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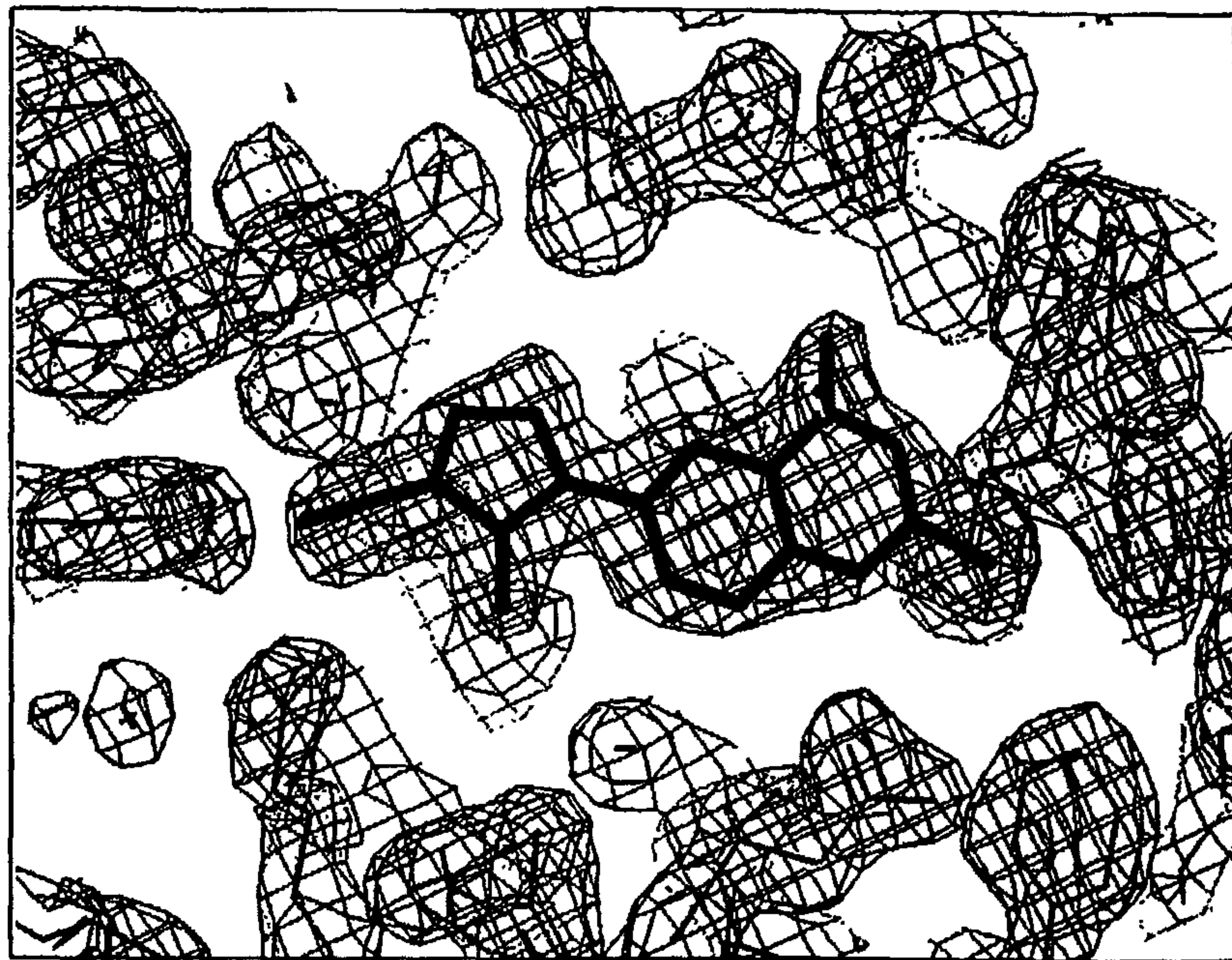
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(54) Title: PROGESTERONE RECEPTOR STRUCTURE



(57) Abrégé/Abstract:

This invention relates to progesterone receptor/ligand complexes, and related methods and software systems.



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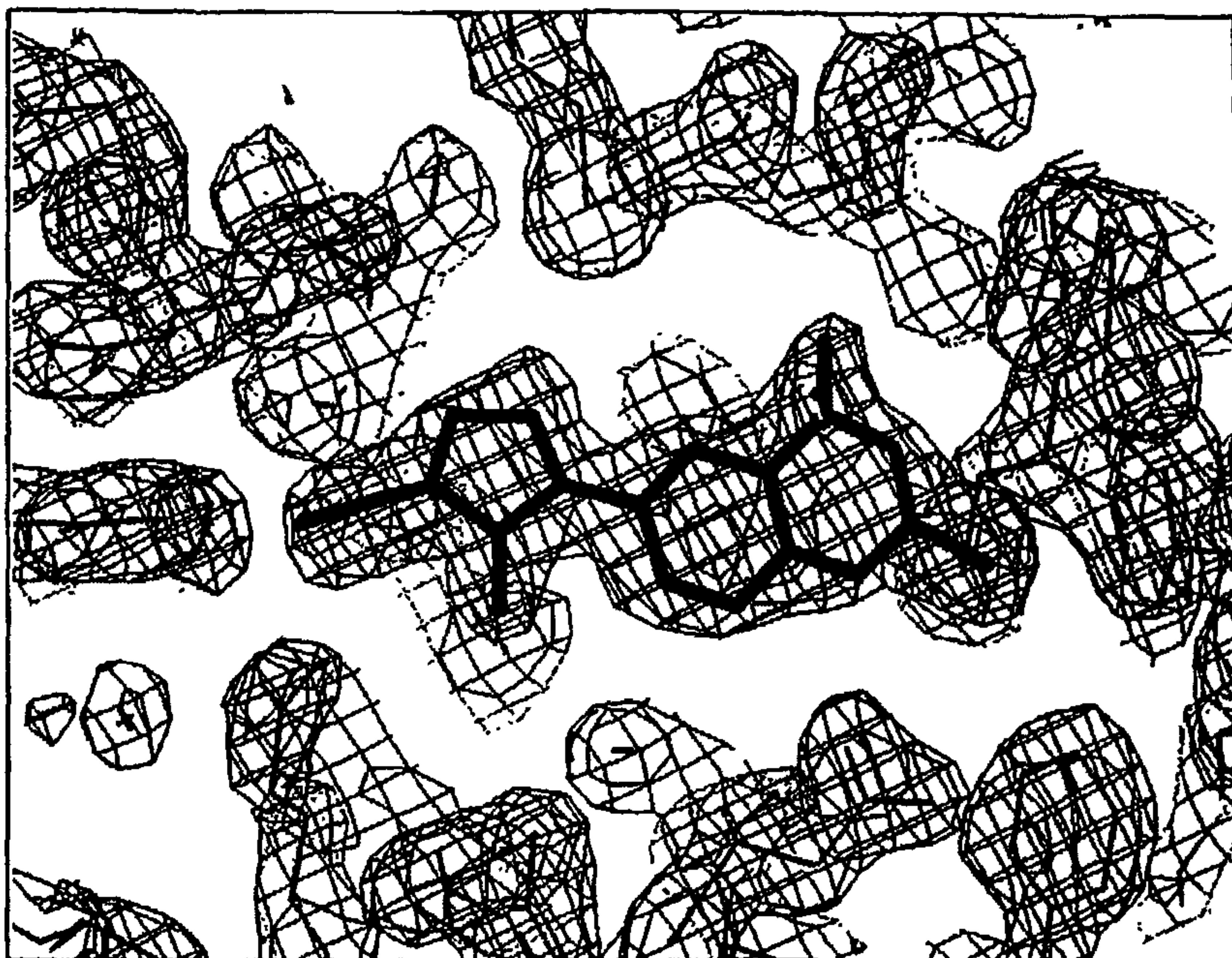
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(54) Title: PROGESTERONE RECEPTOR STRUCTURE



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PROGESTERONE RECEPTOR STRUCTURE

RELATED APPLICATIONS

This application claims the benefit of U.S. Provisional Application No. 60/603,242, filed August 20, 2004, which is incorporated herein by reference in its entirety.

TECHNICAL FIELD

This invention relates to progesterone receptor/ligand complexes, and related methods and software systems.

BACKGROUND

Progesterone is a steroidal hormone that regulates many biological processes. Many of the physiological effects of progesterone are mediated by progesterone receptors (PRs). Interaction of progesterone with progesterone receptor can cause activation of the receptor. This can cause the progesterone receptor to be transported from the cytoplasm into the nucleus. In the nucleus, the progesterone receptor can function as a transcriptional activator, which can cause increased expression of specific gene targets.

SUMMARY

In general, the invention relates to crystalline protein/ligand complexes that include a PR polypeptide bound to a non-steroidal ligand. The PR polypeptide can include the ligand binding domain of the PR, and the non-steroidal ligand can be an agonist or antagonist of the receptor. The invention also relates to methods of using a three-dimensional model of a PR polypeptide/non-steroidal ligand complex to design an agent, such as an agonist or antagonist, that can interact with a PR polypeptide. The invention also features related software methods.

In one aspect, the invention features a crystallized protein-ligand complex that includes a progesterone receptor polypeptide and a non-steroidal ligand. The non-steroidal ligand is an agonist or antagonist of the progesterone receptor polypeptide.

In another aspect, the invention features a crystallized protein-ligand complex that includes a progesterone receptor polypeptide, which includes the amino acid sequence of SEQ ID NO:2, and a non-steroidal ligand. The crystallized protein-ligand complex diffracts X-rays to a resolution of at least about 3.5 Å. The non-steroidal ligand is an agonist or antagonist of the progesterone receptor polypeptide.

In another aspect, the invention features a composition that includes a crystal, which includes a progesterone receptor polypeptide and a non-steroidal ligand. The non-steroidal ligand is an agonist or antagonist of the progesterone receptor polypeptide.

In yet another aspect, the invention features a method that includes using a three-dimensional model to design an agent that interacts with a progesterone receptor polypeptide. The three-dimensional model includes the progesterone receptor polypeptide bound to a non-steroidal ligand that is an agonist or antagonist of the receptor polypeptide.

Another aspect of the invention features a method that includes selecting an agent by performing rational drug design with a three-dimensional structure of a crystalline complex. The complex includes a progesterone receptor polypeptide bound to a non-steroidal ligand that is an agonist or antagonist of the receptor polypeptide, and the method includes contacting the agent with a receptor polypeptide and detecting the ability of the agent to bind the polypeptide.

In another aspect, the invention features a method of growing a crystal that includes a progesterone receptor polypeptide and a non-steroidal ligand that is an agonist or antagonist of the polypeptide. The method includes contacting the receptor polypeptide with the non-steroidal ligand, and the resulting crystal can diffract X-rays to a resolution of at least about 3.5 Å.

Another aspect of the invention features a software system for determining binding characteristics of a candidate agent to a progesterone receptor polypeptide. The software system includes instructions for causing a computer system to accept information relating to the structure of a progesterone receptor polypeptide bound to a non-steroidal ligand that is an agonist or antagonist of the progesterone receptor polypeptide, and to accept information relating to a candidate agent. The determination of binding characteristics is based on the information relating to the structure of the receptor polypeptide and the information relating to the candidate agent.

Another aspect of the invention features a computer program for determining the binding characteristics of a candidate agent to a progesterone receptor polypeptide. The computer program resides on a computer readable medium that includes a plurality of instructions. When executed by one or more processors, the plurality of instructions causes
5 the one or more processors to accept information relating to the structure of a progesterone receptor polypeptide bound to a non-steroidal ligand that is an agonist or antagonist of the progesterone receptor polypeptide, and to accept information relating to a candidate agent. The determination of binding characteristics is based on the information relating to the structure of the receptor polypeptide and the information relating to the candidate agent.

10 In another aspect, the invention features a method for modeling the binding characteristics of a progesterone receptor polypeptide with a candidate agent. The method includes a software system that models the binding characteristics by accepting information relating to the structure of a progesterone receptor polypeptide bound to a non-steroidal ligand that is an agonist or antagonist of the progesterone receptor polypeptide.

15 In yet another aspect, the invention features a computer program for modeling the binding characteristics of a progesterone receptor polypeptide with a candidate agent. The computer program resides on a computer readable medium on which is stored a plurality of instructions. When the instructions are executed by one or more processors, the processors accept information relating to the structure of a progesterone receptor polypeptide bound to a
20 non-steroidal ligand that is an agonist or antagonist of the progesterone receptor polypeptide and the processors model the binding characteristics of the receptor polypeptide with the candidate agent.

In another aspect, the invention features a software system for modeling the binding characteristics of a progesterone receptor polypeptide with a candidate agent. The software
25 system includes instructions for causing a computer system to accept information relating to the structure of a progesterone receptor polypeptide bound to a non-steroidal ligand that is an agonist or antagonist of the progesterone receptor polypeptide and to model the binding characteristics of the receptor polypeptide with a candidate agent.

30 Structural information of a polypeptide can lead to a greater understanding of how the polypeptide functions *in vivo*. For example, knowledge of the structure of a protein can reveal properties that facilitate the interaction of the protein with its ligands, including other

proteins, effector molecules (*e.g.*, hormones), and nucleic acids. In the case of a progesterone receptor, an understanding of such interactions can facilitate the design or selection of ligands (*e.g.*, drugs) that can be useful for modulating the activity of the progesterone receptor *in vivo*, and can therefore be useful for treating a human. Structure based modeling can be used to identify ligands capable of interacting with a PR polypeptide, thus eliminating the need for screening assays, which can be expensive and time-consuming. Structural information can also be used to direct the modification of a ligand known to interact with a PR polypeptide to generate an alternative ligand with more desirable properties, such as tighter binding or greater specificity.

Unless otherwise defined, all technical and scientific terms used herein have the same meaning as commonly understood by one of ordinary skill in the art to which this invention pertains. Although methods and materials similar or equivalent to those described herein can be used in the practice or testing of the present invention, useful methods and materials are described below. The materials, methods, and examples are illustrative only and not intended to be limiting. Other features and advantages of the invention will be apparent from the accompanying drawings and description, and from the claims. The contents of all references, pending patent applications and published patents, cited throughout this application are hereby expressly incorporated by reference. In case of conflict, the present specification, including definitions, will control.

DESCRIPTION OF DRAWINGS

FIG. 1A is an electron density map showing tanaproget bound to the human PR-LBD. The A, B, and C rings of tanaproget are as designated. The benzoxazine moiety of tanaproget is formed of rings B and C.

FIG. 1B is an electron density map showing tanaproget bound to the human PR-LBD.

FIG. 2A shows the amino acid sequence of the human progesterone receptor ligand binding domain (human PR-LBD) (sequence underlined) fused to glutathione-S-transferase (GST) (sequence not underlined) (SEQ ID NO:1). A thrombin cleavage site (LVPRG (SEQ ID NO:3), marked in bold) occurs at the junction between the GST and PR-LBD sequences.

FIG. 2B shows the amino acid sequence (SEQ ID NO:2) of the human PR-LBD. Amino acids are numbered according to the amino acid sequence of the full-length human progesterone receptor (see FIG. 2C).

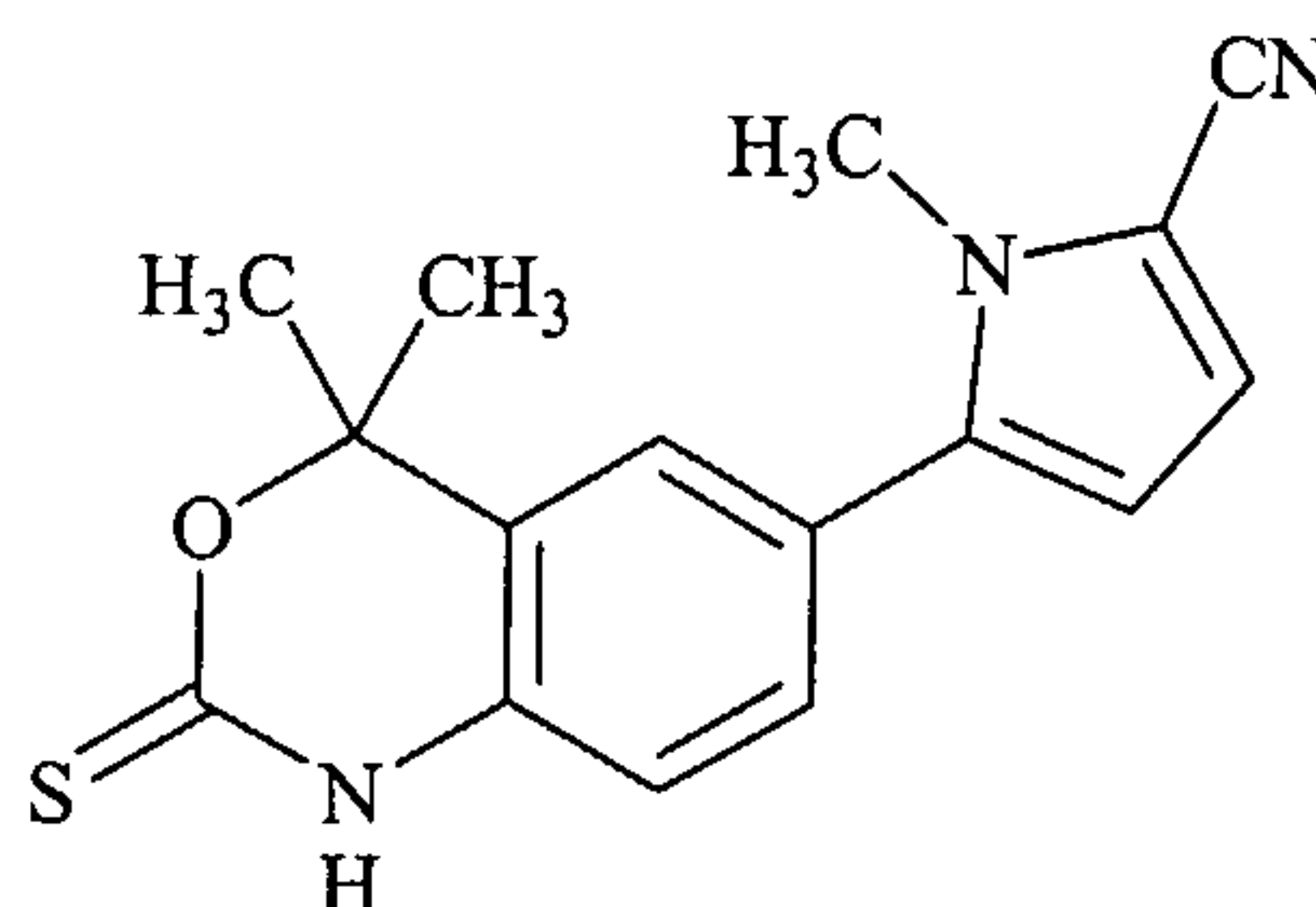
FIG. 2C is the full-length sequence of human progesterone receptor (GenBank
5 Accession Number NM_000926; SEQ ID NO:4). Amino acids of the human PR-LBD are underlined.

DETAILED DESCRIPTION

The structure of the human progesterone receptor ligand binding domain (PR-LBD) bound to the non-steroidal hormone tanaproget (IUPAC name: 5-(4,4-dimethyl-2-thioxo-1,4-dihydro-2H-3,1-benzoxazin-6-yl)-1-methyl-1H-pyrrole-2-carbonitrile; tanaproget is the
10 United States Adopted Name (USAN)) was determined by X-ray crystallography and is described herein. FIGs. 1A and 1B are electron density maps illustrating the structure of the PR-LBD/tanaproget complex. The electron density maps provide evidence indicating that the tertiary structure of the human PR-LBD bound to tanaproget is very similar to that of the
15 human PR-LBD bound to its natural ligand, progesterone. It is therefore believed that the crystal structure of the human PR-LBD/tanaproget complex (see Table 2 below) can be useful for designing or identifying other ligands, such as, for example, non-steroidal ligands, that can also interact with a PR-LBD.

FIGs. 2A and 2B provide information regarding the amino acid sequence of the
20 human PR-LBD, and FIG. 2C provides information regarding the full length sequence of human PR.

The chemical structure of tanaproget is shown below:



In general, a complex of the human PR-LBD bound to tanaproget can be prepared as desired. In some embodiments, such a complex can be prepared as follows. The human PR-LBD is expressed from a DNA plasmid. The expression can be driven by a promoter, such as an inducible promoter. The human PR-LBD can be expressed as a fusion protein with a suitable tag, such as a glutathione-S-transferase (GST), myc, HA, hexahistidine, or FLAG tag. The tag can facilitate isolation of the human PR-LBD from cells. A fusion protein can be cleaved at a protease site engineered into the fusion protein, such as at or near the site of fusion between the polypeptide and the tag. Following cleavage and purification, the human PR-LBD can be contacted with tanaproget. For example, the human PR-LBD can be mixed with tanaproget prior to purification (*e.g.*, prior to cleavage of a polypeptide tag), or the human PR-LBD can be mixed with tanaproget after purification. In some embodiments, tanaproget can be mixed with the human PR-LBD prior to purification and again following purification.

The human PR-LBD and tanaproget can be combined in a solution for collecting spectral data for the human PR-LBD/tanaproget complex, NMR data for the human PR-LBD/tanaproget complex, or for growing a crystal of the human PR-LBD/tanaproget complex. For example, the human PR-LBD/tanaproget complex can be crystallized in the presence of a salt (*e.g.*, a sodium salt), a polymer (*e.g.*, polyethylene glycol (PEG)), and/or an organic solvent. Crystals can be grown by various methods, such as, for example, sitting or hanging drop vapor diffusion. In general, crystallization can be performed at a temperature of from about 4°C to about 60°C (*e.g.*, from about 4°C to about 45°C, such as at about 4°C, about 15°C, about 18°C, about 20°C, about 25°C, about 30°C, about 32°C, about 35°C, about 37°C).

In general, a crystal of the human PR-LBD bound to tanaproget can diffract X-rays to a resolution of about 3.5 Å or less (*e.g.*, about 3.2 Å or less, about 3.0 Å or less, about 2.5 Å or less, about 2.4 Å or less, about 2.3 Å or less, about 2.2 Å or less, about 2.1 Å or less, about 2.0 Å or less, about 1.9 Å or less, about 1.8 Å or less, about 1.7 Å or less, about 1.6 Å or less, about 1.5 Å or less, or about 1.4 Å or less). In some embodiments, a crystal of the human

PR-LBD bound to tanaproget can diffract X-rays to a resolution of from about 1.6 Å to about 2.5 Å (*e.g.*, from about 1.8 Å to about 2.2 Å).

In some embodiments, a crystal of the human PR-LBD bound to tanaproget belongs to space group $P2_1$ with unit cell parameters $a = 57.52$ Å, $b = 64.50$ Å, $c = 70.41$ Å, and $b = 95.76^\circ$. In certain embodiments, a crystal of the human PR-LBD bound to tanaproget can further contain two molecules of the human PR-LBD in the asymmetric unit.

Structural data describing a crystal can be obtained, for example, by X-ray diffraction. X-ray diffraction data can be collected by a variety of sources, X-ray wavelengths and detectors. In some embodiments, rotating anodes and synchrotron sources (*e.g.*, Advanced Light Source (ALS), Berkeley, California; or Advanced Photon Source (APS), Argonne, Illinois) can be used as the source(s) of X-rays. In certain embodiments, X-rays for generating diffraction data can have a wavelength of from about 0.5 Å to about 1.6 Å (*e.g.*, about 0.7 Å, about 0.9 Å, about 1.1 Å, about 1.3 Å, about 1.4 Å, about 1.5 Å, or about 1.6 Å). In some embodiments, area detectors and/or charge-couple devices (CCDs) can be used as the detector(s).

X-ray diffraction data of a crystal of a complex of the human PR-LBD bound to tanaproget can be used to obtain the structural coordinates of the atoms in the complex. The structural coordinates are Cartesian coordinates that describe the location of atoms in three-dimensional space in relation to other atoms in the complex. For example, the structural coordinates listed in Table 2 are the structural coordinates of a crystalline complex of the human PR-LBD bound to tanaproget. These structural coordinates describe the location of atoms of the human PR-LBD in relation to each other, the location of atoms in the human PR-LBD in relation to the atoms in tanaproget, and the location of atoms in tanaproget in relation to each other. The structural coordinates of the complex can be modified by mathematical manipulation, such as by inversion or integer additions or subtractions. As such, structural coordinates are relative coordinates. For example, structural coordinates describing the location of atoms in a PR-LBD bound to tanaproget are not specifically limited by the actual x, y, and z coordinates of Table 2.

The structural coordinates of a complex of the human PR-LBD bound to tanaproget can be used to derive a representation (*e.g.*, a two dimensional representation or three dimensional representation) of the complex, a fragment of the complex, the PR-LBD or a

fragment of the PR-LBD. Such a representation can be useful for a number of applications, including, for example, the visualization, identification and characterization of an active site of the polypeptide. In certain embodiments, a three-dimensional representation can include the structural coordinates of the human PR-LBD according to Table 2 $\pm$ a root mean square deviation from the alpha carbon atoms of amino acids of not more than about 1.5 Å (*e.g.*, not more than about 1.0 Å, not more than about 0.5 Å). Root mean square deviation is the square root of the arithmetic mean of the squares of the deviations from the mean, and is a way of expressing deviation or variation from structural coordinates. Conservative substitutions (see discussion below) of amino acids can result in a molecular representation having structural coordinates within the stated root mean square deviation. For example, two molecular models of polypeptides that differ from one another by conservative amino acid substitutions can have coordinates of backbone atoms within a stated rms deviation, such as less than about 1.5 Å (*e.g.*, less than about 1.0 Å, less than about 0.5 Å). Backbone atoms of a polypeptide include the alpha carbon (C_{α} or CA) atoms, carbonyl carbon (C) atoms, and amide nitrogen (N) atoms.

Various software programs allow for the graphical representation of a set of structural coordinates to obtain a representation of a complex of the human PR-LBD bound to tanaproget or a fragment thereof. In general, such a representation should accurately reflect (relatively and/or absolutely) structural coordinates, or information derived from structural coordinates, such as distances or angles between features. In some embodiments, the representation is a two-dimensional figure, such as a stereoscopic two-dimensional figure. In certain embodiments, the representation is an interactive two-dimensional display, such as an interactive stereoscopic two-dimensional display. An interactive two-dimensional display can be, for example, a computer display that can be rotated to show different faces of a polypeptide, a fragment of a polypeptide, a complex and/or a fragment of a complex. In some embodiments, the representation is a three-dimensional representation. As an example, a three-dimensional model can be a physical model of a molecular structure (*e.g.*, a ball-and-stick model). As another example, a three dimensional representation can be a graphical representation of a molecular structure (*e.g.*, a drawing or a figure presented on a computer display). A two-dimensional graphical representation (*e.g.*, a drawing) can correspond to a three-dimensional representation when the two-dimensional representation reflects three-

dimensional information, for example, through the use of perspective, shading, or the obstruction of features more distant from the viewer by features closer to the viewer. In some embodiments, a representation can be modeled at more than one level. As an example, when the three-dimensional representation includes a polypeptide, such as a complex of the human PR-LBD bound to tanaproget, the polypeptide can be represented at one or more different levels of structure, such as primary (amino acid sequence), secondary (*e.g.*, α -helices and β -sheets), tertiary (overall fold), and quaternary (oligomerization state) structure. A representation can include different levels of detail. For example, the representation can include the relative locations of secondary structural features of a protein without specifying the positions of atoms. A more detailed representation could, for example, include the positions of atoms.

In some embodiments, a representation can include information in addition to the structural coordinates of the atoms in a complex of the human PR-LBD bound to tanaproget. For example, a representation can provide information regarding the shape of a solvent accessible surface, the van der Waals radii of the atoms of the model, and the van der Waals radius of a solvent (*e.g.*, water). Other features that can be derived from a representation include, for example, electrostatic potential, the location of voids or pockets within a macromolecular structure, and the location of hydrogen bonds and salt bridges.

An agent that interacts with a human PR-LBD can be identified or designed by a method that includes using a representation of the human PR-LBD or a fragment thereof, or a complex of human PR-LBD bound to tanaproget or a fragment thereof. Exemplary types of representations include the representations discussed above. In some embodiments, the representation can be of an analog polypeptide, polypeptide fragment, complex or fragment of a complex. A candidate agent that interacts with the representation can be designed or identified by performing computer fitting analysis of the candidate agent with the representation. In general, an agent is a molecule. Examples of agents include polypeptides, nucleic acids (including DNA or RNA), steroids and non-steroidal organic compounds. An agent can be a ligand, and can act as an agonist or antagonist. An agent that interacts with a polypeptide (*e.g.*, a PR polypeptide) can interact transiently or stably with the polypeptide. The interaction can be mediated by any of the forces noted herein, including, for example,

hydrogen bonding, electrostatic forces, hydrophobic interactions, and van der Waals interactions.

As noted above, X-ray crystallography can be used to obtain structural coordinates of a complex of human PR-LBD bound to tanaproget. However, such structural coordinates
5 can be obtained using other techniques including NMR techniques. Additional structural information can be obtained from spectral techniques (*e.g.*, optical rotary dispersion (ORD), circular dichroism (CD)), homology modeling, and computational methods (*e.g.*, computational methods that can include data from molecular mechanics, computational methods that include data from dynamics assays).

10 In some embodiments, the X-ray diffraction data can be used to construct an electron density map of a complex of human PR-LBD bound to tanaproget or a fragment thereof, and the electron density map can be used to derive a representation (*e.g.*, a two dimensional representation, a three dimensional representation) of human PR-LBD bound to tanaproget or a fragment thereof. Creation of an electron density map typically involves using information
15 regarding the phase of the X-ray scatter. Phase information can be extracted, for example, either from the diffraction data or from supplementing diffraction experiments to complete the construction of the electron density map. Methods for calculating phase from X-ray diffraction data include, for example, multiwavelength anomalous dispersion (MAD), multiple isomorphous replacement (MIR), multiple isomorphous replacement with
20 anomalous scattering (MIRAS), single isomorphous replacement with anomalous scattering (SIRAS), reciprocal space solvent flattening, molecular replacement, or a combination thereof. These methods generate phase information by making isomorphous structural modifications to the native protein, such as by including a heavy atom or changing the scattering strength of a heavy atom already present, and then measuring the diffraction
25 amplitudes for the native protein and each of the modified cases. If the position of the additional heavy atom or the change in its scattering strength is known, then the phase of each diffracted X-ray can be determined by solving a set of simultaneous phase equations. The location of heavy atom sites can be identified using a computer program, such as SHELXS (Sheldrick, Institut Anorg. Chemie, Göttingen, Germany), and diffraction data can
30 be processed using computer programs such as MOSFLM, SCALA, SOLOMON, and SHARP ("The CCP4 Suite: Programs for Protein Crystallography," *Acta Crystallogr. Sect.*

D, 54:905-921, 1997; deLa Fortelle and Brigogne, *Meth. Enzym.* 276:472-494, 1997). Upon determination of the phase, an electron density map of the polypeptide or the complex can be constructed.

The electron density map can be used to derive a representation of a polypeptide or a complex, or a fragment of a polypeptide or complex, by aligning a three-dimensional model of a previously known polypeptide or a previously known complex (e.g., a complex containing a polypeptide bound to a ligand) with the electron density map. This process results in a comparative model that shows the degree to which the calculated electron density map varies from the model of the previously known polypeptide or the previously known complex. The comparative model is then refined over one or more cycles (e.g., two cycles, three cycles, four cycles, five cycles, six cycles, seven cycles, eight cycles, nine cycles, 10 cycles) to generate a better fit with the electron density map. A software program such as CNS (Brunger *et al.*, *Acta Crystallogr.* D54:905-921, 1998) can be used to refine the model. The quality of fit in the comparative model can be measured by, for example, an R_{work} or R_{free} value. A smaller value of R_{work} or R_{free} generally indicates a better fit. Misalignments in the comparative model can be adjusted to provide a modified comparative model and a lower R_{work} or R_{free} value. The adjustments can be based on information (e.g., sequence information) relating to human PR-LBD, tanaproget, the previously known polypeptide and/or the previously known complex. As an example, in embodiments in which a model of a previously known complex of a polypeptide bound to a ligand is used, an adjustment can include replacing the ligand in the previously known complex with tanaproget. As another example, in certain embodiments, an adjustment can include replacing an amino acid in the previously known polypeptide with the amino acid in the corresponding site of human PR-LBD. When adjustments to the modified comparative model satisfy a best fit to the electron density map, the resulting model is that which is determined to describe the polypeptide or complex from which the X-ray data was derived (e.g., the PR-LBD/tanaproget complex). Methods of such processes are disclosed, for example, in Carter and Sweet, eds., "Macromolecular Crystallography" in *Methods in Enzymology*, Vol. 277, Part B, New York: Academic Press, 1997, and articles therein, e.g., Jones and Kjeldgaard, "Electron-Density Map Interpretation," p. 173, and Kleywegt and Jones, "Model Building and Refinement Practice," p. 208.

In some embodiments, a representation of human PR-LBD bound to tanaproget can be derived by aligning a previously determined structural model of progesterone bound to human PR-LBD (e.g., Protein Databank Identification No. 1a28) with the electron density map of human PR-LBD bound to tanaproget derived from X-ray diffraction data. One
5 adjustment that can be used in the modeling process can include replacing progesterone with tanaproget.

A machine, such as a computer, can be programmed in memory with the structural coordinates of a complex of the human PR-LBD bound to tanaproget, together with a program capable of generating a graphical representation of the structural coordinates on a
10 display connected to the machine. Alternatively or additionally, a software system can be designed and/or utilized to accept and store the structural coordinates. The software system can be capable of generating a graphical representation of the structural coordinates. The software system can also be capable of accessing external databases to identify compounds (e.g., polypeptides) with similar structural features as human PR-LBD, and/or to identify one
15 or more candidate agents with characteristics that may render the candidate agent(s) likely to interact with human PR-LBD.

A machine having a memory containing structure data or a software system containing such data can aid in the rational design or selection of PR agonists and/or PR antagonists. For example, such a machine or software system can aid in the evaluation of the
20 ability of an agent to associate with a complex of the human PR-LBD bound to tanaproget, or can aid in the modeling of compounds or proteins related by structural or sequence homology to a PR-LBD.

The machine can produce a representation (e.g., a two dimensional representation, a three dimensional representation) of a complex of the human PR-LBD bound to tanaproget or a fragment thereof. A software system, for example, can cause the machine to produce
25 such information. The machine can include a machine-readable data storage medium including a data storage material encoded with machine-readable data. The machine-readable data can include structural coordinates of atoms of a complex of the human PR-LBD bound to tanaproget or a fragment thereof. Machine-readable storage media (e.g., data
30 storage material) include, for example, conventional computer hard drives, floppy disks, DAT tape, CD-ROM, DVD, and other magnetic, magneto-optical, optical, and other media which

may be adapted for use with a machine (*e.g.*, a computer). The machine can also have a working memory for storing instructions for processing the machine-readable data, as well as a central processing unit (CPU) coupled to the working memory and to the machine-readable data storage medium for the purpose of processing the machine-readable data into the desired three-dimensional representation. A display can be connected to the CPU so that the three-dimensional representation can be visualized by the user. Accordingly, when used with a machine programmed with instructions for using the data (*e.g.*, a computer loaded with one or more programs of the sort described herein) the machine is capable of displaying a graphical representation (*e.g.*, a two dimensional graphical representation, a three-dimensional graphical representation) of any of the polypeptides, polypeptide fragments, complexes, or complex fragments described herein.

A display (*e.g.*, a computer display) can show a representation of a complex of human PR-LBD bound to tanaproget or a fragment thereof. The user can inspect the representation and, using information gained from the representation, generate a model of a complex or fragment thereof that includes an agent other than tanaproget. The model can be generated, for example, by altering a previously existing representation of a human PR-LBD/tanaproget complex. Optionally, the user can superimpose a three-dimensional model of an agent on the representation of human PR-LBD bound to tanaproget. The agent can be an agonist (*e.g.*, a candidate agonist) of human PR-LBD or an antagonist (*e.g.*, a candidate antagonist) of human PR-LBD. In some embodiments, the agent can be a known compound or fragment of a compound. In certain embodiments, the agent can be a previously unknown compound, or a fragment of a previously unknown compound.

It can be desirable for the agent to have a shape that complements the shape of the active site. There can be a preferred distance, or range of distances, between atoms of the agent and atoms of the PR polypeptide. Distances longer than a preferred distance may be associated with a weak interaction between the agent and active site (*e.g.*, human PR-LBD). Distances shorter than a preferred distance may be associated with repulsive forces that can weaken the interaction between the agent and the polypeptide. A steric clash can occur when distances between atoms are too short. A steric clash occurs when the locations of two atoms are unreasonably close together, for example, when two atoms are separated by a distance less than the sum of their van der Waals radii. If a steric clash exists, the user can adjust the

position of the agent relative to the PR polypeptide (*e.g.*, a rigid body translation or rotation of the agent), until the steric clash is relieved. The user can adjust the conformation of the agent or of the PR polypeptide in the vicinity of the agent in order to relieve a steric clash. Steric clashes can also be removed by altering the structure of the agent, for example, by changing a “bulky group,” such as an aromatic ring, to a smaller group, such as to a methyl or hydroxyl group, or by changing a rigid group to a flexible group that can accommodate a conformation that does not produce a steric clash. Electrostatic forces can also influence an interaction between an agent and a ligand-binding domain. For example, electrostatic properties can be associated with repulsive forces that can weaken the interaction between the agent and the PR polypeptide. Electrostatic repulsion can be relieved by altering the charge of the agent, *e.g.*, by replacing a positively charged group with a neutral group.

Forces that influence binding strength between tanaproget and human PR-LBD can be evaluated in the polypeptide/agent model. These can include, for example, hydrogen bonding, electrostatic forces, hydrophobic interactions, van der Waals interactions, dipole-dipole interactions, π -stacking forces, and cation- π interactions. The user can evaluate these forces visually, for example by noting a hydrogen bond donor/acceptor pair arranged with a distance and angle suitable for a hydrogen bond. Based on the evaluation, the user can alter the model to find a more favorable interaction between the PR polypeptide and the agent. Altering the model can include changing the three-dimensional structure of the polypeptide without altering its chemical structure, for example by altering the conformation of amino acid side chains or backbone dihedral angles. Altering the model can include altering the position or conformation of the agent, as described above. Altering the model can also include altering the chemical structure of the agent, for example by substituting, adding, or removing groups. For example, if a hydrogen bond donor on the PR polypeptide is located near a hydrogen bond donor on the agent, the user can replace the hydrogen bond donor on the agent with a hydrogen bond acceptor.

The relative locations of an agent and the PR polypeptide, or their conformations, can be adjusted to find an optimized binding geometry for a particular agent to the PR polypeptide. An optimized binding geometry is characterized by, for example, favorable hydrogen bond distances and angles, maximal electrostatic attractions, minimal electrostatic repulsions, the sequestration of hydrophobic moieties away from an aqueous environment,

and the absence of steric clashes. The optimized geometry can have the lowest calculated energy of a family of possible geometries for a PR polypeptide/agent complex. An optimized geometry can be determined, for example, through molecular mechanics or molecular dynamics calculations.

5 A series of representations of complexes of human PR-LBD bound to tanaproget, where tanaproget is replaced or overlaid with different agents, can be generated. A score can be calculated for each representation. The score can describe, for example, an expected strength of interaction between human PR-LBD and the agent. The score can reflect one of the factors described above that influence binding strength. The score can be an aggregate
10 score that reflects more than one of the factors. The different agents can be ranked according to their scores.

 Steps in the design of the agent can be carried out in an automated fashion by a machine. For example, a representation of PR-LBD can be programmed in the machine, along with representations of candidate agents. The machine can find an optimized binding
15 geometry for each of the candidate agents to the active site, and calculate a score to determine which of the agents in the series is likely to interact most strongly with human PR-LBD.

 A software system can be designed and/or implemented to facilitate these steps. Software systems (*e.g.*, computer programs) used to generate such three-dimensional models
20 or perform the necessary fitting analyses include, but are not limited to: MCSS, Ludi, QUANTA, Insight II, Cerius2, CHARMm, and Modeler from Accelrys, Inc. (San Diego, CA); SYBYL, Unity, FleXX, and LEAPFROG from TRIPOS, Inc. (St. Louis, MO); AUTODOCK (Scripps Research Institute, La Jolla, CA); GRID (Oxford University, Oxford, UK); DOCK (University of California, San Francisco, CA); and Flo+ and Flo99 (Thistlesoft,
25 Morris Township, NJ). Other useful programs include ROCS, ZAP, FRED, Vida, and Szybki from Openeye Scientific Software (Santa Fe, NM); Maestro, Macromodel, and Glide from Schrodinger, LLC (Portland, OR); MOE (Chemical Computing Group, Montreal, Quebec), Allegrow (Boston De Novo, Boston, MA), CNS (Brunger, *et al.*, *Acta Crystall.* Sect. D 54:905-921, 1997) and GOLD (Jones *et al.*, *J. Mol. Biol.* 245:43-53, 1995). The structural
30 coordinates can also be used to visualize the three-dimensional structure of PKC θ using MOLSCRIPT, RASTER3D, or PYMOL (Kraulis, *J. Appl. Crystallogr.* 24: 946-950, 1991;

Bacon and Anderson, *J. Mol. Graph.* 6: 219-220, 1998; DeLano, The PYMOL Molecular Graphics System (2002) DeLano Scientific, San Carlos, CA).

The agent, whether an agonist or antagonist, can, for example, be selected by screening an appropriate database, can be designed *de novo* by analyzing the steric configurations and charge potentials of unbound human PR-LBD in conjunction with the appropriate software systems, and/or can be designed using characteristics of known agonists or antagonists of progesterone receptors or other hormone receptors. The method can be used to design or select agonists or antagonists of human PR-LBD. A software system can be designed and/or implemented to facilitate database searching, and/or agent selection and design.

Once an agent has been designed or identified, it can be obtained or synthesized and further evaluated for its effect on human PR-LBD activity. For example, the agent can be evaluated by contacting it with human PR-LBD and measuring the effect of the agent on polypeptide activity. A method for evaluating the agent can include an activity assay performed *in vitro* or *in vivo*. An activity assay can be a cell-based assay, for example. Depending upon the action of the agent on human PR-LBD, the agent can act either as an agonist or antagonist of human PR-LBD activity. The agent also can be contacted with the polypeptide in the presence of progesterone in order to determine whether or not the agent inhibits binding of progesterone to the polypeptide. A crystal containing human PR-LBD bound to the identified agent can be grown and the structure determined by X-ray crystallography. A second agent can be designed or identified based on the interaction of the first agent with human PR-LBD.

Various molecular analysis and rational drug design techniques are further disclosed in, for example, U.S. Patent Nos. 5,834,228, 5,939,528 and 5,856,116, as well as in PCT Application No. PCT/US98/16879, published as WO 99/09148.

While certain embodiments have been described, other embodiments are also contemplated.

As an example, while embodiments involving the human PR-LBD and tanaproget have been described, the description herein is more generally directed to any PR polypeptide and any non-steroidal ligand.

A PR polypeptide can be a full-length, mature polypeptide, including the full-length amino acid sequence of any isoform of a PR polypeptide. An isoform is any of several multiple forms of a protein that differ in their primary structure. For example, human progesterone receptor exists in at least two isoforms, Pr-B (full-length PR) and Pr-A (N-terminally truncated PR). The two isoforms are transcribed from a single gene, but have different translation start sites. Thus the isoforms are identical except that Pr-B contains an additional 164 N-terminal amino acids. The isoforms have an identical centrally located DNA binding domain, which is flanked at the N-terminus by a transcriptional activation function-1 (AF-1) domain, and at the C-terminus by a hinge region containing nuclear localization signals and a ligand binding domain (PR-LBD). A second transcriptional activation function domain (AF-2) is located in the PR-LBD.

A PR polypeptide can be a fragment of a PR, such as a ligand binding domain, a DNA-binding domain, a protein-interaction domain (*e.g.*, an activation domain), or a combination thereof.

A PR polypeptide can have an active site. In general, an active site can include a site of ligand binding, or a site of phosphorylation, glycosylation, alkylation, acylation, or other covalent modification. A ligand binding site can include accessory binding sites adjacent or proximal to the actual site of binding that may affect activity upon interaction with the ligand. An active site of a PR polypeptide can include amino acids of SEQ ID NO:2. For example, an active site of a PR-polypeptide can include one or more of amino acids Ile699, Ala701, Leu714, Leu715, Leu718, Asn719, Leu721, Gln725, Trp755, Met756, Met759, Val760, Leu763, Arg766, Ser767, Tyr777, Phe778, Ala779, Leu782, Phe794, Leu797, Lys798, Met801, Ile804, Leu887, His888, Tyr890, Cys891, Asn893, Thr894, Phe895, Ser898, Leu901, Val903, Phe905, Met909, Ile913, and Leu917 as defined by SEQ ID NO:2.

The numbering of the amino acids of a PR polypeptide may be different than that set forth herein, and the sequence of the PR polypeptide may contain certain conservative amino acid substitutions that yield the same three-dimensional structure. For example, the numbering of a PR-LBD may be different than that set forth in FIG. 2B, and the sequence of the PR-LBD may contain conservative amino acid substitutions but yield the same structure as that defined by the coordinates of Table 2 and illustrated in FIGs. 1A and 1B.

Corresponding amino acids and conservative substitutions in other isoforms or analogs are

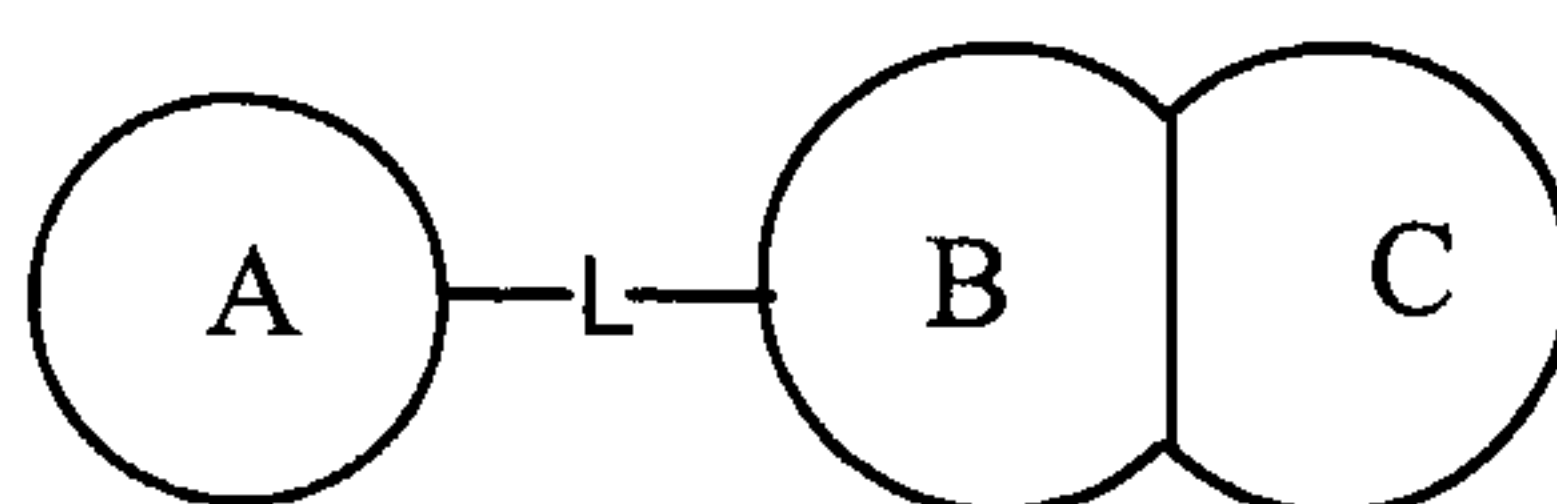
easily identified by visual inspection of the relevant amino acid sequences or by using commercially available homology software programs (*e.g.*, MODELLAR, MSI, San Diego, CA).

An analog is a polypeptide having conservative amino acid substitutions. A conservative substitution can include switching one amino acid for another with similar polarity, steric arrangement, or of the same class (*e.g.*, hydrophobic, acidic or basic), and includes substitutions having an inconsequential effect on the three-dimensional structure of the PR polypeptide with respect to identification and design of agents that interact with the polypeptide (*e.g.*, a PR-LBD), as well as for molecular replacement analyses and/or for homology modeling.

A PR polypeptide can originate from a nonmammalian or mammalian species. A mammalian PR polypeptide can originate from a human, for example. Exemplary nonhuman mammals include, a nonhuman primate (such as a monkey or ape), a mouse, rat, goat, cow, bull, pig, horse, sheep, wild boar, sea otter, cat, and dog. Exemplary nonmammalian species include chicken, turkey, shrimp, alligator, and fish.

As another example, while embodiments have been described in which tanaproget is a ligand, more generally other non-steroidal compounds may also be used as ligands. For example, based on a representation of the human PR-LBD bound to tanaproget derived from the structure of the crystalline complex, without wishing to be bound by theory it is believed that: the carbonitrilo nitrogen of tanaproget forms hydrogen bonds with the side chains of Gln725 and Arg766 of the human PR-LBD; the benzoxazine nitrogen of tanaproget forms hydrogen bonds with the side chain oxygen of Asn719 of the human PR-LBD; hydrophobic interactions occur between Leu797 of the human PR-LBD and the hydrophobic region of the benzoxazine moiety (which includes the pair of methyl substituents in the 4 position) of tanaproget; and an electrostatic interaction occurs between Thr894 of the human PR-LBD and the sulfur of tanaproget.

Based on this information, without wishing to be bound by theory, it is believed that other non-steroidal compounds capable of having one or more similar interactions with the human PR-LBD may also be capable of acting as ligands (*e.g.*, agonists, antagonists) for the human PR-LBD. Such non-steroidal compounds may have the structure:



where A, B and C represent ring systems, B and C are fused rings, and L is a linker moiety.

In general, rings A, B and C are each independently formed of at least four atoms (e.g., five atoms, six atoms, seven atoms, eight atoms, nine atoms, 10 atoms, 11 atoms, 12 atoms, 13 atoms, 14 atoms). One or more atoms (e.g., one atom, two atoms, three atoms, four atoms) in rings A, B and/or C can independently be heteroatoms (e.g., N, S, O). In some embodiments, rings B and C form an indole, an oxindole, a thioindole, a benzothiophene, a benzofuran, a benzothiazole, a benzimidazole, a benzoxazine or a benzthiazine. In one embodiment rings B and C can form a benzoxazine ring that can have at least one hydrophobic substituent at the 4 position. In another embodiment the benzoxazine ring can have at least one hydrophobic substituent near the 4 position e.g. at the 5 position. Benzoxazine derivatives are described, for example, in U.S. Patent No. 6,562,857, which is hereby incorporated by reference. Ring A can be, for example, a pyrrole, a furan, a thiophene, an imidazole, an oxazole, or a phenyl. In some embodiments, rings A, B and/or C can each independently include one or more (e.g., one, two, three, four) substituents (e.g., one or more substituents that provide favorable interaction with the human PR-LBD, such as, for example, through hydrogen bonding, hydrophobic interaction and/or electrostatic interaction). Examples of substituents include hydroxy substituents, amino substituents, cyano substituents, nitro substituents, oxime substituents, thiol substituents, amido substituents, oxo substituents, alkyl substituents e.g. having 1-6 carbon atoms, alkenyl substituents e.g. having 2-6 carbon atoms, alkynyl substituents e.g. having 2-6 carbon atoms, aryl substituents e.g. an aromatic carbocyclic mono- or polycyclic ring system having from 6-20 ring carbon atoms, cyclyl substituents e.g. a saturated or partially saturated mono- or polycyclic carbocyclic ring system having from 3-14 ring atoms, heteroaryl substituents e.g. an aromatic heterocyclic mono- or polycyclic ring system having from 5-14 ring atoms wherein 1, 2, 3 or 4 of the ring atoms are selected from N, O or S, heterocyclyl substituents e.g. a saturated or partially saturated mono- or polycyclic heterocyclic ring system having from 3-14 ring atoms wherein 1, 2, 3 or 4 of the ring atoms are selected from N, O or S, and halogens (e.g., fluorine, chlorine, bromine, iodine). While in some embodiments, a

substituent itself may be a hydrogen bond donor or acceptor with the human PR-LBD, in other embodiments, the substituent may form a hydrogen bond with a portion of the human PR-LBD through one or more solvent molecules such as water.

In general, L can be a direct chemical bond, or L can be formed of a chemical moiety, such as, for example, an alkyl moiety e.g. having 1-6 carbon atoms, an alkenyl moiety e.g. having 2-6 carbon atoms, an alkynyl moiety e.g. having 2-6 carbon atoms, an ether moiety, a thioether moiety, an amido moiety, a carbonyl moiety or a sulfonyl moiety. In some embodiments, L can be formed of multiple moieties (e.g., a sulfonyl moiety bonded to an alkyl moiety).

Although embodiments have been described in which the non-steroidal compound includes rings B and C fused together, in some embodiments, rings B and C can be joined by a chemical linker. Examples of linkers are noted above. In certain embodiments, ring B is not present. For example, ring B can be replaced with a linker moiety that connects ring C with ring A. The linker moiety can, for example, be of sufficient length to allow favorable interactions between ring A and one or both of Glu725 or Arg766 of the human PR-LBD, and between ring C and one or more of Asn719, Thr894, or Cys891 of the human PR-LBD. For example, ring B can be replaced with an alkenyl linker such as a branched alkene, which can provide sufficient length, structural rigidity, and, where desired, bulk (e.g., the linker moiety can include a branched alkenyl moiety).

The following example is illustrative and not intended as limiting.

EXAMPLE

Human progesterone ligand binding domain (PR-LBD) was expressed as an amino terminal glutathione-S-transferase (GST) fusion protein from Escherichia coli BL21 (Stratagene). The PR-LBD domain coding sequence was cloned into the pGEX plasmid (Amersham Pharmacia Biotech) under tac transcriptional control. A thrombin cleavage site (LVPRG, SEQ ID #3) was present at the boundary of the GST and PR-LBD regions (thrombin cleaves between the R and the G). The sequence of this fusion protein is shown in FIG. 2A. The sequence of the PR-LBD polypeptide following thrombin cleavage is shown in FIG. 2B.

Bacterial growth and protein expression were performed in a Biostat 10 liter fermenter (B. Braun Biotech). A 100 mL preculture was used to inoculate 10 liters of media (fermenter salts, glucose, ampicillin, trace metals and yeast extract media) and expanded overnight at 25°C. Fifteen minutes prior to induction, the vessel temperature was lowered to 15°C and 5 mls of 66 mM progesterone (Sigma-Aldrich, St. Louis, MO) in 100% ethanol was added. The culture was induced at a density of 5.4 OD600 absorbance units with addition of isopropyl-beta-D-thiogalactopyranoside (IPTG, Fisher) to a final concentration of 1.0 mM. Progesterone was again added in 5ml aliquots of 66mM at the time of induction and every fifteen minutes thereafter, for the duration of expression (4 hours total, 660 µM final concentration of progesterone). After 4 hours of induction, the culture was harvested yielding 158.76g of wet cell weight. The protein of interest represented 5-7% of total cell protein, as estimated by SDS-PAGE. Successful isolation of PR-LBD depended strongly on inclusion of a PR ligand during expression (possibly to ensure proper protein folding) and purification. See, for example, Williams and Sigler, *Nature* 393:392-396, 1998; Tanenbaum *et al.*, *Proc. Natl. Acad. Sci. USA* 95:5998-6003, 1998; and Matias *et al.*, *J. Biol. Chem.* 275: 26164-26171, 2000. Tanaproget was exchanged for progesterone during purification.

20 g of frozen cells were suspended in 300 mL of 50 mM HEPES pH 7.3, 150 mM NaCl, 5 mM EDTA, 10% glycerol, 5 mM dithiothreitol (DTT) with 0.33 mM of the protease inhibitor aminoethylbenzenesulfonyl fluoride (AEBSF, Sigma-Aldrich), 0.3 mL of protease inhibitor cocktail (Sigma-Aldrich catalog number 8849) and 5 µM progesterone (Progesterone was stored as a 50 mM stock solution in dimethylsulfoxide). Cells were broken by passage through a microfluidizer (Microfluidics, Newton, MA). Cell debris and aggregated GST/PR-LBD were removed by centrifugation for 2.5 hrs at approximately 40,000 g. CHAPS (Sigma) was added to 1.5% and the solution was passed through a 0.45 micron cellulose nitrate filter and stored overnight.

An initial purification of GST/PR-LBD fusion protein was carried out by affinity chromatography. The filtered solution was passed over two 5 mL columns (in tandem) of GSTrap FF glutathione-Sepharose chromatography media (Amersham Bioscience) at flow rate of about 1 mL/min. Resin was washed with 50 mL of 50 mM HEPES pH 7.3, 150 mM NaCl, 5 mM EDTA, 10% glycerol, then with 50 mL of same solution containing 50 µM tanaproget. GST/PR-LBD was eluted with 12 mM reduced glutathione (Sigma) in

50 mM HEPES pH 7.3, 100 mM NaCl, 10% glycerol, 0.1% octyl- β -glucoside, and 50 μ M tanaproget. Fractions of 5 mL were collected. Those fractions containing GST/PR-LBD were identified by SDS-PAGE and pooled. Typically the pooled fractions had a total volume of 30-40 mL. Thrombin was added to 25,000 NIH units/mL. The solution was incubated overnight for specific proteolysis.

The solution was diluted with 4 volumes of 10 mM HEPES pH 7.3, 10% glycerol, 5 mM DTT, 0.1% octyl- β -glucoside, and 50 μ M tanaproget. The solution was passed over a 1 mL column of HiTrap SP FF sulfopropyl-Sepharose (Amersham Bioscience) at a flow rate of 1 mL/min. The column was washed with 5 mL of 10 mM HEPES pH 7.3, 20 mM NaCl, 10% glycerol, 0.1% octyl- β -glucoside, and 1 μ M tanaproget (tanaproget was stored as a 50 mM stock solution in dimethylsulfoxide). PR-LBD was eluted from the column with a 15 mL gradient of sodium chloride, running from 20 mM to 220 mM (other components as above). Fractions of 1 mL were collected, PR-LBD was located by SDS-PAGE and those fractions containing PR/LBD at a concentration of 1 to 2 mg/mL were used directly for crystallization.

Prior to crystallization, the PR-LBD/tanaproget complex was determined to be homogeneous by SDS-PAGE. The protein had the expected mass as determined by MALDI mass spectrometry (~29,800 Da). The protein behaved as a single species during size-exclusion chromatography. The retention volume, as compared with reference proteins, was consistent with a dimer of PR-LBD. Only those preparations of the PR-LBD/tanaproget complex without any detectable progesterone were used for crystallization. Bound ligand was analyzed by reverse-phase chromatography following protein denaturation in the presence of guanidine-HCl.

Crystals were grown by hanging drop vapor diffusion at 18°C. The drops contained 2.0 μ L protein stock solution (5 mg/mL protein, 10 mM HEPES pH 7.3, 10% glycerol, 5 mM DTT, ~100 mM NaCl, 0.1% octyl- β -glucoside, 1 μ M tanaproget) mixed with 1.0 μ L well solution (8% PEG 3350 (Hampton Research), 300 mM MgSO₄, 50 mM PIPES pH 6.5, 10% glycerol) and 0.5 μ L 1,3-propanediol (40% v/v, Hampton Research) and equilibrated against a 1 mL well solution. Diamond shaped crystals grew in 2-6 weeks, measuring ~50 μ m across.

Showers of small crystals grew in the conditions described above with a variety of sulfate salts. The number of nucleation events was reduced by the addition of 1,3-propanediol (40% v/v) to drops, enabling the growth of fewer, larger, single crystals. The crystals belonged to space group $P2_1$ with unit cell parameters $a = 57.52 \text{ \AA}$, $b = 64.50 \text{ \AA}$, $c = 70.41 \text{ \AA}$, and $\beta = 95.76^\circ$, and contained two molecules of PR-LBD in the asymmetric unit, implying a solvent content of 44%. Crystals were drawn through a cryoprotectant solution of 20% ethylene glycol and 80% well solution, and cooled rapidly in liquid nitrogen. Diffraction data were recorded on an R-axis 4 detector. Intensities were integrated and scaled using the programs Denzo and Scalepack (Otwinowski and Minor, *Methods Enzymol.* 276: 307-326, 1997).

The structure was solved by molecular replacement using the protein model of the PR-LBD/progesterone structure (Williams and Sigler, *Nature* 393:392-396, 1998) as the search model. After several iterative cycles of refinement using CNS (Brunger *et al.*, *Acta Crystallogr.* D54:905-921, 1998) and model improvement, tanaproget was placed and refined. The final values of R_{work} and R_{free} were 19.62% and 23.74%, respectively. Table 1 summarizes the data collection parameters and results.

Table 1. Statistics of X-Ray Diffraction Data Collection

Data Collection	
Crystal System	monoclinic
Space Group	P2 ₁
Unit Cell Dimensions	A=57.52 Å, b=64.50 Å, c=70.41 Å, β=95.76°
Data Collection Temperature	-180°C
Number of crystals	1
Radiation Source	Rigaku rotating anode X-ray generator
X-ray wavelength	1.54179 Å
Resolution range of data	30.0-2.0 Å
Maximum Resolution	2.0 Å
R _{merge} ^a	4.9 % (17.6 %)
Completeness	100.0 % (99.9 %)
Total reflections	147,224
Unique reflections	34,825
I/σ(I)	26.9 (8.3)
Phasing and Refinement	
Model for molecular refinement	1a28.pdb (PR-LBD/progesterone)
Construct (aa)	PR-LBD (675-933)
Compound (ligand)	tanaproget
PR-LBD molecules per asymmetric unit	2
Resolution range of refinement	20.0 – 2.0 Å
R _{work}	19.62 %
R _{free}	23.74 %
Number of non-hydrogen protein atoms	4072
Number of water molecules	179
RMS deviations from ideal bond lengths	0.0057 Å
RMS deviations from ideal bond angles	1.132°
^a R _{merge} = I _h - <I _h > / I _h , where <I _h > is the average intensity over symmetry equivalents. Numbers in parentheses reflect statistics for the last shell. ^b R _{work} = F _{obs} - F _{calc} / F _{obs} ^c R _{free} is equivalent to R _{work} , but calculated for a randomly chosen 5% of reflections omitted from the refinement process.	

The refined model included two PR-LBD molecules in the asymmetric unit of the crystal, each bound to one agonist. Tanaproget fit into the buried hydrophobic ligand binding pocket, occupying roughly the same area as progesterone.

The principle features of nuclear receptor ligand binding domains were conserved in the PR-LBD. There were ten helices (following standard steroid receptor nomenclature, helix 2 is missing, and helices 10 and 11 are contiguous), of which helices 3, 5, 7, 11 and 12 contributed to the ligand binding pocket. The two PR-LBD molecules in the crystal formed a

dimer centered around interactions between helix 11 of one subunit with helix 12 of the other.

The tertiary structure of PR-LBD/tanaproget was very similar to that of PR-LBD/progesterone. Tanaproget occupied the same binding pocket as progesterone. See
5 FIGs. 1A and 1B, which present views of a $3F_{\text{obs}}-2F_{\text{calc}}$ experimental map of tanaproget bound to PR-LBD unbiased by ligand phases and contoured at 1.2σ . Superposition of the structures of the PR-LBD/tanaproget complex and the PR-LBD/progesterone complex revealed that the 1-methyl-1H-pyrrole-2-carbonitrile ring lay roughly between the A and B rings of progesterone, and the 1,4-dihydro-3,1-benzoxazine-2-thione moiety ("benzoxazine")
10 lay just above the C and D rings of progesterone in the direction of the protruding methyl groups of progesterone.

Tanaproget mimicked the interaction of progesterone with the ligand binding pocket of PR-LBD in many ways. The nitrile group, positioned approximately 0.6 Å from the 3-keto substituent of the progesterone A ring, formed hydrogen bonds with the side chains of
15 Gln725 and Arg766. Similarly, the progesterone 3-keto group interacted with the side chains of Gln725 and Arg766, and maintained the hydrogen bonding network that provides specificity for steroids with an oxygen atom at the 3-position of the A ring. The benzoxazine moiety occupied approximately the same space as rings C and D of progesterone with similar hydrophobic interactions. The sulfur of the benzoxazine appeared to extend beyond the
20 methyl-ketone substituent at C17 of progesterone. Tanaproget had an additional favorable interaction with the protein in the hydrogen bond formed between the benzoxazine nitrogen and the side chain oxygen of Asn719. The loop between helix 6 and helix 7, including amino acids 788-794, was rearranged with respect to the PR-LBD/progesterone structure. This rearrangement did not appear to be directly due to the different ligand, however, as the
25 shortest distance between tanaproget and PR-LBD in this region is 5 Å, from one tanaproget methyl substituent of the benzoxazine to the side chain of Phe794. The structure indicated that the sulfur atom of tanaproget may form a weak interaction with Thr894 of the PR-LBD, and a hydrophobic region on the benzoxazine molecule forms a favorable hydrophobic interaction with Leu797 of the receptor LBD.

30 Several side chains were well defined by the experimental electron density in one molecule of the asymmetric unit (molecule "A"), but not in the other (molecule "B"). These

side chains include: Met908, Phe794, Trp755, and Leu714. Met908 is somewhat disordered in molecule "A", with more than one rotamer represented in the electron density.

