.05
ATOM	2133	C	VAL	A	276	13.321	46.329	14.248	1.00	21.61
ATOM	2134	O	VAL	A	276	13.311	45.099	14.279	1.00	20.83
ATOM	2135	CB	VAL	A	276	11.728	47.875	15.386	1.00	21.69
ATOM	2136	CGl	VAL	A	276	10.619	46.859	15.123	1.00	21.73
ATOM	2137	CG2	VAL	A	276	11.428	48.665	16.659	1.00	22.52

ATOM 2138 N LEU A 277 13.543 47.014 13.130 1.00 20.72 N
ATOM 2139 CA LEU A 277 13.771 46.321 11.870 1.00 22.27 C
ATOM 2140 C LEU A 277 15.129 45.626 11.870 1.00 21.36 C
ATOM 2141 O LEU A 277 15.255 44.498 '11.399 1.00 21.98 O
ATOM 2142 CB LEU A 277 13.692 47.296 10.691 1.00 24.52 C
ATOM 2143 CG LEU A 277 13.883 46.645 9.318 1.00 25.33 C
ATOM 2144 CDl LEU A 277 12.808 45.587 9.096 1.00 26.74 C
ATOM 2145 CD2 LEU A 277 13.822 47.712 8.233 1.00 27.84 C
ATOM 2146 N SER A 278 16.137 46.305 12.405 1.00 22.10 N
ATOM 2147 CA SER A 278 17.480 45.746 12.469 1.00 23.40 C
ATOM 2148 C SER A 278 17.514 44.477 13.306 1.00 21.97 C
ATOM 2149 O SER A 278 18.111 43.480 12.901 1.00 21.04 O
ATOM 2150 CB SER A 278 18.449 46.771 13.048 1.00 25.34 C
ATOM 2151 OG SER A 278 18.690 47.796 12.099 1.00 31.33 O
ATOM 2152 N GLY A 279 16.868 44.513 14.469 1.00 22.02 N
ATOM 2153 CA GLY A 279 16.844 43.346 15.332 1.00 22.08 C
ATOM 2154 C GLY A 279 16.119 42.177 14.693 1.00 22.07 C
ATOM 2155 O GLY A 279 16.580 41.036 14.745 1.00 20.27 O
ATOM 2156 N LEU A 280 14.973 42.461 14.081 1.00 21.26 N
ATOM 2157 CA LEU A 280 14.190 41.427 13.423 1.00 21.19 C
ATOM 2158 C LEU A 280 14.968 40.813 12.263 1.00 20.28 C
ATOM 2159 O LEU A 280 14.901 39.606 12.030 1.00 22.36 O
ATOM 2160 CB LEU A 280 12.878 42.015 12.895 1.00 22.62 C
ATOM 2161 CG LEU A 280 11.983 41.051 12.111 1.00 24.65 C
ATOM 2162 CDl LEU A 280 11.531 39.907 13.012 1.00 25.92 C
ATOM 2163 CD2 LEU A 280 10.771 41.821 11.571 1.00 24.96 C
ATOM 2164 N THR A 281 15.714 41.646 11.542 1.00 20.78 N
ATOM 2165 CA THR A 281 16.488 41.175 10.401 1.00 21.49 C
ATOM 2166 C THR A 281 17.614 40.252 10.855 1.00 21.11 C
ATOM 2167 O THR A 281 17.835 39.195 10.267 1.00 22.11 O

ATOM	2168	CB	THR	A	281	17.080	42.359	9.594	1.00	22.10
C										
ATOM	2169	OGl	THR	A	281	16.014	43.169	9.074	1.00	23.91
O										
ATOM	2170	CG2	THR	A	281	17.912	41.848	8.427	1.00	22.02
C										
ATOM	2171	N	ALA	A	282	18.326	40.649	11.903	1.00	21.94
N										
ATOM	2172	CA	ALA	A	282	19.415	39.818	12.412	1.00	21.80
C										
ATOM	2173	C	ALA	A	282	18.850	38.471	12.847	1.00	21.47
C										
ATOM	2174	O	ALA	A	282	19.425	37.422	12.559	1.00	21.15
O										
ATOM	2175	CB	ALA	A	282	20.098	40.503	13.584	1.00	22.93
C										
ATOM	2176	N	ALA	A	283	17.715	38.506	13.538	1.00	20.30
N										
ATOM	2177	CA	ALA	A	283	17.075	37.290	14.015	1.00	19.82
C										
ATOM	2178	C	ALA	A	283	16.623	36.397	12.862	1.00	20.92
C										
ATOM	2179	O	ALA	A	283	16.781	35.178	12.914	1.00	18.79
O										
ATOM	2180	CB	ALA	A	283	15.885	37.642	14.902	1.00	20.28
C										
ATOM	2181	N	THR	A	284	16.053	37.008	11.828	1.00	20.73
N										
ATOM	2182	CA	THR	A	284	15.579	36.257	10.670	1.00	22.68
C										
ATOM	2183	C	THR	A	284	16.736	35.652	9.896	1.00	20.36
C										
ATOM	2184	O	THR	A	284	16.646	34.525	9.422	1.00	20.36
O										
ATOM	2185	CB	THR	A	284	14.754	37.153	9.726	1.00	24.05
C										
ATOM	2186	OGl	THR	A	284	13.589	37.611	10.419	1.00	28.99
O										
ATOM	2187	CG2	THR	A	284	14.324	36.371	8.491	1.00	28.17
C										
ATOM	2188	N	LEU	A	285	17.819	36.405	9.755	1.00	20.44
N										
ATOM	2189	CA	LEU	A	285	18.989	35.900	9.052	1.00	20.56
C										
ATOM	2190	C	LEU	A	285	19.533	34.687	9.799	1.00	19.61
C										
ATOM	2191	O	LEU	A	285	19.941	33.701	9.189	1.00	19.88
O										
ATOM	2192	CB	LEU	A	285	20.071	36.979	8.963	1.00	21.04
C										
ATOM	2193	CG	LEU	A	285	19.852	38.093	7.938	1.00	24.02
C										
ATOM	2194	CDl	LEU	A	285	20.936	39.148	8.101	1.00	21.73
C										
ATOM	2195	CD2	LEU	A	285	19.875	37.505	6.524	1.00	25.47
C										
ATOM	2196	N	ASN	A	286	19.532	34.749	11.126	1.00	18.81
N										
ATOM	2197	CA	ASN	A	286	20.033	33.622	11.892	1.00	18.65
C										

ATOM	2198	C	ASN	A	286	19.163	32.398	11.680	1.00	18.76
C										
ATOM	2199	O	ASN	A	286	19.667	31.292	11.497	1.00	17.99
O										
ATOM	2200	CB	ASN	A	286	20.062	33.914	13.390	1.00	17.53
C										
ATOM	2201	CG	ASN	A	286	20.538	32.716	14.187	1.00	19.00
C										
ATOM	2202	ODl	ASN	A	286	21.729	32.408	14.203	1.00	17.32
O										
ATOM	2203	ND2	ASN	A	286	19.606	32.015	14.827	1.00	19.74
N										
ATOM	2204	N	GLU	A	287	17.850	32.596	11.721	1.00	18.77
N										
ATOM	2205	CA	GLU	A	287	16.936	31.482	11.540	1.00	20.40
C										
ATOM	2206	C	GLU	A	287	17.054	30.829	10.176	1.00	20.86
C										
ATOM	2207	O	GLU	A	287	16.951	29.606	10.063	1.00	22.58
O										
ATOM	2208	CB	GLU	A	287	15.498	31.928	11.809	1.00	22.00
C										
ATOM	2209	CG	GLU	A	287	15.277	32.268	13.270	1.00	23.41
C										
ATOM	2210	CD	GLU	A	287	15.814	31.183	14.197	1.00	23.30
C										
ATOM	2211	OEl	GLU	A	287	15.380	30.022	14.068	1.00	25.04
O										
ATOM	2212	OE2	GLU	A	287	16.670	31.490	15.050	1.00	24.39
O										
ATOM	2213	N	LYS	A	288	17.275	31.628	9.139	1.00	22.99
N										
ATOM	2214	CA	LYS	A	288	17.428	31.067	7.807	1.00	23.08
C										
ATOM	2215	C	LYS	A	288	18.712	30.254	7.765	1.00	23.87
C										
ATOM	2216	O	LYS	A	288	18.745	29.160	7.205	1.00	24.00
O										
ATOM	2217	CB	LYS	A	288	17.479	32.175	6.755	1.00	24.65
C										
ATOM	2218	CG	LYS	A	288	16.149	32.880	6.554	1.00	28.77
C										
ATOM	2219	CD	LYS	A	288	16.246	33.951	5.478	1.00	32.52
C										
ATOM	2220	CE	LYS	A	288	14.933	34.707	5.344	1.00	35.63
C										
ATOM	2221	NZ	LYS	A	288	15.039	35.839	4.383	1.00	37.02
N										
ATOM	2222	N	ALA	A	289	19.768	30.789	8.371	1.00	21.98
N										
ATOM	2223	CA	ALA	A	289	21.053	30.102	8.391	1.00	22.42
C										
ATOM	2224	C	ALA	A	289	20.961	28.820	9.209	1.00	23.38
C										
ATOM	2225	O	ALA	A	289	21.639	27.835	8.922	1.00	24.84
O										
ATOM	2226	CB	ALA	A	289	22.133	31.022	8.965	1.00	21.92
C										
ATOM	2227	N	GLU	A	290	20.111	28.831	10.227	1.00	21.66
N										

ATOM 2228 CA GLU A 290 19.941 27.664 11.076 1.00 20.13 C
ATOM 2229 C GLU A 290 19.092 26.562 10.451 1.00 21.73 C
ATOM 2230 O GLU A 290 19.568 25.454 10.231 1.00 20.20 O
ATOM 2231 CB GLU A 290 19.318 28.076 12.413 1.00 21.07 C
ATOM 2232 CG GLU A 290 19.037 26.913 13.355 1.00 21.90 C
ATOM 2233 CD GLU A 290 19.492 27.210 14.772 1.00 21.65 C
ATOM 2234 OEl GLU A 290 18.692 27.020 15.717 1.00 22.19 O
ATOM 2235 OE2 GLU A 290 20.658 27.631 14.935 1.00 20.40 O
ATOM 2236 N VAL A 291 17.834 26.869 10.155 1.00 21.80 N
ATOM 2237 CA VAL A 291 16.939 25.858 9.609 1.00 23.93 C
ATOM 2238 C VAL A 291 17.157 25.506 8.145 1.00 24.47 C
ATOM 2239 O VAL A 291 16.995 24.352 7.759 1.00 26.60 O
ATOM 2240 CB VAL A 291 15.456 26.255 9.825 1.00 24.65 C
ATOM 2241 CGl VAL A 291 15.222 26.572 11.293 1.00 24.19 C
ATOM 2242 CG2 VAL A 291 15.088 27.436 8.949 1.00 25.34 C
ATOM 2243 N ILE A 292 17.535 26.484 7.331 1.00 24.22 N
ATOM 2244 CA ILE A 292 17.757 26.221 5.915 1.00 25.14 C
ATOM 2245 C ILE A 292 19.160 25.704 5.601 1.00 24.84 C
ATOM 2246 O ILE A 292 19.317 24.729 4.865 1.00 26.33 O
ATOM 2247 CB ILE A 292 17.509 27.483 5.070 1.00 27.45 C
ATOM 2248 CGl ILE A 292 16.086 27.996 5.307 1.00 29.02 C
ATOM 2249 CG2 ILE A 292 17.717 27.165 3.591 1.00 28.54 C
ATOM 2250 CDl ILE A 292 15.782 29.297 4.596 1.00 31.64 C
ATOM 2251 N LEU A 293 20.181 26.350 6.154 1.00 22.70 N
ATOM 2252 CA LEU A 293 21.551 25.933 5.885 1.00 22.44 C
ATOM 2253 C LEU A 293 22.050 24.868 6.860 1.00 22.33 C
ATOM 2254 O LEU A 293 22.455 23.781 6.443 1.00 23.46 O
ATOM 2255 CB LEU A 293 22.477 27.157 5.893 1.00 22.36 C
ATOM 2256 CG LEU A 293 22.096 28.237 4.867 1.00 24.30 C
ATOM 2257 CDl LEU A 293 23.069 29.402 4.945 1.00 25.44 C

ATOM	2258	CD2	LEU	A	293	22.103	27.639	3.468	1.00	24.37	C
ATOM	2259	N	GLY	A	294	22.011	25.166	8.154	1.00	21.61	N
ATOM	2260	CA	GLY	A	294	22.469	24.193	9.134	1.00	21.25	C
ATOM	2261	C	GLY	A	294	21.639	22.922	9.105	1.00	21.95	C
ATOM	2262	O	GLY	A	294	22.166	21.812	9.207	1.00	20.86	O
ATOM	2263	N	GLY	A	295	20.332	23.080	8.947	1.00	21.62	N
ATOM	2264	CA	GLY	A	295	19.454	21.925	8.917	1.00	21.32	C
ATOM	2265	C	GLY	A	295	19.582	21.069	7.672	1.00	22.03	C
ATOM	2266	O	GLY	A	295	19.233	19.888	7.698	1.00	23.90	O
ATOM	2267	N	SER	A	296	20.100	21.645	6.591	1.00	22.25	N
ATOM	2268	CA	SER	A	296	20.229	20.913	5.330	1.00	22.45	C
ATOM	2269	C	SER	A	296	21.587	20.269	5.053	1.00	22.61	C
ATOM	2270	O	SER	A	296	21.766	19.632	4.011	1.00	23.33	O
ATOM	2271	CB	SER	A	296	19.872	21.832	4.160	1.00	24.63	C
ATOM	2272	OG	SER	A	296	18.545	22.318	4.279	1.00	25.72	O
ATOM	2273	N	ILE	A	297	22.545	20.425	5.964	1.00	21.92	N
ATOM	2274	CA	ILE	A	297	23.858	19.829	5.742	1.00	21.73	C
ATOM	2275	C	ILE	A	297	24.071	18.499	6.470	1.00	22.28	C
ATOM	2276	O	ILE	A	297	24.039	17.435	5.854	1.00	22.77	O
ATOM	2277	CB	ILE	A	297	24.994	20.817	6.138	1..00	20.90	C
ATOM	2278	CGl	ILE	A	297	24.935	22.052	5.238	1.00	20.24	C
ATOM	2279	CG2	ILE	A	297	26.365	20.142	6.004	1.00	20.92	C
ATOM	2280	CDl	ILE	A	297	25.870	23.173	5.662	1.00	20.34	C
ATOM	2281	N	SER	A	298	24.262	18.562	7.782	1.00	22.01	N
ATOM	2282	CA	SER	A	298	24.530	17.379	{3.596	1.00	23.01	C
ATOM	2283	C	SER	A	298	23.471	16.282	{3.611	1.00	22.91	C
ATOM	2284	O	SER	A	298	23.780	15.111	{3.380	1.00	22.41	O
ATOM	2285	CB	SER	A	298	24.815	17.815	10.036	1.00	23.96	C
ATOM	2286	OG	SER	A	298	25.808	18.823	10.044	1.00	32.54	O
ATOM	2287	N	ILE	A	299	22.230	16.652	8.903	1.00	23.33	N

ATOM	2288	CA	ILE	A	299	21.154	15.670	8.964	1.00	24.62
ATOM	2289	C	ILE	A	299	20.899	14.953	7.640	1.00	24.26
ATOM	2290	O	ILE	A	299	20.851	13.724	7.603	1.00	25.03
ATOM	2291	CB	ILE	A	299	19.836	16.307	9.465	1.00	26.86
ATOM	2292	CGl	ILE	A	299	19.990	16.720	10.930	1.00	29.00
ATOM	2293	CG2	ILE	A	299	18.679	15.321	9.309	1.00	27.98
ATOM	2294	CDl	ILE	A	299	20.417	15.594	11.845	1.00	31.34
ATOM	2295	N	PRO	A	300	20.725	15.704	6.540	1.00	22.92
ATOM	2296	CA	PRO	A	300	20.482	15.038	5.257	1.00	22.55
ATOM	2297	C	PRO	A	300	21.641	14.130	4.853	1.00	23.08
ATOM	2298	O	PRO	A	300	21.429	13.054	4.299	1.00	21.95
ATOM	2299	CB	PRO	A	300	20.286	16.207	4.297	1.00	22.88
ATOM	2300	CG	PRO	A	300	19.634	17.235	5.178	1.00	24.54
ATOM	2301	CD	PRO	A	300	20.499	17.154	6.418	1.00	24.52
ATOM	2302	N	ALA	A	301	22.869	14.554	5.138	1.00	19.81
ATOM	2303	CA	ALA	A	301	24.027	13.734	4.787	1.00	19.94
ATOM	2304	C	ALA	A	301	24.023	12.437	5.589	1.00	19.55
ATOM	2305	O	ALA	A	301	24.223	11.352	5.038	1.00	19.33
ATOM	2306	CB	ALA	A	301	25.322	14.506	5.039	1.00	19.22
ATOM	2307	N	ALA	A	302	23.794	12.548	6.894	1.00	20.22
ATOM	2308	CA	ALA	A	302	23.769	11.381	7.767	1.00	21.57
ATOM	2309	C	ALA	A	302	22.630	10.429	7.402	1.00	22.00
ATOM	2310	O	ALA	A	302	22.815	9.214	7.346	1.00	22.91
ATOM	2311	CB	ALA	A	302	23.635	11.822	9.226	1.00	21.47
ATOM	2312	N	VAL	A	303	21.450	10.981	7.152	1.00	23.15
ATOM	2313	CA	VAL	A	303	20.309	10.147	6.805	1.00	24.53
ATOM	2314	C	VAL	A	303	20.505	9.461	5.455	1.00	25.22
ATOM	2315	O	VAL	A	303	20.129	8.299	5.283	1.00	25.75
ATOM	2316	CB	VAL	A	303	19.003	10.972	6.776	1.00	24.74
ATOM	2317	CGl	VAL	A	303	17.846	10.102	6.293	1.00	27.70

ATOM	2318	CG2	VAL	A	303	18.708	11.512	8.165	1.00	24.19
ATOM	2319	N	ALA	A	304	21.093	10.174	4.499	1.00	24.71
ATOM	2320	CA	ALA	A	304	21.323	9.605	3.173	1.00	25.02
ATOM	2321	C	ALA	A	304	22.249	8.397	3.244	1.00	26.80
ATOM	2322	O	ALA	A	304	22.006	7.379	2.594	1.00	26.86
ATOM	2323	CB	ALA	A	304	21.916	10.660	2.238	1.00	24.86
ATOM	2324	N	PHE	A	305	23.304	8.503	4.045	1.00	24.88
ATOM	2325	CA	PHE	A	305	24.265	7.416	4.168	1.00	26.54
ATOM	2326	C	PHE	A	305	23.906	6.296	5.136	1.00	26.76
ATOM	2327	O	PHE	A	305	24.237	5.137	4.886	1.00	26.85
ATOM	2328	CB	PHE	A	305	25.642	7.968	4.551	1.00	27.08
ATOM	2329	CG	PHE	A	305	26.529	8.248	3.374	1.00	30.41
ATOM	2330	CDl	PHE	A	305	26.198	9.238	2.455	1.00	31.27
ATOM	2331	CD2	PHE	A	305	27.688	7.508	3.174	1.00	30.60
ATOM	2332	CEl	PHE	A	305	27.010	9.486	1.352	1.00	32.91
ATOM	2333	CE2	PHE	A	305	28.509	7.747	2.076	1.00	33.12
ATOM	2334	CZ	PHE	A	305	28.169	8.739	1.162	1.00	33.77
ATOM	2335	N	PHE	A	306	23.233	6.636	6.231	1.00	27.70
ATOM	2336	CA	PHE	A	306	22.889	5.651	7.257	1.00	28.83
ATOM	2337	C	PHE	A	306	21.404	5.391	7.473	1.00	29.82
ATOM	2338	O	PHE	A	306	21.036	4.407	8.114	1.00	31.15
ATOM	2339	CB	PHE	A	306	23.488	6.082	8.598	1.00	28.86
ATOM	2340	CG	PHE	A	306	24.980	6.204	8.588	1.00	30.32
ATOM	2341	CDl	PHE	A	306	25.783	-5.069	8.566	1.00	31.70
ATOM	2342	CD2	PHE	A	306	25.587	7.457	8.595	1.00	29.46
ATOM	2343	CEl	PHE	A	306	27.172	5.178	8.553	1.00	32.90
ATOM	2344	CE2	PHE	A	306	26.971	7.578	8.580	1.00	29.82
ATOM	2345	CZ	PHE	A	306	27.768	6.435	8.560	1.00	31.35
ATOM	2346	N	GLY	A	307	20.554	6.266	6.955	1.00	30.44
ATOM	2347	CA	GLY	A	307	19.128	6.093	7.165	1.00	30.63

ATOM	2348	C	GLY	A	307	18.748	6.874	8.411	1.00 31.51 C
ATOM	2349	O	GLY	A	307	19.623	7.257	9.188	1.00 29.79 O
ATOM	2350	N	VAL	A	308	17.455	7.101	8.619	1.00 32.55 N
ATOM	2351	CA	VAL	A	308	16.992	7.870	9.770	1.00 33.42 C
ATOM	2352	C	VAL	A	308	17.325	7.285	11.143	1.00 34.06 C
ATOM	2353	O	VAL	A	308	17.896	7.975	11.992	1.00 33.82 O
ATOM	2354	CB	VAL	A	308	15.467	8.107	9.699	1.00 34.48 C
ATOM	2355	CGl	VAL	A	308	15.011	8.935	10.898	1.00 34.54 C
ATOM	2356	CG2	VAL	A	308	15.114	8.820	8.405	1.00 34.01 C
ATOM	2357	N	ALA	A	309	16. 970	6.025	11.368	1.00 34.24 N
ATOM	2358	CA	ALA	A	309	17.225	5.387	12.656	1.00 34.46 C
ATOM	2359	C	ALA	A	309	18.673	5.512	13.114	1.00 33.98 C
ATOM	2360	O	ALA	A	309	18.935	5.861	14.267	1.00 32.90 O
ATOM	2361	CB	ALA	A	309	16.823	3.919	12.604	1.00 35.24 C
ATOM	2362	N	ASN	A	310	19.611	5.220	12.217	1.00 33.82 N
ATOM	2363	CA	ASN	A	310	21.028	5.299	12.551	1.00 33.52 C
ATOM	2364	C	ASN	A	310	21.504	6.735	12.706	1.00 32.47 C
ATOM	2365	O	ASN	A	310	22.376	7.017	13.526	1.00 31.48 O
ATOM	2366	CB	ASN	A	310	21. 873	4.595	11. 488	1.00 37.08 C
ATOM	2367	CG	ASN	A	310	21.736	3.091	11.543	1.00 39. 07 C
ATOM	2368	ODl	ASN	A	310	21.817	2.491	12.614	1.00 42.22 O
ATOM	2369	ND2	ASN	A	310	21.538	2.470	10.387	1.00 42.56 N
ATOM	2370	N	ALA	A	311	20.936	7.636	11.910	1.00 32.82 N
ATOM	2371	CA	ALA	A	311	21.304	9.045	11.978	1.00 31.97 C
ATOM	2372	C	ALA	A	311	20.921	9.588	13.349	1.00 31.97 C
ATOM	2373	O	ALA	A	311	21.702	10.291	13.992	1.00 32.34 O
ATOM	2374	CB	ALA	A	311	20.590	9.828	10.881	1.00 32.09 C
ATOM	2375	N	VAL	A	312	19.716	9.253	13.800	1.00 31.17 N
ATOM	2376	CA	VAL	A	312	19.251	9.706	15.106	1.00 31.20 C
ATOM	2377	C	VAL	A	312	20.145	9.152	16. 212	1.00 31.70 C

ATOM	2378	O	VAL	A	312	20.483	9.861	17.162	1.00	31.48
ATOM	2379	CB	VAL	A	312	17.796	9.264	15.368	1.00	31.07
ATOM	2380	CGl	VAL	A	312	17.404	9.582	16.802	1.00	31.52
ATOM	2381	CG2	VAL	A	312	16.864	9.972	14.402	1.00	30.92
ATOM	2382	N	ALA	A	313	20.527	7.883	16.084	1.00	31.22
ATOM	2383	CA	ALA	A	313	21.386	7.247	17.075	1.00	31.89
ATOM	2384	C	ALA	A	313	22.733	7.960	17.135	1.00	31.74
ATOM	2385	O	ALA	A	313	23.337	8.081	18.200	1.00	31.03
ATOM	2386	CB	ALA	A	313	21.585	5.774	16.731	1.00	33.01
ATOM	2387	N	ILE	A	314	23.199	8.430	15.983	1.00	31.97
ATOM	2388	CA	ILE	A	314	24.468	9.145	15.906	1.00	33.03
ATOM	2389	C	ILE	A	314	24.370	10.488	16.627	1.00	32.11
ATOM	2390	O	ILE	A	314	25.282	10.880	17.352	1.00	34.80
ATOM	2391	CB	ILE	A	314	24.880	9.384	14.433	1.00	33.15
ATOM	2392	CGl	ILE	A	314	25.290	8.052	13.794	1.00	34.16
ATOM	2393	CG2	ILE	A	314	26.014	10.405	14.359	1.00	33.96
ATOM	2394	CDl	ILE	A	314	25.622	8.147	12.316	1.00	34.78
ATOM	2395	N	ALA	A	315	23.259	11.189	16.424	1.00	32.70
ATOM	2396	CA	ALA	A	315	23.051	12.484	17.061	1.00	33.30
ATOM	2397	C	ALA	A	315	22.990	12.335	18.577	1.00	33.96
ATOM	2398	O	ALA	A	315	23.520	13.168	19.313	1.00	34.01
ATOM	2399	CB	ALA	A	315	21.768	13.118-	16.548	1.00	33.24
ATOM	2400	N	LYS	A	316	22.345	11.269	19.040	1.00	33.85
ATOM	2401	CA	LYS	A	316	22.221	11.017	20.471	1.00	35.02
ATOM	2402	C	LYS	A	316	23.542	10.575	21.094	1.00	35.83
ATOM	2403	O	LYS	A	316	23.706	10.616	22.314	1.00	36.36
ATOM	2404	CB	LYS	A	316	21.154	9.949	20.726	1.00	35.40
ATOM	2405	CG	LYS	A	316	19.738	10.397	20.400	1.00	38.07
ATOM	2406	CD	LYS	A	316	18.733	9.293	20.693	1.00	40.20
ATOM	2407	CE	LYS	A	316	17.312	9.752	20.418	1.00	41.92

ATOM	2408	NZ	LYS	A	316	16.922	10.889	21.297	1.00	44.76
ATOM	2409	N	ALA	A	317	24.481	10.160	20.249	1.00	36.21
ATOM	2410	CA	ALA	A	317	25.790	9.697	20.707	1.00	37.97
ATOM	2411	C	ALA	A	317	26.564	10.768	21.466	1.00	38.44
ATOM	2412	O	ALA	A	317	27.168	10.494	22.504	1.00	40.66
ATOM	2413	CB	ALA	A	317	26.611	9.211	19.518	1.00	37.61
ATOM	2414	N	GLY	A	318	26.554	11.985	20.936	1.00	37.85
ATOM	2415	CA	GLY	A	318	27.261	13.078	21.574	1.00	36.50
ATOM	2416	C	GLY	A	318	26.957	14.380	20.865	1.00	35.38
ATOM	2417	O	GLY	A	318	26.243	14.397	19.866	1.00	36.63
ATOM	2418	N	ALA	A	319	27.495	15.481	21.371	1.00	33.21
ATOM	2419	CA	ALA	A	319	27.241	16.767	20.743	1.00	31.30
ATOM	2420	C	ALA	A	319	28.192	16.998	19.572	1.00	29.58
ATOM	2421	O	ALA	A	319	27.934	17.843	18.717	1.00	29.84
ATOM	2422	CB	ALA	A	319	27.403	17.883	21.768	1.00	32.49
ATOM	2423	N	PHE	A	320	29.274	16.228	19.527	1.00	26.86
ATOM	2424	CA	PHE	A	320	30.287	16.403	18.491	1.00	24.32
ATOM	2425	C	PHE	A	320	30.426	15.287	17.466	1.00	24.63
ATOM	2426	O	PHE	A	320	31.135	15.447	16.471	1.00	24.08
ATOM	2427	CB	PHE	A	320	31.647	16.634	19.160	1.00	23.52
ATOM	2428	CG	PHE	A	320	31.649	17.765	20.143	1.00	23.10
ATOM	2429	CDl	PHE	A	320	31.430	19.073	19.717	1.00	22.02
ATOM	2430	CD2	PHE	A	320	31.840	17.524	21.500	1.00	24.58
ATOM	2431	CEl	PHE	A	320	31.398	20.121	20.625	1.00	22.36
ATOM	2432	CE2	PHE	A	320	31.808	18.572	22.421	1.00	25.17
ATOM	2433	CZ	PHE	A	320	31.587	19.871	21.981	1.00	22.37
ATOM	2434	N	ASN	A	321	29.756	14.165	17.696	1.00	22.92
ATOM	2435	CA	ASN	A	321	29.852	13.034	16.781	1.00	26.49
ATOM	2436	C	ASN	A	321	29.433	13.357	15.354	1.00	24.84
ATOM	2437	O	ASN	A	321	30.139	13.031	14.400	1.00	25.22

ATOM 2438 CB ASN A 321 29.009 11.870 17.301 1.00 29.82 C
ATOM 2439 CG ASN A 321 29.628 11.198 18.505 1.00 35.81 C
ATOM 2440 ODl ASN A 321 30.262 10.150 18.386 1.00 42.55 O
ATOM 2441 ND2 ASN A 321 29.458 11.803 19.674 1.00 39.55 N
ATOM 2442 N LEU A 322 28.284 14.002 15.207 1.00 21.89 N
ATOM 2443 CA LEU A 322 27.776 14.325 13.884 1.00 21.71 C
ATOM 2444 C LEU A 322 28.669 15.264 13.078 1.00 21.56 C
ATOM 2445 O LEU A 322 28.990 14.986 11.920 1.00 22.02 O
ATOM 2446 CB LEU A 322 26.376 14.929 14.011 1.00 23.65 C
ATOM 2447 CG LEU A 322 25.620 15.209 12.714 1.00 25.57 C
ATOM 2448 CDl LEU A 322 25.488 13.927 11.900 1.00 27.64 C
ATOM 2449 CD2 LEU A 322 24.247 15.772 13.057 1.00 26.38 C
ATOM 2450 N GLY A 323 29.084 16.365 13.697 1.00 19.99 N
ATOM 2451 CA GLY A 323 29.896 17.343 12.996 1.00 18.03 C
ATOM 2452 C GLY A 323 31.385 17.101 12.844 1.00 18.41 C
ATOM 2453 O GLY A 323 31.971 17.513 11.847 1.00 18.70 O
ATOM 2454 N PHE A 324 32.007 16.439 13.812 1.00 17.52 N
ATOM 2455 CA PHE A 324 33.445 16.208 13.752 1.00 18.48 C
ATOM 2456 C PHE A 324 33.857 14.807 13.334 1.00 18.40 C
ATOM 2457 O PHE A 324 35.011 14.582 12.972 1.00 20.77 O
ATOM 2458 CB PHE A 324 34.081 16.518 15.112 1.00 17.06 C
ATOM 2459 CG PHE A 324 34.160 17.985 15.428 1.00 18.45 C
ATOM 2460 CDl PHE A 324 35.265 18.736 15.038 1.00 18.12 C
ATOM 2461 CD2 PHE A 324 33.124 18.620 16.114 1.00 18.02 C
ATOM 2462 CEl PHE A 324 35.341 20.102 15.327 1.00 17.26 C
ATOM 2463 CE2 PHE A 324 33.185 19.985 16.409 1.00 17.47 C
ATOM 2464 CZ PHE A 324 34.296 20.729 16.015 1.00 18.82 C
ATOM 2465 N ILE A 325 32.927 13.863 13.384 1.00 18.03 N
ATOM 2466 CA ILE A 325 33.254 12.492 13.031 1.00 19.05 C
ATOM 2467 C ILE A 325 32.452 11.984 11.848 1.00 19.82 C