Table 2. Structure coordinates

5		#	Name	Res.	Chain	Res #	X	Y	Z	occ	B	SegID
	ATOM	1	CB	GLN	A	682	-7.348	13.179	57.749	1.00	59.37	A
	ATOM	2	CG	GLN	A	682	-6.839	14.229	58.725	1.00	62.50	A
	ATOM	3	CD	GLN	A	682	-6.509	13.648	60.089	1.00	64.16	A
10	ATOM	4	OE1	GLN	A	682	-7.383	13.129	60.785	1.00	65.34	A
	ATOM	5	NE2	GLN	A	682	-5.240	13.732	60.476	1.00	64.49	A
	ATOM	6	C	GLN	A	682	-6.989	11.007	56.577	1.00	54.95	A
	ATOM	7	O	GLN	A	682	-6.920	9.824	56.915	1.00	55.50	A
	ATOM	8	N	GLN	A	682	-5.169	12.697	56.667	1.00	58.18	A
15	ATOM	9	CA	GLN	A	682	-6.321	12.097	57.404	1.00	57.18	A
	ATOM	10	N	LEU	A	683	-7.640	11.412	55.493	1.00	51.76	A
	ATOM	11	CA	LEU	A	683	-8.315	10.464	54.618	1.00	48.27	A
	ATOM	12	CB	LEU	A	683	-9.448	11.156	53.851	1.00	50.10	A
	ATOM	13	CG	LEU	A	683	-10.757	11.418	54.603	1.00	52.21	A
20	ATOM	14	CD1	LEU	A	683	-11.685	12.275	53.749	1.00	52.58	A
	ATOM	15	CD2	LEU	A	683	-11.420	10.091	54.945	1.00	51.94	A
	ATOM	16	C	LEU	A	683	-7.338	9.846	53.627	1.00	43.82	A
	ATOM	17	O	LEU	A	683	-7.630	8.815	53.027	1.00	43.05	A
	ATOM	18	N	ILE	A	684	-6.175	10.471	53.470	1.00	39.89	A
25	ATOM	19	CA	ILE	A	684	-5.173	9.983	52.526	1.00	35.45	A
	ATOM	20	CB	ILE	A	684	-4.119	11.060	52.215	1.00	35.60	A
	ATOM	21	CG2	ILE	A	684	-3.298	10.633	51.014	1.00	34.67	A
	ATOM	22	CG1	ILE	A	684	-4.798	12.400	51.921	1.00	34.80	A
	ATOM	23	CD1	ILE	A	684	-5.754	12.361	50.761	1.00	35.65	A
30	ATOM	24	C	ILE	A	684	-4.435	8.732	52.996	1.00	33.40	A
	ATOM	25	O	ILE	A	684	-3.823	8.724	54.063	1.00	32.14	A
	ATOM	26	N	PRO	A	685	-4.482	7.657	52.190	1.00	31.08	A
	ATOM	27	CD	PRO	A	685	-5.212	7.563	50.914	1.00	29.47	A
	ATOM	28	CA	PRO	A	685	-3.823	6.386	52.497	1.00	29.34	A
35	ATOM	29	CB	PRO	A	685	-4.051	5.566	51.230	1.00	28.42	A
	ATOM	30	CG	PRO	A	685	-5.360	6.071	50.745	1.00	29.55	A
	ATOM	31	C	PRO	A	685	-2.341	6.604	52.777	1.00	28.94	A
	ATOM	32	O	PRO	A	685	-1.685	7.395	52.099	1.00	27.20	A
	ATOM	33	N	PRO	A	686	-1.795	5.892	53.776	1.00	28.63	A
40	ATOM	34	CD	PRO	A	686	-2.499	4.881	54.583	1.00	30.74	A
	ATOM	35	CA	PRO	A	686	-0.388	5.983	54.178	1.00	28.46	A
	ATOM	36	CB	PRO	A	686	-0.225	4.796	55.122	1.00	29.48	A
	ATOM	37	CG	PRO	A	686	-1.565	4.697	55.750	1.00	30.51	A
	ATOM	38	C	PRO	A	686	0.615	5.941	53.026	1.00	26.34	A
45	ATOM	39	O	PRO	A	686	1.448	6.836	52.897	1.00	27.12	A
	ATOM	40	N	LEU	A	687	0.538	4.907	52.192	1.00	23.00	A
	ATOM	41	CA	LEU	A	687	1.474	4.782	51.077	1.00	21.26	A
	ATOM	42	CB	LEU	A	687	1.145	3.552	50.228	1.00	19.41	A
	ATOM	43	CG	LEU	A	687	2.091	3.305	49.047	1.00	18.40	A
50	ATOM	44	CD1	LEU	A	687	3.537	3.370	49.521	1.00	17.99	A
	ATOM	45	CD2	LEU	A	687	1.788	1.944	48.420	1.00	17.48	A
	ATOM	46	C	LEU	A	687	1.484	6.022	50.194	1.00	21.24	A

Table 2. (cont'd)

		#	Name	Res.	Chain	Res #	X	Y	Z	occ	B	SegID
	ATOM	47	O	LEU	A	687	2.535	6.432	49.700	1.00	21.10	A
5	ATOM	48	N	ILE	A	688	0.317	6.623	49.994	1.00	20.14	A
	ATOM	49	CA	ILE	A	688	0.234	7.818	49.168	1.00	20.01	A
	ATOM	50	CB	ILE	A	688	-1.243	8.179	48.845	1.00	20.19	A
	ATOM	51	CG2	ILE	A	688	-1.321	9.546	48.196	1.00	19.71	A
	ATOM	52	CG1	ILE	A	688	-1.833	7.114	47.907	1.00	20.43	A
10	ATOM	53	CD1	ILE	A	688	-3.294	7.332	47.534	1.00	20.19	A
	ATOM	54	C	ILE	A	688	0.938	8.983	49.862	1.00	20.11	A
	ATOM	55	O	ILE	A	688	1.686	9.725	49.225	1.00	20.42	A
	ATOM	56	N	ASN	A	689	0.712	9.146	51.164	1.00	21.73	A
	ATOM	57	CA	ASN	A	689	1.370	10.227	51.901	1.00	22.53	A
15	ATOM	58	CB	ASN	A	689	0.967	10.200	53.380	1.00	28.18	A
	ATOM	59	CG	ASN	A	689	-0.417	10.782	53.627	1.00	32.46	A
	ATOM	60	OD1	ASN	A	689	-1.037	10.513	54.659	1.00	37.47	A
	ATOM	61	ND2	ASN	A	689	-0.901	11.594	52.693	1.00	35.14	A
	ATOM	62	C	ASN	A	689	2.884	10.040	51.790	1.00	22.06	A
20	ATOM	63	O	ASN	A	689	3.634	10.997	51.609	1.00	20.86	A
	ATOM	64	N	LEU	A	690	3.325	8.793	51.888	1.00	20.88	A
	ATOM	65	CA	LEU	A	690	4.746	8.497	51.794	1.00	21.42	A
	ATOM	66	CB	LEU	A	690	4.982	7.013	52.057	1.00	21.51	A
	ATOM	67	CG	LEU	A	690	6.427	6.547	52.240	1.00	22.35	A
25	ATOM	68	CD1	LEU	A	690	6.409	5.229	52.969	1.00	26.08	A
	ATOM	69	CD2	LEU	A	690	7.129	6.416	50.897	1.00	23.08	A
	ATOM	70	C	LEU	A	690	5.259	8.895	50.411	1.00	20.43	A
	ATOM	71	O	LEU	A	690	6.299	9.545	50.293	1.00	20.25	A
	ATOM	72	N	LEU	A	691	4.523	8.524	49.366	1.00	19.54	A
30	ATOM	73	CA	LEU	A	691	4.931	8.873	48.008	1.00	18.70	A
	ATOM	74	CB	LEU	A	691	3.908	8.357	46.989	1.00	16.88	A
	ATOM	75	CG	LEU	A	691	3.852	6.840	46.763	1.00	16.04	A
	ATOM	76	CD1	LEU	A	691	2.834	6.533	45.671	1.00	15.95	A
	ATOM	77	CD2	LEU	A	691	5.230	6.311	46.355	1.00	16.73	A
35	ATOM	78	C	LEU	A	691	5.088	10.385	47.868	1.00	19.45	A
	ATOM	79	O	LEU	A	691	6.028	10.870	47.238	1.00	18.17	A
	ATOM	80	N	MET	A	692	4.166	11.136	48.459	1.00	20.70	A
	ATOM	81	CA	MET	A	692	4.243	12.588	48.380	1.00	23.63	A
	ATOM	82	CB	MET	A	692	2.998	13.232	49.000	1.00	25.77	A
40	ATOM	83	CG	MET	A	692	2.988	14.751	48.917	1.00	29.26	A
	ATOM	84	SD	MET	A	692	3.036	15.361	47.206	1.00	35.42	A
	ATOM	85	CE	MET	A	692	4.716	16.016	47.096	1.00	34.93	A
	ATOM	86	C	MET	A	692	5.484	13.105	49.104	1.00	23.94	A
	ATOM	87	O	MET	A	692	6.139	14.033	48.636	1.00	22.01	A
45	ATOM	88	N	SER	A	693	5.804	12.496	50.243	1.00	23.84	A
	ATOM	89	CA	SER	A	693	6.953	12.925	51.036	1.00	25.43	A
	ATOM	90	CB	SER	A	693	6.960	12.218	52.397	1.00	26.51	A
	ATOM	91	OG	SER	A	693	7.373	10.868	52.268	1.00	30.46	A
	ATOM	92	C	SER	A	693	8.310	12.716	50.370	1.00	23.96	A
50	ATOM	93	O	SER	A	693	9.257	13.432	50.677	1.00	22.54	A
	ATOM	94	N	ILE	A	694	8.415	11.745	49.465	1.00	22.45	A
	ATOM	95	CA	ILE	A	694	9.694	11.492	48.814	1.00	21.42	A
	ATOM	96	CB	ILE	A	694	10.001	9.976	48.740	1.00	20.54	A
	ATOM	97	CG2	ILE	A	694	10.052	9.393	50.153	1.00	18.76	A
55	ATOM	98	CG1	ILE	A	694	8.947	9.261	47.896	1.00	20.09	A
	ATOM	99	CD1	ILE	A	694	9.257	7.790	47.648	1.00	19.61	A

Table 2. (cont'd)

		#	Name	Res.	Chain	Res #	X	Y	Z	occ	B	SegID
	ATOM	100	C	ILE	A	694	9.828	12.100	47.422	1.00	23.09	A
5	ATOM	101	O	ILE	A	694	10.756	11.767	46.677	1.00	23.23	A
	ATOM	102	N	GLU	A	695	8.904	12.989	47.069	1.00	23.79	A
	ATOM	103	CA	GLU	A	695	8.956	13.658	45.773	1.00	24.75	A
	ATOM	104	CB	GLU	A	695	7.691	14.489	45.544	1.00	23.00	A
	ATOM	105	CG	GLU	A	695	6.538	13.671	45.009	1.00	22.30	A
10	ATOM	106	CD	GLU	A	695	6.766	13.243	43.574	1.00	22.70	A
	ATOM	107	OE1	GLU	A	695	6.637	14.100	42.679	1.00	24.09	A
	ATOM	108	OE2	GLU	A	695	7.082	12.060	43.339	1.00	20.49	A
	ATOM	109	C	GLU	A	695	10.181	14.563	45.739	1.00	26.09	A
	ATOM	110	O	GLU	A	695	10.596	15.097	46.762	1.00	24.44	A
15	ATOM	111	N	PRO	A	696	10.775	14.746	44.554	1.00	27.98	A
	ATOM	112	CD	PRO	A	696	10.513	13.991	43.318	1.00	30.08	A
	ATOM	113	CA	PRO	A	696	11.964	15.589	44.402	1.00	29.41	A
	ATOM	114	CB	PRO	A	696	12.419	15.286	42.974	1.00	30.04	A
	ATOM	115	CG	PRO	A	696	11.895	13.887	42.729	1.00	31.56	A
20	ATOM	116	C	PRO	A	696	11.692	17.072	44.592	1.00	30.11	A
	ATOM	117	O	PRO	A	696	10.561	17.527	44.436	1.00	28.96	A
	ATOM	118	N	ASP	A	697	12.737	17.819	44.941	1.00	31.22	A
	ATOM	119	CA	ASP	A	697	12.624	19.264	45.093	1.00	32.61	A
	ATOM	120	CB	ASP	A	697	13.829	19.834	45.852	1.00	36.05	A
25	ATOM	121	CG	ASP	A	697	13.550	20.037	47.328	1.00	39.53	A
	ATOM	122	OD1	ASP	A	697	12.602	20.786	47.654	1.00	40.51	A
	ATOM	123	OD2	ASP	A	697	14.281	19.458	48.160	1.00	40.91	A
	ATOM	124	C	ASP	A	697	12.641	19.794	43.661	1.00	32.25	A
	ATOM	125	O	ASP	A	697	12.689	19.012	42.712	1.00	29.97	A
30	ATOM	126	N	VAL	A	698	12.609	21.114	43.506	1.00	32.44	A
	ATOM	127	CA	VAL	A	698	12.640	21.722	42.180	1.00	32.25	A
	ATOM	128	CB	VAL	A	698	12.444	23.260	42.257	1.00	34.46	A
	ATOM	129	CG1	VAL	A	698	12.766	23.896	40.918	1.00	36.09	A
	ATOM	130	CG2	VAL	A	698	11.014	23.587	42.653	1.00	35.95	A
35	ATOM	131	C	VAL	A	698	13.995	21.435	41.543	1.00	30.21	A
	ATOM	132	O	VAL	A	698	15.025	21.495	42.217	1.00	30.12	A
	ATOM	133	N	ILE	A	699	13.990	21.114	40.253	1.00	27.42	A
	ATOM	134	CA	ILE	A	699	15.226	20.835	39.526	1.00	25.67	A
	ATOM	135	CB	ILE	A	699	15.239	19.399	38.956	1.00	25.17	A
40	ATOM	136	CG2	ILE	A	699	16.491	19.190	38.091	1.00	23.70	A
	ATOM	137	CG1	ILE	A	699	15.196	18.387	40.102	1.00	23.56	A
	ATOM	138	CD1	ILE	A	699	14.904	16.973	39.652	1.00	24.85	A
	ATOM	139	C	ILE	A	699	15.384	21.810	38.366	1.00	25.34	A
	ATOM	140	O	ILE	A	699	14.507	21.912	37.503	1.00	22.56	A
45	ATOM	141	N	TYR	A	700	16.504	22.526	38.349	1.00	25.69	A
	ATOM	142	CA	TYR	A	700	16.769	23.486	37.286	1.00	26.30	A
	ATOM	143	CB	TYR	A	700	17.538	24.689	37.830	1.00	29.84	A
	ATOM	144	CG	TYR	A	700	16.802	25.473	38.890	1.00	33.46	A
	ATOM	145	CD1	TYR	A	700	16.630	24.956	40.173	1.00	35.57	A
50	ATOM	146	CE1	TYR	A	700	15.977	25.685	41.161	1.00	36.93	A
	ATOM	147	CD2	TYR	A	700	16.296	26.744	38.617	1.00	35.62	A
	ATOM	148	CE2	TYR	A	700	15.640	27.484	39.600	1.00	37.08	A
	ATOM	149	CZ	TYR	A	700	15.487	26.947	40.868	1.00	37.98	A
	ATOM	150	OH	TYR	A	700	14.857	27.677	41.849	1.00	42.60	A
55	ATOM	151	C	TYR	A	700	17.573	22.845	36.165	1.00	26.05	A

Table 2. (cont'd)

		#	Name	Res.	Chain	Res #	X	Y	Z	occ	B	SegID
5	ATOM	152	O	TYR	A	700	18.347	21.911	36.395	1.00	25.35	A
	ATOM	153	N	ALA	A	701	17.384	23.352	34.949	1.00	25.26	A
	ATOM	154	CA	ALA	A	701	18.092	22.845	33.781	1.00	24.29	A
	ATOM	155	CB	ALA	A	701	17.270	23.101	32.518	1.00	24.28	A
	ATOM	156	C	ALA	A	701	19.457	23.510	33.650	1.00	25.20	A
10	ATOM	157	O	ALA	A	701	20.378	22.947	33.053	1.00	23.68	A
	ATOM	158	N	GLY	A	702	19.576	24.711	34.212	1.00	26.21	A
	ATOM	159	CA	GLY	A	702	20.824	25.453	34.141	1.00	26.56	A
	ATOM	160	C	GLY	A	702	20.991	26.136	32.794	1.00	27.49	A
	ATOM	161	O	GLY	A	702	22.113	26.367	32.342	1.00	25.92	A
15	ATOM	162	N	HIS	A	703	19.875	26.456	32.147	1.00	25.65	A
	ATOM	163	CA	HIS	A	703	19.911	27.106	30.841	1.00	28.02	A
	ATOM	164	CB	HIS	A	703	18.604	26.829	30.090	1.00	26.86	A
	ATOM	165	CG	HIS	A	703	18.596	27.332	28.681	1.00	28.60	A
	ATOM	166	CD2	HIS	A	703	18.915	26.723	27.515	1.00	27.33	A
20	ATOM	167	ND1	HIS	A	703	18.233	28.621	28.354	1.00	28.67	A
	ATOM	168	CE1	HIS	A	703	18.325	28.782	27.046	1.00	29.35	A
	ATOM	169	NE2	HIS	A	703	18.738	27.646	26.513	1.00	29.47	A
	ATOM	170	C	HIS	A	703	20.155	28.615	30.961	1.00	29.77	A
	ATOM	171	O	HIS	A	703	19.651	29.265	31.873	1.00	27.82	A
25	ATOM	172	N	ASP	A	704	20.931	29.159	30.027	1.00	32.72	A
	ATOM	173	CA	ASP	A	704	21.275	30.579	30.019	1.00	37.35	A
	ATOM	174	CB	ASP	A	704	22.110	30.896	28.767	1.00	40.24	A
	ATOM	175	CG	ASP	A	704	21.321	30.733	27.468	1.00	42.83	A
	ATOM	176	OD1	ASP	A	704	20.357	31.498	27.263	1.00	41.93	A
30	ATOM	177	OD2	ASP	A	704	21.664	29.847	26.646	1.00	42.26	A
	ATOM	178	C	ASP	A	704	20.082	31.542	30.110	1.00	39.25	A
	ATOM	179	O	ASP	A	704	19.964	32.310	31.070	1.00	42.51	A
	ATOM	180	N	ASN	A	705	19.204	31.487	29.115	1.00	40.19	A
	ATOM	181	CA	ASN	A	705	18.023	32.347	29.018	1.00	39.83	A
35	ATOM	182	CB	ASN	A	705	17.213	32.328	30.318	1.00	39.65	A
	ATOM	183	CG	ASN	A	705	16.404	31.052	30.482	1.00	39.53	A
	ATOM	184	OD1	ASN	A	705	15.623	30.677	29.602	1.00	38.94	A
	ATOM	185	ND2	ASN	A	705	16.582	30.382	31.614	1.00	37.25	A
	ATOM	186	C	ASN	A	705	18.358	33.791	28.637	1.00	40.65	A
40	ATOM	187	O	ASN	A	705	17.479	34.540	28.206	1.00	40.21	A
	ATOM	188	N	THR	A	706	19.619	34.186	28.792	1.00	40.22	A
	ATOM	189	CA	THR	A	706	20.024	35.542	28.429	1.00	41.37	A
	ATOM	190	CB	THR	A	706	21.211	36.046	29.276	1.00	41.45	A
	ATOM	191	OG1	THR	A	706	22.376	35.273	28.974	1.00	42.94	A
45	ATOM	192	CG2	THR	A	706	20.899	35.930	30.760	1.00	42.56	A
	ATOM	193	C	THR	A	706	20.449	35.555	26.963	1.00	41.48	A
	ATOM	194	O	THR	A	706	20.735	36.609	26.398	1.00	42.00	A
	ATOM	195	N	LYS	A	707	20.493	34.373	26.355	1.00	39.94	A
	ATOM	196	CA	LYS	A	707	20.882	34.246	24.957	1.00	39.25	A
50	ATOM	197	CB	LYS	A	707	22.080	33.303	24.805	1.00	40.35	A
	ATOM	198	CG	LYS	A	707	23.378	33.794	25.420	1.00	43.83	A
	ATOM	199	CD	LYS	A	707	24.534	32.911	24.963	1.00	45.58	A
	ATOM	200	CE	LYS	A	707	25.874	33.379	25.514	1.00	48.00	A
	ATOM	201	NZ	LYS	A	707	25.993	33.156	26.982	1.00	50.15	A
55	ATOM	202	C	LYS	A	707	19.727	33.690	24.146	1.00	36.97	A
	ATOM	203	O	LYS	A	707	18.858	33.009	24.684	1.00	37.69	A
	ATOM	204	N	PRO	A	708	19.703	33.978	22.838	1.00	35.45	A

Table 2. (cont'd)

		#	Name	Res.	Chain	Res #	X	Y	Z	occ	B	SegID
5	ATOM	205	CD	PRO	A	708	20.543	34.966	22.141	1.00	36.01	A
	ATOM	206	CA	PRO	A	708	18.640	33.487	21.954	1.00	33.79	A
	ATOM	207	CB	PRO	A	708	18.937	34.194	20.632	1.00	33.78	A
	ATOM	208	CG	PRO	A	708	19.611	35.460	21.065	1.00	35.82	A
	ATOM	209	C	PRO	A	708	18.745	31.966	21.824	1.00	32.66	A
10	ATOM	210	O	PRO	A	708	19.848	31.420	21.802	1.00	31.44	A
	ATOM	211	N	ASP	A	709	17.605	31.289	21.738	1.00	30.13	A
	ATOM	212	CA	ASP	A	709	17.596	29.835	21.613	1.00	27.78	A
	ATOM	213	CB	ASP	A	709	16.164	29.288	21.594	1.00	26.98	A
	ATOM	214	CG	ASP	A	709	15.494	29.335	22.941	1.00	26.45	A
15	ATOM	215	OD1	ASP	A	709	16.180	29.603	23.947	1.00	27.85	A
	ATOM	216	OD2	ASP	A	709	14.271	29.086	22.989	1.00	27.12	A
	ATOM	217	C	ASP	A	709	18.257	29.357	20.337	1.00	27.24	A
	ATOM	218	O	ASP	A	709	18.204	30.026	19.310	1.00	25.71	A
	ATOM	219	N	THR	A	710	18.877	28.187	20.413	1.00	25.67	A
20	ATOM	220	CA	THR	A	710	19.480	27.565	19.245	1.00	26.35	A
	ATOM	221	CB	THR	A	710	21.025	27.716	19.195	1.00	26.29	A
	ATOM	222	OG1	THR	A	710	21.616	26.958	20.255	1.00	24.75	A
	ATOM	223	CG2	THR	A	710	21.433	29.182	19.329	1.00	25.04	A
	ATOM	224	C	THR	A	710	19.129	26.097	19.428	1.00	27.11	A
25	ATOM	225	O	THR	A	710	18.912	25.640	20.555	1.00	26.86	A
	ATOM	226	N	SER	A	711	19.052	25.364	18.328	1.00	26.94	A
	ATOM	227	CA	SER	A	711	18.725	23.950	18.395	1.00	30.05	A
	ATOM	228	CB	SER	A	711	18.857	23.323	17.004	1.00	30.48	A
	ATOM	229	OG	SER	A	711	18.600	21.934	17.046	1.00	35.04	A
30	ATOM	230	C	SER	A	711	19.644	23.227	19.382	1.00	29.29	A
	ATOM	231	O	SER	A	711	19.187	22.424	20.197	1.00	30.34	A
	ATOM	232	N	SER	A	712	20.937	23.529	19.326	1.00	27.88	A
	ATOM	233	CA	SER	A	712	21.891	22.870	20.207	1.00	27.73	A
	ATOM	234	CB	SER	A	712	23.322	23.089	19.706	1.00	30.70	A
35	ATOM	235	OG	SER	A	712	23.692	24.451	19.784	1.00	37.15	A
	ATOM	236	C	SER	A	712	21.803	23.264	21.678	1.00	25.40	A
	ATOM	237	O	SER	A	712	21.922	22.401	22.544	1.00	23.44	A
	ATOM	238	N	SER	A	713	21.593	24.547	21.970	1.00	23.22	A
	ATOM	239	CA	SER	A	713	21.519	24.983	23.363	1.00	23.17	A
40	ATOM	240	CB	SER	A	713	21.554	26.516	23.466	1.00	23.10	A
	ATOM	241	OG	SER	A	713	20.364	27.104	22.976	1.00	27.55	A
	ATOM	242	C	SER	A	713	20.277	24.442	24.068	1.00	21.24	A
	ATOM	243	O	SER	A	713	20.332	24.077	25.246	1.00	20.24	A
	ATOM	244	N	LEU	A	714	19.159	24.391	23.351	1.00	20.03	A
45	ATOM	245	CA	LEU	A	714	17.922	23.871	23.924	1.00	18.97	A
	ATOM	246	CB	LEU	A	714	16.734	24.100	22.978	1.00	17.28	A
	ATOM	247	CG	LEU	A	714	16.139	25.503	22.873	1.00	20.44	A
	ATOM	248	CD1	LEU	A	714	14.961	25.473	21.901	1.00	16.61	A
	ATOM	249	CD2	LEU	A	714	15.682	25.978	24.245	1.00	21.04	A
50	ATOM	250	C	LEU	A	714	18.039	22.378	24.215	1.00	17.72	A
	ATOM	251	O	LEU	A	714	17.733	21.927	25.322	1.00	19.37	A
	ATOM	252	N	LEU	A	715	18.476	21.610	23.222	1.00	16.17	A
	ATOM	253	CA	LEU	A	715	18.611	20.163	23.396	1.00	16.51	A
	ATOM	254	CB	LEU	A	715	18.941	19.497	22.054	1.00	15.83	A
55	ATOM	255	CG	LEU	A	715	17.839	19.637	20.990	1.00	17.05	A
	ATOM	256	CD1	LEU	A	715	18.291	19.026	19.668	1.00	17.78	A
	ATOM	257	CD2	LEU	A	715	16.566	18.953	21.489	1.00	17.52	A

Table 2. (cont'd)

		#	Name	Res.	Chain	Res #	X	Y	Z	occ	B	SegID
5	ATOM	258	C	LEU	A	715	19.676	19.842	24.444	1.00	17.19	A
	ATOM	259	O	LEU	A	715	19.526	18.905	25.233	1.00	15.94	A
	ATOM	260	N	THR	A	716	20.755	20.618	24.456	1.00	16.23	A
	ATOM	261	CA	THR	A	716	21.807	20.405	25.444	1.00	16.41	A
	ATOM	262	CB	THR	A	716	23.002	21.353	25.192	1.00	17.33	A
10	ATOM	263	OG1	THR	A	716	23.719	20.901	24.039	1.00	18.63	A
	ATOM	264	CG2	THR	A	716	23.946	21.383	26.393	1.00	18.48	A
	ATOM	265	C	THR	A	716	21.254	20.625	26.855	1.00	17.19	A
	ATOM	266	O	THR	A	716	21.569	19.873	27.777	1.00	17.56	A
	ATOM	267	N	SER	A	717	20.422	21.649	27.025	1.00	17.82	A
15	ATOM	268	CA	SER	A	717	19.836	21.917	28.334	1.00	17.93	A
	ATOM	269	CB	SER	A	717	19.142	23.282	28.349	1.00	18.40	A
	ATOM	270	OG	SER	A	717	20.099	24.315	28.459	1.00	20.04	A
	ATOM	271	C	SER	A	717	18.840	20.826	28.699	1.00	17.68	A
	ATOM	272	O	SER	A	717	18.774	20.399	29.849	1.00	17.99	A
20	ATOM	273	N	LEU	A	718	18.060	20.372	27.723	1.00	18.63	A
	ATOM	274	CA	LEU	A	718	17.092	19.312	27.987	1.00	18.40	A
	ATOM	275	CB	LEU	A	718	16.256	19.022	26.733	1.00	18.14	A
	ATOM	276	CG	LEU	A	718	15.122	20.027	26.496	1.00	17.83	A
	ATOM	277	CD1	LEU	A	718	14.466	19.780	25.139	1.00	18.47	A
25	ATOM	278	CD2	LEU	A	718	14.096	19.894	27.626	1.00	19.81	A
	ATOM	279	C	LEU	A	718	17.835	18.057	28.447	1.00	19.24	A
	ATOM	280	O	LEU	A	718	17.357	17.320	29.317	1.00	18.56	A
	ATOM	281	N	ASN	A	719	19.012	17.821	27.872	1.00	17.74	A
	ATOM	282	CA	ASN	A	719	19.811	16.664	28.259	1.00	18.99	A
30	ATOM	283	CB	ASN	A	719	20.880	16.359	27.207	1.00	19.92	A
	ATOM	284	CG	ASN	A	719	20.300	15.715	25.964	1.00	21.70	A
	ATOM	285	OD1	ASN	A	719	19.264	15.051	26.023	1.00	22.14	A
	ATOM	286	ND2	ASN	A	719	20.975	15.888	24.834	1.00	21.49	A
	ATOM	287	C	ASN	A	719	20.464	16.870	29.625	1.00	19.54	A
35	ATOM	288	O	ASN	A	719	20.631	15.915	30.383	1.00	18.51	A
	ATOM	289	N	GLN	A	720	20.833	18.111	29.946	1.00	20.24	A
	ATOM	290	CA	GLN	A	720	21.438	18.383	31.248	1.00	20.89	A
	ATOM	291	CB	GLN	A	720	22.024	19.804	31.299	1.00	24.62	A
	ATOM	292	CG	GLN	A	720	22.851	20.080	32.562	1.00	29.69	A
40	ATOM	293	CD	GLN	A	720	23.710	21.344	32.462	1.00	34.45	A
	ATOM	294	OE1	GLN	A	720	23.197	22.465	32.431	1.00	36.61	A
	ATOM	295	NE2	GLN	A	720	25.024	21.159	32.409	1.00	34.00	A
	ATOM	296	C	GLN	A	720	20.345	18.211	32.303	1.00	20.76	A
	ATOM	297	O	GLN	A	720	20.571	17.608	33.355	1.00	18.85	A
45	ATOM	298	N	LEU	A	721	19.156	18.736	32.007	1.00	18.88	A
	ATOM	299	CA	LEU	A	721	18.018	18.611	32.909	1.00	19.76	A
	ATOM	300	CB	LEU	A	721	16.783	19.313	32.317	1.00	20.61	A
	ATOM	301	CG	LEU	A	721	15.529	19.375	33.197	1.00	21.89	A
	ATOM	302	CD1	LEU	A	721	15.845	20.126	34.491	1.00	17.83	A
50	ATOM	303	CD2	LEU	A	721	14.389	20.058	32.435	1.00	17.08	A
	ATOM	304	C	LEU	A	721	17.743	17.115	33.063	1.00	18.66	A
	ATOM	305	O	LEU	A	721	17.457	16.626	34.157	1.00	18.65	A
	ATOM	306	N	GLY	A	722	17.839	16.392	31.953	1.00	18.59	A
	ATOM	307	CA	GLY	A	722	17.623	14.959	31.981	1.00	18.69	A
55	ATOM	308	C	GLY	A	722	18.591	14.261	32.922	1.00	19.59	A
	ATOM	309	O	GLY	A	722	18.184	13.426	33.735	1.00	21.70	A
	ATOM	310	N	GLU	A	723	19.874	14.598	32.817	1.00	18.22	A

Table 2. (cont'd)

		#	Name	Res.	Chain	Res	#	X	Y	Z	occ	B	SegID
5	ATOM	311	CA	GLU	A	723		20.898	13.998	33.674	1.00	18.14	A
	ATOM	312	CB	GLU	A	723		22.271	14.631	33.400	1.00	18.39	A
	ATOM	313	CG	GLU	A	723		23.409	14.008	34.198	1.00	19.11	A
	ATOM	314	CD	GLU	A	723		23.922	12.713	33.588	1.00	22.52	A
	ATOM	315	OE1	GLU	A	723		23.277	12.184	32.655	1.00	22.75	A
10	ATOM	316	OE2	GLU	A	723		24.979	12.220	34.040	1.00	22.45	A
	ATOM	317	C	GLU	A	723		20.549	14.209	35.145	1.00	18.01	A
	ATOM	318	O	GLU	A	723		20.691	13.296	35.967	1.00	16.59	A
	ATOM	319	N	ARG	A	724		20.110	15.422	35.474	1.00	17.42	A
	ATOM	320	CA	ARG	A	724		19.742	15.756	36.850	1.00	19.72	A
15	ATOM	321	CB	ARG	A	724		19.551	17.266	36.987	1.00	20.72	A
	ATOM	322	CG	ARG	A	724		20.820	18.047	36.693	1.00	21.86	A
	ATOM	323	CD	ARG	A	724		20.602	19.549	36.744	1.00	23.18	A
	ATOM	324	NE	ARG	A	724		21.855	20.245	36.465	1.00	23.39	A
	ATOM	325	CZ	ARG	A	724		22.021	21.563	36.505	1.00	25.86	A
20	ATOM	326	NH1	ARG	A	724		21.008	22.362	36.813	1.00	24.78	A
	ATOM	327	NH2	ARG	A	724		23.217	22.079	36.252	1.00	23.92	A
	ATOM	328	C	ARG	A	724		18.476	15.029	37.292	1.00	20.26	A
	ATOM	329	O	ARG	A	724		18.383	14.546	38.422	1.00	18.14	A
	ATOM	330	N	GLN	A	725		17.493	14.947	36.405	1.00	19.29	A
25	ATOM	331	CA	GLN	A	725		16.271	14.256	36.762	1.00	21.28	A
	ATOM	332	CB	GLN	A	725		15.191	14.504	35.705	1.00	23.07	A
	ATOM	333	CG	GLN	A	725		14.691	15.955	35.716	1.00	27.51	A
	ATOM	334	CD	GLN	A	725		13.556	16.210	34.743	1.00	30.36	A
	ATOM	335	OE1	GLN	A	725		13.084	17.341	34.600	1.00	33.13	A
30	ATOM	336	NE2	GLN	A	725		13.111	15.161	34.068	1.00	31.54	A
	ATOM	337	C	GLN	A	725		16.570	12.769	36.918	1.00	21.14	A
	ATOM	338	O	GLN	A	725		15.952	12.087	37.731	1.00	21.59	A
	ATOM	339	N	LEU	A	726		17.542	12.276	36.156	1.00	20.47	A
	ATOM	340	CA	LEU	A	726		17.919	10.870	36.232	1.00	20.31	A
35	ATOM	341	CB	LEU	A	726		18.928	10.547	35.126	1.00	21.56	A
	ATOM	342	CG	LEU	A	726		19.070	9.108	34.622	1.00	22.31	A
	ATOM	343	CD1	LEU	A	726		17.705	8.482	34.346	1.00	20.98	A
	ATOM	344	CD2	LEU	A	726		19.908	9.127	33.346	1.00	22.17	A
	ATOM	345	C	LEU	A	726		18.512	10.607	37.621	1.00	21.15	A
40	ATOM	346	O	LEU	A	726		18.190	9.611	38.272	1.00	19.58	A
	ATOM	347	N	LEU	A	727		19.375	11.509	38.077	1.00	19.81	A
	ATOM	348	CA	LEU	A	727		19.972	11.376	39.400	1.00	20.36	A
	ATOM	349	CB	LEU	A	727		20.927	12.535	39.662	1.00	23.93	A
	ATOM	350	CG	LEU	A	727		22.304	12.433	39.009	1.00	26.70	A
45	ATOM	351	CD1	LEU	A	727		23.092	13.712	39.259	1.00	30.45	A
	ATOM	352	CD2	LEU	A	727		23.037	11.231	39.586	1.00	27.44	A
	ATOM	353	C	LEU	A	727		18.862	11.384	40.455	1.00	18.86	A
	ATOM	354	O	LEU	A	727		18.910	10.637	41.437	1.00	17.62	A
	ATOM	355	N	SER	A	728		17.863	12.229	40.223	1.00	17.97	A
50	ATOM	356	CA	SER	A	728		16.724	12.376	41.115	1.00	19.31	A
	ATOM	357	CB	SER	A	728		15.836	13.523	40.625	1.00	21.26	A
	ATOM	358	OG	SER	A	728		14.794	13.788	41.542	1.00	24.60	A
	ATOM	359	C	SER	A	728		15.916	11.083	41.180	1.00	19.09	A
	ATOM	360	O	SER	A	728		15.465	10.675	42.251	1.00	18.25	A
55	ATOM	361	N	VAL	A	729		15.730	10.445	40.027	1.00	18.98	A
	ATOM	362	CA	VAL	A	729		14.990	9.190	39.962	1.00	17.54	A
	ATOM	363	CB	VAL	A	729		14.814	8.720	38.498	1.00	17.32	A

Table 2. (cont'd)

		#	Name	Res.	Chain	Res	#	X	Y	Z	occ	B	SegID
5	ATOM	364	CG1	VAL	A	729		14.261	7.312	38.460	1.00	17.30	A
	ATOM	365	CG2	VAL	A	729		13.875	9.676	37.770	1.00	19.41	A
	ATOM	366	C	VAL	A	729		15.718	8.112	40.765	1.00	17.34	A
	ATOM	367	O	VAL	A	729		15.095	7.382	41.537	1.00	16.18	A
	ATOM	368	N	VAL	A	730		17.033	8.015	40.590	1.00	15.92	A
10	ATOM	369	CA	VAL	A	730		17.812	7.024	41.330	1.00	16.21	A
	ATOM	370	CB	VAL	A	730		19.321	7.098	40.957	1.00	17.70	A
	ATOM	371	CG1	VAL	A	730		20.151	6.236	41.909	1.00	17.59	A
	ATOM	372	CG2	VAL	A	730		19.518	6.592	39.533	1.00	19.79	A
	ATOM	373	C	VAL	A	730		17.628	7.234	42.840	1.00	18.41	A
15	ATOM	374	O	VAL	A	730		17.364	6.282	43.582	1.00	20.77	A
	ATOM	375	N	LYS	A	731		17.747	8.480	43.290	1.00	18.40	A
	ATOM	376	CA	LYS	A	731		17.571	8.809	44.707	1.00	19.11	A
	ATOM	377	CB	LYS	A	731		17.806	10.307	44.915	1.00	22.06	A
	ATOM	378	CG	LYS	A	731		17.424	10.842	46.297	1.00	26.05	A
20	ATOM	379	CD	LYS	A	731		18.409	10.437	47.379	1.00	30.61	A
	ATOM	380	CE	LYS	A	731		18.029	11.072	48.717	1.00	32.42	A
	ATOM	381	NZ	LYS	A	731		19.059	10.845	49.766	1.00	35.26	A
	ATOM	382	C	LYS	A	731		16.158	8.435	45.179	1.00	19.62	A
	ATOM	383	O	LYS	A	731		15.973	7.778	46.209	1.00	19.40	A
25	ATOM	384	N	TRP	A	732		15.164	8.873	44.417	1.00	18.65	A
	ATOM	385	CA	TRP	A	732		13.767	8.595	44.714	1.00	16.92	A
	ATOM	386	CB	TRP	A	732		12.905	9.226	43.617	1.00	18.08	A
	ATOM	387	CG	TRP	A	732		11.453	8.863	43.602	1.00	16.59	A
	ATOM	388	CD2	TRP	A	732		10.791	8.069	42.612	1.00	18.88	A
30	ATOM	389	CE2	TRP	A	732		9.412	8.062	42.931	1.00	19.08	A
	ATOM	390	CE3	TRP	A	732		11.228	7.366	41.478	1.00	16.99	A
	ATOM	391	CD1	TRP	A	732		10.481	9.286	44.469	1.00	19.57	A
	ATOM	392	NE1	TRP	A	732		9.250	8.810	44.069	1.00	18.44	A
	ATOM	393	CZ2	TRP	A	732		8.467	7.375	42.157	1.00	19.26	A
35	ATOM	394	CZ3	TRP	A	732		10.289	6.685	40.710	1.00	17.20	A
	ATOM	395	CH2	TRP	A	732		8.923	6.697	41.054	1.00	18.84	A
	ATOM	396	C	TRP	A	732		13.508	7.090	44.808	1.00	16.34	A
	ATOM	397	O	TRP	A	732		12.876	6.611	45.754	1.00	17.11	A
	ATOM	398	N	SER	A	733		14.016	6.341	43.838	1.00	16.51	A
40	ATOM	399	CA	SER	A	733		13.803	4.901	43.813	1.00	18.54	A
	ATOM	400	CB	SER	A	733		14.448	4.287	42.561	1.00	18.74	A
	ATOM	401	OG	SER	A	733		15.861	4.291	42.643	1.00	18.35	A
	ATOM	402	C	SER	A	733		14.319	4.202	45.072	1.00	19.10	A
	ATOM	403	O	SER	A	733		13.749	3.196	45.508	1.00	18.34	A
45	ATOM	404	N	LYS	A	734		15.385	4.741	45.658	1.00	18.85	A
	ATOM	405	CA	LYS	A	734		15.958	4.160	46.865	1.00	19.80	A
	ATOM	406	CB	LYS	A	734		17.295	4.831	47.200	1.00	22.02	A
	ATOM	407	CG	LYS	A	734		18.381	4.547	46.178	1.00	24.28	A
	ATOM	408	CD	LYS	A	734		19.678	5.259	46.517	1.00	29.24	A
50	ATOM	409	CE	LYS	A	734		20.717	5.021	45.429	1.00	30.96	A
	ATOM	410	NZ	LYS	A	734		21.974	5.767	45.688	1.00	34.40	A
	ATOM	411	C	LYS	A	734		15.012	4.275	48.054	1.00	19.01	A
	ATOM	412	O	LYS	A	734		15.107	3.500	49.000	1.00	18.14	A
	ATOM	413	N	SER	A	735		14.099	5.240	47.998	1.00	19.77	A
55	ATOM	414	CA	SER	A	735		13.131	5.445	49.075	1.00	20.89	A
	ATOM	415	CB	SER	A	735		13.032	6.931	49.418	1.00	21.77	A
	ATOM	416	OG	SER	A	735		14.270	7.412	49.899	1.00	26.19	A

Table 2. (cont'd)

		#	Name	Res.	Chain	Res #	X	Y	Z	occ	B	SegID
5	ATOM	417	C	SER	A	735	11.741	4.928	48.735	1.00	18.31	A
	ATOM	418	O	SER	A	735	10.864	4.888	49.594	1.00	17.33	A
	ATOM	419	N	LEU	A	736	11.544	4.544	47.480	1.00	18.55	A
	ATOM	420	CA	LEU	A	736	10.258	4.036	47.007	1.00	16.70	A
	ATOM	421	CB	LEU	A	736	10.280	3.936	45.478	1.00	16.07	A
10	ATOM	422	CG	LEU	A	736	9.049	3.372	44.766	1.00	17.19	A
	ATOM	423	CD1	LEU	A	736	7.807	4.227	45.062	1.00	16.11	A
	ATOM	424	CD2	LEU	A	736	9.328	3.338	43.270	1.00	12.10	A
	ATOM	425	C	LEU	A	736	9.954	2.670	47.622	1.00	16.59	A
	ATOM	426	O	LEU	A	736	10.643	1.686	47.341	1.00	14.96	A
15	ATOM	427	N	PRO	A	737	8.906	2.588	48.461	1.00	16.50	A
	ATOM	428	CD	PRO	A	737	7.985	3.652	48.900	1.00	15.57	A
	ATOM	429	CA	PRO	A	737	8.564	1.306	49.092	1.00	18.45	A
	ATOM	430	CB	PRO	A	737	7.215	1.593	49.753	1.00	18.84	A
	ATOM	431	CG	PRO	A	737	7.356	3.040	50.154	1.00	16.58	A
20	ATOM	432	C	PRO	A	737	8.510	0.127	48.126	1.00	20.18	A
	ATOM	433	O	PRO	A	737	7.839	0.181	47.090	1.00	18.72	A
	ATOM	434	N	GLY	A	738	9.244	-0.928	48.468	1.00	19.99	A
	ATOM	435	CA	GLY	A	738	9.269	-2.122	47.643	1.00	20.37	A
	ATOM	436	C	GLY	A	738	10.379	-2.222	46.609	1.00	21.67	A
25	ATOM	437	O	GLY	A	738	10.883	-3.314	46.344	1.00	22.52	A
	ATOM	438	N	PHE	A	739	10.784	-1.094	46.033	1.00	20.61	A
	ATOM	439	CA	PHE	A	739	11.807	-1.113	44.988	1.00	19.83	A
	ATOM	440	CB	PHE	A	739	12.028	0.300	44.431	1.00	19.10	A
	ATOM	441	CG	PHE	A	739	12.605	0.322	43.035	1.00	19.43	A
30	ATOM	442	CD1	PHE	A	739	11.907	-0.252	41.972	1.00	20.73	A
	ATOM	443	CD2	PHE	A	739	13.835	0.925	42.782	1.00	21.00	A
	ATOM	444	CE1	PHE	A	739	12.426	-0.225	40.669	1.00	20.34	A
	ATOM	445	CE2	PHE	A	739	14.366	0.961	41.482	1.00	20.08	A
	ATOM	446	CZ	PHE	A	739	13.653	0.381	40.424	1.00	18.50	A
35	ATOM	447	C	PHE	A	739	13.154	-1.703	45.404	1.00	20.67	A
	ATOM	448	O	PHE	A	739	13.695	-2.555	44.708	1.00	19.78	A
	ATOM	449	N	ARG	A	740	13.690	-1.248	46.532	1.00	21.77	A
	ATOM	450	CA	ARG	A	740	14.990	-1.716	47.010	1.00	22.39	A
	ATOM	451	CB	ARG	A	740	15.355	-1.009	48.321	1.00	21.37	A
40	ATOM	452	CG	ARG	A	740	14.409	-1.304	49.480	1.00	21.34	A
	ATOM	453	CD	ARG	A	740	14.946	-0.719	50.780	1.00	19.50	A
	ATOM	454	NE	ARG	A	740	14.050	-0.960	51.908	1.00	20.23	A
	ATOM	455	CZ	ARG	A	740	14.351	-0.652	53.165	1.00	20.17	A
	ATOM	456	NH1	ARG	A	740	15.520	-0.095	53.442	1.00	18.30	A
45	ATOM	457	NH2	ARG	A	740	13.488	-0.900	54.144	1.00	19.12	A
	ATOM	458	C	ARG	A	740	15.092	-3.225	47.213	1.00	24.06	A
	ATOM	459	O	ARG	A	740	16.195	-3.776	47.272	1.00	24.88	A
	ATOM	460	N	ASN	A	741	13.953	-3.899	47.308	1.00	24.13	A
	ATOM	461	CA	ASN	A	741	13.962	-5.340	47.531	1.00	26.03	A
50	ATOM	462	CB	ASN	A	741	12.744	-5.736	48.373	1.00	27.83	A
	ATOM	463	CG	ASN	A	741	12.650	-4.931	49.660	1.00	29.37	A
	ATOM	464	OD1	ASN	A	741	13.637	-4.780	50.381	1.00	29.40	A
	ATOM	465	ND2	ASN	A	741	11.464	-4.409	49.952	1.00	30.58	A
	ATOM	466	C	ASN	A	741	14.042	-6.172	46.253	1.00	25.13	A
55	ATOM	467	O	ASN	A	741	14.128	-7.401	46.305	1.00	24.44	A
	ATOM	468	N	LEU	A	742	14.012	-5.504	45.104	1.00	22.83	A
	ATOM	469	CA	LEU	A	742	14.135	-6.197	43.831	1.00	21.37	A

Table 2. (cont'd)

		#	Name	Res.	Chain	Res #	X	Y	Z	occ	B	SegID
5	ATOM	470	CB	LEU	A	742	13.496	-5.384	42.698	1.00	21.88	A
	ATOM	471	CG	LEU	A	742	12.009	-5.019	42.812	1.00	21.52	A
	ATOM	472	CD1	LEU	A	742	11.613	-4.138	41.624	1.00	21.95	A
	ATOM	473	CD2	LEU	A	742	11.159	-6.284	42.840	1.00	19.89	A
	ATOM	474	C	LEU	A	742	15.637	-6.311	43.597	1.00	21.92	A
10	ATOM	475	O	LEU	A	742	16.406	-5.514	44.130	1.00	21.09	A
	ATOM	476	N	HIS	A	743	16.057	-7.302	42.818	1.00	23.00	A
	ATOM	477	CA	HIS	A	743	17.477	-7.485	42.527	1.00	23.50	A
	ATOM	478	CB	HIS	A	743	17.652	-8.612	41.507	1.00	25.73	A
	ATOM	479	CG	HIS	A	743	19.071	-9.056	41.328	1.00	29.22	A
15	ATOM	480	CD2	HIS	A	743	19.697	-10.202	41.690	1.00	29.68	A
	ATOM	481	ND1	HIS	A	743	20.025	-8.277	40.708	1.00	28.89	A
	ATOM	482	CE1	HIS	A	743	21.177	-8.925	40.694	1.00	31.58	A
	ATOM	483	NE2	HIS	A	743	21.005	-10.096	41.283	1.00	31.35	A
	ATOM	484	C	HIS	A	743	18.011	-6.170	41.961	1.00	24.00	A
20	ATOM	485	O	HIS	A	743	17.290	-5.459	41.252	1.00	22.58	A
	ATOM	486	N	ILE	A	744	19.260	-5.840	42.276	1.00	22.45	A
	ATOM	487	CA	ILE	A	744	19.854	-4.598	41.791	1.00	23.13	A
	ATOM	488	CB	ILE	A	744	21.316	-4.437	42.286	1.00	24.13	A
	ATOM	489	CG2	ILE	A	744	22.158	-5.623	41.829	1.00	23.77	A
25	ATOM	490	CG1	ILE	A	744	21.908	-3.128	41.751	1.00	25.51	A
	ATOM	491	CD1	ILE	A	744	21.194	-1.865	42.234	1.00	27.84	A
	ATOM	492	C	ILE	A	744	19.819	-4.496	40.263	1.00	21.80	A
	ATOM	493	O	ILE	A	744	19.639	-3.406	39.715	1.00	19.60	A
	ATOM	494	N	ASP	A	745	19.990	-5.622	39.574	1.00	21.91	A
30	ATOM	495	CA	ASP	A	745	19.945	-5.609	38.112	1.00	21.89	A
	ATOM	496	CB	ASP	A	745	20.271	-6.987	37.526	1.00	25.03	A
	ATOM	497	CG	ASP	A	745	21.706	-7.415	37.776	1.00	27.05	A
	ATOM	498	OD1	ASP	A	745	22.562	-6.546	38.028	1.00	28.56	A
	ATOM	499	OD2	ASP	A	745	21.973	-8.632	37.703	1.00	31.09	A
35	ATOM	500	C	ASP	A	745	18.545	-5.210	37.653	1.00	20.59	A
	ATOM	501	O	ASP	A	745	18.386	-4.530	36.637	1.00	19.07	A
	ATOM	502	N	ASP	A	746	17.530	-5.656	38.391	1.00	19.31	A
	ATOM	503	CA	ASP	A	746	16.154	-5.332	38.043	1.00	18.60	A
	ATOM	504	CB	ASP	A	746	15.160	-6.124	38.903	1.00	19.50	A
40	ATOM	505	CG	ASP	A	746	15.187	-7.620	38.620	1.00	20.87	A
	ATOM	506	OD1	ASP	A	746	15.631	-8.029	37.530	1.00	24.46	A
	ATOM	507	OD2	ASP	A	746	14.743	-8.391	39.493	1.00	22.73	A
	ATOM	508	C	ASP	A	746	15.901	-3.842	38.232	1.00	18.23	A
	ATOM	509	O	ASP	A	746	15.283	-3.201	37.383	1.00	16.68	A
45	ATOM	510	N	GLN	A	747	16.379	-3.294	39.347	1.00	16.31	A
	ATOM	511	CA	GLN	A	747	16.196	-1.877	39.635	1.00	16.33	A
	ATOM	512	CB	GLN	A	747	16.870	-1.505	40.965	1.00	17.68	A
	ATOM	513	CG	GLN	A	747	16.402	-2.330	42.158	1.00	16.41	A
	ATOM	514	CD	GLN	A	747	17.039	-1.894	43.471	1.00	19.86	A
50	ATOM	515	OE1	GLN	A	747	17.270	-2.714	44.361	1.00	21.96	A
	ATOM	516	NE2	GLN	A	747	17.307	-0.601	43.605	1.00	13.08	A
	ATOM	517	C	GLN	A	747	16.790	-1.025	38.519	1.00	16.94	A
	ATOM	518	O	GLN	A	747	16.158	-0.083	38.032	1.00	16.26	A
	ATOM	519	N	ILE	A	748	18.011	-1.360	38.119	1.00	17.19	A
55	ATOM	520	CA	ILE	A	748	18.694	-0.621	37.067	1.00	17.75	A
	ATOM	521	CB	ILE	A	748	20.133	-1.136	36.867	1.00	18.93	A
	ATOM	522	CG2	ILE	A	748	20.736	-0.537	35.591	1.00	19.15	A

Table 2. (cont'd)

		#	Name	Res.	Chain	Res #	X	Y	Z	occ	B	SegID
	ATOM	523	CG1	ILE	A	748	20.979	-0.780	38.094	1.00	19.91	A
5	ATOM	524	CD1	ILE	A	748	22.419	-1.268	38.003	1.00	26.17	A
	ATOM	525	C	ILE	A	748	17.951	-0.726	35.745	1.00	16.60	A
	ATOM	526	O	ILE	A	748	17.801	0.263	35.035	1.00	17.71	A
	ATOM	527	N	THR	A	749	17.490	-1.926	35.415	1.00	16.86	A
	ATOM	528	CA	THR	A	749	16.772	-2.128	34.166	1.00	17.95	A
10	ATOM	529	CB	THR	A	749	16.441	-3.618	33.942	1.00	18.55	A
	ATOM	530	OG1	THR	A	749	17.657	-4.358	33.776	1.00	19.19	A
	ATOM	531	CG2	THR	A	749	15.589	-3.794	32.695	1.00	19.51	A
	ATOM	532	C	THR	A	749	15.479	-1.317	34.114	1.00	17.38	A
	ATOM	533	O	THR	A	749	15.178	-0.690	33.099	1.00	17.28	A
15	ATOM	534	N	LEU	A	750	14.720	-1.327	35.206	1.00	16.72	A
	ATOM	535	CA	LEU	A	750	13.455	-0.591	35.259	1.00	16.64	A
	ATOM	536	CB	LEU	A	750	12.727	-0.887	36.576	1.00	15.87	A
	ATOM	537	CG	LEU	A	750	12.229	-2.334	36.712	1.00	17.09	A
	ATOM	538	CD1	LEU	A	750	11.660	-2.569	38.111	1.00	13.60	A
20	ATOM	539	CD2	LEU	A	750	11.166	-2.604	35.642	1.00	15.56	A
	ATOM	540	C	LEU	A	750	13.675	0.911	35.097	1.00	17.48	A
	ATOM	541	O	LEU	A	750	12.894	1.599	34.423	1.00	16.71	A
	ATOM	542	N	ILE	A	751	14.737	1.427	35.706	1.00	16.32	A
	ATOM	543	CA	ILE	A	751	15.026	2.850	35.581	1.00	17.20	A
25	ATOM	544	CB	ILE	A	751	16.123	3.289	36.576	1.00	18.58	A
	ATOM	545	CG2	ILE	A	751	16.583	4.694	36.251	1.00	17.18	A
	ATOM	546	CG1	ILE	A	751	15.581	3.223	38.010	1.00	17.86	A
	ATOM	547	CD1	ILE	A	751	16.642	3.467	39.092	1.00	20.51	A
	ATOM	548	C	ILE	A	751	15.464	3.190	34.151	1.00	17.20	A
30	ATOM	549	O	ILE	A	751	15.093	4.234	33.613	1.00	16.21	A
	ATOM	550	N	GLN	A	752	16.241	2.306	33.534	1.00	17.94	A
	ATOM	551	CA	GLN	A	752	16.714	2.543	32.169	1.00	18.41	A
	ATOM	552	CB	GLN	A	752	17.844	1.571	31.824	1.00	19.20	A
	ATOM	553	CG	GLN	A	752	19.052	1.687	32.760	1.00	21.33	A
35	ATOM	554	CD	GLN	A	752	20.237	0.850	32.311	1.00	22.26	A
	ATOM	555	OE1	GLN	A	752	20.075	-0.214	31.717	1.00	21.77	A
	ATOM	556	NE2	GLN	A	752	21.439	1.323	32.614	1.00	22.92	A
	ATOM	557	C	GLN	A	752	15.600	2.435	31.128	1.00	19.31	A
	ATOM	558	O	GLN	A	752	15.657	3.088	30.082	1.00	19.71	A
40	ATOM	559	N	TYR	A	753	14.594	1.609	31.408	1.00	16.40	A
	ATOM	560	CA	TYR	A	753	13.468	1.445	30.488	1.00	17.45	A
	ATOM	561	CB	TYR	A	753	12.649	0.189	30.812	1.00	16.91	A
	ATOM	562	CG	TYR	A	753	13.220	-1.160	30.420	1.00	18.88	A
	ATOM	563	CD1	TYR	A	753	14.312	-1.280	29.560	1.00	19.37	A
45	ATOM	564	CE1	TYR	A	753	14.775	-2.542	29.158	1.00	19.99	A
	ATOM	565	CD2	TYR	A	753	12.609	-2.329	30.874	1.00	20.86	A
	ATOM	566	CE2	TYR	A	753	13.058	-3.579	30.483	1.00	19.71	A
	ATOM	567	CZ	TYR	A	753	14.134	-3.685	29.628	1.00	21.49	A
	ATOM	568	OH	TYR	A	753	14.546	-4.944	29.251	1.00	22.20	A
50	ATOM	569	C	TYR	A	753	12.480	2.606	30.583	1.00	18.38	A
	ATOM	570	O	TYR	A	753	11.925	3.053	29.578	1.00	20.69	A
	ATOM	571	N	SER	A	754	12.263	3.080	31.804	1.00	16.00	A
	ATOM	572	CA	SER	A	754	11.259	4.108	32.070	1.00	17.01	A
	ATOM	573	CB	SER	A	754	10.514	3.731	33.349	1.00	16.69	A
55	ATOM	574	OG	SER	A	754	11.362	3.939	34.477	1.00	14.48	A
	ATOM	575	C	SER	A	754	11.651	5.574	32.195	1.00	16.37	A

Table 2. (cont'd)

		#	Name	Res.	Chain	Res #	X	Y	Z	occ	B	SegID
	ATOM	576	O	SER	A	754	10.774	6.425	32.338	1.00	15.97	A
5	ATOM	577	N	TRP	A	755	12.934	5.896	32.141	1.00	16.30	A
	ATOM	578	CA	TRP	A	755	13.310	7.289	32.333	1.00	16.48	A
	ATOM	579	CB	TRP	A	755	14.828	7.468	32.235	1.00	17.08	A
	ATOM	580	CG	TRP	A	755	15.389	7.268	30.884	1.00	19.06	A
	ATOM	581	CD2	TRP	A	755	15.593	8.276	29.890	1.00	18.43	A
10	ATOM	582	CE2	TRP	A	755	16.138	7.640	28.757	1.00	18.03	A
	ATOM	583	CE3	TRP	A	755	15.364	9.657	29.848	1.00	20.60	A
	ATOM	584	CD1	TRP	A	755	15.807	6.093	30.333	1.00	21.01	A
	ATOM	585	NE1	TRP	A	755	16.260	6.308	29.053	1.00	21.00	A
	ATOM	586	CZ2	TRP	A	755	16.462	8.336	27.590	1.00	20.14	A
15	ATOM	587	CZ3	TRP	A	755	15.686	10.351	28.687	1.00	23.49	A
	ATOM	588	CH2	TRP	A	755	16.229	9.686	27.572	1.00	20.73	A
	ATOM	589	C	TRP	A	755	12.608	8.330	31.461	1.00	16.13	A
	ATOM	590	O	TRP	A	755	12.208	9.372	31.970	1.00	15.92	A
	ATOM	591	N	MET	A	756	12.450	8.073	30.165	1.00	15.54	A
20	ATOM	592	CA	MET	A	756	11.791	9.066	29.314	1.00	15.68	A
	ATOM	593	CB	MET	A	756	11.881	8.677	27.832	1.00	15.94	A
	ATOM	594	CG	MET	A	756	11.294	9.720	26.872	1.00	15.93	A
	ATOM	595	SD	MET	A	756	12.195	11.300	26.820	1.00	20.03	A
	ATOM	596	CE	MET	A	756	13.530	10.864	25.738	1.00	18.29	A
25	ATOM	597	C	MET	A	756	10.327	9.249	29.710	1.00	15.47	A
	ATOM	598	O	MET	A	756	9.837	10.379	29.778	1.00	15.06	A
	ATOM	599	N	SER	A	757	9.627	8.150	29.983	1.00	16.31	A
	ATOM	600	CA	SER	A	757	8.226	8.258	30.371	1.00	17.31	A
	ATOM	601	CB	SER	A	757	7.569	6.872	30.481	1.00	19.17	A
30	ATOM	602	OG	SER	A	757	8.121	6.111	31.537	1.00	23.52	A
	ATOM	603	C	SER	A	757	8.087	9.005	31.690	1.00	16.83	A
	ATOM	604	O	SER	A	757	7.166	9.798	31.855	1.00	16.08	A
	ATOM	605	N	LEU	A	758	8.998	8.765	32.632	1.00	16.85	A
	ATOM	606	CA	LEU	A	758	8.918	9.456	33.915	1.00	15.97	A
35	ATOM	607	CB	LEU	A	758	9.940	8.899	34.911	1.00	17.47	A
	ATOM	608	CG	LEU	A	758	9.748	7.461	35.401	1.00	18.97	A
	ATOM	609	CD1	LEU	A	758	10.879	7.100	36.362	1.00	19.01	A
	ATOM	610	CD2	LEU	A	758	8.408	7.324	36.094	1.00	18.02	A
	ATOM	611	C	LEU	A	758	9.156	10.950	33.730	1.00	15.21	A
40	ATOM	612	O	LEU	A	758	8.469	11.774	34.333	1.00	14.38	A
	ATOM	613	N	MET	A	759	10.131	11.301	32.895	1.00	15.87	A
	ATOM	614	CA	MET	A	759	10.424	12.707	32.650	1.00	15.98	A
	ATOM	615	CB	MET	A	759	11.675	12.855	31.784	1.00	18.16	A
	ATOM	616	CG	MET	A	759	12.968	12.528	32.506	1.00	20.79	A
45	ATOM	617	SD	MET	A	759	14.388	12.785	31.431	1.00	26.08	A
	ATOM	618	CE	MET	A	759	15.672	11.980	32.416	1.00	25.95	A
	ATOM	619	C	MET	A	759	9.266	13.441	31.981	1.00	16.81	A
	ATOM	620	O	MET	A	759	8.900	14.542	32.392	1.00	18.56	A
	ATOM	621	N	VAL	A	760	8.688	12.837	30.949	1.00	17.28	A
50	ATOM	622	CA	VAL	A	760	7.590	13.483	30.241	1.00	17.08	A
	ATOM	623	CB	VAL	A	760	7.290	12.761	28.897	1.00	18.35	A
	ATOM	624	CG1	VAL	A	760	6.511	11.486	29.137	1.00	19.74	A
	ATOM	625	CG2	VAL	A	760	6.545	13.699	27.964	1.00	20.50	A
	ATOM	626	C	VAL	A	760	6.330	13.548	31.111	1.00	18.39	A
55	ATOM	627	O	VAL	A	760	5.547	14.499	31.017	1.00	19.10	A
	ATOM	628	N	PHE	A	761	6.140	12.545	31.963	1.00	16.68	A

Table 2. (cont'd)

		#	Name	Res.	Chain	Res	#	X	Y	Z	occ	B	SegID
	ATOM	629	CA	PHE	A	761		4.986	12.523	32.857	1.00	16.45	A
5	ATOM	630	CB	PHE	A	761		4.897	11.174	33.575	1.00	16.18	A
	ATOM	631	CG	PHE	A	761		3.529	10.861	34.130	1.00	15.95	A
	ATOM	632	CD1	PHE	A	761		2.420	10.794	33.290	1.00	13.24	A
	ATOM	633	CD2	PHE	A	761		3.359	10.588	35.485	1.00	15.65	A
	ATOM	634	CE1	PHE	A	761		1.164	10.457	33.791	1.00	14.74	A
10	ATOM	635	CE2	PHE	A	761		2.104	10.248	35.997	1.00	16.67	A
	ATOM	636	CZ	PHE	A	761		1.007	10.183	35.148	1.00	16.46	A
	ATOM	637	C	PHE	A	761		5.155	13.651	33.876	1.00	16.84	A
	ATOM	638	O	PHE	A	761		4.205	14.377	34.175	1.00	17.63	A
	ATOM	639	N	GLY	A	762		6.372	13.798	34.400	1.00	15.02	A
15	ATOM	640	CA	GLY	A	762		6.644	14.853	35.363	1.00	15.08	A
	ATOM	641	C	GLY	A	762		6.480	16.213	34.706	1.00	15.77	A
	ATOM	642	O	GLY	A	762		5.978	17.158	35.316	1.00	16.20	A
	ATOM	643	N	LEU	A	763		6.920	16.317	33.457	1.00	15.32	A
	ATOM	644	CA	LEU	A	763		6.796	17.559	32.706	1.00	17.12	A
20	ATOM	645	CB	LEU	A	763		7.346	17.373	31.294	1.00	17.85	A
	ATOM	646	CG	LEU	A	763		6.960	18.409	30.236	1.00	18.06	A
	ATOM	647	CD1	LEU	A	763		7.544	19.779	30.588	1.00	17.06	A
	ATOM	648	CD2	LEU	A	763		7.473	17.931	28.878	1.00	16.76	A
	ATOM	649	C	LEU	A	763		5.316	17.906	32.627	1.00	17.25	A
25	ATOM	650	O	LEU	A	763		4.920	19.064	32.795	1.00	16.63	A
	ATOM	651	N	GLY	A	764		4.511	16.883	32.365	1.00	17.94	A
	ATOM	652	CA	GLY	A	764		3.077	17.067	32.265	1.00	19.00	A
	ATOM	653	C	GLY	A	764		2.510	17.652	33.540	1.00	19.54	A
	ATOM	654	O	GLY	A	764		1.750	18.621	33.497	1.00	18.93	A
30	ATOM	655	N	TRP	A	765		2.890	17.073	34.677	1.00	19.11	A
	ATOM	656	CA	TRP	A	765		2.408	17.539	35.971	1.00	20.62	A
	ATOM	657	CB	TRP	A	765		2.930	16.632	37.092	1.00	21.33	A
	ATOM	658	CG	TRP	A	765		2.414	17.012	38.449	1.00	23.29	A
	ATOM	659	CD2	TRP	A	765		1.078	16.833	38.937	1.00	23.57	A
35	ATOM	660	CE2	TRP	A	765		1.034	17.368	40.242	1.00	25.22	A
	ATOM	661	CE3	TRP	A	765		-0.088	16.272	38.396	1.00	25.69	A
	ATOM	662	CD1	TRP	A	765		3.107	17.630	39.449	1.00	24.56	A
	ATOM	663	NE1	TRP	A	765		2.284	17.848	40.532	1.00	25.99	A
	ATOM	664	CZ2	TRP	A	765		-0.132	17.362	41.016	1.00	27.48	A
40	ATOM	665	CZ3	TRP	A	765		-1.248	16.266	39.166	1.00	24.65	A
	ATOM	666	CH2	TRP	A	765		-1.259	16.808	40.460	1.00	25.43	A
	ATOM	667	C	TRP	A	765		2.794	18.988	36.255	1.00	19.81	A
	ATOM	668	O	TRP	A	765		1.928	19.812	36.546	1.00	19.54	A
	ATOM	669	N	ARG	A	766		4.087	19.299	36.174	1.00	19.47	A
45	ATOM	670	CA	ARG	A	766		4.556	20.666	36.421	1.00	19.40	A
	ATOM	671	CB	ARG	A	766		6.080	20.763	36.247	1.00	18.97	A
	ATOM	672	CG	ARG	A	766		6.882	20.041	37.320	1.00	19.48	A
	ATOM	673	CD	ARG	A	766		8.363	20.419	37.252	1.00	17.56	A
	ATOM	674	NE	ARG	A	766		8.984	20.012	35.994	1.00	18.67	A
50	ATOM	675	CZ	ARG	A	766		9.269	18.755	35.666	1.00	20.53	A
	ATOM	676	NH1	ARG	A	766		8.996	17.761	36.502	1.00	19.81	A
	ATOM	677	NH2	ARG	A	766		9.822	18.488	34.492	1.00	17.68	A
	ATOM	678	C	ARG	A	766		3.884	21.687	35.505	1.00	19.03	A
	ATOM	679	O	ARG	A	766		3.505	22.774	35.944	1.00	19.25	A
55	ATOM	680	N	SER	A	767		3.741	21.348	34.229	1.00	18.79	A
	ATOM	681	CA	SER	A	767		3.108	22.265	33.281	1.00	18.18	A

Table 2. (cont'd)

		#	Name	Res.	Chain	Res #	X	Y	Z	occ	B	SegID
5	ATOM	682	CB	SER	A	767	3.140	21.671	31.875	1.00	19.63	A
	ATOM	683	OG	SER	A	767	4.472	21.475	31.433	1.00	20.37	A
	ATOM	684	C	SER	A	767	1.662	22.507	33.708	1.00	20.50	A
	ATOM	685	O	SER	A	767	1.156	23.638	33.670	1.00	17.64	A
	ATOM	686	N	TYR	A	768	1.008	21.427	34.123	1.00	21.00	A
10	ATOM	687	CA	TYR	A	768	-0.375	21.465	34.579	1.00	22.52	A
	ATOM	688	CB	TYR	A	768	-0.845	20.027	34.853	1.00	24.84	A
	ATOM	689	CG	TYR	A	768	-2.213	19.874	35.490	1.00	26.80	A
	ATOM	690	CD1	TYR	A	768	-3.330	20.524	34.968	1.00	27.94	A
	ATOM	691	CE1	TYR	A	768	-4.601	20.319	35.505	1.00	28.43	A
15	ATOM	692	CD2	TYR	A	768	-2.401	19.012	36.577	1.00	28.57	A
	ATOM	693	CE2	TYR	A	768	-3.672	18.799	37.119	1.00	29.44	A
	ATOM	694	CZ	TYR	A	768	-4.765	19.455	36.575	1.00	30.55	A
	ATOM	695	OH	TYR	A	768	-6.024	19.238	37.092	1.00	32.27	A
	ATOM	696	C	TYR	A	768	-0.545	22.328	35.834	1.00	23.30	A
20	ATOM	697	O	TYR	A	768	-1.411	23.202	35.884	1.00	23.03	A
	ATOM	698	N	LYS	A	769	0.296	22.100	36.836	1.00	24.38	A
	ATOM	699	CA	LYS	A	769	0.195	22.834	38.097	1.00	25.93	A
	ATOM	700	CB	LYS	A	769	0.828	22.013	39.228	1.00	29.02	A
	ATOM	701	CG	LYS	A	769	0.293	20.591	39.364	1.00	33.47	A
25	ATOM	702	CD	LYS	A	769	-1.225	20.546	39.541	1.00	36.41	A
	ATOM	703	CE	LYS	A	769	-1.671	21.179	40.850	1.00	37.62	A
	ATOM	704	NZ	LYS	A	769	-3.160	21.214	40.952	1.00	38.42	A
	ATOM	705	C	LYS	A	769	0.759	24.255	38.155	1.00	25.94	A
	ATOM	706	O	LYS	A	769	0.248	25.085	38.908	1.00	25.87	A
30	ATOM	707	N	HIS	A	770	1.799	24.549	37.380	1.00	25.10	A
	ATOM	708	CA	HIS	A	770	2.405	25.881	37.425	1.00	25.51	A
	ATOM	709	CB	HIS	A	770	3.928	25.770	37.294	1.00	28.44	A
	ATOM	710	CG	HIS	A	770	4.572	24.979	38.389	1.00	32.15	A
	ATOM	711	CD2	HIS	A	770	5.154	23.755	38.383	1.00	33.76	A
35	ATOM	712	ND1	HIS	A	770	4.641	25.427	39.691	1.00	36.27	A
	ATOM	713	CE1	HIS	A	770	5.236	24.515	40.439	1.00	35.37	A
	ATOM	714	NE2	HIS	A	770	5.557	23.490	39.670	1.00	34.58	A
	ATOM	715	C	HIS	A	770	1.893	26.879	36.390	1.00	25.25	A
	ATOM	716	O	HIS	A	770	1.779	28.073	36.679	1.00	25.06	A
40	ATOM	717	N	VAL	A	771	1.601	26.404	35.185	1.00	22.32	A
	ATOM	718	CA	VAL	A	771	1.132	27.300	34.134	1.00	22.97	A
	ATOM	719	CB	VAL	A	771	2.213	27.486	33.043	1.00	23.19	A
	ATOM	720	CG1	VAL	A	771	3.326	28.385	33.575	1.00	23.98	A
	ATOM	721	CG2	VAL	A	771	2.786	26.134	32.630	1.00	23.30	A
45	ATOM	722	C	VAL	A	771	-0.179	26.869	33.491	1.00	21.91	A
	ATOM	723	O	VAL	A	771	-0.411	27.101	32.305	1.00	23.10	A
	ATOM	724	N	SER	A	772	-1.036	26.247	34.291	1.00	20.67	A
	ATOM	725	CA	SER	A	772	-2.340	25.796	33.825	1.00	22.11	A
	ATOM	726	CB	SER	A	772	-3.226	27.012	33.532	1.00	23.44	A
50	ATOM	727	OG	SER	A	772	-3.245	27.902	34.643	1.00	22.81	A
	ATOM	728	C	SER	A	772	-2.222	24.923	32.583	1.00	21.42	A
	ATOM	729	O	SER	A	772	-3.157	24.830	31.781	1.00	21.19	A
	ATOM	730	N	GLY	A	773	-1.060	24.292	32.426	1.00	21.10	A
	ATOM	731	CA	GLY	A	773	-0.820	23.415	31.292	1.00	19.40	A
55	ATOM	732	C	GLY	A	773	-0.654	24.099	29.944	1.00	20.22	A
	ATOM	733	O	GLY	A	773	-0.603	23.426	28.911	1.00	21.05	A
	ATOM	734	N	GLN	A	774	-0.541	25.423	29.935	1.00	19.35	A

Table 2. (cont'd)

		#	Name	Res.	Chain	Res #	X	Y	Z	occ	B	SegID
	ATOM	735	CA	GLN	A	774	-0.422	26.144	28.669	1.00	19.19	A
5	ATOM	736	CB	GLN	A	774	-1.335	27.372	28.703	1.00	19.43	A
	ATOM	737	CG	GLN	A	774	-2.793	26.987	28.931	1.00	19.08	A
	ATOM	738	CD	GLN	A	774	-3.187	25.750	28.136	1.00	18.95	A
	ATOM	739	OE1	GLN	A	774	-3.122	25.739	26.904	1.00	18.16	A
	ATOM	740	NE2	GLN	A	774	-3.590	24.697	28.842	1.00	18.81	A
10	ATOM	741	C	GLN	A	774	0.992	26.527	28.224	1.00	18.56	A
	ATOM	742	O	GLN	A	774	1.178	27.356	27.337	1.00	18.81	A
	ATOM	743	N	MET	A	775	1.981	25.911	28.855	1.00	19.20	A
	ATOM	744	CA	MET	A	775	3.385	26.105	28.520	1.00	19.64	A
	ATOM	745	CB	MET	A	775	4.009	27.253	29.323	1.00	20.86	A
15	ATOM	746	CG	MET	A	775	3.522	28.652	28.959	1.00	21.16	A
	ATOM	747	SD	MET	A	775	4.507	29.907	29.799	1.00	25.84	A
	ATOM	748	CE	MET	A	775	3.216	30.919	30.610	1.00	25.72	A
	ATOM	749	C	MET	A	775	4.061	24.803	28.921	1.00	18.35	A
	ATOM	750	O	MET	A	775	3.516	24.050	29.727	1.00	20.32	A
20	ATOM	751	N	LEU	A	776	5.224	24.521	28.349	1.00	17.82	A
	ATOM	752	CA	LEU	A	776	5.955	23.317	28.721	1.00	18.54	A
	ATOM	753	CB	LEU	A	776	6.723	22.741	27.526	1.00	18.50	A
	ATOM	754	CG	LEU	A	776	5.844	22.027	26.490	1.00	19.83	A
	ATOM	755	CD1	LEU	A	776	6.711	21.491	25.367	1.00	19.70	A
25	ATOM	756	CD2	LEU	A	776	5.068	20.890	27.149	1.00	18.31	A
	ATOM	757	C	LEU	A	776	6.912	23.762	29.813	1.00	18.66	A
	ATOM	758	O	LEU	A	776	7.886	24.471	29.551	1.00	19.30	A
	ATOM	759	N	TYR	A	777	6.611	23.354	31.040	1.00	16.71	A
	ATOM	760	CA	TYR	A	777	7.401	23.719	32.203	1.00	17.38	A
30	ATOM	761	CB	TYR	A	777	6.459	23.907	33.405	1.00	18.98	A
	ATOM	762	CG	TYR	A	777	7.056	24.636	34.591	1.00	22.23	A
	ATOM	763	CD1	TYR	A	777	7.970	24.008	35.439	1.00	23.96	A
	ATOM	764	CE1	TYR	A	777	8.500	24.670	36.550	1.00	25.16	A
	ATOM	765	CD2	TYR	A	777	6.689	25.954	34.878	1.00	22.47	A
35	ATOM	766	CE2	TYR	A	777	7.216	26.626	35.984	1.00	24.25	A
	ATOM	767	CZ	TYR	A	777	8.118	25.978	36.816	1.00	25.97	A
	ATOM	768	OH	TYR	A	777	8.632	26.629	37.918	1.00	25.81	A
	ATOM	769	C	TYR	A	777	8.440	22.641	32.500	1.00	16.79	A
	ATOM	770	O	TYR	A	777	8.290	21.867	33.443	1.00	16.14	A
40	ATOM	771	N	PHE	A	778	9.479	22.575	31.675	1.00	17.41	A
	ATOM	772	CA	PHE	A	778	10.533	21.590	31.890	1.00	18.04	A
	ATOM	773	CB	PHE	A	778	11.592	21.668	30.780	1.00	17.18	A
	ATOM	774	CG	PHE	A	778	11.076	21.299	29.414	1.00	19.92	A
	ATOM	775	CD1	PHE	A	778	10.664	22.284	28.520	1.00	19.96	A
45	ATOM	776	CD2	PHE	A	778	11.017	19.967	29.016	1.00	18.19	A
	ATOM	777	CE1	PHE	A	778	10.206	21.946	27.244	1.00	20.84	A
	ATOM	778	CE2	PHE	A	778	10.561	19.620	27.745	1.00	20.50	A
	ATOM	779	CZ	PHE	A	778	10.155	20.611	26.855	1.00	19.47	A
	ATOM	780	C	PHE	A	778	11.178	21.873	33.245	1.00	17.23	A
50	ATOM	781	O	PHE	A	778	11.393	20.961	34.049	1.00	15.16	A
	ATOM	782	N	ALA	A	779	11.479	23.149	33.486	1.00	17.50	A
	ATOM	783	CA	ALA	A	779	12.091	23.588	34.738	1.00	18.81	A
	ATOM	784	CB	ALA	A	779	13.599	23.329	34.708	1.00	16.57	A
	ATOM	785	C	ALA	A	779	11.816	25.083	34.940	1.00	20.23	A
55	ATOM	786	O	ALA	A	779	11.372	25.771	34.021	1.00	18.79	A
	ATOM	787	N	PRO	A	780	12.068	25.603	36.151	1.00	22.34	A

Table 2. (cont'd)

		#	Name	Res.	Chain	Res #	X	Y	Z	occ	B	SegID
5	ATOM	788	CD	PRO	A	780	12.432	24.933	37.411	1.00	22.01	A
	ATOM	789	CA	PRO	A	780	11.815	27.031	36.373	1.00	23.57	A
	ATOM	790	CB	PRO	A	780	12.236	27.232	37.825	1.00	25.03	A
	ATOM	791	CG	PRO	A	780	11.911	25.906	38.448	1.00	23.19	A
	ATOM	792	C	PRO	A	780	12.610	27.911	35.406	1.00	23.67	A
10	ATOM	793	O	PRO	A	780	12.154	28.982	35.018	1.00	22.71	A
	ATOM	794	N	ASP	A	781	13.795	27.442	35.017	1.00	23.34	A
	ATOM	795	CA	ASP	A	781	14.657	28.182	34.098	1.00	21.94	A
	ATOM	796	CB	ASP	A	781	16.107	28.136	34.594	1.00	21.93	A
	ATOM	797	CG	ASP	A	781	16.646	26.718	34.718	1.00	23.63	A
15	ATOM	798	OD1	ASP	A	781	15.843	25.769	34.856	1.00	22.19	A
	ATOM	799	OD2	ASP	A	781	17.883	26.554	34.693	1.00	24.73	A
	ATOM	800	C	ASP	A	781	14.569	27.676	32.653	1.00	21.19	A
	ATOM	801	O	ASP	A	781	15.390	28.032	31.806	1.00	20.19	A
	ATOM	802	N	LEU	A	782	13.572	26.847	32.369	1.00	19.89	A
20	ATOM	803	CA	LEU	A	782	13.385	26.343	31.013	1.00	20.33	A
	ATOM	804	CB	LEU	A	782	14.151	25.028	30.802	1.00	18.43	A
	ATOM	805	CG	LEU	A	782	14.176	24.494	29.361	1.00	19.40	A
	ATOM	806	CD1	LEU	A	782	14.784	25.536	28.434	1.00	20.75	A
	ATOM	807	CD2	LEU	A	782	14.981	23.203	29.300	1.00	19.07	A
25	ATOM	808	C	LEU	A	782	11.895	26.139	30.768	1.00	19.43	A
	ATOM	809	O	LEU	A	782	11.377	25.027	30.848	1.00	18.09	A
	ATOM	810	N	ILE	A	783	11.211	27.240	30.486	1.00	19.42	A
	ATOM	811	CA	ILE	A	783	9.779	27.208	30.233	1.00	20.01	A
	ATOM	812	CB	ILE	A	783	9.036	28.186	31.172	1.00	20.25	A
30	ATOM	813	CG2	ILE	A	783	7.536	28.162	30.877	1.00	23.95	A
	ATOM	814	CG1	ILE	A	783	9.298	27.803	32.632	1.00	20.97	A
	ATOM	815	CD1	ILE	A	783	8.914	28.885	33.646	1.00	21.41	A
	ATOM	816	C	ILE	A	783	9.531	27.614	28.786	1.00	19.86	A
	ATOM	817	O	ILE	A	783	9.954	28.686	28.352	1.00	18.73	A
35	ATOM	818	N	LEU	A	784	8.861	26.752	28.032	1.00	18.35	A
	ATOM	819	CA	LEU	A	784	8.577	27.073	26.642	1.00	18.52	A
	ATOM	820	CB	LEU	A	784	9.040	25.946	25.709	1.00	18.59	A
	ATOM	821	CG	LEU	A	784	10.420	25.291	25.813	1.00	20.62	A
	ATOM	822	CD1	LEU	A	784	10.716	24.600	24.479	1.00	19.63	A
40	ATOM	823	CD2	LEU	A	784	11.496	26.306	26.120	1.00	21.85	A
	ATOM	824	C	LEU	A	784	7.090	27.303	26.389	1.00	18.16	A
	ATOM	825	O	LEU	A	784	6.290	26.373	26.513	1.00	17.61	A
	ATOM	826	N	ASN	A	785	6.714	28.536	26.058	1.00	18.24	A
	ATOM	827	CA	ASN	A	785	5.323	28.809	25.708	1.00	18.38	A
45	ATOM	828	CB	ASN	A	785	4.970	30.302	25.866	1.00	19.86	A
	ATOM	829	CG	ASN	A	785	5.922	31.220	25.127	1.00	21.17	A
	ATOM	830	OD1	ASN	A	785	6.473	30.861	24.091	1.00	22.33	A
	ATOM	831	ND2	ASN	A	785	6.104	32.428	25.654	1.00	21.27	A
	ATOM	832	C	ASN	A	785	5.257	28.377	24.242	1.00	18.94	A
50	ATOM	833	O	ASN	A	785	6.286	28.051	23.655	1.00	19.11	A
	ATOM	834	N	GLU	A	786	4.077	28.376	23.637	1.00	20.82	A
	ATOM	835	CA	GLU	A	786	3.974	27.919	22.256	1.00	20.94	A
	ATOM	836	CB	GLU	A	786	2.513	27.923	21.792	1.00	23.70	A
	ATOM	837	CG	GLU	A	786	2.345	27.424	20.366	1.00	24.17	A
55	ATOM	838	CD	GLU	A	786	0.935	26.968	20.058	1.00	26.71	A
	ATOM	839	OE1	GLU	A	786	-0.012	27.549	20.630	1.00	20.59	A
	ATOM	840	OE2	GLU	A	786	0.781	26.037	19.235	1.00	23.53	A

Table 2. (cont'd)

		#	Name	Res.	Chain	Res #	X	Y	Z	occ	B	SegID
5	ATOM	841	C	GLU	A	786	4.839	28.649	21.239	1.00	22.11	A
	ATOM	842	O	GLU	A	786	5.375	28.023	20.330	1.00	21.62	A
	ATOM	843	N	GLN	A	787	4.978	29.963	21.370	1.00	22.98	A
	ATOM	844	CA	GLN	A	787	5.799	30.702	20.417	1.00	24.73	A
	ATOM	845	CB	GLN	A	787	5.738	32.207	20.698	1.00	26.16	A
10	ATOM	846	CG	GLN	A	787	6.457	33.064	19.652	1.00	29.65	A
	ATOM	847	CD	GLN	A	787	5.977	32.785	18.233	1.00	34.00	A
	ATOM	848	OE1	GLN	A	787	4.771	32.732	17.967	1.00	35.14	A
	ATOM	849	NE2	GLN	A	787	6.920	32.613	17.313	1.00	35.97	A
	ATOM	850	C	GLN	A	787	7.251	30.218	20.487	1.00	25.27	A
15	ATOM	851	O	GLN	A	787	7.916	30.078	19.457	1.00	23.55	A
	ATOM	852	N	ARG	A	788	7.740	29.957	21.696	1.00	24.46	A
	ATOM	853	CA	ARG	A	788	9.113	29.488	21.856	1.00	23.62	A
	ATOM	854	CB	ARG	A	788	9.512	29.486	23.332	1.00	23.38	A
	ATOM	855	CG	ARG	A	788	11.013	29.406	23.555	1.00	22.19	A
20	ATOM	856	CD	ARG	A	788	11.371	29.462	25.035	1.00	22.56	A
	ATOM	857	NE	ARG	A	788	12.817	29.466	25.241	1.00	21.14	A
	ATOM	858	CZ	ARG	A	788	13.410	29.478	26.433	1.00	25.92	A
	ATOM	859	NH1	ARG	A	788	14.737	29.481	26.514	1.00	26.50	A
	ATOM	860	NH2	ARG	A	788	12.682	29.482	27.546	1.00	26.08	A
25	ATOM	861	C	ARG	A	788	9.224	28.081	21.270	1.00	23.70	A
	ATOM	862	O	ARG	A	788	10.282	27.683	20.769	1.00	23.15	A
	ATOM	863	N	MET	A	789	8.122	27.335	21.331	1.00	23.02	A
	ATOM	864	CA	MET	A	789	8.072	25.987	20.776	1.00	23.37	A
	ATOM	865	CB	MET	A	789	6.746	25.298	21.124	1.00	23.06	A
30	ATOM	866	CG	MET	A	789	6.543	24.933	22.592	1.00	21.04	A
	ATOM	867	SD	MET	A	789	4.957	24.068	22.811	1.00	21.30	A
	ATOM	868	CE	MET	A	789	4.293	24.917	24.247	1.00	21.48	A
	ATOM	869	C	MET	A	789	8.185	26.074	19.255	1.00	25.50	A
	ATOM	870	O	MET	A	789	8.940	25.325	18.636	1.00	25.04	A
35	ATOM	871	N	LYS	A	790	7.423	26.992	18.664	1.00	27.11	A
	ATOM	872	CA	LYS	A	790	7.408	27.190	17.214	1.00	29.59	A
	ATOM	873	CB	LYS	A	790	6.447	28.322	16.833	1.00	32.00	A
	ATOM	874	CG	LYS	A	790	4.976	27.980	16.967	1.00	37.02	A
	ATOM	875	CD	LYS	A	790	4.103	29.124	16.456	1.00	38.59	A
40	ATOM	876	CE	LYS	A	790	2.628	28.840	16.698	1.00	41.04	A
	ATOM	877	NZ	LYS	A	790	1.753	29.958	16.236	1.00	42.99	A
	ATOM	878	C	LYS	A	790	8.770	27.498	16.609	1.00	30.18	A
	ATOM	879	O	LYS	A	790	9.068	27.073	15.493	1.00	28.32	A
	ATOM	880	N	GLU	A	791	9.591	28.251	17.330	1.00	30.15	A
45	ATOM	881	CA	GLU	A	791	10.908	28.597	16.813	1.00	33.53	A
	ATOM	882	CB	GLU	A	791	11.149	30.101	16.988	1.00	34.94	A
	ATOM	883	CG	GLU	A	791	10.733	30.663	18.334	1.00	37.89	A
	ATOM	884	CD	GLU	A	791	10.597	32.179	18.320	1.00	38.69	A
	ATOM	885	OE1	GLU	A	791	9.722	32.700	17.596	1.00	40.52	A
50	ATOM	886	OE2	GLU	A	791	11.366	32.851	19.035	1.00	39.54	A
	ATOM	887	C	GLU	A	791	12.048	27.790	17.435	1.00	33.31	A
	ATOM	888	O	GLU	A	791	13.198	28.230	17.440	1.00	34.67	A
	ATOM	889	N	SER	A	792	11.726	26.595	17.926	1.00	32.17	A
	ATOM	890	CA	SER	A	792	12.710	25.722	18.572	1.00	32.29	A
55	ATOM	891	CB	SER	A	792	12.011	24.823	19.595	1.00	31.21	A
	ATOM	892	OG	SER	A	792	11.197	23.862	18.942	1.00	25.26	A
	ATOM	893	C	SER	A	792	13.514	24.827	17.624	1.00	33.43	A

Table 2. (cont'd)

		#	Name	Res.	Chain	Res #	X	Y	Z	occ	B	SegID
5	ATOM	894	O	SER	A	792	14.676	24.512	17.902	1.00	34.87	A
	ATOM	895	N	SER	A	793	12.871	24.417	16.531	1.00	32.81	A
	ATOM	896	CA	SER	A	793	13.421	23.528	15.495	1.00	31.80	A
	ATOM	897	CB	SER	A	793	14.955	23.396	15.571	1.00	34.40	A
	ATOM	898	OG	SER	A	793	15.367	22.397	16.494	1.00	32.53	A
10	ATOM	899	C	SER	A	793	12.774	22.151	15.648	1.00	30.98	A
	ATOM	900	O	SER	A	793	12.882	21.299	14.764	1.00	32.51	A
	ATOM	901	N	PHE	A	794	12.101	21.933	16.775	1.00	27.80	A
	ATOM	902	CA	PHE	A	794	11.408	20.669	17.012	1.00	26.68	A
	ATOM	903	CB	PHE	A	794	12.221	19.764	17.954	1.00	24.25	A
15	ATOM	904	CG	PHE	A	794	12.685	20.437	19.221	1.00	21.22	A
	ATOM	905	CD1	PHE	A	794	11.961	20.308	20.400	1.00	23.19	A
	ATOM	906	CD2	PHE	A	794	13.870	21.166	19.241	1.00	21.45	A
	ATOM	907	CE1	PHE	A	794	12.412	20.893	21.586	1.00	24.05	A
	ATOM	908	CE2	PHE	A	794	14.333	21.756	20.420	1.00	20.76	A
20	ATOM	909	CZ	PHE	A	794	13.606	21.619	21.593	1.00	23.61	A
	ATOM	910	C	PHE	A	794	9.996	20.928	17.552	1.00	26.57	A
	ATOM	911	O	PHE	A	794	9.566	20.356	18.555	1.00	26.01	A
	ATOM	912	N	TYR	A	795	9.285	21.803	16.847	1.00	25.69	A
	ATOM	913	CA	TYR	A	795	7.920	22.192	17.191	1.00	24.51	A
25	ATOM	914	CB	TYR	A	795	7.382	23.150	16.120	1.00	24.31	A
	ATOM	915	CG	TYR	A	795	5.983	23.675	16.365	1.00	27.22	A
	ATOM	916	CD1	TYR	A	795	5.605	24.166	17.619	1.00	27.70	A
	ATOM	917	CE1	TYR	A	795	4.331	24.688	17.834	1.00	27.85	A
	ATOM	918	CD2	TYR	A	795	5.048	23.718	15.330	1.00	27.80	A
30	ATOM	919	CE2	TYR	A	795	3.771	24.239	15.534	1.00	29.91	A
	ATOM	920	CZ	TYR	A	795	3.419	24.723	16.788	1.00	30.25	A
	ATOM	921	OH	TYR	A	795	2.159	25.242	16.988	1.00	30.87	A
	ATOM	922	C	TYR	A	795	6.991	20.993	17.336	1.00	23.82	A
	ATOM	923	O	TYR	A	795	6.283	20.872	18.335	1.00	21.37	A
35	ATOM	924	N	SER	A	796	7.001	20.100	16.349	1.00	23.12	A
	ATOM	925	CA	SER	A	796	6.132	18.928	16.385	1.00	23.80	A
	ATOM	926	CB	SER	A	796	6.296	18.106	15.104	1.00	27.03	A
	ATOM	927	OG	SER	A	796	7.659	17.796	14.869	1.00	30.34	A
	ATOM	928	C	SER	A	796	6.372	18.043	17.605	1.00	24.28	A
40	ATOM	929	O	SER	A	796	5.430	17.470	18.163	1.00	23.18	A
	ATOM	930	N	LEU	A	797	7.631	17.927	18.014	1.00	22.88	A
	ATOM	931	CA	LEU	A	797	7.973	17.124	19.176	1.00	22.93	A
	ATOM	932	CB	LEU	A	797	9.492	17.019	19.327	1.00	26.10	A
	ATOM	933	CG	LEU	A	797	9.992	15.840	20.163	1.00	27.87	A
45	ATOM	934	CD1	LEU	A	797	9.676	14.545	19.430	1.00	28.16	A
	ATOM	935	CD2	LEU	A	797	11.491	15.966	20.392	1.00	27.90	A
	ATOM	936	C	LEU	A	797	7.386	17.809	20.407	1.00	20.98	A
	ATOM	937	O	LEU	A	797	6.837	17.151	21.287	1.00	20.95	A
	ATOM	938	N	CYS	A	798	7.513	19.133	20.461	1.00	20.57	A
50	ATOM	939	CA	CYS	A	798	6.973	19.903	21.579	1.00	20.61	A
	ATOM	940	CB	CYS	A	798	7.265	21.399	21.404	1.00	20.74	A
	ATOM	941	SG	CYS	A	798	8.989	21.866	21.726	1.00	21.60	A
	ATOM	942	C	CYS	A	798	5.469	19.690	21.678	1.00	20.72	A
	ATOM	943	O	CYS	A	798	4.926	19.504	22.773	1.00	19.17	A
55	ATOM	944	N	LEU	A	799	4.793	19.722	20.533	1.00	19.90	A
	ATOM	945	CA	LEU	A	799	3.349	19.526	20.518	1.00	21.06	A
	ATOM	946	CB	LEU	A	799	2.798	19.688	19.099	1.00	21.78	A

Table 2. (cont'd)

		#	Name	Res.	Chain	Res #	X	Y	Z	occ	B	SegID
	ATOM	947	CG	LEU	A	799	2.933	21.096	18.505	1.00	21.95	A
5	ATOM	948	CD1	LEU	A	799	2.376	21.100	17.093	1.00	24.69	A
	ATOM	949	CD2	LEU	A	799	2.194	22.114	19.377	1.00	21.59	A
	ATOM	950	C	LEU	A	799	3.007	18.146	21.060	1.00	22.12	A
	ATOM	951	O	LEU	A	799	2.035	17.984	21.797	1.00	23.00	A
	ATOM	952	N	THR	A	800	3.813	17.153	20.698	1.00	21.35	A
10	ATOM	953	CA	THR	A	800	3.593	15.789	21.170	1.00	22.13	A
	ATOM	954	CB	THR	A	800	4.621	14.818	20.539	1.00	22.94	A
	ATOM	955	OG1	THR	A	800	4.413	14.770	19.124	1.00	22.16	A
	ATOM	956	CG2	THR	A	800	4.469	13.414	21.116	1.00	24.15	A
	ATOM	957	C	THR	A	800	3.696	15.727	22.693	1.00	20.94	A
15	ATOM	958	O	THR	A	800	2.861	15.125	23.361	1.00	21.14	A
	ATOM	959	N	MET	A	801	4.723	16.356	23.247	1.00	21.63	A
	ATOM	960	CA	MET	A	801	4.890	16.363	24.691	1.00	20.90	A
	ATOM	961	CB	MET	A	801	6.251	16.960	25.059	1.00	21.60	A
	ATOM	962	CG	MET	A	801	7.439	16.115	24.604	1.00	22.22	A
20	ATOM	963	SD	MET	A	801	9.029	16.740	25.194	1.00	24.57	A
	ATOM	964	CE	MET	A	801	9.415	17.955	23.949	1.00	24.02	A
	ATOM	965	C	MET	A	801	3.770	17.165	25.363	1.00	22.02	A
	ATOM	966	O	MET	A	801	3.265	16.786	26.421	1.00	21.68	A
	ATOM	967	N	TRP	A	802	3.373	18.259	24.720	1.00	21.19	A
25	ATOM	968	CA	TRP	A	802	2.337	19.155	25.232	1.00	21.40	A
	ATOM	969	CB	TRP	A	802	2.214	20.360	24.290	1.00	20.55	A
	ATOM	970	CG	TRP	A	802	1.627	21.606	24.910	1.00	21.30	A
	ATOM	971	CD2	TRP	A	802	1.238	22.802	24.219	1.00	21.96	A
	ATOM	972	CE2	TRP	A	802	0.797	23.727	25.193	1.00	20.55	A
30	ATOM	973	CE3	TRP	A	802	1.225	23.182	22.869	1.00	22.42	A
	ATOM	974	CD1	TRP	A	802	1.409	21.847	26.239	1.00	21.16	A
	ATOM	975	NE1	TRP	A	802	0.910	23.121	26.416	1.00	20.99	A
	ATOM	976	CZ2	TRP	A	802	0.343	25.011	24.860	1.00	21.73	A
	ATOM	977	CZ3	TRP	A	802	0.775	24.461	22.536	1.00	23.05	A
35	ATOM	978	CH2	TRP	A	802	0.342	25.359	23.531	1.00	23.08	A
	ATOM	979	C	TRP	A	802	0.974	18.479	25.419	1.00	21.76	A
	ATOM	980	O	TRP	A	802	0.126	18.973	26.168	1.00	21.60	A
	ATOM	981	N	GLN	A	803	0.766	17.350	24.747	1.00	21.02	A
	ATOM	982	CA	GLN	A	803	-0.496	16.619	24.856	1.00	21.96	A
40	ATOM	983	CB	GLN	A	803	-0.488	15.404	23.921	1.00	23.91	A
	ATOM	984	CG	GLN	A	803	-0.267	15.756	22.447	1.00	27.15	A
	ATOM	985	CD	GLN	A	803	-0.209	14.537	21.537	1.00	31.34	A
	ATOM	986	OE1	GLN	A	803	0.116	14.648	20.352	1.00	35.35	A
	ATOM	987	NE2	GLN	A	803	-0.526	13.372	22.084	1.00	32.57	A
45	ATOM	988	C	GLN	A	803	-0.759	16.152	26.289	1.00	23.03	A
	ATOM	989	O	GLN	A	803	-1.898	16.173	26.759	1.00	21.44	A
	ATOM	990	N	ILE	A	804	0.299	15.736	26.980	1.00	21.25	A
	ATOM	991	CA	ILE	A	804	0.170	15.242	28.344	1.00	22.31	A
	ATOM	992	CB	ILE	A	804	1.532	14.758	28.891	1.00	21.58	A
50	ATOM	993	CG2	ILE	A	804	1.381	14.289	30.331	1.00	22.10	A
	ATOM	994	CG1	ILE	A	804	2.051	13.609	28.020	1.00	25.42	A
	ATOM	995	CD1	ILE	A	804	3.379	13.044	28.464	1.00	28.79	A
	ATOM	996	C	ILE	A	804	-0.432	16.270	29.297	1.00	21.32	A
	ATOM	997	O	ILE	A	804	-1.415	15.984	29.981	1.00	21.18	A
55	ATOM	998	N	PRO	A	805	0.153	17.476	29.366	1.00	21.85	A
	ATOM	999	CD	PRO	A	805	1.379	17.971	28.716	1.00	19.76	A

Table 2. (cont'd)

		#	Name	Res.	Chain	Res #	X	Y	Z	occ	B	SegID
	ATOM	1000	CA	PRO	A	805	-0.409	18.484	30.270	1.00	22.32	A
5	ATOM	1001	CB	PRO	A	805	0.439	19.718	29.981	1.00	23.10	A
	ATOM	1002	CG	PRO	A	805	1.758	19.134	29.593	1.00	24.27	A
	ATOM	1003	C	PRO	A	805	-1.880	18.716	29.932	1.00	22.86	A
	ATOM	1004	O	PRO	A	805	-2.726	18.842	30.820	1.00	21.86	A
	ATOM	1005	N	GLN	A	806	-2.178	18.767	28.637	1.00	21.67	A
10	ATOM	1006	CA	GLN	A	806	-3.549	18.991	28.199	1.00	24.13	A
	ATOM	1007	CB	GLN	A	806	-3.601	19.119	26.669	1.00	25.09	A
	ATOM	1008	CG	GLN	A	806	-2.740	20.270	26.116	1.00	25.65	A
	ATOM	1009	CD	GLN	A	806	-3.241	21.661	26.516	1.00	29.07	A
	ATOM	1010	OE1	GLN	A	806	-3.896	21.832	27.546	1.00	26.16	A
15	ATOM	1011	NE2	GLN	A	806	-2.914	22.666	25.701	1.00	30.40	A
	ATOM	1012	C	GLN	A	806	-4.481	17.882	28.696	1.00	23.92	A
	ATOM	1013	O	GLN	A	806	-5.624	18.152	29.062	1.00	23.37	A
	ATOM	1014	N	GLU	A	807	-3.998	16.640	28.726	1.00	24.30	A
	ATOM	1015	CA	GLU	A	807	-4.818	15.532	29.215	1.00	25.08	A
20	ATOM	1016	CB	GLU	A	807	-4.175	14.180	28.893	1.00	27.80	A
	ATOM	1017	CG	GLU	A	807	-4.461	13.676	27.495	1.00	32.53	A
	ATOM	1018	CD	GLU	A	807	-5.951	13.489	27.238	1.00	34.70	A
	ATOM	1019	OE1	GLU	A	807	-6.570	12.623	27.893	1.00	35.52	A
	ATOM	1020	OE2	GLU	A	807	-6.501	14.211	26.381	1.00	36.62	A
25	ATOM	1021	C	GLU	A	807	-5.025	15.641	30.723	1.00	24.42	A
	ATOM	1022	O	GLU	A	807	-6.056	15.222	31.251	1.00	22.60	A
	ATOM	1023	N	PHE	A	808	-4.034	16.189	31.418	1.00	23.73	A
	ATOM	1024	CA	PHE	A	808	-4.143	16.357	32.860	1.00	23.36	A
	ATOM	1025	CB	PHE	A	808	-2.818	16.857	33.443	1.00	24.21	A
30	ATOM	1026	CG	PHE	A	808	-1.785	15.774	33.622	1.00	25.04	A
	ATOM	1027	CD1	PHE	A	808	-2.118	14.433	33.439	1.00	26.18	A
	ATOM	1028	CD2	PHE	A	808	-0.490	16.091	34.010	1.00	26.53	A
	ATOM	1029	CE1	PHE	A	808	-1.173	13.422	33.648	1.00	27.84	A
	ATOM	1030	CE2	PHE	A	808	0.462	15.088	34.222	1.00	27.25	A
35	ATOM	1031	CZ	PHE	A	808	0.119	13.754	34.040	1.00	25.53	A
	ATOM	1032	C	PHE	A	808	-5.264	17.349	33.150	1.00	22.79	A
	ATOM	1033	O	PHE	A	808	-6.074	17.142	34.057	1.00	22.62	A
	ATOM	1034	N	VAL	A	809	-5.312	18.418	32.359	1.00	22.34	A
	ATOM	1035	CA	VAL	A	809	-6.345	19.440	32.512	1.00	22.35	A
40	ATOM	1036	CB	VAL	A	809	-6.140	20.590	31.500	1.00	21.96	A
	ATOM	1037	CG1	VAL	A	809	-7.325	21.541	31.545	1.00	22.83	A
	ATOM	1038	CG2	VAL	A	809	-4.863	21.346	31.818	1.00	20.25	A
	ATOM	1039	C	VAL	A	809	-7.734	18.844	32.285	1.00	23.40	A
	ATOM	1040	O	VAL	A	809	-8.658	19.059	33.073	1.00	22.44	A
45	ATOM	1041	N	LYS	A	810	-7.880	18.088	31.204	1.00	24.89	A
	ATOM	1042	CA	LYS	A	810	-9.168	17.493	30.873	1.00	26.91	A
	ATOM	1043	CB	LYS	A	810	-9.105	16.836	29.491	1.00	29.69	A
	ATOM	1044	CG	LYS	A	810	-8.893	17.826	28.355	1.00	33.08	A
	ATOM	1045	CD	LYS	A	810	-8.741	17.116	27.014	1.00	38.27	A
50	ATOM	1046	CE	LYS	A	810	-8.498	18.114	25.881	1.00	40.99	A
	ATOM	1047	NZ	LYS	A	810	-8.286	17.433	24.568	1.00	43.19	A
	ATOM	1048	C	LYS	A	810	-9.663	16.486	31.907	1.00	27.41	A
	ATOM	1049	O	LYS	A	810	-10.855	16.444	32.214	1.00	26.62	A
	ATOM	1050	N	LEU	A	811	-8.753	15.677	32.440	1.00	24.95	A
55	ATOM	1051	CA	LEU	A	811	-9.123	14.683	33.438	1.00	25.56	A
	ATOM	1052	CB	LEU	A	811	-8.217	13.458	33.318	1.00	25.67	A

Table 2. (cont'd)

		#	Name	Res.	Chain	Res #	X	Y	Z	occ	B	SegID
	ATOM	1053	CG	LEU	A	811	-8.421	12.595	32.078	1.00	26.38	A
5	ATOM	1054	CD1	LEU	A	811	-7.289	11.591	31.949	1.00	26.98	A
	ATOM	1055	CD2	LEU	A	811	-9.760	11.893	32.186	1.00	26.29	A
	ATOM	1056	C	LEU	A	811	-9.044	15.220	34.863	1.00	24.44	A
	ATOM	1057	O	LEU	A	811	-9.522	14.579	35.793	1.00	24.86	A
	ATOM	1058	N	GLN	A	812	-8.458	16.401	35.026	1.00	25.33	A
10	ATOM	1059	CA	GLN	A	812	-8.288	16.989	36.351	1.00	26.61	A
	ATOM	1060	CB	GLN	A	812	-9.635	17.477	36.905	1.00	30.42	A
	ATOM	1061	CG	GLN	A	812	-10.100	18.777	36.256	1.00	35.79	A
	ATOM	1062	CD	GLN	A	812	-11.386	19.328	36.849	1.00	40.76	A
	ATOM	1063	OE1	GLN	A	812	-11.736	20.489	36.621	1.00	45.20	A
15	ATOM	1064	NE2	GLN	A	812	-12.099	18.499	37.608	1.00	42.16	A
	ATOM	1065	C	GLN	A	812	-7.655	15.950	37.281	1.00	24.37	A
	ATOM	1066	O	GLN	A	812	-8.185	15.625	38.348	1.00	22.99	A
	ATOM	1067	N	VAL	A	813	-6.513	15.423	36.846	1.00	22.72	A
	ATOM	1068	CA	VAL	A	813	-5.776	14.422	37.607	1.00	20.15	A
20	ATOM	1069	CB	VAL	A	813	-4.501	13.989	36.853	1.00	21.18	A
	ATOM	1070	CG1	VAL	A	813	-3.707	12.977	37.694	1.00	19.93	A
	ATOM	1071	CG2	VAL	A	813	-4.882	13.388	35.506	1.00	19.31	A
	ATOM	1072	C	VAL	A	813	-5.380	14.998	38.958	1.00	20.32	A
	ATOM	1073	O	VAL	A	813	-4.906	16.134	39.042	1.00	18.09	A
25	ATOM	1074	N	SER	A	814	-5.579	14.220	40.016	1.00	18.44	A
	ATOM	1075	CA	SER	A	814	-5.235	14.690	41.353	1.00	20.30	A
	ATOM	1076	CB	SER	A	814	-6.143	14.057	42.408	1.00	18.76	A
	ATOM	1077	OG	SER	A	814	-5.858	12.674	42.549	1.00	17.92	A
	ATOM	1078	C	SER	A	814	-3.794	14.348	41.687	1.00	21.13	A
30	ATOM	1079	O	SER	A	814	-3.173	13.496	41.050	1.00	21.63	A
	ATOM	1080	N	GLN	A	815	-3.276	15.024	42.700	1.00	21.79	A
	ATOM	1081	CA	GLN	A	815	-1.916	14.807	43.164	1.00	23.69	A
	ATOM	1082	CB	GLN	A	815	-1.648	15.736	44.349	1.00	27.86	A
	ATOM	1083	CG	GLN	A	815	-0.226	15.755	44.851	1.00	34.98	A
35	ATOM	1084	CD	GLN	A	815	-0.029	16.804	45.927	1.00	38.93	A
	ATOM	1085	OE1	GLN	A	815	1.084	17.036	46.386	1.00	42.97	A
	ATOM	1086	NE2	GLN	A	815	-1.120	17.448	46.333	1.00	42.31	A
	ATOM	1087	C	GLN	A	815	-1.748	13.348	43.585	1.00	21.52	A
	ATOM	1088	O	GLN	A	815	-0.710	12.729	43.325	1.00	21.53	A
40	ATOM	1089	N	GLU	A	816	-2.782	12.794	44.215	1.00	19.19	A
	ATOM	1090	CA	GLU	A	816	-2.744	11.410	44.682	1.00	19.04	A
	ATOM	1091	CB	GLU	A	816	-3.946	11.116	45.582	1.00	20.60	A
	ATOM	1092	CG	GLU	A	816	-3.983	11.908	46.885	1.00	22.06	A
	ATOM	1093	CD	GLU	A	816	-4.344	13.374	46.692	1.00	24.05	A
45	ATOM	1094	OE1	GLU	A	816	-4.903	13.729	45.632	1.00	21.48	A
	ATOM	1095	OE2	GLU	A	816	-4.078	14.171	47.615	1.00	26.29	A
	ATOM	1096	C	GLU	A	816	-2.720	10.408	43.534	1.00	18.03	A
	ATOM	1097	O	GLU	A	816	-2.003	9.409	43.586	1.00	16.07	A
	ATOM	1098	N	GLU	A	817	-3.516	10.664	42.503	1.00	17.72	A
50	ATOM	1099	CA	GLU	A	817	-3.553	9.772	41.352	1.00	18.37	A
	ATOM	1100	CB	GLU	A	817	-4.700	10.163	40.413	1.00	19.36	A
	ATOM	1101	CG	GLU	A	817	-6.089	10.025	41.036	1.00	18.88	A
	ATOM	1102	CD	GLU	A	817	-7.186	10.619	40.164	1.00	20.98	A
	ATOM	1103	OE1	GLU	A	817	-6.934	11.652	39.510	1.00	19.85	A
55	ATOM	1104	OE2	GLU	A	817	-8.305	10.067	40.143	1.00	20.28	A
	ATOM	1105	C	GLU	A	817	-2.214	9.869	40.615	1.00	17.45	A

Table 2. (cont'd)

		#	Name	Res.	Chain	Res #	X	Y	Z	occ	B	SegID
	ATOM	1106	O	GLU	A	817	-1.654	8.859	40.203	1.00	18.12	A
5	ATOM	1107	N	PHE	A	818	-1.710	11.092	40.464	1.00	17.39	A
	ATOM	1108	CA	PHE	A	818	-0.443	11.339	39.778	1.00	17.67	A
	ATOM	1109	CB	PHE	A	818	-0.108	12.836	39.820	1.00	18.87	A
	ATOM	1110	CG	PHE	A	818	1.307	13.158	39.396	1.00	20.11	A
	ATOM	1111	CD1	PHE	A	818	1.697	13.039	38.065	1.00	21.04	A
10	ATOM	1112	CD2	PHE	A	818	2.255	13.551	40.337	1.00	22.59	A
	ATOM	1113	CE1	PHE	A	818	3.018	13.306	37.673	1.00	21.13	A
	ATOM	1114	CE2	PHE	A	818	3.577	13.821	39.961	1.00	22.38	A
	ATOM	1115	CZ	PHE	A	818	3.959	13.696	38.624	1.00	21.87	A
	ATOM	1116	C	PHE	A	818	0.690	10.543	40.423	1.00	17.61	A
15	ATOM	1117	O	PHE	A	818	1.426	9.828	39.745	1.00	17.85	A
	ATOM	1118	N	LEU	A	819	0.820	10.668	41.739	1.00	17.17	A
	ATOM	1119	CA	LEU	A	819	1.857	9.966	42.476	1.00	16.75	A
	ATOM	1120	CB	LEU	A	819	1.712	10.259	43.972	1.00	17.20	A
	ATOM	1121	CG	LEU	A	819	2.030	11.713	44.349	1.00	17.53	A
20	ATOM	1122	CD1	LEU	A	819	1.682	11.970	45.816	1.00	18.42	A
	ATOM	1123	CD2	LEU	A	819	3.509	11.989	44.089	1.00	18.88	A
	ATOM	1124	C	LEU	A	819	1.844	8.456	42.217	1.00	18.00	A
	ATOM	1125	O	LEU	A	819	2.890	7.864	41.954	1.00	17.24	A
	ATOM	1126	N	CYS	A	820	0.665	7.840	42.273	1.00	16.25	A
25	ATOM	1127	CA	CYS	A	820	0.549	6.400	42.034	1.00	16.35	A
	ATOM	1128	CB	CYS	A	820	-0.851	5.911	42.419	1.00	13.68	A
	ATOM	1129	SG	CYS	A	820	-1.192	5.999	44.186	1.00	18.53	A
	ATOM	1130	C	CYS	A	820	0.837	6.027	40.580	1.00	17.21	A
	ATOM	1131	O	CYS	A	820	1.516	5.027	40.305	1.00	16.67	A
30	ATOM	1132	N	MET	A	821	0.318	6.826	39.652	1.00	15.37	A
	ATOM	1133	CA	MET	A	821	0.530	6.573	38.234	1.00	16.27	A
	ATOM	1134	CB	MET	A	821	-0.265	7.573	37.392	1.00	17.92	A
	ATOM	1135	CG	MET	A	821	-1.771	7.383	37.460	1.00	17.69	A
	ATOM	1136	SD	MET	A	821	-2.643	8.818	36.774	1.00	19.79	A
35	ATOM	1137	CE	MET	A	821	-2.555	8.439	35.021	1.00	15.33	A
	ATOM	1138	C	MET	A	821	2.015	6.677	37.897	1.00	15.93	A
	ATOM	1139	O	MET	A	821	2.531	5.902	37.097	1.00	14.16	A
	ATOM	1140	N	LYS	A	822	2.707	7.628	38.515	1.00	14.88	A
	ATOM	1141	CA	LYS	A	822	4.130	7.774	38.239	1.00	16.59	A
40	ATOM	1142	CB	LYS	A	822	4.698	9.016	38.936	1.00	16.10	A
	ATOM	1143	CG	LYS	A	822	6.140	9.301	38.551	1.00	16.38	A
	ATOM	1144	CD	LYS	A	822	6.486	10.792	38.596	1.00	17.94	A
	ATOM	1145	CE	LYS	A	822	6.423	11.366	40.004	1.00	16.34	A
	ATOM	1146	NZ	LYS	A	822	7.308	10.632	40.944	1.00	18.00	A
45	ATOM	1147	C	LYS	A	822	4.892	6.516	38.664	1.00	15.81	A
	ATOM	1148	O	LYS	A	822	5.834	6.104	37.992	1.00	14.75	A
	ATOM	1149	N	VAL	A	823	4.487	5.894	39.772	1.00	16.36	A
	ATOM	1150	CA	VAL	A	823	5.160	4.672	40.203	1.00	14.72	A
	ATOM	1151	CB	VAL	A	823	4.703	4.200	41.613	1.00	15.84	A
50	ATOM	1152	CG1	VAL	A	823	5.305	2.824	41.917	1.00	15.64	A
	ATOM	1153	CG2	VAL	A	823	5.167	5.197	42.684	1.00	14.56	A
	ATOM	1154	C	VAL	A	823	4.889	3.550	39.204	1.00	14.32	A
	ATOM	1155	O	VAL	A	823	5.776	2.753	38.899	1.00	13.04	A
	ATOM	1156	N	LEU	A	824	3.668	3.484	38.684	1.00	13.35	A
55	ATOM	1157	CA	LEU	A	824	3.340	2.437	37.725	1.00	14.01	A
	ATOM	1158	CB	LEU	A	824	1.834	2.433	37.434	1.00	13.91	A

Table 2. (cont'd)

		#	Name	Res.	Chain	Res #	X	Y	Z	occ	B	SegID
	ATOM	1159	CG	LEU	A	824	0.993	2.089	38.671	1.00	16.39	A
5	ATOM	1160	CD1	LEU	A	824	-0.493	2.176	38.350	1.00	15.94	A
	ATOM	1161	CD2	LEU	A	824	1.360	0.683	39.158	1.00	15.40	A
	ATOM	1162	C	LEU	A	824	4.152	2.572	36.437	1.00	11.71	A
	ATOM	1163	O	LEU	A	824	4.466	1.573	35.792	1.00	13.59	A
	ATOM	1164	N	LEU	A	825	4.497	3.800	36.062	1.00	12.33	A
10	ATOM	1165	CA	LEU	A	825	5.301	4.012	34.862	1.00	12.91	A
	ATOM	1166	CB	LEU	A	825	5.418	5.507	34.542	1.00	12.32	A
	ATOM	1167	CG	LEU	A	825	4.228	6.126	33.799	1.00	14.73	A
	ATOM	1168	CD1	LEU	A	825	4.491	7.612	33.545	1.00	16.34	A
	ATOM	1169	CD2	LEU	A	825	4.023	5.389	32.478	1.00	12.28	A
15	ATOM	1170	C	LEU	A	825	6.698	3.407	35.058	1.00	13.79	A
	ATOM	1171	O	LEU	A	825	7.252	2.791	34.147	1.00	13.59	A
	ATOM	1172	N	LEU	A	826	7.262	3.583	36.251	1.00	12.61	A
	ATOM	1173	CA	LEU	A	826	8.576	3.027	36.554	1.00	14.11	A
	ATOM	1174	CB	LEU	A	826	8.977	3.375	37.994	1.00	14.02	A
20	ATOM	1175	CG	LEU	A	826	10.211	2.635	38.531	1.00	17.91	A
	ATOM	1176	CD1	LEU	A	826	11.464	3.153	37.824	1.00	16.45	A
	ATOM	1177	CD2	LEU	A	826	10.333	2.838	40.038	1.00	17.97	A
	ATOM	1178	C	LEU	A	826	8.526	1.501	36.391	1.00	14.93	A
	ATOM	1179	O	LEU	A	826	9.505	0.875	35.995	1.00	15.99	A
25	ATOM	1180	N	LEU	A	827	7.364	0.918	36.676	1.00	15.65	A
	ATOM	1181	CA	LEU	A	827	7.168	-0.528	36.590	1.00	15.35	A
	ATOM	1182	CB	LEU	A	827	6.430	-1.000	37.848	1.00	15.51	A
	ATOM	1183	CG	LEU	A	827	6.949	-0.493	39.202	1.00	16.57	A
	ATOM	1184	CD1	LEU	A	827	5.966	-0.846	40.304	1.00	15.59	A
30	ATOM	1185	CD2	LEU	A	827	8.320	-1.110	39.486	1.00	18.43	A
	ATOM	1186	C	LEU	A	827	6.350	-0.952	35.362	1.00	17.65	A
	ATOM	1187	O	LEU	A	827	5.749	-2.031	35.361	1.00	16.15	A
	ATOM	1188	N	ASN	A	828	6.346	-0.131	34.314	1.00	18.51	A
	ATOM	1189	CA	ASN	A	828	5.520	-0.424	33.141	1.00	16.99	A
35	ATOM	1190	CB	ASN	A	828	4.881	0.877	32.649	1.00	17.83	A
	ATOM	1191	CG	ASN	A	828	3.418	0.703	32.307	1.00	20.51	A
	ATOM	1192	OD1	ASN	A	828	2.743	-0.175	32.858	1.00	17.90	A
	ATOM	1193	ND2	ASN	A	828	2.912	1.541	31.411	1.00	17.96	A
	ATOM	1194	C	ASN	A	828	6.126	-1.180	31.958	1.00	17.76	A
40	ATOM	1195	O	ASN	A	828	5.448	-1.412	30.960	1.00	17.82	A
	ATOM	1196	N	THR	A	829	7.391	-1.566	32.066	1.00	16.44	A
	ATOM	1197	CA	THR	A	829	8.056	-2.318	31.013	1.00	16.99	A
	ATOM	1198	CB	THR	A	829	8.866	-1.396	30.056	1.00	18.11	A
	ATOM	1199	OG1	THR	A	829	8.008	-0.394	29.494	1.00	17.42	A
45	ATOM	1200	CG2	THR	A	829	9.474	-2.219	28.920	1.00	20.30	A
	ATOM	1201	C	THR	A	829	9.031	-3.292	31.673	1.00	17.73	A
	ATOM	1202	O	THR	A	829	9.717	-2.930	32.629	1.00	17.99	A
	ATOM	1203	N	ILE	A	830	9.071	-4.531	31.189	1.00	17.90	A
	ATOM	1204	CA	ILE	A	830	10.002	-5.519	31.724	1.00	18.71	A
50	ATOM	1205	CB	ILE	A	830	9.311	-6.520	32.685	1.00	19.83	A
	ATOM	1206	CG2	ILE	A	830	8.568	-5.753	33.781	1.00	20.83	A
	ATOM	1207	CG1	ILE	A	830	8.338	-7.423	31.922	1.00	18.24	A
	ATOM	1208	CD1	ILE	A	830	7.762	-8.554	32.782	1.00	19.69	A
	ATOM	1209	C	ILE	A	830	10.661	-6.278	30.572	1.00	19.02	A
55	ATOM	1210	O	ILE	A	830	10.193	-6.224	29.434	1.00	18.72	A
	ATOM	1211	N	PRO	A	831	11.771	-6.981	30.849	1.00	19.69	A

Table 2. (cont'd)

		#	Name	Res.	Chain	Res #	X	Y	Z	occ	B	SegID
5	ATOM	1212	CD	PRO	A	831	12.515	-7.077	32.118	1.00	17.13	A
	ATOM	1213	CA	PRO	A	831	12.451	-7.725	29.789	1.00	20.61	A
	ATOM	1214	CB	PRO	A	831	13.691	-8.289	30.491	1.00	20.77	A
	ATOM	1215	CG	PRO	A	831	13.920	-7.336	31.637	1.00	19.58	A
	ATOM	1216	C	PRO	A	831	11.555	-8.830	29.256	1.00	21.97	A
10	ATOM	1217	O	PRO	A	831	10.610	-9.247	29.922	1.00	21.43	A
	ATOM	1218	N	LEU	A	832	11.855	-9.297	28.051	1.00	23.36	A
	ATOM	1219	CA	LEU	A	832	11.082	-10.371	27.448	1.00	25.72	A
	ATOM	1220	CB	LEU	A	832	11.617	-10.676	26.047	1.00	26.92	A
	ATOM	1221	CG	LEU	A	832	11.334	-9.596	25.003	1.00	28.15	A
15	ATOM	1222	CD1	LEU	A	832	12.033	-9.942	23.699	1.00	30.17	A
	ATOM	1223	CD2	LEU	A	832	9.827	-9.476	24.801	1.00	28.94	A
	ATOM	1224	C	LEU	A	832	11.180	-11.619	28.318	1.00	26.21	A
	ATOM	1225	O	LEU	A	832	10.217	-12.373	28.447	1.00	25.46	A
	ATOM	1226	N	GLU	A	833	12.348	-11.822	28.918	1.00	25.70	A
20	ATOM	1227	CA	GLU	A	833	12.592	-12.982	29.770	1.00	27.45	A
	ATOM	1228	CB	GLU	A	833	14.083	-13.354	29.741	1.00	29.43	A
	ATOM	1229	CG	GLU	A	833	15.009	-12.303	30.357	1.00	32.13	A
	ATOM	1230	CD	GLU	A	833	15.437	-11.215	29.378	1.00	33.98	A
	ATOM	1231	OE1	GLU	A	833	14.668	-10.884	28.454	1.00	33.06	A
25	ATOM	1232	OE2	GLU	A	833	16.550	-10.675	29.545	1.00	36.26	A
	ATOM	1233	C	GLU	A	833	12.156	-12.739	31.219	1.00	27.20	A
	ATOM	1234	O	GLU	A	833	12.334	-13.599	32.081	1.00	27.90	A
	ATOM	1235	N	GLY	A	834	11.583	-11.569	31.480	1.00	25.12	A
	ATOM	1236	CA	GLY	A	834	11.153	-11.246	32.827	1.00	24.64	A
30	ATOM	1237	C	GLY	A	834	12.292	-10.725	33.687	1.00	23.57	A
	ATOM	1238	O	GLY	A	834	13.425	-10.611	33.225	1.00	23.20	A
	ATOM	1239	N	LEU	A	835	11.992	-10.409	34.941	1.00	22.62	A
	ATOM	1240	CA	LEU	A	835	12.994	-9.896	35.868	1.00	23.78	A
	ATOM	1241	CB	LEU	A	835	12.384	-8.781	36.718	1.00	21.76	A
35	ATOM	1242	CG	LEU	A	835	11.886	-7.540	35.965	1.00	22.76	A
	ATOM	1243	CD1	LEU	A	835	11.025	-6.680	36.888	1.00	21.31	A
	ATOM	1244	CD2	LEU	A	835	13.072	-6.745	35.448	1.00	21.97	A
	ATOM	1245	C	LEU	A	835	13.517	-11.011	36.772	1.00	23.97	A
	ATOM	1246	O	LEU	A	835	12.925	-12.085	36.847	1.00	23.94	A
40	ATOM	1247	N	ARG	A	836	14.632	-10.761	37.451	1.00	25.83	A
	ATOM	1248	CA	ARG	A	836	15.198	-11.760	38.352	1.00	27.17	A
	ATOM	1249	CB	ARG	A	836	16.594	-11.346	38.828	1.00	30.08	A
	ATOM	1250	CG	ARG	A	836	17.643	-11.247	37.733	1.00	36.54	A
	ATOM	1251	CD	ARG	A	836	19.056	-11.242	38.313	1.00	41.84	A
45	ATOM	1252	NE	ARG	A	836	19.633	-12.586	38.408	1.00	48.33	A
	ATOM	1253	CZ	ARG	A	836	19.195	-13.552	39.214	1.00	50.99	A
	ATOM	1254	NH1	ARG	A	836	18.164	-13.342	40.021	1.00	53.00	A
	ATOM	1255	NH2	ARG	A	836	19.783	-14.741	39.205	1.00	52.15	A
	ATOM	1256	C	ARG	A	836	14.286	-11.915	39.565	1.00	26.30	A
50	ATOM	1257	O	ARG	A	836	14.091	-13.021	40.068	1.00	25.88	A
	ATOM	1258	N	SER	A	837	13.735	-10.797	40.029	1.00	23.15	A
	ATOM	1259	CA	SER	A	837	12.840	-10.797	41.181	1.00	23.00	A
	ATOM	1260	CB	SER	A	837	13.198	-9.644	42.128	1.00	23.75	A
	ATOM	1261	OG	SER	A	837	14.548	-9.705	42.557	1.00	23.11	A
55	ATOM	1262	C	SER	A	837	11.403	-10.628	40.693	1.00	22.34	A
	ATOM	1263	O	SER	A	837	10.647	-9.822	41.233	1.00	19.84	A
	ATOM	1264	N	GLN	A	838	11.035	-11.398	39.671	1.00	23.15	A

Table 2. (cont'd)