ATOM	2468	O	ILE	A	325	33.012	11.618	10.813	1.00	19.26
ATOM	2469	CB	ILE	A	325	33.011	11.542	14.234	1.00	19.31
ATOM	2470	CGl	ILE	A	325	33.935	11.931	15.390	1.00	18.88
ATOM	2471	CG2	ILE	A	325	33.255	10.085	13.824	1.00	20.21
ATOM	2472	CDl	ILE	A	325	33.688	11.142	16.664	1.00	21.00
ATOM	2473	N	THR	A	326	31.135	11.976	12.002	1.00	19.17
ATOM	2474	CA	THR	A	326	30.260	11.459	10.963	1.00	19.59
ATOM	2475	C	THR	A	326	30.297	12.193	9.630	1.00	19.74
ATOM	2476	O	THR	A	326	30.471	11.558	8.586	1.00	21.06
ATOM	2477	CB	THR	A	326	28.806	11.399	11.458	1.00	21.68
ATOM	2478	OGl	THR	A	326	28.748	10.591	12.639	1.00	23.54
ATOM	2479	CG2	THR	A	326	27.902	10.778	10.393	1.00	21.35
ATOM	2480	N	LEU	A	327	30.139	13.513	9.642	1.00	19.17
ATOM	2481	CA	LEU	A	327	30.139	14.245	8.381	1.00	19.96
ATOM	2482	C	LEU	A	327	31.449	14.091	7.604	1.00	21.41
ATOM	2483	O	LEU	A	327	31.426	13.805	6.406	1.00	20.03
ATOM	2484	CB	LEU	A	327	29.819	15.724	8.600	1.00	20.72
ATOM	2485	CG	LEU	A	327	29.482	16.476	7.309	1.00	22.46
ATOM	2486	CDl	LEU	A	327	28.294	15.813	6.613	1.00	23.06
ATOM	2487	CD2	LEU	A	327	29.161	17.924	7.627	1.00	22.84
ATOM	2488	N	PRO	A	328	32.608	14.285	8.262	1.00	21.41
ATOM	2489	CA	PRO	A	328	33.832	14.114	7.468	1.00	20.55
ATOM	2490	C	PRO	A	328	34.005	12.673	6.974	1.00	19.98
ATOM	2491	O	PRO	A	328	34.565	12.445	5.902	1.00	19.29
ATOM	2492	CB	PRO	A	328	34.945	14.563	8.422	1.00	22.75
ATOM	2493	CG	PRO	A	328	34.351	14.389	9.789	1.00	22.72
ATOM	2494	CD	PRO	A	328	32.917	14.828	9.598	1.00	20.72
ATOM	2495	N	ALA	A	329	33.517	11.705	7.748	1.00	18.63
ATOM	2496	CA	ALA	A	329	33.606	10.300	7.354	1.00	18.81
ATOM	2497	C	ALA	A	329	32.778	10.097	6.092	1.00	19.97

ATOM	2498	O	ALA	A	329	33.217	9.437	5.148	1.00	20.03
O										
ATOM	2499	CB	ALA	A	329	33.088	9.396	8.474	1.00	18.86
C										
ATOM	2500	N	ILE	A	330	31.576	10.667	6.077	1.00	17.34
N										
ATOM	2501	CA	ILE	A	330	30.701	10.561	4.917	1.00	18.84
C										
ATOM	2502	C	ILE	A	330	31.377	11.229	3.724	1.00	20.19
C										
ATOM	2503	O	ILE	A	330	31.449	10.653	2.638	1.00	21.73
O										
ATOM	2504	CB	ILE	A	330	29.341	11.249	5.185	1.00	19.53
C										
ATOM	2505	CGl	ILE	A	330	28.521	10.397	6.154	1.00	19.59
C										
ATOM	2506	CG2	ILE	A	330	28.580	11.464	3.868	1.00	20.32
C										
ATOM	2507	CDl	ILE	A	330	27.278	11.103	6.689	1.00	21.12
C										
ATOM	2508	N	PHE	A	331	31.885	12.440	3.929	1.00	19.19
N										
ATOM	2509	CA	PHE	A	331	32.547	13.164	2.845	1.00	20.98
C										
ATOM	2510	C	PHE	A	331	33.724	12.387	2.265	1.00	22.14
C										
ATOM	2511	O	PHE	A	331	33.984	12.458	1.063	1.00	21.94
O										
ATOM	2512	CB	PHE	A	331	33.044	14.530	3.328	1.00	22.21
C										
ATOM	2513	CG	PHE	A	331	31.950	15.550	3.520	1.00	24.15
C										
ATOM	2514	CDl	PHE	A	331	30.633	15.265	3.166	1.00	25.56
C										
ATOM	2515	CD2	PHE	A	331	32.244	16.802	4.045	1.00	26.18
C										
ATOM	2516	CEl	PHE	A	331	29.626	16.217	3.332	1.00	28.79
C										
ATOM	2517	CE2	PHE	A	331	31.243	17.761	4.216	1.00	27.74
C										
ATOM	2518	CZ	PHE	A	331	29.933	17.467	3.859	1.00	27.28
C										
ATOM	2519	N	SER	A	332	34.428	11.647	3.117	1.00	21.07
N										
ATOM	2520	CA	SER	A	332	35.593	10.873	2.684	1.00	22.95
C										
ATOM	2521	C	SER	A	332	35.253	9.823	1.634	1.00	24.76
C										
ATOM	2522	O	SER	A	332	36.136	9.335	0.929	1.00	25.03
O										
ATOM	2523	CB	SER	A	332	36.245	10.173	3.876	1.00	23.30
C										
ATOM	2524	OG	SER	A	332	35.522	9.005	4.233	1.00	25.56
O										
ATOM	2525	N	GLN	A	333	33.977	9.471	1.541	1.00	24.55
N										
ATOM	2526	CA	GLN	A	333	33.530	8.467	0.585	1.00	26.96
C										
ATOM	2527	C	GLN	A	333	33.188	9.066	-0.776	1.00	27.41
C										

ATOM	2528	O	GLN	A	333	32.674	8.372	-1.654	1.00	29.30
O										
ATOM	2529	CB	GLN	A	333	32.311	7.730	1.142	1.00	28.01
C										
ATOM	2530	CG	GLN	A	333	32.572	6.975	2.437	1.00	29.83
C										
ATOM	2531	CD	GLN	A	333	33.698	5.965	2.309	1.00	32.04
C										
ATOM	2532	OEl	GLN	A	333	34.824	6.205	2.756	1.00	33.59
O										
ATOM	2533	NE2	GLN	A	333	33.403	4.832	1.684	1.00	34.33
N										
ATOM	2534	N	THR	A	334	33.469	10.354	-0.948	1.00	27.45
N										
ATOM	2535	CA	THR	A	334	33.187	11.036	-2.207	1.00	28.21
C										
ATOM	2536	C	THR	A	334	34.451	11.670	-2.780	1.00	27.53
C										
ATOM	2537	O	THR	A	334	35.398	11.964	-2.048	1.00	25.45
O										
ATOM	2538	CB	THR	A	334	32.137	12.152	-2.021	1.00	30.13
C										
ATOM	2539	OGl	THR	A	334	32.685	13.198	-1.205	1.00	32.12
O										
ATOM	2540	CG2	THR	A	334	30.885	11.601	-1.353	1.00	32.28
C										
ATOM	2541	N	ALA	A	335	34.459	11.879	-4.093	1.00	26.83
N										
ATOM	2542	CA	ALA	A	335	35.602	12.489	-4.763	1.00	25.70
C										
ATOM	2543	C	ALA	A	335	35.779	13.911	-4.257	1.00	22.54
C										
ATOM	2544	O	ALA	A	335	34.828	14.690	-4.253	1.00	24.81
O										
ATOM	2545	CB	ALA	A	335	35.381	12.492	-6.278	1.00	26.99
C										
ATOM	2546	N	GLY	A	336	36.996	14.244	-3.832	1.00	21.88
N										
ATOM	2547	CA	GLY	A	336	37.269	15.575	-3.321	1.00	21.53
C										
ATOM	2548	C	GLY	A	336	36.709	15.743	-1.918	1.00	20.72
C										
ATOM	2549	O	GLY	A	336	36.596	16.863	-1.422	1.00	20.81
O										
ATOM	2550	N	GLY	A	337	36.385	14.620	-1.282	1.00	21.38
N										
ATOM	2551	CA	GLY	A	337	35.806	14.633	0.056	1.00	21.83
C										
ATOM	2552	C	GLY	A	337	36.628	15.260	1.165	1.00	22.80
C										
ATOM	2553	O	GLY	A	337	36.073	15.792	2.136	1.00	19.50
O										
ATOM	2554	N	THR	A	338	37.948	15.192	1.047	1.00	21.19
N										
ATOM	2555	CA	THR	A	338	38.818	15.775	2.057	1.00	21.70
C										
ATOM	2556	C	THR	A	338	38.734	17.298	1.972	1.00	21.72
C										
ATOM	2557	O	THR	A	338	38.720	17.996	2.995	1.00	21.06
O										

ATOM 2558 CB THR A 338 40.274 15.310 1.855 1.00 24.22 C
ATOM 2559 OGl THR A 338 40.325 13.881 1.940 1.00 25.35 O
ATOM 2560 CG2 THR A 338 41.182 15.908 2.920 1.00 26.30 C
ATOM 2561 N PHE A 339 38.665 17.817 0.751 1.00 19.60 N
ATOM 2562 CA PHE A 339 38.555 19.253 0.558 1.00 18.76 C
ATOM 2563 C PHE A 339 37.165 19.708 1.018 1.00 19.23 C
ATOM 2564 O PHE A 339 37.002 20.804 1.541 1.00 18.34 O
ATOM 2565 CB PHE A 339 38.752 19.612 -0.916 1.00 20.54 C
ATOM 2566 CG PHE A 339 38.891 21.081 -1.160 1.00 20.48 C
ATOM 2567 CDl PHE A 339 40.066 21.744 -0.822 1.00 20.34 C
ATOM 2568 CD2 PHE A 339 37.840 21.813 -1.707 1.00 21.59 C
ATOM 2569 CEl PHE A 339 40.192 23.111 -1.022 1.00 22.20 C
ATOM 2570 CE2 PHE A 339 37.958 23.184 -1.910 1.00 21.72 C
ATOM 2571 CZ PHE A 339 39.134 23.834 -1.567 1.00 22.78 C
ATOM 2572 N LEU A 340 36.158 18.864 0.808 1.00 18.44 N
ATOM 2573 CA LEU A 340 34.806 19.205 1.239 1.00 19.70 C
ATOM 2574 C LEU A 340 34.822 19.290 2.772 1.00 18.05 C
ATOM 2575 O LEU A 340 34.127 20.117 3.371 1.00 18.63 O
ATOM 2576 CB LEU A 340 33.816 18.133 0.778 1.00 22.29 C
ATOM 2577 CG LEU A 340 32.333 18.481 0.897 1.00 27.46 C
ATOM 2578 CDl LEU A 340 32.042 19.741 0.094 1.00 30.29 C
ATOM 2579 CD2 LEU A 340 31.493 17.311 0.380 1.00 29.45 C
ATOM 2580 N GLY A 341 35.621 18.428 3.395 1.00 16.83 N
ATOM 2581 CA GLY A 341 35.749 18.440 4.845 1.00 17.43 C
ATOM 2582 C GLY A 341 36.397 19.744 5.267 1.00 17.75 C
ATOM 2583 O GLY A 341 35.995 20.364 6.254 1.00 16.02 O
ATOM 2584 N PHE A 342 37.415 20.163 4.518 1.00 14.95 N
ATOM 2585 CA PHE A 342 38.094 21.421 4.794 1.00 14.99 C
ATOM 2586 C PHE A 342 37.079 22.562 4.743 1.00 16.25 C
ATOM 2587 O PHE A 342 37.024 23.393 5.643 1.00 15.51 O

ATOM	2588	CB	PHE	A	342	39.188	21.687	3.757	1.00	16.38
C										
ATOM	2589	CG	PHE	A	342	39.540	23.142	3.618	1.00	16.67
C										
ATOM	2590	CDl	PHE	A	342	40.174	23.825	4.654	1.00	17.48
C										
ATOM	2591	CD2	PHE	A	342	39.207	23.843	2.459	1.00	17.96
C										
ATOM	2592	CEl	PHE	A	342	40.469	25.184	4.539	1.00	17.67
C										
ATOM	2593	CE2	PHE	A	342	39.498	25.199	2.336	1.00	20.37
C										
ATOM	2594	CZ	PHE	A	342	40.130	25.871	3.379	1.00	18.17
C										
ATOM	2595	N	LEU	A	343	36.278	22.597	3.683	1.00	14.36
N										
ATOM	2596	CA	LEU	A	343	35.277	23.647	3.528	1.00	15.15
C										
ATOM	2597	C	LEU	A	343	34.294	23.681	4.693	1.00	15.49
C										
ATOM	2598	O	LEU	A	343	33.885	24.754	5.136	1.00	17.04
O										
ATOM	2599	CB	LEU	A	343	34.503	23.465	2.218	1.00	17.38
C										
ATOM	2600	CG	LEU	A	343	35.312	23.667	0.932	1.00	18.13
C										
ATOM	2601	CDl	LEU	A	343	34.394	23.442	-0.269	1.00	20.67
C										
ATOM	2602	CD2	LEU	A	343	35.902	25.065	0.889	1.00	18.76
C										
ATOM	2603	N	TRP	A	344	33.904	22.500	5.164	1.00	15.44
N										
ATOM	2604	CA	TRP	A	344	32.984	22.374	6.293	1.00	15.50
C										
ATOM	2605	C	TRP	A	344	33.611	22.957	7.560	1.00	16.32
C										
ATOM	2606	O	TRP	A	344	32.997	23.768	8.260	1.00	14.23
O										
ATOM	2607	CB	TRP	A	344	32.639	20.896	6.492	1.00	15.46
C										
ATOM	2608	CG	TRP	A	344	32.011	20.538	7.816	1.00	15.33
C										
ATOM	2609	CDl	TRP	A	344	32.526	19.693	8.755	1.00	14.20
C										
ATOM	2610	CD2	TRP	A	344	30.722	20.943	8.307	1.00	14.56
C										
ATOM	2611	NEl	TRP	A	344	31.638	19.535	9.794	1.00	14.52
N										
ATOM	2612	CE2	TRP	A	344	30.524	20.291	9.545	1.00	15.18
C										
ATOM	2613	CE3	TRP	A	344	29.716	21.786	7.817	1.00	15.91
C										
ATOM	2614	CZ2	TRP	A	344	29.361	20.456	10.304	1.00	14.50
C										
ATOM	2615	CZ3	TRP	A	344	28.555	21.952	8.573	1.00	17.37
C										
ATOM	2616	CH2	TRP	A	344	28.388	21.288	9.802	1.00	17.75
C										
ATOM	2617	N	PHE	A	345	34.841	22.561	7.857	1.00	14.52
N										

ATOM 2618 CA PHE A 345 35.484 23.091 9.050 1.00 14.87 C
ATOM 2619 C PHE A 345 35.847 24.565 8.926 1.00 16.46 C
ATOM 2620 O PHE A 345 35.864 25.289 9.927 1.00 15.61 O
ATOM 2621 CB PHE A 345 36.686 22.217 9.426 1.00 15.78 C
ATOM 2622 CG PHE A 345 36.280 20.854 9.905 1.00 16.61 C
ATOM 2623 CDl PHE A 345 35.526 20.714 11.070 1.00 17.79 C
ATOM 2624 CD2 PHE A 345 36.566 19.718 9.152 1.00 17.14 C
ATOM 2625 CEl PHE A 345 35.052 19.466 11.473 1.00 16.97 C
ATOM 2626 CE2 PHE A 345 36.099 18.464 9.546 1.00 16.98 C
ATOM 2627 CZ PHE A 345 35.337 18.338 10.711 1.00 18.76 C
ATOM 2628 N PHE A 346 36.101 25.030 7.704 1.00 16.53 N
ATOM 2629 CA PHE A 346 36.410 26.442 7.520 1.00 18.60 C
ATOM 2630 C PHE A 346 35.114 27.212 7.795 1.00 16.98 C
ATOM 2631 O PHE A 346 35.122 28.268 8.430 1.00 17.05 O
ATOM 2632 CB PHE A 346 36.878 26.729 6.095 1.00 21.63 C
ATOM 2633 CG PHE A 346 37.461 28.100 5.932 1.00 28.99 C
ATOM 2634 CDl PHE A 346 38.784 28.350 6.277 1.00 32.45 C
ATOM 2635 CD2 PHE A 346 36.669 29.158 5.496 1.00 32.91 C
ATOM 2636 CEl PHE A 346 39.314 29.638 6.192 1.00 35.95 C
ATOM 2637 CE2 PHE A 346 37.186 30.450 5.408 1.00 34.44 C
ATOM 2638 CZ PHE A 346 38.511 30.690 5.757 1.00 36.29 C
ATOM 2639 N LEU A 347 34.000 26.669 7.310 1.00 16.23 N
ATOM 2640 CA LEU A 347 32.691 27.275 7.536 1.00 16.65 C
ATOM 2641 C LEU A 347 32.456 27.371 9.044 1.00 15.19 C
ATOM 2642 O LEU A 347 32.084 28.425 9.561 1.00 16.47 O
ATOM 2643 CB LEU A 347 31.590 26.417 6.898 1.00 17.50 C
ATOM 2644 CG LEU A 347 30.141 26.736 7.291 1.00 20.68 C
ATOM 2645 CDl LEU A 347 29.795 28.159 6.907 1.00 23.70 C
ATOM 2646 CD2 LEU A 347 29.195 25.757 6.606 1.00 22.85 C
ATOM 2647 N LEU A 348 32.681 26.268 9.750 1.00 15.07 N

ATOM	2648	CA	LEU	A	348	32.480	26.263	11.199	1.00	14.75
ATOM	2649	C	LEU	A	348	33.395	27.265	11.888	1.00	15.36
ATOM	2650	O	LEU	A	348	32.989	27.932	12.845	1.00	16.23
ATOM	2651	CB	LEU	A	348	32.724	24.863	11.782	1.00	14.84
ATOM	2652	CG	LEU	A	348	31.762	23.741	11.364	1.00	16.67
ATOM	2653	CDl	LEU	A	348	32.129	22.466	12.102	1.00	18.83
ATOM	2654	CD2	LEU	A	348	30.321	24.132	11.693	1.00	18.23
ATOM	2655	N	PHE	A	349	34.632	27.379	11.415	1.00	15.52
ATOM	2656	CA	PHE	A	349	35.556	28.317	12.032	1.00	15.44
ATOM	2657	C	PHE	A	349	35.080	29.763	11.900	1.00	16.67
ATOM	2658	O	PHE	A	349	35.091	30.512	12.877	1.00	16.35
ATOM	2659	CB	PHE	A	349	36.961	28.184	11.440	1.00	16.45
ATOM	2660	CG	PHE	A	349	37.941	29.151	12.029	1.00	17.96
ATOM	2661	CDl	PHE	A	349	38.236	29.113	13.388	1.00	16.86
ATOM	2662	CD2	PHE	A	349	38.530	30.134	11.243	1.00	19.09
ATOM	2663	CEl	PHE	A	349	39.100	30.042	13.956	1.00	16.66
ATOM	2664	CE2	PHE	A	349	39.396	31.066	11.807	1.00	18.84
ATOM	2665	CZ	PHE	A	349	39.678	31.017	13.163	1.00	18.49
ATOM	2666	N	PHE	A	350	34.674	30.167	10.699	1.00	16.00
ATOM	2667	CA	PHE	A	350	34.189	31.533	10.515	1.00	17.68
ATOM	2668	C	PHE	A	350	32.900	31.756	11.294	1.00	17.83
ATOM	2669	O	PHE	A	350	32.684	32.836	11.845	1.00	17.15
ATOM	2670	CB	PHE	A	350	33.989	31.836	9.023	1.00	19.50
ATOM	2671	CG	PHE	A	350	35.132	32.598	8.407	1.00	23.98
ATOM	2672	CDl	PHE	A	350	36.418	32.486	8.924	1.00	26.15
ATOM	2673	CD2	PHE	A	350	34.922	33.428	7.310	1.00	26.21
ATOM	2674	CEl	PHE	A	350	37.486	33.192	8.358	1.00	28.50
ATOM	2675	CE2	PHE	A	350	35.979	34.136	6.734	1.00	26.45
ATOM	2676	CZ	PHE	A	350	37.261	34.019	7.261	1.00	27.78
ATOM	2677	N	ALA	A	351	32.051	30.733	11.353	1.00	16.09

ATOM	2678	CA	ALA	A	351	30.804	30.840	12.106	1.00	16.99
ATOM	2679	C	ALA	A	351	31.145	31.024	13.585	1.00	16.41
ATOM	2680	O	ALA	A	351	30.584	31.885	14.266	1.00	16.45
ATOM	2681	CB	ALA	A	351	29.958	29.580	11.908	1.00	17.19
ATOM	2682	N	GLY	A	352	32.078	30.218	14.079	1.00	15.21
ATOM	2683	CA	GLY	A	352	32.462	30.339	15.473	1.00	14.32
ATOM	2684	C	GLY	A	352	33.165	31.651	15.779	1.00	15.88
ATOM	2685	O	GLY	A	352	32.840	32.314	16.755	1.00	16.50
ATOM	2686	N	LEU	A	353	34.115	32.043	14.935	1.00	14.78
ATOM	2687	CA	LEU	A	353	34.880	33.270	15.153	1.00	14.53
ATOM	2688	C	LEU	A	353	34.011	34.525	15.268	1.00	16.41
ATOM	2689	O	LEU	A	353	34.225	35.363	16.150	1.00	17.33
ATOM	2690	CB	LEU	A	353	35.900	33.441	14.024	1.00	16.30
ATOM	2691	CG	LEU	A	353	36.822	34.657	14.053	1.00	16.78
ATOM	2692	CDl	LEU	A	353	37.536	34.753	15.400	1.00	18.13
ATOM	2693	CD2	LEU	A	353	37.835	34.518	12.913	1.00	17.20
ATOM	2694	N	THR	A	354	33.038	34.660	14.374	1.00	15.96
ATOM	2695	CA	THR	A	354	32.153	35.818	14.412	1.00	17.05
ATOM	2696	C	THR	A	354	31.289	35.816	15.669	1.00	17.43
ATOM	2697	O	THR	A	354	30.765	36.857	16.070	1.00	18.67
ATOM	2698	CB	THR	A	354	31.244	35.873	13.171	1.00	17.57
ATOM	2699	OGl	THR	A	354	30.613	34.602	12.982	1.00	18.83
ATOM	2700	CG2	THR	A	354	32.065	36.228	11.932	1.00	19.35
ATOM	2701	N	SER	A	355	31.133	34.652	16.294	1.00	16.62
ATOM	2702	CA	SER	A	355	30.343	34.571	17.516	1.00	15.78
ATOM	2703	C	SER	A	355	31.207	34.717	18.758	1.00	15.96
ATOM	2704	O	SER	A	355	30.787	35.329	19.735	1.00	16.03
ATOM	2705	CB	SER	A	355	29.574	33.250	17.586	1.00	15.30
ATOM	2706	OG	SER	A	355	28.526	33.230	16.630	1.00	16.94
ATOM	2707	N	SER	A	356	32.416	34.163	18.729	1.00	15.27

ATOM 2708 CA SER A 356 33.275 34.267 19.898 1.00 16.75 C
ATOM 2709 C SER A 356 33.694 35.708 20.175 1.00 17.51 C
ATOM 2710 O SER A 356 33.801 36.108 21.336 1.00 17.39 O
ATOM 2711 CB SER A 356 34.501 33.352 19.755 1.00 16.77 C
ATOM 2712 OG SER A 356 35.316 33.717 18.657 1.00 18.43 O
ATOM 2713 N ILE A 357 33.915 36.505 19.135 1.00 17.29 N
ATOM 2714 CA ILE A 357 34.295 37.890 19.387 1.00 18.11 C
ATOM 2715 C ILE A 357 33.116 38.604 20.065 1.00 19.02 C
ATOM 2716 O ILE A 357 33.312 39.496 20.883 1.00 19.35 O
ATOM 2717 CB ILE A 357 34.693 38.629 18.086 1.00 17.96 C
ATOM 2718 CGl ILE A 357 33.563 38.540 17.053 1.00 19.69 C
ATOM 2719 CG2 ILE A 357 35.997 38.042 17.545 1.00 17.69 C
ATOM 2720 CDl ILE A 357 33.912 39.164 15.704 1.00 21.13 C
ATOM 2721 N ALA A 358 31.897 38.172 19.755 1.00 17.88 N
ATOM 2722 CA ALA A 358 30.701 38.769 20.350 1.00 18.44 C
ATOM 2723 C ALA A 358 30.537 38.432 21.837 1.00 19.85 C
ATOM 2724 O ALA A 358 30.013 39.251 22.600 1.00 19.41 O
ATOM 2725 CB ALA A 358 29.450 38.333 19.580 1.00 18.22 C
ATOM 2726 N ILE A 359 30.947 37.236 22.260 1.00 18.42 N
ATOM 2727 CA ILE A 359 30.810 36.913 23.677 1.00 19.68 C
ATOM 2728 C ILE A 359 31.993 37.358 24.517 1.00 18.41 C
ATOM 2729 O ILE A 359 31.966 37.249 25.741 1.00 19.34 O
ATOM 2730 CB ILE A 359 30.510 35.412 23.952 1.00 22.38 C
ATOM 2731 CGl ILE A 359 31.380 34.510 23.088 1.00 21.99 C
ATOM 2732 CG2 ILE A 359 29.022 35.150 23.753 1.00 24.85 C
ATOM 2733 CDl ILE A 359 31.156 33.028 23.373 1.00 26.52 C
ATOM 2734 N MET A 360 33.040 37.863 23.871 1.00 16.50 N
ATOM 2735 CA MET A 360 34.160 38.391 24.637 1.00 17.03 C
ATOM 2736 C MET A 360 34.009 39.906 24.757 1.00 17.86 C
ATOM 2737 O MET A 360 34.531 40.518 25.688 1.00 17.07 O

ATOM 2738 CB MET A 360 35.499 38.033 23.987 1.00 20.64 C
ATOM 2739 CG MET A 360 35.881 36.583 24.241 1.00 25.14 C
ATOM 2740 SD MET A 360 37.530 36.162 23.690 1.00 30.87 S
ATOM 2741 CE MET A 360 37.247 35.892 21.997 1.00 28.97 C
ATOM 2742 N GLN A 361 33.264 40.514 23.833 1.00 17.66 N
ATOM 2743 CA GLN A 361 33.080 41.962 23.882 1.00 16.60 C
ATOM 2744 C GLN A 361 32.397 42.477 25.160 1.00 16.38 C
ATOM 2745 O GLN A 361 32.667 43.596 25.580 1.00 16.73 O
ATOM 2746 CB GLN A 361 32.335 42.465 22.630 1.00 18.07 C
ATOM 2747 CG GLN A 361 32.185 44.000 22.551 1.00 18.49 C
ATOM 2748 CD GLN A 361 33.508 44.764 22.444 1.00 16.49 C
ATOM 2749 OEl GLN A 361 33.585 45.939 22.816 1.00 22.25 O
ATOM 2750 NE2 GLN A 361 34.536 44.116 21.928 1.00 16.09 N
ATOM 2751 N PRO A 362 31.508 41.680 25.795 1.00 15.91 N
ATOM 2752 CA PRO A 362 30.886 42.208 27.019 1.00 17.07 C
ATOM 2753 C PRO A 362 31.915 42.508 28.112 1.00 18.10 C
ATOM 2754 O PRO A 362 31.853 43.551 28.766 1.00 16.91 O
ATOM 2755 CB PRO A 362 29.922 41.099 27.427 1.00 18.21 C
ATOM 2756 CG PRO A 362 29.505 40.526 26.103 1.00 16.94 C
ATOM 2757 CD PRO A 362 30.820 40.454 25.351 1.00 16.00 C
ATOM 2758 N MET A 363 32.859 41.592 28.318 1.00 16.96 N
ATOM 2759 CA MET A 363 33.891 41.807 29.330 1.00 18.05 C
ATOM 2760 C MET A 363 34.760 42.993 28.905 1.00 15.99 C
ATOM 2761 O MET A 363 35.169 43.812 29.733 1.00 17.04 O
ATOM 2762 CB MET A 363 34.756 40.551 29.486 1.00 20.04 C
ATOM 2763 CG MET A 363 35.817 40.670 30.571 1.00 24.38 C
ATOM 2764 SD MET A 363 35.073 40.912 32.209 1.00 33.98 S
ATOM 2765 CE MET A 363 36.527 40.845 33.250 1.00 31.60 C
ATOM 2766 N ILE A 364 35.044 43.088 27.610 1.00 14.78 N
ATOM 2767 CA ILE A 364 35.850 44.190 27.100 1.00 17.02 C

ATOM	2768	C	ILE	A	364	35.128	45.517	27.354	1.00	17.22
C										
ATOM	2769	O	ILE	A	364	35.728	46.473	27.848	1.00	17.61
O										
ATOM	2770	CB	ILE	A	364	36.118	44.014	25.589	1.00	17.53
C										
ATOM	2771	CGl	ILE	A	364	37.065	42.823	25.381	1.00	17.32
C										
ATOM	2772	CG2	ILE	A	364	36.712	45.293	24.996	1.00	16.91
C										
ATOM	2773	CDl	ILE	A	364	37.055	42.275	23.963	1.00	16.99
C										
ATOM	2774	N	ALA	A	365	33.839	45.560	27.027	1.00	17.05
N										
ATOM	2775	CA	ALA	A	365	33.035	46.767	27.219	1.00	16.88
C										
ATOM	2776	C	ALA	A	365	32.945	47.142	28.694	1.00	18.84
C										
ATOM	2777	O	ALA	A	365	32.973	48.323	29.043	1.00	19.34
O										
ATOM	2778	CB	ALA	A	365	31.637	46.570	26.645	1.00	17.24
C										
ATOM	2779	N	PHE	A	366	32.834	46.143	29.564	1.00	17.32
N										
ATOM	2780	CA	PHE	A	366	32.761	46.432	30.993	1.00	18.32
C										
ATOM	2781	C	PHE	A	366	34.060	47.081	31.461	1.00	19.18
C										
ATOM	2782	O	PHE	A	366	34.040	48.089	32.169	1.00	19.58
O										
ATOM	2783	CB	PHE	A	366	32.531	45.158	31.808	1.00	17.47
C										
ATOM	2784	CG	PHE	A	366	32.680	45.366	33.293	1.00	18.94
C										
ATOM	2785	CDl	PHE	A	366	31.663	45.960	34.031	1.00	20.69
C										
ATOM	2786	CD2	PHE	A	366	33.867	45.029	33.935	1.00	20.69
C										
ATOM	2787	CEl	PHE	A	366	31.823	46.224	35.394	1.00	21.93
C										
ATOM	2788	CE2	PHE	A	366	34.043	45.288	35.298	1.00	22.01
C										
ATOM	2789	CZ	PHE	A	366	33.016	45.889	36.027	1.00	20.98
C										
ATOM	2790	N	LEU	A	367	35.191	46.496	31.077	1.00	18.42
N										
ATOM	2791	CA	LEU	A	367	36.479	47.039	31.490	1.00	18.48
C										
ATOM	2792	C	LEU	A	367	36.685	48.449	30.943	1.00	19.77
C										
ATOM	2793	O	LEU	A	367	37.232	49.306	31.632	1.00	20.02
O										
ATOM	2794	CB	LEU	A	367	37.621	46.122	31.036	1.00	17.50
C										
ATOM	2795	CG	LEU	A	367	37.624	44.729	31.674	1.00	17.01
C										
ATOM	2796	CDl	LEU	A	367	38.705	43.860	31.033	1.00	19.45
C										
ATOM	2797	CD2	LEU	A	367	37.861	44.868	33.178	1.00	19.61
C										