		#	Name	Res.	Chain	Res #	X	Y	Z	occ	B	SegID
5	ATOM	1265	CA	GLN	A	838	9.698	-11.326	39.081	1.00	24.26	A
	ATOM	1266	CB	GLN	A	838	9.527	-12.422	38.020	1.00	25.27	A
	ATOM	1267	CG	GLN	A	838	8.289	-12.273	37.134	1.00	22.45	A
	ATOM	1268	CD	GLN	A	838	8.307	-10.999	36.290	1.00	25.56	A
	ATOM	1269	OE1	GLN	A	838	9.336	-10.627	35.725	1.00	24.82	A
10	ATOM	1270	NE2	GLN	A	838	7.157	-10.338	36.187	1.00	23.08	A
	ATOM	1271	C	GLN	A	838	8.565	-11.423	40.094	1.00	24.82	A
	ATOM	1272	O	GLN	A	838	7.569	-10.706	39.983	1.00	23.75	A
	ATOM	1273	N	THR	A	839	8.702	-12.314	41.074	1.00	26.33	A
	ATOM	1274	CA	THR	A	839	7.662	-12.474	42.088	1.00	26.16	A
15	ATOM	1275	CB	THR	A	839	8.004	-13.597	43.088	1.00	28.64	A
	ATOM	1276	OG1	THR	A	839	8.256	-14.816	42.378	1.00	30.75	A
	ATOM	1277	CG2	THR	A	839	6.845	-13.817	44.050	1.00	26.66	A
	ATOM	1278	C	THR	A	839	7.475	-11.179	42.873	1.00	25.53	A
	ATOM	1279	O	THR	A	839	6.358	-10.681	43.010	1.00	25.17	A
20	ATOM	1280	N	GLN	A	840	8.576	-10.637	43.385	1.00	24.47	A
	ATOM	1281	CA	GLN	A	840	8.526	-9.404	44.157	1.00	24.83	A
	ATOM	1282	CB	GLN	A	840	9.912	-9.072	44.721	1.00	26.45	A
	ATOM	1283	CG	GLN	A	840	10.482	-10.137	45.663	1.00	30.94	A
	ATOM	1284	CD	GLN	A	840	11.324	-11.185	44.951	1.00	33.60	A
25	ATOM	1285	OE1	GLN	A	840	10.894	-11.795	43.966	1.00	32.51	A
	ATOM	1286	NE2	GLN	A	840	12.534	-11.405	45.456	1.00	35.22	A
	ATOM	1287	C	GLN	A	840	8.010	-8.242	43.307	1.00	23.05	A
	ATOM	1288	O	GLN	A	840	7.231	-7.417	43.780	1.00	23.69	A
	ATOM	1289	N	PHE	A	841	8.447	-8.180	42.052	1.00	21.65	A
30	ATOM	1290	CA	PHE	A	841	8.006	-7.123	41.145	1.00	20.44	A
	ATOM	1291	CB	PHE	A	841	8.640	-7.311	39.763	1.00	19.26	A
	ATOM	1292	CG	PHE	A	841	8.031	-6.441	38.697	1.00	18.62	A
	ATOM	1293	CD1	PHE	A	841	8.448	-5.125	38.528	1.00	18.04	A
	ATOM	1294	CD2	PHE	A	841	7.021	-6.932	37.877	1.00	19.63	A
35	ATOM	1295	CE1	PHE	A	841	7.865	-4.314	37.569	1.00	17.16	A
	ATOM	1296	CE2	PHE	A	841	6.428	-6.123	36.913	1.00	18.19	A
	ATOM	1297	CZ	PHE	A	841	6.855	-4.811	36.758	1.00	17.63	A
	ATOM	1298	C	PHE	A	841	6.489	-7.195	41.007	1.00	20.37	A
	ATOM	1299	O	PHE	A	841	5.790	-6.186	41.078	1.00	15.98	A
40	ATOM	1300	N	GLU	A	842	5.987	-8.405	40.797	1.00	20.47	A
	ATOM	1301	CA	GLU	A	842	4.557	-8.607	40.635	1.00	23.77	A
	ATOM	1302	CB	GLU	A	842	4.274	-10.091	40.400	1.00	27.79	A
	ATOM	1303	CG	GLU	A	842	3.228	-10.343	39.345	1.00	32.65	A
	ATOM	1304	CD	GLU	A	842	3.644	-9.861	37.961	1.00	32.93	A
45	ATOM	1305	OE1	GLU	A	842	4.434	-10.554	37.291	1.00	36.77	A
	ATOM	1306	OE2	GLU	A	842	3.179	-8.786	37.542	1.00	33.52	A
	ATOM	1307	C	GLU	A	842	3.800	-8.095	41.866	1.00	23.22	A
	ATOM	1308	O	GLU	A	842	2.794	-7.399	41.740	1.00	22.93	A
	ATOM	1309	N	GLU	A	843	4.293	-8.429	43.053	1.00	23.18	A
50	ATOM	1310	CA	GLU	A	843	3.658	-7.982	44.290	1.00	24.02	A
	ATOM	1311	CB	GLU	A	843	4.334	-8.640	45.499	1.00	27.96	A
	ATOM	1312	CG	GLU	A	843	3.980	-10.118	45.676	1.00	33.63	A
	ATOM	1313	CD	GLU	A	843	4.660	-10.752	46.880	1.00	37.86	A
	ATOM	1314	OE1	GLU	A	843	4.585	-10.176	47.986	1.00	41.00	A
55	ATOM	1315	OE2	GLU	A	843	5.265	-11.833	46.725	1.00	41.92	A
	ATOM	1316	C	GLU	A	843	3.713	-6.457	44.426	1.00	21.45	A
	ATOM	1317	O	GLU	A	843	2.748	-5.825	44.848	1.00	20.19	A

Table 2. (cont'd)

		#	Name	Res.	Chain	Res #	X	Y	Z	occ	B	SegID
	ATOM	1318	N	MET	A	844	4.842	-5.869	44.055	1.00	19.19	A
5	ATOM	1319	CA	MET	A	844	5.005	-4.418	44.143	1.00	19.24	A
	ATOM	1320	CB	MET	A	844	6.454	-4.032	43.832	1.00	19.91	A
	ATOM	1321	CG	MET	A	844	6.747	-2.542	43.974	1.00	19.06	A
	ATOM	1322	SD	MET	A	844	8.449	-2.108	43.505	1.00	21.31	A
	ATOM	1323	CE	MET	A	844	8.364	-0.338	43.669	1.00	16.72	A
10	ATOM	1324	C	MET	A	844	4.064	-3.703	43.172	1.00	18.33	A
	ATOM	1325	O	MET	A	844	3.332	-2.793	43.558	1.00	17.42	A
	ATOM	1326	N	ARG	A	845	4.087	-4.121	41.910	1.00	18.70	A
	ATOM	1327	CA	ARG	A	845	3.230	-3.511	40.894	1.00	19.90	A
	ATOM	1328	CB	ARG	A	845	3.474	-4.180	39.539	1.00	20.02	A
15	ATOM	1329	CG	ARG	A	845	2.649	-3.614	38.385	1.00	21.73	A
	ATOM	1330	CD	ARG	A	845	3.201	-4.107	37.053	1.00	24.38	A
	ATOM	1331	NE	ARG	A	845	2.496	-3.542	35.903	1.00	28.68	A
	ATOM	1332	CZ	ARG	A	845	1.308	-3.950	35.474	1.00	29.80	A
	ATOM	1333	NH1	ARG	A	845	0.677	-4.939	36.096	1.00	31.71	A
20	ATOM	1334	NH2	ARG	A	845	0.750	-3.369	34.419	1.00	32.30	A
	ATOM	1335	C	ARG	A	845	1.754	-3.631	41.284	1.00	19.74	A
	ATOM	1336	O	ARG	A	845	1.004	-2.657	41.227	1.00	18.83	A
	ATOM	1337	N	SER	A	846	1.341	-4.824	41.692	1.00	18.87	A
	ATOM	1338	CA	SER	A	846	-0.044	-5.025	42.083	1.00	19.72	A
25	ATOM	1339	CB	SER	A	846	-0.275	-6.491	42.452	1.00	21.67	A
	ATOM	1340	OG	SER	A	846	-0.127	-7.322	41.306	1.00	21.71	A
	ATOM	1341	C	SER	A	846	-0.420	-4.107	43.247	1.00	20.41	A
	ATOM	1342	O	SER	A	846	-1.524	-3.563	43.291	1.00	19.34	A
	ATOM	1343	N	SER	A	847	0.506	-3.923	44.184	1.00	19.04	A
30	ATOM	1344	CA	SER	A	847	0.247	-3.063	45.329	1.00	18.35	A
	ATOM	1345	CB	SER	A	847	1.408	-3.137	46.323	1.00	20.48	A
	ATOM	1346	OG	SER	A	847	1.220	-2.210	47.372	1.00	24.25	A
	ATOM	1347	C	SER	A	847	0.016	-1.612	44.918	1.00	17.69	A
	ATOM	1348	O	SER	A	847	-0.853	-0.938	45.465	1.00	16.70	A
35	ATOM	1349	N	TYR	A	848	0.794	-1.120	43.960	1.00	16.16	A
	ATOM	1350	CA	TYR	A	848	0.615	0.258	43.525	1.00	16.48	A
	ATOM	1351	CB	TYR	A	848	1.873	0.740	42.804	1.00	16.12	A
	ATOM	1352	CG	TYR	A	848	2.954	1.112	43.796	1.00	15.32	A
	ATOM	1353	CD1	TYR	A	848	2.862	2.292	44.541	1.00	15.55	A
40	ATOM	1354	CE1	TYR	A	848	3.817	2.616	45.507	1.00	15.99	A
	ATOM	1355	CD2	TYR	A	848	4.031	0.264	44.040	1.00	16.08	A
	ATOM	1356	CE2	TYR	A	848	4.993	0.579	45.005	1.00	15.10	A
	ATOM	1357	CZ	TYR	A	848	4.878	1.756	45.733	1.00	17.33	A
	ATOM	1358	OH	TYR	A	848	5.825	2.076	46.682	1.00	16.56	A
45	ATOM	1359	C	TYR	A	848	-0.643	0.428	42.674	1.00	16.19	A
	ATOM	1360	O	TYR	A	848	-1.233	1.509	42.636	1.00	16.16	A
	ATOM	1361	N	ILE	A	849	-1.060	-0.640	42.003	1.00	16.12	A
	ATOM	1362	CA	ILE	A	849	-2.286	-0.588	41.209	1.00	17.53	A
	ATOM	1363	CB	ILE	A	849	-2.487	-1.883	40.375	1.00	16.60	A
50	ATOM	1364	CG2	ILE	A	849	-3.915	-1.928	39.806	1.00	11.46	A
	ATOM	1365	CG1	ILE	A	849	-1.443	-1.943	39.255	1.00	16.24	A
	ATOM	1366	CD1	ILE	A	849	-1.505	-3.204	38.413	1.00	17.37	A
	ATOM	1367	C	ILE	A	849	-3.419	-0.459	42.232	1.00	17.52	A
	ATOM	1368	O	ILE	A	849	-4.350	0.331	42.062	1.00	19.29	A
55	ATOM	1369	N	ARG	A	850	-3.327	-1.237	43.306	1.00	18.62	A
	ATOM	1370	CA	ARG	A	850	-4.337	-1.179	44.356	1.00	19.04	A

Table 2. (cont'd)

		#	Name	Res.	Chain	Res #	X	Y	Z	occ	B	SegID
	ATOM	1371	CB	ARG	A	850	-4.081	-2.252	45.425	1.00	17.63	A
5	ATOM	1372	CG	ARG	A	850	-4.325	-3.677	44.942	1.00	20.04	A
	ATOM	1373	CD	ARG	A	850	-4.508	-4.651	46.104	1.00	19.34	A
	ATOM	1374	NE	ARG	A	850	-3.302	-4.816	46.905	1.00	21.22	A
	ATOM	1375	CZ	ARG	A	850	-2.261	-5.569	46.558	1.00	23.77	A
	ATOM	1376	NH1	ARG	A	850	-2.266	-6.246	45.413	1.00	20.56	A
10	ATOM	1377	NH2	ARG	A	850	-1.202	-5.641	47.360	1.00	23.31	A
	ATOM	1378	C	ARG	A	850	-4.333	0.206	45.002	1.00	18.72	A
	ATOM	1379	O	ARG	A	850	-5.384	0.717	45.410	1.00	17.53	A
	ATOM	1380	N	GLU	A	851	-3.158	0.825	45.080	1.00	17.58	A
	ATOM	1381	CA	GLU	A	851	-3.049	2.154	45.687	1.00	16.80	A
15	ATOM	1382	CB	GLU	A	851	-1.580	2.476	45.987	1.00	17.63	A
	ATOM	1383	CG	GLU	A	851	-1.378	3.485	47.117	1.00	18.50	A
	ATOM	1384	CD	GLU	A	851	-1.946	2.995	48.444	1.00	17.77	A
	ATOM	1385	OE1	GLU	A	851	-2.123	1.767	48.597	1.00	17.44	A
	ATOM	1386	OE2	GLU	A	851	-2.198	3.834	49.340	1.00	18.22	A
20	ATOM	1387	C	GLU	A	851	-3.657	3.222	44.768	1.00	16.79	A
	ATOM	1388	O	GLU	A	851	-4.258	4.200	45.235	1.00	20.29	A
	ATOM	1389	N	LEU	A	852	-3.497	3.040	43.462	1.00	15.37	A
	ATOM	1390	CA	LEU	A	852	-4.063	3.973	42.493	1.00	16.55	A
	ATOM	1391	CB	LEU	A	852	-3.708	3.554	41.063	1.00	15.51	A
25	ATOM	1392	CG	LEU	A	852	-4.438	4.310	39.941	1.00	16.71	A
	ATOM	1393	CD1	LEU	A	852	-4.188	5.810	40.076	1.00	14.65	A
	ATOM	1394	CD2	LEU	A	852	-3.972	3.807	38.582	1.00	16.68	A
	ATOM	1395	C	LEU	A	852	-5.576	3.934	42.666	1.00	17.16	A
	ATOM	1396	O	LEU	A	852	-6.251	4.959	42.593	1.00	17.80	A
30	ATOM	1397	N	ILE	A	853	-6.102	2.734	42.890	1.00	17.86	A
	ATOM	1398	CA	ILE	A	853	-7.535	2.563	43.078	1.00	18.24	A
	ATOM	1399	CB	ILE	A	853	-7.898	1.061	43.173	1.00	17.18	A
	ATOM	1400	CG2	ILE	A	853	-9.353	0.880	43.639	1.00	18.01	A
	ATOM	1401	CG1	ILE	A	853	-7.700	0.415	41.797	1.00	15.66	A
35	ATOM	1402	CD1	ILE	A	853	-7.798	-1.103	41.795	1.00	15.60	A
	ATOM	1403	C	ILE	A	853	-8.003	3.322	44.316	1.00	18.88	A
	ATOM	1404	O	ILE	A	853	-9.065	3.946	44.294	1.00	20.72	A
	ATOM	1405	N	LYS	A	854	-7.207	3.290	45.385	1.00	19.21	A
	ATOM	1406	CA	LYS	A	854	-7.559	4.009	46.609	1.00	19.73	A
40	ATOM	1407	CB	LYS	A	854	-6.574	3.697	47.739	1.00	19.29	A
	ATOM	1408	CG	LYS	A	854	-6.560	2.276	48.255	1.00	23.21	A
	ATOM	1409	CD	LYS	A	854	-5.459	2.177	49.304	1.00	25.78	A
	ATOM	1410	CE	LYS	A	854	-5.237	0.771	49.787	1.00	27.22	A
	ATOM	1411	NZ	LYS	A	854	-4.022	0.746	50.645	1.00	27.63	A
45	ATOM	1412	C	LYS	A	854	-7.530	5.517	46.352	1.00	18.40	A
	ATOM	1413	O	LYS	A	854	-8.353	6.267	46.882	1.00	17.47	A
	ATOM	1414	N	ALA	A	855	-6.559	5.956	45.554	1.00	18.32	A
	ATOM	1415	CA	ALA	A	855	-6.414	7.371	45.216	1.00	19.46	A
	ATOM	1416	CB	ALA	A	855	-5.177	7.574	44.332	1.00	18.11	A
50	ATOM	1417	C	ALA	A	855	-7.668	7.854	44.486	1.00	20.08	A
	ATOM	1418	O	ALA	A	855	-8.194	8.931	44.771	1.00	20.31	A
	ATOM	1419	N	ILE	A	856	-8.138	7.054	43.535	1.00	21.87	A
	ATOM	1420	CA	ILE	A	856	-9.341	7.393	42.779	1.00	22.21	A
	ATOM	1421	CB	ILE	A	856	-9.663	6.312	41.720	1.00	21.32	A
55	ATOM	1422	CG2	ILE	A	856	-11.043	6.574	41.106	1.00	22.81	A
	ATOM	1423	CG1	ILE	A	856	-8.591	6.318	40.626	1.00	21.10	A

Table 2. (cont'd)

		#	Name	Res.	Chain	Res #	X	Y	Z	occ	B	SegID
	ATOM	1424	CD1	ILE	A	856	-8.721	5.169	39.625	1.00	17.78	A
5	ATOM	1425	C	ILE	A	856	-10.525	7.495	43.739	1.00	23.75	A
	ATOM	1426	O	ILE	A	856	-11.333	8.417	43.651	1.00	23.51	A
	ATOM	1427	N	GLY	A	857	-10.617	6.539	44.657	1.00	24.69	A
	ATOM	1428	CA	GLY	A	857	-11.712	6.531	45.611	1.00	25.96	A
	ATOM	1429	C	GLY	A	857	-11.791	7.754	46.508	1.00	27.36	A
10	ATOM	1430	O	GLY	A	857	-12.818	7.993	47.145	1.00	25.78	A
	ATOM	1431	N	LEU	A	858	-10.713	8.533	46.566	1.00	28.12	A
	ATOM	1432	CA	LEU	A	858	-10.687	9.733	47.400	1.00	29.63	A
	ATOM	1433	CB	LEU	A	858	-9.275	10.330	47.437	1.00	28.28	A
	ATOM	1434	CG	LEU	A	858	-8.196	9.521	48.153	1.00	27.33	A
15	ATOM	1435	CD1	LEU	A	858	-6.867	10.264	48.070	1.00	27.66	A
	ATOM	1436	CD2	LEU	A	858	-8.611	9.294	49.606	1.00	27.32	A
	ATOM	1437	C	LEU	A	858	-11.663	10.807	46.921	1.00	32.53	A
	ATOM	1438	O	LEU	A	858	-12.139	11.621	47.714	1.00	31.16	A
	ATOM	1439	N	ARG	A	859	-11.956	10.816	45.626	1.00	35.00	A
20	ATOM	1440	CA	ARG	A	859	-12.864	11.814	45.076	1.00	40.11	A
	ATOM	1441	CB	ARG	A	859	-12.079	12.810	44.218	1.00	41.59	A
	ATOM	1442	CG	ARG	A	859	-10.950	13.477	44.983	1.00	45.19	A
	ATOM	1443	CD	ARG	A	859	-10.168	14.479	44.149	1.00	46.94	A
	ATOM	1444	NE	ARG	A	859	-9.060	15.024	44.929	1.00	49.30	A
25	ATOM	1445	CZ	ARG	A	859	-8.256	16.000	44.524	1.00	50.75	A
	ATOM	1446	NH1	ARG	A	859	-8.426	16.560	43.333	1.00	52.23	A
	ATOM	1447	NH2	ARG	A	859	-7.278	16.418	45.317	1.00	50.68	A
	ATOM	1448	C	ARG	A	859	-13.964	11.169	44.251	1.00	43.10	A
	ATOM	1449	O	ARG	A	859	-15.145	11.469	44.429	1.00	43.32	A
30	ATOM	1450	N	GLN	A	860	-13.568	10.282	43.346	1.00	45.83	A
	ATOM	1451	CA	GLN	A	860	-14.521	9.592	42.493	1.00	48.83	A
	ATOM	1452	CB	GLN	A	860	-13.782	8.786	41.424	1.00	49.90	A
	ATOM	1453	CG	GLN	A	860	-12.820	9.633	40.604	1.00	50.95	A
	ATOM	1454	CD	GLN	A	860	-13.514	10.785	39.901	1.00	51.85	A
35	ATOM	1455	OE1	GLN	A	860	-12.874	11.756	39.498	1.00	52.01	A
	ATOM	1456	NE2	GLN	A	860	-14.829	10.677	39.742	1.00	52.02	A
	ATOM	1457	C	GLN	A	860	-15.386	8.682	43.346	1.00	50.16	A
	ATOM	1458	O	GLN	A	860	-15.055	7.519	43.580	1.00	51.05	A
	ATOM	1459	N	LYS	A	861	-16.496	9.235	43.821	1.00	50.99	A
40	ATOM	1460	CA	LYS	A	861	-17.425	8.497	44.657	1.00	51.23	A
	ATOM	1461	CB	LYS	A	861	-18.081	9.450	45.657	1.00	52.22	A
	ATOM	1462	CG	LYS	A	861	-17.072	10.173	46.543	1.00	53.62	A
	ATOM	1463	CD	LYS	A	861	-17.738	11.203	47.441	1.00	56.57	A
	ATOM	1464	CE	LYS	A	861	-18.380	12.322	46.629	1.00	57.51	A
45	ATOM	1465	NZ	LYS	A	861	-19.063	13.320	47.501	1.00	57.72	A
	ATOM	1466	C	LYS	A	861	-18.469	7.844	43.763	1.00	50.75	A
	ATOM	1467	O	LYS	A	861	-19.079	8.499	42.917	1.00	51.25	A
	ATOM	1468	N	GLY	A	862	-18.660	6.544	43.950	1.00	48.78	A
	ATOM	1469	CA	GLY	A	862	-19.614	5.815	43.139	1.00	46.59	A
50	ATOM	1470	C	GLY	A	862	-18.891	4.728	42.371	1.00	45.09	A
	ATOM	1471	O	GLY	A	862	-17.832	4.966	41.789	1.00	42.61	A
	ATOM	1472	N	VAL	A	863	-19.464	3.532	42.367	1.00	43.94	A
	ATOM	1473	CA	VAL	A	863	-18.859	2.401	41.678	1.00	44.09	A
	ATOM	1474	CB	VAL	A	863	-19.721	1.130	41.853	1.00	44.83	A
55	ATOM	1475	CG1	VAL	A	863	-19.897	0.829	43.334	1.00	46.10	A
	ATOM	1476	CG2	VAL	A	863	-21.074	1.319	41.193	1.00	45.96	A

Table 2. (cont'd)

		#	Name	Res.	Chain	Res #	X	Y	Z	occ	B	SegID
5	ATOM	1477	C	VAL	A	863	-18.624	2.641	40.186	1.00	42.90	A
	ATOM	1478	O	VAL	A	863	-17.542	2.357	39.671	1.00	43.15	A
	ATOM	1479	N	VAL	A	864	-19.628	3.168	39.493	1.00	40.87	A
	ATOM	1480	CA	VAL	A	864	-19.506	3.414	38.061	1.00	39.53	A
	ATOM	1481	CB	VAL	A	864	-20.878	3.775	37.430	1.00	39.71	A
10	ATOM	1482	CG1	VAL	A	864	-21.395	5.075	38.002	1.00	40.62	A
	ATOM	1483	CG2	VAL	A	864	-20.745	3.874	35.921	1.00	41.26	A
	ATOM	1484	C	VAL	A	864	-18.500	4.519	37.748	1.00	37.88	A
	ATOM	1485	O	VAL	A	864	-17.720	4.403	36.806	1.00	37.34	A
	ATOM	1486	N	SER	A	865	-18.518	5.585	38.540	1.00	35.74	A
15	ATOM	1487	CA	SER	A	865	-17.598	6.696	38.338	1.00	35.39	A
	ATOM	1488	CB	SER	A	865	-17.972	7.865	39.251	1.00	37.79	A
	ATOM	1489	OG	SER	A	865	-17.071	8.943	39.081	1.00	41.84	A
	ATOM	1490	C	SER	A	865	-16.153	6.283	38.614	1.00	33.45	A
	ATOM	1491	O	SER	A	865	-15.262	6.529	37.800	1.00	31.58	A
20	ATOM	1492	N	SER	A	866	-15.927	5.654	39.764	1.00	30.19	A
	ATOM	1493	CA	SER	A	866	-14.584	5.224	40.136	1.00	29.83	A
	ATOM	1494	CB	SER	A	866	-14.567	4.714	41.584	1.00	30.55	A
	ATOM	1495	OG	SER	A	866	-15.330	3.528	41.733	1.00	35.07	A
	ATOM	1496	C	SER	A	866	-14.073	4.142	39.186	1.00	28.90	A
25	ATOM	1497	O	SER	A	866	-12.871	4.046	38.925	1.00	26.65	A
	ATOM	1498	N	SER	A	867	-14.991	3.338	38.661	1.00	28.37	A
	ATOM	1499	CA	SER	A	867	-14.634	2.268	37.732	1.00	30.83	A
	ATOM	1500	CB	SER	A	867	-15.815	1.313	37.549	1.00	32.58	A
	ATOM	1501	OG	SER	A	867	-15.419	0.156	36.834	1.00	39.29	A
30	ATOM	1502	C	SER	A	867	-14.214	2.845	36.376	1.00	30.15	A
	ATOM	1503	O	SER	A	867	-13.253	2.376	35.760	1.00	29.63	A
	ATOM	1504	N	GLN	A	868	-14.940	3.857	35.912	1.00	29.59	A
	ATOM	1505	CA	GLN	A	868	-14.616	4.501	34.643	1.00	30.50	A
	ATOM	1506	CB	GLN	A	868	-15.735	5.459	34.225	1.00	33.42	A
35	ATOM	1507	CG	GLN	A	868	-17.027	4.768	33.798	1.00	40.79	A
	ATOM	1508	CD	GLN	A	868	-18.021	5.727	33.160	1.00	44.38	A
	ATOM	1509	OE1	GLN	A	868	-17.714	6.387	32.164	1.00	48.14	A
	ATOM	1510	NE2	GLN	A	868	-19.219	5.806	33.729	1.00	47.00	A
	ATOM	1511	C	GLN	A	868	-13.306	5.279	34.780	1.00	28.76	A
40	ATOM	1512	O	GLN	A	868	-12.501	5.339	33.847	1.00	28.37	A
	ATOM	1513	N	ARG	A	869	-13.106	5.875	35.952	1.00	25.54	A
	ATOM	1514	CA	ARG	A	869	-11.904	6.651	36.239	1.00	23.93	A
	ATOM	1515	CB	ARG	A	869	-12.001	7.257	37.643	1.00	24.14	A
	ATOM	1516	CG	ARG	A	869	-10.842	8.165	38.026	1.00	24.38	A
45	ATOM	1517	CD	ARG	A	869	-10.865	9.446	37.230	1.00	26.98	A
	ATOM	1518	NE	ARG	A	869	-9.901	10.419	37.734	1.00	26.60	A
	ATOM	1519	CZ	ARG	A	869	-9.722	11.624	37.209	1.00	27.32	A
	ATOM	1520	NH1	ARG	A	869	-10.443	12.002	36.159	1.00	27.79	A
	ATOM	1521	NH2	ARG	A	869	-8.831	12.453	37.734	1.00	26.20	A
50	ATOM	1522	C	ARG	A	869	-10.667	5.760	36.142	1.00	21.71	A
	ATOM	1523	O	ARG	A	869	-9.640	6.159	35.589	1.00	21.09	A
	ATOM	1524	N	PHE	A	870	-10.767	4.553	36.689	1.00	20.52	A
	ATOM	1525	CA	PHE	A	870	-9.657	3.607	36.649	1.00	21.95	A
	ATOM	1526	CB	PHE	A	870	-10.030	2.313	37.380	1.00	23.09	A
55	ATOM	1527	CG	PHE	A	870	-8.945	1.273	37.361	1.00	23.44	A
	ATOM	1528	CD1	PHE	A	870	-7.878	1.342	38.252	1.00	24.31	A
	ATOM	1529	CD2	PHE	A	870	-8.975	0.237	36.432	1.00	23.49	A

Table 2. (cont'd)

		#	Name	Res.	Chain	Res #	X	Y	Z	occ	B	SegID
	ATOM	1530	CE1	PHE	A	870	-6.858	0.391	38.215	1.00	23.31	A
5	ATOM	1531	CE2	PHE	A	870	-7.960	-0.717	36.388	1.00	23.17	A
	ATOM	1532	CZ	PHE	A	870	-6.902	-0.639	37.281	1.00	22.88	A
	ATOM	1533	C	PHE	A	870	-9.316	3.290	35.192	1.00	22.30	A
	ATOM	1534	O	PHE	A	870	-8.145	3.189	34.818	1.00	19.13	A
	ATOM	1535	N	TYR	A	871	-10.346	3.131	34.367	1.00	22.40	A
10	ATOM	1536	CA	TYR	A	871	-10.132	2.835	32.957	1.00	23.09	A
	ATOM	1537	CB	TYR	A	871	-11.466	2.628	32.234	1.00	25.44	A
	ATOM	1538	CG	TYR	A	871	-11.291	2.436	30.743	1.00	29.50	A
	ATOM	1539	CD1	TYR	A	871	-10.944	1.192	30.216	1.00	31.45	A
	ATOM	1540	CE1	TYR	A	871	-10.709	1.027	28.846	1.00	34.54	A
15	ATOM	1541	CD2	TYR	A	871	-11.404	3.516	29.865	1.00	30.74	A
	ATOM	1542	CE2	TYR	A	871	-11.168	3.362	28.499	1.00	33.34	A
	ATOM	1543	CZ	TYR	A	871	-10.821	2.117	27.998	1.00	34.38	A
	ATOM	1544	OH	TYR	A	871	-10.579	1.966	26.650	1.00	38.83	A
	ATOM	1545	C	TYR	A	871	-9.388	3.986	32.285	1.00	21.64	A
20	ATOM	1546	O	TYR	A	871	-8.399	3.778	31.587	1.00	20.89	A
	ATOM	1547	N	GLN	A	872	-9.881	5.200	32.501	1.00	21.08	A
	ATOM	1548	CA	GLN	A	872	-9.295	6.394	31.899	1.00	21.63	A
	ATOM	1549	CB	GLN	A	872	-10.088	7.627	32.309	1.00	23.97	A
	ATOM	1550	CG	GLN	A	872	-11.548	7.594	31.907	1.00	29.50	A
25	ATOM	1551	CD	GLN	A	872	-12.270	8.844	32.344	1.00	32.02	A
	ATOM	1552	OE1	GLN	A	872	-12.344	9.148	33.536	1.00	35.43	A
	ATOM	1553	NE2	GLN	A	872	-12.800	9.585	31.381	1.00	36.11	A
	ATOM	1554	C	GLN	A	872	-7.833	6.626	32.263	1.00	20.95	A
	ATOM	1555	O	GLN	A	872	-6.998	6.879	31.392	1.00	17.56	A
30	ATOM	1556	N	LEU	A	873	-7.533	6.557	33.553	1.00	18.12	A
	ATOM	1557	CA	LEU	A	873	-6.175	6.791	34.007	1.00	19.84	A
	ATOM	1558	CB	LEU	A	873	-6.145	6.878	35.538	1.00	19.94	A
	ATOM	1559	CG	LEU	A	873	-6.994	8.036	36.083	1.00	20.53	A
	ATOM	1560	CD1	LEU	A	873	-6.851	8.145	37.598	1.00	20.93	A
35	ATOM	1561	CD2	LEU	A	873	-6.551	9.336	35.417	1.00	23.05	A
	ATOM	1562	C	LEU	A	873	-5.221	5.724	33.500	1.00	20.65	A
	ATOM	1563	O	LEU	A	873	-4.110	6.033	33.062	1.00	19.40	A
	ATOM	1564	N	THR	A	874	-5.656	4.468	33.542	1.00	20.04	A
	ATOM	1565	CA	THR	A	874	-4.811	3.382	33.077	1.00	20.77	A
40	ATOM	1566	CB	THR	A	874	-5.361	2.017	33.538	1.00	20.85	A
	ATOM	1567	OG1	THR	A	874	-6.725	1.878	33.126	1.00	21.70	A
	ATOM	1568	CG2	THR	A	874	-5.279	1.905	35.062	1.00	20.63	A
	ATOM	1569	C	THR	A	874	-4.689	3.425	31.553	1.00	22.66	A
	ATOM	1570	O	THR	A	874	-3.623	3.132	30.992	1.00	23.26	A
45	ATOM	1571	N	LYS	A	875	-5.773	3.806	30.885	1.00	22.44	A
	ATOM	1572	CA	LYS	A	875	-5.752	3.915	29.431	1.00	23.45	A
	ATOM	1573	CB	LYS	A	875	-7.129	4.316	28.890	1.00	24.25	A
	ATOM	1574	CG	LYS	A	875	-7.208	4.331	27.369	1.00	27.73	A
	ATOM	1575	CD	LYS	A	875	-6.942	2.944	26.792	1.00	30.15	A
50	ATOM	1576	CE	LYS	A	875	-6.923	2.964	25.270	1.00	31.96	A
	ATOM	1577	NZ	LYS	A	875	-6.757	1.594	24.705	1.00	35.36	A
	ATOM	1578	C	LYS	A	875	-4.722	4.976	29.047	1.00	22.41	A
	ATOM	1579	O	LYS	A	875	-3.984	4.810	28.079	1.00	23.26	A
	ATOM	1580	N	LEU	A	876	-4.679	6.066	29.813	1.00	22.49	A
55	ATOM	1581	CA	LEU	A	876	-3.728	7.149	29.565	1.00	22.37	A
	ATOM	1582	CB	LEU	A	876	-3.914	8.264	30.606	1.00	22.36	A

Table 2. (cont'd)

		#	Name	Res.	Chain	Res #	X	Y	Z	occ	B	SegID
5	ATOM	1583	CG	LEU	A	876	-3.128	9.579	30.483	1.00	24.28	A
	ATOM	1584	CD1	LEU	A	876	-3.717	10.604	31.439	1.00	24.81	A
	ATOM	1585	CD2	LEU	A	876	-1.654	9.362	30.796	1.00	23.97	A
	ATOM	1586	C	LEU	A	876	-2.305	6.589	29.640	1.00	22.30	A
	ATOM	1587	O	LEU	A	876	-1.469	6.875	28.777	1.00	19.88	A
10	ATOM	1588	N	LEU	A	877	-2.033	5.788	30.668	1.00	20.81	A
	ATOM	1589	CA	LEU	A	877	-0.708	5.198	30.814	1.00	20.51	A
	ATOM	1590	CB	LEU	A	877	-0.609	4.409	32.125	1.00	18.01	A
	ATOM	1591	CG	LEU	A	877	-0.722	5.272	33.391	1.00	19.57	A
	ATOM	1592	CD1	LEU	A	877	-0.644	4.381	34.623	1.00	19.95	A
15	ATOM	1593	CD2	LEU	A	877	0.397	6.318	33.422	1.00	19.10	A
	ATOM	1594	C	LEU	A	877	-0.404	4.300	29.614	1.00	20.50	A
	ATOM	1595	O	LEU	A	877	0.714	4.322	29.085	1.00	17.23	A
	ATOM	1596	N	ASP	A	878	-1.389	3.518	29.177	1.00	20.16	A
	ATOM	1597	CA	ASP	A	878	-1.191	2.651	28.014	1.00	21.77	A
20	ATOM	1598	CB	ASP	A	878	-2.474	1.885	27.657	1.00	22.61	A
	ATOM	1599	CG	ASP	A	878	-2.712	0.658	28.530	1.00	24.90	A
	ATOM	1600	OD1	ASP	A	878	-1.883	0.338	29.408	1.00	20.69	A
	ATOM	1601	OD2	ASP	A	878	-3.756	-0.002	28.323	1.00	27.24	A
	ATOM	1602	C	ASP	A	878	-0.802	3.518	26.813	1.00	21.54	A
25	ATOM	1603	O	ASP	A	878	0.132	3.194	26.076	1.00	22.58	A
	ATOM	1604	N	ASN	A	879	-1.524	4.620	26.625	1.00	21.91	A
	ATOM	1605	CA	ASN	A	879	-1.275	5.529	25.509	1.00	24.62	A
	ATOM	1606	CB	ASN	A	879	-2.361	6.612	25.432	1.00	23.63	A
	ATOM	1607	CG	ASN	A	879	-3.730	6.054	25.063	1.00	26.89	A
30	ATOM	1608	OD1	ASN	A	879	-3.840	4.973	24.486	1.00	26.87	A
	ATOM	1609	ND2	ASN	A	879	-4.781	6.807	25.381	1.00	26.39	A
	ATOM	1610	C	ASN	A	879	0.098	6.203	25.549	1.00	25.62	A
	ATOM	1611	O	ASN	A	879	0.593	6.658	24.517	1.00	26.49	A
	ATOM	1612	N	LEU	A	880	0.711	6.276	26.727	1.00	24.07	A
35	ATOM	1613	CA	LEU	A	880	2.028	6.900	26.838	1.00	25.83	A
	ATOM	1614	CB	LEU	A	880	2.456	7.033	28.298	1.00	25.52	A
	ATOM	1615	CG	LEU	A	880	1.906	8.225	29.081	1.00	29.53	A
	ATOM	1616	CD1	LEU	A	880	2.583	8.268	30.450	1.00	27.82	A
	ATOM	1617	CD2	LEU	A	880	2.170	9.524	28.315	1.00	28.47	A
40	ATOM	1618	C	LEU	A	880	3.112	6.146	26.078	1.00	25.34	A
	ATOM	1619	O	LEU	A	880	4.035	6.760	25.549	1.00	25.19	A
	ATOM	1620	N	HIS	A	881	3.007	4.818	26.038	1.00	26.40	A
	ATOM	1621	CA	HIS	A	881	3.987	3.995	25.335	1.00	26.00	A
	ATOM	1622	CB	HIS	A	881	3.520	2.532	25.290	1.00	27.74	A
45	ATOM	1623	CG	HIS	A	881	3.805	1.765	26.548	1.00	29.80	A
	ATOM	1624	CD2	HIS	A	881	4.934	1.656	27.289	1.00	29.97	A
	ATOM	1625	ND1	HIS	A	881	2.866	0.962	27.162	1.00	31.29	A
	ATOM	1626	CE1	HIS	A	881	3.404	0.391	28.226	1.00	30.71	A
	ATOM	1627	NE2	HIS	A	881	4.659	0.796	28.325	1.00	32.87	A
50	ATOM	1628	C	HIS	A	881	4.235	4.508	23.916	1.00	26.38	A
	ATOM	1629	O	HIS	A	881	5.379	4.641	23.483	1.00	25.86	A
	ATOM	1630	N	ASP	A	882	3.159	4.816	23.203	1.00	25.87	A
	ATOM	1631	CA	ASP	A	882	3.267	5.303	21.835	1.00	25.66	A
	ATOM	1632	CB	ASP	A	882	1.891	5.273	21.179	1.00	31.45	A
55	ATOM	1633	CG	ASP	A	882	1.262	3.900	21.238	1.00	35.82	A
	ATOM	1634	OD1	ASP	A	882	1.688	3.017	20.460	1.00	37.06	A
	ATOM	1635	OD2	ASP	A	882	0.359	3.699	22.081	1.00	39.76	A

Table 2. (cont'd)

		#	Name	Res.	Chain	Res #	X	Y	Z	occ	B	SegID
	ATOM	1636	C	ASP	A	882	3.853	6.706	21.757	1.00	23.14	A
5	ATOM	1637	O	ASP	A	882	4.692	6.990	20.904	1.00	23.94	A
	ATOM	1638	N	LEU	A	883	3.412	7.583	22.648	1.00	20.96	A
	ATOM	1639	CA	LEU	A	883	3.914	8.950	22.671	1.00	20.25	A
	ATOM	1640	CB	LEU	A	883	3.146	9.759	23.719	1.00	20.75	A
	ATOM	1641	CG	LEU	A	883	3.408	11.260	23.836	1.00	23.11	A
10	ATOM	1642	CD1	LEU	A	883	2.206	11.911	24.517	1.00	24.84	A
	ATOM	1643	CD2	LEU	A	883	4.692	11.525	24.624	1.00	24.63	A
	ATOM	1644	C	LEU	A	883	5.414	8.925	22.989	1.00	19.01	A
	ATOM	1645	O	LEU	A	883	6.209	9.615	22.354	1.00	16.78	A
	ATOM	1646	N	VAL	A	884	5.794	8.116	23.971	1.00	18.69	A
15	ATOM	1647	CA	VAL	A	884	7.193	7.987	24.370	1.00	16.95	A
	ATOM	1648	CB	VAL	A	884	7.301	7.148	25.666	1.00	17.81	A
	ATOM	1649	CG1	VAL	A	884	8.753	6.772	25.953	1.00	15.34	A
	ATOM	1650	CG2	VAL	A	884	6.724	7.954	26.831	1.00	15.89	A
	ATOM	1651	C	VAL	A	884	8.061	7.377	23.261	1.00	17.62	A
20	ATOM	1652	O	VAL	A	884	9.264	7.631	23.189	1.00	17.21	A
	ATOM	1653	N	LYS	A	885	7.458	6.585	22.384	1.00	18.89	A
	ATOM	1654	CA	LYS	A	885	8.227	5.995	21.296	1.00	19.66	A
	ATOM	1655	CB	LYS	A	885	7.388	4.976	20.532	1.00	22.16	A
	ATOM	1656	CG	LYS	A	885	8.142	4.308	19.388	1.00	24.56	A
25	ATOM	1657	CD	LYS	A	885	7.292	3.222	18.738	1.00	27.97	A
	ATOM	1658	CE	LYS	A	885	7.977	2.647	17.506	1.00	30.89	A
	ATOM	1659	NZ	LYS	A	885	7.178	1.532	16.917	1.00	33.14	A
	ATOM	1660	C	LYS	A	885	8.741	7.078	20.341	1.00	19.41	A
	ATOM	1661	O	LYS	A	885	9.855	6.976	19.820	1.00	17.34	A
30	ATOM	1662	N	GLN	A	886	7.943	8.117	20.114	1.00	20.30	A
	ATOM	1663	CA	GLN	A	886	8.368	9.208	19.237	1.00	20.05	A
	ATOM	1664	CB	GLN	A	886	7.214	10.175	18.982	1.00	24.07	A
	ATOM	1665	CG	GLN	A	886	6.098	9.593	18.119	1.00	31.54	A
	ATOM	1666	CD	GLN	A	886	4.942	10.566	17.914	1.00	36.15	A
35	ATOM	1667	OE1	GLN	A	886	3.995	10.271	17.188	1.00	41.20	A
	ATOM	1668	NE2	GLN	A	886	5.016	11.728	18.557	1.00	38.67	A
	ATOM	1669	C	GLN	A	886	9.546	9.963	19.863	1.00	20.53	A
	ATOM	1670	O	GLN	A	886	10.483	10.365	19.168	1.00	17.99	A
	ATOM	1671	N	LEU	A	887	9.495	10.153	21.178	1.00	18.09	A
40	ATOM	1672	CA	LEU	A	887	10.568	10.849	21.880	1.00	17.27	A
	ATOM	1673	CB	LEU	A	887	10.163	11.118	23.336	1.00	17.29	A
	ATOM	1674	CG	LEU	A	887	8.846	11.886	23.520	1.00	19.30	A
	ATOM	1675	CD1	LEU	A	887	8.660	12.252	24.997	1.00	16.99	A
	ATOM	1676	CD2	LEU	A	887	8.850	13.137	22.661	1.00	16.70	A
45	ATOM	1677	C	LEU	A	887	11.835	9.999	21.825	1.00	16.42	A
	ATOM	1678	O	LEU	A	887	12.927	10.507	21.574	1.00	18.79	A
	ATOM	1679	N	HIS	A	888	11.678	8.700	22.048	1.00	15.31	A
	ATOM	1680	CA	HIS	A	888	12.799	7.771	22.006	1.00	15.69	A
	ATOM	1681	CB	HIS	A	888	12.316	6.343	22.279	1.00	13.45	A
50	ATOM	1682	CG	HIS	A	888	12.170	6.018	23.733	1.00	16.95	A
	ATOM	1683	CD2	HIS	A	888	12.609	6.662	24.840	1.00	16.73	A
	ATOM	1684	ND1	HIS	A	888	11.553	4.869	24.180	1.00	18.43	A
	ATOM	1685	CE1	HIS	A	888	11.622	4.816	25.498	1.00	19.06	A
	ATOM	1686	NE2	HIS	A	888	12.259	5.892	25.924	1.00	19.99	A
55	ATOM	1687	C	HIS	A	888	13.546	7.802	20.677	1.00	14.55	A
	ATOM	1688	O	HIS	A	888	14.776	7.862	20.654	1.00	15.76	A

Table 2. (cont'd)

		#	Name	Res.	Chain	Res #	X	Y	Z	occ	B	SegID
5	ATOM	1689	N	LEU	A	889	12.807	7.751	19.571	1.00	14.95	A
	ATOM	1690	CA	LEU	A	889	13.426	7.763	18.247	1.00	15.66	A
	ATOM	1691	CB	LEU	A	889	12.371	7.551	17.146	1.00	15.15	A
	ATOM	1692	CG	LEU	A	889	12.885	7.571	15.693	1.00	16.45	A
	ATOM	1693	CD1	LEU	A	889	13.998	6.548	15.523	1.00	14.91	A
10	ATOM	1694	CD2	LEU	A	889	11.751	7.283	14.712	1.00	15.91	A
	ATOM	1695	C	LEU	A	889	14.171	9.069	18.000	1.00	16.20	A
	ATOM	1696	O	LEU	A	889	15.296	9.061	17.498	1.00	15.72	A
	ATOM	1697	N	TYR	A	890	13.544	10.189	18.353	1.00	15.89	A
	ATOM	1698	CA	TYR	A	890	14.167	11.497	18.165	1.00	15.42	A
15	ATOM	1699	CB	TYR	A	890	13.181	12.612	18.545	1.00	16.23	A
	ATOM	1700	CG	TYR	A	890	13.720	14.017	18.336	1.00	19.79	A
	ATOM	1701	CD1	TYR	A	890	14.631	14.580	19.232	1.00	17.47	A
	ATOM	1702	CE1	TYR	A	890	15.146	15.863	19.026	1.00	20.88	A
	ATOM	1703	CD2	TYR	A	890	13.336	14.775	17.225	1.00	20.09	A
20	ATOM	1704	CE2	TYR	A	890	13.851	16.059	17.009	1.00	20.17	A
	ATOM	1705	CZ	TYR	A	890	14.754	16.593	17.912	1.00	21.65	A
	ATOM	1706	OH	TYR	A	890	15.283	17.846	17.694	1.00	22.11	A
	ATOM	1707	C	TYR	A	890	15.432	11.604	19.022	1.00	14.92	A
	ATOM	1708	O	TYR	A	890	16.451	12.143	18.584	1.00	15.02	A
25	ATOM	1709	N	CYS	A	891	15.355	11.092	20.246	1.00	13.56	A
	ATOM	1710	CA	CYS	A	891	16.488	11.125	21.164	1.00	13.38	A
	ATOM	1711	CB	CYS	A	891	16.060	10.621	22.549	1.00	15.61	A
	ATOM	1712	SG	CYS	A	891	17.401	10.546	23.778	1.00	17.44	A
	ATOM	1713	C	CYS	A	891	17.634	10.272	20.625	1.00	12.47	A
30	ATOM	1714	O	CYS	A	891	18.789	10.704	20.604	1.00	14.79	A
	ATOM	1715	N	LEU	A	892	17.322	9.061	20.178	1.00	13.99	A
	ATOM	1716	CA	LEU	A	892	18.366	8.190	19.646	1.00	13.42	A
	ATOM	1717	CB	LEU	A	892	17.802	6.798	19.325	1.00	14.16	A
	ATOM	1718	CG	LEU	A	892	18.817	5.779	18.779	1.00	16.50	A
35	ATOM	1719	CD1	LEU	A	892	19.976	5.645	19.750	1.00	17.30	A
	ATOM	1720	CD2	LEU	A	892	18.146	4.430	18.564	1.00	15.85	A
	ATOM	1721	C	LEU	A	892	19.035	8.786	18.408	1.00	13.65	A
	ATOM	1722	O	LEU	A	892	20.259	8.745	18.286	1.00	14.68	A
	ATOM	1723	N	ASN	A	893	18.244	9.331	17.486	1.00	13.74	A
40	ATOM	1724	CA	ASN	A	893	18.817	9.921	16.284	1.00	15.86	A
	ATOM	1725	CB	ASN	A	893	17.726	10.436	15.337	1.00	18.00	A
	ATOM	1726	CG	ASN	A	893	17.040	9.322	14.578	1.00	19.28	A
	ATOM	1727	OD1	ASN	A	893	17.694	8.407	14.081	1.00	20.97	A
	ATOM	1728	ND2	ASN	A	893	15.716	9.403	14.465	1.00	21.13	A
45	ATOM	1729	C	ASN	A	893	19.733	11.071	16.663	1.00	16.82	A
	ATOM	1730	O	ASN	A	893	20.837	11.205	16.124	1.00	14.75	A
	ATOM	1731	N	THR	A	894	19.273	11.898	17.600	1.00	14.78	A
	ATOM	1732	CA	THR	A	894	20.061	13.037	18.046	1.00	16.39	A
	ATOM	1733	CB	THR	A	894	19.258	13.912	19.033	1.00	18.69	A
50	ATOM	1734	OG1	THR	A	894	18.055	14.371	18.394	1.00	18.55	A
	ATOM	1735	CG2	THR	A	894	20.091	15.113	19.484	1.00	18.34	A
	ATOM	1736	C	THR	A	894	21.359	12.566	18.715	1.00	17.20	A
	ATOM	1737	O	THR	A	894	22.425	13.153	18.501	1.00	15.61	A
	ATOM	1738	N	PHE	A	895	21.269	11.501	19.509	1.00	14.74	A
55	ATOM	1739	CA	PHE	A	895	22.435	10.947	20.199	1.00	16.10	A
	ATOM	1740	CB	PHE	A	895	22.004	9.768	21.080	1.00	18.24	A
	ATOM	1741	CG	PHE	A	895	23.129	9.135	21.849	1.00	17.59	A

Table 2. (cont'd)

		#	Name	Res.	Chain	Res	#	X	Y	Z	occ	B	SegID
5	ATOM	1742	CD1	PHE	A	895		23.674	9.767	22.964	1.00	19.36	A
	ATOM	1743	CD2	PHE	A	895		23.637	7.900	21.464	1.00	18.77	A
	ATOM	1744	CE1	PHE	A	895		24.712	9.173	23.691	1.00	19.72	A
	ATOM	1745	CE2	PHE	A	895		24.676	7.295	22.181	1.00	20.89	A
	ATOM	1746	CZ	PHE	A	895		25.214	7.933	23.298	1.00	19.53	A
10	ATOM	1747	C	PHE	A	895		23.470	10.472	19.170	1.00	17.01	A
	ATOM	1748	O	PHE	A	895		24.665	10.740	19.300	1.00	16.55	A
	ATOM	1749	N	ILE	A	896		22.993	9.754	18.157	1.00	16.61	A
	ATOM	1750	CA	ILE	A	896		23.843	9.243	17.084	1.00	18.06	A
	ATOM	1751	CB	ILE	A	896		22.997	8.447	16.052	1.00	18.72	A
15	ATOM	1752	CG2	ILE	A	896		23.783	8.231	14.758	1.00	20.23	A
	ATOM	1753	CG1	ILE	A	896		22.575	7.106	16.649	1.00	18.11	A
	ATOM	1754	CD1	ILE	A	896		21.537	6.382	15.811	1.00	19.50	A
	ATOM	1755	C	ILE	A	896		24.542	10.394	16.360	1.00	18.68	A
	ATOM	1756	O	ILE	A	896		25.724	10.310	16.029	1.00	19.12	A
20	ATOM	1757	N	GLN	A	897		23.807	11.477	16.132	1.00	17.29	A
	ATOM	1758	CA	GLN	A	897		24.349	12.637	15.427	1.00	19.03	A
	ATOM	1759	CB	GLN	A	897		23.305	13.146	14.427	1.00	19.67	A
	ATOM	1760	CG	GLN	A	897		22.667	12.039	13.596	1.00	21.81	A
	ATOM	1761	CD	GLN	A	897		21.462	12.510	12.804	1.00	22.65	A
25	ATOM	1762	OE1	GLN	A	897		20.568	11.720	12.483	1.00	23.76	A
	ATOM	1763	NE2	GLN	A	897		21.434	13.793	12.476	1.00	21.56	A
	ATOM	1764	C	GLN	A	897		24.743	13.780	16.366	1.00	18.17	A
	ATOM	1765	O	GLN	A	897		24.892	14.922	15.925	1.00	17.24	A
	ATOM	1766	N	SER	A	898		24.927	13.475	17.646	1.00	19.29	A
30	ATOM	1767	CA	SER	A	898		25.256	14.498	18.641	1.00	19.48	A
	ATOM	1768	CB	SER	A	898		25.482	13.857	20.016	1.00	19.59	A
	ATOM	1769	OG	SER	A	898		26.612	13.015	20.014	1.00	23.61	A
	ATOM	1770	C	SER	A	898		26.431	15.428	18.321	1.00	20.34	A
	ATOM	1771	O	SER	A	898		26.339	16.629	18.563	1.00	19.85	A
35	ATOM	1772	N	ARG	A	899		27.528	14.892	17.790	1.00	20.10	A
	ATOM	1773	CA	ARG	A	899		28.679	15.736	17.468	1.00	23.31	A
	ATOM	1774	CB	ARG	A	899		29.880	14.876	17.052	1.00	27.16	A
	ATOM	1775	CG	ARG	A	899		30.420	13.995	18.169	1.00	33.57	A
	ATOM	1776	CD	ARG	A	899		31.727	13.320	17.775	1.00	39.72	A
40	ATOM	1777	NE	ARG	A	899		32.308	12.568	18.885	1.00	45.23	A
	ATOM	1778	CZ	ARG	A	899		33.516	12.013	18.862	1.00	48.88	A
	ATOM	1779	NH1	ARG	A	899		33.963	11.345	19.919	1.00	50.43	A
	ATOM	1780	NH2	ARG	A	899		34.282	12.126	17.784	1.00	49.70	A
	ATOM	1781	C	ARG	A	899		28.359	16.743	16.363	1.00	24.46	A
45	ATOM	1782	O	ARG	A	899		28.630	17.938	16.497	1.00	23.89	A
	ATOM	1783	N	ALA	A	900		27.781	16.254	15.271	1.00	23.66	A
	ATOM	1784	CA	ALA	A	900		27.424	17.113	14.150	1.00	25.41	A
	ATOM	1785	CB	ALA	A	900		26.821	16.276	13.022	1.00	24.80	A
	ATOM	1786	C	ALA	A	900		26.436	18.198	14.576	1.00	25.89	A
50	ATOM	1787	O	ALA	A	900		26.536	19.341	14.141	1.00	24.07	A
	ATOM	1788	N	LEU	A	901		25.496	17.836	15.446	1.00	24.94	A
	ATOM	1789	CA	LEU	A	901		24.471	18.765	15.908	1.00	25.72	A
	ATOM	1790	CB	LEU	A	901		23.180	17.993	16.198	1.00	26.87	A
	ATOM	1791	CG	LEU	A	901		22.684	17.065	15.088	1.00	26.25	A
55	ATOM	1792	CD1	LEU	A	901		21.458	16.312	15.569	1.00	26.78	A
	ATOM	1793	CD2	LEU	A	901		22.361	17.869	13.841	1.00	28.03	A
	ATOM	1794	C	LEU	A	901		24.852	19.587	17.139	1.00	26.55	A

Table 2. (cont'd)

		#	Name	Res.	Chain	Res #	X	Y	Z	occ	B	SegID
5	ATOM	1795	O	LEU	A	901	24.058	20.402	17.610	1.00	25.12	A
	ATOM	1796	N	SER	A	902	26.058	19.374	17.660	1.00	25.57	A
	ATOM	1797	CA	SER	A	902	26.526	20.094	18.846	1.00	25.20	A
	ATOM	1798	CB	SER	A	902	26.683	21.589	18.549	1.00	26.76	A
	ATOM	1799	OG	SER	A	902	27.664	21.806	17.552	1.00	32.11	A
10	ATOM	1800	C	SER	A	902	25.595	19.922	20.042	1.00	24.98	A
	ATOM	1801	O	SER	A	902	25.303	20.874	20.768	1.00	22.85	A
	ATOM	1802	N	VAL	A	903	25.121	18.702	20.247	1.00	23.89	A
	ATOM	1803	CA	VAL	A	903	24.244	18.430	21.375	1.00	22.49	A
	ATOM	1804	CB	VAL	A	903	22.960	17.712	20.917	1.00	21.00	A
15	ATOM	1805	CG1	VAL	A	903	22.100	17.373	22.115	1.00	20.35	A
	ATOM	1806	CG2	VAL	A	903	22.190	18.601	19.942	1.00	21.63	A
	ATOM	1807	C	VAL	A	903	25.004	17.551	22.357	1.00	22.22	A
	ATOM	1808	O	VAL	A	903	25.462	16.468	22.004	1.00	22.99	A
	ATOM	1809	N	GLU	A	904	25.149	18.023	23.588	1.00	22.49	A
20	ATOM	1810	CA	GLU	A	904	25.863	17.261	24.605	1.00	22.99	A
	ATOM	1811	CB	GLU	A	904	26.494	18.201	25.636	1.00	26.54	A
	ATOM	1812	CG	GLU	A	904	27.496	19.191	25.070	1.00	32.93	A
	ATOM	1813	CD	GLU	A	904	27.985	20.166	26.123	1.00	35.69	A
	ATOM	1814	OE1	GLU	A	904	28.416	19.703	27.203	1.00	38.41	A
25	ATOM	1815	OE2	GLU	A	904	27.939	21.390	25.872	1.00	36.80	A
	ATOM	1816	C	GLU	A	904	24.947	16.294	25.344	1.00	22.46	A
	ATOM	1817	O	GLU	A	904	23.801	16.624	25.660	1.00	21.31	A
	ATOM	1818	N	PHE	A	905	25.467	15.102	25.621	1.00	19.52	A
	ATOM	1819	CA	PHE	A	905	24.736	14.088	26.370	1.00	20.13	A
30	ATOM	1820	CB	PHE	A	905	24.483	12.833	25.521	1.00	17.67	A
	ATOM	1821	CG	PHE	A	905	23.378	12.993	24.517	1.00	20.01	A
	ATOM	1822	CD1	PHE	A	905	23.611	13.625	23.299	1.00	18.40	A
	ATOM	1823	CD2	PHE	A	905	22.095	12.519	24.795	1.00	16.55	A
	ATOM	1824	CE1	PHE	A	905	22.589	13.785	22.373	1.00	18.70	A
35	ATOM	1825	CE2	PHE	A	905	21.066	12.675	23.877	1.00	18.48	A
	ATOM	1826	CZ	PHE	A	905	21.311	13.309	22.660	1.00	18.42	A
	ATOM	1827	C	PHE	A	905	25.604	13.715	27.565	1.00	19.48	A
	ATOM	1828	O	PHE	A	905	26.663	13.115	27.395	1.00	18.97	A
	ATOM	1829	N	PRO	A	906	25.179	14.083	28.786	1.00	19.52	A
40	ATOM	1830	CD	PRO	A	906	24.084	15.010	29.128	1.00	20.38	A
	ATOM	1831	CA	PRO	A	906	25.963	13.756	29.981	1.00	19.87	A
	ATOM	1832	CB	PRO	A	906	25.157	14.397	31.108	1.00	19.03	A
	ATOM	1833	CG	PRO	A	906	24.561	15.594	30.442	1.00	20.40	A
	ATOM	1834	C	PRO	A	906	26.147	12.252	30.170	1.00	20.93	A
45	ATOM	1835	O	PRO	A	906	25.532	11.448	29.471	1.00	19.74	A
	ATOM	1836	N	GLU	A	907	26.982	11.892	31.138	1.00	22.35	A
	ATOM	1837	CA	GLU	A	907	27.317	10.504	31.435	1.00	23.45	A
	ATOM	1838	CB	GLU	A	907	28.243	10.457	32.656	1.00	28.12	A
	ATOM	1839	CG	GLU	A	907	29.018	9.154	32.788	1.00	34.86	A
50	ATOM	1840	CD	GLU	A	907	29.942	9.140	33.993	1.00	38.06	A
	ATOM	1841	OE1	GLU	A	907	30.637	10.154	34.220	1.00	41.07	A
	ATOM	1842	OE2	GLU	A	907	29.978	8.114	34.706	1.00	38.81	A
	ATOM	1843	C	GLU	A	907	26.166	9.517	31.646	1.00	21.79	A
	ATOM	1844	O	GLU	A	907	26.042	8.543	30.908	1.00	21.49	A
55	ATOM	1845	N	MET	A	908	25.344	9.742	32.665	1.00	22.08	A
	ATOM	1846	CA	MET	A	908	24.241	8.822	32.937	1.00	23.28	A
	ATOM	1847	CB	MET	A	908	23.538	9.193	34.245	1.00	27.12	A

Table 2. (cont'd)

		#	Name	Res.	Chain	Res #	X	Y	Z	occ	B	SegID
5	ATOM	1848	CG	MET	A	908	24.346	8.860	35.489	1.00	34.62	A
	ATOM	1849	SD	MET	A	908	23.440	9.197	37.025	1.00	43.74	A
	ATOM	1850	CE	MET	A	908	22.199	7.897	36.981	1.00	38.86	A
	ATOM	1851	C	MET	A	908	23.230	8.757	31.799	1.00	20.83	A
	ATOM	1852	O	MET	A	908	22.700	7.686	31.504	1.00	20.86	A
10	ATOM	1853	N	MET	A	909	22.967	9.898	31.166	1.00	18.93	A
	ATOM	1854	CA	MET	A	909	22.036	9.958	30.041	1.00	19.79	A
	ATOM	1855	CB	MET	A	909	21.883	11.402	29.542	1.00	21.27	A
	ATOM	1856	CG	MET	A	909	20.947	12.269	30.359	1.00	20.34	A
	ATOM	1857	SD	MET	A	909	19.199	11.802	30.150	1.00	26.91	A
15	ATOM	1858	CE	MET	A	909	18.993	12.166	28.374	1.00	23.59	A
	ATOM	1859	C	MET	A	909	22.576	9.087	28.910	1.00	19.04	A
	ATOM	1860	O	MET	A	909	21.854	8.282	28.330	1.00	19.89	A
	ATOM	1861	N	SER	A	910	23.858	9.251	28.604	1.00	18.89	A
	ATOM	1862	CA	SER	A	910	24.484	8.469	27.546	1.00	20.47	A
20	ATOM	1863	CB	SER	A	910	25.938	8.908	27.364	1.00	20.19	A
	ATOM	1864	OG	SER	A	910	25.998	10.249	26.900	1.00	20.62	A
	ATOM	1865	C	SER	A	910	24.427	6.976	27.869	1.00	21.20	A
	ATOM	1866	O	SER	A	910	24.210	6.153	26.982	1.00	19.29	A
	ATOM	1867	N	GLU	A	911	24.610	6.638	29.142	1.00	22.27	A
25	ATOM	1868	CA	GLU	A	911	24.587	5.244	29.578	1.00	24.86	A
	ATOM	1869	CB	GLU	A	911	24.965	5.149	31.060	1.00	29.31	A
	ATOM	1870	CG	GLU	A	911	24.950	3.736	31.626	1.00	35.80	A
	ATOM	1871	CD	GLU	A	911	25.165	3.700	33.136	1.00	40.80	A
	ATOM	1872	OE1	GLU	A	911	26.207	4.204	33.609	1.00	45.47	A
30	ATOM	1873	OE2	GLU	A	911	24.290	3.166	33.854	1.00	43.61	A
	ATOM	1874	C	GLU	A	911	23.231	4.574	29.347	1.00	23.81	A
	ATOM	1875	O	GLU	A	911	23.164	3.493	28.756	1.00	22.59	A
	ATOM	1876	N	VAL	A	912	22.151	5.202	29.807	1.00	20.88	A
	ATOM	1877	CA	VAL	A	912	20.827	4.613	29.623	1.00	22.23	A
35	ATOM	1878	CB	VAL	A	912	19.718	5.404	30.374	1.00	22.28	A
	ATOM	1879	CG1	VAL	A	912	20.025	5.441	31.868	1.00	23.61	A
	ATOM	1880	CG2	VAL	A	912	19.602	6.807	29.819	1.00	23.21	A
	ATOM	1881	C	VAL	A	912	20.454	4.535	28.149	1.00	20.96	A
	ATOM	1882	O	VAL	A	912	19.876	3.546	27.699	1.00	21.47	A
40	ATOM	1883	N	ILE	A	913	20.794	5.571	27.392	1.00	20.47	A
	ATOM	1884	CA	ILE	A	913	20.477	5.589	25.969	1.00	21.45	A
	ATOM	1885	CB	ILE	A	913	20.875	6.949	25.330	1.00	21.91	A
	ATOM	1886	CG2	ILE	A	913	20.829	6.862	23.810	1.00	21.47	A
	ATOM	1887	CG1	ILE	A	913	19.926	8.042	25.830	1.00	19.94	A
45	ATOM	1888	CD1	ILE	A	913	20.320	9.446	25.420	1.00	23.22	A
	ATOM	1889	C	ILE	A	913	21.188	4.448	25.249	1.00	22.68	A
	ATOM	1890	O	ILE	A	913	20.570	3.694	24.503	1.00	23.60	A
	ATOM	1891	N	ALA	A	914	22.486	4.313	25.492	1.00	23.11	A
	ATOM	1892	CA	ALA	A	914	23.276	3.270	24.857	1.00	24.55	A
50	ATOM	1893	CB	ALA	A	914	24.757	3.453	25.203	1.00	24.17	A
	ATOM	1894	C	ALA	A	914	22.823	1.878	25.268	1.00	24.85	A
	ATOM	1895	O	ALA	A	914	22.738	0.973	24.441	1.00	24.84	A
	ATOM	1896	N	ALA	A	915	22.532	1.715	26.551	1.00	26.25	A
	ATOM	1897	CA	ALA	A	915	22.119	0.425	27.077	1.00	27.16	A
55	ATOM	1898	CB	ALA	A	915	22.155	0.460	28.602	1.00	26.43	A
	ATOM	1899	C	ALA	A	915	20.759	-0.093	26.616	1.00	27.28	A
	ATOM	1900	O	ALA	A	915	20.627	-1.277	26.315	1.00	28.47	A

Table 2. (cont'd)