ATOM	2798	N	GLU	A	368	36.239	48.688	29.710	1.00	18.69
ATOM	2799	CA	GLU	A	368	36.375	50.010	29.099	1.00	19.80
ATOM	2800	C	GLU	A	368	35.417	51.024	29.724	1.00	20.15
ATOM	2801	O	GLU	A	368	35.830	52.109	30.141	1.00	21.51
ATOM	2802	CB	GLU	A	368	36.076	49.949	27.596	1.00	19.44
ATOM	2803	CG	GLU	A	368	36.985	49.047	26.790	1.00	23.03
ATOM	2804	CD	GLU	A	368	36.526	48.918	25.346	1.00	25.17
ATOM	2805	OEl	GLU	A	368	35.305	48.996	25.109	1.00	28.53
ATOM	2806	OE2	GLU	A	368	37.373	48.725	24.453	1.00	28.96
ATOM	2807	N	ASP	A	369	34.139	50.659	29.775	1.00	20.87
ATOM	2808	CA	ASP	A	369	33.084	51.528	30.294	1.00	21.81
ATOM	2809	C	ASP	A	369	33.113	51.803	31.790	1.00	22.57
ATOM	2810	O	ASP	A	369	32.955	52.945	32.217	1.00	24.05
ATOM	2811	CB	ASP	A	369	31.692	50.954	29.987	1.00	22.02
ATOM	2812	CG	ASP	A	369	31.439	50.733	28.504	1.00	23.16
ATOM	2813	ODl	ASP	A	369	32.140	51.321	27.660	1.00	25.19
ATOM	2814	OD2	ASP	A	369	30.505	49.966	28.188	1.00	23.15
ATOM	2815	N	GLU	A	370	33.292	50.755	32.588	1.00	22.20
ATOM	2816	CA	GLU	A	370	33.252	50.908	34.038	1.00	22.80
ATOM	2817	C	GLU	A	370	34.587	51.059	34.756	1.00	22.71
ATOM	2818	O	GLU	A	370	34.665	51.757	35.764	1.00	24.07
ATOM	2819	CB	GLU	A	370	32.469	49.745	34.658	1.00	22.08
ATOM	2820	CG	GLU	A	370	31.194	49.330	33.910	1.00	24.86
ATOM	2821	CD	GLU	A	370	30.251	50.488	33.605	1.00	28.33
ATOM	2822	OEl	GLU	A	370	30.251	51.488	34.355	1.00	29.31
ATOM	2823	OE2	GLU	A	370	29.491	50.387	32.617	1.00	30.00
ATOM	2824	N	LEU	A	371	35.633	50.406	34.265	1.00	22.27
ATOM	2825	CA	LEU	A	371	36.936	50.531	34.905	1.00	23.56
ATOM	2826	C	LEU	A	371	37.853	51.454	34.117	1.00	24.48
ATOM	2827	O	LEU	A	371	39.001	51.686	34.498	1.00	25.47

ATOM 2828 CB LEU A 371 37.578 49.156 35.104 1.00 23.37 C
ATOM 2829 CG LEU A 371 36.883 48.295 36.165 1.00 23.86 C
ATOM 2830 CDl LEU A 371 37.677 47.017 36.370 1.00 23.43 C
ATOM 2831 CD2 LEU A 371 36.772 49.064 37.482 1.00 24.31 C
ATOM 2832 N LYS A 372 37.330 51.970 33.008 1.00 24.51 N
ATOM 2833 CA LYS A 372 38.049 52.918 32.167 1.00 25.18 C
ATOM 2834 C LYS A 372 39.371 52.453 31.569 1.00 24.97 C
ATOM 2835 O LYS A 372 40.289 53.254 31.389 1.00 26.14 O
ATOM 2836 CB LYS A 372 38.272 54.220 32.953 1.00 28.11 C
ATOM 2837 CG LYS A 372 36.986 54.889 33.422 1.00 30.31 C
ATOM 2838 CD LYS A 372 36.089 55.253 32.249 1.00 33.59 C
ATOM 2839 CE LYS A 372 34.857 56.028 32.701 1.00 36.54 C
ATOM 2840 NZ LYS A 372 33.992 55.245 33.628 1.00 39.85 N
ATOM 2841 N LEU A 373 39.481 51.167 31.261 1.00 23.03 N
ATOM 2842 CA LEU A 373 40.702 50.662 30.650 1.00 21.76 C
ATOM 2843 C LEU A 373 40.674 51.015 29.173 1.00 21.27 C
ATOM 2844 O LEU A 373 39.601 51.187 28.589 1.00 20.88 O
ATOM 2845 CB LEU A 373 40.796 49.136 30.772 1.00 22.16 C
ATOM 2846 CG LEU A 373 41.237 48.526 32.104 1.00 27.19 C
ATOM 2847 CDl LEU A 373 40.234 48.851 33.180 1.00 28.12 C
ATOM 2848 CD2 LEU A 373 41.381 47.017 31.941 1.00 25.36 C
ATOM 2849 N SER A 374 41.854 51.118 28.574 1.00 22.01 N
ATOM 2850 CA SER A 374 41.959 51.400 27.152 1.00 22.80 C
ATOM 2851 C SER A 374 41.462 50.137 26.454 1.00 22.10 C
ATOM 2852 O SER A 374 41.435 49.065 27.059 1.00 22.50 O
ATOM 2853 CB SER A 374 43.417 51.644 26.766 1.00 23.77 C
ATOM 2854 OG SER A 374 44.195 50.473 26.970 1.00 23.09 O
ATOM 2855 N ARG A 375 41.075 50.251 25.191 1.00 20.72 N
ATOM 2856 CA ARG A 375 40.603 49.082 24.459 1.00 20.76 C
ATOM 2857 C ARG A 375 41.689 48.006 24.419 1.00 21.44 C

ATOM	2858	O	ARG	A	375	41.406	46.827	24.619	1.00	19.84	
ATOM	2859	CB	ARG	A	375	40.193	49.467	23.035	1.00	22.68	
ATOM	2860	CG	ARG	A	375	39.743	48.293	22.174	1.00	23.85	
ATOM	2861	CD	ARG	A	375	39.154	48.790	20.860	1.00	27.21	
ATOM	2862	NE	ARG	A	375	40.155	49.459	20.041	1.00	30.59	
ATOM	2863	CZ	ARG	A	375	39.906	50.501	19.254	1.00	33.71	
ATOM	2864	NHl	ARG	A	375	38.681	51.005	19.179	1.00	33.70	
ATOM	2865	NH2	ARG	A	375	40.883	51.037	18.535	1.00	36.01	
ATOM	2866	N	LYS	A	376	42.929	48.420	24.169	1.00	20.04	
ATOM	2867	CA	LYS	A	376	44.051	47.487	24.108	1.00	21.23	
ATOM	2868	C	LYS	A	376	44.167	46.668	25.389	1.00	20.74	
ATOM	2869	O	LYS	A	376	44.253	45.443	25.344	1.00	21.99	
ATOM	2870	CB	LYS	A	376	45.362	48.240	23.875	1.00	23.10	
ATOM	2871	CG	LYS	A	376	46.591	47.344	23.862	1.00	28.00	
ATOM	2872	CD	LYS	A	376	47.873	48.160	23.782	1.00	31.63	
ATOM	2873	CE	LYS	A	376	49.092	47.256	23.765	1.00	35.58	
ATOM	2874	NZ	LYS	A	376	50.358	48.041	23.681	1.00	40.86	
ATOM	2875	N	HIS	A	377	44.172	47.351	26.527	1.00	20.04	
ATOM	2876	CA	HIS	A	377	44.282	46.670	27.811	1.00	19.72	
ATOM	2877	C	HIS	A	377	43.059	45.817	28.118	1.00	19.95	
ATOM	2878	O	HIS	A	377	43.194	44.719	28.648	1.00	18.85	
ATOM	2879	CB	HIS	A	377	44.511	47.695	28.924	1.00	22.92	
ATOM	2880	CG	HIS	A	377	45.858	48.343	28.870	1.00	26.77	
ATOM	2881	NDl	HIS	A	377	46.175	49.474	29.596	1.00	28.91	
ATOM	2882	CD2	HIS	A	377	46.979	48.013	28.187	1.00	29.35	
ATOM	2883	CEl	HIS	A	377	47.428	49.809	29.361	1.00	30.94	
ATOM	2884	NE2	HIS	A	377	47.941	48.938	28.507	1.00	30.18	
ATOM	2885	N	ALA	A	378	41.872	46.318	27.782	1.00	18.30	
ATOM	2886	CA	ALA	A	378	40.639	45.577	28.037	1.00	18.36	
ATOM	2887	C	ALA	A	378	40.619	44.277	27.242	1.00	18.16	

ATOM	2888	O	ALA	A	378	40.248	43.225	27.762	1.00	18.21
ATOM	2889	CB	ALA	A	378	39.426	46.422	27.675	1.00	16.14
ATOM	2890	N	VAL	A	379	41.007	44.354	25.975	1.00	19.54
ATOM	2891	CA	VAL	A	379	41.026	43.174	25.124	1.00	18.59
ATOM	2892	C	VAL	A	379	42.074	42.174	25.599	1.00	18.55
ATOM	2893	O	VAL	A	379	41.794	40.980	25.706	1.00	18.22
ATOM	2894	CB	VAL	A	379	41.316	43.554	23.650	1.00	18.18
ATOM	2895	CGl	VAL	A	379	41.509	42.299	22.804	1.00	18.64
ATOM	2896	CG2	VAL	A	379	40.160	44.384	23.101	1.00	17.50
ATOM	2897	N	LEU	A	380	43.277	42.658	25.900	1.00	18.77
ATOM	2898	CA	LEU	A	380	44.336	41.752	26.332	1.00	18.79
ATOM	2899	C	LEU	A	380	44.020	41.052	27.650	1.00	18.81
ATOM	2900	O	LEU	A	380	44.265	39.856	27.784	1.00	19.48
ATOM	2901	CB	LEU	A	380	45.675	42.489	26.418	1.00	19.29
ATOM	2902	CG	LEU	A	380	46.211	42.963	25.059	1.00	22.31
ATOM	2903	CDl	LEU	A	380	47.538	43.698	25.253	1.00	21.79
ATOM	2904	CD2	LEU	A	380	46.394	41.774	24.124	1.00	23.36
ATOM	2905	N	TRP	A	381	43.477	41.781	28.622	1.00	18.53
ATOM	2906	CA	TRP	A	381	43.133	41.149	29.889	1.00	18.43
ATOM	2907	C	TRP	A	381	41.992	40.166	29.714	1.00	18.79
ATOM	2908	O	TRP	A	381	41.971	39.122	30.357	1.00	19.06
ATOM	2909	CB	TRP	A	381	42.755	42.186	30.941	1.00	18.67
ATOM	2910	CG	TRP	A	381	43.948	42.767	31.616	1.00	21.20
ATOM	2911	CDl	TRP	A	381	44.447	44.025	31.461	1.00	21.44
ATOM	2912	CD2	TRP	A	381	44.816	42.097	32.539	1.00	22.13
ATOM	2913	NEl	TRP	A	381	45.576	44.183	32.232	1.00	23.13
ATOM	2914	CE2	TRP	A	381	45.824	43.016	32.905	1.00	23.21
ATOM	2915	CE3	TRP	A	381	44.839	40.810	33.094	1.00	23.25
ATOM	2916	CZ2	TRP	A	381	46.849	42.691	33.803	1.00	23.39
ATOM	2917	CZ3	TRP	A	381	45.860	40.484	33.989	1.00	23.68

ATOM	2918	CH2	TRP	A	381		46.849	41.424	34.333	1.00	24.04
C											
ATOM	2919	N	THR	A	382		41.035	40.496	28.848	1.00	17.24
N											
ATOM	2920	CA	THR	A	382	i	39.919	39.592	28.623	1.00	17.31
C											
ATOM	2921	C	THR	A	382		40.448	38.305	27.991	1.00	18.33
C											
ATOM	2922	O	THR	A	382		40.053	37.203	28.379	1.00	17.21
O											
ATOM	2923	CB	THR	A	382		38.849	40.246	27.713	1.00	17.09
C											
ATOM	2924	OGl	THR	A	382		38.259	41.353	28.412	1.00	17.19
O											
ATOM	2925	CG2	THR	A	382		37.743	39.241	27.354	1.00	17.56
C											
ATOM	2926	N	ALA	A	383		41.356	38.442	27.031	1.00	17.40
N											
ATOM	2927	CA	ALA	A	383		41.929	37.273	26.370	1.00	18.74
C											
ATOM	2928	C	ALA	A	383		42.723	36.435	27.368	1.00	19.72
C											
ATOM	2929	O	ALA	A	383		42.672	35.206	27.335	1.00	20.42
O											
ATOM	2930	CB	ALA	A	383		42.824	37.706	25.213	1.00	19.63
C											
ATOM	2931	N	ALA	A	384		43.442	37.109	28.263	1.00	19.13
N											
ATOM	2932	CA	ALA	A	384		44.244	36.425	29.276	1.00	19.35
C											
ATOM	2933	C	ALA	A	384		43.357	35.577	30.187	1.00	19.11
C											
ATOM	2934	O	ALA	A	384		43.682	34.431	30.485	1.00	19.22
O											
ATOM	2935	CB	ALA	A	384		45.025	37.449	30.110	1.00	20.85
C											
ATOM	2936	N	ILE	A	385		42.246	36.147	30.641	1.00	17.68
N											
ATOM	2937	CA	ILE	A	385		41.329	35.426	31.518	1.00	19.36
C											
ATOM	2938	C	ILE	A	385		40.709	34.230	30.797	1.00	18.49
C											
ATOM	2939	O	ILE	A	385		40.591	33.141	31.370	1.00	18.07
O											
ATOM	2940	CB	ILE	A	385		40.194	36.346	32.027	1.00	20.59
C											
ATOM	2941	CGl	ILE	A	385		40.788	37.499	32.844	1.00	24.35
C											
ATOM	2942	CG2	ILE	A	385		39.215	35.540	32.877	1.00	25.20
C											
ATOM	2943	CDl	ILE	A	385		39.783	38.585	33.210	1.00	27.03
C											
ATOM	2944	N	VAL	A	386		40.311	34.424	29.541	1.00	16.87
N											
ATOM	2945	CA	VAL	A	386		39.717	33.331	28.775	1.00	17.21
C											
ATOM	2946	C	VAL	A	386		40.760	32.243	28.491	1.00	16.37
C											
ATOM	2947	o .	VAL	A	386		40.502	31.054	28.691	1.00	16.61
O											

ATOM	2948	CB	VAL	A	386	39.123	33.841	27.430	1.00	17.33
C										
ATOM	2949	CGl	VAL	A	386	38.650	32.664	26.580	1.00	18.29
C										
ATOM	2950	CG2	VAL	A	386	37.950	34.776	27.710	1.00	17.45
C										
ATOM	2951	N	PHE	A	387	41.942	32.655	28.043	1.00	17.12
N										
ATOM	2952	CA	PHE	A	387	43.012	31.704	27.741	1.00	18.72
C										
ATOM	2953	C	PHE	A	387	43.377	30.874	28.971	1.00	17.40
C										
ATOM	2954	O	PHE	A	387	43.466	29.649	28.901	1.00	17.37
O										
ATOM	2955	CB	PHE	A	387	44.255	32.441	27.235	1.00	19.53
C										
ATOM	2956	CG	PHE	A	387	45.429	31.536	26.990	1.00	24.95
C										
ATOM	2957	CDl	PHE	A	387	45.413	30.629	25.939	1.00	25.42
C										
ATOM	2958	CD2	PHE	A	387	46.528	31.556	27.842	1.00	25.70
C										
ATOM	2959	CEl	PHE	A	387	46.479	29.747	25.737	1.00	27.53
C										
ATOM	2960	CE2	PHE	A	387	47.596	30.680	27.652	1.00	26.91
C										
ATOM	2961	CZ	PHE	A	387	47.569	29.774	26.597	1.00	26.35
C										
ATOM	2962	N	PHE	A	388	43.587	31.543	30.098	1.00	15.88
N										
ATOM	2963	CA	PHE	A	388	43.927	30.837	31.328	1.00	16.87
C										
ATOM	2964	C	PHE	A	388	42.817	29.863	31.732	1.00	17.13
C										
ATOM	2965	O	PHE	A	388	43.055	28.671	31.947	1.00	15.49
O										
ATOM	2966	CB	PHE	A	388	44.140	31.832	32.468	1.00	18.12
C										
ATOM	2967	CG	PHE	A	388	44.252	31.180	33.812	1.00	20.76
C										
ATOM	2968	CDl	PHE	A	388	45.401	30.484	34.168	1.00	22.99
C										
ATOM	2969	CD2	PHE	A	388	43.189	31.223	34.706	1.00	22.13
C										
ATOM	2970	CEl	PHE	A	388	45.486	29.837	35.401	1.00	22.70
C										
ATOM	2971	CE2	PHE	A	388	43.268	30.580	35.937	1.00	22.82
C										
ATOM	2972	CZ	PHE	A	388	44.419	29.888	36.280	1.00	22.19
C										
ATOM	2973	N	SER	A	389	41.602	30.388	31.839	1.00	15.95
N										
ATOM	2974	CA	SER	A	389	40.450	29.590	32.242	1.00	15.16
C										
ATOM	2975	C	SER	A	389	40.202	28.382	31.357	1.00	15.89
C										
ATOM	2976	O	SER	A	389	39.756	27.343	31.832	1.00	16.90
O										
ATOM	2977	CB	SER	A	389	39.192	30.465	32.250	1.00	17.24
C										

ATOM 2978 OG SER A 389 39.314 31.509 33.199 1.00 19.39 O
ATOM 2979 N ALA A 390 40.466 28.534 30.066 1.00 15.51 N
ATOM 2980 CA ALA A 390 40.243 27.452 29.110 1.00 16.15 C
ATOM 2981 C ALA A 390 41.053 26.194 29.411 1.00 16.15 C
ATOM 2982 O ALA A 390 40.707 25.113 28.949 1.00 16.58 O
ATOM 2983 CB ALA A 390 40.543 27.936 27.696 1.00 16.24 C
ATOM 2984 N HIS A 391 42.130 26.323 30.175 1.00 15.83 N
ATOM 2985 CA HIS A 391 42.919 25.140 30.495 1.00 16.67 C
ATOM 2986 C HIS A 391 42.075 24.127 31.267 1.00 17.09 C
ATOM 2987 O HIS A 391 42.324 22.923 31.212 1.00 18.18 O
ATOM 2988 CB HIS A 391 44.176 25.530 31.270 1.00 17.03 C
ATOM 2989 CG HIS A 391 45.216 26.173 30.410 1.00 17.96 C
ATOM 2990 NDl HIS A 391 45.093 27.459 29.931 1.00 19.89 N
ATOM 2991 CD2 HIS A 391 46.361 25.682 29.877 1.00 18.88 C
ATOM 2992 CEl HIS A 391 46.116 27.733 29.142 1.00 20.51 C
ATOM 2993 NE2 HIS A 391 46.900 26.672 29.092 1.00 19.65 N
ATOM 2994 N LEU A 392 41.052 24.607 31.966 1.00 16.38 N
ATOM 2995 CA LEU A 392 40.182 23.705 32.701 1.00 17.37 C
ATOM 2996 C LEU A 392 39.378 22.858 31.704 1.00 18.99 C
ATOM 2997 O LEU A 392 39.214 21.646 31.876 1.00 18.75 O
ATOM 2998 CB LEU A 392 39.241 24.510 33.605 1.00 19.70 C
ATOM 2999 CG LEU A 392 38.328 23.740 34.560 1.00 23.03 C
ATOM 3000 CDl LEU A 392 39.148 22.792 35.408 1.00 25.12 C
ATOM 3001 CD2 LEU A 392 37.580 24.724 35.449 1.00 22.02 C
ATOM 3002 N VAL A 393 38.884 23.500 30.651 1.00 16.92 N
ATOM 3003 CA VAL A 393 38.108 22.797 29.637 1.00 17.07 C
ATOM 3004 C VAL A 393 38.997 21.904 28.763 1.00 16.35 C
ATOM 3005 O VAL A 393 38.548 20.871 28.257 1.00 17.43 O
ATOM 3006 CB VAL A 393 37.354 23.801 28.736 1.00 20.23 C
ATOM 3007 CGl VAL A 393 36.682 23.084 27.585 1.00 23.68 C

ATOM	3008	CG2	VAL	A	393	36.315	24.540	29.568	1.00	20.67
C										
ATOM	3009	N	MET	A	394	40.250	22.302	28.574	1.00	15.45
N										
ATOM	3010	CA	MET	A	394	41.157	21.502	27.748	1.00	15.50
C										
ATOM	3011	C	MET	A	394	41.684	20.246	28.449	1.00	16.75
C										
ATOM	3012	O	MET	A	394	41.977	19.245	27.794	1.00	16.85
O										
ATOM	3013	CB	MET	A	394	42.359	22.344	27.293	1.00	17.42
C										
ATOM	3014	CG	MET	A	394	42.004	23.542	26.420	1.00	21.89
C										
ATOM	3015	SD	MET	A	394	43.458	24.365	25.709	1.00	29.11
S										
ATOM	3016	CE	MET	A	394	43.933	25.438	27.057	1.00	25.89
C										
ATOM	3017	N	PHE	A	395	41.786	20.289	29.775	1.00	16.11
N										
ATOM	3018	CA	PHE	A	395	42.352	19.162	30.514	1.00	16.47
C										
ATOM	3019	C	PHE	A	395	41.446	18.348	31.430	1.00	16.05
C										
ATOM	3020	O	PHE	A	395	41.796	17.228	31.793	1.00	17.23
O										
ATOM	3021	CB	PHE	A	395	43.562	19.661	31.307	1.00	16.15
C										
ATOM	3022	CG	PHE	A	395	44.723	20.041	30.444	1.00	18.99
C										
ATOM	3023	CDl	PHE	A	395	45.561	19.060	29.924	1.00	19.96
C										
ATOM	3024	CD2	PHE	A	395	44.948	21.369	30.098	1.00	20.95
C										
ATOM	3025	CEl	PHE	A	395	46.607	19.398	29.065	1.00	22.57
C										
ATOM	3026	CE2	PHE	A	395	45.989	21.715	29.242	1.00	23.01
C										
ATOM	3027	CZ	PHE	A	395	46.819	20.724	28.723	1.00	21.85
C										
ATOM	3028	N	LEU	A	396	40.296	18.889	31.819	1.00	16.48
N										
ATOM	3029	CA	LEU	A	396	39.398	18.139	32.695	1.00	16.43
C										
ATOM	3030	C	LEU	A	396	38.214	17.597	31.908	1.00	17.61
C										
ATOM	3031	O	LEU	A	396	37.401	18.361	31.379	1.00	17.67
O										
ATOM	3032	CB	LEU	A	396	38.903	19.023	33.844	1.00	17.64
C										
ATOM	3033	CG	LEU	A	396	38.008	18.327	34.880	1.00	17.78
C										
ATOM	3034	CDl	LEU	A	396	38.771	17.202	35.576	1.00	20.63
C										
ATOM	3035	CD2	LEU	A	396	37.538	19.348	35.902	1.00	20.63
C										
ATOM	3036	N	ASN	A	397	38.116	16.275	31.828	1.00	19.32
N										
ATOM	3037	CA	ASN	A	397	37.031	15.647	31.086	1.00	19.22
C										

ATOM	3038	C	ASN	A	397	35.659	16.087	31.603	1.00	20.83
C										
ATOM	3039	O	ASN	A	397	35.397	16.085	32.808	1.00	20.14
O										
ATOM	3040	CB	ASN	A	397	37.163	14.119	31.153	1.00	21.84
C										
ATOM	3041	CG	ASN	A	397	36.248	13.412	30.176	1.00	23.17
C										
ATOM	3042	ODl	ASN	A	397	36.122	13.825	29.025	1.00	26.54
O										
ATOM	3043	ND2	ASN	A	397	35.611	12.336	30.627	1.00	26.29
N										
ATOM	3044	N	LYS	A	398	34.806	16.493	30.669	1.00	20.20
N										
ATOM	3045	CA	LYS	A	398	33.445	16.939	30.955	1.00	21.89
C										
ATOM	3046	C	LYS	A	398	33.310	18.302	31.627	1.00	20.36
C										
ATOM	3047	O	LYS	A	398	32.210	18.685	32.029	1.00	20.63
O										
ATOM	3048	CB	LYS	A	398	32.689	15.885	31.775	1.00	24.61
C										
ATOM	3049	CG	LYS	A	398	32.609	14.511	31.109	1.00	29.22
C										
ATOM	3050	CD	LYS	A	398	32.137	14.606	29.665	1.00	32.55
C										
ATOM	3051	CE	LYS	A	398	32.112	13.238	28.995	1.00	36.15
C										
ATOM	3052	NZ	LYS	A	398	31.805	13.343	27.542	1.00	38.80
N										
ATOM	3053	N	SER	A	399	34.411	19.037	31.756	1.00	18.38
N										
ATOM	3054	CA	SER	A	399	34.344	20.373	32.342	1.00	18.06
C										
ATOM	3055	C	SER	A	399	33.540	21.235	31.370	1.00	18.72
C										
ATOM	3056	O	SER	A	399	32.714	22.058	31.767	1.00	17.12
C										
ATOM	3057	CB	SER	A	399	35.747	20.962	32.509	1.00	16.10
C										
ATOM	3058	OG	SER	A	399	35.687	22.285	33.020	1.00	20.37
O										
ATOM	3059	N	LEU	A	400	33.793	21.038	30.081	1.00	18.40
N										
ATOM	3060	CA	LEU	A	400	33.084	21.776	29.040	1.00	20.34
C										
ATOM	3061	C	LEU	A	400	31.572	21.596	29.205	1.00	20.55
C										
ATOM	3062	O	LEU	A	400	30.807	22.555	29.121	1.00	19.32
O										
ATOM	3063	CB	LEU	A	400	33.540	21.263	27.667	1.00	24.88
C										
ATOM	3064	CG	LEU	A	400	32.949	21.845	26.382	1.00	29.42
C										
ATOM	3065	CDl	LEU	A	400	33.887	21.512	25.224	1.00	32.06
C										
ATOM	3066	CD2	LEU	A	400	31.557	21.283	26.135	1.00	30.62
C										
ATOM	3067	N	ASP	A	401	31.155	20.357	29.455	1.00	20.93
N										

ATOM	3068	CA	ASP	A	401	29.746	20.024	29.622	1.00	22.67
C										
ATOM	3069	C	ASP	A	401	29.117	20.759	30.806	1.00	21.90
C										
ATOM	3070	O	ASP	A	401	27.977	21.223	30.733	1.00	21.22
O										
ATOM	3071	CB	ASP	A	401	29.592	18.515	29.827	1.00	25.33
C										
ATOM	3072	CG	ASP	A	401	30.197	17.704	28.694	1.00	29.68
C										
ATOM	3073	ODl	ASP	A	401	31.384	17.917	28.362	1.00	30.97
O										
ATOM	3074	OD2	ASP	A	401	29.483	16.842	28.138	1.00	33.86
O										
ATOM	3075	N	GLU	A	402	29.865	20.844	31.900	1.00	19.70
N										
ATOM	3076	CA	GLU	A	402	29.393	21.511	33.106	1.00	19.35
C										
ATOM	3077	C	GLU	A	402	29.224	23.013	32.871	1.00	17.86
C										
ATOM	3078	O	GLU	A	402	28.236	23.608	33.299	1.00	19.05
O										
ATOM	3079-	CB	GLU	A	402	30.387	21.268	34.245	1.00	21.21
C										
ATOM	3080	CG	GLU	A	402	29.865	21.583	35.630	1.00	24.51
C										
ATOM	3081	CD	GLU	A	402	28.668	20.734	36.016	1.00	25.30
C										
ATOM	3082	OEl	GLU	A	402	28.433	19.683	35.382	1.00	30.04
O										
ATOM	3083	OE2	GLU	A	402	27.967	21.114	36.966	1.00	28.06
O										
ATOM	3084	N	MET	A	403	30.198	23.634	32.209	1.00	17.59
N										
ATOM	3085	CA	MET	A	403	30.106	25.061	31.927	1.00	17.31
C										
ATOM	3086	C	MET	A	403	28.949	25.332	30.979	1.00	17.88
C										
ATOM	3087	O	MET	A	403	28.188	26.284	31.166	1.00	17.12
O										
ATOM	3088	CB	MET	A	403	31.398	25.578	31.294	1.00	15.84
C										
ATOM	3089	CG	MET	A	403	32.595	25.515	32.217	1.00	16.56
C										
ATOM	3090	SD	MET	A	403	33.966	26.459	31.555	1.00	19.56
S										
ATOM	3091	CE	MET	A	403	35.290	25.905	32.639	1.00	19.19
C										
ATOM	3092	N	ASP	A	404	28.820	24.492	29.959	1.00	18.20
N										
ATOM	3093	CA	ASP	A	404	27.751	24.658	28.984	1.00	18.46
C										
ATOM	3094	C	ASP	A	404	26.396	24.545	29.667	1.00	19.45
C										
ATOM	3095	O	ASP	A	404	25.427	25.187	29.260	1.00	20.89
O										
ATOM	3096	CB	ASP	A	404	27.857	23.605	27.887	1.00	19.38
C										
ATOM	3097	CG	ASP	A	404	26.724	23.701	26.886	1.00	20.32
C										

ATOM 3098 ODl ASP A 404 26.705 24.675 26.103 1.00 21.41
O
ATOM 3099 OD2 ASP A 404 25.849 22.809 26.899 1.00 21.23
O
ATOM 3100 N PHE A 405 26.322 23.730 30.711 1.00 20.19
N
ATOM 3101 CA PHE A 405 25.059 23.581 31.413 1.00 19.77
C
ATOM 3102 C PHE A 405 24.674 24.797 32.253 1.00 20.70
C
ATOM 3103 O PHE A 405 23.620 25.402 32.037 1.00 22.14
O
ATOM 3104 CB PHE A 405 25.076 22.350 32.313 1.00 21.32
C
ATOM 3105 CG PHE A 405 23.818 22.192 33.115 1.00 24.39
C
ATOM 3106 CDl PHE A 405 22.612 21.902 32.483 1.00 27.77
C
ATOM 3107 CD2 PHE A 405 23.825 22.393 34.489 1.00 26.33
C
ATOM 3108 CEl PHE A 405 21.426 21.819 33.211 1.00 29.27
C
ATOM 3109 CE2 PHE A 405 22.649 22.313 35.227 1.00 29.09
C
ATOM 3110 CZ PHE A 405 21.446 22.025 34.585 1.00 29.31
C
ATOM 3111 N TRP A 406 25.521 25.166 33.208 1.00 19.16
N
ATOM 3112 CA TRP A 406 25.200 26.293 34.080 1.00 20.73
C
ATOM 3113 C TRP A 406 25.119 27.649 33.401 1.00 20.29
C
ATOM 3114 O TRP A 406 24.219 28.438 33.688 1.00 20.46
O
ATOM 3115 CB TRP A 406 26.188 26.370 35.248 1.00 20.05
C
ATOM 3116 CG TRP A 406 26.092 25.181 36.144 1.00 21.07
C
ATOM 3117 CDl TRP A 406 26.957 24.126 36.204 1.00 21.22
C
ATOM 3118 CD2 TRP A 406 25.029 24.882 37.058 1.00 23.58
C
ATOM 3119 NEl TRP A 406 26.496 23.187 37.095 1.00 22.35
N
ATOM 3120 CE2 TRP A 406 25.315 23.625 37.633 1.00 23.36
C
ATOM 3121 CE3 TRP A 406 23.859 25.554 37.442 1.00 26.54
C
ATOM 3122 CZ2 TRP A 406 24.473 23.022 38.575 1.00 26.00
C
ATOM 3123 CZ3 TRP A 406 23.019 24.952 38.380 1.00 27.66
C
ATOM 3124 CH2 TRP A 406 23.334 23.698 38.935 1.00 26.21
C
ATOM 3125 N ALA A 407 26.054 27.925 32.503 1.00 19.92
N
ATOM 3126 CA ALA A 407 26.056 29.213 31.828 1.00 21.15
C
ATOM 3127 C ALA A 407 25.249 29.201 30.542 1.00 22.18
C

ATOM	3128	O	ALA	A	407	24.321	29.997	30.377	1.00	22.68
O										
ATOM	3129	CB	ALA	A	407	27.502	29.652	31.537	1.00	21.73
C										
ATOM	3130	N	GLY	A	408	25.590	28.275	29.649	1.00	21.72
N										
ATOM	3131	CA	GLY	A	408	24.934	28.201	28.354	1.00	22.70
C										
ATOM	3132	C	GLY	A	408	23.555	27.579	28.246	1.00	23.18
C										
ATOM	3133	O	GLY	A	408	22.939	27.645	27.187	1.00	23.70
O										
ATOM	3134	N	THR	A	409	23.063	26.975	29.319	1.00	22.76
N										
ATOM	3135	CA	THR	A	409	21.751	26.351	29.275	1.00	25.65
C										
ATOM	3136	C	THR	A	409	20.818	26.961	30.318	1.00	25.69
C										
ATOM	3137	O	THR	A	409	19.883	27.682	29.970	1.00	27.69
O										
ATOM	3138	CB	THR	A	409	21.875	24.826	29.477	1.00	26.28
C										
ATOM	3139	OGl	THR	A	409	22.765	24.291	28.488	1.00	28.28
O										
ATOM	3140	CG2	THR	A	409	20.526	24.150	29.320	1.00	29.37
C										
ATOM	3141	N	ILE	A	410	21.083	26.695	31.593	1.00	25.04
N										
ATOM	3142	CA	ILE	A	410	20.260	27.233	32.673	1.00	26.89
C										
ATOM	3143	C	ILE	A	410	20.435	28.739	32.813	1.00	25.35
C										
ATOM	3144	O	ILE	A	410	19.461	29.489	32.882	1.00	23.56
O										
ATOM	3145	CB	ILE	A	410	20.626	26.597	34.038	1.00	29.69
C										
ATOM	3146	CGl	ILE	A	410	20.465	25.081	33.968	1.00	32.84
C										
ATOM	3147	CG2	ILE	A	410	19.742	27.179	35.138	1.00	32.43
C										
ATOM	3148	CDl	ILE	A	410	19.067	24.620	33.609	1.00	34.79
C										
ATOM	3149	N	GLY	A	411	21.691	29.172	32.856	1.00	23.30
N										
ATOM	3150	CA	GLY	A	411	21.992	30.578	33.015	1.00	21.38
C										
ATOM	3151	C	GLY	A	411	21.303	31.517	32.048	1.00	20.77
C										
ATOM	3152	O	GLY	A	411	20.720	32.516	32.471	1.00	20.03
O										
ATOM	3153	N	VAL	A	412	21.363	31.213	30.754	1.00	19.99
N										
ATOM	3154	CA	VAL	A	412	20.745	32.092	29.766	1.00	20.66
C										
ATOM	3155	C	VAL	A	412	19.230	32.190	29.887	1.00	20.47
C										
ATOM	3156	O	VAL	A	412	18.665	33.253	29.647	1.00	20.47
O										
ATOM	3157	CB	VAL	A	412	21.106	31.680	28.314	1.00	20.66
C										

ATOM	3158	CGl	VAL	A	412	22.618	31.730	28.125	1.00	23.41
ATOM	3159	CG2	VAL	A	412	20.565	30.300	28.004	1.00	22.78
ATOM	3160	N	VAL	A	413	18.563	31.100	30.251	1.00	20.85
ATOM	3161	CA	VAL	A	413	17.110	31.167	30.382	1.00	22.11
ATOM	3162	C	VAL	A	413	16.771	32.002	31.611	1.00	23.85
ATOM	3163	O	VAL	A	413	15.870	32.842	31.578	1.00	21.96
ATOM	3164	CB	VAL	A	413	16.478	29.761	30.492	1.00	22.81
ATOM	3165	CGl	VAL	A	413	14.968	29.883	30.692	1.00	25.43
ATOM	3166	CG2	VAL	A	413	16.767	28.967	29.227	1.00	24.16
ATOM	3167	N	PHE	A	414	17.509	31.776	32.694	1.00	23.73
ATOM	3168	CA	PHE	A	414	17.314	32.536	33.923	1.00	24.96
ATOM	3169	C	PHE	A	414	17.584	34.019	33.668	1.00	24.38
ATOM	3170	O	PHE	A	414	16.831	34.883	34.119	1.00	24.21
ATOM	3171	CB	PHE	A	414	18.265	32.026	35.013	1.00	28.57
ATOM	3172	CG	PHE	A	414	18.406	32.960	36.184	1.00	33.21
ATOM	3173	CDl	PHE	A	414	17.372	33.108	37.107	1.00	35.79
ATOM	3174	CD2	PHE	A	414	19.567	33.713	36.352	1.00	35.05
ATOM	3175	CEl	PHE	A	414	17.494	33.993	38.181	1.00	37.24
ATOM	3176	CE2	PHE	A	414	19.697	34.600	37.420	1.00	36.18
ATOM	3177	CZ	PHE	A	414	18.660	34.741	38.336	1.00	36.43
ATOM	3178	N	PHE	A	415	18.662	34.316	32.944	1.00	22.28
ATOM	3179	CA	PHE	A	415	19.013	35.701	32.665	1.00	22.32
ATOM	3180	C	PHE	A	415	18.015	36.358	31.717	1.00	21.15
ATOM	3181	O	PHE	A	415	17.741	37.549	31.834	1.00	20.75
ATOM	3182	CB	PHE	A	415	20.427	35.797	32.078	1.00	22.37
ATOM	3183	CG	PHE	A	415	21.038	37.166	32.195	1.00	22.50
ATOM	3184	CDl	PHE	A	415	21.170	37.773	33.446	1.00	23.29
ATOM	3185	CD2	PHE	A	415	21.487	37.849	31.069	1.00	23.39
ATOM	3186	CEl	PHE	A	415	21.739	39.033	33.573	1.00	23.51
ATOM	3187	CE2	PHE	A	415	22.062	39.119	31.187	1.00	24.14

ATOM	3188	CZ	PHE	A	415	22.187	39.710	32.445	1.00	23.67
C										
ATOM	3189	N	GLY	A	416	17.481	35.584	30.776	1.00	21.00
N										
ATOM	3190	CA	GLY	A	416	16.502	36.133	29.853	1.00	20.92
C										
ATOM	3191	C	GLY	A	416	15.263	36.565	30.626	1.00	22.76
C										
ATOM	3192	O	GLY	A	416	14.701	37.638	30.385	1.00	23.62
O										
ATOM	3193	N	LEU	A	417	14.835	35.725	31.560	1.00	23.34
N										
ATOM	3194	CA	LEU	A	417	13.668	36.030	32.379	1.00	24.81
C										
ATOM	3195	C	LEU	A	417	13.966	37.240	33.256	1.00	25.70
C										
ATOM	3196	O	LEU	A	417	13.113	38.111	33.449	1.00	26.35
O										
ATOM	3197	CB	LEU	A	417	13.306	34.829	33.258	1.00	26.30
C										
ATOM	3198	CG	LEU	A	417	12.158	35.081	34.240	1.00	28.36
C										
ATOM	3199	CDl	LEU	A	417	10.908	35.508	33.470	1.00	27.54
C										
ATOM	3200	CD2	LEU	A	417	11.894	33.822	35.054	1.00	29.43
C										
ATOM	3201	N	THR	A	418	15.186	37.293	33.781	1.00	25.46
N										
ATOM	3202	CA	THR	A	418	15.608	38.395	34.635	1.00	25.99
C										
ATOM	3203	C	THR	A	418	15.613	39.731	33.891	1.00	27.56
C										
ATOM	3204	O	THR	A	418	15.088	40.727	34.392	1.00	27.64
O										
ATOM	3205	CB	THR	A	418	17.019	38.134	35.215	1.00	26.05
C										
ATOM	3206	OGl	THR	A	418	16.977	36.971	36.053	1.00	27.68
O										
ATOM	3207	CG2	THR	A	418	17.497	39.326	36.031	1.00	28.68
C										
ATOM	3208	N	GLU	A	419	16.201	39.761	32.699	1.00	26.55
N										
ATOM	3209	CA	GLU	A	419	16.244	41.006	31.942	1.00	26.65
C										
ATOM	3210	C	GLU	A	419	14.841	41.450	31.545	1.00	26.79
C										
ATOM	3211	O	GLU	A	419	14.554	42.644	31.513	1.00	27.02
O										
ATOM	3212	CB	GLU	A	419	17.136	40.865	30.699	1.00	26.73
C										
ATOM	3213	CG	GLU	A	419	16.801	39.697	29.802	1.00	29.79
C										
ATOM	3214	CD	GLU	A	419	17.788	39.538	28.651	1.00	28.93
C										
ATOM	3215	OEl	GLU	A	419	18.949	39.984	28.782	1.00	28.72
O										
ATOM	3216	OE2	GLU	A	419	17.399	38.953	27.622	1.00	31.19
O										
ATOM	3217	N	LEU	A	420	13.963	40.493	31.263	1.00	26.95
N										

ATOM	3218	CA	LEU	A	420	12.595	40.825	30.879	1.00	28.96
ATOM	3219	C	LEU	A	420	11.837	41.440	32.056	1.00	29.05
ATOM	3220	O	LEU	A	420	11.110	42.422	31.888	1.00	30.29
ATOM	3221	CB	LEU	A	420	11.859	39.578	30.376	1.00	29.71
ATOM	3222	CG	LEU	A	420	10.481	39.823	29.747	1.00	32.98
ATOM	3223	CDl	LEU	A	420	10.095	38.639	28.889	1.00	34.57
ATOM	3224	CD2	LEU	A	420	9.442	40.064	30.832	1.00	34.63
ATOM	3225	N	ILE	A	421	12.006	40.861	33.242	1.00	27.70
ATOM	3226	CA	ILE	A	421	11.336	41.369	34.440	1.00	27.20
ATOM	3227	C	ILE	A	421	11.834	42.769	34.781	1.00	27.86
ATOM	3228	O	ILE	A	421	11.042	43.670	35.067	1.00	29.17
ATOM	3229	CB	ILE	A	421	11.575	40.436	35.656	1.00	27.70
ATOM	3230	CGl	ILE	A	421	10.830	39.115	35.452	1.00	27.02
ATOM	3231	CG2	ILE	A	421	11.105	41.114	36.947	1.00	26.90
ATOM	3232	CDl	ILE	A	421	11.155	38.057	36.499	1.00	28.18
ATOM	3233	N	ILE	A	422	13.148	42.956	34.745	1.00	26.88
ATOM	3234	CA	ILE	A	422	13.727	44.253	35.058	1.00	26.80
ATOM	3235	C	ILE	A	422	13.323	45.333	34.055	1.00	26.87
ATOM	3236	O	ILE	A	422	13.013	46.460	34.438	1.00	26.17
ATOM	3237	CB	ILE	A	422	15.269	44.169	35.119	1.00	27.65
ATOM	3238	CGl	ILE	A	422	15.685	43.314	36.319	1.00	29.44
ATOM	3239	CG2	ILE	A	422	15.870	45.568	35.207	1.00	27.61
ATOM	3240	CDl	ILE	A	422	17.189	43.215	36.530	1.00	28.88
ATOM	3241	N	PHE	A	423	13.309	44.985	32.773	1.00	24.96
ATOM	3242	CA	PHE	A	423	12.969	45.955	31.739	1.00	26.14
ATOM	3243	C	PHE	A	423	11.474	46.181	31.541	1.00	28.36
ATOM	3244	O	PHE	A	423	11.015	47.326	31.478	1.00	28.71
ATOM	3245	CB	PHE	A	423	13.600	45.527	30.410	1.00	24.78
ATOM	3246	CG	PHE	A	423	13.520	46.568	29.324	1.00	25.07
ATOM	3247	CDl	PHE	A	423	14.047	47.843	29.517	1.00	25.43

ATOM	3248	CD2	PHE	A	423	12.954	46.257	28.092	1.00	24.13
C										
ATOM	3249	CEl	PHE	A	423	14.015	48.792	28.494	1.00	25.45
C										
ATOM	3250	CE2	PHE	A	423	12.918	47.196	27.063	1.00	23.86
C										
ATOM	3251	CZ	PHE	A	423	13.449	48.465	27.265	1.00	24.95
C										
ATOM	3252	N	PHE	A	424	10.708	45.100	31.458	1.00	29.42
N										
ATOM	3253	CA	PHE	A	424	9.278	45.220	31.217	1.00	31.53
C										
ATOM	3254	C	PHE	A	424	8.366	45.309	32.434	1.00	32.84
C										
ATOM	3255	O	PHE	A	424	7.210	45.714	32.312	1.00	34.87
O										
ATOM	3256	CB	PHE	A	424	8.805	44.080	30.317	1.00	30.99
C										
ATOM	3257	CG	PHE	A	424	8.178	44.551	29.043	1.00	30.89
C										
ATOM	3258	CDl	PHE	A	424	8.966	45.021	27.997	1.00	30.66
C										
ATOM	3259	CD2	PHE	A	424	6.794	44.582	28.908	1.00	30.33
C										
ATOM	3260	CEl	PHE	A	424	8.383	45.520	26.836	1.00	30.75
C										
ATOM	3261	CE2	PHE	A	42*1	6.203	45.079	27.751	1.00	30.19
C										
ATOM	3262	CZ	PHE	A	424	6.998	45.550	26.715	1.00	31.05
C										
ATOM	3263	N	TRP	A	425	8.869	44.938	33.604	1.00	32.86
N										
ATOM	3264	CA	TRP	A	425	8.051	44.998	34.808	1.00	32.84
C										
ATOM	3265	C	TRP	A	425	8.512	46.083	35.770	1.00	33.25
C										
ATOM	3266	O	TRP	A	425	7.731	46.954	36.150	1.00	34.52
O										
ATOM	3267	CB	TRP	A	425	8.053	43.645	35.524	1.00	33.17
C										
ATOM	3268	CG	TRP	A	425	7.255	42.575	34.833	1.00	34.48
C										
ATOM	3269	CDl	TRP	A	425	6.653	42.652	33.610	1.00	34.79
C										
ATOM	3270	CD2	TRP	A	425	6.973	41.264	35.336	1.00	34.97
C										
ATOM	3271	NEl	TRP	A	425	6.010	41.471	33.321	1.00	34.04
NNT										
ATOM	3272	CE2	TRP	A	425	6.192	40.602	34.365	1.00	34.95
C										
ATOM	3273	CE3	TRP	A	425	7.306	40.585	36.516	1.00	35.92
C										
ATOM	3274	CZ2	TRP	A	425	5.735	39.291	34.536	1.00	34.74
C										
ATOM	3275	CZ3	TRP	A	425	6.851	39.278	36.687	1.00	36.18
C										
ATOM	3276	CH2	TRP	A	425	6.074	38.648	35.700	1.00	35.94
C										
ATOM	3277	N	ILE	A	426	9.781	46.035	36.157	1.00	31.04
N										

ATOM 3278 CA ILE A 426 10.323 47.011 37.093 1.00 30.91 C
ATOM 3279 C ILE A 426 10.532 48.381 36.456 1.00 31.41 C
ATOM 3280 O ILE A 426 10.021 49.387 36.955 1.00 31.07 O
ATOM 3281 CB ILE A 426 11.647 46.504 37.704 1.00 30.63 C
ATOM 3282 CGl ILE A 426 11.393 45.177 38.431 1.00 31.52 C
ATOM 3283 CG2 ILE A 426 12.210 47.539 38.665 1.00 30.97 C
ATOM 3284 CDl ILE A 426 12.624 44.570 39.092 1.00 31.98 C
ATOM 3285 N PHE A 427 11.275 48.426 35.356 1.00 29.90 N
ATOM 3286 CA PHE A 427 11.521 49.683 34.661 1.00 30.27 C
ATOM 3287 C PHE A 427 10.178 50.271 34.227 1.00 30.83 C
ATOM 3288 O PHE A 427 9.954 51.476 34.330 1.00 31.84 O
ATOM 3289 CB PHE A 427 12.409 49.437 33.438 1.00 29.13 C
ATOM 3290 CG PHE A 427 12.719 50.675 32.643 1.00 29.32 C
ATOM 3291 CDl PHE A 427 13.396 51.742 33.222 1.00 29.53 C
ATOM 3292 CD2 PHE A 427 12.367 50.754 31.297 1.00 28.44 C
ATOM 3293 CEl PHE A 427 13.725 52.869 32.473 1.00 28.86 C
ATOM 3294 CE2 PHE A 427 12.690 51.876 30.539 1.00 29.55 C
ATOM 3295 CZ PHE A 427 13.372 52.936 31.127 1.00 29.33 C
ATOM 3296 N GLY A 428 9.288 49.409 33.746 1.00 30.54 N
ATOM 3297 CA GLY A 428 7.979 49.861 33.312 1.00 29.72 C
ATOM 3298 C GLY A 428 7.635 49.374 31.920 1.00 28.63 C
ATOM 3299 O GLY A 428 8.325 49.695 30.958 1.00 29.26 O
ATOM 3300 N ALA A 429 6.563 48.598 31.814 1.00 28.42 N
ATOM 3301 CA ALA A 429 6.129 48.057 30.533 1.00 27.67 C
ATOM 3302 C ALA A 429 5.940 49.136 29.471 1.00 27.25 C
ATOM 3303 O ALA A 429 6.391 48.991 28.337 1.00 26.02 O
ATOM 3304 CB ALA A 429 4.834 47.271 30.713 1.00 27.21 C
ATOM 3305 N ASP A 430 5.276 50.229 29.832 1.00 27.59 N
ATOM 3306 CA ASP A 430 5.045 51.286 28.860 1.00 28.31 C
ATOM 3307 C ASP A 430 6.311 52.061 28.509 1.00 25.86 C

ATOM	3308	O	ASP	A	430	6.493	52.475	27.365	1.00	26.18
ATOM	3309	CB	ASP	A	430	3.936	52.214	29.363	1.00	31.33
ATOM	3310	CG	ASP	A	430	2.642	51.463	29.625	1.00	34.48
ATOM	3311	ODl	ASP	A	430	2.193	50.730	28.720	1.00	37.11
ATOM	3312	OD2	ASP	A	430	2.074	51.595	30.731	1.00	38.22
ATOM	3313	N	LYS	A	431	7.193	52.249	29.482	1.00	25.64
ATOM	3314	CA	LYS	A	431	8.450	52.944	29.225	1.00	26.41
ATOM	3315	C	LYS	A	431	9.306	52.049	28.329	1.00	25.30
ATOM	3316	O	LYS	A	431	9.967	52.522	27.404	1.00	25.77
ATOM	3317	CB	LYS	A	431	9.206	53.198	30.527	1.00	29.13
ATOM	3318	CG	LYS	A	431	8.489	54.091	31.514	1.00	34.26
ATOM	3319	CD	LYS	A	431	9.234	54.115	32.839	1.00	36.97
ATOM	3320	CE	LYS	A	431	10.597	54.767	32.713	1.00	38.85
ATOM	3321	NZ	LYS	A	431	11.303	54.760	34.024	1.00	43.23
ATOM	3322	N	ALA	A	432	9.291	50.753	28.623	1.00	25.03
ATOM	3323	CA	ALA	A	432	10.062	49.781	27.849	1.00	24.58
ATOM	3324	C	ALA	A	432	9.561	49.729	26.409	1.00	24.31
ATOM	3325	O	ALA	A	432	10.348	49.754	25.464	1.00	24.09
ATOM	3326	CB	ALA	A	432	9.959	48.399	28.492	1.00	23.55
ATOM	3327	N	TRP	A	433	8.243	49.667	26.248	1.00	25.48
ATOM	3328	CA	TRP	A	433	7.633	49.615	24.928	1.00	25.31
ATOM	3329	C	TRP	A	433	8.022	50.852	24.122	1.00	26.18
ATOM	3330	O	TRP	A	433	8.365	50.757	22.945	1.00	25.60
ATOM	3331	CB	TRP	A	433	6.111	49.517	25.073	1.00	26.14
ATOM	3332	CG	TRP	A	433	5.372	49.379	23.779	1.00	27.33
ATOM	3333	CDl	TRP	A	433	4.629	50.339	23.152	1.00	27.35
ATOM	3334	CD2	TRP	A	433	5.283	48.206	22.961	1.00	26.62
ATOM	3335	NEl	TRP	A	433	4.081	49.836	21.997	1.00	26.68
ATOM	3336	CE2	TRP	A	433	4.466	48.529	21.855	1.00	26.90
ATOM	3337	CE3	TRP	A	433	5.814	46.912	23.056	1.00	26.95

ATOM 3338 CZ2 TRP A 433 4.166 47.605 20.849 1.00 26.06 C
ATOM 3339 CZ3 TRP A 433 5.515 45.992 22.055 1.00 25.66 C
ATOM 3340 CH2 TRP A 433 4.698 46.345 20.966 1.00 27.58 C
ATOM 3341 N GLU A 434 7.971 52.011 24.769 1.00 27.43 N
ATOM 3342 CA GLU A 434 8.331 53.271 24.132 1.00 29.57 C
ATOM 3343 C GLU A 434 9.792 53.256 23.690 1.00 28.77 C
ATOM 3344 O GLU A 434 10.127 53.678 22.582 1.00 27.54 O
ATOM 3345 CB GLU A 434 8.120 54.429 25.111 1.00 33.01 C
ATOM 3346 CG GLU A 434 8.652 55.761 24.609 1.00 39.58 C
ATOM 3347 CD GLU A 434 7.705 56.445 23.645 1.00 44.09 C
ATOM 3348 OEl GLU A 434 7.100 55.751 22.801 1.00 48.29 O
ATOM 3349 OE2 GLU A 434 7.572 57.683 23.728 1.00 46.27 O
ATOM 3350 N GLU A 435 10.660 52.767 24.570 1.00 27.96 N
ATOM 3351 CA GLU A 435 12.089 52.708 24.288 1.00 27.82 C
ATOM 3352 C GLU A 435 12.400 51.797 23.105 1.00 26.53 C
ATOM 3353 O GLU A 435 13.214 52.139 22.253 1.00 27.95 O
ATOM 3354 CB GLU A 435 12.842 52.233 25.534 1.00 30.60 C
ATOM 3355 CG GLU A 435 14.359 52.311 25.434 1.00 31.79 C
ATOM 3356 CD GLU A 435 14.857 53.715 25.157 1.00 32.92 C
ATOM 3357 OEl GLU A 435 14.275 54.672 25.712 1.00 35.80 O
ATOM 3358 OE2 GLU A 435 15.840 53.864 24.399 1.00 31.87 O
ATOM 3359 N ILE A 436 11.743 50.642 23.052 1.00 25.29 N
ATOM 3360 CA ILE A 436 11.955 49.693 21.965 1.00 23.70 C
ATOM 3361 C ILE A 436 11.575 50.294 20.614 1.00 24.78 C
ATOM 3362 O ILE A 436 12.328 50.207 19.649 1.00 23.10 O
ATOM 3363 CB ILE A 436 11.105 48.420 22.159 1.00 23.27 C
ATOM 3364 CGl ILE A 436 11.558 47.677 23.418 1.00 24.73 C
ATOM 3365 CG2 ILE A 436 11.203 47.535 20.918 1.00 24.27 C
ATOM 3366 CDl ILE A 436 10.614 46.571 23.846 1.00 24.79 C
ATOM 3367 N ASN A 437 10.401 50.914 20.564 1.00 24.80 N

ATOM	3368	CA	ASN	A	437	9.891	51.493	19.326	1.00	26.03	C
ATOM	3369	C	ASN	A	437	10.476	52.835	18.896	1.00	26.30	C
ATOM	3370	O	ASN	A	437	10.355	53.218	17.732	1.00	26.44	O
ATOM	3371	CB	ASN	A	437	8.364	51,588	19.410	1.00	26.52	C
ATOM	3372	CG	ASN	A	437	7.695	50.231	19.289	1.00	27.02	C
ATOM	3373	ODl	ASN	A	437	7.744	49.599	18.234	1.00	28.56	O
ATOM	3374	ND2	ASN	A	437	7.078	49.770	20.370	1.00	29.04	N
ATOM	3375	N	ARG	A	438	11.112	53.545	19.820	1.00	26.74	N
ATOM	3376	CA	ARG	A	438	11.702	54.839	19.497	1.00	27.84	C
ATOM	3377	C	ARG	A	438	12.706	54.714	18.346	1.00	28.96	C
ATOM	3378	O	ARG	A	438	13.607	53.874	18.382	1.00	28.06	O
ATOM	3379	CB	ARG	A	438	12.385	55.421	20.740	1.00	28.58	C
ATOM	3380	CG	ARG	A	438	12.909	56.841	20.570	1.00	30.89	C
ATOM	3381	CD	ARG	A	438	13.451	57.374	21.890	1.00	32.74	C
ATOM	3382	NE	ARG	A	438	14.514	56.523	22.424	1.00	32.65	N
ATOM	3383	CZ	ARG	A	438	15.687	56.342	21.828	1.00	32.80	C
ATOM	3384	NHl	ARG	A	438	15.948	56.957	20.681	1.00	34.51	N
ATOM	3385	NH2	ARG	A	438	16.595	55.541	22.371	1.00	30.83	N
ATOM	3386	N	GLY	A	439	12.529	55.537	17.313	1.00	27.94	N
ATOM	3387	CA	GLY	A	439	13.425	55.513	16.170	1.00	28.01	C
ATOM	3388	C	GLY	A	439	13.232	54.345	15.220	1.00	27.31	C
ATOM	3389	O	GLY	A	439	13.941	54.227	14.222	1.00	29.59	O
ATOM	3390	N	GLY	A	440	12.268	53.483	15.516	1.00	27.69	N
ATOM	3391	CA	GLY	A	440	12.031	52.328	14.670'	1.00	28.27	C
ATOM	3392	C	GLY	A	440	11.566	52.630	13.256	1.00	29.98	C
ATOM	3393	O	GLY	A	440	10.731	53.512	13.039	1.00	30.44	O
ATOM	3394	N	ILE	A	441	12.116	51.896	12.293	1.00	29.75	N
ATOM	3395	CA	ILE	A	441	11.749	52.045	10.890	1.00	31.03	C
ATOM	3396	C	ILE	A	441	10.350	51.456	10.757	1.00	32.17	C
ATOM	3397	O	ILE	A	441	9.553	51.873	9.914	1.00	32.74	O

ATOM 3398 CB ILE A 441 12.734 51.289 9.979 1.00 31.40 C
ATOM 3399 CGl ILE A 441 14.100 51.979 10.027 1.00 32.38 C
ATOM 3400 CG2 ILE A 441 12.207 51.236 8.555 1.00 31.25 C
ATOM 3401 CDl ILE A 441 15.179 51.256 9.250 1.00 32.80 C
ATOM 3402 N ILE A 442 10.069 50.477 11.610 1.00 31.57 N
ATOM 3403 CA ILE A 442 8.763 49.834 11.673 1.00 31.78 C
ATOM 3404 C ILE A 442 8.475 49.748 13.163 1.00 30.82 C
ATOM 3405 O ILE A 442 9.386 49.879 13.978 1.00 29.12 O
ATOM 3406 CB ILE A 442 8.773 48.401 11.090 1.00 33.41 C
ATOM 3407 CGl ILE A 442 9.788 47.537 11.843 1.00 34.78 C
ATOM 3408 CG2 ILE A 442 9.088 48.442 9.603 1.00 34.52 C
ATOM 3409 CDl ILE A 442 9.769 46.076 11.436 1.00 35.86 C
ATOM 3410 N LYS A 443 7.217 49.548 13.527 1.00 31.11 N
ATOM 3411 CA LYS A 443 6.878 49.436 14.934 1.00 31.44 C
ATOM 3412 C LYS A 443 6.650 47.977 15.277 1.00 29.31 C
ATOM 3413 O LYS A 443 6.304 47.172 14.415 1.00 27.02 O
ATOM 3414 CB LYS A 443 5.620 50.243 15.264 1.00 34.61 C
ATOM 3415 CG LYS A 443 5.823 51.747 15.261 1.00 39.15 C
ATOM 3416 CD LYS A 443 4.620 52.458 15.854 1.00 42.49 C
ATOM 3417 CE LYS A 443 4.840 53.963 15.902 1.00 44.44 C
ATOM 3418 NZ LYS A 443 3.685 54.664 16.525 1.00 46.07 N
ATOM 3419 N VAL A 444 6.862 47.633 16.539 1.00 28.05 N
ATOM 3420 CA VAL A 444 6.638 46.266 16.968 1.00 27.27 C
ATOM 3421 C VAL A 444 5.131 46.047 16.957 1.00 28.22 C
ATOM 3422 O VAL A 444 4.374 46.890 17.442 1.00 27.14 O
ATOM 3423 CB VAL A 444 7.165 46.031 18.395 1.00 27.41 C
ATOM 3424 CGl VAL A 444 6.841 44.615 18.839 1.00 26.56 C
ATOM 3425 CG2 VAL A 444 8.660 46.270 18.438 1.00 27.57 C
ATOM 3426 N PRO A 445 4.673 44.927 16.377 1.00 28.52 N
ATOM 3427 CA PRO A 445 3.236 44.643 16.334 1.00 28.20 C

ATOM	3428	C	PRO	A	445	2.644	44.770	17.733	1.00	28.05
C										
ATOM	3429	O	PRO	A	445	3.215	44.279	18.705	1.00	26.39
O										
ATOM	3430	CB	PRO	A	445	3.189	43.216	15.801	1.00	29.04
C										
ATOM	3431	CG	PRO	A	445	4.348	43.196	14.851	1.00	29.21
C										
ATOM	3432	CD	PRO	A	445	5.435	43.904	15.637	1.00	27.97
C										
ATOM	3433	N	ARG	A	446	1.500	45.436	17.831	1.00	27.25
N										
ATOM	3434	CA	ARG	A	446	0.840	45.650	19.111	1.00	28.05
C										
ATOM	3435	C	ARG	A	446	0.683	44.403	19.979	1.00	26.86
C										
ATOM	3436	O	ARG	A	446	0.827	44.472	21.198	1.00	26.26
O										
ATOM	3437	CB	ARG	A	446	-0.539	46.284	18.889	1.00	31.47
C										
ATOM	3438	CG	ARG	A	446	-1.270	46.627	20.178	1.00	37.03
C										
ATOM	3439	CD	ARG	A	446	-2.720	47.007	19.910	1.00	42.44
C										
ATOM	3440	NE	ARG	A	446	-3.456	47.265	21.148	1.00	46.77
N										
ATOM	3441	CZ	ARG	A	446	-3.291	48.344	21.908	1.00	48.28
C										
ATOM	3442	NHl	ARG	A	446	-2.415	49.280	21.560	1.00	48.43
N										
ATOM	3443	NH2	ARG	A	446	-4.001	48.486	23.020	1.00	48.54
N										
ATOM	3444	N	ILE	A	447	0.387	43.267	19.357	1.00	26.75
N										
ATOM	3445	CA	ILE	A	447	0.192	42.028	20.102	1.00	27.47
C										
ATOM	3446	C	ILE	A	447	1.418	41.639	20.929	1.00	26.41
C										
ATOM	3447	O	ILE	A	447	1.287	41.018	21.985	1.00	25.38
O										
ATOM	3448	CB	ILE	A	447	-0.174	40.854	19.157	1.00	30.04
C										
ATOM	3449	CGl	ILE	A	447	-0.556	39.621	19.978	1.00	32.33
C										
ATOM	3450	CG2	ILE	A	447	0.999	40.523	18.247	1.00	30.71
C										
ATOM	3451	CDl	ILE	A	447	-1.739	39.836	20.905	1.00	36.08
C										
ATOM	3452	N	TYR	A	448	2.605	42.017	20.461	1.00	24.45
N										
ATOM	3453	CA	TYR	A	448	3.828	41.686	21.183	1.00	24.50
C										
ATOM	3454	C	TYR	A	448	3.975	42.393	22.527	1.00	24.11
C										
ATOM	3455	O	TYR	A	448	4.758	41.969	23.373	1.00	23.58
O										
ATOM	3456	CB	TYR	A	448	5.056	41.944	20.305	1.00	23.75
C										
ATOM	3457	CG	TYR	A	448	5.500	40.705	19.560	1.00	24.00
C										

ATOM	3458	CDl	TYR	A	448	5.473	40.648	18.165	1.00	23.63	C
ATOM	3459	CD2	TYR	A	448	5.921	39.573	20.260	1.00	23.06	C
ATOM	3460	CEl	TYR	A	448	5.855	39.486	17.486	1.00	24.33	C
ATOM	3461	CE2	TYR	A	448	6.302	38.414	19.594	1.00	24.13	C
ATOM	3462	CZ	TYR	A	448	6.267	38.373	18.216	1.00	23.96	C
ATOM	3463	OH	TYR	A	448	6.640	37.216	17.573	1.00	23.92	O
ATOM	3464	N	TYR	A	449	3.225	43.470	22.738	1.00	24.88	N
ATOM	3465	CA	TYR	A	449	3.297	44.158	24.019	1.00	24.50	C
ATOM	3466	C	TYR	A	449	2.792	43.186	25.079	1.00	24.66	C
ATOM	3467	O	TYR	A	449	3.364	43.062	26.157	1.00	24.32	O
ATOM	3468	CB	TYR	A	449	2.412	45.406	24.025	1.00	24.08	C
ATOM	3469	CG	TYR	A	449	2.245	46.001	25.403	1.00	25.01	C
ATOM	3470	CDl	TYR	A	449	3.155	46.934	25.901	1.00	25.79	C
ATOM	3471	CD2	TYR	A	449	1.188	45.609	26.221	1.00	25.10	C
ATOM	3472	CEl	TYR	A	449	3.011	47.463	27.182	1.00	26.72	C
ATOM	3473	CE2	TYR	A	449	1.036	46.125	27.496	1.00	25.61	C
ATOM	3474	CZ	TYR	A	449	1.945	47.052	27.972	1.00	28.42	C
ATOM	3475	OH	TYR	A	449	1.772	47.576	29.230	1.00	29.96	O
ATOM	3476	N	TYR	A	450	1.705	42.497	24.755	1.00	24.18	N
ATOM	3477	CA	TYR	A	450	1.105	41.537	25.670	1.00	26.75	C
ATOM	3478	C	TYR	A	450	1.942	40.268	25.770	1.00	25.66	C
ATOM	3479	O	TYR	A	450	1.994	39.633	26.821	1.00	26.24	O
ATOM	3480	CB	TYR	A	450	-0.314	41.222	25.203	1.00	28.52	C
ATOM	3481	CG	TYR	A	450	-1.170	42.465	25.187	1.00	32.79	C
ATOM	3482	CDl	TYR	A	450	-1.714	42.971	26.366	1.00	33.74	C
ATOM	3483	CD2	TYR	A	450	-1.357	43.190	24.010	1.00	33.71	C
ATOM	3484	CEl	TYR	A	450	-2.417	44.170	26.380	1.00	35.95	C
ATOM	3485	CE2	TYR	A	450	-2.059	44.,395	24.012	1.00	36.71	C
ATOM	3486	CZ	TYR	A	450	-2.583	44..878	25.202	1.00	37.07	C
ATOM	3487	OH	TYR	A	450	-3.256	46..080	25.220	1.00	39.96	O