		#	Name	Res.	Chain	Res #	X	Y	Z	occ	B	SegID
	ATOM	1901	N	GLN	A	916	19.754	0.773	26.526	1.00	24.56	A
5	ATOM	1902	CA	GLN	A	916	18.429	0.272	26.178	1.00	23.88	A
	ATOM	1903	CB	GLN	A	916	17.529	0.337	27.418	1.00	23.68	A
	ATOM	1904	CG	GLN	A	916	18.134	-0.202	28.704	1.00	25.94	A
	ATOM	1905	CD	GLN	A	916	18.337	-1.704	28.688	1.00	28.66	A
	ATOM	1906	OE1	GLN	A	916	17.808	-2.408	27.828	1.00	29.30	A
10	ATOM	1907	NE2	GLN	A	916	19.101	-2.206	29.654	1.00	29.87	A
	ATOM	1908	C	GLN	A	916	17.622	0.830	25.011	1.00	21.93	A
	ATOM	1909	O	GLN	A	916	16.766	0.119	24.496	1.00	20.48	A
	ATOM	1910	N	LEU	A	917	17.856	2.073	24.588	1.00	21.01	A
	ATOM	1911	CA	LEU	A	917	17.030	2.639	23.518	1.00	21.54	A
15	ATOM	1912	CB	LEU	A	917	17.484	4.062	23.150	1.00	24.24	A
	ATOM	1913	CG	LEU	A	917	16.864	5.165	24.010	1.00	27.14	A
	ATOM	1914	CD1	LEU	A	917	17.113	6.536	23.371	1.00	25.74	A
	ATOM	1915	CD2	LEU	A	917	15.367	4.913	24.147	1.00	27.44	A
	ATOM	1916	C	LEU	A	917	16.846	1.826	22.243	1.00	21.71	A
20	ATOM	1917	O	LEU	A	917	15.717	1.662	21.771	1.00	22.26	A
	ATOM	1918	N	PRO	A	918	17.939	1.315	21.656	1.00	20.55	A
	ATOM	1919	CD	PRO	A	918	19.368	1.494	21.970	1.00	21.89	A
	ATOM	1920	CA	PRO	A	918	17.764	0.530	20.429	1.00	20.41	A
	ATOM	1921	CB	PRO	A	918	19.190	0.106	20.082	1.00	21.03	A
25	ATOM	1922	CG	PRO	A	918	20.017	1.247	20.622	1.00	21.48	A
	ATOM	1923	C	PRO	A	918	16.851	-0.670	20.683	1.00	19.91	A
	ATOM	1924	O	PRO	A	918	15.918	-0.932	19.924	1.00	18.25	A
	ATOM	1925	N	LYS	A	919	17.132	-1.386	21.766	1.00	19.57	A
	ATOM	1926	CA	LYS	A	919	16.356	-2.561	22.154	1.00	19.46	A
30	ATOM	1927	CB	LYS	A	919	16.944	-3.152	23.436	1.00	22.54	A
	ATOM	1928	CG	LYS	A	919	16.263	-4.419	23.930	1.00	27.11	A
	ATOM	1929	CD	LYS	A	919	16.667	-4.723	25.374	1.00	28.80	A
	ATOM	1930	CE	LYS	A	919	18.180	-4.789	25.536	1.00	29.86	A
	ATOM	1931	NZ	LYS	A	919	18.598	-4.886	26.971	1.00	33.98	A
35	ATOM	1932	C	LYS	A	919	14.882	-2.213	22.375	1.00	20.15	A
	ATOM	1933	O	LYS	A	919	13.986	-2.941	21.944	1.00	19.14	A
	ATOM	1934	N	ILE	A	920	14.631	-1.099	23.057	1.00	20.31	A
	ATOM	1935	CA	ILE	A	920	13.262	-0.669	23.321	1.00	18.33	A
	ATOM	1936	CB	ILE	A	920	13.242	0.552	24.267	1.00	20.86	A
40	ATOM	1937	CG2	ILE	A	920	11.820	1.098	24.402	1.00	22.14	A
	ATOM	1938	CG1	ILE	A	920	13.781	0.138	25.640	1.00	18.33	A
	ATOM	1939	CD1	ILE	A	920	13.903	1.284	26.619	1.00	23.66	A
	ATOM	1940	C	ILE	A	920	12.540	-0.328	22.025	1.00	19.54	A
	ATOM	1941	O	ILE	A	920	11.424	-0.788	21.788	1.00	19.13	A
45	ATOM	1942	N	LEU	A	921	13.180	0.472	21.179	1.00	20.13	A
	ATOM	1943	CA	LEU	A	921	12.585	0.851	19.904	1.00	20.63	A
	ATOM	1944	CB	LEU	A	921	13.503	1.829	19.167	1.00	21.68	A
	ATOM	1945	CG	LEU	A	921	13.416	3.266	19.680	1.00	22.69	A
	ATOM	1946	CD1	LEU	A	921	14.462	4.139	18.995	1.00	21.07	A
50	ATOM	1947	CD2	LEU	A	921	12.005	3.796	19.409	1.00	20.56	A
	ATOM	1948	C	LEU	A	921	12.304	-0.362	19.022	1.00	21.94	A
	ATOM	1949	O	LEU	A	921	11.324	-0.386	18.280	1.00	24.08	A
	ATOM	1950	N	ALA	A	922	13.162	-1.372	19.107	1.00	20.43	A
	ATOM	1951	CA	ALA	A	922	12.989	-2.578	18.305	1.00	21.49	A
55	ATOM	1952	CB	ALA	A	922	14.294	-3.354	18.243	1.00	20.05	A
	ATOM	1953	C	ALA	A	922	11.889	-3.466	18.866	1.00	22.02	A

Table 2. (cont'd)

		#	Name	Res.	Chain	Res #	X	Y	Z	occ	B	SegID
5	ATOM	1954	O	ALA	A	922	11.546	-4.489	18.274	1.00	21.77	A
	ATOM	1955	N	GLY	A	923	11.342	-3.075	20.012	1.00	21.48	A
	ATOM	1956	CA	GLY	A	923	10.286	-3.860	20.629	1.00	21.95	A
	ATOM	1957	C	GLY	A	923	10.794	-5.142	21.266	1.00	21.42	A
	ATOM	1958	O	GLY	A	923	10.031	-6.092	21.456	1.00	22.31	A
10	ATOM	1959	N	MET	A	924	12.080	-5.179	21.601	1.00	19.45	A
	ATOM	1960	CA	MET	A	924	12.658	-6.364	22.215	1.00	20.79	A
	ATOM	1961	CB	MET	A	924	14.091	-6.580	21.722	1.00	22.02	A
	ATOM	1962	CG	MET	A	924	14.178	-6.895	20.238	1.00	25.40	A
	ATOM	1963	SD	MET	A	924	13.141	-8.295	19.764	1.00	28.65	A
15	ATOM	1964	CE	MET	A	924	14.164	-9.661	20.270	1.00	27.15	A
	ATOM	1965	C	MET	A	924	12.631	-6.293	23.737	1.00	20.36	A
	ATOM	1966	O	MET	A	924	13.603	-6.635	24.404	1.00	20.04	A
	ATOM	1967	N	VAL	A	925	11.499	-5.829	24.259	1.00	20.45	A
	ATOM	1968	CA	VAL	A	925	11.235	-5.718	25.689	1.00	19.83	A
20	ATOM	1969	CB	VAL	A	925	11.571	-4.319	26.262	1.00	19.54	A
	ATOM	1970	CG1	VAL	A	925	13.067	-4.040	26.133	1.00	18.25	A
	ATOM	1971	CG2	VAL	A	925	10.745	-3.252	25.555	1.00	17.24	A
	ATOM	1972	C	VAL	A	925	9.730	-5.924	25.773	1.00	20.81	A
	ATOM	1973	O	VAL	A	925	9.053	-5.958	24.739	1.00	17.16	A
25	ATOM	1974	N	LYS	A	926	9.206	-6.052	26.986	1.00	20.03	A
	ATOM	1975	CA	LYS	A	926	7.776	-6.271	27.157	1.00	22.62	A
	ATOM	1976	CB	LYS	A	926	7.532	-7.544	27.977	1.00	24.15	A
	ATOM	1977	CG	LYS	A	926	6.062	-7.903	28.123	1.00	27.68	A
	ATOM	1978	CD	LYS	A	926	5.884	-9.233	28.839	1.00	32.47	A
30	ATOM	1979	CE	LYS	A	926	4.412	-9.611	28.927	1.00	33.32	A
	ATOM	1980	NZ	LYS	A	926	4.224	-10.923	29.603	1.00	35.99	A
	ATOM	1981	C	LYS	A	926	7.037	-5.103	27.803	1.00	22.57	A
	ATOM	1982	O	LYS	A	926	7.076	-4.921	29.026	1.00	22.63	A
	ATOM	1983	N	PRO	A	927	6.367	-4.280	26.986	1.00	23.30	A
35	ATOM	1984	CD	PRO	A	927	6.374	-4.224	25.516	1.00	23.83	A
	ATOM	1985	CA	PRO	A	927	5.629	-3.149	27.551	1.00	23.76	A
	ATOM	1986	CB	PRO	A	927	5.220	-2.339	26.316	1.00	24.30	A
	ATOM	1987	CG	PRO	A	927	6.229	-2.751	25.265	1.00	25.51	A
	ATOM	1988	C	PRO	A	927	4.417	-3.750	28.253	1.00	24.23	A
40	ATOM	1989	O	PRO	A	927	3.801	-4.686	27.740	1.00	22.94	A
	ATOM	1990	N	LEU	A	928	4.081	-3.241	29.427	1.00	22.92	A
	ATOM	1991	CA	LEU	A	928	2.930	-3.773	30.132	1.00	24.28	A
	ATOM	1992	CB	LEU	A	928	3.200	-3.825	31.640	1.00	22.59	A
	ATOM	1993	CG	LEU	A	928	4.419	-4.655	32.060	1.00	24.35	A
45	ATOM	1994	CD1	LEU	A	928	4.460	-4.776	33.579	1.00	23.99	A
	ATOM	1995	CD2	LEU	A	928	4.350	-6.038	31.426	1.00	26.06	A
	ATOM	1996	C	LEU	A	928	1.726	-2.896	29.824	1.00	25.03	A
	ATOM	1997	O	LEU	A	928	1.826	-1.666	29.812	1.00	27.49	A
	ATOM	1998	N	LEU	A	929	0.596	-3.533	29.549	1.00	24.29	A
50	ATOM	1999	CA	LEU	A	929	-0.627	-2.809	29.234	1.00	24.19	A
	ATOM	2000	CB	LEU	A	929	-1.107	-3.163	27.825	1.00	25.39	A
	ATOM	2001	CG	LEU	A	929	-0.272	-2.680	26.640	1.00	23.43	A
	ATOM	2002	CD1	LEU	A	929	-0.739	-3.371	25.363	1.00	23.68	A
	ATOM	2003	CD2	LEU	A	929	-0.397	-1.166	26.520	1.00	23.94	A
55	ATOM	2004	C	LEU	A	929	-1.722	-3.150	30.226	1.00	25.66	A
	ATOM	2005	O	LEU	A	929	-1.820	-4.286	30.699	1.00	23.46	A
	ATOM	2006	N	PHE	A	930	-2.541	-2.152	30.535	1.00	26.75	A

Table 2. (cont'd)

		#	Name	Res.	Chain	Res #	X	Y	Z	occ	B	SegID
5	ATOM	2007	CA	PHE	A	930	-3.657	-2.315	31.451	1.00	28.37	A
	ATOM	2008	CB	PHE	A	930	-3.949	-0.987	32.151	1.00	25.94	A
	ATOM	2009	CG	PHE	A	930	-2.857	-0.545	33.093	1.00	24.34	A
	ATOM	2010	CD1	PHE	A	930	-2.662	-1.198	34.306	1.00	24.73	A
	ATOM	2011	CD2	PHE	A	930	-2.015	0.511	32.758	1.00	22.44	A
10	ATOM	2012	CE1	PHE	A	930	-1.641	-0.802	35.175	1.00	24.82	A
	ATOM	2013	CE2	PHE	A	930	-0.994	0.914	33.617	1.00	23.39	A
	ATOM	2014	CZ	PHE	A	930	-0.805	0.256	34.828	1.00	23.89	A
	ATOM	2015	C	PHE	A	930	-4.880	-2.776	30.660	1.00	30.68	A
	ATOM	2016	O	PHE	A	930	-5.794	-3.391	31.215	1.00	29.02	A
15	ATOM	2017	N	HIS	A	931	-4.881	-2.476	29.362	1.00	33.18	A
	ATOM	2018	CA	HIS	A	931	-5.976	-2.856	28.475	1.00	38.68	A
	ATOM	2019	CB	HIS	A	931	-6.909	-1.666	28.238	1.00	39.02	A
	ATOM	2020	CG	HIS	A	931	-7.356	-0.994	29.497	1.00	40.32	A
	ATOM	2021	CD2	HIS	A	931	-7.249	0.292	29.906	1.00	40.17	A
20	ATOM	2022	ND1	HIS	A	931	-7.976	-1.674	30.523	1.00	40.39	A
	ATOM	2023	CE1	HIS	A	931	-8.229	-0.836	31.513	1.00	40.76	A
	ATOM	2024	NE2	HIS	A	931	-7.798	0.363	31.164	1.00	41.79	A
	ATOM	2025	C	HIS	A	931	-5.439	-3.341	27.134	1.00	41.55	A
	ATOM	2026	O	HIS	A	931	-4.304	-3.045	26.762	1.00	41.94	A
25	ATOM	2027	N	LYS	A	932	-6.264	-4.087	26.409	1.00	45.37	A
	ATOM	2028	CA	LYS	A	932	-5.871	-4.607	25.107	1.00	49.31	A
	ATOM	2029	CB	LYS	A	932	-6.553	-5.953	24.850	1.00	51.25	A
	ATOM	2030	CG	LYS	A	932	-8.041	-5.969	25.159	1.00	53.19	A
	ATOM	2031	CD	LYS	A	932	-8.607	-7.375	25.030	1.00	55.91	A
30	ATOM	2032	CE	LYS	A	932	-10.000	-7.477	25.642	1.00	57.08	A
	ATOM	2033	NZ	LYS	A	932	-10.971	-6.540	25.010	1.00	58.49	A
	ATOM	2034	C	LYS	A	932	-6.219	-3.625	23.997	1.00	50.69	A
	ATOM	2035	O	LYS	A	932	-6.726	-2.528	24.316	1.00	51.64	A
	ATOM	2036	OXT	LYS	A	932	-5.971	-3.965	22.820	1.00	53.42	A
35	ATOM	2037	CB	GLN	B	682	18.994	-21.280	-25.886	1.00	64.64	B
	ATOM	2038	CG	GLN	B	682	20.304	-21.103	-26.640	1.00	67.42	B
	ATOM	2039	CD	GLN	B	682	20.213	-21.557	-28.085	1.00	69.58	B
	ATOM	2040	OE1	GLN	B	682	19.707	-22.642	-28.379	1.00	70.69	B
	ATOM	2041	NE2	GLN	B	682	20.711	-20.728	-28.997	1.00	70.72	B
40	ATOM	2042	C	GLN	B	682	17.739	-20.948	-23.741	1.00	60.54	B
	ATOM	2043	O	GLN	B	682	16.624	-20.450	-23.891	1.00	61.01	B
	ATOM	2044	N	GLN	B	682	20.194	-20.628	-23.821	1.00	62.94	B
	ATOM	2045	CA	GLN	B	682	18.922	-20.478	-24.585	1.00	62.30	B
	ATOM	2046	N	LEU	B	683	17.986	-21.915	-22.863	1.00	57.86	B
45	ATOM	2047	CA	LEU	B	683	16.949	-22.424	-21.976	1.00	54.52	B
	ATOM	2048	CB	LEU	B	683	17.296	-23.831	-21.481	1.00	56.05	B
	ATOM	2049	CG	LEU	B	683	17.347	-24.973	-22.497	1.00	56.91	B
	ATOM	2050	CD1	LEU	B	683	17.763	-26.253	-21.789	1.00	57.17	B
	ATOM	2051	CD2	LEU	B	683	15.988	-25.149	-23.158	1.00	57.28	B
50	ATOM	2052	C	LEU	B	683	16.906	-21.464	-20.797	1.00	51.41	B
	ATOM	2053	O	LEU	B	683	15.849	-21.218	-20.214	1.00	51.78	B
	ATOM	2054	N	ILE	B	684	18.074	-20.923	-20.458	1.00	46.89	B
	ATOM	2055	CA	ILE	B	684	18.197	-19.974	-19.360	1.00	42.41	B
	ATOM	2056	CB	ILE	B	684	19.665	-19.802	-18.918	1.00	42.31	B
55	ATOM	2057	CG2	ILE	B	684	19.742	-18.819	-17.754	1.00	41.95	B
	ATOM	2058	CG1	ILE	B	684	20.259	-21.152	-18.516	1.00	43.99	B
	ATOM	2059	CD1	ILE	B	684	19.612	-21.778	-17.297	1.00	44.53	B

Table 2. (cont'd)

		#	Name	Res.	Chain	Res #	X	Y	Z	occ	B	SegID
5	ATOM	2060	C	ILE	B	684	17.685	-18.616	-19.825	1.00	38.54	B
	ATOM	2061	O	ILE	B	684	18.255	-18.010	-20.729	1.00	36.91	B
	ATOM	2062	N	PRO	B	685	16.598	-18.123	-19.213	1.00	35.60	B
	ATOM	2063	CD	PRO	B	685	15.838	-18.725	-18.103	1.00	35.69	B
	ATOM	2064	CA	PRO	B	685	16.032	-16.824	-19.587	1.00	33.16	B
10	ATOM	2065	CB	PRO	B	685	15.030	-16.555	-18.469	1.00	33.62	B
	ATOM	2066	CG	PRO	B	685	14.553	-17.922	-18.121	1.00	34.50	B
	ATOM	2067	C	PRO	B	685	17.134	-15.763	-19.652	1.00	30.56	B
	ATOM	2068	O	PRO	B	685	18.029	-15.738	-18.808	1.00	29.11	B
	ATOM	2069	N	PRO	B	686	17.081	-14.880	-20.658	1.00	28.12	B
15	ATOM	2070	CD	PRO	B	686	16.116	-14.858	-21.772	1.00	28.97	B
	ATOM	2071	CA	PRO	B	686	18.083	-13.823	-20.822	1.00	27.69	B
	ATOM	2072	CB	PRO	B	686	17.532	-13.010	-21.990	1.00	28.13	B
	ATOM	2073	CG	PRO	B	686	16.862	-14.063	-22.820	1.00	29.95	B
	ATOM	2074	C	PRO	B	686	18.321	-12.967	-19.575	1.00	25.10	B
20	ATOM	2075	O	PRO	B	686	19.464	-12.648	-19.247	1.00	25.19	B
	ATOM	2076	N	LEU	B	687	17.252	-12.601	-18.878	1.00	22.87	B
	ATOM	2077	CA	LEU	B	687	17.396	-11.771	-17.685	1.00	22.31	B
	ATOM	2078	CB	LEU	B	687	16.025	-11.372	-17.141	1.00	20.28	B
	ATOM	2079	CG	LEU	B	687	16.037	-10.547	-15.848	1.00	21.32	B
25	ATOM	2080	CD1	LEU	B	687	16.936	-9.323	-16.015	1.00	21.04	B
	ATOM	2081	CD2	LEU	B	687	14.616	-10.132	-15.501	1.00	22.03	B
	ATOM	2082	C	LEU	B	687	18.207	-12.467	-16.592	1.00	21.06	B
	ATOM	2083	O	LEU	B	687	19.025	-11.840	-15.921	1.00	23.05	B
	ATOM	2084	N	ILE	B	688	17.974	-13.760	-16.409	1.00	21.09	B
30	ATOM	2085	CA	ILE	B	688	18.702	-14.512	-15.399	1.00	20.07	B
	ATOM	2086	CB	ILE	B	688	18.120	-15.927	-15.252	1.00	21.05	B
	ATOM	2087	CG2	ILE	B	688	19.059	-16.808	-14.438	1.00	21.46	B
	ATOM	2088	CG1	ILE	B	688	16.741	-15.831	-14.594	1.00	20.53	B
	ATOM	2089	CD1	ILE	B	688	15.968	-17.135	-14.567	1.00	20.95	B
35	ATOM	2090	C	ILE	B	688	20.166	-14.572	-15.804	1.00	21.10	B
	ATOM	2091	O	ILE	B	688	21.056	-14.491	-14.960	1.00	18.80	B
	ATOM	2092	N	ASN	B	689	20.411	-14.696	-17.104	1.00	21.37	B
	ATOM	2093	CA	ASN	B	689	21.776	-14.743	-17.613	1.00	24.08	B
	ATOM	2094	CB	ASN	B	689	21.770	-14.963	-19.132	1.00	28.04	B
40	ATOM	2095	CG	ASN	B	689	23.165	-15.126	-19.700	1.00	34.12	B
	ATOM	2096	OD1	ASN	B	689	23.885	-16.064	-19.350	1.00	37.11	B
	ATOM	2097	ND2	ASN	B	689	23.560	-14.210	-20.582	1.00	37.70	B
	ATOM	2098	C	ASN	B	689	22.451	-13.415	-17.288	1.00	22.87	B
	ATOM	2099	O	ASN	B	689	23.612	-13.370	-16.873	1.00	23.07	B
45	ATOM	2100	N	LEU	B	690	21.712	-12.332	-17.482	1.00	22.51	B
	ATOM	2101	CA	LEU	B	690	22.232	-11.000	-17.200	1.00	21.77	B
	ATOM	2102	CB	LEU	B	690	21.199	-9.942	-17.587	1.00	21.00	B
	ATOM	2103	CG	LEU	B	690	21.628	-8.481	-17.421	1.00	24.94	B
	ATOM	2104	CD1	LEU	B	690	20.798	-7.601	-18.349	1.00	26.36	B
50	ATOM	2105	CD2	LEU	B	690	21.469	-8.047	-15.963	1.00	23.11	B
	ATOM	2106	C	LEU	B	690	22.570	-10.893	-15.715	1.00	20.64	B
	ATOM	2107	O	LEU	B	690	23.637	-10.395	-15.347	1.00	20.56	B
	ATOM	2108	N	LEU	B	691	21.666	-11.376	-14.866	1.00	20.00	B
	ATOM	2109	CA	LEU	B	691	21.882	-11.331	-13.421	1.00	18.30	B
55	ATOM	2110	CB	LEU	B	691	20.669	-11.906	-12.675	1.00	14.83	B
	ATOM	2111	CG	LEU	B	691	19.385	-11.068	-12.715	1.00	16.41	B
	ATOM	2112	CD1	LEU	B	691	18.292	-11.772	-11.925	1.00	14.23	B

Table 2. (cont'd)

		#	Name	Res.	Chain	Res	#	X	Y	Z	occ	B	SegID
	ATOM	2113	CD2	LEU	B	691		19.648	-9.672	-12.136	1.00	16.13	B
5	ATOM	2114	C	LEU	B	691		23.145	-12.097	-13.029	1.00	18.65	B
	ATOM	2115	O	LEU	B	691		23.826	-11.728	-12.079	1.00	17.99	B
	ATOM	2116	N	MET	B	692		23.450	-13.167	-13.757	1.00	19.64	B
	ATOM	2117	CA	MET	B	692		24.646	-13.956	-13.470	1.00	21.71	B
	ATOM	2118	CB	MET	B	692		24.676	-15.237	-14.319	1.00	23.95	B
10	ATOM	2119	CG	MET	B	692		23.620	-16.280	-13.983	1.00	28.81	B
	ATOM	2120	SD	MET	B	692		23.860	-17.830	-14.932	1.00	34.88	B
	ATOM	2121	CE	MET	B	692		22.791	-17.547	-16.333	1.00	34.64	B
	ATOM	2122	C	MET	B	692		25.887	-13.130	-13.793	1.00	20.55	B
	ATOM	2123	O	MET	B	692		26.827	-13.062	-13.003	1.00	19.66	B
15	ATOM	2124	N	SER	B	693		25.872	-12.490	-14.959	1.00	20.66	B
	ATOM	2125	CA	SER	B	693		27.003	-11.691	-15.417	1.00	22.33	B
	ATOM	2126	CB	SER	B	693		26.811	-11.303	-16.888	1.00	24.97	B
	ATOM	2127	OG	SER	B	693		25.751	-10.374	-17.040	1.00	29.96	B
	ATOM	2128	C	SER	B	693		27.298	-10.430	-14.609	1.00	21.68	B
20	ATOM	2129	O	SER	B	693		28.428	-9.938	-14.623	1.00	21.77	B
	ATOM	2130	N	ILE	B	694		26.305	-9.891	-13.912	1.00	20.69	B
	ATOM	2131	CA	ILE	B	694		26.559	-8.674	-13.141	1.00	20.69	B
	ATOM	2132	CB	ILE	B	694		25.397	-7.667	-13.264	1.00	19.13	B
	ATOM	2133	CG2	ILE	B	694		25.199	-7.291	-14.732	1.00	19.95	B
25	ATOM	2134	CG1	ILE	B	694		24.115	-8.262	-12.685	1.00	18.02	B
	ATOM	2135	CD1	ILE	B	694		22.973	-7.256	-12.567	1.00	16.95	B
	ATOM	2136	C	ILE	B	694		26.833	-8.939	-11.667	1.00	20.67	B
	ATOM	2137	O	ILE	B	694		27.035	-8.009	-10.888	1.00	20.17	B
	ATOM	2138	N	GLU	B	695		26.840	-10.212	-11.288	1.00	21.75	B
30	ATOM	2139	CA	GLU	B	695		27.104	-10.583	-9.908	1.00	24.75	B
	ATOM	2140	CB	GLU	B	695		27.027	-12.100	-9.745	1.00	24.51	B
	ATOM	2141	CG	GLU	B	695		27.077	-12.547	-8.310	1.00	28.80	B
	ATOM	2142	CD	GLU	B	695		25.739	-12.415	-7.615	1.00	28.02	B
	ATOM	2143	OE1	GLU	B	695		24.997	-11.445	-7.898	1.00	25.16	B
35	ATOM	2144	OE2	GLU	B	695		25.436	-13.288	-6.776	1.00	29.89	B
	ATOM	2145	C	GLU	B	695		28.502	-10.086	-9.541	1.00	26.27	B
	ATOM	2146	O	GLU	B	695		29.416	-10.100	-10.368	1.00	25.29	B
	ATOM	2147	N	PRO	B	696		28.681	-9.625	-8.296	1.00	29.47	B
	ATOM	2148	CD	PRO	B	696		27.624	-9.400	-7.293	1.00	31.49	B
40	ATOM	2149	CA	PRO	B	696		29.968	-9.116	-7.812	1.00	30.81	B
	ATOM	2150	CB	PRO	B	696		29.662	-8.727	-6.366	1.00	30.96	B
	ATOM	2151	CG	PRO	B	696		28.228	-8.311	-6.433	1.00	32.91	B
	ATOM	2152	C	PRO	B	696		31.122	-10.113	-7.891	1.00	30.70	B
	ATOM	2153	O	PRO	B	696		30.926	-11.327	-7.848	1.00	29.38	B
45	ATOM	2154	N	ASP	B	697		32.331	-9.578	-8.005	1.00	31.64	B
	ATOM	2155	CA	ASP	B	697		33.531	-10.396	-8.051	1.00	32.72	B
	ATOM	2156	CB	ASP	B	697		34.676	-9.592	-8.668	1.00	37.63	B
	ATOM	2157	CG	ASP	B	697		35.443	-10.374	-9.710	1.00	41.79	B
	ATOM	2158	OD1	ASP	B	697		34.805	-10.892	-10.655	1.00	43.16	B
50	ATOM	2159	OD2	ASP	B	697		36.684	-10.464	-9.585	1.00	44.61	B
	ATOM	2160	C	ASP	B	697		33.833	-10.722	-6.587	1.00	29.84	B
	ATOM	2161	O	ASP	B	697		33.262	-10.101	-5.693	1.00	28.09	B
	ATOM	2162	N	VAL	B	698		34.706	-11.694	-6.344	1.00	28.32	B
	ATOM	2163	CA	VAL	B	698		35.069	-12.083	-4.981	1.00	27.02	B
55	ATOM	2164	CB	VAL	B	698		36.205	-13.140	-4.974	1.00	28.37	B
	ATOM	2165	CG1	VAL	B	698		36.747	-13.323	-3.560	1.00	28.43	B

Table 2. (cont'd)

		#	Name	Res.	Chain	Res	#	X	Y	Z	occ	B	SegID
	ATOM	2166	CG2	VAL	B	698		35.682	-14.470	-5.502	1.00	28.67	B
5	ATOM	2167	C	VAL	B	698		35.532	-10.881	-4.168	1.00	25.36	B
	ATOM	2168	O	VAL	B	698		36.328	-10.076	-4.639	1.00	25.06	B
	ATOM	2169	N	ILE	B	699		35.030	-10.767	-2.944	1.00	24.97	B
	ATOM	2170	CA	ILE	B	699		35.397	-9.658	-2.071	1.00	22.14	B
	ATOM	2171	CB	ILE	B	699		34.156	-8.823	-1.679	1.00	20.66	B
10	ATOM	2172	CG2	ILE	B	699		34.545	-7.726	-0.690	1.00	20.23	B
	ATOM	2173	CG1	ILE	B	699		33.545	-8.188	-2.931	1.00	21.51	B
	ATOM	2174	CD1	ILE	B	699		32.271	-7.432	-2.666	1.00	19.96	B
	ATOM	2175	C	ILE	B	699		36.089	-10.142	-0.800	1.00	21.77	B
	ATOM	2176	O	ILE	B	699		35.546	-10.957	-0.044	1.00	16.92	B
15	ATOM	2177	N	TYR	B	700		37.296	-9.636	-0.579	1.00	20.63	B
	ATOM	2178	CA	TYR	B	700		38.069	-9.988	0.602	1.00	23.86	B
	ATOM	2179	CB	TYR	B	700		39.566	-10.003	0.285	1.00	26.68	B
	ATOM	2180	CG	TYR	B	700		39.969	-11.095	-0.676	1.00	32.41	B
	ATOM	2181	CD1	TYR	B	700		39.640	-11.018	-2.027	1.00	34.57	B
20	ATOM	2182	CE1	TYR	B	700		39.979	-12.036	-2.909	1.00	38.16	B
	ATOM	2183	CD2	TYR	B	700		40.651	-12.224	-0.228	1.00	33.94	B
	ATOM	2184	CE2	TYR	B	700		40.993	-13.251	-1.104	1.00	37.69	B
	ATOM	2185	CZ	TYR	B	700		40.652	-13.149	-2.442	1.00	38.33	B
	ATOM	2186	OH	TYR	B	700		40.974	-14.165	-3.315	1.00	43.13	B
25	ATOM	2187	C	TYR	B	700		37.798	-8.979	1.706	1.00	23.63	B
	ATOM	2188	O	TYR	B	700		37.501	-7.816	1.439	1.00	24.64	B
	ATOM	2189	N	ALA	B	701		37.892	-9.427	2.949	1.00	23.12	B
	ATOM	2190	CA	ALA	B	701		37.664	-8.541	4.080	1.00	23.90	B
	ATOM	2191	CB	ALA	B	701		37.177	-9.345	5.276	1.00	21.97	B
30	ATOM	2192	C	ALA	B	701		38.947	-7.795	4.439	1.00	25.27	B
	ATOM	2193	O	ALA	B	701		38.907	-6.764	5.117	1.00	23.66	B
	ATOM	2194	N	GLY	B	702		40.078	-8.316	3.971	1.00	26.40	B
	ATOM	2195	CA	GLY	B	702		41.361	-7.706	4.282	1.00	30.27	B
	ATOM	2196	C	GLY	B	702		41.693	-7.977	5.740	1.00	33.57	B
35	ATOM	2197	O	GLY	B	702		42.346	-7.170	6.410	1.00	32.31	B
	ATOM	2198	N	HIS	B	703		41.238	-9.130	6.229	1.00	35.31	B
	ATOM	2199	CA	HIS	B	703		41.441	-9.529	7.616	1.00	39.69	B
	ATOM	2200	CB	HIS	B	703		40.355	-10.529	8.021	1.00	39.47	B
	ATOM	2201	CG	HIS	B	703		40.516	-11.070	9.406	1.00	40.61	B
40	ATOM	2202	CD2	HIS	B	703		39.934	-10.715	10.575	1.00	41.64	B
	ATOM	2203	ND1	HIS	B	703		41.390	-12.092	9.707	1.00	42.57	B
	ATOM	2204	CE1	HIS	B	703		41.338	-12.345	11.003	1.00	42.52	B
	ATOM	2205	NE2	HIS	B	703		40.462	-11.523	11.553	1.00	42.74	B
	ATOM	2206	C	HIS	B	703		42.824	-10.107	7.909	1.00	43.10	B
45	ATOM	2207	O	HIS	B	703		43.437	-10.747	7.058	1.00	42.57	B
	ATOM	2208	N	ASP	B	704		43.301	-9.876	9.130	1.00	48.46	B
	ATOM	2209	CA	ASP	B	704		44.613	-10.353	9.561	1.00	53.34	B
	ATOM	2210	CB	ASP	B	704		45.215	-9.389	10.588	1.00	55.90	B
	ATOM	2211	CG	ASP	B	704		45.145	-7.941	10.147	1.00	59.16	B
50	ATOM	2212	OD1	ASP	B	704		44.020	-7.417	9.988	1.00	60.18	B
	ATOM	2213	OD2	ASP	B	704		46.219	-7.326	9.963	1.00	61.84	B
	ATOM	2214	C	ASP	B	704		44.552	-11.745	10.187	1.00	55.32	B
	ATOM	2215	O	ASP	B	704		44.445	-11.872	11.407	1.00	55.54	B
	ATOM	2216	N	ASN	B	705		44.619	-12.785	9.362	1.00	57.68	B
55	ATOM	2217	CA	ASN	B	705		44.593	-14.148	9.881	1.00	60.68	B
	ATOM	2218	CB	ASN	B	705		44.482	-15.162	8.738	1.00	60.99	B

Table 2. (cont'd)

		#	Name	Res.	Chain	Res	#	X	Y	Z	occ	B	SegID
	ATOM	2219	CG	ASN	B	705		43.096	-15.201	8.126	1.00	61.69	B
5	ATOM	2220	OD1	ASN	B	705		42.623	-14.215	7.561	1.00	61.90	B
	ATOM	2221	ND2	ASN	B	705		42.434	-16.345	8.241	1.00	62.70	B
	ATOM	2222	C	ASN	B	705		45.878	-14.391	10.665	1.00	62.22	B
	ATOM	2223	O	ASN	B	705		45.965	-15.311	11.478	1.00	62.97	B
	ATOM	2224	N	THR	B	706		46.870	-13.544	10.410	1.00	63.73	B
10	ATOM	2225	CA	THR	B	706		48.166	-13.629	11.069	1.00	64.99	B
	ATOM	2226	CB	THR	B	706		49.068	-12.445	10.655	1.00	64.95	B
	ATOM	2227	OG1	THR	B	706		50.196	-12.373	11.534	1.00	65.67	B
	ATOM	2228	CG2	THR	B	706		48.293	-11.132	10.710	1.00	65.66	B
	ATOM	2229	C	THR	B	706		48.064	-13.652	12.591	1.00	65.48	B
15	ATOM	2230	O	THR	B	706		48.428	-14.636	13.233	1.00	65.69	B
	ATOM	2231	N	LYS	B	707		47.559	-12.561	13.158	1.00	66.27	B
	ATOM	2232	CA	LYS	B	707		47.419	-12.424	14.604	1.00	66.72	B
	ATOM	2233	CB	LYS	B	707		47.443	-10.944	14.983	1.00	67.27	B
	ATOM	2234	CG	LYS	B	707		48.563	-10.151	14.333	1.00	68.66	B
20	ATOM	2235	CD	LYS	B	707		48.407	-8.666	14.617	1.00	69.39	B
	ATOM	2236	CE	LYS	B	707		49.468	-7.847	13.901	1.00	69.82	B
	ATOM	2237	NZ	LYS	B	707		49.310	-6.392	14.181	1.00	70.19	B
	ATOM	2238	C	LYS	B	707		46.127	-13.043	15.125	1.00	66.65	B
	ATOM	2239	O	LYS	B	707		45.153	-13.186	14.385	1.00	66.82	B
25	ATOM	2240	N	PRO	B	708		46.106	-13.422	16.414	1.00	66.47	B
	ATOM	2241	CD	PRO	B	708		47.218	-13.402	17.381	1.00	66.43	B
	ATOM	2242	CA	PRO	B	708		44.908	-14.019	17.011	1.00	65.90	B
	ATOM	2243	CB	PRO	B	708		45.291	-14.151	18.482	1.00	66.34	B
	ATOM	2244	CG	PRO	B	708		46.763	-14.410	18.413	1.00	66.16	B
30	ATOM	2245	C	PRO	B	708		43.727	-13.075	16.799	1.00	64.68	B
	ATOM	2246	O	PRO	B	708		43.917	-11.868	16.654	1.00	64.70	B
	ATOM	2247	N	ASP	B	709		42.514	-13.615	16.781	1.00	63.45	B
	ATOM	2248	CA	ASP	B	709		41.341	-12.781	16.563	1.00	62.09	B
	ATOM	2249	CB	ASP	B	709		40.410	-13.430	15.527	1.00	64.40	B
35	ATOM	2250	CG	ASP	B	709		39.736	-14.691	16.047	1.00	65.90	B
	ATOM	2251	OD1	ASP	B	709		40.448	-15.647	16.421	1.00	67.51	B
	ATOM	2252	OD2	ASP	B	709		38.487	-14.726	16.079	1.00	66.80	B
	ATOM	2253	C	ASP	B	709		40.565	-12.493	17.841	1.00	59.94	B
	ATOM	2254	O	ASP	B	709		40.223	-13.405	18.595	1.00	60.20	B
40	ATOM	2255	N	THR	B	710		40.300	-11.212	18.081	1.00	56.60	B
	ATOM	2256	CA	THR	B	710		39.538	-10.786	19.247	1.00	52.69	B
	ATOM	2257	CB	THR	B	710		40.152	-9.532	19.901	1.00	53.13	B
	ATOM	2258	OG1	THR	B	710		40.264	-8.488	18.925	1.00	52.57	B
	ATOM	2259	CG2	THR	B	710		41.527	-9.843	20.466	1.00	52.58	B
45	ATOM	2260	C	THR	B	710		38.125	-10.460	18.781	1.00	50.35	B
	ATOM	2261	O	THR	B	710		37.880	-10.302	17.586	1.00	48.41	B
	ATOM	2262	N	SER	B	711		37.196	-10.361	19.721	1.00	48.24	B
	ATOM	2263	CA	SER	B	711		35.816	-10.060	19.376	1.00	46.44	B
	ATOM	2264	CB	SER	B	711		34.943	-10.057	20.634	1.00	47.23	B
50	ATOM	2265	OG	SER	B	711		33.572	-9.910	20.303	1.00	49.85	B
	ATOM	2266	C	SER	B	711		35.709	-8.711	18.668	1.00	43.95	B
	ATOM	2267	O	SER	B	711		34.900	-8.544	17.757	1.00	43.72	B
	ATOM	2268	N	SER	B	712		36.531	-7.753	19.081	1.00	41.06	B
	ATOM	2269	CA	SER	B	712		36.502	-6.429	18.475	1.00	38.56	B
55	ATOM	2270	CB	SER	B	712		37.143	-5.402	19.417	1.00	39.63	B
	ATOM	2271	OG	SER	B	712		38.524	-5.659	19.593	1.00	42.74	B

Table 2. (cont'd)

		#	Name	Res.	Chain	Res #	X	Y	Z	occ	B	SegID
	ATOM	2272	C	SER	B	712	37.207	-6.400	17.117	1.00	35.92	B
5	ATOM	2273	O	SER	B	712	36.779	-5.695	16.201	1.00	33.99	B
	ATOM	2274	N	SER	B	713	38.285	-7.167	16.983	1.00	32.54	B
	ATOM	2275	CA	SER	B	713	39.025	-7.200	15.728	1.00	30.34	B
	ATOM	2276	CB	SER	B	713	40.357	-7.934	15.904	1.00	31.13	B
	ATOM	2277	OG	SER	B	713	40.161	-9.335	15.964	1.00	31.92	B
10	ATOM	2278	C	SER	B	713	38.186	-7.912	14.673	1.00	28.11	B
	ATOM	2279	O	SER	B	713	38.265	-7.607	13.487	1.00	24.98	B
	ATOM	2280	N	LEU	B	714	37.380	-8.864	15.125	1.00	26.38	B
	ATOM	2281	CA	LEU	B	714	36.517	-9.626	14.240	1.00	26.52	B
	ATOM	2282	CB	LEU	B	714	35.972	-10.848	14.986	1.00	29.55	B
15	ATOM	2283	CG	LEU	B	714	35.155	-11.892	14.226	1.00	31.86	B
	ATOM	2284	CD1	LEU	B	714	35.842	-12.254	12.917	1.00	34.03	B
	ATOM	2285	CD2	LEU	B	714	34.997	-13.129	15.106	1.00	32.83	B
	ATOM	2286	C	LEU	B	714	35.373	-8.746	13.745	1.00	25.49	B
	ATOM	2287	O	LEU	B	714	35.045	-8.749	12.557	1.00	22.75	B
20	ATOM	2288	N	LEU	B	715	34.770	-7.982	14.652	1.00	23.34	B
	ATOM	2289	CA	LEU	B	715	33.679	-7.101	14.266	1.00	22.41	B
	ATOM	2290	CB	LEU	B	715	33.040	-6.480	15.509	1.00	23.20	B
	ATOM	2291	CG	LEU	B	715	32.283	-7.511	16.358	1.00	25.47	B
	ATOM	2292	CD1	LEU	B	715	31.802	-6.887	17.658	1.00	25.60	B
25	ATOM	2293	CD2	LEU	B	715	31.110	-8.056	15.551	1.00	24.95	B
	ATOM	2294	C	LEU	B	715	34.203	-6.021	13.318	1.00	21.60	B
	ATOM	2295	O	LEU	B	715	33.537	-5.655	12.346	1.00	20.68	B
	ATOM	2296	N	THR	B	716	35.406	-5.527	13.595	1.00	19.50	B
	ATOM	2297	CA	THR	B	716	36.021	-4.513	12.750	1.00	18.98	B
30	ATOM	2298	CB	THR	B	716	37.385	-4.066	13.337	1.00	18.83	B
	ATOM	2299	OG1	THR	B	716	37.155	-3.304	14.531	1.00	20.73	B
	ATOM	2300	CG2	THR	B	716	38.156	-3.220	12.345	1.00	18.41	B
	ATOM	2301	C	THR	B	716	36.210	-5.059	11.330	1.00	20.03	B
	ATOM	2302	O	THR	B	716	35.944	-4.365	10.350	1.00	18.15	B
35	ATOM	2303	N	SER	B	717	36.657	-6.306	11.217	1.00	20.54	B
	ATOM	2304	CA	SER	B	717	36.857	-6.901	9.898	1.00	21.70	B
	ATOM	2305	CB	SER	B	717	37.588	-8.241	10.010	1.00	23.38	B
	ATOM	2306	OG	SER	B	717	38.960	-8.031	10.299	1.00	28.56	B
	ATOM	2307	C	SER	B	717	35.533	-7.090	9.168	1.00	20.61	B
40	ATOM	2308	O	SER	B	717	35.466	-6.914	7.952	1.00	20.71	B
	ATOM	2309	N	LEU	B	718	34.484	-7.449	9.905	1.00	18.62	B
	ATOM	2310	CA	LEU	B	718	33.164	-7.638	9.306	1.00	18.51	B
	ATOM	2311	CB	LEU	B	718	32.193	-8.240	10.321	1.00	18.50	B
	ATOM	2312	CG	LEU	B	718	32.302	-9.746	10.585	1.00	19.89	B
45	ATOM	2313	CD1	LEU	B	718	31.510	-10.098	11.833	1.00	20.48	B
	ATOM	2314	CD2	LEU	B	718	31.781	-10.517	9.369	1.00	18.28	B
	ATOM	2315	C	LEU	B	718	32.625	-6.294	8.826	1.00	18.13	B
	ATOM	2316	O	LEU	B	718	31.889	-6.220	7.837	1.00	16.53	B
	ATOM	2317	N	ASN	B	719	32.985	-5.229	9.534	1.00	18.23	B
50	ATOM	2318	CA	ASN	B	719	32.528	-3.902	9.144	1.00	17.99	B
	ATOM	2319	CB	ASN	B	719	32.704	-2.907	10.292	1.00	19.22	B
	ATOM	2320	CG	ASN	B	719	31.682	-3.107	11.390	1.00	20.19	B
	ATOM	2321	OD1	ASN	B	719	30.611	-3.667	11.156	1.00	20.66	B
	ATOM	2322	ND2	ASN	B	719	31.997	-2.632	12.593	1.00	19.69	B
55	ATOM	2323	C	ASN	B	719	33.294	-3.432	7.915	1.00	19.00	B
	ATOM	2324	O	ASN	B	719	32.745	-2.727	7.067	1.00	16.93	B

Table 2. (cont'd)

		#	Name	Res.	Chain	Res #	X	Y	Z	occ	B	SegID
	ATOM	2325	N	GLN	B	720	34.562	-3.834	7.820	1.00	17.58	B
5	ATOM	2326	CA	GLN	B	720	35.391	-3.463	6.679	1.00	18.94	B
	ATOM	2327	CB	GLN	B	720	36.851	-3.859	6.925	1.00	19.50	B
	ATOM	2328	CG	GLN	B	720	37.736	-3.733	5.695	1.00	22.84	B
	ATOM	2329	CD	GLN	B	720	37.784	-2.318	5.149	1.00	23.37	B
	ATOM	2330	OE1	GLN	B	720	37.894	-2.117	3.941	1.00	21.74	B
10	ATOM	2331	NE2	GLN	B	720	37.711	-1.332	6.038	1.00	22.07	B
	ATOM	2332	C	GLN	B	720	34.846	-4.200	5.463	1.00	19.76	B
	ATOM	2333	O	GLN	B	720	34.714	-3.636	4.372	1.00	15.95	B
	ATOM	2334	N	LEU	B	721	34.526	-5.474	5.665	1.00	18.87	B
	ATOM	2335	CA	LEU	B	721	33.973	-6.293	4.599	1.00	18.03	B
15	ATOM	2336	CB	LEU	B	721	33.763	-7.726	5.102	1.00	18.09	B
	ATOM	2337	CG	LEU	B	721	33.182	-8.735	4.113	1.00	19.65	B
	ATOM	2338	CD1	LEU	B	721	34.094	-8.844	2.893	1.00	16.27	B
	ATOM	2339	CD2	LEU	B	721	33.033	-10.090	4.810	1.00	18.08	B
	ATOM	2340	C	LEU	B	721	32.643	-5.660	4.204	1.00	17.35	B
20	ATOM	2341	O	LEU	B	721	32.301	-5.592	3.027	1.00	17.63	B
	ATOM	2342	N	GLY	B	722	31.901	-5.188	5.202	1.00	16.11	B
	ATOM	2343	CA	GLY	B	722	30.622	-4.547	4.942	1.00	17.12	B
	ATOM	2344	C	GLY	B	722	30.780	-3.281	4.109	1.00	19.60	B
	ATOM	2345	O	GLY	B	722	29.948	-2.985	3.239	1.00	17.68	B
25	ATOM	2346	N	GLU	B	723	31.847	-2.526	4.366	1.00	17.38	B
	ATOM	2347	CA	GLU	B	723	32.095	-1.296	3.612	1.00	17.59	B
	ATOM	2348	CB	GLU	B	723	33.322	-0.563	4.162	1.00	16.95	B
	ATOM	2349	CG	GLU	B	723	33.590	0.782	3.490	1.00	16.70	B
	ATOM	2350	CD	GLU	B	723	32.710	1.898	4.032	1.00	18.40	B
30	ATOM	2351	OE1	GLU	B	723	31.667	1.582	4.637	1.00	18.46	B
	ATOM	2352	OE2	GLU	B	723	33.057	3.092	3.847	1.00	15.57	B
	ATOM	2353	C	GLU	B	723	32.340	-1.629	2.143	1.00	17.94	B
	ATOM	2354	O	GLU	B	723	31.844	-0.946	1.241	1.00	18.69	B
	ATOM	2355	N	ARG	B	724	33.122	-2.679	1.910	1.00	18.32	B
35	ATOM	2356	CA	ARG	B	724	33.451	-3.099	0.555	1.00	18.63	B
	ATOM	2357	CB	ARG	B	724	34.591	-4.125	0.586	1.00	18.71	B
	ATOM	2358	CG	ARG	B	724	35.845	-3.613	1.289	1.00	19.29	B
	ATOM	2359	CD	ARG	B	724	36.992	-4.604	1.193	1.00	20.38	B
	ATOM	2360	NE	ARG	B	724	38.173	-4.123	1.903	1.00	22.22	B
40	ATOM	2361	CZ	ARG	B	724	39.355	-4.728	1.892	1.00	23.91	B
	ATOM	2362	NH1	ARG	B	724	39.526	-5.849	1.205	1.00	22.36	B
	ATOM	2363	NH2	ARG	B	724	40.372	-4.205	2.568	1.00	26.01	B
	ATOM	2364	C	ARG	B	724	32.230	-3.683	-0.148	1.00	18.31	B
	ATOM	2365	O	ARG	B	724	32.021	-3.465	-1.339	1.00	16.69	B
45	ATOM	2366	N	GLN	B	725	31.414	-4.422	0.590	1.00	17.60	B
	ATOM	2367	CA	GLN	B	725	30.227	-5.000	-0.011	1.00	18.87	B
	ATOM	2368	CB	GLN	B	725	29.637	-6.073	0.908	1.00	17.78	B
	ATOM	2369	CG	GLN	B	725	30.538	-7.305	1.030	1.00	23.54	B
	ATOM	2370	CD	GLN	B	725	29.853	-8.468	1.714	1.00	25.93	B
50	ATOM	2371	OE1	GLN	B	725	30.443	-9.532	1.901	1.00	29.72	B
	ATOM	2372	NE2	GLN	B	725	28.599	-8.274	2.088	1.00	28.88	B
	ATOM	2373	C	GLN	B	725	29.195	-3.920	-0.332	1.00	18.08	B
	ATOM	2374	O	GLN	B	725	28.440	-4.036	-1.298	1.00	18.14	B
	ATOM	2375	N	LEU	B	726	29.172	-2.855	0.459	1.00	18.05	B
55	ATOM	2376	CA	LEU	B	726	28.227	-1.777	0.203	1.00	18.04	B
	ATOM	2377	CB	LEU	B	726	28.323	-0.727	1.314	1.00	20.54	B

Table 2. (cont'd)

		#	Name	Res.	Chain	Res #	X	Y	Z	occ	B	SegID
5	ATOM	2378	CG	LEU	B	726	27.263	0.376	1.383	1.00	20.94	B
	ATOM	2379	CD1	LEU	B	726	25.859	-0.216	1.325	1.00	19.79	B
	ATOM	2380	CD2	LEU	B	726	27.472	1.171	2.681	1.00	21.03	B
	ATOM	2381	C	LEU	B	726	28.551	-1.172	-1.167	1.00	18.14	B
	ATOM	2382	O	LEU	B	726	27.658	-0.933	-1.986	1.00	17.87	B
10	ATOM	2383	N	LEU	B	727	29.836	-0.950	-1.426	1.00	16.39	B
	ATOM	2384	CA	LEU	B	727	30.259	-0.401	-2.706	1.00	18.19	B
	ATOM	2385	CB	LEU	B	727	31.775	-0.179	-2.715	1.00	19.81	B
	ATOM	2386	CG	LEU	B	727	32.387	0.233	-4.060	1.00	22.06	B
	ATOM	2387	CD1	LEU	B	727	31.828	1.578	-4.498	1.00	24.00	B
15	ATOM	2388	CD2	LEU	B	727	33.905	0.309	-3.932	1.00	24.38	B
	ATOM	2389	C	LEU	B	727	29.868	-1.334	-3.860	1.00	18.39	B
	ATOM	2390	O	LEU	B	727	29.457	-0.872	-4.929	1.00	18.62	B
	ATOM	2391	N	SER	B	728	29.986	-2.644	-3.646	1.00	17.14	B
	ATOM	2392	CA	SER	B	728	29.643	-3.598	-4.696	1.00	19.54	B
20	ATOM	2393	CB	SER	B	728	30.125	-5.013	-4.343	1.00	20.37	B
	ATOM	2394	OG	SER	B	728	29.369	-5.558	-3.280	1.00	27.70	B
	ATOM	2395	C	SER	B	728	28.138	-3.610	-4.943	1.00	17.78	B
	ATOM	2396	O	SER	B	728	27.698	-3.747	-6.079	1.00	18.32	B
	ATOM	2397	N	VAL	B	729	27.352	-3.476	-3.880	1.00	17.66	B
25	ATOM	2398	CA	VAL	B	729	25.895	-3.446	-4.020	1.00	18.18	B
	ATOM	2399	CB	VAL	B	729	25.201	-3.329	-2.642	1.00	19.59	B
	ATOM	2400	CG1	VAL	B	729	23.712	-3.029	-2.816	1.00	19.79	B
	ATOM	2401	CG2	VAL	B	729	25.381	-4.630	-1.869	1.00	22.69	B
	ATOM	2402	C	VAL	B	729	25.467	-2.261	-4.888	1.00	18.00	B
30	ATOM	2403	O	VAL	B	729	24.630	-2.402	-5.781	1.00	18.81	B
	ATOM	2404	N	VAL	B	730	26.040	-1.092	-4.624	1.00	16.70	B
	ATOM	2405	CA	VAL	B	730	25.694	0.092	-5.401	1.00	18.31	B
	ATOM	2406	CB	VAL	B	730	26.364	1.364	-4.822	1.00	17.54	B
	ATOM	2407	CG1	VAL	B	730	25.962	2.587	-5.646	1.00	20.82	B
35	ATOM	2408	CG2	VAL	B	730	25.940	1.561	-3.363	1.00	20.52	B
	ATOM	2409	C	VAL	B	730	26.102	-0.086	-6.865	1.00	17.87	B
	ATOM	2410	O	VAL	B	730	25.331	0.230	-7.770	1.00	21.04	B
	ATOM	2411	N	LYS	B	731	27.303	-0.598	-7.108	1.00	17.34	B
	ATOM	2412	CA	LYS	B	731	27.739	-0.803	-8.485	1.00	18.71	B
40	ATOM	2413	CB	LYS	B	731	29.190	-1.289	-8.527	1.00	22.00	B
	ATOM	2414	CG	LYS	B	731	30.213	-0.192	-8.223	1.00	23.19	B
	ATOM	2415	CD	LYS	B	731	31.632	-0.719	-8.378	1.00	28.30	B
	ATOM	2416	CE	LYS	B	731	32.657	0.390	-8.185	1.00	30.48	B
	ATOM	2417	NZ	LYS	B	731	34.053	-0.126	-8.247	1.00	34.47	B
45	ATOM	2418	C	LYS	B	731	26.825	-1.808	-9.183	1.00	19.77	B
	ATOM	2419	O	LYS	B	731	26.421	-1.605	-10.331	1.00	17.95	B
	ATOM	2420	N	TRP	B	732	26.509	-2.887	-8.473	1.00	17.50	B
	ATOM	2421	CA	TRP	B	732	25.630	-3.937	-8.975	1.00	17.41	B
	ATOM	2422	CB	TRP	B	732	25.438	-4.996	-7.883	1.00	16.91	B
50	ATOM	2423	CG	TRP	B	732	24.321	-5.985	-8.112	1.00	15.88	B
	ATOM	2424	CD2	TRP	B	732	23.100	-6.073	-7.371	1.00	15.43	B
	ATOM	2425	CE2	TRP	B	732	22.388	-7.191	-7.863	1.00	16.91	B
	ATOM	2426	CE3	TRP	B	732	22.539	-5.317	-6.331	1.00	14.91	B
	ATOM	2427	CD1	TRP	B	732	24.299	-7.019	-9.011	1.00	16.77	B
55	ATOM	2428	NE1	TRP	B	732	23.140	-7.751	-8.863	1.00	16.21	B
	ATOM	2429	CZ2	TRP	B	732	21.140	-7.571	-7.350	1.00	16.15	B
	ATOM	2430	CZ3	TRP	B	732	21.299	-5.694	-5.818	1.00	14.22	B

Table 2. (cont'd)

		#	Name	Res.	Chain	Res #	X	Y	Z	occ	B	SegID
5	ATOM	2431	CH2	TRP	B	732	20.614	-6.813	-6.330	1.00	16.68	B
	ATOM	2432	C	TRP	B	732	24.279	-3.350	-9.378	1.00	16.02	B
	ATOM	2433	O	TRP	B	732	23.783	-3.617	-10.472	1.00	16.45	B
	ATOM	2434	N	SER	B	733	23.699	-2.541	-8.495	1.00	16.26	B
	ATOM	2435	CA	SER	B	733	22.390	-1.939	-8.749	1.00	17.13	B
10	ATOM	2436	CB	SER	B	733	21.945	-1.105	-7.543	1.00	15.29	B
	ATOM	2437	OG	SER	B	733	22.713	0.081	-7.434	1.00	16.35	B
	ATOM	2438	C	SER	B	733	22.365	-1.068	-10.009	1.00	18.91	B
	ATOM	2439	O	SER	B	733	21.318	-0.901	-10.633	1.00	18.17	B
	ATOM	2440	N	LYS	B	734	23.519	-0.524	-10.383	1.00	18.91	B
15	ATOM	2441	CA	LYS	B	734	23.612	0.329	-11.564	1.00	21.91	B
	ATOM	2442	CB	LYS	B	734	24.952	1.073	-11.576	1.00	26.10	B
	ATOM	2443	CG	LYS	B	734	25.042	2.153	-10.518	1.00	30.52	B
	ATOM	2444	CD	LYS	B	734	26.320	2.954	-10.644	1.00	35.02	B
	ATOM	2445	CE	LYS	B	734	26.159	4.306	-9.974	1.00	37.63	B
20	ATOM	2446	NZ	LYS	B	734	25.095	5.122	-10.632	1.00	39.56	B
	ATOM	2447	C	LYS	B	734	23.444	-0.447	-12.863	1.00	21.73	B
	ATOM	2448	O	LYS	B	734	23.125	0.133	-13.905	1.00	19.82	B
	ATOM	2449	N	SER	B	735	23.659	-1.758	-12.798	1.00	19.96	B
	ATOM	2450	CA	SER	B	735	23.517	-2.616	-13.969	1.00	19.76	B
25	ATOM	2451	CB	SER	B	735	24.748	-3.519	-14.126	1.00	19.35	B
	ATOM	2452	OG	SER	B	735	25.918	-2.756	-14.356	1.00	23.17	B
	ATOM	2453	C	SER	B	735	22.267	-3.488	-13.878	1.00	18.19	B
	ATOM	2454	O	SER	B	735	21.932	-4.189	-14.833	1.00	17.56	B
	ATOM	2455	N	LEU	B	736	21.589	-3.446	-12.731	1.00	17.46	B
30	ATOM	2456	CA	LEU	B	736	20.375	-4.239	-12.503	1.00	16.58	B
	ATOM	2457	CB	LEU	B	736	19.991	-4.193	-11.017	1.00	16.96	B
	ATOM	2458	CG	LEU	B	736	18.736	-4.939	-10.547	1.00	19.34	B
	ATOM	2459	CD1	LEU	B	736	18.886	-6.439	-10.793	1.00	18.13	B
	ATOM	2460	CD2	LEU	B	736	18.525	-4.679	-9.058	1.00	18.75	B
35	ATOM	2461	C	LEU	B	736	19.230	-3.680	-13.344	1.00	17.27	B
	ATOM	2462	O	LEU	B	736	18.776	-2.562	-13.111	1.00	16.74	B
	ATOM	2463	N	PRO	B	737	18.738	-4.458	-14.322	1.00	18.08	B
	ATOM	2464	CD	PRO	B	737	19.117	-5.847	-14.643	1.00	17.66	B
	ATOM	2465	CA	PRO	B	737	17.643	-4.005	-15.188	1.00	18.21	B
40	ATOM	2466	CB	PRO	B	737	17.247	-5.275	-15.943	1.00	18.86	B
	ATOM	2467	CG	PRO	B	737	18.556	-6.022	-16.035	1.00	17.53	B
	ATOM	2468	C	PRO	B	737	16.470	-3.390	-14.438	1.00	18.80	B
	ATOM	2469	O	PRO	B	737	15.890	-4.013	-13.544	1.00	19.03	B
	ATOM	2470	N	GLY	B	738	16.145	-2.152	-14.800	1.00	18.43	B
45	ATOM	2471	CA	GLY	B	738	15.031	-1.455	-14.187	1.00	17.85	B
	ATOM	2472	C	GLY	B	738	15.338	-0.574	-12.991	1.00	16.86	B
	ATOM	2473	O	GLY	B	738	14.678	0.444	-12.791	1.00	15.62	B
	ATOM	2474	N	PHE	B	739	16.350	-0.932	-12.205	1.00	15.96	B
	ATOM	2475	CA	PHE	B	739	16.662	-0.163	-11.010	1.00	14.50	B
50	ATOM	2476	CB	PHE	B	739	17.791	-0.829	-10.216	1.00	14.29	B
	ATOM	2477	CG	PHE	B	739	17.917	-0.307	-8.818	1.00	14.77	B
	ATOM	2478	CD1	PHE	B	739	17.021	-0.712	-7.832	1.00	17.58	B
	ATOM	2479	CD2	PHE	B	739	18.916	0.601	-8.483	1.00	16.38	B
	ATOM	2480	CE1	PHE	B	739	17.116	-0.217	-6.528	1.00	19.63	B
55	ATOM	2481	CE2	PHE	B	739	19.022	1.102	-7.187	1.00	18.02	B
	ATOM	2482	CZ	PHE	B	739	18.120	0.689	-6.205	1.00	15.95	B
	ATOM	2483	C	PHE	B	739	17.031	1.296	-11.247	1.00	15.95	B

Table 2. (cont'd)

		#	Name	Res.	Chain	Res #	X	Y	Z	occ	B	SegID
5	ATOM	2484	O	PHE	B	739	16.554	2.180	-10.532	1.00	15.43	B
	ATOM	2485	N	ARG	B	740	17.893	1.542	-12.233	1.00	14.92	B
	ATOM	2486	CA	ARG	B	740	18.336	2.898	-12.546	1.00	18.27	B
	ATOM	2487	CB	ARG	B	740	19.414	2.868	-13.631	1.00	20.12	B
	ATOM	2488	CG	ARG	B	740	18.933	2.276	-14.956	1.00	20.07	B
10	ATOM	2489	CD	ARG	B	740	19.951	2.489	-16.074	1.00	20.49	B
	ATOM	2490	NE	ARG	B	740	19.432	2.001	-17.347	1.00	21.32	B
	ATOM	2491	CZ	ARG	B	740	20.021	2.190	-18.524	1.00	22.16	B
	ATOM	2492	NH1	ARG	B	740	21.164	2.862	-18.601	1.00	20.37	B
	ATOM	2493	NH2	ARG	B	740	19.460	1.704	-19.625	1.00	20.63	B
15	ATOM	2494	C	ARG	B	740	17.185	3.783	-13.013	1.00	18.64	B
	ATOM	2495	O	ARG	B	740	17.324	5.001	-13.090	1.00	18.88	B
	ATOM	2496	N	ASN	B	741	16.048	3.167	-13.315	1.00	18.88	B
	ATOM	2497	CA	ASN	B	741	14.883	3.904	-13.786	1.00	19.14	B
	ATOM	2498	CB	ASN	B	741	14.088	3.015	-14.742	1.00	22.68	B
20	ATOM	2499	CG	ASN	B	741	14.904	2.633	-15.964	1.00	23.46	B
	ATOM	2500	OD1	ASN	B	741	14.743	1.551	-16.533	1.00	25.91	B
	ATOM	2501	ND2	ASN	B	741	15.798	3.530	-16.371	1.00	22.56	B
	ATOM	2502	C	ASN	B	741	14.001	4.448	-12.666	1.00	18.84	B
	ATOM	2503	O	ASN	B	741	13.090	5.241	-12.906	1.00	18.36	B
25	ATOM	2504	N	LEU	B	742	14.282	4.034	-11.436	1.00	16.78	B
	ATOM	2505	CA	LEU	B	742	13.529	4.532	-10.293	1.00	17.18	B
	ATOM	2506	CB	LEU	B	742	13.660	3.583	-9.090	1.00	17.93	B
	ATOM	2507	CG	LEU	B	742	13.275	2.111	-9.273	1.00	19.23	B
	ATOM	2508	CD1	LEU	B	742	13.651	1.333	-8.019	1.00	20.55	B
30	ATOM	2509	CD2	LEU	B	742	11.782	1.993	-9.554	1.00	21.11	B
	ATOM	2510	C	LEU	B	742	14.125	5.886	-9.919	1.00	17.11	B
	ATOM	2511	O	LEU	B	742	15.287	6.171	-10.219	1.00	16.40	B
	ATOM	2512	N	HIS	B	743	13.323	6.720	-9.273	1.00	17.11	B
	ATOM	2513	CA	HIS	B	743	13.779	8.030	-8.826	1.00	20.34	B
35	ATOM	2514	CB	HIS	B	743	12.670	8.667	-7.981	1.00	22.04	B
	ATOM	2515	CG	HIS	B	743	12.930	10.087	-7.590	1.00	26.50	B
	ATOM	2516	CD2	HIS	B	743	12.372	11.244	-8.018	1.00	28.30	B
	ATOM	2517	ND1	HIS	B	743	13.842	10.439	-6.617	1.00	27.58	B
	ATOM	2518	CE1	HIS	B	743	13.832	11.751	-6.461	1.00	28.99	B
40	ATOM	2519	NE2	HIS	B	743	12.948	12.263	-7.299	1.00	27.82	B
	ATOM	2520	C	HIS	B	743	15.046	7.777	-7.990	1.00	20.44	B
	ATOM	2521	O	HIS	B	743	15.121	6.782	-7.264	1.00	18.79	B
	ATOM	2522	N	ILE	B	744	16.041	8.652	-8.109	1.00	20.57	B
	ATOM	2523	CA	ILE	B	744	17.289	8.483	-7.365	1.00	19.99	B
45	ATOM	2524	CB	ILE	B	744	18.279	9.638	-7.666	1.00	21.19	B
	ATOM	2525	CG2	ILE	B	744	19.513	9.538	-6.760	1.00	19.18	B
	ATOM	2526	CG1	ILE	B	744	18.701	9.569	-9.138	1.00	20.37	B
	ATOM	2527	CD1	ILE	B	744	19.690	10.646	-9.566	1.00	25.65	B
	ATOM	2528	C	ILE	B	744	17.086	8.352	-5.857	1.00	20.50	B
50	ATOM	2529	O	ILE	B	744	17.802	7.595	-5.196	1.00	20.10	B
	ATOM	2530	N	ASP	B	745	16.114	9.073	-5.304	1.00	19.58	B
	ATOM	2531	CA	ASP	B	745	15.857	8.974	-3.868	1.00	21.19	B
	ATOM	2532	CB	ASP	B	745	14.768	9.952	-3.416	1.00	24.33	B
	ATOM	2533	CG	ASP	B	745	15.233	11.387	-3.413	1.00	27.99	B
55	ATOM	2534	OD1	ASP	B	745	16.458	11.622	-3.380	1.00	30.68	B
	ATOM	2535	OD2	ASP	B	745	14.364	12.280	-3.426	1.00	30.97	B
	ATOM	2536	C	ASP	B	745	15.400	7.566	-3.517	1.00	19.87	B