ATOM	3488	N	VAL	A	451	2.599	39.902	24.678	1.00	25.17
N										
ATOM	3489	CA	VAL	A	451	3.444	38.715	24.698	1.00	24.58
C										
ATOM	3490	C	VAL	A	451	4.608	38.993	25.644	1.00	24.42
C										
ATOM	3491	O	VAL	A	451	4.892	38.201	26.540	1.00	25.40
O										
ATOM	3492	CB	VAL	A	451	3.979	38.376	23.280	1.00	24.16
C										
ATOM	3493	CGl	VAL	A	451	5.025	37.256	23.355	1.00	25.01
C										
ATOM	3494	CG2	VAL	A	451	2.827	37.937	22.390	1.00	24.26
C										
ATOM	3495	N	MET	A	452	5.261	40.137	25.462	1.00	26.08
N										
ATOM	3496	CA	MET	A	452	6.399	40.507	26.298	1.00	26.48
C										
ATOM	3497	C	MET	A	452	6.058	40.673	27.772	1.00	27.39
C										
ATOM	3498	O	MET	A	452	6.790	40.212	28.640	1.00	26.56
O										
ATOM	3499	CB	MET	A	452	7.023	41.813	25.813	1.00	27.20
C										
ATOM	3500	CG	MET	A	452	7.565	41.788	24.398	1.00	27.88
C										
ATOM	3501	SD	MET	A	452	8.195	43.414	23.932	1.00	28.35
S										
ATOM	3502	CE	MET	A	452	9.084	43.003	22.423	1.00	28.71
C										
ATOM	3503	N	ARG	A	453	4.949	41.344	28.057	1.00	26.93
N										
ATOM	3504	CA	ARG	A	453	4.567	41.586	29.438	1.00	27.79
C										
ATOM	3505	C	ARG	A	453	4.005	40.386	30.191	1.00	27.04
C										
ATOM	3506	O	ARG	A	453	4.263	40.230	31.382	1.00	29.14
O										
ATOM	3507	CB	ARG	A	453	3.563	42.743	29.497	1.00	28.06
C										
ATOM	3508	CG	ARG	A	453	3.212	43.185	30.907	1.00	29.81
C										
ATOM	3509	CD	ARG	A	453	2.398	44.471	30.900	1.00	31.83
C										
ATOM	3510	NE	ARG	A	453	2.097	44.916	32.257	1.00	33.76
N										
ATOM	3511	CZ	ARG	A	453	1.490	46.061	32.555	1.00	35.42
C										
ATOM	3512	NHl	ARG	A	453	1.115	46.888	31.587	1.00	35.22
N										
ATOM	3513	NH2	ARG	A	453	1.256	46.376	33.822	1.00	36.80
N										
ATOM	3514	N	TYR	A	454	3.252	39.533	29.504	1.00	28.17
N										
ATOM	3515	CA	TYR	A	454	2.628	38.389	30.163	1.00	30.28
C										
ATOM	3516	C	TYR	A	454	3.063	36.993	29.716	1.00	30.92
C										
ATOM	3517	O	TYR	A	454	3.446	36.160	30.542	1.00	33.11
O										

ATOM	3518	CB	TYR	A	454	1.108	38.496	30.013	1.00	32.40
C										
ATOM	3519	CG	TYR	A	454	0.551	39.838	30.428	1.00	34.06
C										
ATOM	3520	CDl	TYR	A	454	0.574	40.242	31.761	1.00	36.02
C										
ATOM	3521	CD2	TYR	A	454	0.019	40.714	29.482	1.00	35.82
C										
ATOM	3522	CEl	TYR	A	454	0.082	41.490	32.143	1.00	37.11
C										
ATOM	3523	CE2	TYR	A	454	-0.474	41.964	29.854	1.00	37.42
C										
ATOM	3524	CZ	TYR	A	454	-0.438	42.343	31.186	1.00	37.20
C										
ATOM	3525	OH	TYR	A	454	-0.915	43.579	31.556	1.00	39.77
O										
ATOM	3526	N	ILE	A	455	3.000	36.742	28.413	1.00	30.19
N										
ATOM	3527	CA	ILE	A	455	3.332	35.434	27.857	1.00	30.30
C										
ATOM	3528	C	ILE	A	455	4.777	34.968	28.031	1.00	29.70
C										
ATOM	3529	O	ILE	A	455	5.026	33.925	28.639	1.00	29.59
O										
ATOM	3530	CB	ILE	A	455	2.973	35.376	26.356	1.00	30.83
C										
ATOM	3531	CGl	ILE	A	455	1.525	35.833	26.150	1.00	32.34
C										
ATOM	3532	CG2	ILE	A	455	3.157	33.960	25.825	1.00	30.15
C										
ATOM	3533	CDl	ILE	A	455	0.499	35.002	26.891	1.00	34.18
C										
ATOM	3534	N	THR	A	456	5.726	35.731	27.501	1.00	26.91
N										
ATOM	3535	CA	THR	A	456	7.132	35.352	27.597	1.00	28.92
C										
ATOM	3536	C	THR	A	456	7.597	35.032	29.023	1.00	28.62
C										
ATOM	3537	O	THR	A	456	8.184	33.975	29.268	1.00	27.89
O										
ATOM	3538	CB	THR	A	456	8.042	36.445	26.999	1.00	27.96
C										
ATOM	3539	OGl	THR	A	456	7.585	36.776	25.679	1.00	28.31
O										
ATOM	3540	CG2	THR	A	456	9.484	35.948	26.911	1.00	28.64
C										
ATOM	3541	N	PRO	A	457	7.336	35.931	29.988	1.00	29.45
N										
ATOM	3542	CA	PRO	A	457	7.775	35.639	31.359	1.00	29.67
C										
ATOM	3543	C	PRO	A	457	7.115	34.400	31.969	1.00	31.34
C										
ATOM	3544	O	PRO	A	457	7.771	33.612	32.649	1.00	30.72
O										
ATOM	3545	CB	PRO	A	457	7.435	36.925	32.113	1.00	30.40
C										
ATOM	3546	CG	PRO	A	457	6.268	37.472	31.346	1.00	30.36
C										
ATOM	3547	CD	PRO	A	457	6.675	37.245	29.914	1.00	27.60
C										

ATOM	3548	N	ALA	A	458	5.820	34.228	31.725	1.00	32.37
N										
ATOM	3549	CA	ALA	A	458	5.107	33.071	32.257	1.00	33.66
C										
ATOM	3550	C	ALA	A	458	5.686	31.808	31.629	1.00	34.31
C										
ATOM	3551	O	ALA	A	458	5.900	30.800	32.304	1.00	36.25
O										
ATOM	3552	CB	ALA	A	458	3.620	33.182	31.945	1.00	33.21
C										
ATOM	3553	N	PHE	A	459	5.943	31.883	30.328	1.00	34.54
N										
ATOM	3554	CA	PHE	A	459	6.502	30.775	29.563	1.00	34.52
C										
ATOM	3555	C	PHE	A	459	7.846	30.347	30.151	1.00	33.29
C										
ATOM	3556	O	PHE	A	459	8.055	29.170	30.460	1.00	34.62
O										
ATOM	3557	CB	PHE	A	459	6.686	31.210	28.107	1.00	37.43
C										
ATOM	3558	CG	PHE	A	459	6.958	30.081	27.155	1.00	40.95
C										
ATOM	3559	CDl	PHE	A	459	5.980	29.131	26.882	1.00	43.20
C										
ATOM	3560	CD2	PHE	A	459	8.185	29.984	26.509	1.00	41.77
C										
ATOM	3561	CEl	PHE	A	459	6.219	28.098	25.972	1.00	44.95
C										
ATOM	3562	CE2	PHE	A	459	8.436	28.958	25.599	1.00	43.19
C										
ATOM	3563	CZ	PHE	A	459	7.452	28.014	25.329	1.00	43.83
C										
ATOM	3564	N	LEU	A	460	8.750	31.309	30.309	1.00	31.11
N										
ATOM	3565	CA	LEU	A	460	10.076	31.038	30.852	1.00	29.66
C										
ATOM	3566	C	LEU	A	460	10.034	30.588	32.311	1.00	31.18
C										
ATOM	3567	O	LEU	A	460	10.781	29.694	32.709	1.00	29.77
O										
ATOM	3568	CB	LEU	A	460	10.965	32.276	30.719	1.00	29.16
C										
ATOM	3569	CG	LEU	A	460	11.234	32.761	29.290	1.00	28.98
C										
ATOM	3570	CDl	LEU	A	460	12.190	33.943	29.332	1.00	29.05
C										
ATOM	3571	CD2	LEU	A	460	11.822	31.625	28.455	1.00	27.28
C										
ATOM	3572	N	ALA	A	461	9.164	31.205	33.106	1.00	31.32
N										
ATOM	3573	CA	ALA	A	461	9.056	30.843	34.514	1.00	32.54
C										
ATOM	3574	C	ALA	A	461	8.677	29.371	34.654	1.00	33.58
C										
ATOM	3575	O	ALA	A	461	9.285	28.637	35.432	1.00	32.44
O										
ATOM	3576	CB	ALA	A	461	8.023	31.723	35.209	1.00	30.88
C										
ATOM	3577	N	VAL	A	462	7.673	28.943	33.895	1.00	34.62
N										

ATOM	3578	CA	VAL	A	462	7.229	27.555	33.941	1.00	37.33
C										
ATOM	3579	C	VAL	A	462	8.367	26.631	33.517	1.00	38.33
C										
ATOM	3580	O	VAL	A	462	8.621	25.608	34.152	1.00	38.47
O										
ATOM	3581	CB	VAL	A	462	6.027	27.319	33.002	1.00	38.08
C										
ATOM	3582	CGl	VAL	A	462	5.625	25.854	33.036	1.00	39.81
C										
ATOM	3583	CG2	VAL	A	462	4.859	28.198	33.418	1.00	38.67
C										
ATOM	3584	N	LEU	A	463	9.051	27.008	32.442	1.00	38.90
N										
ATOM	3585	CA	LEU	A	463	10.165	26.229	31.918	1.00	40.27
C										
ATOM	3586	C	LEU	A	463	11.239	26.024	32.981	1.00	40.13
C										
ATOM	3587	O	LEU	A	463	11.733	24.912	33.172	1.00	40.48
O										
ATOM	3588	CB	LEU	A	463	10.774	26.943	30.708	1.00	42.75
C										
ATOM	3589	CG	LEU	A	463	11.872	26.211	29.934	1.00	44.98
C										
ATOM	3590	CDl	LEU	A	463	11.267	25.030	29.189	1.00	46.10
C										
ATOM	3591	CD2	LEU	A	463	12.529	27.171	28.955	1.00	45.71
C										
ATOM	3592	N	LEU	A	464	11.600	27.102	33.669	1.00	38.92
N										
ATOM	3593	CA	LEU	A	464	12.619	27.039	34.707	1.00	39.22
C										
ATOM	3594	C	LEU	A	464	12.205	26.172	35.893	1.00	39.92
C										
ATOM	3595	O	LEU	A	464	13.026	25.445	36.453	1.00	39.34
O										
ATOM	3596	CB	LEU	A	464	12.964	28.449	35.189	1.00	38.95
C										
ATOM	3597	CG	LEU	A	464	13.761	29.297	34.193	1.00	37.92
C										
ATOM	3598	CDl	LEU	A	464	13.920	30.715	34.718	1.00	39.31
C										
ATOM	3599	CD2	LEU	A	464	15.124	28.654	33.966	1.00	38.49
C										
ATOM	3600	N	VAL	A	465	10.934	26.250	36.277	1.00	39.96
N										
ATOM	3601	CA	VAL	A	465	10.437	25.460	37.398	1.00	42.10
C										
ATOM	3602	C	VAL	A	465	10.511	23.973	37.072	1.00	43.74
C										
ATOM	3603	O	VAL	A	465	10.966	23.171	37.887	1.00	43.56
O										
ATOM	3604	CB	VAL	A	465	8.975	25.822	37.741	1.00	41.37
C										
ATOM	3605	CGl	VAL	A	465	8.453	24.898	38.836	1.00	42.13
C										
ATOM	3606	CG2	VAL	A	465	8.894	27.269	38.195	1.00	40.08
C										
ATOM	3607	N	VAL	A	466	10.060	23.611	35.876	1.00	45.94
N										

ATOM	3608	CA	VAL	A	466	10.080	22.221	35.445	1.00	48.24
C										
ATOM	3609	C	VAL	A	466	11.516	21.723	35.336	1.00	49.90
C										
ATOM	3610	O	VAL	A	466	11.795	20.545	35.563	1.00	50.09
O										
ATOM	3611	CB	VAL	A	466	9.384	22.055	34.077	1.00	48.40
C										
ATOM	3612	CGl	VAL	A	466	9.481	20.609	33.613	1.00	49.17
C										
ATOM	3613	CG2	VAL	A	466	7.929	22.481	34.185	1.00	47.82
C										
ATOM	3614	N	TRP	A	467	12.425	22.630	34.994	1.00	51.34
N										
ATOM	3615	CA	TRP	A	467	13.835	22.289	34.854	1.00	52.63
C										
ATOM	3616	C	TRP	A	467	14.431	21.918	36.207	1.00	53.16
C										
ATOM	3617	O	TRP	A	467	15.106	20.897	36.346	1.00	53.23
O										
ATOM	3618	CB	TRP	A	467	14.612	23.476	34.282	1.00	53.63
C										
ATOM	3619	CG	TRP	A	467	15.652	23.086	33.283	1.00	54.32
C										
ATOM	3620	CDl	TRP	A	467	16.501	22.020	33.351	1.00	54.75
C										
ATOM	3621	CD2	TRP	A	467	15.958	23.766	32.061	1.00	54.77
C										
ATOM	3622	NEl	TRP	A	467	17.316	21.991	32.246	1.00	54.54
N										
ATOM	3623	CE2	TRP	A	467	17.004	23.052	31.437	1.00	55.14
C										
ATOM	3624	CE3	TRP	A	467	15.449	24.910	31.432	1.00	55.15
C										
ATOM	3625	CZ2	TRP	A	467	17.552	23.444	30.213	1.00	55.95
C										
ATOM	3626	CZ3	TRP	A	467	15.995	25.302	30.213	1.00	56.30
C										
ATOM	3627	CH2	TRP	A	467	17.037	24.568	29.617	1.00	56.93
C										
ATOM	3628	N	ALA	A	468	14.175	22.759	37.202	1.00	53.27
N										
ATOM	3629	CA	ALA	A	468	14.691	22.541	38.545	1.00	54.30
C										
ATOM	3630	C	ALA	A	468	14.020	21.374	39.261	1.00	55.07
C										
ATOM	3631	O	ALA	A	468	14.519	20.898	40.280	1.00	55.19
O										
ATOM	3632	CB	ALA	A	468	14.535	23.811	39.370	1.00	54.31
C										
ATOM	3633	N	ARG	A	469	12.897	20.908	38.725	1.00	55.93
N										
ATOM	3634	CA	ARG	A	469	12.165	19.810	39.346	1.00	57.53
C										
ATOM	3635	C	ARG	A	469	12.369	18.440	38.712	1.00	58.86
C										
ATOM	3636	O	ARG	A	469	12.622	17.460	39.413	1.00	59.03
O										
ATOM	3637	CB	ARG	A	469	10.666	20.118	39.357	1.00	57.47
C										

ATOM	3638	CG	ARG	A	469	10.252	21.237	40.291	1.00	57.97
C										
ATOM	3639	CD	ARG	A	469	8.747	21.422	40.246	1.00	57.93
C										
ATOM	3640	NE	ARG	A	469	8.284	22.449	41.172	1.00	58.58
N										
ATOM	3641	CZ	ARG	A	469	7.014	22.822	41.292	1.00	58.82
C										
ATOM	3642	NHl	ARG	A	469	6.081	22.249	40.542	1.00	58.90
N										
ATOM	3643	NH2	ARG	A	469	6.676	23.765	42.160	1.00	59.09
N										
ATOM	3644	N	GLU	A	470	12.258	18.371	37.390	1.00	60.04
N										
ATOM	3645	CA	GLU	A	470	12.384	17.099	36.688	1.00	61.76
C										
ATOM	3646	C	GLU	A	470	13.675	16.879	35.906	1.00	62.15
C										
ATOM	3647	O	GLU	A	470	13.732	15.975	35.072	1.00	62.72
O										
ATOM	3648	CB	GLU	A	470	11.202	16.928	35.729	1.00	62.80
C										
ATOM	3649	CG	GLU	A	470	9.836	17.053	36.380	1.00	64.74
C										
ATOM	3650	CD	GLU	A	470	9.582	15.974	37.412	1.00	65.95
C										
ATOM	3651	OEl	GLU	A	470	9.636	14.780	37.049	1.00	66.80
O										
ATOM	3652	OE2	GLU	A	470	9.328	16.320	38.586	1.00	67.05
O										
ATOM	3653	N	TYR	A	471	14.712	17.673	36.161	1.00	62.17
N										
ATOM	3654	CA	TYR	A	471	15.952	17.496	35.410	1.00	62.20
C										
ATOM	3655	C	TYR	A	471	17.268	17.775	36.133	1.00	62.42
C										
ATOM	3656	O	TYR	A	471	18.169	16.937	36.119	1.00	62.65
O										
ATOM	3657	CB	TYR	A	471	15.890	18.326	34.122	1.00	62.57
C										
ATOM	3658	CG	TYR	A	471	14.844	17.835	33.145	1.00	63.09
C										
ATOM	3659	CDl	TYR	A	471	15.002	16.621	32.476	1.00	63.03
C										
ATOM	3660	CD2	TYR	A	471	13.677	18.564	32.916	1.00	63.18
C										
ATOM	3661	CEl	TYR	A	471	14.025	16.144	31.606	1.00	63.19
C										
ATOM	3662	CE2	TYR	A	471	12.693	18.095	32.049	1.00	63.34
C										
ATOM	3663	CZ	TYR	A	471	12.873	16.885	31.399	1.00	63.31
C										
ATOM	3664	OH	TYR	A	471	11.900	16.415	30.547	1.00	63.60
O										
ATOM	3665	N	ILE	A	472	17.391	18.938	36.764	1.00	62.42
N										
ATOM	3666	CA	ILE	A	472	18.633	19.277	37.453	1.00	62.82
C										
ATOM	3667	C	ILE	A	472	18.976	18.433	38.687	1.00	62.90
C										

ATOM	3668	O	ILE	A	472	20.149	18.301	39.040	1.00	62.49
O										
ATOM	3669	CB	ILE	A	472	18.670	20.771	37.859	1.00	63.47
C										
ATOM	3670	CGl	ILE	A	472	17.687	21.038	38.998	1.00	64.09
C										
ATOM	3671	CG2	ILE	A	472	18.334	21.640	36.656	1.00	63.29
C										
ATOM	3672	CDl	ILE	A	472	17.799	22.436	39.575	1.00	65.26
C										
ATOM	3673	N	PRO	A	473	17.968	17.855	39.365	1.00	62.71
N										
ATOM	3674	CA	PRO	A	473	18.313	17.049	40.542	1.00	62.67
C										
ATOM	3675	C	PRO	A	473	19.241	15.883	40.200	1.00	62.47
C										
ATOM	3676	O	PRO	A	473	20.087	15.495	41.006	1.00	62.13
O										
ATOM	3677	CB	PRO	A	473	16.948	16.589	41.055	1.00	62.82
C										
ATOM	3678	CG	PRO	A	473	16.118	16.539	39.809	1.00	63.16
C										
ATOM	3679	CD	PRO	A	473	16.516	17.818	39.120	1.00	62.89
C										
ATOM	3680	N	LYS	A	474	19.078	15.335	39.000	1.00	62.10
N										
ATOM	3681	CA	LYS	A	474	19.902	14.220	38.544	1.00	62.62
C										
ATOM	3682	C	LYS	A	474	21.319	14.713	38.264	1.00	62.29
C										
ATOM	3683	O	LYS	A	474	22.290	13.970	38.410	1.00	62.35
O										
ATOM	3684	CB	LYS	A	474	19.308	13.620	37.268	1.00	63.12
C										
ATOM	3685	CG	LYS	A	474	17.836	13.265	37.380	1.00	64.47
C										
ATOM	3686	CD	LYS	A	474	17.251	12.895	36.026	1.00	65.27
C										
ATOM	3687	CE	LYS	A	474	15.747	12.691	36.115	1.00	65.91
C										
ATOM	3688	NZ	LYS	A	474	15.137	12.434	34.779	1.00	66.78
N										
ATOM	3689	N	ILE	A	475	21.425	15.975	37.860	1.00	61.50
N										
ATOM	3690	CA	ILE	A	475	22.712	16.584	37.549	1.00	60.50
C										
ATOM	3691	C	ILE	A	475	23.470	16.946	38.825	1.00	59.92
C										
ATOM	3692	O	ILE	A	475	24.692	17.100	38.811	1.00	59.62
O										
ATOM	3693	CB	ILE	A	475	22.516	17.851	36.685	1.00	60.93
C										
ATOM	3694	CGl	ILE	A	475	21.799	17.474	35.385	1.00	61.13
C										
ATOM	3695	CG2	ILE	A	475	23.860	18.498	36.379	1.00	61.05
C										
ATOM	3696	CDl	ILE	A	475	21.510	18.644	34.473	1.00	61.54
C										
ATOM	3697	N	MET	A	476	22.741	17.073	39.929	1.00	58.88
N										

ATOM	3698	CA	MET	A	476	23.353	17.411	41.208	1.00	58.37
ATOM	3699	C	MET	A	476	23.699	16.172	42.029	1.00	58.08
ATOM	3700	O	MET	A	476	24.508	16.244	42.957	1.00	58.04
ATOM	3701	CB	MET	A	476	22.415	18.308	42.024	1.00	58.04
ATOM	3702	CG	MET	A	476	22.241	19.713	41.468	1.00	57.80
ATOM	3703	SD	MET	A	476	23.782	20.651	41.468	1.00	56.57
ATOM	3704	CE	MET	A	476	23.810	21.268	43.147	1.00	56.56
ATOM	3705	N	GLU	A	477	23.101	15.036	41.684	1.00	57.86
ATOM	3706	CA	GLU	A	477	23.349	13.807	42.430	1.00	57.37
ATOM	3707	C	GLU	A	477	23.879	12.630	41.608	1.00	56.51
ATOM	3708	O	GLU	A	477	24.389	11.664	42.176	1.00	56.82
ATOM	3709	CB	GLU	A	477	22.071	13.382	43.159	1.00	58.14
ATOM	3710	CG	GLU	A	477	22.266	12.232	44.132	1.00	59.74
ATOM	3711	CD	GLU	A	477	20.977	11.816	44.807	1.00	60.04
ATOM	3712	OEl	GLU	A	477	20.331	12.677	45.441	1.00	61.22
ATOM	3713	OE2	GLU	A	477	20.611	10.626	44.706	1.00	59.48
ATOM	3714	N	GLU	A	478	23.777	12.706	40.284	1.00	54.87
ATOM	3715	CA	GLU	A	478	24.248	11.612	39.436	1.00	53.31
ATOM	3716	C	GLU	A	478	25.472	11.925	38.578	1.00	51.07
ATOM	3717	O	GLU	A	478	25.655	11.323	37.518	1.00	51.43
ATOM	3718	CB	GLU	A	478	23.119	11.120	38.522	1.00	55.04
ATOM	3719	CG	GLU	A	478	22.039	10.297	39.215	1.00	57.61
ATOM	3720	CD	GLU	A	478	22.574	9.011	39.827	1.00	58.89
ATOM	3721	OEl	GLU	A	478	23.274	8.253	39.121	1.00	59.83
ATOM	3722	OE2	GLU	A	478	22.286	8.755	41.015	1.00	59.47
ATOM	3723	N	THR	A	479	26.313	12.855	39.021	1.00	47.49
ATOM	3724	CA	THR	A	479	27.509	13.192	38.252	1.00	43.82
ATOM	3725	C	THR	A	479	28.788	12.861	39.016	1.00	40.17
ATOM	3726	O	THR	A	479	28.771	12.710	40.237	1.00	40.06
ATOM	3727	CB	THR	A	479	27.533	14.693	37.861	1.00	44.02

ATOM 3728 OGl THR A 479 27.410 15.497 39.038 1.00 45.77
O
ATOM 3729 CG2 THR A 479 26.394 15.018 36.909 1.00 45.21
C
ATOM 3730 N HIS A 480 29.891 12.745 38.281 1.00 36.13
N
ATOM 3731 CA HIS A 480 31.200 12.439 38.855 1.00 32.02
C
ATOM 3732 C HIS A 480 31.640 13.597 39.757 1.00 28.82
C
ATOM 3733 O HIS A 480 31.301 14.750 39.494 1.00 26.40
O
ATOM 3734 CB HIS A 480 32.205 12.216 37.719 1.00 31.55
C
ATOM 3735 CG HIS A 480 33.530 11.682 38.169 1.00 34.03
C
ATOM 3736 NDl HIS A 480 34.653 12.472 38.280 1.00 31.74
N
ATOM 3737 CD2 HIS A 480 33.913 10.432 38.524 1.00 33.60
C
ATOM 3738 CEl HIS A 480 35.672 11.733 38.681 1.00 33.42
C
ATOM 3739 NE2 HIS A 480 35.250 10.492 38.836 1.00 35.53
N
ATOM 3740 N TRP A 481 32.404 13.296 40.805 1.00 25.50
N
ATOM 3741 CA TRP A 481 32.839 14.334 41.737 1.00 23.16
C
ATOM 3742 C TRP A 481 33.606 15.489 41.102 1.00 22.78
C
ATOM 3743 O TRP A 481 33.586 16.610 41.623 1.00 20.95
O
ATOM 3744 CB TRP A 481 33.689 13.739 42.870 1.00 25.27
C
ATOM 3745 CG TRP A 481 35.057 13.259 42.467 1.00 23.97
C
ATOM 3746 CDl TRP A 481 35.410 11.987 42.117 1.00 26.19
C
ATOM 3747 CD2 TRP A 481 36.255 14.045 42.384 1.00 23.24
C
ATOM 3748 NEl TRP A 481 36.753 11.931 41.824 1.00 25.28
N
ATOM 3749 CE2 TRP A 481 37.296 13.178 41.978 1.00 24.91
C
ATOM 3750 CE3 TRP A 481 36.550 15.395 42.611 1.00 22.96
C
ATOM 3751 CZ2 TRP A 481 38.613 13.619 41.794 1.00 23.86
C
ATOM 3752 CZ3 TRP A 481 37.865 15.835 42.428 1.00 22.27
C
ATOM 3753 CH2 TRP A 481 38.877 14.945 42.023 1.00 24.00
C
ATOM 3754 N THR A 482 34.276 15.231 39.984 1.00 18.88
N
ATOM 3755 CA THR A 482 35.047 16.289 39.338 1.00 17.60
C
ATOM 3756 C THR A 482 34.207 17.456 38.835 1.00 17.05
C
ATOM 3757 O THR A 482 34.757 18.504 38.502 1.00 17.21
O

ATOM	3758	CB	THR	A	482	35.893	15.752	38.170	1.00	18.37
ATOM	3759	OGl	THR	A	482	35.059	15.003	37.274	1.00	21.73
ATOM	3760	CG2	THR	A	482	37.015	14.868	38.695	1.00	18.08
ATOM	3761	N	VAL	A	483	32.889	17.296	38.768	1.00	16.94
ATOM	3762	CA	VAL	A	483	32.062	18.416	38.317	1.00	17.48
ATOM	3763	C	VAL	A	483	32.221	19.563	39.315	1.00	16.65
ATOM	3764	O	VAL	A	483	32.076	20.727	38.956	1.00	17.59
ATOM	3765	CB	VAL	A	483	30.551	18.060	38.217	1.00	19.65
ATOM	3766	CGl	VAL	A	483	30.342	16.929	37.225	1.00	22.97
ATOM	3767	CG2	VAL	A	483	30.006	17.702	39.586	1.00	20.38
ATOM	3768	N	TRP	A	484	32.538	19.238	40.565	1.00	16.81
ATOM	3769	CA	TRP	A	484	32.711	20.279	41.569	1.00	16.96
ATOM	3770	C	TRP	A	484	33.944	21.139	41.326	1.00	17.96
ATOM	3771	O	TRP	A	484	34.033	22.254	41.838	1.00	17.38
ATOM	3772	CB	TRP	A	484	32.744	19.679	42.978	1.00	19.02
ATOM	3773	CG	TRP	A	484	31.388	19.291	43.450	1.00	23.29
ATOM	3774	CDl	TRP	A	484	30.870	18.034	43.523	1.00	26.35
ATOM	3775	CD2	TRP	A	484	30.345	20.182	43.864	1.00	25.76
ATOM	3776	NEl	TRP	A	484	29.564	18.084	43.960	1.00	28.37
ATOM	3777	CE2	TRP	A	484	29.219	19.391	44.176	1.00	27.72
ATOM	3778	CE3	TRP	A	484	30.253	21.572	43.999	1.00	27.06
ATOM	3779	CZ2	TRP	A	484	28.012	19.945	44.618	1.00	30.40
ATOM	3780	CZ3	TRP	A	484	29.049	22.125	44.440	1.00	30.82
ATOM	3781	CH2	TRP	A	484	27.948	21.309	44.743	1.00	29.75
ATOM	3782	N	ILE	A	485	34.898	20.631	40.549	1.00	16.25
ATOM	3783	CA	ILE	A	485	36.088	21.418	40.241	1.00	15.86
ATOM	3784	C	ILE	A	485	35.639	22.569	39.341	1.00	16.47
ATOM	3785	O	ILE	A	485	36.019	23.722	39.529	1.00	15.60
ATOM	3786	CB	ILE	A	485	37.140	20.590	39.475	1.00	17.27
ATOM	3787	CGl	ILE	A	485	37.595	19.401	40.327	1.00	19.62

ATOM 3788 CG2 ILE A 485 38.326 21.481 39.095 1.00 17.07 C
ATOM 3789 GDI ILE A 485 38.456 18.401 39.557 1.00 21.23 C
ATOM 3790 N THR A 486 34.823 22.245 38.349 1.00 15.58 N
ATOM 3791 CA THR A 486 34.339 23.266 37.438 1.00 15.51 C
ATOM 3792 C THR A 486 33.383 24.223 38.140 1.00 15.63 C
ATOM 3793 O THR A 486 33.463 25.435 37.954 1.00 15.52 O
ATOM 3794 CB THR A 486 33.651 22.616 36.234 1.00 17.73 C
ATOM 3795 OGl THR A 486 34.607 21.790 35.558 1.00 18.15 O
ATOM 3796 CG2 THR A 486 33.131 23.674 35.268 1.00 18.27 C
ATOM 3797 N ARG A 487 32.479 23.678 38.946 1.00 14.79 N
ATOM 3798 CA ARG A 487 31.525 24.513 39.672 1.00 14.77 C
ATOM 3799 C ARG A 487 32.266 25.501 40.566 1.00 16.15 C
ATOM 3800 O ARG A 487 31.955 26.691 40.597 1.00 16.15 O
ATOM 3801 CB ARG A 487 30.603 23.637 40.510 1.00 13.98 C
ATOM 3802 CG ARG A 487 29.675 22.793 39.658 1.00 16.60 C
ATOM 3803 CD ARG A 487 28.861 21.832 40.506 1.00 18.99 C
ATOM 3804 NE ARG A 487 28.009 20.985 39.676 1.00 20.93 N
ATOM 3805 CZ ARG A 487 27.263 19.992 40.147 1.00 24.45 C
ATOM 3806 NHl ARG A 487 27.256 19.723 41.446 1.00 25.04 N
ATOM 3807 NH2 ARG A 487 26.543 19.250 39.317 1.00 25.44 N
ATOM 3808 N PHE A 488 33.253 24.997 41.295 1.00 15.02 N
ATOM 3809 CA PHE A 488 34.059 25.831 42.177 1.00 16.72 C
ATOM 3810 C PHE A 488 34.714 26.951 41.378 1.00 16.80 C
ATOM 3811 O PHE A 488 34.643 28.122 41.752 1.00 16.33 O
ATOM 3812 CB PHE A 488 35.144 24.979 42.839 1.00 17.12 C
ATOM 3813 CG PHE A 488 36.135 25.767 43.647 1.00 18.78 C
ATOM 3814 CDl PHE A 488 35.770 26.328 44.866 1.00 20.34 C
ATOM 3815 CD2 PHE A 488 37.443 25.931 43.194 1.00 20.01 C
ATOM 3816 CEl PHE A 488 36.696 27.042 45.628 1.00 22.06 C
ATOM 3817 CE2 PHE A 488 38.376 26.645 43.950 1.00 22.15 C

ATOM	3818	CZ	PHE	A	488	37.998	27.198	45.168	1.00	21.32
C										
ATOM	3819	N	TYR	A	489	35.347	26.594	40.266	1.00	15.24
N										
ATOM	3820	CA	TYR	A	489	36.024	27.606	39.475	1.00	16.02
C										
ATOM	3821	C	TYR	A	489	35.092	28.670	38.912	1.00	15.21
C										
ATOM	3822	O	TYR	A	489	35.393	29.861	39.009	1.00	16.59
O										
ATOM	3823	CB	TYR	A	489	36.808	26.981	38.327	1.00	16.65
C										
ATOM	3824	CG	TYR	A	489	37.641	28.008	37.600	1.00	19.32
C										
ATOM	3825	CDl	TYR	A	489	38.750	28.582	38.214	1.00	21.71
C										
ATOM	3826	CD2	TYR	A	489	37.286	28.453	36.328	1.00	20.04
C										
ATOM	3827	CEl	TYR	A	489	39.487	29.579	37.588	1.00	22.66
C										
ATOM	3828	CE2	TYR	A	489	38.021	29.456	35.687	1.00	22.49
C										
ATOM	3829	CZ	TYR	A	489	39.115	30.013	36.325	1.00	22.29
C										
ATOM	3830	OH	TYR	A	489	39.825	31.017	35.715	1.00	25.04
O										
ATOM	3831	N	ILE	A	490	33.975	28.265	38.314	1.00	15.39
N										
ATOM	3832	CA	ILE	A	490	33.081	29.272	37.752	1.00	15.08
C										
ATOM	3833	C	ILE	A	490	32.368	30.088	38.824	1.00	15.36
C										
ATOM	3834	O	ILE	A	490	31.980	31.221	38.575	1.00	17.15
O										
ATOM	3835	CB	ILE	A	490	32.074	28.671	36.722	1.00	16.24
C										
ATOM	3836	CGl	ILE	A	490	31.113	27.686	37.382	1.00	17.20
C										
ATOM	3837	CG2	ILE	A	490	32.863	28.005	35.587	1.00	17.86
C										
ATOM	3838	CDl	ILE	A	490	30.090	27.097	36.407	1.00	19.93
C										
ATOM	3839	N	ILE	A	491	32.205	29.531	40.022	1.00	16.61
N										
ATOM	3840	CA	ILE	A	491	31.597	30.308	41.095	1.00	17.47
C										
ATOM	3841	C	ILE	A	491	32.645	31.364	41.466	1.00	16.89
C										
ATOM	3842	O	ILE	A	491	32.312	32.508	41.771	1.00	18.68
O										
ATOM	3843	CB	ILE	A	491	31.264	29.426	42.319	1.00	18.00
C										
ATOM	3844	CGl	ILE	A	491	30.069	28.531	41.985	1.00	18.33
C										
ATOM	3845	CG2	ILE	A	491	30.938	30.301	43.532	1.00	20.21
C										
ATOM	3846	CDl	ILE	A	491	29.765	27.485	43.041	1.00	21.30
C										
ATOM	3847	N	GLY	A	492	33.918	30.968	41.426	1.00	16.85
N										

ATOM	3848	CA	GLY	A	492	34.998	31.897	41.720	1.00	15.18
C										
ATOM	3849	C	GLY	A	492	34.985	33.028	40.702	1.00	18.89
C										
ATOM	3850	O	GLY	A	492	35.181	34.192	41.050	1.00	17.11
O										
ATOM	3851	N	LEU	A	493	34.755	32.690	39.436	1.00	17.57
N										
ATOM	3852	CA	LEU	A	493	34.698	33.710	38.396	1.00	17.64
C										
ATOM	3853	C	LEU	A	493	33.563	34.689	38.683	1.00	16.77
C										
ATOM	3854	O	LEU	A	493	33.692	35.885	38.434	1.00	17.75
O										
ATOM	3855	CB	LEU	A	493	34.491	33.072	37.020	1.00	19.68
C										
ATOM	3856	CG	LEU	A	493	35.681	32.349	36.389	1.00	23.58
C										
ATOM	3857	CDl	LEU	A	493	35.234	31.700	35.082	1.00	24.26
C										
ATOM	3858	CD2	LEU	A	493	36.820	33.338	36.136	1.00	25.13
C										
ATOM	3859	N	PHE	A	494	32.450	34.191	39.211	1.00	16.16
N										
ATOM	3860	CA	PHE	A	494	31.331	35.079	39.516	1.00	16.75
C										
ATOM	3861	C	PHE	A	494	31.719	36.045	40.633	1.00	18.52
C										
ATOM	3862	O	PHE	A	494	31.382	37.227	40.585	1.00	18.41
O										
ATOM	3863	CB	PHE	A	494	30.095	34.283	39.943	1.00	17.77
C										
ATOM	3864	CG	PHE	A	494	28.861	35.125	40.072	1.00	19.67
C										
ATOM	3865	CDl	PHE	A	494	28.008	35.303	38.990	1.00	19.25
C										
ATOM	3866	CD2	PHE	A	494	28.581	35.788	41.263	1.00	21.05
C										
ATOM	3867	CEl	PHE	A	494	26.890	36.133	39.089	1.00	20.98
C										
ATOM	3868	CE2	PHE	A	494	27.467	36.620	41.370	1.00	21.92
C										
ATOM	3869	CZ	PHE	A	494	26.624	36.791	40.280	1.00	19.85
C										
ATOM	3870	N	LEU	A	495	32.429	35.536	41.637	1.00	17.45
N										
ATOM	3871	CA	LEU	A	495	32.863	36.361	42.765	1.00	18.84
C										
ATOM	3872	C	LEU	A	495	33.879	37.400	42.304	1.00	17.53
C										
ATOM	3873	O	LEU	A	495	33.879	38.537	42.779	1.00	17.71
O										
ATOM	3874	CB	LEU	A	495	33.459	35.476	43.866	1.00	20.63
C										
ATOM	3875	CG	LEU	A	495	32.428	34.516	44.471	1.00	25.65
C										
ATOM	3876	CDl	LEU	A	495	33.103	33.590	45.465	1.00	28.58
C										
ATOM	3877	CD2	LEU	A	495	31.317	35.313	45.151	1.00	29.30
C										

ATOM	3878	N	PHE	A	496	34.740	37.006	41.373	1.00	16.19
ATOM	3879	CA	PHE	A	496	35.744	37.908	40.814	1.00	17.42
ATOM	3880	C	PHE	A	496	35.044	39.067	40.095	1.00	17.42
ATOM	3881	O	PHE	A	496	35.383	40.233	40.290	1.00	16.68
ATOM	3882	CB	PHE	A	496	36.626	37.135	39.826	1.00	20.01
ATOM	3883	CG	PHE	A	496	37.414	38.008	38.884	1.00	21.70
ATOM	3884	CDl	PHE	A	496	38.428	38.833	39.354	1.00	24.24
ATOM	3885	CD2	PHE	A	496	37.147	37.986	37.517	1.00	24.14
ATOM	3886	CEl	PHE	A	496	39.171	39.624	38.473	1.00	24.21
ATOM	3887	CE2	PHE	A	496	37.883	38.773	36.630	1.00	26.26
ATOM	3888	CZ	PHE	A	496	38.896	39.591	37.110	1.00	25.76
ATOM	3889	N	LEU	A	497	34.065	38.735	39.260	1.00	17.81
ATOM	3890	CA	LEU	A	497	33.333	39.756	38.521	1.00	16.73
ATOM	3891	C	LEU	A	497	32.545	40.658	39.462	1.00	17.43
ATOM	3892	O	LEU	A	497	32.426	41.858	39.221	1.00	18.23
ATOM	3893	CB	LEU	A	497	32.406	39.094	37.502	1.00	16.31
ATOM	3894	CG	LEU	A	497	33.183	38.366	36.397	1.00	18.13
ATOM	3895	CDl	LEU	A	497	32.232	37.497	35.584	1.00	17.55
ATOM	3896	CD2	LEU	A	497	33.879	39.378	35.497	1.00	19.41
ATOM	3897	N	THR	A	498	32.000	40.084	40.529	1.00	18.91
ATOM	3898	CA	THR	A	498	31.254	40.884	41.493	1.00	19.09
ATOM	3899	C	THR	A	498	32.228	41.879	42.127	1.00	18.62
ATOM	3900	O	THR	A	498	31.887	43.043	42.338	1.00	19.10
ATOM	3901	CB	THR	A	498	30.621	39.992	42.576	1.00	19.75
ATOM	3902	OGl	THR	A	498	29.701	39.082	41.954	1.00	21.45
ATOM	3903	CG2	THR	A	498	29.870	40.834	43.605	1.00	22.41
ATOM	3904	N	PHE	A	499	33.444	41.423	42.422	1.00	16.73
ATOM	3905	CA	PHE	A	499	34.450	42.300	43.015	1.00	17.88
ATOM	3906	C	PHE	A	499	34.776	43.445	42.056	1.00	18.38
ATOM	3907	O	PHE	A	499	34.942	44.586	42.481	1.00	18.46

ATOM	3908	CB	PHE	A	499	35.734	41.527	43.351	1.00	18.83
C										
ATOM	3909	CG	PHE	A	499	36.782	42.370	44.025	1.00	20.14
C										
ATOM	3910	CDl	PHE	A	499	36.494	43.028	45.218	1.00	20.08
C										
ATOM	3911	CD2	PHE	A	499	38.043	42.527	43.460	1.00	21.69
C										
ATOM	3912	CEl	PHE	A	499	37.449	43.835	45.844	1.00	21.32
C										
ATOM	3913	CE2	PHE	A	499	39.007	43.330	44.076	1.00	25.29
C										
ATOM	3914	CZ	PHE	A	499	38.708	43.985	45.269	1.00	22.41
C										
ATOM	3915	N	LEU	A	500	34.863	43.145	40.761	1.00	17.87
N										
ATOM	3916	CA	LEU	A	500	35.152	44.183	39.773	1.00	17.37
C										
ATOM	3917	C	LEU	A	500	34.028	45.212	39.690	1.00	17.91
C										
ATOM	3918	O	LEU	A	500	34.283	46.397	39.483	1.00	18.44
O										
ATOM	3919	CB	LEU	A	500	35.383	43.572	38.385	1.00	18.57
C										
ATOM	3920	CG	LEU	A	500	36.630	42.698	38.236	1.00	18.28
C										
ATOM	3921	CDl	LEU	A	500	36.857	42.401	36.754	1.00	21.57
C										
ATOM	3922	CD2	LEU	A	500	37.844	43.413	38.824	1.00	19.39
C										
ATOM	3923	N	VAL	A	501	32.787	44.757	39.842	1.00	18.13
N										
ATOM	3924	CA	VAL	A	501	31.639	45.664	39.805	1.00	19.09
C										
ATOM	3925	C	VAL	A	501	31.710	46.554	41.045	1.00	19.42
C										
ATOM	392 6	O	VAL	A	501	31.384	47.741	40.997	1.00	20.87
O										
ATOM	3927	CB	VAL	A	501	30.306	44.874	39.767	1.00	20.18
C										
ATOM	3928	CGl	VAL	A	501	29.120	45.802	39.994	1.00	21.34
C										
ATOM	3929	CG2	VAL	A	501	30.166	44.192	38.410	1.00	21.18
C										
ATOM	3930	N	PHE	A	502	32.155	45.969	42.153	1.00	19.36
N										
ATOM	3931	CA	PHE	A	502	32.323	46.699	43.404	1.00	20.09
C										
ATOM	3932	C	PHE	A	502	33.388	47.787	43.195	1.00	20.03
C										
ATOM	3933	O	PHE	A	502	33.206	48.941	43.596	1.00	20.33
O										
ATOM	3934	CB	PHE	A	502	32.770	45.736	44.508	1.00	21.51
C										
ATOM	3935	CG	PHE	A	502	33.197	46.419	45.772	1.00	22.58
C										
ATOM	3936	CDl	PHE	A	502	32.257	46.809	46.719	1.00	23.81
C										
ATOM	3937	CD2	PHE	A	502	34.538	46.698	46.002	1.00	24.48
C										

ATOM 3938 CEl PHE A 502 32.649 47.469 47.882 1.00 25.13 C
ATOM 3939 CE2 PHE A 502 34.942 47.362 47.164 1.00 25.71 C
ATOM 3940 CZ PHE A 502 33.993 47.745 48.103 1.00 24.58 C
ATOM 3941 N LEU A 503 34.502 47.420 42.565 1.00 19.61 N
ATOM 3942 CA LEU A 503 35.571 48.384 42.311 1.00 20.23 C
ATOM 3943 C LEU A 503 35.102 49.480 41.360 1.00 21.15 C
ATOM 3944 O LEU A 503 35.477 50.646 41.505 1.00 22.63 O
ATOM 3945 CB LEU A 503 36.803 47.689 41.717 1.00 20.87 C
ATOM 3946 CG LEU A 503 37.557 46.730 42.638 1.00 22.07 C
ATOM 3947 CDl LEU A 503 38.772 46.162 41.901 1.00 23.29 C
ATOM 3948 CD2 LEU A 503 37.994 47.471 43.906 1.00 23.41 C
ATOM 3949 N ALA A 504 34.284 49.102 40.383 1.00 19.57 N
ATOM 3950 CA ALA A 504 33.765 50.064 39.422 1.00 21.78 C
ATOM 3951 C ALA A 504 32.895 51.107 40.126 1.00 23.51 C
ATOM 3952 O ALA A 504 32.971 52.295 39.813 1.00 24.23 O
ATOM 3953 CB ALA A 504 32.956 49.350 38.346 1.00 20.59 C
ATOM 3954 N GLU A 505 32.067 50.666 41.070 1.00 25.25 N
ATOM 3955 CA GLU A 505 31.205 51.599 41.788 1.00 30.00 C
ATOM 3956 C GLU A 505 32.010 52.486 42.728 1.00 31.36 C
ATOM 3957 O GLU A 505 31.621 53.623 43.003 1.00 31.93 O
ATOM 3958 CB GLU A 505 30.102 50.856 42.559 1.00 33.54 C
ATOM 3959 CG GLU A 505 30.544 49.627 43.323 1.00 41.41 C
ATOM 3960 CD GLU A 505 29.400 48.972 44.085 1.00 44.26 C
ATOM 3961 OEl GLU A 505 28.324 48.762 43.484 1.00 48.06 O
ATOM 3962 OE2 GLU A 505 29.576 48.660 45.281 1.00 45.71 O
ATOM 3963 N ARG A 506 33.135 51.976 43.215 1.00 31.63 N
ATOM 3964 CA ARG A 506 33.979 52.768 44.098 1.00 34.43 C
ATOM 3965 C ARG A 506 34.722 53.817 43.274 1.00 35.36 C
ATOM 3966 O ARG A 506 34.932 54.938 43.734 1.00 34.97 O
ATOM 3967 CB ARG A 506 34.963 51.868 44.855 1.00 35.66 C

ATOM	3968	CG	ARG	A	506	34.283	51.002	45.912	1.00	39.17
C										
ATOM	3969	CD	ARG	A	506	33.575	51.882	46.933	1.00	43.34
C										
ATOM	3970	NE	ARG	A	506	32.612	51.156	47.757	1.00	46.57
N										
ATOM	3971	CZ	ARG	A	506	31.534	50.541	47.282	1.00	48.19
C										
ATOM	3972	NHl	ARG	A	506	31.276	50.556	45.983	1.00	48.60
N1										
ATOM	3973	NH2	ARG	A	506	30.703	49.921	48.109	1.00	49.91
N										
ATOM	3974	N	ARG	A	507	35.112	53.459	42.053	1.00	35.53
N										
ATOM	3975	CA	ARG	A	507	35.806	54.406	41.186	1.00	37.77
C1.										
ATOM	3976	C	ARG	A	507	34.843	55.526	40.808	1.00	39.17
e										
ATOM	3977	O	ARG	A	507	35.222	56.696	40.755	1.00	38.85
6·										
ATOM	3978	CB	ARG	A	507	36.299	53.726	39.908	1.00	38.73
e,										
ATOM	3979	CG	ARG	A	507	36.945	54.697	38.925	1.00	40.43
C										
ATOM	3980	CD	ARG	A	507	36.988	54.121	37.520	1.00	42.39
e-										
ATOM	3981	NE	ARG	A	507	35.669	53.657	37.098	1.00	46.30
N										
ATOM	3982	CZ	ARG	A	507	34.605	54.439	36.933	1.00	48.04
C										
ATOM	3983	NHl	ARG	A	507	34.688	55.746	37.147	1.00	48.43
N1										
ATOM	3984	NH2	ARG	A	507	33.446	53.906	36.569	1.00	48.27
N										
ATOM	3985	N	ARG	A	508	33.597	55.153	40.536	1.00	40.40
N										
ATOM	3986	CA	ARG	A	508	32.566	56.115	40.167	1.00	43.35
e										
ATOM	3987	C	ARG	A	508	32.353	57.103	41.310	1.00	44.83
C										
ATOM	3988	O	ARG	A	508	32.228	58.309	41.091	1.00	44.30
c.										
ATOM	3989	CB	ARG	A	508	31.254	55.390	39.865	1.00	44.46
C										
ATOM	3990	CG	ARG	A	508	30.091	56.317	39.572	1.00	47.64
C										
ATOM	3991	CD	ARG	A	508	28.765	55.596	39.724	1.00	50.01
C										
ATOM	3992	NE	ARG	A	508	27.639	56.525	39.708	1.00	53.36
N										
ATOM	3993	CZ	ARG	A	508	26.398	56.197	40.053	1.00	54.41
C										
ATOM	3994	NHl	ARG	A	508	26.122	54.959	40.442	1.00	55.20
N										
ATOM	3995	NH2	ARG	A	508	25.433	57.106	40.011	1.00	55.32
N										
ATOM	3996	N	ASN	A	509	32.310	56.581	42.531	1.00	46.05
N										
ATOM	3997	CA	ASN	A	509	32.120	57.406	43.717	1.00	48.74
C										

ATOM 3998 C ASN A 509 33.253 58.416 43.864 1.00 50.32 C
ATOM 3999 O ASN A 509 33.014 59.599 44.101 1.00 50.36 O
ATOM 4000 CB ASN A 509 32.056 56.523 44.966 1.00 48.82 C
ATOM 4001 CG ASN A 509 30.808 55.667 45.012 1.00 49.43 C
ATOM 4002 ODl ASN A 509 30.667 54.801 45.876 1.00 50.30 O
ATOM 4003 ND2 ASN A 509 29.888 55.910 44.086 1.00 49.75 N
ATOM 4004 N HIS A 510 34.487 57.941 43.725 1.00 52.74 N
ATOM 4005 CA HIS A 510 35.653 58.806 43.846 1.00 55.11 C
ATOM 4006 C HIS A 510 35.721 59.810 42.701 1.00 56.20 C
ATOM 4007 O HIS A 510 36.191 60.934 42.877 1.00 56.05 O
ATOM 4008 CB HIS A 510 36.934 57.969 43.877 1.00 56.04 C
ATOM 4009 CG HIS A 510 38.186 58.785 43.953 1.00 58.50 C
ATOM 4010 NDl HIS A 510 38.628 59.570 42.908 1.00 59.07 N
ATOM 4011 CD2 HIS A 510 39.077 58.962 44.957 1.00 59.19 C
ATOM 4012 CEl HIS A 510 39.735 60.193 43.266 1.00 59.75 C
ATOM 4013 NE2 HIS A 510 40.030 59.842 44.506 1.00 59.59 N
ATOM 4014 N GLU A 511 35.252 59.400 41.528 1.00 57.57 N
ATOM 4015 CA GLU A 511 35.258 60.270 40.360 1.00 59.47 C
ATOM 4016 C GLU A 511 34.212 61.368 40.533 1.00 60.34 C
ATOM 4017 O GLU A 511 34.452 62.526 40.194 1.00 59.93 O
ATOM 4018 CB GLU A 511 34.960 59.459 39.097 1.00 60.01 C
ATOM 4019 CG GLU A 511 34.964 60.275 37.814 1.00 61.94 C
ATOM 4020 CD GLU A 511 34.680 59.430 36.586 1.00 63.07 C
ATOM 4021 OEl GLU A 511 33.615 58.776 36.544 1.00 63.48 O
ATOM 4022 OE2 GLU A 511 35.521 59.420 35.661 1.00 64.04 O
ATOM 4023 N SER A 512 33.054 60.996 41.069 1.00 61.38 N
ATOM 4024 CA SER A 512 31.973 61.947 41.293 1.00 62.99 C
ATOM 4025 C SER A 512 32.368 62.961 42.361 1.00 63.91 C
ATOM 4026 O SER A 512 32.029 64.141 42.266 1.00 64.29 O
ATOM 4027 CB SER A 512 30.703 61.211 41.725 1.00 62.76 C

ATOM	4028	OG	SER	A	512	30.272	60.306	40.723	1.00	63.60
ATOM	4029	N	ALA	A	513	33.089	62.493	43.376	1.00	64.86
ATOM	4030	CA	ALA	A	513	33.536	63.356	44.463	1.00	65.80
ATOM	4031	C	ALA	A	513	34.530	64.391	43.946	1.00	66.48
ATOM	4032	O	ALA	A	513	34.624	65.497	44.480	1.00	66.37
ATOM	4033	CB	ALA	A	513	34.178	62.517	45.563	1.00	65.39
ATOM	4034	N	GLY	A	514	35.270	64.023	42.904	1.00	67.05
ATOM	4035	CA	GLY	A	514	36.244	64.932	42.330	1.00	67.58
ATOM	4036	C	GLY	A	514	35.646	65.788	41.230	1.00	68.05
ATOM	4037	O	GLY	A	514	36.353	66.547	40.569	1.00	68.23
ATOM	4038	N	THR	A	515	34.338	65.663	41.033	1.00	68.41
ATOM	4039	CA	THR	A	515	33.639	66.429	40.008	1.00	68.83
ATOM	4040	C	THR	A	515	32.438	67.162	40.596	1.00	68.81
ATOM	4041	O	THR	A	515	32.400	68.391	40.619	1.00	69.16
ATOM	4042	CB	THR	A	515	33.146	65.518	38.867	1.00	69.01
ATOM	4043	OGl	THR	A	515	32.280	64.509	39.401	1.00	69.48
ATOM	4044	CG2	THR	A	515	34.323	64.854	38.170	1.00	69.34
TER	4045		THR	A	515					
HETATM	4046	Cl	BOG		701	-0.375	42.351	12.575	1.00	48.25
HETATM	4047	Ol	BOG		701	-0.015	41.051	13.048	1.00	49.00
HETATM	4048	C2	BOG		701	-1.925	42.456	12.478	1.00	48.04
HETATM	4049	02	BOG		701	-2.416	41.450	11.596	1.00	49.44
HETATM	4050	C3	BOG		701	-2.319	43.876	11.977	1.00	47.50
HETATM	4051	03	BOG		701	-3.734	43.990	11.885	1.00	46.97
HETATM	4052	C4	BOG		701	-1.764	44.924	12.967	1.00	46.59
HETATM	4053	04	BOG		701	-2.115	46.246	12.541	1.00	47.11
HETATM	4054	C5	BOG		701	-0.203	44.784	13.063	1.00	46.21
HETATM	4055	05	BOG		701	0.128	43.416	13.487	1.00	47.25
HETATM	4056	C6	BOG		701	0.378	45.801	14.065	1.00	44.83
HETATM	4057	06	BOG		701	-0.063	45.547	15.404	1.00	41.79
HETATM	4058	Cl'	BOG		701	1.396	40.858	13.161	1.00	50.24