Table 2. (cont'd)

		#	Name	Res.	Chain	Res #	X	Y	Z	occ	B	SegID
5	ATOM	2537	O	ASP	B	745	15.752	7.044	-2.462	1.00	20.15	B
	ATOM	2538	N	ASP	B	746	14.591	6.971	-4.389	1.00	19.04	B
	ATOM	2539	CA	ASP	B	746	14.097	5.618	-4.152	1.00	18.78	B
	ATOM	2540	CB	ASP	B	746	13.055	5.201	-5.197	1.00	18.11	B
	ATOM	2541	CG	ASP	B	746	11.817	6.078	-5.191	1.00	21.37	B
10	ATOM	2542	OD1	ASP	B	746	11.580	6.816	-4.207	1.00	19.54	B
	ATOM	2543	OD2	ASP	B	746	11.065	6.004	-6.188	1.00	22.68	B
	ATOM	2544	C	ASP	B	746	15.261	4.631	-4.213	1.00	17.19	B
	ATOM	2545	O	ASP	B	746	15.319	3.689	-3.423	1.00	18.41	B
	ATOM	2546	N	GLN	B	747	16.176	4.836	-5.157	1.00	16.73	B
15	ATOM	2547	CA	GLN	B	747	17.320	3.936	-5.282	1.00	16.32	B
	ATOM	2548	CB	GLN	B	747	18.227	4.357	-6.439	1.00	16.06	B
	ATOM	2549	CG	GLN	B	747	17.570	4.282	-7.815	1.00	14.64	B
	ATOM	2550	CD	GLN	B	747	18.478	4.787	-8.916	1.00	16.67	B
	ATOM	2551	OE1	GLN	B	747	18.021	5.411	-9.874	1.00	18.54	B
20	ATOM	2552	NE2	GLN	B	747	19.775	4.518	-8.789	1.00	12.03	B
	ATOM	2553	C	GLN	B	747	18.116	3.929	-3.984	1.00	15.90	B
	ATOM	2554	O	GLN	B	747	18.426	2.870	-3.445	1.00	15.22	B
	ATOM	2555	N	ILE	B	748	18.441	5.119	-3.486	1.00	15.67	B
	ATOM	2556	CA	ILE	B	748	19.199	5.247	-2.250	1.00	14.76	B
25	ATOM	2557	CB	ILE	B	748	19.447	6.726	-1.901	1.00	17.21	B
	ATOM	2558	CG2	ILE	B	748	20.131	6.831	-0.544	1.00	18.09	B
	ATOM	2559	CG1	ILE	B	748	20.314	7.376	-2.981	1.00	16.97	B
	ATOM	2560	CD1	ILE	B	748	20.562	8.874	-2.767	1.00	19.77	B
	ATOM	2561	C	ILE	B	748	18.459	4.588	-1.094	1.00	15.63	B
30	ATOM	2562	O	ILE	B	748	19.046	3.826	-0.320	1.00	15.86	B
	ATOM	2563	N	THR	B	749	17.166	4.884	-0.984	1.00	14.70	B
	ATOM	2564	CA	THR	B	749	16.336	4.323	0.072	1.00	14.94	B
	ATOM	2565	CB	THR	B	749	14.891	4.858	-0.037	1.00	16.72	B
	ATOM	2566	OG1	THR	B	749	14.894	6.268	0.218	1.00	18.70	B
35	ATOM	2567	CG2	THR	B	749	13.974	4.173	0.969	1.00	17.71	B
	ATOM	2568	C	THR	B	749	16.320	2.793	0.055	1.00	14.91	B
	ATOM	2569	O	THR	B	749	16.499	2.151	1.096	1.00	15.12	B
	ATOM	2570	N	LEU	B	750	16.117	2.204	-1.122	1.00	13.93	B
	ATOM	2571	CA	LEU	B	750	16.073	0.745	-1.232	1.00	14.49	B
40	ATOM	2572	CB	LEU	B	750	15.667	0.327	-2.654	1.00	14.19	B
	ATOM	2573	CG	LEU	B	750	14.214	0.702	-2.987	1.00	16.47	B
	ATOM	2574	CD1	LEU	B	750	13.922	0.449	-4.476	1.00	16.09	B
	ATOM	2575	CD2	LEU	B	750	13.272	-0.115	-2.101	1.00	14.27	B
	ATOM	2576	C	LEU	B	750	17.407	0.108	-0.853	1.00	14.83	B
45	ATOM	2577	O	LEU	B	750	17.437	-0.924	-0.177	1.00	15.56	B
	ATOM	2578	N	ILE	B	751	18.508	0.719	-1.277	1.00	14.16	B
	ATOM	2579	CA	ILE	B	751	19.824	0.179	-0.942	1.00	16.07	B
	ATOM	2580	CB	ILE	B	751	20.952	0.904	-1.719	1.00	15.86	B
	ATOM	2581	CG2	ILE	B	751	22.326	0.534	-1.138	1.00	15.95	B
50	ATOM	2582	CG1	ILE	B	751	20.874	0.525	-3.202	1.00	15.28	B
	ATOM	2583	CD1	ILE	B	751	21.803	1.311	-4.093	1.00	20.05	B
	ATOM	2584	C	ILE	B	751	20.077	0.298	0.561	1.00	16.75	B
	ATOM	2585	O	ILE	B	751	20.543	-0.650	1.196	1.00	16.19	B
	ATOM	2586	N	GLN	B	752	19.763	1.454	1.136	1.00	17.86	B
55	ATOM	2587	CA	GLN	B	752	19.976	1.646	2.567	1.00	18.49	B
	ATOM	2588	CB	GLN	B	752	19.788	3.120	2.950	1.00	17.93	B
	ATOM	2589	CG	GLN	B	752	20.754	4.049	2.212	1.00	19.72	B

Table 2. (cont'd)

		#	Name	Res.	Chain	Res #	X	Y	Z	occ	B	SegID
5	ATOM	2590	CD	GLN	B	752	20.823	5.449	2.800	1.00	21.05	B
	ATOM	2591	OE1	GLN	B	752	19.825	5.986	3.282	1.00	22.57	B
	ATOM	2592	NE2	GLN	B	752	22.006	6.056	2.742	1.00	20.90	B
	ATOM	2593	C	GLN	B	752	19.067	0.748	3.407	1.00	19.34	B
	ATOM	2594	O	GLN	B	752	19.457	0.315	4.488	1.00	19.27	B
10	ATOM	2595	N	TYR	B	753	17.865	0.461	2.909	1.00	17.95	B
	ATOM	2596	CA	TYR	B	753	16.919	-0.407	3.616	1.00	16.98	B
	ATOM	2597	CB	TYR	B	753	15.519	-0.316	2.994	1.00	19.29	B
	ATOM	2598	CG	TYR	B	753	14.634	0.837	3.424	1.00	18.86	B
	ATOM	2599	CD1	TYR	B	753	15.116	1.891	4.204	1.00	19.58	B
15	ATOM	2600	CE1	TYR	B	753	14.275	2.973	4.552	1.00	20.49	B
	ATOM	2601	CD2	TYR	B	753	13.304	0.884	3.007	1.00	20.96	B
	ATOM	2602	CE2	TYR	B	753	12.472	1.943	3.342	1.00	20.37	B
	ATOM	2603	CZ	TYR	B	753	12.956	2.980	4.106	1.00	19.88	B
	ATOM	2604	OH	TYR	B	753	12.108	4.021	4.401	1.00	21.79	B
20	ATOM	2605	C	TYR	B	753	17.318	-1.888	3.574	1.00	18.67	B
	ATOM	2606	O	TYR	B	753	17.142	-2.612	4.555	1.00	17.27	B
	ATOM	2607	N	SER	B	754	17.845	-2.327	2.431	1.00	17.61	B
	ATOM	2608	CA	SER	B	754	18.198	-3.736	2.215	1.00	17.75	B
	ATOM	2609	CB	SER	B	754	17.769	-4.150	0.807	1.00	16.13	B
25	ATOM	2610	OG	SER	B	754	18.566	-3.484	-0.156	1.00	17.94	B
	ATOM	2611	C	SER	B	754	19.659	-4.129	2.392	1.00	17.86	B
	ATOM	2612	O	SER	B	754	20.004	-5.303	2.253	1.00	17.64	B
	ATOM	2613	N	TRP	B	755	20.513	-3.157	2.678	1.00	17.38	B
	ATOM	2614	CA	TRP	B	755	21.941	-3.410	2.853	1.00	19.81	B
30	ATOM	2615	CB	TRP	B	755	22.569	-2.169	3.497	1.00	24.07	B
	ATOM	2616	CG	TRP	B	755	23.816	-2.413	4.246	1.00	30.04	B
	ATOM	2617	CD2	TRP	B	755	23.997	-2.283	5.656	1.00	31.44	B
	ATOM	2618	CE2	TRP	B	755	25.333	-2.639	5.942	1.00	33.80	B
	ATOM	2619	CE3	TRP	B	755	23.159	-1.900	6.709	1.00	30.73	B
35	ATOM	2620	CD1	TRP	B	755	25.013	-2.826	3.739	1.00	33.58	B
	ATOM	2621	NE1	TRP	B	755	25.934	-2.966	4.754	1.00	35.50	B
	ATOM	2622	CZ2	TRP	B	755	25.850	-2.625	7.239	1.00	34.63	B
	ATOM	2623	CZ3	TRP	B	755	23.673	-1.886	7.998	1.00	31.07	B
	ATOM	2624	CH2	TRP	B	755	25.007	-2.247	8.251	1.00	32.77	B
40	ATOM	2625	C	TRP	B	755	22.263	-4.683	3.662	1.00	18.91	B
	ATOM	2626	O	TRP	B	755	22.919	-5.599	3.160	1.00	18.50	B
	ATOM	2627	N	MET	B	756	21.794	-4.745	4.903	1.00	16.98	B
	ATOM	2628	CA	MET	B	756	22.054	-5.902	5.765	1.00	16.75	B
	ATOM	2629	CB	MET	B	756	21.488	-5.652	7.169	1.00	15.08	B
45	ATOM	2630	CG	MET	B	756	21.834	-6.735	8.207	1.00	18.13	B
	ATOM	2631	SD	MET	B	756	23.609	-6.843	8.597	1.00	21.78	B
	ATOM	2632	CE	MET	B	756	23.790	-5.506	9.806	1.00	22.86	B
	ATOM	2633	C	MET	B	756	21.477	-7.205	5.205	1.00	16.39	B
	ATOM	2634	O	MET	B	756	22.135	-8.243	5.236	1.00	16.19	B
50	ATOM	2635	N	SER	B	757	20.251	-7.155	4.694	1.00	15.29	B
	ATOM	2636	CA	SER	B	757	19.619	-8.349	4.150	1.00	17.08	B
	ATOM	2637	CB	SER	B	757	18.174	-8.055	3.728	1.00	20.88	B
	ATOM	2638	OG	SER	B	757	18.141	-7.124	2.662	1.00	28.77	B
	ATOM	2639	C	SER	B	757	20.401	-8.895	2.960	1.00	17.10	B
55	ATOM	2640	O	SER	B	757	20.589	-10.101	2.846	1.00	17.47	B
	ATOM	2641	N	LEU	B	758	20.861	-8.013	2.078	1.00	17.47	B
	ATOM	2642	CA	LEU	B	758	21.620	-8.452	0.911	1.00	17.62	B

Table 2. (cont'd)

		#	Name	Res.	Chain	Res	#	X	Y	Z	occ	B	SegID
5	ATOM	2643	CB	LEU	B	758		21.922	-7.270	-0.018	1.00	17.52	B
	ATOM	2644	CG	LEU	B	758		20.713	-6.633	-0.715	1.00	21.15	B
	ATOM	2645	CD1	LEU	B	758		21.172	-5.516	-1.651	1.00	21.27	B
	ATOM	2646	CD2	LEU	B	758		19.964	-7.696	-1.500	1.00	21.66	B
	ATOM	2647	C	LEU	B	758		22.922	-9.103	1.356	1.00	16.78	B
10	ATOM	2648	O	LEU	B	758		23.342	-10.114	0.795	1.00	16.30	B
	ATOM	2649	N	MET	B	759		23.556	-8.529	2.373	1.00	14.76	B
	ATOM	2650	CA	MET	B	759		24.808	-9.077	2.863	1.00	17.48	B
	ATOM	2651	CB	MET	B	759		25.458	-8.126	3.863	1.00	19.24	B
	ATOM	2652	CG	MET	B	759		26.046	-6.892	3.211	1.00	25.62	B
15	ATOM	2653	SD	MET	B	759		27.036	-5.967	4.372	1.00	30.32	B
	ATOM	2654	CE	MET	B	759		27.629	-4.686	3.275	1.00	31.96	B
	ATOM	2655	C	MET	B	759		24.659	-10.452	3.494	1.00	16.79	B
	ATOM	2656	O	MET	B	759		25.465	-11.344	3.229	1.00	17.13	B
	ATOM	2657	N	VAL	B	760		23.639	-10.626	4.329	1.00	16.12	B
20	ATOM	2658	CA	VAL	B	760		23.429	-11.912	4.980	1.00	16.70	B
	ATOM	2659	CB	VAL	B	760		22.425	-11.788	6.163	1.00	18.09	B
	ATOM	2660	CG1	VAL	B	760		21.012	-11.598	5.652	1.00	18.30	B
	ATOM	2661	CG2	VAL	B	760		22.524	-13.005	7.059	1.00	18.55	B
	ATOM	2662	C	VAL	B	760		22.945	-12.966	3.972	1.00	17.46	B
25	ATOM	2663	O	VAL	B	760		23.260	-14.146	4.098	1.00	16.23	B
	ATOM	2664	N	PHE	B	761		22.195	-12.533	2.963	1.00	15.44	B
	ATOM	2665	CA	PHE	B	761		21.700	-13.451	1.938	1.00	15.94	B
	ATOM	2666	CB	PHE	B	761		20.686	-12.732	1.040	1.00	13.58	B
	ATOM	2667	CG	PHE	B	761		19.770	-13.657	0.281	1.00	15.45	B
30	ATOM	2668	CD1	PHE	B	761		18.904	-14.516	0.957	1.00	15.98	B
	ATOM	2669	CD2	PHE	B	761		19.745	-13.643	-1.110	1.00	14.81	B
	ATOM	2670	CE1	PHE	B	761		18.028	-15.343	0.261	1.00	16.60	B
	ATOM	2671	CE2	PHE	B	761		18.867	-14.470	-1.815	1.00	15.63	B
	ATOM	2672	CZ	PHE	B	761		18.009	-15.319	-1.125	1.00	14.90	B
35	ATOM	2673	C	PHE	B	761		22.907	-13.922	1.116	1.00	15.74	B
	ATOM	2674	O	PHE	B	761		23.038	-15.110	0.812	1.00	15.94	B
	ATOM	2675	N	GLY	B	762		23.788	-12.986	0.767	1.00	14.42	B
	ATOM	2676	CA	GLY	B	762		24.979	-13.330	0.003	1.00	15.82	B
	ATOM	2677	C	GLY	B	762		25.858	-14.267	0.822	1.00	15.85	B
40	ATOM	2678	O	GLY	B	762		26.462	-15.198	0.293	1.00	15.53	B
	ATOM	2679	N	LEU	B	763		25.934	-14.005	2.123	1.00	13.94	B
	ATOM	2680	CA	LEU	B	763		26.709	-14.838	3.033	1.00	14.37	B
	ATOM	2681	CB	LEU	B	763		26.599	-14.290	4.460	1.00	14.34	B
	ATOM	2682	CG	LEU	B	763		26.948	-15.255	5.596	1.00	13.19	B
45	ATOM	2683	CD1	LEU	B	763		28.420	-15.626	5.511	1.00	13.63	B
	ATOM	2684	CD2	LEU	B	763		26.631	-14.599	6.948	1.00	14.36	B
	ATOM	2685	C	LEU	B	763		26.163	-16.270	2.985	1.00	13.49	B
	ATOM	2686	O	LEU	B	763		26.921	-17.244	2.939	1.00	13.17	B
	ATOM	2687	N	GLY	B	764		24.841	-16.392	2.992	1.00	13.47	B
50	ATOM	2688	CA	GLY	B	764		24.230	-17.708	2.943	1.00	15.22	B
	ATOM	2689	C	GLY	B	764		24.621	-18.453	1.677	1.00	16.83	B
	ATOM	2690	O	GLY	B	764		24.932	-19.647	1.718	1.00	14.60	B
	ATOM	2691	N	TRP	B	765		24.615	-17.747	0.550	1.00	15.62	B
	ATOM	2692	CA	TRP	B	765		24.974	-18.360	-0.729	1.00	16.29	B
55	ATOM	2693	CB	TRP	B	765		24.776	-17.364	-1.877	1.00	17.83	B
	ATOM	2694	CG	TRP	B	765		25.067	-17.960	-3.226	1.00	19.06	B
	ATOM	2695	CD2	TRP	B	765		24.298	-18.961	-3.901	1.00	21.11	B

Table 2. (cont'd)

		#	Name	Res.	Chain	Res #	X	Y	Z	occ	B	SegID
5	ATOM	2696	CE2	TRP	B	765	24.981	-19.278	-5.097	1.00	22.22	B
	ATOM	2697	CE3	TRP	B	765	23.099	-19.625	-3.610	1.00	20.70	B
	ATOM	2698	CD1	TRP	B	765	26.149	-17.711	-4.017	1.00	21.91	B
	ATOM	2699	NE1	TRP	B	765	26.107	-18.500	-5.146	1.00	21.48	B
	ATOM	2700	CZ2	TRP	B	765	24.504	-20.231	-6.003	1.00	20.86	B
10	ATOM	2701	CZ3	TRP	B	765	22.625	-20.574	-4.515	1.00	21.28	B
	ATOM	2702	CH2	TRP	B	765	23.331	-20.866	-5.695	1.00	20.63	B
	ATOM	2703	C	TRP	B	765	26.413	-18.863	-0.727	1.00	14.88	B
	ATOM	2704	O	TRP	B	765	26.676	-20.009	-1.079	1.00	14.96	B
	ATOM	2705	N	ARG	B	766	27.350	-18.010	-0.329	1.00	15.86	B
15	ATOM	2706	CA	ARG	B	766	28.755	-18.414	-0.293	1.00	15.20	B
	ATOM	2707	CB	ARG	B	766	29.645	-17.219	0.059	1.00	15.13	B
	ATOM	2708	CG	ARG	B	766	29.681	-16.130	-1.027	1.00	14.72	B
	ATOM	2709	CD	ARG	B	766	30.770	-15.102	-0.715	1.00	17.05	B
	ATOM	2710	NE	ARG	B	766	30.520	-14.418	0.553	1.00	15.75	B
20	ATOM	2711	CZ	ARG	B	766	29.649	-13.424	0.706	1.00	17.31	B
	ATOM	2712	NH1	ARG	B	766	28.939	-12.992	-0.327	1.00	14.99	B
	ATOM	2713	NH2	ARG	B	766	29.499	-12.847	1.889	1.00	15.66	B
	ATOM	2714	C	ARG	B	766	29.031	-19.569	0.678	1.00	14.85	B
	ATOM	2715	O	ARG	B	766	29.819	-20.463	0.371	1.00	15.12	B
25	ATOM	2716	N	SER	B	767	28.396	-19.556	1.846	1.00	14.72	B
	ATOM	2717	CA	SER	B	767	28.605	-20.623	2.826	1.00	15.93	B
	ATOM	2718	CB	SER	B	767	27.876	-20.284	4.128	1.00	16.70	B
	ATOM	2719	OG	SER	B	767	28.307	-19.035	4.638	1.00	17.22	B
	ATOM	2720	C	SER	B	767	28.071	-21.941	2.253	1.00	16.52	B
30	ATOM	2721	O	SER	B	767	28.680	-23.007	2.397	1.00	17.28	B
	ATOM	2722	N	TYR	B	768	26.918	-21.842	1.604	1.00	16.21	B
	ATOM	2723	CA	TYR	B	768	26.255	-22.969	0.966	1.00	15.35	B
	ATOM	2724	CB	TYR	B	768	24.914	-22.476	0.405	1.00	16.96	B
	ATOM	2725	CG	TYR	B	768	24.224	-23.359	-0.615	1.00	17.34	B
35	ATOM	2726	CD1	TYR	B	768	23.962	-24.707	-0.358	1.00	16.25	B
	ATOM	2727	CE1	TYR	B	768	23.226	-25.481	-1.263	1.00	16.76	B
	ATOM	2728	CD2	TYR	B	768	23.742	-22.811	-1.805	1.00	17.37	B
	ATOM	2729	CE2	TYR	B	768	23.009	-23.569	-2.705	1.00	17.14	B
	ATOM	2730	CZ	TYR	B	768	22.749	-24.896	-2.432	1.00	16.64	B
40	ATOM	2731	OH	TYR	B	768	21.970	-25.608	-3.309	1.00	17.70	B
	ATOM	2732	C	TYR	B	768	27.148	-23.536	-0.140	1.00	17.02	B
	ATOM	2733	O	TYR	B	768	27.427	-24.737	-0.174	1.00	16.79	B
	ATOM	2734	N	LYS	B	769	27.627	-22.665	-1.021	1.00	14.67	B
	ATOM	2735	CA	LYS	B	769	28.474	-23.086	-2.132	1.00	16.86	B
45	ATOM	2736	CB	LYS	B	769	28.599	-21.944	-3.151	1.00	16.98	B
	ATOM	2737	CG	LYS	B	769	27.302	-21.576	-3.852	1.00	18.50	B
	ATOM	2738	CD	LYS	B	769	26.917	-22.586	-4.943	1.00	19.38	B
	ATOM	2739	CE	LYS	B	769	27.840	-22.500	-6.161	1.00	17.86	B
	ATOM	2740	NZ	LYS	B	769	27.399	-23.425	-7.249	1.00	15.11	B
50	ATOM	2741	C	LYS	B	769	29.885	-23.579	-1.782	1.00	18.73	B
	ATOM	2742	O	LYS	B	769	30.337	-24.590	-2.318	1.00	18.48	B
	ATOM	2743	N	HIS	B	770	30.577	-22.874	-0.889	1.00	17.78	B
	ATOM	2744	CA	HIS	B	770	31.961	-23.219	-0.546	1.00	18.94	B
	ATOM	2745	CB	HIS	B	770	32.750	-21.937	-0.241	1.00	20.02	B
55	ATOM	2746	CG	HIS	B	770	32.825	-20.982	-1.391	1.00	21.63	B
	ATOM	2747	CD2	HIS	B	770	32.090	-19.883	-1.685	1.00	21.95	B
	ATOM	2748	ND1	HIS	B	770	33.712	-21.142	-2.434	1.00	22.29	B

Table 2. (cont'd)

		#	Name	Res.	Chain	Res #	X	Y	Z	occ	B	SegID
5	ATOM	2749	CE1	HIS	B	770	33.517	-20.183	-3.324	1.00	23.77	B
	ATOM	2750	NE2	HIS	B	770	32.539	-19.407	-2.894	1.00	23.71	B
	ATOM	2751	C	HIS	B	770	32.214	-24.202	0.592	1.00	19.97	B
	ATOM	2752	O	HIS	B	770	33.203	-24.935	0.564	1.00	19.99	B
	ATOM	2753	N	VAL	B	771	31.341	-24.212	1.592	1.00	19.79	B
10	ATOM	2754	CA	VAL	B	771	31.532	-25.080	2.746	1.00	20.09	B
	ATOM	2755	CB	VAL	B	771	31.993	-24.242	3.968	1.00	21.67	B
	ATOM	2756	CG1	VAL	B	771	33.355	-23.626	3.691	1.00	21.97	B
	ATOM	2757	CG2	VAL	B	771	30.988	-23.132	4.246	1.00	22.98	B
	ATOM	2758	C	VAL	B	771	30.274	-25.864	3.110	1.00	19.76	B
15	ATOM	2759	O	VAL	B	771	30.047	-26.194	4.280	1.00	20.09	B
	ATOM	2760	N	SER	B	772	29.465	-26.162	2.099	1.00	17.17	B
	ATOM	2761	CA	SER	B	772	28.225	-26.903	2.294	1.00	18.29	B
	ATOM	2762	CB	SER	B	772	28.539	-28.381	2.525	1.00	18.92	B
	ATOM	2763	OG	SER	B	772	29.220	-28.907	1.397	1.00	20.36	B
20	ATOM	2764	C	SER	B	772	27.370	-26.361	3.433	1.00	17.67	B
	ATOM	2765	O	SER	B	772	26.645	-27.116	4.092	1.00	17.83	B
	ATOM	2766	N	GLY	B	773	27.448	-25.049	3.651	1.00	16.98	B
	ATOM	2767	CA	GLY	B	773	26.665	-24.407	4.700	1.00	18.02	B
	ATOM	2768	C	GLY	B	773	27.068	-24.727	6.134	1.00	19.19	B
25	ATOM	2769	O	GLY	B	773	26.385	-24.322	7.080	1.00	19.19	B
	ATOM	2770	N	GLN	B	774	28.181	-25.436	6.307	1.00	18.16	B
	ATOM	2771	CA	GLN	B	774	28.637	-25.820	7.640	1.00	18.57	B
	ATOM	2772	CB	GLN	B	774	29.293	-27.200	7.579	1.00	18.50	B
	ATOM	2773	CG	GLN	B	774	28.375	-28.248	6.987	1.00	22.02	B
30	ATOM	2774	CD	GLN	B	774	27.010	-28.250	7.647	1.00	26.61	B
	ATOM	2775	OE1	GLN	B	774	26.879	-28.545	8.841	1.00	27.59	B
	ATOM	2776	NE2	GLN	B	774	25.980	-27.907	6.875	1.00	28.16	B
	ATOM	2777	C	GLN	B	774	29.566	-24.817	8.328	1.00	19.18	B
	ATOM	2778	O	GLN	B	774	29.995	-25.033	9.460	1.00	18.70	B
35	ATOM	2779	N	MET	B	775	29.879	-23.730	7.634	1.00	17.50	B
	ATOM	2780	CA	MET	B	775	30.705	-22.653	8.176	1.00	18.41	B
	ATOM	2781	CB	MET	B	775	32.182	-22.814	7.790	1.00	19.65	B
	ATOM	2782	CG	MET	B	775	32.922	-23.895	8.558	1.00	23.25	B
	ATOM	2783	SD	MET	B	775	34.702	-23.859	8.249	1.00	27.85	B
40	ATOM	2784	CE	MET	B	775	35.070	-25.630	8.200	1.00	29.77	B
	ATOM	2785	C	MET	B	775	30.159	-21.370	7.569	1.00	16.57	B
	ATOM	2786	O	MET	B	775	29.460	-21.414	6.559	1.00	15.67	B
	ATOM	2787	N	LEU	B	776	30.452	-20.233	8.189	1.00	16.83	B
	ATOM	2788	CA	LEU	B	776	29.976	-18.963	7.657	1.00	15.86	B
45	ATOM	2789	CB	LEU	B	776	29.558	-18.022	8.797	1.00	15.81	B
	ATOM	2790	CG	LEU	B	776	28.302	-18.480	9.556	1.00	15.03	B
	ATOM	2791	CD1	LEU	B	776	27.886	-17.440	10.586	1.00	16.94	B
	ATOM	2792	CD2	LEU	B	776	27.167	-18.709	8.565	1.00	17.07	B
	ATOM	2793	C	LEU	B	776	31.089	-18.355	6.817	1.00	16.39	B
50	ATOM	2794	O	LEU	B	776	32.086	-17.856	7.342	1.00	16.45	B
	ATOM	2795	N	TYR	B	777	30.907	-18.421	5.502	1.00	15.59	B
	ATOM	2796	CA	TYR	B	777	31.885	-17.923	4.544	1.00	14.70	B
	ATOM	2797	CB	TYR	B	777	31.792	-18.764	3.264	1.00	16.31	B
	ATOM	2798	CG	TYR	B	777	32.970	-18.650	2.316	1.00	18.23	B
55	ATOM	2799	CD1	TYR	B	777	33.118	-17.544	1.476	1.00	19.16	B
	ATOM	2800	CE1	TYR	B	777	34.175	-17.469	0.559	1.00	19.47	B
	ATOM	2801	CD2	TYR	B	777	33.910	-19.676	2.222	1.00	19.79	B

Table 2. (cont'd)

		#	Name	Res.	Chain	Res #	X	Y	Z	occ	B	SegID
	ATOM	2802	CE2	TYR	B	777	34.969	-19.610	1.307	1.00	18.50	B
5	ATOM	2803	CZ	TYR	B	777	35.091	-18.509	0.480	1.00	18.83	B
	ATOM	2804	OH	TYR	B	777	36.109	-18.463	-0.446	1.00	19.32	B
	ATOM	2805	C	TYR	B	777	31.662	-16.441	4.236	1.00	16.02	B
	ATOM	2806	O	TYR	B	777	31.095	-16.089	3.200	1.00	13.24	B
	ATOM	2807	N	PHE	B	778	32.098	-15.578	5.149	1.00	15.22	B
10	ATOM	2808	CA	PHE	B	778	31.950	-14.141	4.953	1.00	16.74	B
	ATOM	2809	CB	PHE	B	778	32.370	-13.377	6.217	1.00	14.02	B
	ATOM	2810	CG	PHE	B	778	31.427	-13.571	7.382	1.00	16.42	B
	ATOM	2811	CD1	PHE	B	778	31.654	-14.568	8.328	1.00	17.13	B
	ATOM	2812	CD2	PHE	B	778	30.282	-12.784	7.504	1.00	16.49	B
15	ATOM	2813	CE1	PHE	B	778	30.752	-14.779	9.382	1.00	17.43	B
	ATOM	2814	CE2	PHE	B	778	29.374	-12.986	8.553	1.00	17.31	B
	ATOM	2815	CZ	PHE	B	778	29.612	-13.987	9.493	1.00	16.02	B
	ATOM	2816	C	PHE	B	778	32.798	-13.719	3.758	1.00	16.59	B
	ATOM	2817	O	PHE	B	778	32.343	-12.974	2.887	1.00	18.01	B
20	ATOM	2818	N	ALA	B	779	34.028	-14.216	3.714	1.00	17.78	B
	ATOM	2819	CA	ALA	B	779	34.940	-13.918	2.620	1.00	19.19	B
	ATOM	2820	CB	ALA	B	779	35.589	-12.556	2.833	1.00	18.30	B
	ATOM	2821	C	ALA	B	779	36.010	-15.004	2.550	1.00	20.69	B
	ATOM	2822	O	ALA	B	779	36.133	-15.832	3.456	1.00	19.06	B
25	ATOM	2823	N	PRO	B	780	36.790	-15.028	1.462	1.00	22.12	B
	ATOM	2824	CD	PRO	B	780	36.645	-14.287	0.196	1.00	22.83	B
	ATOM	2825	CA	PRO	B	780	37.834	-16.050	1.353	1.00	22.26	B
	ATOM	2826	CB	PRO	B	780	38.468	-15.747	-0.004	1.00	23.89	B
	ATOM	2827	CG	PRO	B	780	37.306	-15.222	-0.795	1.00	25.92	B
30	ATOM	2828	C	PRO	B	780	38.838	-15.949	2.502	1.00	22.45	B
	ATOM	2829	O	PRO	B	780	39.424	-16.950	2.916	1.00	22.14	B
	ATOM	2830	N	ASP	B	781	39.014	-14.740	3.029	1.00	21.57	B
	ATOM	2831	CA	ASP	B	781	39.954	-14.512	4.126	1.00	21.92	B
	ATOM	2832	CB	ASP	B	781	40.814	-13.282	3.820	1.00	23.49	B
35	ATOM	2833	CG	ASP	B	781	39.991	-12.017	3.661	1.00	24.54	B
	ATOM	2834	OD1	ASP	B	781	38.772	-12.117	3.393	1.00	22.71	B
	ATOM	2835	OD2	ASP	B	781	40.571	-10.920	3.795	1.00	24.49	B
	ATOM	2836	C	ASP	B	781	39.267	-14.340	5.476	1.00	21.74	B
	ATOM	2837	O	ASP	B	781	39.888	-13.917	6.451	1.00	22.77	B
40	ATOM	2838	N	LEU	B	782	37.979	-14.664	5.526	1.00	20.36	B
	ATOM	2839	CA	LEU	B	782	37.210	-14.557	6.756	1.00	19.59	B
	ATOM	2840	CB	LEU	B	782	36.619	-13.151	6.893	1.00	20.63	B
	ATOM	2841	CG	LEU	B	782	35.970	-12.802	8.232	1.00	22.29	B
	ATOM	2842	CD1	LEU	B	782	36.949	-13.088	9.370	1.00	25.24	B
45	ATOM	2843	CD2	LEU	B	782	35.567	-11.325	8.237	1.00	21.90	B
	ATOM	2844	C	LEU	B	782	36.095	-15.603	6.761	1.00	19.08	B
	ATOM	2845	O	LEU	B	782	34.954	-15.320	6.389	1.00	15.84	B
	ATOM	2846	N	ILE	B	783	36.452	-16.815	7.179	1.00	18.17	B
	ATOM	2847	CA	ILE	B	783	35.525	-17.941	7.257	1.00	17.98	B
50	ATOM	2848	CB	ILE	B	783	36.062	-19.142	6.446	1.00	17.80	B
	ATOM	2849	CG2	ILE	B	783	35.093	-20.311	6.551	1.00	20.50	B
	ATOM	2850	CG1	ILE	B	783	36.282	-18.723	4.988	1.00	18.65	B
	ATOM	2851	CD1	ILE	B	783	37.092	-19.720	4.155	1.00	20.07	B
	ATOM	2852	C	ILE	B	783	35.407	-18.340	8.725	1.00	19.08	B
55	ATOM	2853	O	ILE	B	783	36.402	-18.697	9.358	1.00	19.55	B
	ATOM	2854	N	LEU	B	784	34.200	-18.289	9.269	1.00	19.91	B

Table 2. (cont'd)

		#	Name	Res.	Chain	Res #	X	Y	Z	occ	B	SegID
5	ATOM	2855	CA	LEU	B	784	34.021	-18.618	10.676	1.00	22.66	B
	ATOM	2856	CB	LEU	B	784	33.276	-17.490	11.401	1.00	21.59	B
	ATOM	2857	CG	LEU	B	784	33.858	-16.076	11.358	1.00	24.80	B
	ATOM	2858	CD1	LEU	B	784	32.937	-15.138	12.135	1.00	23.29	B
	ATOM	2859	CD2	LEU	B	784	35.257	-16.062	11.941	1.00	24.21	B
10	ATOM	2860	C	LEU	B	784	33.291	-19.917	10.953	1.00	24.35	B
	ATOM	2861	O	LEU	B	784	32.305	-20.251	10.300	1.00	22.70	B
	ATOM	2862	N	ASN	B	785	33.799	-20.645	11.939	1.00	26.14	B
	ATOM	2863	CA	ASN	B	785	33.186	-21.885	12.376	1.00	28.52	B
	ATOM	2864	CB	ASN	B	785	34.158	-23.058	12.240	1.00	30.54	B
15	ATOM	2865	CG	ASN	B	785	35.509	-22.761	12.841	1.00	31.69	B
	ATOM	2866	OD1	ASN	B	785	35.606	-22.104	13.875	1.00	33.80	B
	ATOM	2867	ND2	ASN	B	785	36.564	-23.253	12.204	1.00	34.71	B
	ATOM	2868	C	ASN	B	785	32.835	-21.648	13.843	1.00	29.93	B
	ATOM	2869	O	ASN	B	785	33.155	-20.597	14.409	1.00	28.08	B
20	ATOM	2870	N	GLU	B	786	32.190	-22.625	14.458	1.00	31.08	B
	ATOM	2871	CA	GLU	B	786	31.771	-22.516	15.845	1.00	33.20	B
	ATOM	2872	CB	GLU	B	786	31.169	-23.849	16.286	1.00	37.40	B
	ATOM	2873	CG	GLU	B	786	30.217	-23.750	17.455	1.00	42.11	B
	ATOM	2874	CD	GLU	B	786	29.476	-25.050	17.696	1.00	46.15	B
25	ATOM	2875	OE1	GLU	B	786	28.841	-25.555	16.743	1.00	46.80	B
	ATOM	2876	OE2	GLU	B	786	29.529	-25.563	18.836	1.00	48.79	B
	ATOM	2877	C	GLU	B	786	32.862	-22.088	16.830	1.00	32.26	B
	ATOM	2878	O	GLU	B	786	32.624	-21.246	17.696	1.00	31.14	B
	ATOM	2879	N	GLN	B	787	34.058	-22.651	16.692	1.00	32.38	B
30	ATOM	2880	CA	GLN	B	787	35.151	-22.332	17.604	1.00	34.18	B
	ATOM	2881	CB	GLN	B	787	36.353	-23.235	17.327	1.00	37.31	B
	ATOM	2882	CG	GLN	B	787	37.302	-22.693	16.275	1.00	41.80	B
	ATOM	2883	CD	GLN	B	787	38.555	-23.530	16.137	1.00	45.28	B
	ATOM	2884	OE1	GLN	B	787	39.524	-23.116	15.497	1.00	47.58	B
35	ATOM	2885	NE2	GLN	B	787	38.542	-24.722	16.733	1.00	48.17	B
	ATOM	2886	C	GLN	B	787	35.609	-20.876	17.558	1.00	34.13	B
	ATOM	2887	O	GLN	B	787	36.198	-20.377	18.518	1.00	33.23	B
	ATOM	2888	N	ARG	B	788	35.355	-20.200	16.441	1.00	32.22	B
	ATOM	2889	CA	ARG	B	788	35.767	-18.810	16.294	1.00	31.78	B
40	ATOM	2890	CB	ARG	B	788	36.169	-18.528	14.842	1.00	31.05	B
	ATOM	2891	CG	ARG	B	788	37.322	-19.393	14.343	1.00	32.23	B
	ATOM	2892	CD	ARG	B	788	37.772	-18.988	12.938	1.00	32.79	B
	ATOM	2893	NE	ARG	B	788	38.365	-17.652	12.923	1.00	33.62	B
	ATOM	2894	CZ	ARG	B	788	38.815	-17.036	11.831	1.00	35.26	B
45	ATOM	2895	NH1	ARG	B	788	38.742	-17.630	10.643	1.00	32.75	B
	ATOM	2896	NH2	ARG	B	788	39.349	-15.824	11.929	1.00	33.61	B
	ATOM	2897	C	ARG	B	788	34.670	-17.847	16.733	1.00	31.36	B
	ATOM	2898	O	ARG	B	788	34.773	-16.637	16.532	1.00	32.48	B
	ATOM	2899	N	MET	B	789	33.621	-18.398	17.334	1.00	30.68	B
50	ATOM	2900	CA	MET	B	789	32.490	-17.613	17.824	1.00	31.24	B
	ATOM	2901	CB	MET	B	789	31.200	-18.116	17.178	1.00	29.02	B
	ATOM	2902	CG	MET	B	789	31.266	-18.136	15.660	1.00	29.15	B
	ATOM	2903	SD	MET	B	789	29.905	-19.023	14.891	1.00	27.19	B
	ATOM	2904	CE	MET	B	789	30.378	-18.882	13.161	1.00	27.27	B
55	ATOM	2905	C	MET	B	789	32.430	-17.787	19.339	1.00	31.40	B
	ATOM	2906	O	MET	B	789	31.528	-18.433	19.870	1.00	31.70	B
	ATOM	2907	N	LYS	B	790	33.404	-17.197	20.023	1.00	33.04	B

Table 2. (cont'd)

		#	Name	Res.	Chain	Res #	X	Y	Z	occ	B	SegID
5	ATOM	2908	CA	LYS	B	790	33.520	-17.297	21.474	1.00	34.21	B
	ATOM	2909	CB	LYS	B	790	34.887	-16.759	21.894	1.00	33.75	B
	ATOM	2910	CG	LYS	B	790	36.030	-17.429	21.141	1.00	34.59	B
	ATOM	2911	CD	LYS	B	790	37.368	-16.763	21.407	1.00	35.73	B
	ATOM	2912	CE	LYS	B	790	38.469	-17.425	20.588	1.00	37.42	B
10	ATOM	2913	NZ	LYS	B	790	39.785	-16.747	20.754	1.00	39.03	B
	ATOM	2914	C	LYS	B	790	32.407	-16.605	22.262	1.00	36.08	B
	ATOM	2915	O	LYS	B	790	31.732	-17.241	23.070	1.00	35.56	B
	ATOM	2916	N	GLU	B	791	32.222	-15.308	22.033	1.00	37.31	B
	ATOM	2917	CA	GLU	B	791	31.186	-14.545	22.728	1.00	39.12	B
15	ATOM	2918	CB	GLU	B	791	31.231	-13.080	22.288	1.00	41.76	B
	ATOM	2919	CG	GLU	B	791	31.625	-12.115	23.390	1.00	47.66	B
	ATOM	2920	CD	GLU	B	791	30.594	-12.053	24.508	1.00	50.47	B
	ATOM	2921	OE1	GLU	B	791	29.437	-11.657	24.237	1.00	51.08	B
	ATOM	2922	OE2	GLU	B	791	30.942	-12.401	25.659	1.00	52.17	B
20	ATOM	2923	C	GLU	B	791	29.804	-15.128	22.445	1.00	38.82	B
	ATOM	2924	O	GLU	B	791	29.383	-15.221	21.292	1.00	39.17	B
	ATOM	2925	N	SER	B	792	29.099	-15.513	23.504	1.00	37.75	B
	ATOM	2926	CA	SER	B	792	27.770	-16.102	23.373	1.00	37.53	B
	ATOM	2927	CB	SER	B	792	27.191	-16.390	24.760	1.00	39.01	B
25	ATOM	2928	OG	SER	B	792	27.172	-15.215	25.549	1.00	41.88	B
	ATOM	2929	C	SER	B	792	26.803	-15.220	22.587	1.00	36.19	B
	ATOM	2930	O	SER	B	792	25.936	-15.720	21.869	1.00	35.18	B
	ATOM	2931	N	SER	B	793	26.955	-13.908	22.736	1.00	35.25	B
	ATOM	2932	CA	SER	B	793	26.102	-12.948	22.046	1.00	34.13	B
30	ATOM	2933	CB	SER	B	793	26.415	-11.535	22.542	1.00	35.74	B
	ATOM	2934	OG	SER	B	793	25.504	-10.594	22.006	1.00	40.72	B
	ATOM	2935	C	SER	B	793	26.339	-13.033	20.539	1.00	32.40	B
	ATOM	2936	O	SER	B	793	25.397	-13.100	19.749	1.00	30.32	B
	ATOM	2937	N	PHE	B	794	27.611	-13.029	20.158	1.00	31.57	B
35	ATOM	2938	CA	PHE	B	794	28.010	-13.111	18.759	1.00	31.79	B
	ATOM	2939	CB	PHE	B	794	29.517	-12.856	18.636	1.00	33.58	B
	ATOM	2940	CG	PHE	B	794	30.024	-12.869	17.222	1.00	36.88	B
	ATOM	2941	CD1	PHE	B	794	29.579	-11.926	16.300	1.00	37.56	B
	ATOM	2942	CD2	PHE	B	794	30.950	-13.825	16.812	1.00	38.13	B
40	ATOM	2943	CE1	PHE	B	794	30.048	-11.932	14.986	1.00	38.39	B
	ATOM	2944	CE2	PHE	B	794	31.426	-13.841	15.500	1.00	39.25	B
	ATOM	2945	CZ	PHE	B	794	30.973	-12.890	14.585	1.00	39.67	B
	ATOM	2946	C	PHE	B	794	27.664	-14.487	18.194	1.00	30.57	B
	ATOM	2947	O	PHE	B	794	27.281	-14.615	17.030	1.00	29.77	B
45	ATOM	2948	N	TYR	B	795	27.794	-15.516	19.026	1.00	29.44	B
	ATOM	2949	CA	TYR	B	795	27.490	-16.876	18.606	1.00	27.92	B
	ATOM	2950	CB	TYR	B	795	27.872	-17.872	19.709	1.00	31.37	B
	ATOM	2951	CG	TYR	B	795	27.579	-19.317	19.357	1.00	33.31	B
	ATOM	2952	CD1	TYR	B	795	28.001	-19.860	18.141	1.00	34.81	B
50	ATOM	2953	CE1	TYR	B	795	27.732	-21.185	17.807	1.00	35.57	B
	ATOM	2954	CD2	TYR	B	795	26.878	-20.142	20.237	1.00	35.46	B
	ATOM	2955	CE2	TYR	B	795	26.603	-21.473	19.913	1.00	36.78	B
	ATOM	2956	CZ	TYR	B	795	27.032	-21.984	18.697	1.00	36.92	B
	ATOM	2957	OH	TYR	B	795	26.752	-23.288	18.365	1.00	39.48	B
55	ATOM	2958	C	TYR	B	795	26.008	-17.008	18.267	1.00	26.49	B
	ATOM	2959	O	TYR	B	795	25.644	-17.624	17.268	1.00	23.95	B
	ATOM	2960	N	SER	B	796	25.150	-16.423	19.095	1.00	25.20	B

Table 2. (cont'd)

		#	Name	Res.	Chain	Res #	X	Y	Z	occ	B	SegID
5	ATOM	2961	CA	SER	B	796	23.716	-16.492	18.847	1.00	26.93	B
	ATOM	2962	CB	SER	B	796	22.941	-15.864	20.006	1.00	28.16	B
	ATOM	2963	OG	SER	B	796	23.161	-16.592	21.200	1.00	30.73	B
	ATOM	2964	C	SER	B	796	23.374	-15.770	17.548	1.00	25.62	B
	ATOM	2965	O	SER	B	796	22.499	-16.195	16.795	1.00	25.30	B
10	ATOM	2966	N	LEU	B	797	24.074	-14.673	17.296	1.00	24.05	B
	ATOM	2967	CA	LEU	B	797	23.851	-13.893	16.088	1.00	25.18	B
	ATOM	2968	CB	LEU	B	797	24.720	-12.638	16.112	1.00	24.29	B
	ATOM	2969	CG	LEU	B	797	24.429	-11.600	15.027	1.00	27.01	B
	ATOM	2970	CD1	LEU	B	797	23.024	-11.043	15.197	1.00	27.55	B
15	ATOM	2971	CD2	LEU	B	797	25.447	-10.491	15.128	1.00	28.99	B
	ATOM	2972	C	LEU	B	797	24.196	-14.744	14.870	1.00	22.79	B
	ATOM	2973	O	LEU	B	797	23.429	-14.809	13.907	1.00	23.34	B
	ATOM	2974	N	CYS	B	798	25.354	-15.397	14.920	1.00	22.06	B
	ATOM	2975	CA	CYS	B	798	25.792	-16.253	13.826	1.00	21.40	B
20	ATOM	2976	CB	CYS	B	798	27.205	-16.777	14.102	1.00	22.48	B
	ATOM	2977	SG	CYS	B	798	28.482	-15.490	14.048	1.00	23.41	B
	ATOM	2978	C	CYS	B	798	24.817	-17.414	13.613	1.00	21.32	B
	ATOM	2979	O	CYS	B	798	24.535	-17.793	12.473	1.00	20.28	B
	ATOM	2980	N	LEU	B	799	24.306	-17.981	14.702	1.00	19.81	B
25	ATOM	2981	CA	LEU	B	799	23.341	-19.069	14.588	1.00	19.74	B
	ATOM	2982	CB	LEU	B	799	22.899	-19.559	15.970	1.00	23.55	B
	ATOM	2983	CG	LEU	B	799	23.890	-20.438	16.740	1.00	24.38	B
	ATOM	2984	CD1	LEU	B	799	23.279	-20.850	18.077	1.00	26.86	B
	ATOM	2985	CD2	LEU	B	799	24.226	-21.674	15.911	1.00	26.58	B
30	ATOM	2986	C	LEU	B	799	22.135	-18.550	13.818	1.00	20.29	B
	ATOM	2987	O	LEU	B	799	21.563	-19.255	12.990	1.00	20.26	B
	ATOM	2988	N	THR	B	800	21.756	-17.304	14.086	1.00	20.04	B
	ATOM	2989	CA	THR	B	800	20.629	-16.703	13.387	1.00	20.32	B
	ATOM	2990	CB	THR	B	800	20.289	-15.308	13.967	1.00	21.13	B
35	ATOM	2991	OG1	THR	B	800	19.814	-15.453	15.312	1.00	19.83	B
	ATOM	2992	CG2	THR	B	800	19.218	-14.620	13.131	1.00	21.16	B
	ATOM	2993	C	THR	B	800	20.937	-16.574	11.893	1.00	19.37	B
	ATOM	2994	O	THR	B	800	20.098	-16.882	11.049	1.00	20.15	B
	ATOM	2995	N	MET	B	801	22.140	-16.119	11.564	1.00	18.98	B
40	ATOM	2996	CA	MET	B	801	22.518	-15.969	10.160	1.00	20.07	B
	ATOM	2997	CB	MET	B	801	23.854	-15.229	10.042	1.00	20.74	B
	ATOM	2998	CG	MET	B	801	23.833	-13.802	10.575	1.00	20.42	B
	ATOM	2999	SD	MET	B	801	25.357	-12.924	10.203	1.00	24.80	B
	ATOM	3000	CE	MET	B	801	26.385	-13.408	11.562	1.00	25.72	B
45	ATOM	3001	C	MET	B	801	22.636	-17.336	9.489	1.00	19.47	B
	ATOM	3002	O	MET	B	801	22.326	-17.491	8.310	1.00	17.79	B
	ATOM	3003	N	TRP	B	802	23.075	-18.321	10.264	1.00	20.79	B
	ATOM	3004	CA	TRP	B	802	23.266	-19.690	9.792	1.00	21.60	B
	ATOM	3005	CB	TRP	B	802	23.788	-20.550	10.942	1.00	22.91	B
50	ATOM	3006	CG	TRP	B	802	24.985	-21.360	10.590	1.00	24.57	B
	ATOM	3007	CD2	TRP	B	802	26.211	-21.434	11.323	1.00	25.80	B
	ATOM	3008	CE2	TRP	B	802	27.069	-22.304	10.613	1.00	25.69	B
	ATOM	3009	CE3	TRP	B	802	26.670	-20.847	12.511	1.00	26.80	B
	ATOM	3010	CD1	TRP	B	802	25.140	-22.168	9.497	1.00	25.78	B
55	ATOM	3011	NE1	TRP	B	802	26.390	-22.738	9.506	1.00	25.97	B
	ATOM	3012	CZ2	TRP	B	802	28.365	-22.603	11.053	1.00	27.76	B
	ATOM	3013	CZ3	TRP	B	802	27.962	-21.145	12.949	1.00	26.64	B

Table 2. (cont'd)

		#	Name	Res.	Chain	Res #	X	Y	Z	occ	B	SegID
5	ATOM	3014	CH2	TRP	B	802	28.792	-22.015	12.219	1.00	27.43	B
	ATOM	3015	C	TRP	B	802	22.005	-20.345	9.227	1.00	21.64	B
	ATOM	3016	O	TRP	B	802	22.085	-21.309	8.463	1.00	20.67	B
	ATOM	3017	N	GLN	B	803	20.842	-19.835	9.617	1.00	21.08	B
	ATOM	3018	CA	GLN	B	803	19.575	-20.396	9.161	1.00	20.48	B
10	ATOM	3019	CB	GLN	B	803	18.416	-19.663	9.824	1.00	21.39	B
	ATOM	3020	CG	GLN	B	803	18.558	-19.535	11.323	1.00	23.58	B
	ATOM	3021	CD	GLN	B	803	17.428	-18.743	11.932	1.00	27.19	B
	ATOM	3022	OE1	GLN	B	803	16.344	-19.274	12.181	1.00	29.06	B
	ATOM	3023	NE2	GLN	B	803	17.666	-17.460	12.159	1.00	28.68	B
15	ATOM	3024	C	GLN	B	803	19.412	-20.321	7.651	1.00	21.76	B
	ATOM	3025	O	GLN	B	803	18.786	-21.191	7.039	1.00	21.16	B
	ATOM	3026	N	ILE	B	804	19.964	-19.274	7.048	1.00	20.31	B
	ATOM	3027	CA	ILE	B	804	19.849	-19.107	5.611	1.00	19.18	B
	ATOM	3028	CB	ILE	B	804	20.336	-17.704	5.184	1.00	18.04	B
20	ATOM	3029	CG2	ILE	B	804	20.227	-17.550	3.674	1.00	17.29	B
	ATOM	3030	CG1	ILE	B	804	19.478	-16.633	5.875	1.00	19.81	B
	ATOM	3031	CD1	ILE	B	804	19.859	-15.195	5.524	1.00	20.17	B
	ATOM	3032	C	ILE	B	804	20.602	-20.206	4.849	1.00	20.03	B
	ATOM	3033	O	ILE	B	804	20.019	-20.884	4.005	1.00	21.05	B
25	ATOM	3034	N	PRO	B	805	21.901	-20.400	5.137	1.00	20.99	B
	ATOM	3035	CD	PRO	B	805	22.753	-19.671	6.094	1.00	20.74	B
	ATOM	3036	CA	PRO	B	805	22.667	-21.446	4.440	1.00	21.50	B
	ATOM	3037	CB	PRO	B	805	24.037	-21.390	5.117	1.00	22.20	B
	ATOM	3038	CG	PRO	B	805	24.136	-19.979	5.600	1.00	22.08	B
30	ATOM	3039	C	PRO	B	805	21.998	-22.807	4.649	1.00	22.88	B
	ATOM	3040	O	PRO	B	805	21.897	-23.624	3.730	1.00	22.43	B
	ATOM	3041	N	GLN	B	806	21.547	-23.041	5.877	1.00	22.24	B
	ATOM	3042	CA	GLN	B	806	20.886	-24.291	6.227	1.00	22.01	B
	ATOM	3043	CB	GLN	B	806	20.511	-24.280	7.712	1.00	23.12	B
35	ATOM	3044	CG	GLN	B	806	21.732	-24.418	8.616	1.00	27.21	B
	ATOM	3045	CD	GLN	B	806	21.452	-24.120	10.079	1.00	31.98	B
	ATOM	3046	OE1	GLN	B	806	22.295	-24.379	10.939	1.00	37.38	B
	ATOM	3047	NE2	GLN	B	806	20.276	-23.569	10.370	1.00	32.65	B
	ATOM	3048	C	GLN	B	806	19.656	-24.528	5.356	1.00	23.33	B
40	ATOM	3049	O	GLN	B	806	19.443	-25.639	4.872	1.00	23.30	B
	ATOM	3050	N	GLU	B	807	18.855	-23.487	5.144	1.00	21.25	B
	ATOM	3051	CA	GLU	B	807	17.662	-23.611	4.306	1.00	21.78	B
	ATOM	3052	CB	GLU	B	807	16.770	-22.375	4.441	1.00	25.31	B
	ATOM	3053	CG	GLU	B	807	15.931	-22.353	5.698	1.00	29.26	B
45	ATOM	3054	CD	GLU	B	807	14.962	-23.520	5.762	1.00	32.50	B
	ATOM	3055	OE1	GLU	B	807	14.077	-23.606	4.887	1.00	33.09	B
	ATOM	3056	OE2	GLU	B	807	15.092	-24.353	6.684	1.00	32.53	B
	ATOM	3057	C	GLU	B	807	18.043	-23.805	2.843	1.00	20.58	B
	ATOM	3058	O	GLU	B	807	17.354	-24.519	2.108	1.00	19.42	B
50	ATOM	3059	N	PHE	B	808	19.129	-23.159	2.418	1.00	19.70	B
	ATOM	3060	CA	PHE	B	808	19.602	-23.292	1.042	1.00	18.77	B
	ATOM	3061	CB	PHE	B	808	20.832	-22.408	0.785	1.00	16.63	B
	ATOM	3062	CG	PHE	B	808	20.510	-20.951	0.577	1.00	18.24	B
	ATOM	3063	CD1	PHE	B	808	19.195	-20.495	0.604	1.00	15.60	B
55	ATOM	3064	CD2	PHE	B	808	21.529	-20.030	0.369	1.00	17.34	B
	ATOM	3065	CE1	PHE	B	808	18.905	-19.133	0.431	1.00	17.14	B
	ATOM	3066	CE2	PHE	B	808	21.248	-18.672	0.196	1.00	18.78	B

Table 2. (cont'd)

		#	Name	Res.	Chain	Res #	X	Y	Z	occ	B	SegID
5	ATOM	3067	CZ	PHE	B	808	19.929	-18.227	0.228	1.00	17.21	B
	ATOM	3068	C	PHE	B	808	19.964	-24.751	0.802	1.00	17.37	B
	ATOM	3069	O	PHE	B	808	19.610	-25.322	-0.225	1.00	17.11	B
	ATOM	3070	N	VAL	B	809	20.673	-25.346	1.756	1.00	18.79	B
	ATOM	3071	CA	VAL	B	809	21.054	-26.756	1.655	1.00	19.69	B
10	ATOM	3072	CB	VAL	B	809	21.955	-27.190	2.846	1.00	21.10	B
	ATOM	3073	CG1	VAL	B	809	22.113	-28.704	2.855	1.00	23.52	B
	ATOM	3074	CG2	VAL	B	809	23.330	-26.536	2.742	1.00	19.39	B
	ATOM	3075	C	VAL	B	809	19.800	-27.640	1.646	1.00	21.36	B
	ATOM	3076	O	VAL	B	809	19.685	-28.560	0.830	1.00	21.94	B
15	ATOM	3077	N	LYS	B	810	18.864	-27.364	2.551	1.00	21.13	B
	ATOM	3078	CA	LYS	B	810	17.634	-28.152	2.630	1.00	23.80	B
	ATOM	3079	CB	LYS	B	810	16.748	-27.674	3.786	1.00	27.42	B
	ATOM	3080	CG	LYS	B	810	17.228	-28.037	5.182	1.00	31.68	B
	ATOM	3081	CD	LYS	B	810	16.184	-27.605	6.205	1.00	35.53	B
20	ATOM	3082	CE	LYS	B	810	16.667	-27.793	7.632	1.00	39.05	B
	ATOM	3083	NZ	LYS	B	810	15.639	-27.331	8.608	1.00	38.71	B
	ATOM	3084	C	LYS	B	810	16.801	-28.115	1.355	1.00	23.30	B
	ATOM	3085	O	LYS	B	810	16.407	-29.157	0.829	1.00	20.94	B
	ATOM	3086	N	LEU	B	811	16.514	-26.910	0.871	1.00	22.91	B
25	ATOM	3087	CA	LEU	B	811	15.700	-26.747	-0.331	1.00	21.97	B
	ATOM	3088	CB	LEU	B	811	15.015	-25.374	-0.315	1.00	21.71	B
	ATOM	3089	CG	LEU	B	811	14.081	-25.064	0.861	1.00	22.02	B
	ATOM	3090	CD1	LEU	B	811	13.701	-23.588	0.851	1.00	22.31	B
	ATOM	3091	CD2	LEU	B	811	12.837	-25.939	0.779	1.00	25.00	B
30	ATOM	3092	C	LEU	B	811	16.507	-26.900	-1.619	1.00	22.54	B
	ATOM	3093	O	LEU	B	811	15.938	-26.954	-2.714	1.00	21.82	B
	ATOM	3094	N	GLN	B	812	17.828	-26.980	-1.483	1.00	21.57	B
	ATOM	3095	CA	GLN	B	812	18.720	-27.097	-2.633	1.00	21.27	B
	ATOM	3096	CB	GLN	B	812	18.561	-28.472	-3.308	1.00	20.69	B
35	ATOM	3097	CG	GLN	B	812	19.021	-29.621	-2.404	1.00	22.08	B
	ATOM	3098	CD	GLN	B	812	19.074	-30.985	-3.097	1.00	26.58	B
	ATOM	3099	OE1	GLN	B	812	19.622	-31.944	-2.550	1.00	26.47	B
	ATOM	3100	NE2	GLN	B	812	18.501	-31.076	-4.290	1.00	25.48	B
	ATOM	3101	C	GLN	B	812	18.466	-25.963	-3.627	1.00	20.82	B
40	ATOM	3102	O	GLN	B	812	18.251	-26.189	-4.815	1.00	21.92	B
	ATOM	3103	N	VAL	B	813	18.495	-24.736	-3.114	1.00	19.44	B
	ATOM	3104	CA	VAL	B	813	18.287	-23.537	-3.923	1.00	19.33	B
	ATOM	3105	CB	VAL	B	813	18.438	-22.268	-3.045	1.00	18.90	B
	ATOM	3106	CG1	VAL	B	813	18.280	-21.007	-3.890	1.00	20.26	B
45	ATOM	3107	CG2	VAL	B	813	17.412	-22.297	-1.921	1.00	18.94	B
	ATOM	3108	C	VAL	B	813	19.287	-23.466	-5.086	1.00	18.64	B
	ATOM	3109	O	VAL	B	813	20.486	-23.680	-4.903	1.00	18.83	B
	ATOM	3110	N	SER	B	814	18.793	-23.157	-6.281	1.00	18.80	B
	ATOM	3111	CA	SER	B	814	19.652	-23.061	-7.459	1.00	18.35	B
50	ATOM	3112	CB	SER	B	814	18.863	-23.440	-8.715	1.00	18.95	B
	ATOM	3113	OG	SER	B	814	17.833	-22.498	-8.946	1.00	17.40	B
	ATOM	3114	C	SER	B	814	20.186	-21.638	-7.616	1.00	19.62	B
	ATOM	3115	O	SER	B	814	19.624	-20.695	-7.060	1.00	19.00	B
	ATOM	3116	N	GLN	B	815	21.266	-21.477	-8.375	1.00	21.03	B
55	ATOM	3117	CA	GLN	B	815	21.815	-20.142	-8.589	1.00	22.06	B
	ATOM	3118	CB	GLN	B	815	23.037	-20.177	-9.513	1.00	24.38	B
	ATOM	3119	CG	GLN	B	815	23.720	-18.810	-9.642	1.00	29.34	B

Table 2. (cont'd)