HETATM 4059 C21 BOG 701 1.672 39.383 13.277 1.00 50.53
C
HETATM 4060 C31 BOG 701 2.349 39.117 14.593 1.00 51.52
C
HETATM 4061 C41 BOG 701 2.661 37.649 14.795 1.00 52.59
C
HETATM 4062 C5' BOG 701 3.346 37.426 16.134 1.00 53.62
C
HETATM 4063 C61 BOG 701 2.446 36.664 17.090 1.00 54.84
C
HETATM 4064 C71 BOG 701 3.105 36.435 18.419 1.00 54.26
C
HETATM 4065 C8' BOG 701 2.173 35.679 19.334 1.00 55.53
C
HETATM 4066 Cl BOG 702 54.221 17.561 16.607 1.00 78.16
C
HETATM 4067 Ol BOG 702 53.515 18.745 16.986 1.00 77.54
O
HETATM 4068 C2 BOG 702 53.707 16.357 17.449 1.00 78.11
C
HETATM 4069 02 BOG 702 53.896 16.626 18.836 1.00 77.98
O
HETATM 4070 C3 BOG 702 54.461 15.064 17.022 1.00 78.26
C
HETATM 4071 03 BOG 702 54.000 13.957 17.785 1.00 77.85
O
HETATM 4072 C4 BOG 702 54.216 14.821 15.512 1.00 78.75
C
HETATM 4073 04 BOG 702 54.885 13.634 15.081 1.00 78.98
O
HETATM 4074 C5 BOG 702 54.732 16.056 14.693 1.00 78.81
C
HETATM 4075 05 BOG 702 54.034 17.264 15.161 1.00 78.67
O
HETATM 4076 C6 BOG 702 54.485 15.852 13.187 1.00 79.28
C
HETATM 4077 06 BOG 702 53.104 16.004 12.846 1.00 79.64
O
HETATM 4078 Cl' BOG 702 53.924 19.901 16.259 1.00 76.84
C
HETATM 4079 C2' BOG 702 52.813 20.916 16.299 1.00 75.96
C
HETATM 4080 C3' BOG 702 53.004 21.891 15.166 1.00 75.58
C
HETATM 4081 C4' BOG 702 51.924 22.953 15.139 1.00 75.09
C
HETATM 4082 C5' BOG 702 52.139 23.918 13.989 1.00 74.71
C
HETATM 4083 C6' BOG 702 50.815 24.539 13.579 1.00 74.31
C
HETATM 4084 C71 BOG 702 50.963 25.503 12.440 1.00 74.33
C
HETATM 4085 C8' BOG 702 49.612 26.082 12.080 1.00 73.99
C
HETATM 4086 Cl BOG 703 51.403 21.818 27.283 1.00 45.00
C
HETATM 4087 Ol BOG 703 51.352 22.183 28.664 1.00 46.15
O
HETATM 4088 C2 BOG 703 52.579 20.823 27.069 1.00 45.62
C

```
HETATM 4089  O2  BOG  703      53.802  21.434  27.479  1.00 47.29
O
HETATM 4090  C3  BOG  703      52.641  20.406  25.573  1.00 44.87
C
HETATM 4091  O3  BOG  703      53.715  19.497  25.363  1.00 46.01
O
HETATM 4092  C4  BOG  703      51.295  19.748  25.185  1.00 42.96
C
HETATM 4093  O4  BOG  703      51.315  19.340  23.816  1.00 44.54
O
HETATM 4094  C5  BOG  703      50.123  20.766  25.427  1.00 41.84
C
HETATM 4095  O5  BOG  703      50.135  21.172  26.842  1.00 42.47
O
HETATM 4096  C6  BOG  703      48.766  20.130  25.065  1.00 39.24
C
HETATM 4097  O6  BOG  703      48.426  19.043  25.926  1.00 36.06
O
HETATM 4098  Cl' BOG  703      50.321  23.108  28.992  1.00 48.48
C
HETATM 4099  C2' BOG  703      50.623  23.648  30.365  1.00 51.37
C
HETATM 4100  C3' BOG  703      49.610  24.694  30.723  1.00 53.82
C
HETATM 4101  C4' BOG  703      49.856  25.282  32.100  1.00 56.59
C
HETATM 4102  C5' BOG  703      48.814  26.342  32.433  1.00 58.17
C
HETATM 4103  C6' BOG  703      49.323  27.728  32.065  1.00 59.36
C
HETATM 4104  C7' BOG  703      48.322  28.801  32.378  1.00 59.81
C
HETATM 4105  C8' BOG  703      48.880  30.150  31.992  1.00 60.05
C
HETATM 4106  Cl  BOG  704      51.182  18.755  31.385  1.00 64.57
C
HETATM 4107  Ol  BOG  704      50.344  19.270  32.418  1.00 62.46
O
HETATM 4108  C2  BOG  704      51.981  17.526  31.913  1.00 65.33
C
HETATM 4109  O2  BOG  704      52.768  17.913  33.039  1.00 66.00
O
HETATM 4110  C3  BOG  704      52.877  16.967  30.769  1.00 66.15
C
HETATM 4111  O3  BOG  704      53.618  15.843  31.229  1.00 66.75
O
HETATM 4112  C4  BOG  704      51.971  16.563  29.583  1.00 66.55
C
HETATM 4113  O4  BOG  704      52.756  16.035  28.508  1.00 68.18
O
HETATM 4114  C5  BOG  704      51.160  17.811  29.090  1.00 66.48
C
HETATM 4115  O5  BOG  704      50.375  18.346  30.205  1.00 65.46
O
HETATM 4116  C6  BOG  704      50.231  17.432  27.925  1.00 66.23
C
HETATM 4117  O6  BOG  704      48.978  16.904  28.378  1.00 66.46
O
HETATM 4118  Cl' BOG  704      49.589  20.395  31.988  1.00 59.92
C
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HETATM 4119 C21 BOG 704 49.017 21.089 33.183 1.00 57.80
C
HETATM 4120 C3' BOG 704 47.625 21.533 32.851 1.00 55.53
C
HETATM 4121 C41 BOG 704 46.969 22.248 34.003 1.00 54.40
C
HETATM 4122 C5' BOG 704 45.566 22.678 33.629 1.00 53.50
C
HETATM 4123 C61 BOG 704 44.652 22.558 34.825 1.00 53.36
C
HETATM 4124 C71 BOG 704 43.254 22.973 34.503 1.00 52.42
C
HETATM 4125 C8' BOG 704 42.404 22.828 35.734 1.00 53.14
C
HETATM 4126 Cl BOG 705 50.110 13.926 35.734 1.00 59.47
C
HETATM 4127 Ol BOG 705 49.321 14.361 34.620 1.00 59.31
O
HETATM 4128 C2 BOG 705 51.452 13.334 35.228 1.00 59.89
C
HETATM 4129 02 BOG 705 51.172 12.248 34.353 1.00 60.71
O
HETATM 4130 C3 BOG 705 52.300 12.867 36.450 1.00 59.64
C
HETATM 4131 03 BOG 705 53.530 12.310 36.012 1.00 60.18
O
HETATM 4132 C4 BOG 705 52.566 14.083 37.359 1.00 59.66
C
HETATM 4133 04 BOG 705 53.349 13.705 38.493 1.00 59.38
O
HETATM 4134 C5 BOG 705 51.206 14.692 37.832 1.00 59.62
C
HETATM 4135 05 BOG 705 50.405 15.059 36.658 1.00 59.78
O
HETATM 4136 C6 BOG 705 51.442 15.925 38.723 1.00 59.82
C
HETATM 4137 06 BOG 705 52.331 16.879 38.126 1.00 60.15
O
HETATM 4138 Cl' BOG 705 48.061 14.868 35.039 1.00 57.95
C
HETATM 4139 C2" BOG 705 47.783 16.224 34.461 1.00 56.34
C
HETATM 4140 C3' BOG 705 46.292 16.409 34.551 1.00 55.31
C
HETATM 4141 C4' BOG 705 45.796 17.735 34.031 1.00 54.03
C
HETATM 4142 C5" BOG 705 44.276 17.803 34.153 1.00 53.48
C
HETATM 4143 C6' BOG 705 43.823 18.551 35.398 1.00 51.53
C
HETATM 4144 C7' BOG 705 42.321 18.602 35.487 1.00 51.67
C
HETATM 4145 C81 BOG 705 41.890 19.347 36.729 1.00 52.00
C
HETATM 4146 NA NA 751 29.148 33.657 14.404 1.00 15.78
NA
HETATM 4147 NA NA 752 22.894 31.014 15.960 1.00 17.28
NA
HETATM 4148 CL CL 753 46.339 16.445 16.280 1.00 36.64
CL

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HETATM 4149  N   LEU   601      24.537  32.416  18.866  1.00 15.26
N
HETATM 4150  CA  LEU   601      25.812  31.696  18.815  1.00 16.66
C
HETATM 4151  C   LEU   601      25.693  30.381  18.046  1.00 16.48
C
HETATM 4152  O   LEU   601      26.714  29.668  17.947  1.00 17.32
O
HETATM 4153  CB  LEU   601      26.314  31.407  20.237  1.00 16.91
C
HETATM 4154  CG  LEU   601      26.432  32.590  21.204  1.00 20.41
C
HETATM 4155  CDl LEU   601      26.926  32.087  22.562  1.00 20.45
C
HETATM 4156  CD2 LEU   601      27.391  33.633  20.645  1.00 19.49
C
HETATM 4157  OXT LEU   601      24.586  30.062  17.552  1.00 18.07
O
HETATM 4158  O   HOH   801      42.416  23.235  19.138  1.00 15.54
O
HETATM 4159  O   HOH   802      40.941  18.708  25.260  1.00 17.38
O
HETATM 4160  O   HOH   803      30.169  39.492  15.312  1.00 19.56
O
HETATM 4161  O   HOH   804      36.299  19.640  29.087  1.00 18.24
O
HETATM 4162  O   HOH   805      16.703  51.629  23.292  1.00 21.01
O
HETATM 4163  O   HOH   806      37.228  13.200  12.465  1.00 24.89
O
HETATM 4164  O   HOH   807      32.817  50.078  25.228  1.00 26.02
O
HETATM 4165  O   HOH   808      44.313  51.132  30.588  1.00 23.84
O
HETATM 4166  O   HOH   809      26.343  42.589  29.546  1.00 25.89
O
HETATM 4167  O   HOH   810      26.223  18.447  14.888  1.00 27.14
O
HETATM 4168  O   HOH   811      36.114  47.903  22.199  1.00 23.13
O
HETATM 4169  O   HOH   812      29.532  48.664  30.600  1.00 25.53
O
HETATM 4170  O   HOH   813      48.117  15.687   1.399  1.00 26.13
O
HETATM 4171  O   HOH   814      24.777  21.249   9.733  1.00 23.47
O
HETATM 4172  O   HOH   815      36.641  45.660  20.851  1.00 25.02
O
HETATM 4173  O   HOH   816      32.596  38.569  27.985  1.00 22.25
O
HETATM 4174  O   HOH   817      36.510  13.896   4.610  1.00 24.09
O
HETATM 4175  O   HOH   818      13.656  51.249  17.174  1.00 23.98
O
HETATM 4176  O   HOH   819      37.096  50.621  15.561  1.00 26.68
O
HETATM 4177  O   HOH   820      50.422  17.312  17.799  1.00 25.66
O
HETATM 4178  O   HOH   821      18.443  22.622  23.386  1.00 26.56
O
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HETATM 4179 O HOH 822 26.561 19.125 12.402 1.00 25.61 O
HETATM 4180 O HOH 823 26.008 20.789 28.815 1.00 28.81 O
HETATM 4181 O HOH 824 22.714 38.447 24.671 1.00 24.10 O
HETATM 4182 O HOH 825 43.526 51.175 23.021 1.00 29.01 O
HETATM 4183 O HOH 826 16.482 22.138 6.257 1.00 30.27 O
HETATM 4184 O HOH 827 22.840 54.456 22.043 1.00 28.51 O
HETATM 4185 O HOH 828 28.798 41.764 22.761 1.00 24.72 O
HETATM 4186 O HOH 829 21.356 19.288 9.618 1.00 27.32 O
HETATM 4187 O HOH 830 5.928 52.392 32.372 1.00 30.04 O
HETATM 4188 O HOH 831 41.213 52.948 24.003 1.00 32.67 O
HETATM 4189 O HOH 832 25.786 19.511 18.985 1.00 32.33 O
HETATM 4190 O HOH 833 33.969 19.324 35.752 1.00 31.20 O
HETATM 4191 O HOH 834 21.522 39.155 27.696 1.00 26.53 O
HETATM 4192 O HOH 835 41.977 7.943 31.745 1.00 32.52 O
HETATM 4193 O HOH 836 26.363 14.085 17.341 1.00 30.77 O
HETATM 4194 O HOH 837 -0.645 43.036 16.629 1.00 29.43 O
HETATM 4195 O HOH 838 28.168 17.338 16.203 1.00 30.58 O
HETATM 4196 O HOH 839 44.047 13.792 15.560 1.00 31.10 O
HETATM 4197 O HOH 840 20.537 26.921 26.015 1.00 35.92 O
HETATM 4198 O HOH 841 50.692 15.733 20.656 1.00 31.88 O
HETATM 4199 O HOH 842 35.098 17.295 27.975 1.00 29.18 O
HETATM 4200 O HOH 843 30.242 13.941 20.976 1.00 33.59 O
HETATM 4201 O HOH 844 34.135 16.625 35.264 1.00 26.89 O
HETATM 4202 O HOH 845 42.619 8.150 12.757 1.00 34.60 O
HETATM 4203 O HOH 846 31.925 10.669 20.237 1.00 40.20 O
HETATM 4204 O HOH 847 24.093 19.563 21.221 1.00 35.98 O
HETATM 4205 O HOH 848 35.086 44.773 5.331 1.00 36.43 O
HETATM 4206 O HOH 849 -0.014 51.947 28.467 1.00 31.64 O
HETATM 4207 O HOH 850 23.832 14.380 21.719 1.00 39.76 O
HETATM 4208 O HOH 851 8.579 55.076 20.908 1.00 34.83 O

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HETATM 4209  O   HOH   852      18.961   3.742   9.860  1.00 32.40
O
HETATM 4210  O   HOH   853      17.514  59.820  19.184  1.00 44.98
O
HETATM 4211  O   HOH   854       5.199  47.501  34.379  1.00 44.22
O
HETATM 4212  O   HOH   855      28.263  47.495  33.705  1.00 34.47
O
HETATM 4213  O   HOH   856      27.932  11.826  -4.137  1.00 42.47
O
HETATM 4214  O   HOH   857      30.972  55.352  26.213  1.00 35.21
O
HETATM 4215  O   HOH   858      46.153  13.673  22.366  1.00 37.14
O
HETATM 4216  O   HOH   859      25.262  24.101  23.648  1.00 36.12
O
HETATM 4217  O   HOH   860      19.496  56.218  27.778  1.00 40.25
O
HETATM 4218  O   HOH   861      44.765  43.574  14.713  1.00 43.94
O
HETATM 4219  O   HOH   862      46.774  51.270  26.386  1.00 32.96
O
HETATM 4220  O   HOH   863      42.081   9.404  23.198  1.00 37.29
O
HETATM 4221  O   HOH   864      38.906  12.639   4.088  1.00 38.59
O
HETATM 4222  O   HOH   865      25.936  54.026  21.428  1.00 34.66
O
HETATM 4223  O   HOH   866      33.298  52.487  23.111  1.00 40.05
O
HETATM 4224  O   HOH   867      19.794  49.518  47.023  1.00 40.81
O
HETATM 4225  O   HOH   868      25.153   8.351  -5.682  1.00 38.67
O
HETATM 4226  O   HOH   869      16.338  37.637   6.486  1.00 43.24
O
HETATM 4227  O   HOH   870       2.294  48.347  16.916  1.00 39.10
O
HETATM 4228  O   HOH   871      39.242  12.679  -3.929  1.00 38.01
O
HETATM 4229  O   HOH   872      25.940  10.010  -3.711  1.00 41.32
O
HETATM 4230  O   HOH   873      42.716   7.830  19.001  1.00 40.80
O
HETATM 4231  O   HOH   874      10.848  55.196  27.548  1.00 41.03
O
HETATM 4232  O   HOH   875       5.231  49.371  11.307  1.00 39.34
O
HETATM 4233  O   HOH   876      39.404   1.138   9.392  1.00 40.83
O
HETATM 4234  O   HOH   877      17.981  17.658  23.142  1.00 45.84
O
HETATM 4235  O   HOH   878      18.943   6.187  -2.631  1.00 37.59
O
HETATM 4236  O   HOH   879      10.032  13.375  11.143  1.00 54.11
O
HETATM 4237  O   HOH   880      25.489   3.651   2.593  1.00 50.69
O
HETATM 4238  O   HOH   881       4.028  52.875  25.911  1.00 42.57
O
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HETATM 4239  O   HOH   882      23.167   6.600  20.323  1.00 38.57
O
HETATM 4240  O   HOH   883      27.723  52.456  41.109  1.00 59.41
O
HETATM 4241  O   HOH   884      50.006  16.543  24.004  1.00 32.58
O
HETATM 4242  O   HOH   885      46.789  15.660  30.456  1.00 34.56
O
HETATM 4243  O   HOH   886      33.628  53.320  27.154  1.00 33.25
O
HETATM 4244  O   HOH   887      31.458  55.053  30.032  1.00 48.66
O
HETATM 4245  O   HOH   888      41.241  50.270  14.973  1.00 49.32
O
HETATM 4246  O   HOH   889       1.622  53.461  32.312  1.00 40.97
O
HETATM 4247  O   HOH   890      12.571  10.352   5.763  1.00 41.87
O
HETATM 4248  O   HOH   891      17.687  13.957  -2.419  1.00 43.22
O
HETATM 4249  O   HOH   892       5.923  18.286  17.925  1.00 51.03
O
HETATM 4250  O   HOH   893      39.865  10.314   4.367  1.00 41.50
O
HETATM 4251  O   HOH   894      19.352  12.379  -5.578  1.00 68.38
O
HETATM 4252  O   HOH   895      45.980  52.231  24.019  1.00 44.36
O
HETATM 4253  O   HOH   896      23.950  21.901  25.380  1.00 40.84
O
HETATM 4254  O   HOH   897      24.391  57.967  20.078  1.00 42.84
O
HETATM 4255  O   HOH   898      32.216  14.330  -5.403  1.00 50.25
O
HETATM 4256  O   HOH   899      28.059  49.603   4.207  1.00 42.03
O
HETATM 4257  O   HOH   900      28.412  15.465  24.242  1.00 47.69
O
HETATM 4258  O   HOH   901      30.742  53.523  36.050  1.00 37.72
O
HETATM 4259  O   HOH   902      31.645  49.567   7.859  1.00 44.52
O
HETATM 4260  O   HOH   903      32.571  10.470  -5.780  1.00 43.46
O
HETATM 4261  O   HOH   904      16.262  62.804  20.129  1.00 68.75
O
HETATM 4262  O   HOH   905      44.048  10.747  26.039  1.00 50.58
O
HETATM 4263  O   HOH   906      18.859  20.634  30.476  1.00 52.68
O
HETATM 4264  O   HOH   907      44.354   8.972  15.773  1.00 44.66
O
HETATM 4265  O   HOH   908      15.055  10.467  -3.446  1.00 64.27
O
HETATM 4266  O   HOH   909      43.727  11.674  28.406  1.00 43.52
O
HETATM 4267  O   HOH   910      40.785  47.141  10.406  1.00 51.17
O
HETATM 4268  O   HOH   911      24.690  51.664  12.141  1.00 38.78
O
```

HETATM	4269	O	HOH	912	34.952	52.594	9.650	1.00	62.64
O									
HETATM	4270	O	HOH	913	8.730	12.065	17.047	1.00	62.85
O									
HETATM	4271	O	HOH	914	14.996	55.951	12.464	1.00	69.45
O									
HETATM	4272	O	HOH	915	32.218	10.570	41.816	1.00	43.58
O									
HETATM	4273	O	HOH	916	29.517	42.768	3.041	1.00	41.09
O									
HETATM	4274	O	HOH	917	11.722	56.229	25.383	1.00	41.23
O									
HETATM	4275	O	HOH	918	15.774	6.307	6.351	1.00	44.11
O									
HETATM	4276	O	HOH	919	31.733	54.641	13.656	1.00	43.33
O									
HETATM	4277	O	HOH	920	41.731	18.972	1.234	1.00	30.77
O									
HETATM	4278	O	HOH	921	12.069	14.390	26.071	1.00	62.94
O									
HETATM	4279	O	HOH	922	16.994	45.363	7.359	1.00	40.10
O									
HETATM	4280	O	HOH	923	24.123	17.032	22.603	1.00	40.22
O									
HETATM	4281	O	HOH	924	33.062	15.741	-2.604	1.00	37.68
O									
HETATM	4282	O	HOH	925	16.600	5.893	-1.723	1.00	44.56
O									
HETATM	4283	O	HOH	926	4.486	54.017	23.571	1.00	41.01
O									
HETATM	4284	O	HOH	927	21.689	17.314	23.920	1.00	46.64
O									
HETATM	4285	O	HOH	928	53.214	14.829	20.801	1.00	44.72
O									
HETATM	4286	O	HOH	929	17.595	54.248	11.734	1.00	37.40
O									
HETATM	4287	O	HOH	930	44.228	6.573	32.300	1.00	44.79
O									
HETATM	4288	O	HOH	931	31.782	10.995	44.706	1.00	52.95
O									
HETATM	4289	O	HOH	932	-1.641	40.839	15.486	1.00	48.78
O									
HETATM	4290	O	HOH	933	7.696	55.192	18.468	1.00	52.19
O									
HETATM	4291	O	HOH	934	32.261	12.044	-7.873	1.00	44.59
O									
HETATM	4292	O	HOH	935	20.272	13.392	-2.882	1.00	45.55
O									
HETATM	4293	O	HOH	936	29.105	54.116	42.401	1.00	68.42
O									
HETATM	4294	O	HOH	937	17.444	7.203	4.486	1.00	47.98
O									
HETATM	4295	O	HOH	938	33.852	53.683	16.285	1.00	55.83
O									
HETATM	4296	O	HOH	939	49.750	14.015	18.719	1.00	48.94
O									
HETATM	4297	O	HOH	940	30.438	13.954	23.977	1.00	45.60
O									
HETATM	4298	O	HOH	941	-0.878	47.029	10.135	1.00	50.81
O									

```
HETATM 4299  O   HOH   942      27.735  12.894  -6.883  1.00 55.61
O
HETATM 4300  O   HOH   943      23.318  21.275  28.870  1.00 49.99
O
HETATM 4301  O   HOH   944      29.675  55.889  35.228  1.00 52.05
O
HETATM 4302  O   HOH   945      27.199   7.752  -2.835  1.00 44.04
O
HETATM 4303  O   HOH   946      33.884   8.247  -5.811  1.00 55.63
O
HETATM 4304  O   HOH   947      31.881  40.013  12.988  1.00 37.29
O
HETATM 4305  O   HOH   948      26.908  57.062  23.311  1.00 50.22
O
HETATM 4306  O   HOH   949      24.788  56.283  22.039  1.00 61.52
O
HETATM 4307  O   HOH   950      31.230  13.123 -10.720  1.00 59.57
O
HETATM 4308  O   HOH   951      22.558   9.281  43.472  1.00 65.02
O
HETATM 4309  O   HOH   952      -0.630  53.326  30.883  1.00 48.48
O
HETATM 4310  O   HOH   953      35.566  54.338  28.627  1.00 58.66
O
HETATM 4311  O   HOH   954      10.746  14.412  28.469  1.00 59.54
O
HETATM 4312  O   HOH   955      20.039  58.857  27.411  1.00 49.06
O
HETATM 4313  O   HOH   956      20.660   5.537  20.557  1.00 55.54
O
HETATM 4314  O   HOH   957       3.150  56.894  17.807  1.00 54.46
O
HETATM 4315  O   HOH   958      38.615  52.920  26.743  1.00 45.27
O
HETATM 4316  O   HOH   959       9.418  54.223   8.803  1.00 53.37
O
HETATM 4317  O   HOH   960      32.305  55.696  16.017  1.00 50.52
O
HETATM 4318  O   HOH   961      17.699   5.495  16.594  1.00 45.85
O
HETATM 4319  O   HOH   962      23.665   7.446  22.778  1.00 59.56
O
HETATM 4320  O   HOH   963      42.588  49.615  12.610  1.00 67.27
O
HETATM 4321  O   HOH   964      -2.539  44.734  29.920  1.00 45.35
O
HETATM 4322  O   HOH   965      37.043  57.055  36.420  1.00 56.38
O
HETATM 4323  O   HOH   966      39.414   2.760  17.698  1.00 63.41
O
HETATM 4324  O   HOH   967      38.459  52.982  15.334  1.00 54.70
O
HETATM 4325  O   HOH   968       5.878  53.482  21.423  1.00 45.47
O
HETATM 4326  O   HOH   969      45.189  11.539  14.454  1.00 52.63
O
HETATM 4327  O   HOH   970      36.127  17.008  25.564  1.00 46.67
O
HETATM 4328  O   HOH   971      29.182   6.315  17.793  1.00 60.12
O
```

HETATM	4329	O	HOH	972	8.750	56.524	28.404	1.00	57.50
HETATM	4330	O	HOH	973	14.070	49.505	44.516	1.00	52.60
HETATM	4331	O	HOH	974	22.538	19.457	-5.404	1.00	47.19
HETATM	4332	O	HOH	975	27.305	4.057	0.821	1.00	54.85
HETATM	4333	O	HOH	976	14.498	11.563	17.372	1.00	43.17
HETATM	4334	O	HOH	977	27.280	42.043	2.015	1.00	60.16
HETATM	4335	O	HOH	978	39.903	53.406	17.443	1.00	53.60
HETATM	4336	O	HOH	979	3.921	49.693	18.516	1.00	53.07
HETATM	4337	O	HOH	980	15.504	57.163	25.910	1.00	53.45
HETATM	4338	O	HOH	981	35.650	12.949	26.644	1.00	45.08
HETATM	4339	O	HOH	982	25.149	18.226	28.186	1.00	59.86
HETATM	4340	O	HOH	983	34.602	54.208	11.804	1.00	62.05
HETATM	4341	O	HOH	984	47.357	13.634	11.623	1.00	61.27
HETATM	4342	O	HOH	985	34.599	10.634	27.920	1.00	44.58
HETATM	4343	O	HOH	986	42.339	52.604	10.474	1.00	71.20
HETATM	4344	O	HOH	987	18.113	6.478	18.963	1.00	46.72
HETATM	4345	O	HOH	988	45.982	11.822	24.345	1.00	54.32
HETATM	4346	O	HOH	989	37.653	4.888	29.054	1.00	60.17
HETATM	4347	O	HOH	990	2.348	49.037	13.967	1.00	66.12
HETATM	4348	O	HOH	991	3.872	46.764	12.946	1.00	53.91
HETATM	4349	O	HOH	992	21.387	60.395	25.428	1.00	55.88
HETATM	4350	O	HOH	993	29.859	11.509	24.785	1.00	64.17
HETATM	4351	O	HOH	994	18.945	46.545	47.827	1.00	57.80
HETATM	4352	O	HOH	995	24.467	13.141	24.037	1.00	56.72
HETATM	4353	O	HOH	996	-4.871	44.896	31.416	1.00	69.85
HETATM	4354	O	HOH	997	13.865	10.895	19.862	1.00	52.51
HETATM	4355	O	HOH	998	7.321	55.663	10.004	1.00	66.03
HETATM	4356	O	HOH	999	29.728	13.718	35.571	1.00	50.55
HETATM	4357	O	HOH	1000	4.813	47.046	9.810	1.00	59.24
HETATM	4358	O	HOH	1001	18.610	55.784	33.567	1.00	53.17