		#	Name	Res.	Chain	Res #	X	Y	Z	occ	B	SegID
	ATOM	3120	CD	GLN	B	815	24.757	-18.746	-10.754	1.00	30.23	B
5	ATOM	3121	OE1	GLN	B	815	25.384	-17.709	-10.968	1.00	35.37	B
	ATOM	3122	NE2	GLN	B	815	24.937	-19.850	-11.468	1.00	32.87	B
	ATOM	3123	C	GLN	B	815	20.758	-19.250	-9.228	1.00	21.09	B
	ATOM	3124	O	GLN	B	815	20.639	-18.073	-8.889	1.00	20.44	B
	ATOM	3125	N	GLU	B	816	19.988	-19.813	-10.153	1.00	19.51	B
10	ATOM	3126	CA	GLU	B	816	18.955	-19.038	-10.837	1.00	21.06	B
	ATOM	3127	CB	GLU	B	816	18.333	-19.862	-11.970	1.00	21.97	B
	ATOM	3128	CG	GLU	B	816	19.327	-20.221	-13.073	1.00	23.03	B
	ATOM	3129	CD	GLU	B	816	20.038	-21.547	-12.836	1.00	26.52	B
	ATOM	3130	OE1	GLU	B	816	20.073	-22.025	-11.681	1.00	23.85	B
15	ATOM	3131	OE2	GLU	B	816	20.575	-22.109	-13.813	1.00	28.20	B
	ATOM	3132	C	GLU	B	816	17.877	-18.529	-9.880	1.00	19.82	B
	ATOM	3133	O	GLU	B	816	17.435	-17.383	-9.993	1.00	19.18	B
	ATOM	3134	N	GLU	B	817	17.463	-19.367	-8.932	1.00	17.39	B
	ATOM	3135	CA	GLU	B	817	16.457	-18.956	-7.956	1.00	18.18	B
20	ATOM	3136	CB	GLU	B	817	15.983	-20.159	-7.126	1.00	18.59	B
	ATOM	3137	CG	GLU	B	817	15.397	-21.297	-7.966	1.00	22.22	B
	ATOM	3138	CD	GLU	B	817	15.064	-22.531	-7.145	1.00	23.48	B
	ATOM	3139	OE1	GLU	B	817	15.892	-22.936	-6.296	1.00	22.86	B
	ATOM	3140	OE2	GLU	B	817	13.976	-23.106	-7.363	1.00	25.72	B
25	ATOM	3141	C	GLU	B	817	17.063	-17.906	-7.030	1.00	17.11	B
	ATOM	3142	O	GLU	B	817	16.422	-16.912	-6.700	1.00	16.65	B
	ATOM	3143	N	PHE	B	818	18.305	-18.142	-6.618	1.00	16.93	B
	ATOM	3144	CA	PHE	B	818	19.018	-17.239	-5.723	1.00	16.13	B
	ATOM	3145	CB	PHE	B	818	20.435	-17.769	-5.456	1.00	16.83	B
30	ATOM	3146	CG	PHE	B	818	21.349	-16.761	-4.791	1.00	16.89	B
	ATOM	3147	CD1	PHE	B	818	21.199	-16.445	-3.442	1.00	15.26	B
	ATOM	3148	CD2	PHE	B	818	22.345	-16.115	-5.526	1.00	17.05	B
	ATOM	3149	CE1	PHE	B	818	22.027	-15.499	-2.830	1.00	16.92	B
	ATOM	3150	CE2	PHE	B	818	23.182	-15.164	-4.927	1.00	17.15	B
35	ATOM	3151	CZ	PHE	B	818	23.022	-14.855	-3.576	1.00	16.27	B
	ATOM	3152	C	PHE	B	818	19.122	-15.818	-6.278	1.00	16.33	B
	ATOM	3153	O	PHE	B	818	18.840	-14.849	-5.569	1.00	15.00	B
	ATOM	3154	N	LEU	B	819	19.538	-15.706	-7.538	1.00	14.54	B
	ATOM	3155	CA	LEU	B	819	19.716	-14.404	-8.177	1.00	16.83	B
40	ATOM	3156	CB	LEU	B	819	20.311	-14.581	-9.582	1.00	16.07	B
	ATOM	3157	CG	LEU	B	819	21.722	-15.189	-9.612	1.00	18.18	B
	ATOM	3158	CD1	LEU	B	819	22.082	-15.583	-11.026	1.00	18.54	B
	ATOM	3159	CD2	LEU	B	819	22.737	-14.192	-9.056	1.00	16.82	B
	ATOM	3160	C	LEU	B	819	18.424	-13.597	-8.245	1.00	16.62	B
45	ATOM	3161	O	LEU	B	819	18.436	-12.385	-8.027	1.00	18.04	B
	ATOM	3162	N	CYS	B	820	17.314	-14.266	-8.541	1.00	16.17	B
	ATOM	3163	CA	CYS	B	820	16.021	-13.596	-8.616	1.00	16.66	B
	ATOM	3164	CB	CYS	B	820	14.983	-14.509	-9.271	1.00	16.58	B
	ATOM	3165	SG	CYS	B	820	15.294	-14.853	-11.023	1.00	18.85	B
50	ATOM	3166	C	CYS	B	820	15.551	-13.197	-7.223	1.00	16.30	B
	ATOM	3167	O	CYS	B	820	15.032	-12.094	-7.023	1.00	14.96	B
	ATOM	3168	N	MET	B	821	15.737	-14.099	-6.263	1.00	16.45	B
	ATOM	3169	CA	MET	B	821	15.342	-13.843	-4.880	1.00	15.29	B
	ATOM	3170	CB	MET	B	821	15.607	-15.074	-4.011	1.00	16.65	B
55	ATOM	3171	CG	MET	B	821	14.675	-16.244	-4.269	1.00	17.53	B
	ATOM	3172	SD	MET	B	821	15.242	-17.726	-3.411	1.00	19.94	B

Table 2. (cont'd)

		#	Name	Res.	Chain	Res #	X	Y	Z	occ	B	SegID
	ATOM	3173	CE	MET	B	821	14.783	-17.351	-1.762	1.00	15.63	B
5	ATOM	3174	C	MET	B	821	16.110	-12.661	-4.299	1.00	15.82	B
	ATOM	3175	O	MET	B	821	15.564	-11.868	-3.535	1.00	14.99	B
	ATOM	3176	N	LYS	B	822	17.381	-12.549	-4.663	1.00	16.67	B
	ATOM	3177	CA	LYS	B	822	18.212	-11.473	-4.148	1.00	16.99	B
	ATOM	3178	CB	LYS	B	822	19.679	-11.705	-4.526	1.00	18.26	B
10	ATOM	3179	CG	LYS	B	822	20.635	-10.691	-3.906	1.00	19.96	B
	ATOM	3180	CD	LYS	B	822	22.044	-11.256	-3.763	1.00	20.99	B
	ATOM	3181	CE	LYS	B	822	22.696	-11.541	-5.110	1.00	23.13	B
	ATOM	3182	NZ	LYS	B	822	22.880	-10.302	-5.919	1.00	23.24	B
	ATOM	3183	C	LYS	B	822	17.728	-10.117	-4.644	1.00	17.98	B
15	ATOM	3184	O	LYS	B	822	17.814	-9.128	-3.922	1.00	17.23	B
	ATOM	3185	N	VAL	B	823	17.220	-10.066	-5.872	1.00	17.29	B
	ATOM	3186	CA	VAL	B	823	16.698	-8.814	-6.404	1.00	15.85	B
	ATOM	3187	CB	VAL	B	823	16.379	-8.919	-7.905	1.00	17.02	B
	ATOM	3188	CG1	VAL	B	823	15.756	-7.603	-8.397	1.00	15.78	B
20	ATOM	3189	CG2	VAL	B	823	17.650	-9.228	-8.685	1.00	15.65	B
	ATOM	3190	C	VAL	B	823	15.412	-8.467	-5.653	1.00	15.49	B
	ATOM	3191	O	VAL	B	823	15.155	-7.306	-5.340	1.00	14.04	B
	ATOM	3192	N	LEU	B	824	14.603	-9.478	-5.356	1.00	14.47	B
	ATOM	3193	CA	LEU	B	824	13.361	-9.240	-4.631	1.00	15.65	B
25	ATOM	3194	CB	LEU	B	824	12.525	-10.523	-4.584	1.00	15.79	B
	ATOM	3195	CG	LEU	B	824	11.928	-10.911	-5.942	1.00	18.34	B
	ATOM	3196	CD1	LEU	B	824	11.245	-12.262	-5.835	1.00	17.24	B
	ATOM	3197	CD2	LEU	B	824	10.933	-9.842	-6.393	1.00	16.65	B
	ATOM	3198	C	LEU	B	824	13.667	-8.730	-3.223	1.00	16.46	B
30	ATOM	3199	O	LEU	B	824	12.907	-7.931	-2.662	1.00	17.28	B
	ATOM	3200	N	LEU	B	825	14.781	-9.184	-2.656	1.00	16.24	B
	ATOM	3201	CA	LEU	B	825	15.190	-8.721	-1.324	1.00	17.69	B
	ATOM	3202	CB	LEU	B	825	16.463	-9.419	-0.861	1.00	17.38	B
	ATOM	3203	CG	LEU	B	825	16.366	-10.560	0.141	1.00	23.00	B
35	ATOM	3204	CD1	LEU	B	825	17.767	-10.795	0.695	1.00	19.06	B
	ATOM	3205	CD2	LEU	B	825	15.396	-10.217	1.276	1.00	21.23	B
	ATOM	3206	C	LEU	B	825	15.472	-7.227	-1.360	1.00	15.92	B
	ATOM	3207	O	LEU	B	825	15.111	-6.492	-0.441	1.00	15.49	B
	ATOM	3208	N	LEU	B	826	16.151	-6.793	-2.416	1.00	15.55	B
40	ATOM	3209	CA	LEU	B	826	16.477	-5.380	-2.587	1.00	15.43	B
	ATOM	3210	CB	LEU	B	826	17.235	-5.179	-3.906	1.00	13.00	B
	ATOM	3211	CG	LEU	B	826	17.367	-3.755	-4.447	1.00	17.08	B
	ATOM	3212	CD1	LEU	B	826	18.309	-2.932	-3.565	1.00	15.15	B
	ATOM	3213	CD2	LEU	B	826	17.880	-3.813	-5.893	1.00	15.84	B
45	ATOM	3214	C	LEU	B	826	15.192	-4.552	-2.605	1.00	15.22	B
	ATOM	3215	O	LEU	B	826	15.159	-3.417	-2.123	1.00	15.10	B
	ATOM	3216	N	LEU	B	827	14.134	-5.146	-3.148	1.00	14.61	B
	ATOM	3217	CA	LEU	B	827	12.835	-4.487	-3.287	1.00	17.58	B
	ATOM	3218	CB	LEU	B	827	12.261	-4.795	-4.678	1.00	16.81	B
50	ATOM	3219	CG	LEU	B	827	13.201	-4.610	-5.872	1.00	19.46	B
	ATOM	3220	CD1	LEU	B	827	12.564	-5.176	-7.146	1.00	18.89	B
	ATOM	3221	CD2	LEU	B	827	13.519	-3.131	-6.032	1.00	15.57	B
	ATOM	3222	C	LEU	B	827	11.827	-4.961	-2.253	1.00	16.56	B
	ATOM	3223	O	LEU	B	827	10.625	-4.866	-2.487	1.00	18.58	B
55	ATOM	3224	N	ASN	B	828	12.299	-5.438	-1.106	1.00	15.56	B
	ATOM	3225	CA	ASN	B	828	11.380	-5.998	-0.125	1.00	17.84	B

Table 2. (cont'd)

		#	Name	Res.	Chain	Res #	X	Y	Z	occ	B	SegID
	ATOM	3226	CB	ASN	B	828	11.992	-7.291	0.421	1.00	19.91	B
5	ATOM	3227	CG	ASN	B	828	10.986	-8.423	0.503	1.00	24.26	B
	ATOM	3228	OD1	ASN	B	828	10.082	-8.524	-0.328	1.00	24.73	B
	ATOM	3229	ND2	ASN	B	828	11.153	-9.294	1.495	1.00	24.40	B
	ATOM	3230	C	ASN	B	828	10.894	-5.105	1.022	1.00	17.27	B
	ATOM	3231	O	ASN	B	828	10.137	-5.558	1.879	1.00	16.66	B
10	ATOM	3232	N	THR	B	829	11.323	-3.848	1.037	1.00	14.98	B
	ATOM	3233	CA	THR	B	829	10.896	-2.903	2.063	1.00	18.37	B
	ATOM	3234	CB	THR	B	829	11.914	-2.802	3.232	1.00	18.06	B
	ATOM	3235	OG1	THR	B	829	12.146	-4.102	3.789	1.00	17.88	B
	ATOM	3236	CG2	THR	B	829	11.372	-1.889	4.321	1.00	20.06	B
15	ATOM	3237	C	THR	B	829	10.775	-1.523	1.426	1.00	18.82	B
	ATOM	3238	O	THR	B	829	11.607	-1.151	0.595	1.00	17.50	B
	ATOM	3239	N	ILE	B	830	9.736	-0.775	1.792	1.00	17.45	B
	ATOM	3240	CA	ILE	B	830	9.548	0.572	1.258	1.00	19.79	B
	ATOM	3241	CB	ILE	B	830	8.523	0.594	0.089	1.00	20.43	B
20	ATOM	3242	CG2	ILE	B	830	8.982	-0.346	-1.019	1.00	19.43	B
	ATOM	3243	CG1	ILE	B	830	7.133	0.200	0.592	1.00	21.42	B
	ATOM	3244	CD1	ILE	B	830	6.083	0.164	-0.493	1.00	22.07	B
	ATOM	3245	C	ILE	B	830	9.084	1.522	2.366	1.00	19.09	B
	ATOM	3246	O	ILE	B	830	8.680	1.080	3.440	1.00	21.03	B
25	ATOM	3247	N	PRO	B	831	9.159	2.840	2.126	1.00	19.68	B
	ATOM	3248	CD	PRO	B	831	9.738	3.505	0.949	1.00	18.90	B
	ATOM	3249	CA	PRO	B	831	8.738	3.828	3.129	1.00	21.03	B
	ATOM	3250	CB	PRO	B	831	9.057	5.164	2.460	1.00	20.87	B
	ATOM	3251	CG	PRO	B	831	10.192	4.821	1.528	1.00	22.56	B
30	ATOM	3252	C	PRO	B	831	7.252	3.696	3.428	1.00	22.30	B
	ATOM	3253	O	PRO	B	831	6.498	3.183	2.608	1.00	22.00	B
	ATOM	3254	N	LEU	B	832	6.827	4.161	4.597	1.00	23.69	B
	ATOM	3255	CA	LEU	B	832	5.413	4.088	4.957	1.00	26.10	B
	ATOM	3256	CB	LEU	B	832	5.190	4.686	6.351	1.00	26.82	B
35	ATOM	3257	CG	LEU	B	832	5.745	3.874	7.529	1.00	26.56	B
	ATOM	3258	CD1	LEU	B	832	5.599	4.667	8.820	1.00	28.10	B
	ATOM	3259	CD2	LEU	B	832	5.002	2.551	7.628	1.00	27.65	B
	ATOM	3260	C	LEU	B	832	4.550	4.823	3.929	1.00	26.82	B
	ATOM	3261	O	LEU	B	832	3.442	4.392	3.614	1.00	26.75	B
40	ATOM	3262	N	GLU	B	833	5.070	5.928	3.403	1.00	27.88	B
	ATOM	3263	CA	GLU	B	833	4.347	6.719	2.414	1.00	29.18	B
	ATOM	3264	CB	GLU	B	833	4.808	8.180	2.461	1.00	31.58	B
	ATOM	3265	CG	GLU	B	833	6.300	8.368	2.212	1.00	33.80	B
	ATOM	3266	CD	GLU	B	833	7.141	8.184	3.467	1.00	34.56	B
45	ATOM	3267	OE1	GLU	B	833	6.840	7.282	4.272	1.00	34.98	B
	ATOM	3268	OE2	GLU	B	833	8.119	8.938	3.643	1.00	36.68	B
	ATOM	3269	C	GLU	B	833	4.559	6.163	1.007	1.00	29.05	B
	ATOM	3270	O	GLU	B	833	4.009	6.682	0.032	1.00	30.18	B
	ATOM	3271	N	GLY	B	834	5.354	5.104	0.901	1.00	25.32	B
50	ATOM	3272	CA	GLY	B	834	5.616	4.520	-0.398	1.00	23.75	B
	ATOM	3273	C	GLY	B	834	6.766	5.233	-1.087	1.00	24.18	B
	ATOM	3274	O	GLY	B	834	7.334	6.179	-0.547	1.00	22.28	B
	ATOM	3275	N	LEU	B	835	7.106	4.779	-2.288	1.00	23.91	B
	ATOM	3276	CA	LEU	B	835	8.196	5.368	-3.049	1.00	24.07	B
55	ATOM	3277	CB	LEU	B	835	8.885	4.283	-3.871	1.00	23.41	B
	ATOM	3278	CG	LEU	B	835	9.564	3.167	-3.074	1.00	22.91	B

Table 2. (cont'd)

		#	Name	Res.	Chain	Res #	X	Y	Z	occ	B	SegID
	ATOM	3279	CD1	LEU	B	835	9.954	2.031	-4.003	1.00	21.52	B
5	ATOM	3280	CD2	LEU	B	835	10.778	3.732	-2.361	1.00	22.16	B
	ATOM	3281	C	LEU	B	835	7.697	6.465	-3.982	1.00	25.22	B
	ATOM	3282	O	LEU	B	835	6.494	6.599	-4.214	1.00	23.05	B
	ATOM	3283	N	ARG	B	836	8.625	7.250	-4.518	1.00	25.18	B
	ATOM	3284	CA	ARG	B	836	8.251	8.305	-5.450	1.00	27.41	B
10	ATOM	3285	CB	ARG	B	836	9.410	9.289	-5.629	1.00	29.23	B
	ATOM	3286	CG	ARG	B	836	9.790	9.972	-4.326	1.00	33.63	B
	ATOM	3287	CD	ARG	B	836	10.699	11.168	-4.531	1.00	39.98	B
	ATOM	3288	NE	ARG	B	836	11.086	11.742	-3.244	1.00	46.27	B
	ATOM	3289	CZ	ARG	B	836	11.726	12.897	-3.091	1.00	48.81	B
15	ATOM	3290	NH1	ARG	B	836	12.032	13.327	-1.873	1.00	50.05	B
	ATOM	3291	NH2	ARG	B	836	12.059	13.623	-4.152	1.00	50.02	B
	ATOM	3292	C	ARG	B	836	7.874	7.644	-6.774	1.00	25.29	B
	ATOM	3293	O	ARG	B	836	6.886	8.015	-7.405	1.00	25.23	B
	ATOM	3294	N	SER	B	837	8.652	6.641	-7.174	1.00	23.28	B
20	ATOM	3295	CA	SER	B	837	8.387	5.906	-8.408	1.00	21.91	B
	ATOM	3296	CB	SER	B	837	9.696	5.609	-9.138	1.00	22.60	B
	ATOM	3297	OG	SER	B	837	10.416	6.806	-9.380	1.00	24.64	B
	ATOM	3298	C	SER	B	837	7.693	4.597	-8.046	1.00	21.70	B
	ATOM	3299	O	SER	B	837	8.145	3.518	-8.427	1.00	19.42	B
25	ATOM	3300	N	GLN	B	838	6.593	4.707	-7.307	1.00	21.26	B
	ATOM	3301	CA	GLN	B	838	5.831	3.544	-6.862	1.00	22.08	B
	ATOM	3302	CB	GLN	B	838	4.618	4.004	-6.040	1.00	22.63	B
	ATOM	3303	CG	GLN	B	838	3.915	2.893	-5.259	1.00	26.54	B
	ATOM	3304	CD	GLN	B	838	4.822	2.234	-4.226	1.00	26.15	B
30	ATOM	3305	OE1	GLN	B	838	5.562	2.909	-3.513	1.00	27.61	B
	ATOM	3306	NE2	GLN	B	838	4.755	0.911	-4.135	1.00	27.61	B
	ATOM	3307	C	GLN	B	838	5.368	2.647	-8.012	1.00	21.61	B
	ATOM	3308	O	GLN	B	838	5.515	1.427	-7.949	1.00	20.05	B
	ATOM	3309	N	THR	B	839	4.812	3.249	-9.062	1.00	22.33	B
35	ATOM	3310	CA	THR	B	839	4.336	2.479	-10.207	1.00	22.29	B
	ATOM	3311	CB	THR	B	839	3.694	3.386	-11.276	1.00	24.97	B
	ATOM	3312	OG1	THR	B	839	2.579	4.077	-10.702	1.00	27.76	B
	ATOM	3313	CG2	THR	B	839	3.206	2.555	-12.460	1.00	24.83	B
	ATOM	3314	C	THR	B	839	5.463	1.690	-10.855	1.00	20.46	B
40	ATOM	3315	O	THR	B	839	5.321	0.498	-11.118	1.00	21.42	B
	ATOM	3316	N	GLN	B	840	6.582	2.354	-11.111	1.00	19.38	B
	ATOM	3317	CA	GLN	B	840	7.725	1.690	-11.722	1.00	21.53	B
	ATOM	3318	CB	GLN	B	840	8.831	2.702	-12.013	1.00	25.28	B
	ATOM	3319	CG	GLN	B	840	10.059	2.081	-12.661	1.00	33.27	B
45	ATOM	3320	CD	GLN	B	840	9.737	1.408	-13.983	1.00	37.68	B
	ATOM	3321	OE1	GLN	B	840	9.410	2.073	-14.968	1.00	41.19	B
	ATOM	3322	NE2	GLN	B	840	9.818	0.078	-14.009	1.00	41.64	B
	ATOM	3323	C	GLN	B	840	8.259	0.599	-10.793	1.00	20.93	B
	ATOM	3324	O	GLN	B	840	8.638	-0.477	-11.242	1.00	22.03	B
50	ATOM	3325	N	PHE	B	841	8.287	0.891	-9.498	1.00	18.17	B
	ATOM	3326	CA	PHE	B	841	8.764	-0.065	-8.499	1.00	17.96	B
	ATOM	3327	CB	PHE	B	841	8.654	0.540	-7.097	1.00	16.53	B
	ATOM	3328	CG	PHE	B	841	8.826	-0.464	-5.982	1.00	17.42	B
	ATOM	3329	CD1	PHE	B	841	10.092	-0.912	-5.612	1.00	19.52	B
55	ATOM	3330	CD2	PHE	B	841	7.718	-0.953	-5.296	1.00	16.29	B
	ATOM	3331	CE1	PHE	B	841	10.250	-1.832	-4.570	1.00	15.82	B

Table 2. (cont'd)

		#	Name	Res.	Chain	Res #	X	Y	Z	occ	B	SegID
5	ATOM	3332	CE2	PHE	B	841	7.867	-1.877	-4.253	1.00	18.30	B
	ATOM	3333	CZ	PHE	B	841	9.139	-2.313	-3.893	1.00	16.42	B
	ATOM	3334	C	PHE	B	841	7.938	-1.341	-8.554	1.00	18.36	B
	ATOM	3335	O	PHE	B	841	8.474	-2.447	-8.625	1.00	16.92	B
	ATOM	3336	N	GLU	B	842	6.624	-1.181	-8.524	1.00	18.46	B
10	ATOM	3337	CA	GLU	B	842	5.742	-2.333	-8.552	1.00	20.40	B
	ATOM	3338	CB	GLU	B	842	4.300	-1.874	-8.320	1.00	22.60	B
	ATOM	3339	CG	GLU	B	842	3.992	-1.716	-6.831	1.00	28.47	B
	ATOM	3340	CD	GLU	B	842	2.778	-0.855	-6.553	1.00	33.41	B
	ATOM	3341	OE1	GLU	B	842	1.849	-0.848	-7.387	1.00	35.95	B
15	ATOM	3342	OE2	GLU	B	842	2.748	-0.194	-5.490	1.00	34.10	B
	ATOM	3343	C	GLU	B	842	5.885	-3.159	-9.824	1.00	19.29	B
	ATOM	3344	O	GLU	B	842	5.856	-4.388	-9.769	1.00	18.69	B
	ATOM	3345	N	GLU	B	843	6.053	-2.492	-10.962	1.00	19.28	B
	ATOM	3346	CA	GLU	B	843	6.234	-3.194	-12.229	1.00	20.40	B
20	ATOM	3347	CB	GLU	B	843	6.279	-2.195	-13.391	1.00	23.21	B
	ATOM	3348	CG	GLU	B	843	4.908	-1.670	-13.817	1.00	26.48	B
	ATOM	3349	CD	GLU	B	843	4.993	-0.619	-14.912	1.00	28.27	B
	ATOM	3350	OE1	GLU	B	843	5.906	-0.710	-15.761	1.00	31.59	B
	ATOM	3351	OE2	GLU	B	843	4.140	0.289	-14.933	1.00	30.69	B
25	ATOM	3352	C	GLU	B	843	7.542	-3.984	-12.180	1.00	21.13	B
	ATOM	3353	O	GLU	B	843	7.600	-5.147	-12.580	1.00	20.25	B
	ATOM	3354	N	MET	B	844	8.594	-3.339	-11.684	1.00	20.24	B
	ATOM	3355	CA	MET	B	844	9.892	-3.984	-11.574	1.00	21.25	B
	ATOM	3356	CB	MET	B	844	10.920	-3.004	-11.001	1.00	21.39	B
30	ATOM	3357	CG	MET	B	844	12.315	-3.597	-10.878	1.00	21.13	B
	ATOM	3358	SD	MET	B	844	13.560	-2.448	-10.248	1.00	19.73	B
	ATOM	3359	CE	MET	B	844	14.982	-3.557	-10.182	1.00	17.38	B
	ATOM	3360	C	MET	B	844	9.787	-5.222	-10.679	1.00	21.40	B
	ATOM	3361	O	MET	B	844	10.238	-6.309	-11.045	1.00	21.49	B
35	ATOM	3362	N	ARG	B	845	9.183	-5.056	-9.509	1.00	21.07	B
	ATOM	3363	CA	ARG	B	845	9.026	-6.170	-8.584	1.00	22.63	B
	ATOM	3364	CB	ARG	B	845	8.320	-5.683	-7.317	1.00	23.95	B
	ATOM	3365	CG	ARG	B	845	8.324	-6.666	-6.164	1.00	27.11	B
	ATOM	3366	CD	ARG	B	845	7.705	-6.032	-4.922	1.00	25.54	B
40	ATOM	3367	NE	ARG	B	845	7.297	-7.039	-3.953	1.00	27.61	B
	ATOM	3368	CZ	ARG	B	845	8.134	-7.751	-3.208	1.00	30.27	B
	ATOM	3369	NH1	ARG	B	845	7.654	-8.651	-2.359	1.00	32.12	B
	ATOM	3370	NH2	ARG	B	845	9.447	-7.552	-3.295	1.00	28.99	B
	ATOM	3371	C	ARG	B	845	8.250	-7.329	-9.236	1.00	23.19	B
45	ATOM	3372	O	ARG	B	845	8.662	-8.485	-9.139	1.00	22.55	B
	ATOM	3373	N	SER	B	846	7.144	-7.021	-9.912	1.00	21.82	B
	ATOM	3374	CA	SER	B	846	6.349	-8.057	-10.572	1.00	23.07	B
	ATOM	3375	CB	SER	B	846	5.115	-7.449	-11.252	1.00	24.12	B
	ATOM	3376	OG	SER	B	846	4.220	-6.922	-10.293	1.00	26.05	B
50	ATOM	3377	C	SER	B	846	7.184	-8.791	-11.614	1.00	22.04	B
	ATOM	3378	O	SER	B	846	7.058	-10.003	-11.777	1.00	24.09	B
	ATOM	3379	N	SER	B	847	8.028	-8.048	-12.324	1.00	21.69	B
	ATOM	3380	CA	SER	B	847	8.888	-8.629	-13.345	1.00	22.04	B
	ATOM	3381	CB	SER	B	847	9.734	-7.545	-14.020	1.00	24.55	B
55	ATOM	3382	OG	SER	B	847	8.929	-6.652	-14.771	1.00	31.05	B
	ATOM	3383	C	SER	B	847	9.816	-9.682	-12.748	1.00	20.47	B
	ATOM	3384	O	SER	B	847	9.948	-10.781	-13.281	1.00	21.10	B

Table 2. (cont'd)

		#	Name	Res.	Chain	Res #	X	Y	Z	occ	B	SegID
5	ATOM	3385	N	TYR	B	848	10.468	-9.343	-11.644	1.00	19.70	B
	ATOM	3386	CA	TYR	B	848	11.379	-10.279	-11.010	1.00	18.31	B
	ATOM	3387	CB	TYR	B	848	12.288	-9.526	-10.043	1.00	19.17	B
	ATOM	3388	CG	TYR	B	848	13.362	-8.765	-10.800	1.00	19.76	B
	ATOM	3389	CD1	TYR	B	848	14.496	-9.425	-11.279	1.00	18.70	B
10	ATOM	3390	CE1	TYR	B	848	15.462	-8.756	-12.026	1.00	16.37	B
	ATOM	3391	CD2	TYR	B	848	13.218	-7.407	-11.088	1.00	18.08	B
	ATOM	3392	CE2	TYR	B	848	14.182	-6.726	-11.839	1.00	17.62	B
	ATOM	3393	CZ	TYR	B	848	15.301	-7.409	-12.302	1.00	19.15	B
	ATOM	3394	OH	TYR	B	848	16.272	-6.751	-13.028	1.00	17.87	B
15	ATOM	3395	C	TYR	B	848	10.641	-11.431	-10.338	1.00	18.15	B
	ATOM	3396	O	TYR	B	848	11.180	-12.529	-10.214	1.00	18.25	B
	ATOM	3397	N	ILE	B	849	9.411	-11.191	-9.903	1.00	18.38	B
	ATOM	3398	CA	ILE	B	849	8.631	-12.274	-9.316	1.00	20.21	B
	ATOM	3399	CB	ILE	B	849	7.286	-11.758	-8.723	1.00	21.49	B
20	ATOM	3400	CG2	ILE	B	849	6.368	-12.929	-8.395	1.00	21.35	B
	ATOM	3401	CG1	ILE	B	849	7.557	-10.955	-7.446	1.00	22.56	B
	ATOM	3402	CD1	ILE	B	849	6.316	-10.343	-6.811	1.00	21.72	B
	ATOM	3403	C	ILE	B	849	8.375	-13.255	-10.474	1.00	21.64	B
	ATOM	3404	O	ILE	B	849	8.468	-14.471	-10.309	1.00	22.27	B
25	ATOM	3405	N	ARG	B	850	8.080	-12.724	-11.659	1.00	22.31	B
	ATOM	3406	CA	ARG	B	850	7.849	-13.588	-12.813	1.00	24.41	B
	ATOM	3407	CB	ARG	B	850	7.375	-12.781	-14.030	1.00	26.21	B
	ATOM	3408	CG	ARG	B	850	5.921	-12.320	-13.957	1.00	28.80	B
	ATOM	3409	CD	ARG	B	850	5.417	-11.832	-15.319	1.00	29.74	B
30	ATOM	3410	NE	ARG	B	850	5.971	-10.537	-15.710	1.00	30.41	B
	ATOM	3411	CZ	ARG	B	850	5.629	-9.378	-15.152	1.00	31.78	B
	ATOM	3412	NH1	ARG	B	850	4.733	-9.348	-14.175	1.00	33.98	B
	ATOM	3413	NH2	ARG	B	850	6.178	-8.247	-15.571	1.00	29.88	B
	ATOM	3414	C	ARG	B	850	9.128	-14.329	-13.181	1.00	25.13	B
35	ATOM	3415	O	ARG	B	850	9.090	-15.501	-13.568	1.00	26.48	B
	ATOM	3416	N	GLU	B	851	10.263	-13.649	-13.058	1.00	22.96	B
	ATOM	3417	CA	GLU	B	851	11.541	-14.258	-13.402	1.00	22.01	B
	ATOM	3418	CB	GLU	B	851	12.647	-13.196	-13.394	1.00	22.35	B
	ATOM	3419	CG	GLU	B	851	13.838	-13.513	-14.289	1.00	21.41	B
40	ATOM	3420	CD	GLU	B	851	13.454	-13.712	-15.756	1.00	25.43	B
	ATOM	3421	OE1	GLU	B	851	12.520	-13.035	-16.241	1.00	25.41	B
	ATOM	3422	OE2	GLU	B	851	14.103	-14.540	-16.435	1.00	26.71	B
	ATOM	3423	C	GLU	B	851	11.856	-15.386	-12.423	1.00	22.31	B
	ATOM	3424	O	GLU	B	851	12.408	-16.416	-12.814	1.00	22.61	B
45	ATOM	3425	N	LEU	B	852	11.497	-15.196	-11.155	1.00	22.07	B
	ATOM	3426	CA	LEU	B	852	11.718	-16.226	-10.140	1.00	21.52	B
	ATOM	3427	CB	LEU	B	852	11.274	-15.724	-8.759	1.00	19.90	B
	ATOM	3428	CG	LEU	B	852	11.214	-16.726	-7.598	1.00	18.71	B
	ATOM	3429	CD1	LEU	B	852	12.577	-17.352	-7.373	1.00	20.12	B
50	ATOM	3430	CD2	LEU	B	852	10.747	-16.017	-6.331	1.00	19.80	B
	ATOM	3431	C	LEU	B	852	10.910	-17.468	-10.520	1.00	22.67	B
	ATOM	3432	O	LEU	B	852	11.369	-18.602	-10.354	1.00	20.55	B
	ATOM	3433	N	ILE	B	853	9.699	-17.248	-11.023	1.00	22.76	B
	ATOM	3434	CA	ILE	B	853	8.852	-18.360	-11.429	1.00	23.15	B
55	ATOM	3435	CB	ILE	B	853	7.472	-17.855	-11.899	1.00	23.96	B
	ATOM	3436	CG2	ILE	B	853	6.652	-19.005	-12.471	1.00	22.33	B
	ATOM	3437	CG1	ILE	B	853	6.741	-17.212	-10.714	1.00	22.16	B

Table 2. (cont'd)

		#	Name	Res.	Chain	Res #	X	Y	Z	occ	B	SegID
	ATOM	3438	CD1	ILE	B	853	5.362	-16.673	-11.052	1.00	24.56	B
5	ATOM	3439	C	ILE	B	853	9.559	-19.127	-12.542	1.00	22.87	B
	ATOM	3440	O	ILE	B	853	9.636	-20.357	-12.505	1.00	22.24	B
	ATOM	3441	N	LYS	B	854	10.097	-18.401	-13.519	1.00	23.12	B
	ATOM	3442	CA	LYS	B	854	10.828	-19.033	-14.612	1.00	23.82	B
	ATOM	3443	CB	LYS	B	854	11.408	-17.987	-15.567	1.00	24.73	B
10	ATOM	3444	CG	LYS	B	854	10.411	-17.073	-16.253	1.00	27.55	B
	ATOM	3445	CD	LYS	B	854	11.172	-16.123	-17.173	1.00	29.14	B
	ATOM	3446	CE	LYS	B	854	10.282	-15.067	-17.796	1.00	30.68	B
	ATOM	3447	NZ	LYS	B	854	11.116	-14.097	-18.571	1.00	30.20	B
	ATOM	3448	C	LYS	B	854	11.990	-19.839	-14.025	1.00	24.39	B
15	ATOM	3449	O	LYS	B	854	12.232	-20.987	-14.417	1.00	23.69	B
	ATOM	3450	N	ALA	B	855	12.712	-19.223	-13.089	1.00	22.20	B
	ATOM	3451	CA	ALA	B	855	13.851	-19.872	-12.446	1.00	21.90	B
	ATOM	3452	CB	ALA	B	855	14.454	-18.949	-11.371	1.00	20.12	B
	ATOM	3453	C	ALA	B	855	13.430	-21.197	-11.825	1.00	22.62	B
20	ATOM	3454	O	ALA	B	855	14.129	-22.199	-11.954	1.00	22.66	B
	ATOM	3455	N	ILE	B	856	12.284	-21.196	-11.152	1.00	24.17	B
	ATOM	3456	CA	ILE	B	856	11.765	-22.401	-10.511	1.00	26.32	B
	ATOM	3457	CB	ILE	B	856	10.527	-22.063	-9.646	1.00	25.90	B
	ATOM	3458	CG2	ILE	B	856	9.780	-23.332	-9.263	1.00	26.41	B
25	ATOM	3459	CG1	ILE	B	856	10.962	-21.282	-8.402	1.00	25.34	B
	ATOM	3460	CD1	ILE	B	856	9.812	-20.728	-7.575	1.00	23.16	B
	ATOM	3461	C	ILE	B	856	11.385	-23.455	-11.558	1.00	28.99	B
	ATOM	3462	O	ILE	B	856	11.572	-24.655	-11.342	1.00	29.74	B
	ATOM	3463	N	GLY	B	857	10.864	-22.989	-12.692	1.00	29.48	B
30	ATOM	3464	CA	GLY	B	857	10.446	-23.883	-13.761	1.00	30.13	B
	ATOM	3465	C	GLY	B	857	11.580	-24.580	-14.482	1.00	31.17	B
	ATOM	3466	O	GLY	B	857	11.366	-25.568	-15.188	1.00	30.36	B
	ATOM	3467	N	LEU	B	858	12.792	-24.071	-14.312	1.00	30.74	B
	ATOM	3468	CA	LEU	B	858	13.944	-24.676	-14.954	1.00	33.55	B
35	ATOM	3469	CB	LEU	B	858	15.199	-23.831	-14.713	1.00	30.85	B
	ATOM	3470	CG	LEU	B	858	15.263	-22.461	-15.392	1.00	29.83	B
	ATOM	3471	CD1	LEU	B	858	16.541	-21.749	-14.968	1.00	29.15	B
	ATOM	3472	CD2	LEU	B	858	15.222	-22.628	-16.914	1.00	29.41	B
	ATOM	3473	C	LEU	B	858	14.163	-26.090	-14.424	1.00	36.01	B
40	ATOM	3474	O	LEU	B	858	14.733	-26.933	-15.114	1.00	34.89	B
	ATOM	3475	N	ARG	B	859	13.697	-26.344	-13.204	1.00	38.73	B
	ATOM	3476	CA	ARG	B	859	13.862	-27.652	-12.585	1.00	43.94	B
	ATOM	3477	CB	ARG	B	859	14.929	-27.562	-11.490	1.00	45.40	B
	ATOM	3478	CG	ARG	B	859	16.243	-27.004	-12.026	1.00	47.91	B
45	ATOM	3479	CD	ARG	B	859	17.346	-26.903	-10.988	1.00	50.31	B
	ATOM	3480	NE	ARG	B	859	18.531	-26.277	-11.574	1.00	53.12	B
	ATOM	3481	CZ	ARG	B	859	19.713	-26.166	-10.973	1.00	54.97	B
	ATOM	3482	NH1	ARG	B	859	19.895	-26.641	-9.746	1.00	55.64	B
	ATOM	3483	NH2	ARG	B	859	20.718	-25.573	-11.605	1.00	54.67	B
50	ATOM	3484	C	ARG	B	859	12.555	-28.221	-12.032	1.00	46.55	B
	ATOM	3485	O	ARG	B	859	12.298	-29.420	-12.159	1.00	47.71	B
	ATOM	3486	N	GLN	B	860	11.730	-27.369	-11.427	1.00	49.36	B
	ATOM	3487	CA	GLN	B	860	10.444	-27.812	-10.884	1.00	51.49	B
	ATOM	3488	CB	GLN	B	860	9.925	-26.819	-9.842	1.00	53.00	B
55	ATOM	3489	CG	GLN	B	860	10.879	-26.585	-8.679	1.00	56.02	B
	ATOM	3490	CD	GLN	B	860	11.123	-27.832	-7.849	1.00	57.66	B

Table 2. (cont'd)

		#	Name	Res.	Chain	Res #	X	Y	Z	occ	B	SegID
5	ATOM	3491	OE1	GLN	B	860	11.981	-27.843	-6.963	1.00	59.53	B
	ATOM	3492	NE2	GLN	B	860	10.367	-28.888	-8.125	1.00	58.86	B
	ATOM	3493	C	GLN	B	860	9.453	-27.913	-12.036	1.00	52.06	B
	ATOM	3494	O	GLN	B	860	8.769	-26.945	-12.370	1.00	52.54	B
	ATOM	3495	N	LYS	B	861	9.384	-29.097	-12.633	1.00	52.72	B
10	ATOM	3496	CA	LYS	B	861	8.514	-29.353	-13.775	1.00	53.52	B
	ATOM	3497	CB	LYS	B	861	8.954	-30.648	-14.463	1.00	54.01	B
	ATOM	3498	CG	LYS	B	861	10.407	-30.634	-14.922	1.00	54.24	B
	ATOM	3499	CD	LYS	B	861	10.654	-29.511	-15.920	1.00	55.39	B
	ATOM	3500	CE	LYS	B	861	12.105	-29.470	-16.371	1.00	55.75	B
15	ATOM	3501	NZ	LYS	B	861	12.329	-28.410	-17.394	1.00	54.73	B
	ATOM	3502	C	LYS	B	861	7.017	-29.415	-13.470	1.00	53.18	B
	ATOM	3503	O	LYS	B	861	6.199	-28.967	-14.272	1.00	54.01	B
	ATOM	3504	N	GLY	B	862	6.657	-29.969	-12.318	1.00	53.04	B
	ATOM	3505	CA	GLY	B	862	5.250	-30.072	-11.968	1.00	52.10	B
20	ATOM	3506	C	GLY	B	862	4.610	-28.753	-11.577	1.00	51.07	B
	ATOM	3507	O	GLY	B	862	5.248	-27.909	-10.952	1.00	50.08	B
	ATOM	3508	N	VAL	B	863	3.345	-28.574	-11.946	1.00	50.57	B
	ATOM	3509	CA	VAL	B	863	2.620	-27.352	-11.615	1.00	50.24	B
	ATOM	3510	CB	VAL	B	863	1.237	-27.312	-12.305	1.00	50.56	B
25	ATOM	3511	CG1	VAL	B	863	1.411	-27.323	-13.814	1.00	50.62	B
	ATOM	3512	CG2	VAL	B	863	0.392	-28.498	-11.859	1.00	51.12	B
	ATOM	3513	C	VAL	B	863	2.419	-27.254	-10.104	1.00	49.58	B
	ATOM	3514	O	VAL	B	863	2.575	-26.184	-9.512	1.00	48.75	B
	ATOM	3515	N	VAL	B	864	2.073	-28.379	-9.486	1.00	48.74	B
30	ATOM	3516	CA	VAL	B	864	1.858	-28.430	-8.044	1.00	47.66	B
	ATOM	3517	CB	VAL	B	864	1.255	-29.784	-7.619	1.00	47.83	B
	ATOM	3518	CG1	VAL	B	864	1.003	-29.793	-6.120	1.00	49.12	B
	ATOM	3519	CG2	VAL	B	864	-0.036	-30.036	-8.376	1.00	48.15	B
	ATOM	3520	C	VAL	B	864	3.201	-28.248	-7.346	1.00	46.26	B
35	ATOM	3521	O	VAL	B	864	3.312	-27.514	-6.363	1.00	45.73	B
	ATOM	3522	N	SER	B	865	4.216	-28.928	-7.869	1.00	44.35	B
	ATOM	3523	CA	SER	B	865	5.566	-28.850	-7.331	1.00	42.44	B
	ATOM	3524	CB	SER	B	865	6.481	-29.811	-8.097	1.00	43.32	B
	ATOM	3525	OG	SER	B	865	7.814	-29.753	-7.619	1.00	46.42	B
40	ATOM	3526	C	SER	B	865	6.089	-27.414	-7.455	1.00	40.83	B
	ATOM	3527	O	SER	B	865	6.677	-26.873	-6.519	1.00	38.94	B
	ATOM	3528	N	SER	B	866	5.866	-26.807	-8.617	1.00	39.03	B
	ATOM	3529	CA	SER	B	866	6.302	-25.440	-8.875	1.00	38.13	B
	ATOM	3530	CB	SER	B	866	5.976	-25.041	-10.315	1.00	39.12	B
45	ATOM	3531	OG	SER	B	866	6.795	-25.745	-11.230	1.00	42.05	B
	ATOM	3532	C	SER	B	866	5.655	-24.447	-7.922	1.00	37.24	B
	ATOM	3533	O	SER	B	866	6.320	-23.545	-7.408	1.00	36.71	B
	ATOM	3534	N	SER	B	867	4.357	-24.610	-7.690	1.00	35.62	B
	ATOM	3535	CA	SER	B	867	3.635	-23.716	-6.794	1.00	35.02	B
50	ATOM	3536	CB	SER	B	867	2.132	-23.979	-6.875	1.00	35.17	B
	ATOM	3537	OG	SER	B	867	1.654	-23.704	-8.180	1.00	38.33	B
	ATOM	3538	C	SER	B	867	4.116	-23.882	-5.361	1.00	34.04	B
	ATOM	3539	O	SER	B	867	4.285	-22.900	-4.640	1.00	33.31	B
	ATOM	3540	N	GLN	B	868	4.335	-25.124	-4.945	1.00	31.60	B
55	ATOM	3541	CA	GLN	B	868	4.810	-25.373	-3.592	1.00	32.33	B
	ATOM	3542	CB	GLN	B	868	4.856	-26.871	-3.308	1.00	34.57	B
	ATOM	3543	CG	GLN	B	868	3.502	-27.494	-3.071	1.00	39.81	B

Table 2. (cont'd)

		#	Name	Res.	Chain	Res	#	X	Y	Z	occ	B	SegID
	ATOM	3544	CD	GLN	B	868		3.579	-28.998	-2.949	1.00	42.53	B
5	ATOM	3545	OE1	GLN	B	868		4.411	-29.530	-2.213	1.00	45.19	B
	ATOM	3546	NE2	GLN	B	868		2.709	-29.696	-3.670	1.00	43.84	B
	ATOM	3547	C	GLN	B	868		6.202	-24.779	-3.417	1.00	29.48	B
	ATOM	3548	O	GLN	B	868		6.537	-24.260	-2.355	1.00	28.85	B
	ATOM	3549	N	ARG	B	869		7.003	-24.868	-4.470	1.00	27.65	B
10	ATOM	3550	CA	ARG	B	869		8.364	-24.345	-4.463	1.00	28.67	B
	ATOM	3551	CB	ARG	B	869		9.067	-24.720	-5.766	1.00	27.99	B
	ATOM	3552	CG	ARG	B	869		10.514	-24.264	-5.852	1.00	29.69	B
	ATOM	3553	CD	ARG	B	869		11.378	-25.038	-4.883	1.00	28.24	B
	ATOM	3554	NE	ARG	B	869		12.798	-24.771	-5.076	1.00	30.16	B
15	ATOM	3555	CZ	ARG	B	869		13.765	-25.430	-4.446	1.00	28.86	B
	ATOM	3556	NH1	ARG	B	869		13.452	-26.393	-3.588	1.00	26.30	B
	ATOM	3557	NH2	ARG	B	869		15.040	-25.130	-4.672	1.00	24.34	B
	ATOM	3558	C	ARG	B	869		8.327	-22.825	-4.322	1.00	27.76	B
	ATOM	3559	O	ARG	B	869		9.083	-22.240	-3.548	1.00	29.39	B
20	ATOM	3560	N	PHE	B	870		7.437	-22.195	-5.080	1.00	26.99	B
	ATOM	3561	CA	PHE	B	870		7.286	-20.749	-5.045	1.00	26.48	B
	ATOM	3562	CB	PHE	B	870		6.215	-20.309	-6.041	1.00	26.94	B
	ATOM	3563	CG	PHE	B	870		6.003	-18.824	-6.085	1.00	26.83	B
	ATOM	3564	CD1	PHE	B	870		6.902	-17.999	-6.755	1.00	28.19	B
25	ATOM	3565	CD2	PHE	B	870		4.905	-18.246	-5.450	1.00	27.94	B
	ATOM	3566	CE1	PHE	B	870		6.711	-16.616	-6.796	1.00	27.85	B
	ATOM	3567	CE2	PHE	B	870		4.704	-16.862	-5.483	1.00	28.37	B
	ATOM	3568	CZ	PHE	B	870		5.612	-16.048	-6.161	1.00	27.70	B
	ATOM	3569	C	PHE	B	870		6.889	-20.328	-3.636	1.00	26.34	B
30	ATOM	3570	O	PHE	B	870		7.401	-19.344	-3.101	1.00	25.56	B
	ATOM	3571	N	TYR	B	871		5.974	-21.078	-3.032	1.00	26.21	B
	ATOM	3572	CA	TYR	B	871		5.542	-20.763	-1.682	1.00	27.42	B
	ATOM	3573	CB	TYR	B	871		4.494	-21.767	-1.193	1.00	30.77	B
	ATOM	3574	CG	TYR	B	871		4.073	-21.517	0.234	1.00	33.19	B
35	ATOM	3575	CD1	TYR	B	871		3.055	-20.613	0.532	1.00	35.86	B
	ATOM	3576	CE1	TYR	B	871		2.717	-20.318	1.853	1.00	36.85	B
	ATOM	3577	CD2	TYR	B	871		4.743	-22.126	1.293	1.00	34.60	B
	ATOM	3578	CE2	TYR	B	871		4.416	-21.837	2.615	1.00	36.18	B
	ATOM	3579	CZ	TYR	B	871		3.405	-20.933	2.888	1.00	37.44	B
40	ATOM	3580	OH	TYR	B	871		3.092	-20.633	4.196	1.00	39.18	B
	ATOM	3581	C	TYR	B	871		6.747	-20.818	-0.751	1.00	26.36	B
	ATOM	3582	O	TYR	B	871		6.972	-19.913	0.049	1.00	25.94	B
	ATOM	3583	N	GLN	B	872		7.518	-21.895	-0.865	1.00	25.60	B
	ATOM	3584	CA	GLN	B	872		8.691	-22.091	-0.026	1.00	25.57	B
45	ATOM	3585	CB	GLN	B	872		9.364	-23.421	-0.359	1.00	27.35	B
	ATOM	3586	CG	GLN	B	872		8.531	-24.643	-0.039	1.00	30.68	B
	ATOM	3587	CD	GLN	B	872		9.221	-25.925	-0.453	1.00	31.86	B
	ATOM	3588	OE1	GLN	B	872		9.552	-26.112	-1.624	1.00	34.33	B
	ATOM	3589	NE2	GLN	B	872		9.444	-26.815	0.505	1.00	34.20	B
50	ATOM	3590	C	GLN	B	872		9.713	-20.978	-0.164	1.00	23.41	B
	ATOM	3591	O	GLN	B	872		10.177	-20.430	0.830	1.00	21.76	B
	ATOM	3592	N	LEU	B	873		10.066	-20.644	-1.398	1.00	22.08	B
	ATOM	3593	CA	LEU	B	873		11.061	-19.605	-1.608	1.00	21.86	B
	ATOM	3594	CB	LEU	B	873		11.508	-19.595	-3.074	1.00	18.40	B
55	ATOM	3595	CG	LEU	B	873		12.160	-20.916	-3.522	1.00	20.29	B
	ATOM	3596	CD1	LEU	B	873		12.594	-20.822	-4.972	1.00	17.60	B

Table 2. (cont'd)

		#	Name	Res.	Chain	Res #	X	Y	Z	occ	B	SegID
	ATOM	3597	CD2	LEU	B	873	13.369	-21.236	-2.632	1.00	19.06	B
5	ATOM	3598	C	LEU	B	873	10.576	-18.228	-1.162	1.00	21.93	B
	ATOM	3599	O	LEU	B	873	11.348	-17.461	-0.584	1.00	22.49	B
	ATOM	3600	N	THR	B	874	9.304	-17.917	-1.404	1.00	22.76	B
	ATOM	3601	CA	THR	B	874	8.767	-16.621	-0.999	1.00	23.91	B
	ATOM	3602	CB	THR	B	874	7.423	-16.299	-1.702	1.00	24.32	B
10	ATOM	3603	OG1	THR	B	874	6.458	-17.318	-1.412	1.00	25.03	B
	ATOM	3604	CG2	THR	B	874	7.626	-16.203	-3.209	1.00	26.12	B
	ATOM	3605	C	THR	B	874	8.576	-16.560	0.516	1.00	25.18	B
	ATOM	3606	O	THR	B	874	8.635	-15.483	1.113	1.00	26.18	B
	ATOM	3607	N	LYS	B	875	8.359	-17.713	1.142	1.00	24.45	B
15	ATOM	3608	CA	LYS	B	875	8.194	-17.753	2.592	1.00	23.83	B
	ATOM	3609	CB	LYS	B	875	7.659	-19.116	3.046	1.00	25.61	B
	ATOM	3610	CG	LYS	B	875	7.292	-19.162	4.522	1.00	28.99	B
	ATOM	3611	CD	LYS	B	875	6.156	-18.190	4.830	1.00	33.42	B
	ATOM	3612	CE	LYS	B	875	5.855	-18.135	6.321	1.00	35.92	B
20	ATOM	3613	NZ	LYS	B	875	4.702	-17.238	6.602	1.00	37.34	B
	ATOM	3614	C	LYS	B	875	9.558	-17.506	3.230	1.00	23.31	B
	ATOM	3615	O	LYS	B	875	9.664	-16.887	4.287	1.00	21.67	B
	ATOM	3616	N	LEU	B	876	10.604	-17.999	2.580	1.00	21.64	B
	ATOM	3617	CA	LEU	B	876	11.957	-17.808	3.088	1.00	22.58	B
25	ATOM	3618	CB	LEU	B	876	12.966	-18.543	2.198	1.00	21.81	B
	ATOM	3619	CG	LEU	B	876	14.434	-18.534	2.645	1.00	22.37	B
	ATOM	3620	CD1	LEU	B	876	15.194	-19.641	1.927	1.00	23.69	B
	ATOM	3621	CD2	LEU	B	876	15.059	-17.179	2.358	1.00	22.29	B
	ATOM	3622	C	LEU	B	876	12.248	-16.308	3.100	1.00	21.74	B
30	ATOM	3623	O	LEU	B	876	12.800	-15.782	4.061	1.00	21.27	B
	ATOM	3624	N	LEU	B	877	11.863	-15.625	2.028	1.00	21.67	B
	ATOM	3625	CA	LEU	B	877	12.072	-14.183	1.935	1.00	21.91	B
	ATOM	3626	CB	LEU	B	877	11.643	-13.669	0.556	1.00	20.68	B
	ATOM	3627	CG	LEU	B	877	12.504	-14.111	-0.631	1.00	22.24	B
35	ATOM	3628	CD1	LEU	B	877	11.906	-13.568	-1.916	1.00	22.05	B
	ATOM	3629	CD2	LEU	B	877	13.941	-13.609	-0.466	1.00	20.37	B
	ATOM	3630	C	LEU	B	877	11.287	-13.476	3.040	1.00	20.65	B
	ATOM	3631	O	LEU	B	877	11.817	-12.593	3.709	1.00	19.22	B
	ATOM	3632	N	ASP	B	878	10.028	-13.869	3.233	1.00	19.37	B
40	ATOM	3633	CA	ASP	B	878	9.202	-13.283	4.289	1.00	20.36	B
	ATOM	3634	CB	ASP	B	878	7.866	-14.022	4.415	1.00	21.34	B
	ATOM	3635	CG	ASP	B	878	6.822	-13.532	3.438	1.00	23.18	B
	ATOM	3636	OD1	ASP	B	878	7.165	-12.760	2.516	1.00	24.47	B
	ATOM	3637	OD2	ASP	B	878	5.649	-13.933	3.597	1.00	24.18	B
45	ATOM	3638	C	ASP	B	878	9.918	-13.391	5.631	1.00	20.20	B
	ATOM	3639	O	ASP	B	878	10.034	-12.413	6.371	1.00	18.45	B
	ATOM	3640	N	ASN	B	879	10.397	-14.593	5.940	1.00	19.35	B
	ATOM	3641	CA	ASN	B	879	11.080	-14.836	7.203	1.00	21.08	B
	ATOM	3642	CB	ASN	B	879	11.361	-16.332	7.380	1.00	23.62	B
50	ATOM	3643	CG	ASN	B	879	10.099	-17.166	7.343	1.00	27.77	B
	ATOM	3644	OD1	ASN	B	879	9.044	-16.740	7.819	1.00	29.01	B
	ATOM	3645	ND2	ASN	B	879	10.200	-18.368	6.787	1.00	29.13	B
	ATOM	3646	C	ASN	B	879	12.379	-14.062	7.377	1.00	21.21	B
	ATOM	3647	O	ASN	B	879	12.904	-13.972	8.487	1.00	21.00	B
55	ATOM	3648	N	LEU	B	880	12.910	-13.501	6.297	1.00	20.95	B
	ATOM	3649	CA	LEU	B	880	14.152	-12.752	6.424	1.00	21.38	B

Table 2. (cont'd)

		#	Name	Res.	Chain	Res #	X	Y	Z	occ	B	SegID
5	ATOM	3650	CB	LEU	B	880	14.770	-12.486	5.052	1.00	20.58	B
	ATOM	3651	CG	LEU	B	880	15.371	-13.739	4.406	1.00	24.77	B
	ATOM	3652	CD1	LEU	B	880	16.034	-13.370	3.100	1.00	24.40	B
	ATOM	3653	CD2	LEU	B	880	16.386	-14.364	5.346	1.00	24.56	B
	ATOM	3654	C	LEU	B	880	13.981	-11.445	7.188	1.00	19.74	B
10	ATOM	3655	O	LEU	B	880	14.925	-10.972	7.809	1.00	20.66	B
	ATOM	3656	N	HIS	B	881	12.786	-10.861	7.154	1.00	19.70	B
	ATOM	3657	CA	HIS	B	881	12.562	-9.613	7.876	1.00	19.35	B
	ATOM	3658	CB	HIS	B	881	11.121	-9.123	7.680	1.00	20.71	B
	ATOM	3659	CG	HIS	B	881	10.856	-8.537	6.323	1.00	20.01	B
15	ATOM	3660	CD2	HIS	B	881	11.379	-7.452	5.704	1.00	17.82	B
	ATOM	3661	ND1	HIS	B	881	9.942	-9.076	5.443	1.00	21.77	B
	ATOM	3662	CE1	HIS	B	881	9.909	-8.345	4.341	1.00	18.83	B
	ATOM	3663	NE2	HIS	B	881	10.772	-7.353	4.475	1.00	21.49	B
	ATOM	3664	C	HIS	B	881	12.855	-9.806	9.368	1.00	20.98	B
20	ATOM	3665	O	HIS	B	881	13.581	-9.018	9.974	1.00	18.74	B
	ATOM	3666	N	ASP	B	882	12.299	-10.858	9.958	1.00	22.20	B
	ATOM	3667	CA	ASP	B	882	12.525	-11.130	11.377	1.00	22.92	B
	ATOM	3668	CB	ASP	B	882	11.698	-12.329	11.842	1.00	27.90	B
	ATOM	3669	CG	ASP	B	882	10.216	-12.047	11.853	1.00	33.60	B
25	ATOM	3670	OD1	ASP	B	882	9.816	-10.997	12.399	1.00	34.59	B
	ATOM	3671	OD2	ASP	B	882	9.449	-12.884	11.327	1.00	39.23	B
	ATOM	3672	C	ASP	B	882	13.987	-11.418	11.666	1.00	22.16	B
	ATOM	3673	O	ASP	B	882	14.532	-10.963	12.670	1.00	21.45	B
	ATOM	3674	N	LEU	B	883	14.617	-12.189	10.785	1.00	20.81	B
30	ATOM	3675	CA	LEU	B	883	16.018	-12.554	10.953	1.00	18.58	B
	ATOM	3676	CB	LEU	B	883	16.425	-13.551	9.853	1.00	19.75	B
	ATOM	3677	CG	LEU	B	883	17.801	-14.225	9.926	1.00	22.35	B
	ATOM	3678	CD1	LEU	B	883	17.821	-15.438	8.994	1.00	22.84	B
	ATOM	3679	CD2	LEU	B	883	18.896	-13.235	9.550	1.00	22.64	B
35	ATOM	3680	C	LEU	B	883	16.918	-11.322	10.912	1.00	18.56	B
	ATOM	3681	O	LEU	B	883	17.753	-11.114	11.795	1.00	17.89	B
	ATOM	3682	N	VAL	B	884	16.733	-10.506	9.882	1.00	17.78	B
	ATOM	3683	CA	VAL	B	884	17.523	-9.295	9.702	1.00	18.13	B
	ATOM	3684	CB	VAL	B	884	17.191	-8.640	8.354	1.00	19.53	B
40	ATOM	3685	CG1	VAL	B	884	17.891	-7.298	8.230	1.00	21.68	B
	ATOM	3686	CG2	VAL	B	884	17.618	-9.576	7.227	1.00	18.29	B
	ATOM	3687	C	VAL	B	884	17.329	-8.287	10.826	1.00	18.10	B
	ATOM	3688	O	VAL	B	884	18.237	-7.520	11.145	1.00	18.80	B
	ATOM	3689	N	LYS	B	885	16.151	-8.290	11.436	1.00	18.09	B
45	ATOM	3690	CA	LYS	B	885	15.889	-7.370	12.530	1.00	19.60	B
	ATOM	3691	CB	LYS	B	885	14.469	-7.565	13.054	1.00	23.11	B
	ATOM	3692	CG	LYS	B	885	14.118	-6.649	14.219	1.00	25.74	B
	ATOM	3693	CD	LYS	B	885	12.706	-6.924	14.689	1.00	31.18	B
	ATOM	3694	CE	LYS	B	885	12.381	-6.163	15.961	1.00	31.73	B
50	ATOM	3695	NZ	LYS	B	885	11.051	-6.599	16.474	1.00	38.15	B
	ATOM	3696	C	LYS	B	885	16.898	-7.582	13.667	1.00	19.50	B
	ATOM	3697	O	LYS	B	885	17.378	-6.618	14.265	1.00	17.26	B
	ATOM	3698	N	GLN	B	886	17.225	-8.842	13.955	1.00	19.54	B
	ATOM	3699	CA	GLN	B	886	18.184	-9.149	15.015	1.00	19.86	B
55	ATOM	3700	CB	GLN	B	886	18.248	-10.660	15.273	1.00	25.01	B
	ATOM	3701	CG	GLN	B	886	16.941	-11.267	15.755	1.00	31.58	B
	ATOM	3702	CD	GLN	B	886	16.480	-10.710	17.098	1.00	36.35	B

Table 2. (cont'd)

		#	Name	Res.	Chain	Res #	X	Y	Z	occ	B	SegID
5	ATOM	3703	OE1	GLN	B	886	15.365	-10.988	17.540	1.00	40.85	B
	ATOM	3704	NE2	GLN	B	886	17.337	-9.930	17.754	1.00	38.26	B
	ATOM	3705	C	GLN	B	886	19.572	-8.639	14.634	1.00	18.79	B
	ATOM	3706	O	GLN	B	886	20.328	-8.171	15.491	1.00	16.94	B
	ATOM	3707	N	LEU	B	887	19.910	-8.736	13.352	1.00	17.04	B
10	ATOM	3708	CA	LEU	B	887	21.205	-8.259	12.881	1.00	16.54	B
	ATOM	3709	CB	LEU	B	887	21.445	-8.685	11.427	1.00	18.52	B
	ATOM	3710	CG	LEU	B	887	21.471	-10.184	11.104	1.00	23.04	B
	ATOM	3711	CD1	LEU	B	887	21.992	-10.382	9.682	1.00	22.45	B
	ATOM	3712	CD2	LEU	B	887	22.358	-10.920	12.080	1.00	24.74	B
15	ATOM	3713	C	LEU	B	887	21.245	-6.733	12.988	1.00	15.32	B
	ATOM	3714	O	LEU	B	887	22.251	-6.156	13.396	1.00	16.15	B
	ATOM	3715	N	HIS	B	888	20.142	-6.085	12.620	1.00	14.69	B
	ATOM	3716	CA	HIS	B	888	20.047	-4.631	12.678	1.00	14.50	B
	ATOM	3717	CB	HIS	B	888	18.684	-4.164	12.144	1.00	15.66	B
20	ATOM	3718	CG	HIS	B	888	18.605	-4.093	10.649	1.00	14.62	B
	ATOM	3719	CD2	HIS	B	888	19.574	-4.009	9.706	1.00	15.13	B
	ATOM	3720	ND1	HIS	B	888	17.406	-4.038	9.971	1.00	15.95	B
	ATOM	3721	CE1	HIS	B	888	17.638	-3.919	8.675	1.00	13.80	B
	ATOM	3722	NE2	HIS	B	888	18.945	-3.900	8.487	1.00	17.55	B
25	ATOM	3723	C	HIS	B	888	20.226	-4.141	14.112	1.00	15.95	B
	ATOM	3724	O	HIS	B	888	20.995	-3.215	14.368	1.00	18.20	B
	ATOM	3725	N	LEU	B	889	19.518	-4.762	15.049	1.00	16.97	B
	ATOM	3726	CA	LEU	B	889	19.617	-4.360	16.449	1.00	17.38	B
	ATOM	3727	CB	LEU	B	889	18.647	-5.176	17.306	1.00	16.53	B
30	ATOM	3728	CG	LEU	B	889	18.667	-4.889	18.814	1.00	18.28	B
	ATOM	3729	CD1	LEU	B	889	18.420	-3.402	19.077	1.00	18.15	B
	ATOM	3730	CD2	LEU	B	889	17.604	-5.737	19.494	1.00	19.21	B
	ATOM	3731	C	LEU	B	889	21.042	-4.528	16.971	1.00	17.72	B
	ATOM	3732	O	LEU	B	889	21.590	-3.622	17.597	1.00	17.23	B
35	ATOM	3733	N	TYR	B	890	21.642	-5.687	16.708	1.00	18.99	B
	ATOM	3734	CA	TYR	B	890	23.007	-5.947	17.160	1.00	20.22	B
	ATOM	3735	CB	TYR	B	890	23.442	-7.360	16.747	1.00	21.39	B
	ATOM	3736	CG	TYR	B	890	24.807	-7.772	17.266	1.00	24.48	B
	ATOM	3737	CD1	TYR	B	890	25.974	-7.278	16.688	1.00	23.63	B
40	ATOM	3738	CE1	TYR	B	890	27.230	-7.639	17.172	1.00	26.80	B
	ATOM	3739	CD2	TYR	B	890	24.926	-8.646	18.348	1.00	25.44	B
	ATOM	3740	CE2	TYR	B	890	26.180	-9.016	18.842	1.00	28.35	B
	ATOM	3741	CZ	TYR	B	890	27.326	-8.508	18.247	1.00	27.86	B
	ATOM	3742	OH	TYR	B	890	28.568	-8.865	18.726	1.00	30.29	B
45	ATOM	3743	C	TYR	B	890	23.951	-4.905	16.563	1.00	18.18	B
	ATOM	3744	O	TYR	B	890	24.798	-4.346	17.260	1.00	18.16	B
	ATOM	3745	N	CYS	B	891	23.796	-4.640	15.270	1.00	17.50	B
	ATOM	3746	CA	CYS	B	891	24.646	-3.667	14.596	1.00	16.55	B
	ATOM	3747	CB	CYS	B	891	24.309	-3.612	13.101	1.00	16.50	B
50	ATOM	3748	SG	CYS	B	891	25.362	-2.476	12.150	1.00	18.64	B
	ATOM	3749	C	CYS	B	891	24.517	-2.268	15.211	1.00	16.80	B
	ATOM	3750	O	CYS	B	891	25.522	-1.628	15.511	1.00	17.68	B
	ATOM	3751	N	LEU	B	892	23.291	-1.794	15.402	1.00	15.23	B
	ATOM	3752	CA	LEU	B	892	23.097	-0.466	15.978	1.00	16.77	B
55	ATOM	3753	CB	LEU	B	892	21.610	-0.100	16.003	1.00	16.01	B
	ATOM	3754	CG	LEU	B	892	21.265	1.332	16.428	1.00	15.16	B
	ATOM	3755	CD1	LEU	B	892	22.059	2.342	15.586	1.00	15.59	B

Table 2. (cont'd)