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HETATM 4359  O   HOH  1002       8.204  52.046  36.554  1.00 59.34
O
HETATM 4360  O   HOH  1003      11.951  17.127  42.229  1.00 70.82
O
HETATM 4361  O   HOH  1004      29.592  -4.061   4.473  1.00 59.66
O
HETATM 4362  O   HOH  1005      13.647  55.567  28.806  1.00 55.43
O
HETATM 4363  O   HOH  1006      54.369  21.756  30.169  1.00 56.65
O
HETATM 4364  O   HOH  1007      45.256  13.028   1.941  1.00 47.58
O
HETATM 4365  O   HOH  1008      16.632  20.836  41.890  1.00 60.85
O
HETATM 4366  O   HOH  1009      32.866  16.678  26.515  1.00 55.14
O
HETATM 4367  O   HOH  1010      -0.422  49.782   9.991  1.00 55.60
O
CONECT 4046 4047 4048 4055
CONECT 4047 4046 4058
CONECT 4048 4046 4049 4050
CONECT 4049 4048
CONECT 4050 4048 4051 4052
CONECT 4051 4050
CONECT 4052 4050 4053 4054
CONECT 4053 4052
CONECT 4054 4052 4055 4056
CONECT 4055 4046 4054
CONECT 4056 4054 4057
CONECT 4057 4056
CONECT 4058 4047 4059
CONECT 4059 4058 4060
CONECT 4060 4059 4061
CONECT 4061 4060 4062
CONECT 4062 4061 4063
CONECT 4063 4062 4064
CONECT 4064 4063 4065
CONECT 4065 4064
CONECT 4066 4067 4068 4075
CONECT 4067 4066 4078
CONECT 4068 4066 4069 4070
CONECT 4069 4068
CONECT 4070 4068 4071 4072
CONECT 4071 4070
CONECT 4072 4070 4073 4074
CONECT 4073 4072
CONECT 4074 4072 4075 4076
CONECT 4075 4066 4074
CONECT 4076 4074 4077
CONECT 4077 4076
CONECT 4078 4067 4079
CONECT 4079 4078 4080
CONECT 4080 4079 4081
CONECT 4081 4080 4082
CONECT 4082 4081 4083
CONECT 4083 4082 4084
CONECT 4084 4083 4085
CONECT 4085 4084
CONECT 4086 4087 4088 4095
CONECT 4087 4086 4098
CONECT 4088 4086 4089 4090
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CONECT 4089 4088
CONECT 4090 4088 4091 4092
CONECT 4091 4090
CONECT 4092 4090 4093 4094
CONECT 4093 4092
CONECT 4094 4092 4095 4096
CONECT 4095 4086 4094
CONECT 4096 4094 4097
CONECT 4097 4096
CONECT 4098 4087 4099
CONECT 4099 4098 4100
CONECT 4100 4099 4101
CONECT 4101 4100 4102
CONECT 4102 4101 4103
CONECT 4103 4102 4104
CONECT 4104 4103 4105
CONECT 4105 4104
CONECT 4106 4107 4108 4115
CONECT 4107 4106 4118
CONECT 4108 4106 4109 4110
CONECT 4109 4108
CONECT 4110 4108 4111 4112
CONECT 4111 4110
CONECT 4112 4110 4113 4114
CONECT 4113 4112
CONECT 4114 4112 4115 4116
CONECT 4115 4106 4114
CONECT 4116 4114 4117
CONECT 4117 4116
CONECT 4118 4107 4119
CONECT 4119 4118 4120
CONECT 4120 4119 4121
CONECT 4121 4120 4122
CONECT 4122 4121 4123
CONECT 4123 4122 4124
CONECT 4124 4123 4125
CONECT 4125 4124
CONECT 4126 4127 4128 4135
CONECT 4127 4126 4138
CONECT 4128 4126 4129 4130
CONECT 4129 4128
CONECT 4130 4128 4131 4132
CONECT 4131 4130
CONECT 4132 4130 4133 4134
CONECT 4133 4132
CONECT 4134 4132 4135 4136
CONECT 4135 4126 4134
CONECT 4136 4134 4137
CONECT 4137 4136
CONECT 4138 4127 4139
CONECT 4139 4138 4140
CONECT 4140 4139 4141
CONECT 4141 4140 4142
CONECT 4142 4141 4143
CONECT 4143 4142 4144
CONECT 4144 4143 4145
CONECT 4145 4144
MASTER      276    0    9   28    2    0    0    6 4366    1  100
40
END
```

TABLE 4

X-RAY Materials and Methods Report 2A65

Crystallization

Crystallization Experiments

Method	VAPOR DIFFUSION, HANGING DROP
PH	7.0
Temperature	291.0

Crystal Data

Unit Cell

Length a (A)	87.86	Angle Alpha (°)	90.00
Length b (A)	86.31	Angle Beta (°)	95.73
Length c (A)	81.02	Angle Gamma (°)	90.00

Space Group

Space Group Name	C 2 (C 1 2 1)

Diffraction

Diffraction Detector

Detector	CCD
Type	ADSC QUANTUM 315
Details	n/a
Collection Date	2004-12-12
Detector	CCD
Type	ADSC QUANTUM 315
Details	n/a
Collection Date	2004-12-12

Diffraction Radiation

Monochromator	Double crystal, Si(III)
Diffraction Protocol	MAD
Wavelength	n/a
Wavelength List	0.9793, 0.9795, 0.9641

Diffraction Radiation

Monochromator	Double crystal, Si(III)
Diffraction Protocol	SINGLE WAVELENGTH
Wavelength	n/a
Wavelength List	0.9950

Diffraction Source

Source	SYNCHROTRON
Type	ALS BEAMLINE 8.2.2
Site	ALS
Beamline	8.2.2

Diffraction Source

Source	SYNCHROTRON
Type	ALS BEAMLINE 8.2.2

Site	ALS
Beamline	8.2.2

Data

Reflection Details

Observed Criterion Sigma (F)	**n/a**
Observed Criterion Sigma(I)	-3.0
Resolution(High)	1.65
Resolution(Low)	50.00
Number Reflections(All)	**n/a**
Number Reflections(Observed)	**70306**
Percent Possible(Observed)	97.3
R Merge I(Observed)	**n/a**
Net I Over Average Sigma(I)	**30.5**
B(Isotropic) From Wilson Plot	**23.5**
Redundancy	**4.0**

High Resolution Shell Details

Resolution(High)	**1.65**
Resolution(Low)	**1.71**
Percent Possible(All)	**85.9**
R Merge I(Observed)	**n/a**
Mean I Over Sigma(Observed)	**1.81**
R-Sym I(Observed)	**0.554**
Redundancy	**n/a**
Number Unique Reflections(All)	**6195**

Refinement

Refinement Statistics

Structure Solution Method	MAD
Resolution(High)	1.65
Resolution(Low)	50.00
Cut-off Sigma(I)	n/a
Cut-off Sigma(F)	0.0
Number of Reflections(all)	70306
Number of Reflections(Observed)	70261
Number of Reflections(R-Free)	3563
Percent Reflections(Observed)	97.2
R-Factor(All)	n/a
R-Factor(Observed)	n/a
R-Work	0.20
R-Free	0.22
R-Free **Selection Details**	Random

Temperature Factor Modeling

Isotropic Thermal Model	Restrained
Mean Isotropic B Value	29.213
Anisotropic B[I][I]	-2.561
Anisotropic B[I] [2]	0.0
Anisotropic B[I][3]	2.901
Anisotropic B[2][2]	1.847
Anisotropic B[2][3]	0.0
Anisotropic B[3][3]	0.714

Resolution Shells

Shell Resolution(High)	1.65
Shell Resolution(Low)	1.71
Number of Reflections(Observed)	6104
Number of Reflections(R-Free)	318
R-Factor(R-Work)	5786
R-Factor(R-Free)	0.3199
R-Free Error	n/a
Percent Reflections(Observed)	84.4

RMS Deviations

Parameter Type	**Deviation from Ideal**
c_scangle_it	2.902
c_scbond_it	1.901
c_mcangle_it	1.891
c_mcbond_it	1.223
c_improper_angle_d	0.76
c_dihedral_angle_d	17.96
c_angle_deg	1.11
c_bond_d	0.0050

Coordinate Error

Luzzati ESD(Observed)	0.2

Luzzati Sigma A(Observed)	0.2
Luzzati Resolution Cutoff(Low)	5.0
Luzzati ESD(R-Free Set)	0.21
Luzzati Sigma A(R-Free Set)	0.22

Number of Non-Hydrogen Atoms Used in Refinement

Protein Atoms	4044
Nucleic Acid Atoms	0
Heterogen Atoms	112
Solvent Atoms	210

Software

Programs

Data Collection	Hkl-2000
Data Reduction	**Scalepack**
Structure Solution	**Solve**
Structure Refinement	**Cns**

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Various patents, patent applications, and other publications are cited herein, the contents of which are hereby incorporated by reference in their entireties.

WHAT IS CLAIMED:

1. Atomic coordinates for a $LeuT_{Aa}$ transporter as described in Table 3, in computer readable form.

2. A database containing the atomic coordinates of claim 1.

3. A computer displaying the atomic coordinates of claim 1.

4. A three dimensional computer model of a $LeuT_{Aa}$ transporter.

5. The three dimensional computer model of claim 4, comprising the coordinates of at least two atoms comprised in one or more amino acid residues selected from the following group: G26, L25, Y108, S256, T254, F253, or A22.

6. The three dimensional computer model of claim 5, further comprising the coordinates of at least two atoms comprised in one or more amino acid residues selected from the following group: V104, F259, S355, and I359.

7. The three dimensional computer model of claim 5, further comprising the coordinates of at least two atoms comprised in one or more amino acid residues selected from the following group: T254, N286, N27, V23, G20, T354, A351, and S355.

8. The three dimensional computer model of claim 5, further comprising the coordinates of at least two atoms comprised in one or more amino acid residues selected from the following group: G62, I262, A261, G260, and G258.

9. The three dimensional computer model of claim 5, further comprising the coordinates of at least two atoms comprised in one or more amino acid residues selected from the following group: E290, Y47, Q250, D404, and R30.

10. The three dimensional computer model of claim 9, further comprising the coordinates of at least two atoms comprised in one or more amino acid residues selected from the following group: R5, Y265, A266, S267, Y268, D369, L14, M16, and A17.

11. A computer-based method for identifying binding affinity of a test molecule to a $LeuT_{Aa}$ transporter or a portion thereof, comprising the steps of:

a) entering input data characterizing the atomic coordinates of a LeuTAa transporter, or homologues thereof, into a computer program;

b) generating a three dimensional computer model comprising a model of a functional site of the $LeuTA_a$ transporter;

c) entering input data characterizing the three dimensional structure of at least one test molecule;

d) generating a three dimensional computer model of the test molecules;

e) analyzing the ability of each test molecule to conform to the functional site using the computer program;

f) generating a prediction of a relative binding affinity for each test molecule; and

g) outputting such prediction.

12. A computer based method of using three-dimensional structure of $LeuT_{Aa}$ or a portion thereof in a drug screening assay comprising:

a) performing the method of claim 11 to identify a test molecule with high binding affinity;

b) obtaining the test molecule;

c) contacting the test molecule to a $LeuT_{Aa}$ transporter or homologues thereof; and

d) detecting the binding of the test molecule with the $LeuT_{Aa}$ transporter; wherein binding of the test molecule to the $LeuT_{Aa}$ transporter indicates that the test molecule is a drug candidate.

13. A computer-based method for identifying a potential modulator of a $LeuT_{Aa}$ transporter or a portion thereof, comprising the steps of:

a) entering input data characterizing the atomic coordinates of a $LeuT_{Aa}$ transporter, or homologues thereof, into a computer program;

b) generating a three dimensional computer model comprising a model of a functional site of the LeuTAa transporter;

c) entering input data characterizing the three dimensional structure of a potential modulator;

d) generating a three dimensional computer model of the potential modulator;

e) analyzing the ability of the potential modulator to modulate the functional

site using the computer program;

f) generating a prediction of the ability of the potential modulator to modulator the LeuTAa transporter; and

g) outputting such prediction;

wherein the ability of the potential modulator to change the conformation of the functional site indicates that the potential modulator is an actual modulator.

14. The method of claim 13, further comprising the steps of:

a) obtaining the potential modulator;

b) contacting the potential modulator to a LeuTAa transporter or portions thereof; and

c) detecting the ability of the potential modulator to modulate the $LeuT_A$a transporter;

wherein a potential modulator is selected as a drug if the potential modulator modulates the $LeuT_{Aa}$ transporter, wherein the ability of the potential modulator to increase $LeuT_{Aa}$ activity indicates an agonist, and the ability of the potential modulator to decrease $LeuT_A$a activity indicates an antagonist.

15. The method of claim 13, further comprising the steps of:

a) obtaining the potential modulator;

b) contacting the potential modulator to a homologue of a $LeuTA_a$ transporter, or portions thereof; and

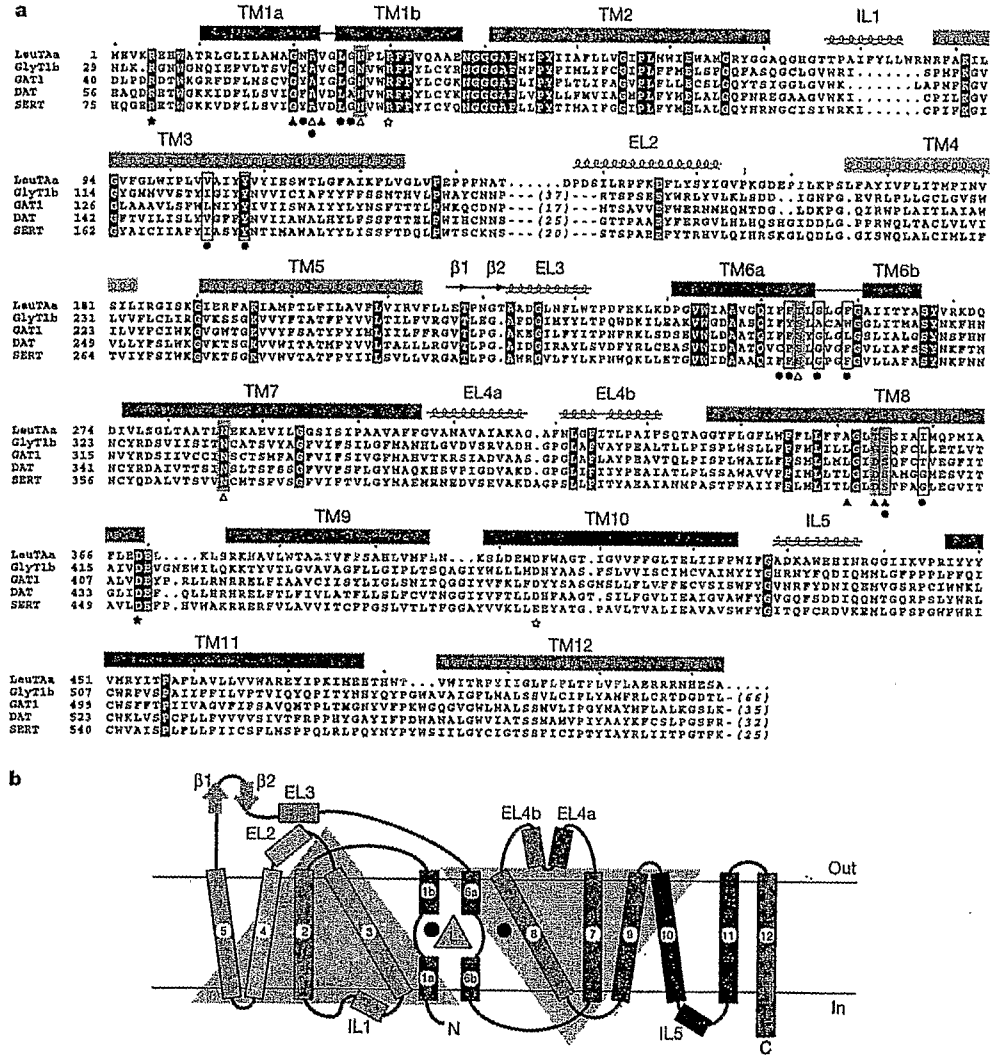
c) detecting the ability of the potential modulator to modulate the $LeuT_{Aa}$ transporter homologue;

wherein a potential modulator is selected as a drug if the potential modulator modulates the $LeuTA_a$ transporter homologue, wherein the ability of the potential modulator to increase $LeuT_{Aa}$ homologue activity indicates an agonist, and the ability of the potential modulator to decrease $LeuT_{Aa}$ homologue activity indicates an antagonist.

16. An isolated, crystalline form of $LeuT_{Aa}$, wherein the crystalline form of $LeuT_{Aa}$ is capable of being used for X-ray crystallographic studies, and wherein the crystalline form of the $LeuT_A$a transporter has a crystal structure with atomic coordinates as set forth in Table 3.

17. The crystalline form of $LeuT_{Aa}$ of claim 11, further comprising leucine.

18. The crystalline form of $LeuT_{Aa}$ of claim 11, further comprising sodium ions.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TM1b
TM2
IL1
TM3
EL2
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TM5
β1
β2
EL3
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EL4a
EL4b
TM8
TM9
TM10
IL5
TM11
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β2
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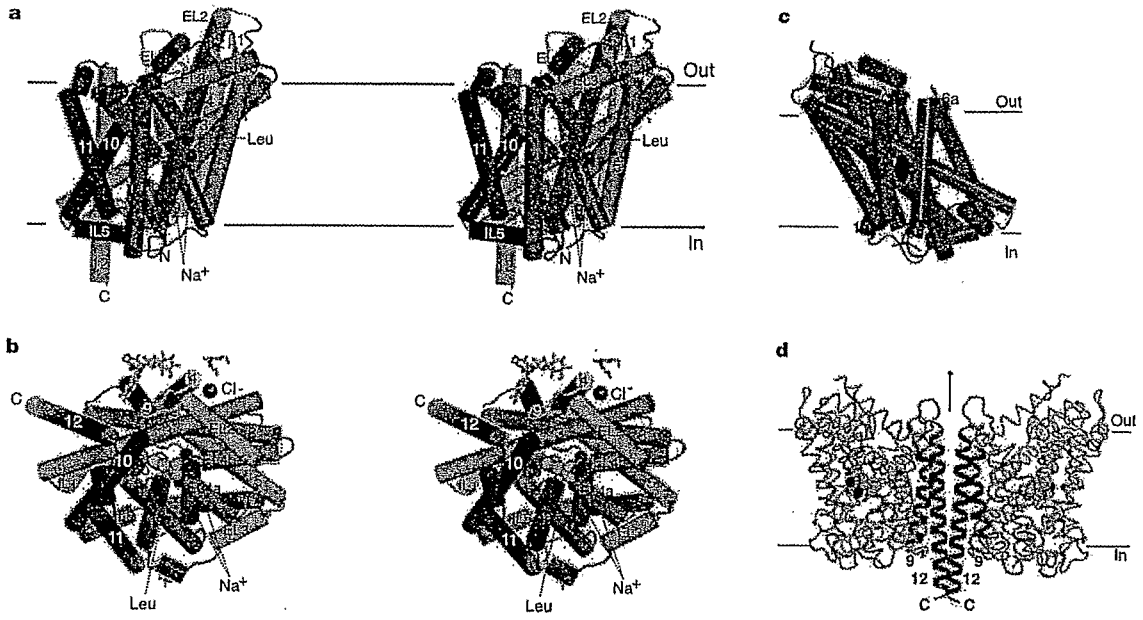
In
IL1
N
IL5
C

Figure 1



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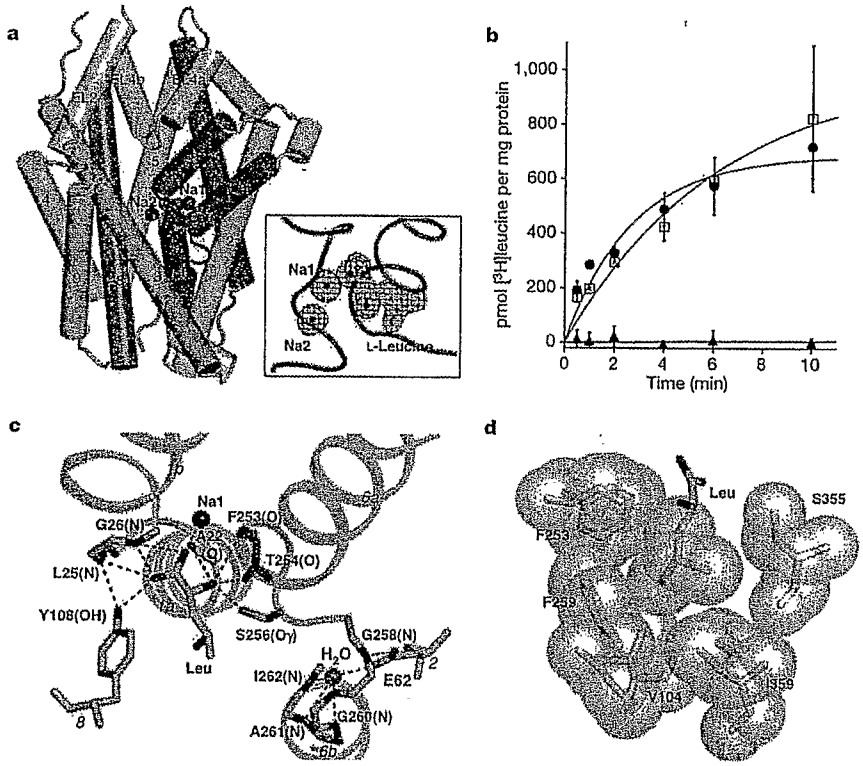
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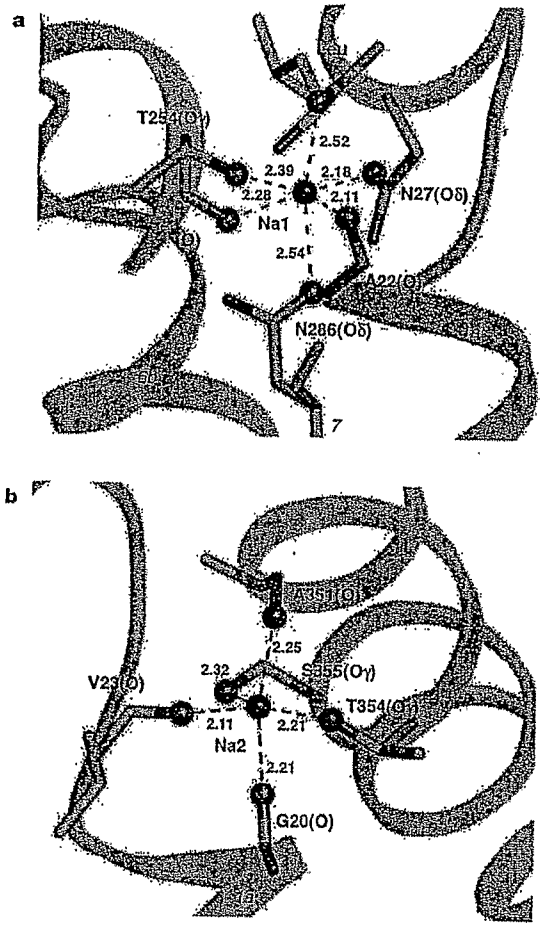
Na1
Na2
L-Leucine
b
pmol [3H]leucine per mg protein
1,000
800
600
400
200
0
0
2
4
6
8
10
Time (min)
c
Na1
G26(N)
F253(O)
T254(O)
L25(N)
Y108(OH)
S256(Oγ)
G258(N)
Leu
H2O
I262(N)
E62
A261(N)
G260(N)
d
Leu
S355
F253
F259
I359
V104

Figure 3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T254(Oγ)
2.52
2.39
2.18
2.28
2.11
N27(Oδ)
Na1
2.54
N286(Oδ)
b
A351(O)
2.25
2.32
S355(Oγ)
V23(O)
T354(Oγ)
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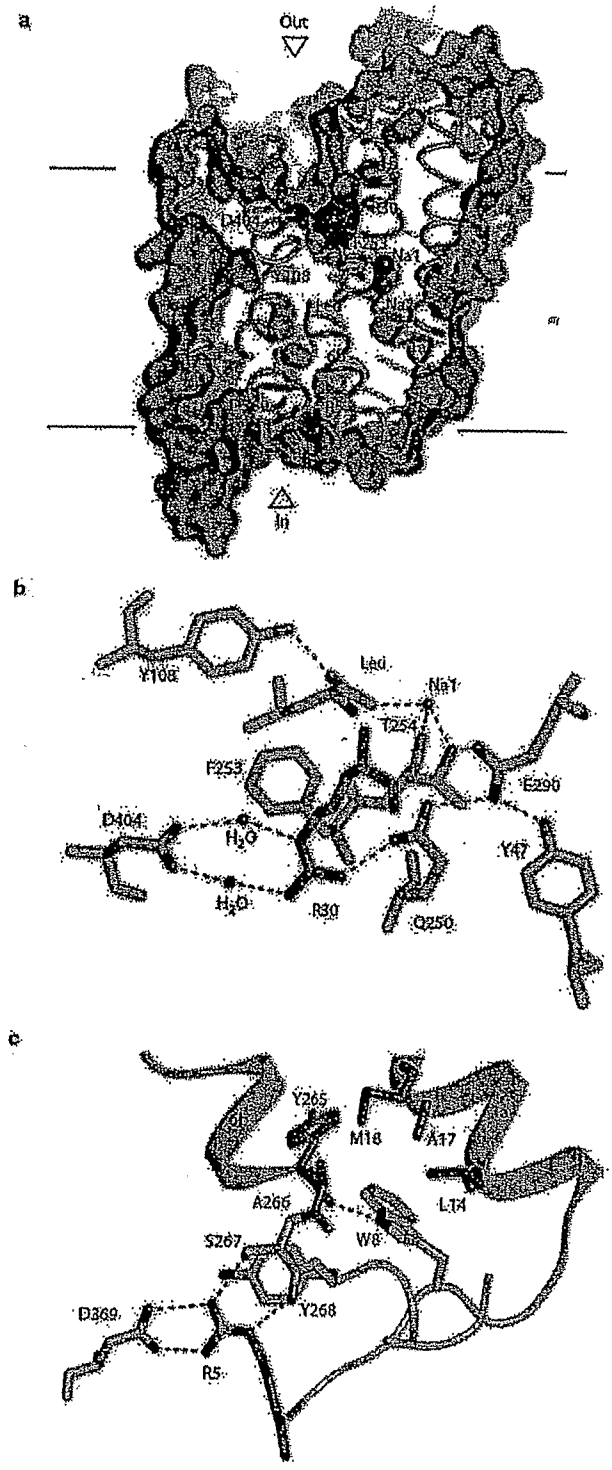
2.21
Na2
2.21
G20(O)

Figure 4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Out
In
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Y108
Leu
Na1
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F253
E290
D404
H_2O
Y47
H_2O
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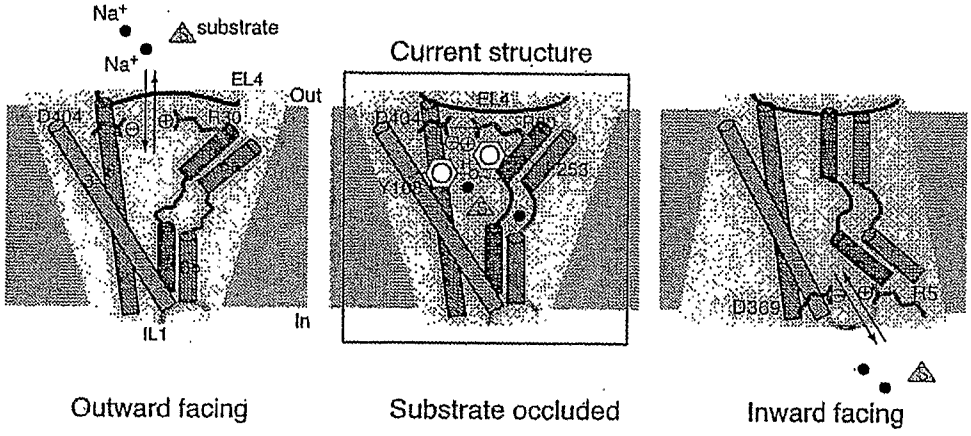
Q250
c
Y265
M18
A17
A266
L14
S267
W8
Y268
D369
R5

Figure 5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substrate
Na+
EL4
Out
D404
H10
IL1
In
Current structure
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EL4
H10
Y106
F253
D369
H5
Outward facing
Substrate occluded
Inward facing

Figure 6

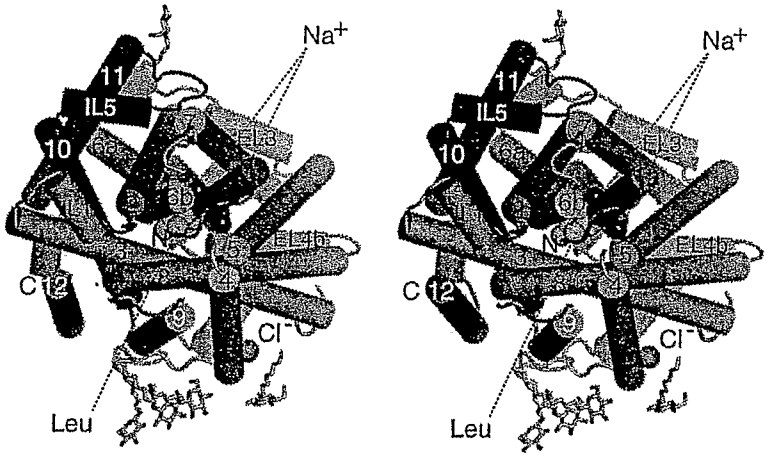
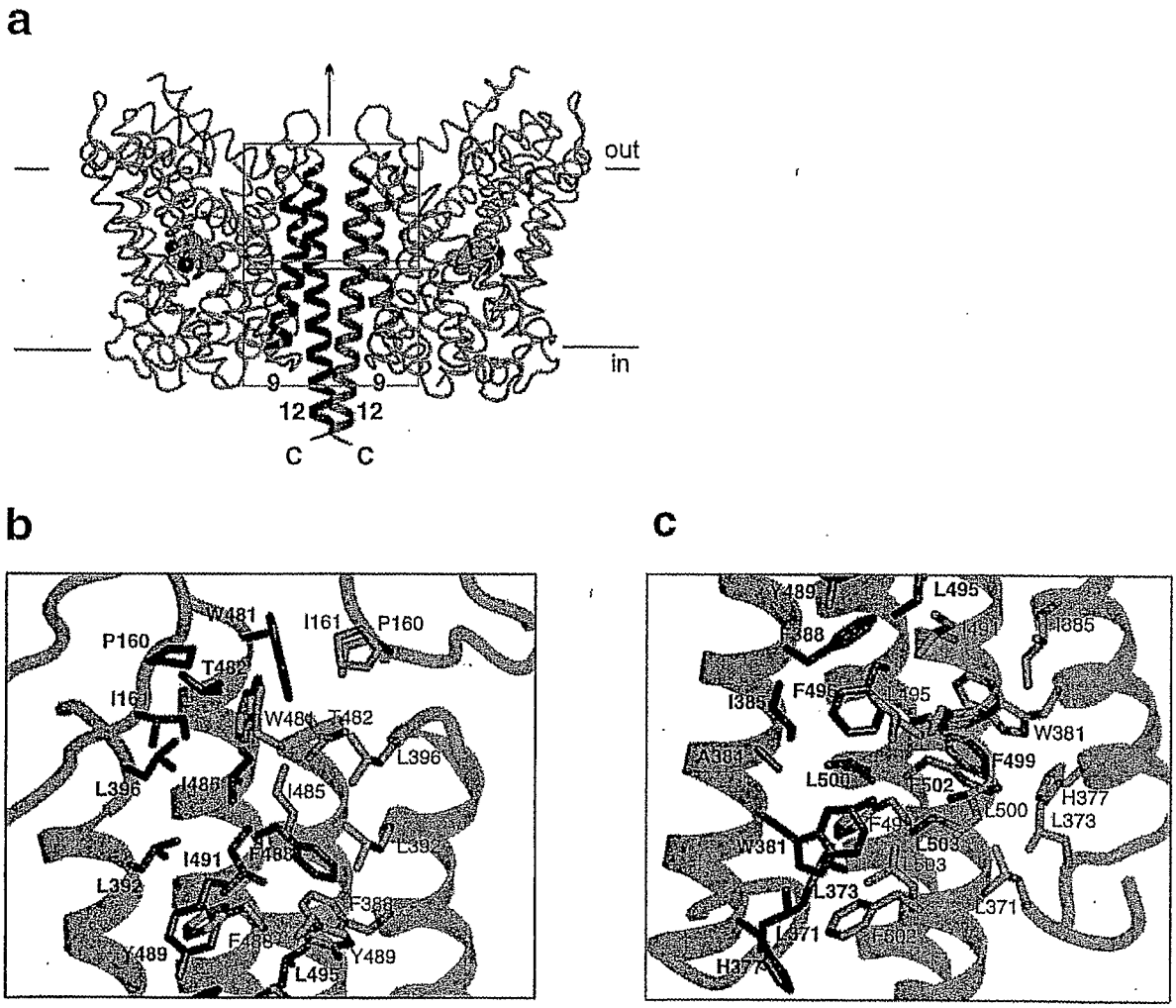


Figure 7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9
9
12
12
C
C
b
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I161
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L396
I485
I485
I491
F488
L392
L392
F388
F488
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Y489
L495
c
Y489
L495
F388
I491
I385
I385
F495
L495
W381
A381
F499
L500
F502
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L371
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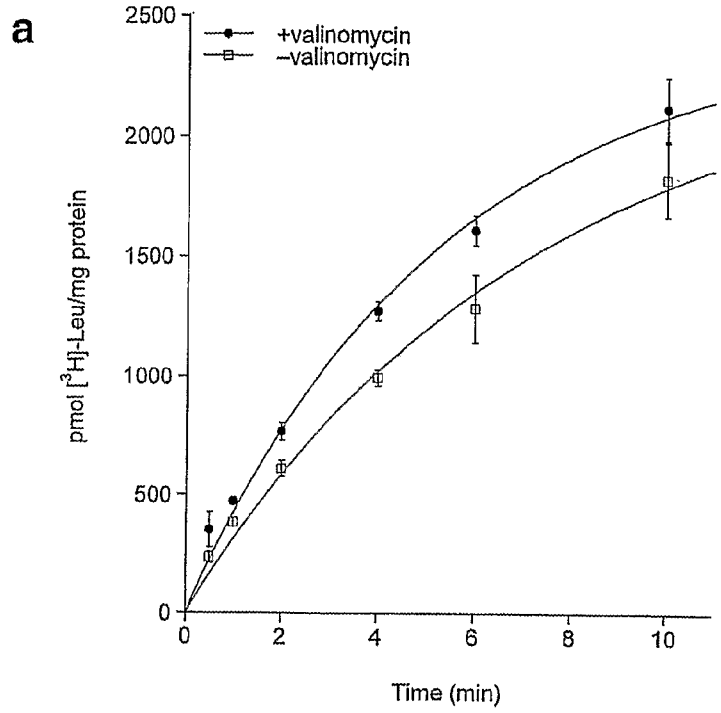
F502
H377

Figure 8



Figure 9


a
+valinomycin
–valinomycin
pmol [3H]-Leu/mg protein
2500
2000
1500
1000
500
0
0
2
4
6
8
10
Time (min)

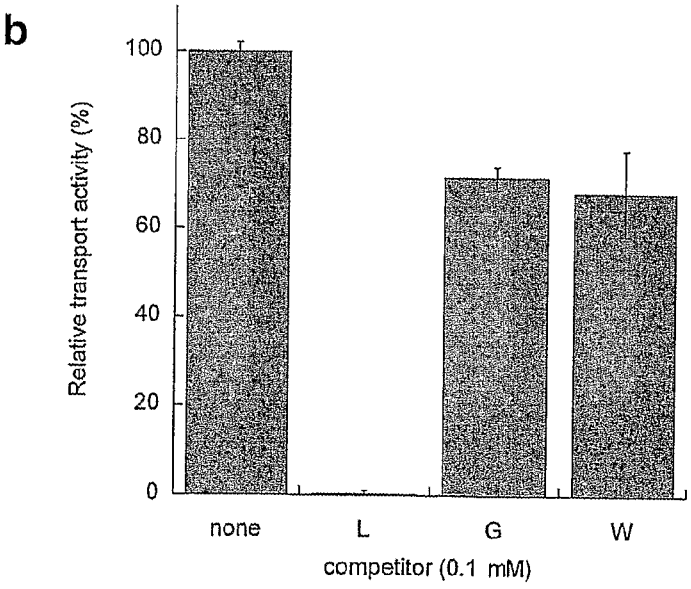

b
Relative transport activity (%)
100
80
60
40
20
0
none
L
G
W
competitor (0.1 mM)

Figure 10

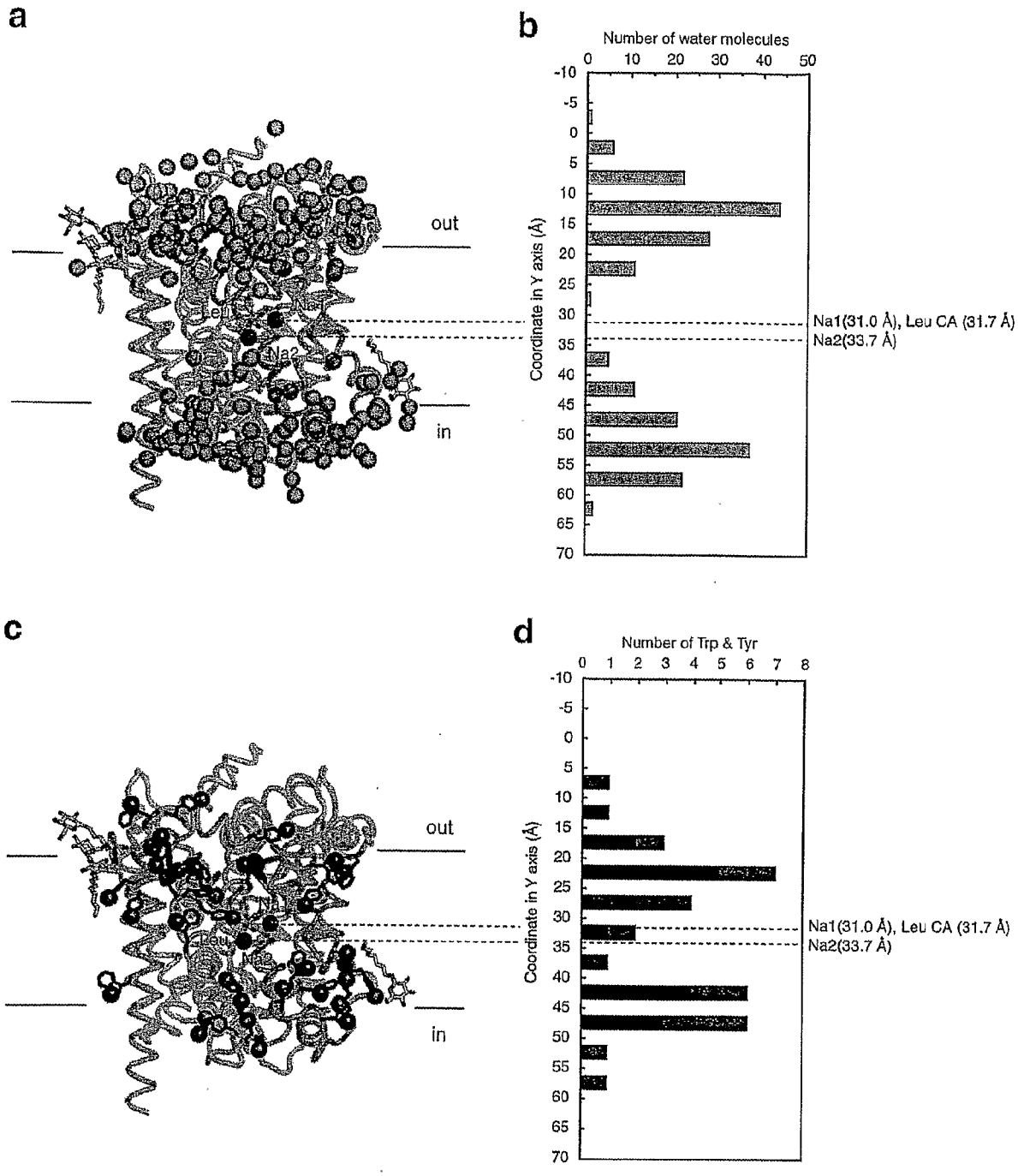

a
out
Leu
Na1
Na2
in
b
Number of water molecules
0 10 20 30 40 50
-10 -5 0 5 10 15 20 25 30 35 40 45 50 55 60 65 70
Coordinate in Y axis (Å)
Na1(31.0 Å), Leu CA (31.7 Å)
Na2(33.7 Å)
c
out
Na1
Leu
Na2
in
d
Number of Trp & Tyr
0 1 2 3 4 5 6 7 8
-10 -5 0 5 10 15 20 25 30 35 40 45 50 55 60 65 70
Coordinate in Y axis (Å)
Na1(31.0 Å), Leu CA (31.7 Å)
Na2(33.7 Å)

Figure 11

INTERNATIONAL SEARCH REPORT

International application No.
PCT/US06/02187

A. CLASSIFICATION OF SUBJECT MATTER
IPC: **G06F 15/00(2006.01);G06G 7/58(2006.01);C07K 14/00(** 2006.01)

USPC: 702/19;703/l l;530/350
According to International Patent Classification (IPC) or to both national classification and IPC

B. FIELDS SEARCHED

Minimum documentation searched (classification system followed by classification symbols)
U.S. : 702/19; 703/1 1; 530/350;

Documentation searched other than minimum documentation to the extent that such documents are included in the fields searched

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

C. DOCUMENTS CONSIDERED TO BE RELEVANT

Category *	Citation of document, with indication, where appropriate, of the relevant passages	Relevant to claim No.
X --- Y	YAMASHITA et al. Crystal Structure of a Bacterial Homologue of Na+/Cl- Dependent Neurotransmitter Transporters. Nature. 8 September 2005. Vol. 437, pp. 215-223. See p. 217, 218, Figures 2 and 3, p. 222, Methods, and p. 223, Author Information (for PDB accession code).	3-10 and 16-17 --- 11-15
X --- Y	PDB Deposit Information for 2A65: atomic coordinates, and deposit information, and displayed 3-D computer model. See all information provided.	3-10 --- 11-15
Y	BOHM, H.J. Towards the Automatic Design of Synthetically Accessible Protein Ligands: Peptides, Amides and Peptidomimetics. Journal of Computer-Aided Molecular Design. 1996. Vol. 10, pp. 265-272. See p. 265-266.	11-15

☒ Further documents are listed in the continuation of Box C. ☐ See patent family annex.

* Special categories of cited documents:

"A" document defining the general state of the art which is not considered to be of particular relevance

"E" earlier application or patent published on or after the international filing date

"L" document which may throw doubts on priority claim(s) or which is cited to establish the publication date of another citation or other special reason (as specified)

"O" document referring to an oral disclosure, use, exhibition or other means

"P" document published prior to the international filing date but later than the priority date claimed

"T" later document published after the international filing date or priority date and not in conflict with the application but cited to understand the principle or theory underlying the invention

"X" document of particular relevance; the claimed invention cannot be considered novel or cannot be considered to involve an inventive step when the document is taken alone

"Y" document of particular relevance; the claimed invention cannot be considered to involve an inventive step when the document is combined with one or more other such documents, such combination being obvious to a person skilled in the art

"&" document member of the same patent family

Date of the actual completion of the international search
18 September 2006 (18.09.2006)

Date of mailing of the international search report
27 NOV 2006

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Form PCT/ISA/210 (second sheet) (April 2005)

INTERNATIONAL SEARCH REPORT

International application No.
PCT/US06/02187

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

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

1. ☒ Claims Nos.: 1 and 2
because they relate to subject matter not required to be searched by this Authority, namely:
Claims drawn to "data" is considered non-statutory subject matter by the USPTO.

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

3. ☐ **Claims Nos.:**
because they are dependent claims and are not drafted in accordance with the second and third sentences of Rule 6.4(a).

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

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

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

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

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

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

Remark on Protest

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

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

☐ No protest accompanied the payment of additional search fees.

INTERNATIONAL SEARCH REPORT

International application No.
PCT/US06/02187

C. (Continuation) DOCUMENTS CONSIDERED TO BE RELEVANT

Category *	Citation of document, with indication, where appropriate, of the relevant passages	Relevant to claim No.
Y	GOODSELL et al. Automated Docking of Flexible Ligands: Application of AutoDock. Journal of Molecular Recognition. 1996. VoI 9, pp. 1-5. See entire document, especially, p. 5, Public availability.	11-15
Y --- A	NELSON, N. The Family of Na+/Cl- Neurotransmitter Transporters. Journal of Neurochemistry. 1998. Vol. 71, pp. 1785-1803. See entire document, especially Abstract and Epilogue.	11-15 --- 3-10 and 16-17
A	YERNOOL et al. Structure of Glutamate Transporter Homologue from Pyrococcus Horikoshii. Nature. 2004. Vol. 431, pp. 811-818. See entire document.	3-17