		#	Name	Res.	Chain	Res #	X	Y	Z	occ	B	SegID
	ATOM	3756	CD2	LEU	B	892	19.769	1.557	16.262	1.00	15.56	B
5	ATOM	3757	C	LEU	B	892	23.693	-0.343	17.384	1.00	17.79	B
	ATOM	3758	O	LEU	B	892	24.342	0.659	17.696	1.00	19.65	B
	ATOM	3759	N	ASN	B	893	23.482	-1.351	18.228	1.00	17.78	B
	ATOM	3760	CA	ASN	B	893	24.030	-1.323	19.585	1.00	19.02	B
	ATOM	3761	CB	ASN	B	893	23.685	-2.604	20.357	1.00	19.78	B
10	ATOM	3762	CG	ASN	B	893	22.266	-2.613	20.870	1.00	22.60	B
	ATOM	3763	OD1	ASN	B	893	21.705	-1.563	21.187	1.00	25.14	B
	ATOM	3764	ND2	ASN	B	893	21.679	-3.804	20.976	1.00	23.61	B
	ATOM	3765	C	ASN	B	893	25.543	-1.189	19.532	1.00	20.12	B
	ATOM	3766	O	ASN	B	893	26.137	-0.380	20.242	1.00	22.59	B
15	ATOM	3767	N	THR	B	894	26.167	-2.000	18.690	1.00	19.05	B
	ATOM	3768	CA	THR	B	894	27.612	-1.974	18.547	1.00	19.44	B
	ATOM	3769	CB	THR	B	894	28.076	-3.079	17.586	1.00	19.42	B
	ATOM	3770	OG1	THR	B	894	27.549	-4.338	18.030	1.00	17.10	B
	ATOM	3771	CG2	THR	B	894	29.595	-3.149	17.545	1.00	18.92	B
20	ATOM	3772	C	THR	B	894	28.076	-0.616	18.023	1.00	21.22	B
	ATOM	3773	O	THR	B	894	29.073	-0.071	18.491	1.00	20.90	B
	ATOM	3774	N	PHE	B	895	27.348	-0.079	17.047	1.00	20.38	B
	ATOM	3775	CA	PHE	B	895	27.677	1.215	16.460	1.00	22.73	B
	ATOM	3776	CB	PHE	B	895	26.662	1.558	15.363	1.00	22.12	B
25	ATOM	3777	CG	PHE	B	895	26.933	2.856	14.664	1.00	21.75	B
	ATOM	3778	CD1	PHE	B	895	28.068	3.014	13.874	1.00	23.50	B
	ATOM	3779	CD2	PHE	B	895	26.043	3.917	14.779	1.00	23.49	B
	ATOM	3780	CE1	PHE	B	895	28.312	4.210	13.206	1.00	23.87	B
	ATOM	3781	CE2	PHE	B	895	26.276	5.121	14.113	1.00	24.35	B
30	ATOM	3782	CZ	PHE	B	895	27.414	5.268	13.326	1.00	23.84	B
	ATOM	3783	C	PHE	B	895	27.643	2.279	17.557	1.00	23.93	B
	ATOM	3784	O	PHE	B	895	28.533	3.121	17.653	1.00	23.95	B
	ATOM	3785	N	ILE	B	896	26.606	2.223	18.384	1.00	26.93	B
	ATOM	3786	CA	ILE	B	896	26.435	3.160	19.488	1.00	31.13	B
35	ATOM	3787	CB	ILE	B	896	25.090	2.900	20.213	1.00	31.72	B
	ATOM	3788	CG2	ILE	B	896	25.012	3.701	21.497	1.00	34.14	B
	ATOM	3789	CG1	ILE	B	896	23.927	3.230	19.277	1.00	33.07	B
	ATOM	3790	CD1	ILE	B	896	24.014	4.596	18.654	1.00	30.60	B
	ATOM	3791	C	ILE	B	896	27.577	3.066	20.508	1.00	33.19	B
40	ATOM	3792	O	ILE	B	896	27.986	4.073	21.085	1.00	35.25	B
	ATOM	3793	N	GLN	B	897	28.089	1.859	20.727	1.00	34.17	B
	ATOM	3794	CA	GLN	B	897	29.169	1.654	21.692	1.00	35.56	B
	ATOM	3795	CB	GLN	B	897	28.817	0.494	22.624	1.00	35.80	B
	ATOM	3796	CG	GLN	B	897	27.338	0.369	22.930	1.00	36.67	B
45	ATOM	3797	CD	GLN	B	897	27.000	-0.946	23.601	1.00	38.80	B
	ATOM	3798	OE1	GLN	B	897	25.836	-1.350	23.657	1.00	39.12	B
	ATOM	3799	NE2	GLN	B	897	28.019	-1.624	24.121	1.00	40.79	B
	ATOM	3800	C	GLN	B	897	30.484	1.337	20.990	1.00	36.74	B
	ATOM	3801	O	GLN	B	897	31.406	0.795	21.605	1.00	36.87	B
50	ATOM	3802	N	SER	B	898	30.569	1.681	19.706	1.00	37.12	B
	ATOM	3803	CA	SER	B	898	31.756	1.407	18.902	1.00	37.09	B
	ATOM	3804	CB	SER	B	898	31.655	2.110	17.544	1.00	36.71	B
	ATOM	3805	OG	SER	B	898	31.802	3.513	17.674	1.00	35.33	B
	ATOM	3806	C	SER	B	898	33.061	1.812	19.575	1.00	38.11	B
55	ATOM	3807	O	SER	B	898	34.007	1.028	19.636	1.00	36.29	B
	ATOM	3808	N	ARG	B	899	33.116	3.039	20.074	1.00	39.88	B

Table 2. (cont'd)

		#	Name	Res.	Chain	Res #	X	Y	Z	occ	B	SegID
	ATOM	3809	CA	ARG	B	899	34.325	3.521	20.724	1.00	42.35	B
5	ATOM	3810	CB	ARG	B	899	34.180	5.000	21.069	1.00	45.76	B
	ATOM	3811	CG	ARG	B	899	35.338	5.530	21.873	1.00	50.91	B
	ATOM	3812	CD	ARG	B	899	35.349	7.042	21.919	1.00	55.56	B
	ATOM	3813	NE	ARG	B	899	36.392	7.501	22.825	1.00	59.98	B
	ATOM	3814	CZ	ARG	B	899	36.755	8.767	22.979	1.00	61.92	B
10	ATOM	3815	NH1	ARG	B	899	37.716	9.067	23.839	1.00	63.21	B
	ATOM	3816	NH2	ARG	B	899	36.166	9.727	22.274	1.00	62.81	B
	ATOM	3817	C	ARG	B	899	34.689	2.731	21.978	1.00	41.68	B
	ATOM	3818	O	ARG	B	899	35.858	2.418	22.202	1.00	41.52	B
	ATOM	3819	N	ALA	B	900	33.686	2.407	22.787	1.00	40.82	B
15	ATOM	3820	CA	ALA	B	900	33.909	1.657	24.018	1.00	40.31	B
	ATOM	3821	CB	ALA	B	900	32.679	1.750	24.910	1.00	39.86	B
	ATOM	3822	C	ALA	B	900	34.246	0.191	23.752	1.00	40.02	B
	ATOM	3823	O	ALA	B	900	34.876	-0.469	24.581	1.00	39.73	B
	ATOM	3824	N	LEU	B	901	33.823	-0.317	22.599	1.00	38.18	B
20	ATOM	3825	CA	LEU	B	901	34.081	-1.706	22.241	1.00	37.31	B
	ATOM	3826	CB	LEU	B	901	32.867	-2.299	21.518	1.00	37.48	B
	ATOM	3827	CG	LEU	B	901	31.545	-2.292	22.285	1.00	38.53	B
	ATOM	3828	CD1	LEU	B	901	30.441	-2.875	21.416	1.00	38.07	B
	ATOM	3829	CD2	LEU	B	901	31.698	-3.095	23.572	1.00	38.86	B
25	ATOM	3830	C	LEU	B	901	35.310	-1.826	21.348	1.00	35.77	B
	ATOM	3831	O	LEU	B	901	35.714	-2.929	20.981	1.00	35.59	B
	ATOM	3832	N	SER	B	902	35.901	-0.685	21.009	1.00	34.11	B
	ATOM	3833	CA	SER	B	902	37.073	-0.645	20.144	1.00	33.24	B
	ATOM	3834	CB	SER	B	902	38.234	-1.415	20.779	1.00	35.64	B
30	ATOM	3835	OG	SER	B	902	38.654	-0.802	21.982	1.00	39.63	B
	ATOM	3836	C	SER	B	902	36.762	-1.230	18.765	1.00	31.15	B
	ATOM	3837	O	SER	B	902	37.620	-1.853	18.137	1.00	29.62	B
	ATOM	3838	N	VAL	B	903	35.532	-1.026	18.301	1.00	28.43	B
	ATOM	3839	CA	VAL	B	903	35.112	-1.525	16.992	1.00	26.89	B
35	ATOM	3840	CB	VAL	B	903	33.725	-2.198	17.059	1.00	26.31	B
	ATOM	3841	CG1	VAL	B	903	33.320	-2.700	15.668	1.00	25.67	B
	ATOM	3842	CG2	VAL	B	903	33.756	-3.350	18.058	1.00	28.50	B
	ATOM	3843	C	VAL	B	903	35.037	-0.377	15.994	1.00	26.42	B
	ATOM	3844	O	VAL	B	903	34.369	0.625	16.243	1.00	26.76	B
40	ATOM	3845	N	GLU	B	904	35.720	-0.524	14.865	1.00	24.57	B
	ATOM	3846	CA	GLU	B	904	35.712	0.513	13.848	1.00	25.03	B
	ATOM	3847	CB	GLU	B	904	37.073	0.595	13.160	1.00	28.92	B
	ATOM	3848	CG	GLU	B	904	38.204	0.987	14.094	1.00	38.82	B
	ATOM	3849	CD	GLU	B	904	39.490	1.288	13.355	1.00	43.68	B
45	ATOM	3850	OE1	GLU	B	904	39.987	0.395	12.633	1.00	47.38	B
	ATOM	3851	OE2	GLU	B	904	40.004	2.419	13.497	1.00	48.28	B
	ATOM	3852	C	GLU	B	904	34.633	0.300	12.797	1.00	23.04	B
	ATOM	3853	O	GLU	B	904	34.418	-0.821	12.326	1.00	19.12	B
	ATOM	3854	N	PHE	B	905	33.957	1.394	12.448	1.00	20.12	B
50	ATOM	3855	CA	PHE	B	905	32.912	1.395	11.431	1.00	20.96	B
	ATOM	3856	CB	PHE	B	905	31.575	1.886	12.006	1.00	20.87	B
	ATOM	3857	CG	PHE	B	905	30.861	0.877	12.856	1.00	21.25	B
	ATOM	3858	CD1	PHE	B	905	31.284	0.613	14.156	1.00	18.95	B
	ATOM	3859	CD2	PHE	B	905	29.761	0.187	12.354	1.00	19.31	B
55	ATOM	3860	CE1	PHE	B	905	30.621	-0.327	14.946	1.00	19.88	B
	ATOM	3861	CE2	PHE	B	905	29.094	-0.751	13.132	1.00	22.00	B

Table 2. (cont'd)

		#	Name	Res.	Chain	Res #	X	Y	Z	occ	B	SegID
	ATOM	3862	CZ	PHE	B	905	29.526	-1.010	14.438	1.00	20.34	B
5	ATOM	3863	C	PHE	B	905	33.340	2.356	10.325	1.00	19.65	B
	ATOM	3864	O	PHE	B	905	33.518	3.550	10.574	1.00	20.10	B
	ATOM	3865	N	PRO	B	906	33.525	1.851	9.096	1.00	19.13	B
	ATOM	3866	CD	PRO	B	906	33.677	0.436	8.715	1.00	19.13	B
	ATOM	3867	CA	PRO	B	906	33.933	2.733	7.994	1.00	18.54	B
10	ATOM	3868	CB	PRO	B	906	34.170	1.762	6.842	1.00	18.01	B
	ATOM	3869	CG	PRO	B	906	34.661	0.526	7.560	1.00	21.07	B
	ATOM	3870	C	PRO	B	906	32.853	3.767	7.687	1.00	17.77	B
	ATOM	3871	O	PRO	B	906	31.698	3.614	8.102	1.00	17.22	B
	ATOM	3872	N	GLU	B	907	33.230	4.800	6.938	1.00	17.56	B
15	ATOM	3873	CA	GLU	B	907	32.330	5.909	6.609	1.00	17.42	B
	ATOM	3874	CB	GLU	B	907	33.106	6.988	5.856	1.00	15.83	B
	ATOM	3875	CG	GLU	B	907	34.261	7.598	6.643	1.00	16.09	B
	ATOM	3876	CD	GLU	B	907	33.823	8.322	7.906	1.00	18.31	B
	ATOM	3877	OE1	GLU	B	907	32.677	8.821	7.962	1.00	17.52	B
20	ATOM	3878	OE2	GLU	B	907	34.643	8.414	8.842	1.00	19.06	B
	ATOM	3879	C	GLU	B	907	31.026	5.634	5.864	1.00	17.19	B
	ATOM	3880	O	GLU	B	907	29.981	6.177	6.227	1.00	16.76	B
	ATOM	3881	N	MET	B	908	31.066	4.819	4.819	1.00	15.73	B
	ATOM	3882	CA	MET	B	908	29.840	4.561	4.076	1.00	17.55	B
25	ATOM	3883	CB	MET	B	908	30.165	3.859	2.755	1.00	17.66	B
	ATOM	3884	CG	MET	B	908	31.054	4.709	1.842	1.00	18.47	B
	ATOM	3885	SD	MET	B	908	31.344	4.017	0.197	1.00	19.83	B
	ATOM	3886	CE	MET	B	908	32.363	2.584	0.608	1.00	20.34	B
	ATOM	3887	C	MET	B	908	28.854	3.756	4.912	1.00	19.27	B
30	ATOM	3888	O	MET	B	908	27.654	4.057	4.944	1.00	18.84	B
	ATOM	3889	N	MET	B	909	29.374	2.741	5.597	1.00	20.63	B
	ATOM	3890	CA	MET	B	909	28.586	1.884	6.477	1.00	21.59	B
	ATOM	3891	CB	MET	B	909	29.498	0.849	7.140	1.00	26.31	B
	ATOM	3892	CG	MET	B	909	29.928	-0.280	6.249	1.00	31.81	B
35	ATOM	3893	SD	MET	B	909	28.744	-1.626	6.369	1.00	41.30	B
	ATOM	3894	CE	MET	B	909	29.012	-2.122	8.117	1.00	35.86	B
	ATOM	3895	C	MET	B	909	27.952	2.732	7.573	1.00	19.52	B
	ATOM	3896	O	MET	B	909	26.767	2.603	7.873	1.00	16.91	B
	ATOM	3897	N	SER	B	910	28.765	3.594	8.178	1.00	19.62	B
40	ATOM	3898	CA	SER	B	910	28.300	4.456	9.254	1.00	18.66	B
	ATOM	3899	CB	SER	B	910	29.438	5.358	9.740	1.00	19.13	B
	ATOM	3900	OG	SER	B	910	30.424	4.602	10.423	1.00	21.89	B
	ATOM	3901	C	SER	B	910	27.108	5.308	8.840	1.00	18.32	B
	ATOM	3902	O	SER	B	910	26.168	5.483	9.610	1.00	17.55	B
45	ATOM	3903	N	GLU	B	911	27.146	5.829	7.618	1.00	18.37	B
	ATOM	3904	CA	GLU	B	911	26.068	6.669	7.112	1.00	17.93	B
	ATOM	3905	CB	GLU	B	911	26.467	7.267	5.759	1.00	18.99	B
	ATOM	3906	CG	GLU	B	911	25.386	8.098	5.091	1.00	23.81	B
	ATOM	3907	CD	GLU	B	911	24.898	9.231	5.965	1.00	26.02	B
50	ATOM	3908	OE1	GLU	B	911	25.737	9.851	6.656	1.00	29.85	B
	ATOM	3909	OE2	GLU	B	911	23.681	9.506	5.954	1.00	28.42	B
	ATOM	3910	C	GLU	B	911	24.769	5.877	6.971	1.00	18.59	B
	ATOM	3911	O	GLU	B	911	23.695	6.353	7.343	1.00	17.69	B
	ATOM	3912	N	VAL	B	912	24.867	4.668	6.433	1.00	17.22	B
55	ATOM	3913	CA	VAL	B	912	23.682	3.837	6.255	1.00	18.22	B
	ATOM	3914	CB	VAL	B	912	24.032	2.532	5.502	1.00	18.83	B

Table 2. (cont'd)

		#	Name	Res.	Chain	Res	#	X	Y	Z	occ	B	SegID
	ATOM	3915	CG1	VAL	B	912		22.898	1.531	5.628	1.00	21.35	B
5	ATOM	3916	CG2	VAL	B	912		24.283	2.850	4.027	1.00	18.17	B
	ATOM	3917	C	VAL	B	912		23.053	3.503	7.599	1.00	17.16	B
	ATOM	3918	O	VAL	B	912		21.831	3.551	7.760	1.00	16.31	B
	ATOM	3919	N	ILE	B	913		23.899	3.165	8.565	1.00	15.65	B
	ATOM	3920	CA	ILE	B	913		23.435	2.821	9.899	1.00	17.18	B
10	ATOM	3921	CB	ILE	B	913		24.614	2.320	10.770	1.00	17.40	B
	ATOM	3922	CG2	ILE	B	913		24.183	2.186	12.225	1.00	16.84	B
	ATOM	3923	CG1	ILE	B	913		25.116	0.972	10.232	1.00	16.47	B
	ATOM	3924	CD1	ILE	B	913		26.470	0.544	10.786	1.00	20.34	B
	ATOM	3925	C	ILE	B	913		22.769	4.030	10.555	1.00	19.14	B
15	ATOM	3926	O	ILE	B	913		21.637	3.946	11.028	1.00	20.38	B
	ATOM	3927	N	ALA	B	914		23.455	5.166	10.555	1.00	20.59	B
	ATOM	3928	CA	ALA	B	914		22.905	6.366	11.175	1.00	21.55	B
	ATOM	3929	CB	ALA	B	914		23.956	7.472	11.191	1.00	20.73	B
	ATOM	3930	C	ALA	B	914		21.635	6.868	10.495	1.00	23.12	B
20	ATOM	3931	O	ALA	B	914		20.707	7.327	11.157	1.00	24.41	B
	ATOM	3932	N	ALA	B	915		21.582	6.766	9.174	1.00	24.15	B
	ATOM	3933	CA	ALA	B	915		20.427	7.263	8.438	1.00	23.02	B
	ATOM	3934	CB	ALA	B	915		20.813	7.496	6.979	1.00	23.13	B
	ATOM	3935	C	ALA	B	915		19.148	6.432	8.498	1.00	22.96	B
25	ATOM	3936	O	ALA	B	915		18.052	6.992	8.515	1.00	23.53	B
	ATOM	3937	N	GLN	B	916		19.268	5.111	8.548	1.00	20.89	B
	ATOM	3938	CA	GLN	B	916		18.074	4.282	8.535	1.00	22.00	B
	ATOM	3939	CB	GLN	B	916		18.010	3.481	7.223	1.00	24.20	B
	ATOM	3940	CG	GLN	B	916		18.095	4.282	5.923	1.00	27.17	B
30	ATOM	3941	CD	GLN	B	916		17.030	5.345	5.801	1.00	29.02	B
	ATOM	3942	OE1	GLN	B	916		15.925	5.205	6.324	1.00	28.23	B
	ATOM	3943	NE2	GLN	B	916		17.353	6.417	5.087	1.00	33.25	B
	ATOM	3944	C	GLN	B	916		17.812	3.292	9.667	1.00	21.39	B
	ATOM	3945	O	GLN	B	916		16.651	3.008	9.959	1.00	22.64	B
35	ATOM	3946	N	LEU	B	917		18.849	2.742	10.295	1.00	19.37	B
	ATOM	3947	CA	LEU	B	917		18.588	1.727	11.317	1.00	18.64	B
	ATOM	3948	CB	LEU	B	917		19.895	1.152	11.885	1.00	18.07	B
	ATOM	3949	CG	LEU	B	917		20.687	0.240	10.936	1.00	20.90	B
	ATOM	3950	CD1	LEU	B	917		21.614	-0.666	11.741	1.00	17.81	B
40	ATOM	3951	CD2	LEU	B	917		19.739	-0.612	10.115	1.00	20.60	B
	ATOM	3952	C	LEU	B	917		17.635	2.090	12.450	1.00	17.99	B
	ATOM	3953	O	LEU	B	917		16.745	1.303	12.777	1.00	19.33	B
	ATOM	3954	N	PRO	B	918		17.793	3.270	13.068	1.00	17.70	B
	ATOM	3955	CD	PRO	B	918		18.853	4.290	12.994	1.00	18.75	B
45	ATOM	3956	CA	PRO	B	918		16.848	3.575	14.148	1.00	18.53	B
	ATOM	3957	CB	PRO	B	918		17.285	4.966	14.596	1.00	19.15	B
	ATOM	3958	CG	PRO	B	918		18.779	4.916	14.375	1.00	17.58	B
	ATOM	3959	C	PRO	B	918		15.400	3.538	13.636	1.00	18.88	B
	ATOM	3960	O	PRO	B	918		14.521	2.939	14.257	1.00	15.75	B
50	ATOM	3961	N	LYS	B	919		15.176	4.173	12.490	1.00	18.61	B
	ATOM	3962	CA	LYS	B	919		13.860	4.234	11.852	1.00	20.51	B
	ATOM	3963	CB	LYS	B	919		13.960	5.063	10.569	1.00	24.87	B
	ATOM	3964	CG	LYS	B	919		12.673	5.155	9.765	1.00	29.78	B
	ATOM	3965	CD	LYS	B	919		12.926	5.776	8.402	1.00	34.28	B
55	ATOM	3966	CE	LYS	B	919		13.531	7.168	8.525	1.00	37.85	B
	ATOM	3967	NZ	LYS	B	919		13.932	7.713	7.194	1.00	42.01	B

Table 2. (cont'd)

		#	Name	Res.	Chain	Res #	X	Y	Z	occ	B	SegID
5	ATOM	3968	C	LYS	B	919	13.317	2.842	11.515	1.00	19.41	B
	ATOM	3969	O	LYS	B	919	12.146	2.540	11.766	1.00	19.67	B
	ATOM	3970	N	ILE	B	920	14.164	2.002	10.925	1.00	17.71	B
	ATOM	3971	CA	ILE	B	920	13.764	0.644	10.573	1.00	17.37	B
	ATOM	3972	CB	ILE	B	920	14.887	-0.077	9.796	1.00	17.05	B
10	ATOM	3973	CG2	ILE	B	920	14.474	-1.515	9.497	1.00	17.48	B
	ATOM	3974	CG1	ILE	B	920	15.171	0.670	8.486	1.00	16.02	B
	ATOM	3975	CD1	ILE	B	920	16.351	0.143	7.705	1.00	15.95	B
	ATOM	3976	C	ILE	B	920	13.411	-0.172	11.825	1.00	17.73	B
	ATOM	3977	O	ILE	B	920	12.357	-0.801	11.891	1.00	19.73	B
15	ATOM	3978	N	LEU	B	921	14.290	-0.153	12.821	1.00	18.28	B
	ATOM	3979	CA	LEU	B	921	14.048	-0.894	14.058	1.00	17.30	B
	ATOM	3980	CB	LEU	B	921	15.256	-0.761	14.991	1.00	17.29	B
	ATOM	3981	CG	LEU	B	921	16.506	-1.550	14.568	1.00	19.30	B
	ATOM	3982	CD1	LEU	B	921	17.685	-1.192	15.458	1.00	20.25	B
20	ATOM	3983	CD2	LEU	B	921	16.212	-3.049	14.650	1.00	18.96	B
	ATOM	3984	C	LEU	B	921	12.779	-0.405	14.759	1.00	18.82	B
	ATOM	3985	O	LEU	B	921	12.060	-1.189	15.386	1.00	18.43	B
	ATOM	3986	N	ALA	B	922	12.506	0.891	14.650	1.00	18.13	B
	ATOM	3987	CA	ALA	B	922	11.316	1.475	15.260	1.00	20.31	B
25	ATOM	3988	CB	ALA	B	922	11.459	2.994	15.329	1.00	18.87	B
	ATOM	3989	C	ALA	B	922	10.062	1.102	14.468	1.00	21.56	B
	ATOM	3990	O	ALA	B	922	8.958	1.530	14.799	1.00	21.69	B
	ATOM	3991	N	GLY	B	923	10.240	0.312	13.415	1.00	21.30	B
	ATOM	3992	CA	GLY	B	923	9.111	-0.104	12.600	1.00	22.52	B
30	ATOM	3993	C	GLY	B	923	8.491	1.015	11.784	1.00	23.20	B
	ATOM	3994	O	GLY	B	923	7.301	0.977	11.474	1.00	24.52	B
	ATOM	3995	N	MET	B	924	9.289	2.010	11.421	1.00	23.73	B
	ATOM	3996	CA	MET	B	924	8.778	3.134	10.651	1.00	24.27	B
	ATOM	3997	CB	MET	B	924	9.433	4.424	11.137	1.00	26.89	B
35	ATOM	3998	CG	MET	B	924	9.330	4.611	12.645	1.00	29.64	B
	ATOM	3999	SD	MET	B	924	7.622	4.544	13.234	1.00	36.14	B
	ATOM	4000	CE	MET	B	924	7.016	6.119	12.590	1.00	32.22	B
	ATOM	4001	C	MET	B	924	8.968	2.973	9.141	1.00	22.97	B
	ATOM	4002	O	MET	B	924	9.237	3.939	8.434	1.00	24.86	B
40	ATOM	4003	N	VAL	B	925	8.834	1.737	8.669	1.00	22.70	B
	ATOM	4004	CA	VAL	B	925	8.945	1.394	7.254	1.00	20.11	B
	ATOM	4005	CB	VAL	B	925	10.357	0.879	6.873	1.00	21.32	B
	ATOM	4006	CG1	VAL	B	925	11.396	1.961	7.137	1.00	18.72	B
	ATOM	4007	CG2	VAL	B	925	10.681	-0.404	7.648	1.00	19.44	B
45	ATOM	4008	C	VAL	B	925	7.951	0.269	7.008	1.00	20.72	B
	ATOM	4009	O	VAL	B	925	7.427	-0.317	7.958	1.00	17.16	B
	ATOM	4010	N	LYS	B	926	7.698	-0.039	5.740	1.00	20.24	B
	ATOM	4011	CA	LYS	B	926	6.756	-1.096	5.405	1.00	22.19	B
	ATOM	4012	CB	LYS	B	926	5.693	-0.583	4.431	1.00	23.49	B
50	ATOM	4013	CG	LYS	B	926	4.697	-1.663	4.034	1.00	27.62	B
	ATOM	4014	CD	LYS	B	926	3.735	-1.209	2.948	1.00	29.56	B
	ATOM	4015	CE	LYS	B	926	2.774	-2.338	2.595	1.00	32.37	B
	ATOM	4016	NZ	LYS	B	926	1.833	-1.961	1.507	1.00	35.72	B
	ATOM	4017	C	LYS	B	926	7.419	-2.320	4.789	1.00	22.27	B
55	ATOM	4018	O	LYS	B	926	7.812	-2.300	3.620	1.00	20.78	B
	ATOM	4019	N	PRO	B	927	7.555	-3.405	5.568	1.00	23.59	B
	ATOM	4020	CD	PRO	B	927	7.287	-3.541	7.009	1.00	23.58	B

Table 2. (cont'd)

		#	Name	Res.	Chain	Res #	X	Y	Z	occ	B	SegID
	ATOM	4021	CA	PRO	B	927	8.177	-4.619	5.035	1.00	23.23	B
5	ATOM	4022	CB	PRO	B	927	8.399	-5.481	6.280	1.00	24.23	B
	ATOM	4023	CG	PRO	B	927	8.372	-4.483	7.429	1.00	26.39	B
	ATOM	4024	C	PRO	B	927	7.156	-5.251	4.095	1.00	23.54	B
	ATOM	4025	O	PRO	B	927	5.968	-5.295	4.417	1.00	23.62	B
	ATOM	4026	N	LEU	B	928	7.598	-5.723	2.935	1.00	21.25	B
10	ATOM	4027	CA	LEU	B	928	6.672	-6.343	2.000	1.00	21.62	B
	ATOM	4028	CB	LEU	B	928	7.083	-6.038	0.553	1.00	20.54	B
	ATOM	4029	CG	LEU	B	928	7.097	-4.547	0.191	1.00	19.73	B
	ATOM	4030	CD1	LEU	B	928	7.385	-4.376	-1.299	1.00	19.70	B
	ATOM	4031	CD2	LEU	B	928	5.751	-3.916	0.530	1.00	19.69	B
15	ATOM	4032	C	LEU	B	928	6.635	-7.845	2.250	1.00	22.19	B
	ATOM	4033	O	LEU	B	928	7.670	-8.481	2.447	1.00	20.86	B
	ATOM	4034	N	LEU	B	929	5.431	-8.404	2.255	1.00	22.00	B
	ATOM	4035	CA	LEU	B	929	5.252	-9.828	2.499	1.00	21.93	B
	ATOM	4036	CB	LEU	B	929	4.480	-10.042	3.804	1.00	20.94	B
20	ATOM	4037	CG	LEU	B	929	5.072	-9.503	5.105	1.00	20.69	B
	ATOM	4038	CD1	LEU	B	929	4.053	-9.654	6.233	1.00	21.83	B
	ATOM	4039	CD2	LEU	B	929	6.350	-10.255	5.429	1.00	18.32	B
	ATOM	4040	C	LEU	B	929	4.498	-10.517	1.370	1.00	23.95	B
	ATOM	4041	O	LEU	B	929	3.556	-9.961	0.799	1.00	22.92	B
25	ATOM	4042	N	PHE	B	930	4.923	-11.736	1.058	1.00	25.00	B
	ATOM	4043	CA	PHE	B	930	4.280	-12.533	0.025	1.00	27.93	B
	ATOM	4044	CB	PHE	B	930	5.275	-13.520	-0.571	1.00	26.70	B
	ATOM	4045	CG	PHE	B	930	6.283	-12.887	-1.474	1.00	27.33	B
	ATOM	4046	CD1	PHE	B	930	5.979	-12.641	-2.807	1.00	26.64	B
30	ATOM	4047	CD2	PHE	B	930	7.531	-12.521	-0.989	1.00	26.19	B
	ATOM	4048	CE1	PHE	B	930	6.910	-12.042	-3.650	1.00	28.73	B
	ATOM	4049	CE2	PHE	B	930	8.470	-11.920	-1.822	1.00	27.94	B
	ATOM	4050	CZ	PHE	B	930	8.158	-11.680	-3.154	1.00	28.06	B
	ATOM	4051	C	PHE	B	930	3.120	-13.302	0.645	1.00	29.58	B
35	ATOM	4052	O	PHE	B	930	2.159	-13.651	-0.039	1.00	30.87	B
	ATOM	4053	N	HIS	B	931	3.220	-13.560	1.944	1.00	31.13	B
	ATOM	4054	CA	HIS	B	931	2.190	-14.303	2.660	1.00	34.65	B
	ATOM	4055	CB	HIS	B	931	2.738	-15.668	3.070	1.00	33.95	B
	ATOM	4056	CG	HIS	B	931	3.394	-16.408	1.948	1.00	35.58	B
40	ATOM	4057	CD2	HIS	B	931	4.685	-16.765	1.751	1.00	35.09	B
	ATOM	4058	ND1	HIS	B	931	2.704	-16.827	0.831	1.00	35.08	B
	ATOM	4059	CE1	HIS	B	931	3.543	-17.408	-0.008	1.00	36.03	B
	ATOM	4060	NE2	HIS	B	931	4.751	-17.384	0.526	1.00	35.91	B
	ATOM	4061	C	HIS	B	931	1.703	-13.556	3.892	1.00	37.35	B
45	ATOM	4062	O	HIS	B	931	2.457	-12.824	4.532	1.00	36.89	B
	ATOM	4063	N	LYS	B	932	0.433	-13.753	4.221	1.00	41.41	B
	ATOM	4064	CA	LYS	B	932	-0.177	-13.105	5.376	1.00	45.14	B
	ATOM	4065	CB	LYS	B	932	-1.702	-13.161	5.241	1.00	46.49	B
	ATOM	4066	CG	LYS	B	932	-2.196	-14.436	4.585	1.00	47.98	B
50	ATOM	4067	CD	LYS	B	932	-3.679	-14.370	4.259	1.00	50.28	B
	ATOM	4068	CE	LYS	B	932	-4.073	-15.492	3.306	1.00	50.95	B
	ATOM	4069	NZ	LYS	B	932	-3.678	-16.832	3.824	1.00	51.90	B
	ATOM	4070	C	LYS	B	932	0.261	-13.748	6.690	1.00	45.88	B
	ATOM	4071	O	LYS	B	932	0.973	-14.774	6.641	1.00	46.33	B
55	ATOM	4072	OXT	LYS	B	932	-0.114	-13.213	7.755	1.00	47.76	B
	ATOM	4073	S	SO4	Z	1	17.414	-1.312	-17.993	1.00	31.48	Z

Table 2. (cont'd)

		#	Name	Res.	Chain	Res #	X	Y	Z	occ	B	SegID
5	ATOM	4074	O1	SO4	Z	1	18.530	-2.281	-17.932	1.00	35.16	Z
	ATOM	4075	O2	SO4	Z	1	17.425	-0.473	-16.787	1.00	32.29	Z
	ATOM	4076	O3	SO4	Z	1	17.593	-0.480	-19.187	1.00	31.61	Z
	ATOM	4077	O4	SO4	Z	1	16.139	-2.038	-18.069	1.00	33.87	Z
10	ATOM	4078	O	HOH	W	1	9.851	-0.179	33.299	1.00	14.73	W
	ATOM	4079	O	HOH	W	2	22.939	-10.562	-9.981	1.00	15.38	W
	ATOM	4080	O	HOH	W	3	2.083	29.100	25.389	1.00	20.40	W
	ATOM	4081	O	HOH	W	4	14.086	-2.560	0.315	1.00	17.07	W
15	ATOM	4082	O	HOH	W	5	27.328	-10.890	1.331	1.00	18.73	W
	ATOM	4083	O	HOH	W	6	13.331	5.641	28.674	1.00	19.86	W
	ATOM	4084	O	HOH	W	7	13.186	1.399	47.673	1.00	13.95	W
	ATOM	4085	O	HOH	W	8	32.971	-11.715	0.505	1.00	14.94	W
20	ATOM	4086	O	HOH	W	9	18.332	-4.869	5.470	1.00	18.48	W
	ATOM	4087	O	HOH	W	10	12.895	-0.329	56.919	1.00	18.21	W
	ATOM	4088	O	HOH	W	11	39.458	-17.312	7.769	1.00	30.23	W
	ATOM	4089	O	HOH	W	12	26.010	-12.904	-3.995	1.00	34.91	W
25	ATOM	4090	O	HOH	W	13	10.307	23.211	14.451	1.00	24.90	W
	ATOM	4091	O	HOH	W	14	33.794	-3.491	-3.298	1.00	24.71	W
	ATOM	4092	O	HOH	W	15	-7.542	-1.149	46.176	1.00	17.56	W
	ATOM	4093	O	HOH	W	16	10.481	5.430	28.973	1.00	16.76	W
30	ATOM	4094	O	HOH	W	17	9.010	1.461	31.392	1.00	20.19	W
	ATOM	4095	O	HOH	W	18	0.442	-1.822	32.126	1.00	27.35	W
	ATOM	4096	O	HOH	W	19	20.106	-2.758	6.202	1.00	22.10	W
	ATOM	4097	O	HOH	W	20	6.858	5.226	-11.172	1.00	19.86	W
35	ATOM	4098	O	HOH	W	21	3.112	31.643	22.889	1.00	22.74	W
	ATOM	4099	O	HOH	W	22	10.057	15.524	34.676	1.00	20.39	W
	ATOM	4100	O	HOH	W	23	28.343	-13.760	-2.951	1.00	27.79	W
	ATOM	4101	O	HOH	W	24	5.302	8.903	42.508	1.00	17.97	W
40	ATOM	4102	O	HOH	W	25	12.929	28.598	20.593	1.00	23.80	W
	ATOM	4103	O	HOH	W	26	-4.534	17.192	43.743	1.00	28.92	W
	ATOM	4104	O	HOH	W	27	9.676	3.409	22.849	1.00	14.96	W
	ATOM	4105	O	HOH	W	28	13.824	-6.363	9.101	1.00	24.33	W
45	ATOM	4106	O	HOH	W	29	19.783	-1.498	23.163	1.00	21.54	W
	ATOM	4107	O	HOH	W	30	7.516	21.308	40.840	1.00	39.46	W
	ATOM	4108	O	HOH	W	31	20.250	-8.806	18.170	1.00	22.74	W
	ATOM	4109	O	HOH	W	32	20.825	-10.938	-8.107	1.00	23.11	W
50	ATOM	4110	O	HOH	W	33	-1.545	-0.716	48.089	1.00	19.38	W
	ATOM	4111	O	HOH	W	34	3.305	-1.599	49.132	1.00	34.02	W
	ATOM	4112	O	HOH	W	35	40.480	-6.360	12.399	1.00	27.56	W
	ATOM	4113	O	HOH	W	36	11.493	20.832	38.950	1.00	38.71	W
55	ATOM	4114	O	HOH	W	37	9.120	1.197	21.414	1.00	23.98	W
	ATOM	4115	O	HOH	W	38	-1.682	3.281	52.013	1.00	22.24	W
	ATOM	4116	O	HOH	W	39	-11.086	22.915	35.681	1.00	32.42	W
	ATOM	4117	O	HOH	W	40	12.002	7.533	-1.688	1.00	30.69	W
	ATOM	4118	O	HOH	W	41	14.518	-13.452	-19.077	1.00	26.25	W
	ATOM	4119	O	HOH	W	42	18.500	30.309	24.738	1.00	37.66	W
	ATOM	4120	O	HOH	W	43	14.005	-7.837	26.712	1.00	24.93	W
	ATOM	4121	O	HOH	W	44	2.873	-1.026	35.419	1.00	35.46	W
	ATOM	4122	O	HOH	W	45	19.791	-5.878	22.089	1.00	24.74	W
	ATOM	4123	O	HOH	W	46	36.617	-7.101	-5.193	1.00	27.22	W
	ATOM	4124	O	HOH	W	47	17.997	16.706	17.050	1.00	23.35	W
	ATOM	4125	O	HOH	W	48	12.818	29.647	30.373	1.00	34.99	W
	ATOM	4126	O	HOH	W	49	35.741	2.637	0.675	1.00	29.22	W

Table 2. (cont'd)

		#	Name	Res.	Chain	Res #	X	Y	Z	occ	B	SegID
5	ATOM	4127	O	HOH	W	50	-0.698	-9.676	42.142	1.00	30.67	W
	ATOM	4128	O	HOH	W	51	-0.525	29.866	21.575	1.00	19.53	W
	ATOM	4129	O	HOH	W	52	18.379	-2.516	47.069	1.00	27.04	W
	ATOM	4130	O	HOH	W	53	8.722	0.737	27.146	1.00	31.04	W
	ATOM	4131	O	HOH	W	54	20.510	8.743	13.356	1.00	23.93	W
10	ATOM	4132	O	HOH	W	55	12.649	20.284	36.357	1.00	16.97	W
	ATOM	4133	O	HOH	W	56	-8.042	11.472	43.548	1.00	24.46	W
	ATOM	4134	O	HOH	W	57	-11.476	3.549	43.258	1.00	25.26	W
	ATOM	4135	O	HOH	W	58	7.056	-16.459	-15.106	1.00	23.80	W
	ATOM	4136	O	HOH	W	59	21.350	-22.318	13.143	1.00	34.05	W
15	ATOM	4137	O	HOH	W	60	28.062	12.099	16.977	1.00	26.29	W
	ATOM	4138	O	HOH	W	61	-22.171	4.158	40.700	1.00	28.15	W
	ATOM	4139	O	HOH	W	62	22.437	24.881	26.553	1.00	20.93	W
	ATOM	4140	O	HOH	W	63	28.474	13.733	32.727	1.00	30.22	W
	ATOM	4141	O	HOH	W	64	1.626	-6.963	38.739	1.00	22.58	W
20	ATOM	4142	O	HOH	W	65	5.955	33.007	28.845	1.00	42.67	W
	ATOM	4143	O	HOH	W	66	7.548	3.514	24.485	1.00	25.19	W
	ATOM	4144	O	HOH	W	67	28.084	10.733	25.158	1.00	32.12	W
	ATOM	4145	O	HOH	W	68	14.819	-4.756	10.909	1.00	22.88	W
	ATOM	4146	O	HOH	W	69	12.512	-3.850	11.912	1.00	30.27	W
25	ATOM	4147	O	HOH	W	70	23.580	-16.334	5.829	1.00	22.52	W
	ATOM	4148	O	HOH	W	71	10.565	-11.166	-16.058	1.00	23.71	W
	ATOM	4149	O	HOH	W	72	2.064	13.163	18.256	1.00	38.01	W
	ATOM	4150	O	HOH	W	73	24.352	27.565	20.778	1.00	29.09	W
	ATOM	4151	O	HOH	W	74	13.534	11.655	46.723	1.00	29.05	W
30	ATOM	4152	O	HOH	W	75	-3.751	1.854	53.213	1.00	24.50	W
	ATOM	4153	O	HOH	W	76	14.249	-6.307	6.318	1.00	33.71	W
	ATOM	4154	O	HOH	W	77	8.346	20.512	13.638	1.00	29.91	W
	ATOM	4155	O	HOH	W	78	10.659	-27.801	-3.102	1.00	25.66	W
	ATOM	4156	O	HOH	W	79	29.300	-5.213	-7.941	1.00	27.88	W
35	ATOM	4157	O	HOH	W	80	23.744	15.309	11.455	1.00	36.84	W
	ATOM	4158	O	HOH	W	81	26.341	-4.131	-16.979	1.00	37.38	W
	ATOM	4159	O	HOH	W	82	-5.101	-2.239	21.176	1.00	49.05	W
	ATOM	4160	O	HOH	W	83	8.948	-10.743	1.764	1.00	25.57	W
	ATOM	4161	O	HOH	W	84	22.426	8.856	3.497	1.00	30.12	W
40	ATOM	4162	O	HOH	W	85	15.590	-6.464	2.357	1.00	20.20	W
	ATOM	4163	O	HOH	W	86	22.984	-28.399	7.053	1.00	43.09	W
	ATOM	4164	O	HOH	W	87	35.903	-1.727	10.279	1.00	24.30	W
	ATOM	4165	O	HOH	W	88	7.456	3.549	31.583	1.00	22.42	W
	ATOM	4166	O	HOH	W	89	7.855	-6.471	46.303	1.00	30.69	W
45	ATOM	4167	O	HOH	W	90	43.114	-4.754	5.804	1.00	31.47	W
	ATOM	4168	O	HOH	W	91	23.688	18.339	28.249	1.00	35.33	W
	ATOM	4169	O	HOH	W	92	8.671	30.830	26.750	1.00	25.23	W
	ATOM	4170	O	HOH	W	93	21.069	9.806	42.796	1.00	22.22	W
	ATOM	4171	O	HOH	W	94	34.235	3.943	13.825	1.00	29.92	W
50	ATOM	4172	O	HOH	W	95	4.325	-12.649	42.865	1.00	33.49	W
	ATOM	4173	O	HOH	W	96	4.905	-14.665	5.831	1.00	30.26	W
	ATOM	4174	O	HOH	W	97	17.850	0.612	51.901	1.00	26.30	W
	ATOM	4175	O	HOH	W	98	29.845	-26.714	-0.530	1.00	32.22	W
	ATOM	4176	O	HOH	W	99	21.826	3.590	34.558	1.00	30.54	W
55	ATOM	4177	O	HOH	W	100	8.730	5.195	6.121	1.00	31.99	W
	ATOM	4178	O	HOH	W	101	-12.510	-0.569	35.114	1.00	39.35	W
	ATOM	4179	O	HOH	W	102	9.974	18.335	15.716	1.00	30.38	W

Table 2. (cont'd)

		#	Name	Res.	Chain	Res #	X	Y	Z	occ	B	SegID
5	ATOM	4180	O	HOH	W	103	-20.727	6.780	40.198	1.00	31.21	W
	ATOM	4181	O	HOH	W	104	17.245	3.775	27.753	1.00	23.95	W
	ATOM	4182	O	HOH	W	105	12.204	31.282	32.900	1.00	47.25	W
	ATOM	4183	O	HOH	W	106	30.849	-13.455	-10.120	1.00	44.05	W
	ATOM	4184	O	HOH	W	107	-31.232	-11.424	-3.737	1.00	34.09	W
10	ATOM	4185	O	HOH	W	108	0.616	0.645	30.187	1.00	19.02	W
	ATOM	4186	O	HOH	W	109	9.969	10.406	39.896	1.00	41.21	W
	ATOM	4187	O	HOH	W	110	4.951	-13.348	36.812	1.00	25.64	W
	ATOM	4188	O	HOH	W	111	24.217	0.126	32.380	1.00	42.27	W
	ATOM	4189	O	HOH	W	112	7.760	3.239	27.484	1.00	31.56	W
15	ATOM	4190	O	HOH	W	113	-13.150	10.929	35.305	1.00	37.37	W
	ATOM	4191	O	HOH	W	114	14.414	10.760	49.023	1.00	25.40	W
	ATOM	4192	O	HOH	W	115	9.753	12.679	37.102	1.00	37.47	W
	ATOM	4193	O	HOH	W	116	-4.457	0.109	25.639	1.00	31.43	W
	ATOM	4194	O	HOH	W	117	31.098	5.122	20.729	1.00	32.11	W
20	ATOM	4195	O	HOH	W	118	9.748	22.778	39.579	1.00	29.38	W
	ATOM	4196	O	HOH	W	119	15.530	-4.123	52.634	1.00	29.51	W
	ATOM	4197	O	HOH	W	120	14.408	-3.786	6.247	1.00	35.75	W
	ATOM	4198	O	HOH	W	121	3.061	16.521	16.785	1.00	25.91	W
	ATOM	4199	O	HOH	W	122	39.801	-19.133	1.482	1.00	26.72	W
25	ATOM	4200	O	HOH	W	123	37.378	-1.402	24.102	1.00	39.79	W
	ATOM	4201	O	HOH	W	124	14.576	12.610	44.487	1.00	30.08	W
	ATOM	4202	O	HOH	W	125	4.145	16.097	43.565	1.00	34.79	W
	ATOM	4203	O	HOH	W	126	7.682	25.781	13.009	1.00	45.48	W
	ATOM	4204	O	HOH	W	127	9.845	-12.141	9.020	1.00	29.42	W
30	ATOM	4205	O	HOH	W	128	15.739	10.997	-9.996	1.00	27.09	W
	ATOM	4206	O	HOH	W	129	6.716	10.052	44.773	1.00	20.65	W
	ATOM	4207	O	HOH	W	130	14.744	-8.445	4.732	1.00	23.00	W
	ATOM	4208	O	HOH	W	131	21.909	24.767	16.946	1.00	31.22	W
	ATOM	4209	O	HOH	W	132	33.120	-12.601	-1.941	1.00	27.91	W
35	ATOM	4210	O	HOH	W	133	23.283	3.901	-16.585	1.00	40.81	W
	ATOM	4211	O	HOH	W	134	27.581	13.334	14.368	1.00	31.58	W
	ATOM	4212	O	HOH	W	135	23.546	-8.108	-4.594	1.00	38.50	W
	ATOM	4213	O	HOH	W	136	3.316	-6.614	1.955	1.00	31.34	W
	ATOM	4214	O	HOH	W	137	17.363	1.926	49.485	1.00	28.70	W
40	ATOM	4215	O	HOH	W	138	38.393	-7.509	-2.153	1.00	31.36	W
	ATOM	4216	O	HOH	W	139	14.920	-4.060	2.471	1.00	31.77	W
	ATOM	4217	O	HOH	W	140	38.118	-0.901	8.667	1.00	31.86	W
	ATOM	4218	O	HOH	W	141	26.383	5.332	2.546	1.00	34.89	W
	ATOM	4219	O	HOH	W	142	35.405	3.798	3.233	1.00	34.38	W
45	ATOM	4220	O	HOH	W	143	11.409	-21.800	-16.697	1.00	35.84	W
	ATOM	4221	O	HOH	W	144	39.725	-6.596	7.646	1.00	38.73	W
	ATOM	4222	O	HOH	W	145	17.070	6.806	11.706	1.00	34.49	W
	ATOM	4223	O	HOH	W	146	3.371	3.664	29.494	1.00	39.22	W
	ATOM	4224	O	HOH	W	147	13.400	6.010	35.121	1.00	36.31	W
50	ATOM	4225	O	HOH	W	148	11.012	18.450	40.465	1.00	37.80	W
	ATOM	4226	O	HOH	W	149	35.666	-17.196	-3.005	1.00	33.54	W
	ATOM	4227	O	HOH	W	150	27.587	-15.335	-11.411	1.00	32.63	W
	ATOM	4228	O	HOH	W	151	24.903	-9.920	-1.819	1.00	37.55	W
	ATOM	4229	O	HOH	W	152	15.833	8.081	-12.357	1.00	42.37	W
55	ATOM	4230	O	HOH	W	153	28.438	16.821	21.396	1.00	44.90	W
	ATOM	4231	O	HOH	W	154	21.332	29.602	23.542	1.00	39.67	W
	ATOM	4232	O	HOH	W	155	12.772	-9.868	3.678	1.00	36.84	W

Table 2. (cont'd)

		#	Name	Res.	Chain	Res #	X	Y	Z	occ	B	SegID
5	ATOM	4233	O	HOH	W	156	16.961	-7.689	35.260	1.00	44.42	W
	ATOM	4234	O	HOH	W	157	10.499	10.751	16.433	1.00	34.39	W
	ATOM	4235	O	HOH	W	158	28.327	-5.237	-10.882	1.00	45.84	W
	ATOM	4236	O	HOH	W	159	36.087	4.558	6.039	1.00	28.34	W
	ATOM	4237	O	HOH	W	160	-0.994	29.266	35.756	1.00	35.83	W
10	ATOM	4238	O	HOH	W	161	0.695	-6.498	29.582	1.00	33.46	W
	ATOM	4239	O	HOH	W	162	26.373	21.757	15.011	1.00	43.14	W
	ATOM	4240	O	HOH	W	163	15.148	32.436	21.985	1.00	36.34	W
	ATOM	4241	O	HOH	W	164	-3.288	-2.573	49.020	1.00	37.67	W
	ATOM	4242	O	HOH	W	165	-1.628	26.470	37.063	1.00	33.28	W
15	ATOM	4243	O	HOH	W	166	27.897	14.312	24.143	1.00	35.59	W
	ATOM	4244	O	HOH	W	167	7.738	17.438	39.142	1.00	46.82	W
	ATOM	4245	O	HOH	W	168	10.899	4.880	52.240	1.00	32.86	W
	ATOM	4246	O	HOH	W	169	10.635	-22.038	3.450	1.00	43.02	W
	ATOM	4247	O	HOH	W	170	25.343	2.041	28.575	1.00	43.36	W
20	ATOM	4248	O	HOH	W	171	4.243	6.461	-2.841	1.00	33.86	W
	ATOM	4249	O	HOH	W	172	4.073	6.130	-9.321	1.00	37.81	W
	ATOM	4250	O	HOH	W	173	7.805	-22.135	-12.033	1.00	33.34	W
	ATOM	4251	O	HOH	W	174	13.170	-15.783	10.760	1.00	40.16	W
	ATOM	4252	O	HOH	W	175	15.268	-15.546	12.623	1.00	39.35	W
25	ATOM	4253	O	HOH	W	176	8.067	-4.029	50.607	1.00	41.24	W
	ATOM	4254	O	HOH	W	177	-2.564	26.998	20.110	1.00	40.38	W
	ATOM	4255	O	HOH	W	178	20.599	-7.598	44.029	1.00	35.32	W
	ATOM	4256	O	HOH	W	179	7.493	-14.259	8.323	1.00	45.07	W
	ATOM	4257	N1	989	C	701	12.950	16.155	29.632	1.00	25.58	C
30	ATOM	4258	C2	989	C	701	12.751	15.346	28.400	1.00	26.75	C
	ATOM	4259	C3	989	C	701	11.423	15.061	28.357	1.00	25.91	C
	ATOM	4260	C4	989	C	701	10.740	15.698	29.489	1.00	26.53	C
	ATOM	4261	C5	989	C	701	11.639	16.305	30.277	1.00	24.85	C
	ATOM	4262	C6	989	C	701	11.345	17.031	31.471	1.00	25.38	C
35	ATOM	4263	N7	989	C	701	11.135	17.620	32.434	1.00	28.13	C
	ATOM	4264	C8	989	C	701	14.187	16.785	30.127	1.00	23.90	C
	ATOM	4265	C12	989	C	701	13.748	15.000	27.362	1.00	26.02	C
	ATOM	4266	C13	989	C	701	15.088	14.717	27.732	1.00	26.27	C
	ATOM	4267	C14	989	C	701	16.102	14.633	26.756	1.00	27.92	C
40	ATOM	4268	C15	989	C	701	15.772	14.704	25.388	1.00	28.20	C
	ATOM	4269	C16	989	C	701	14.419	14.901	24.980	1.00	26.87	C
	ATOM	4270	C17	989	C	701	13.419	15.084	25.984	1.00	27.22	C
	ATOM	4271	N18	989	C	701	16.760	14.547	24.458	1.00	30.23	C
	ATOM	4272	C19	989	C	701	16.515	14.415	23.126	1.00	31.26	C
45	ATOM	4273	O20	989	C	701	15.208	14.452	22.722	1.00	31.21	C
	ATOM	4274	C21	989	C	701	14.108	14.960	23.483	1.00	29.70	C
	ATOM	4275	C22	989	C	701	12.917	14.062	23.101	1.00	28.20	C
	ATOM	4276	C26	989	C	701	13.888	16.419	23.039	1.00	27.96	C
	ATOM	4277	S30	989	C	701	17.846	14.580	22.146	1.00	28.30	C
50	ATOM	4278	N1	989	D	701	28.639	-9.086	6.656	1.00	28.57	D
	ATOM	4279	C2	989	D	701	27.632	-8.815	7.706	1.00	29.39	D
	ATOM	4280	C3	989	D	701	26.668	-9.755	7.546	1.00	27.96	D
	ATOM	4281	C4	989	D	701	26.974	-10.590	6.385	1.00	28.44	D
	ATOM	4282	C5	989	D	701	28.128	-10.194	5.838	1.00	28.00	D
55	ATOM	4283	C6	989	D	701	28.775	-10.812	4.721	1.00	29.08	D
	ATOM	4284	N7	989	D	701	29.314	-11.293	3.826	1.00	32.15	D
	ATOM	4285	C8	989	D	701	30.021	-8.594	6.590	1.00	27.50	D

Table 2. (cont'd)

		#	Name	Res.	Chain	Res	#	X	Y	Z	occ	B	SegID
5	ATOM	4286	C12	989	D	701		27.714	-7.844	8.821	1.00	29.66	D
	ATOM	4287	C13	989	D	701		28.293	-6.561	8.626	1.00	30.33	D
	ATOM	4288	C14	989	D	701		28.500	-5.693	9.723	1.00	32.12	D
	ATOM	4289	C15	989	D	701		28.076	-6.071	11.018	1.00	31.15	D
	ATOM	4290	C16	989	D	701		27.461	-7.340	11.226	1.00	31.11	D
10	ATOM	4291	C17	989	D	701		27.287	-8.212	10.117	1.00	30.39	D
	ATOM	4292	N18	989	D	701		28.293	-5.221	12.072	1.00	33.73	D
	ATOM	4293	C19	989	D	701		27.907	-5.501	13.348	1.00	34.14	D
	ATOM	4294	O20	989	D	701		27.191	-6.652	13.554	1.00	33.18	D
	ATOM	4295	C21	989	D	701		26.998	-7.721	12.626	1.00	32.21	D
15	ATOM	4296	C22	989	D	701		25.485	-8.011	12.650	1.00	32.12	D
	ATOM	4297	C26	989	D	701		27.816	-8.917	13.151	1.00	34.10	D
	ATOM	4298	S30	989	D	701		28.475	-4.462	14.528	1.00	34.00	D

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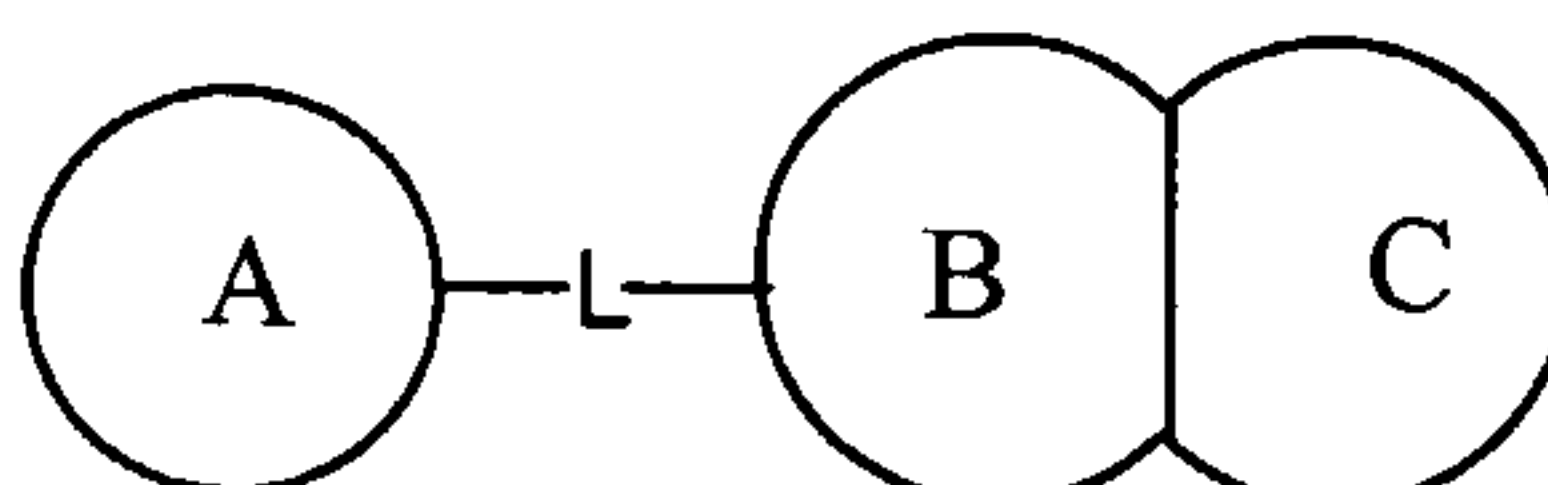
OTHER EMBODIMENTS

A number of embodiments of the invention have been described. Nevertheless, it will be understood that various modifications may be made. For example, a structure of progesterone receptor can be determined where progesterone receptor is bound to a non-steroidal agent other than tanaproget. Accordingly, other embodiments are within the scope of the following claims.

25

WHAT IS CLAIMED IS:

1. A crystallized protein-ligand complex, comprising:
a progesterone receptor polypeptide; and
5 a non-steroidal ligand that is an agonist of the progesterone receptor polypeptide or
an antagonist of the progesterone receptor polypeptide.
- 10 2. The crystallized protein-ligand complex of claim 1, wherein the non-steroidal
ligand is an agonist of the progesterone receptor polypeptide.
3. The crystallized protein-ligand complex of claim 1, wherein the non-steroidal
ligand is an antagonist of the progesterone receptor polypeptide.
- 15 4. The crystallized protein-ligand complex of any one of claims 1 to 3, wherein
the non-steroidal ligand comprises at least two rings.
5. The crystallized protein-ligand complex of claim 4, wherein the at least two
rings are fused.
- 20 6. The crystallized protein-ligand complex of claim 5, wherein the fused rings
comprise at least one ring heteroatom.
7. The crystallized protein-ligand complex of claim 6, wherein the at least one
ring heteroatom is selected from the group consisting of N, O, and S.
- 25 8. The crystallized protein-ligand complex of any one of claims 1 to 7, wherein
the non-steroidal ligand has the structure:



wherein A, B and C represent ring systems, B and C are fused rings, and L is a linker moiety.

9. The crystallized protein-ligand complex of any one of claims 1 to 8, wherein
5 the non-steroidal ligand comprises a benzoxazine derivative.

10. The crystallized protein-ligand complex of claim 9, wherein the benzoxazine derivative comprises an oxo or thio substituent at the 2 position.

10 11. The crystallized protein-ligand complex of claim 9 or 10, wherein the benzoxazine derivative has at least one hydrophobic substituent at or near the 4 position of the benzoxazine ring.

12. The crystallized protein-ligand complex of claim 1, wherein the non-steroidal
15 ligand is tanaproget.

13. The crystallized protein-ligand complex of any one of claims 1 to 12, wherein the crystallized protein-ligand complex has space group $P2_1$.

20 14. The crystallized protein-ligand complex of any one of claims 1 to 13, wherein the crystallized protein-ligand complex has unit cell dimensions $a=57.5 \text{ \AA}$, $b=64.5 \text{ \AA}$, $c=70.4 \text{ \AA}$, and $\beta=95.8^\circ$.

25 15. The crystallized protein-ligand complex of any one of claims 1 to 14, wherein the non-steroidal ligand is bound to the progesterone receptor polypeptide.

16. The crystallized protein-ligand complex of any one of claims 1 to 15, wherein the progesterone receptor polypeptide comprises a ligand binding domain.

30 17. The crystallized protein-ligand complex of claim 16, wherein the non-steroidal ligand is bound to the ligand binding domain.

18. The crystallized protein-ligand complex of any one of claims 1 to 17, wherein the progesterone receptor polypeptide is from a mammalian species.

5 19. The crystallized protein-ligand complex of any one of claims 1 to 17, wherein the progesterone receptor polypeptide is from a non-mammalian species.

20. The crystallized protein-ligand complex of claim 18, wherein the progesterone receptor polypeptide is from a human.

10 21. The crystallized protein-ligand complex of claim 20, wherein the progesterone polypeptide comprises the amino acid sequence of SEQ ID NO:2.

15 22. The crystallized protein-ligand complex of any one of claims 1 to 21, wherein the complex is capable of diffracting X-rays to a resolution of at least about 3.5 Å.

23. The crystallized protein-ligand complex of claim 1, wherein the complex comprises the structural coordinates of Table 2 $\pm$ a root mean square deviation for alpha carbon atoms of not more than 1.5 Å.

20 24. The crystallized protein-ligand complex of any one of claims 1 to 22, wherein the non-steroidal ligand interacts with one or more of Gln725, Leu797, Asn719 and Arg766 of the progesterone receptor polypeptide.

25 25. A composition, comprising a complex according to any one of claims 1 to 24.

26. A method, comprising:

using a three-dimensional model of a progesterone receptor polypeptide bound to a non-steroidal ligand to design an agent that interacts with the progesterone receptor polypeptide,

30

wherein the non-steroidal ligand is an agonist of the progesterone receptor polypeptide or an antagonist of the progesterone receptor polypeptide.

27. The method of claim 26, wherein the three-dimensional model comprises a
5 ligand binding domain of the progesterone receptor polypeptide.

28. The method of claim 26 or 27, wherein the three-dimensional model comprises structural coordinates of atoms of the progesterone receptor polypeptide.

10 29. The method of claim 28, wherein the structural coordinates are experimentally determined coordinates.

30. The method of claim 28 or 29, wherein the atoms include atoms of an active site of the progesterone receptor polypeptide.

15 31. The method of claim 30, wherein the active site is a ligand binding domain.

32. The method of claim 28, wherein the structural coordinates are according to Table 2, $\pm$ a root mean square deviation for alpha carbon atoms of not more than 1.5 Å.

20 33. The method of any one of claims 28 to 32, wherein the three-dimensional model comprises structural coordinates of the non-steroidal ligand.

25 34. The method of claim 33, further comprising altering the non-steroidal ligand of the model.

35. The method of claim 34, wherein altering the non-steroidal ligand comprises changing the structural coordinates of the non-steroidal ligand.

30 36. The method of claim 34, wherein altering the non-steroidal ligand comprises changing the chemical structure of the non-steroidal ligand.

37. The method of any one of claims 28 to 36, wherein the three-dimensional model comprises structural coordinates of an atom selected from the group consisting of atoms of amino acids Gln725 and Arg766 of the progesterone receptor polypeptide as defined by the amino acids of SEQ ID NO:2.

38. The method of any one of claims 28 to 37, wherein the three-dimensional model comprises structural coordinates of an atom selected from the group consisting of atoms of amino acids Ile699, Ala701, Leu714, Leu715, Leu718, Asn719, Leu721, Gln725, Trp755, Met756, Met759, Val760, Leu763, Arg766, Ser767, Tyr777, Phe778, Ala779, Leu782, Phe794, Leu797, Lys798, Met801, Ile804, Leu887, His888, Tyr890, Cys891, Asn893, Thr894, Phe895, Ser898, Leu901, Val903, Phe905, Met909, Ile913, and Leu917 as defined by the amino acids of SEQ ID NO:2.

39. The method of any one of claims 26 to 38, further comprising calculating a distance between an atom of the progesterone receptor polypeptide and an atom of the agent.

40. The method of any one of claims 26 to 39, further comprising comparing a predicted interaction between the agent and the progesterone receptor polypeptide with the interaction between the non-steroidal ligand and the progesterone receptor polypeptide.

41. The method of any one of claims 26 to 40, further comprising providing a composition including the progesterone receptor polypeptide.

42. The method of claim 41, wherein the progesterone receptor polypeptide is crystalline.

43. The method of claim 42, wherein the composition includes the agent that interacts with the progesterone receptor polypeptide.

44. The method of claim 43, further comprising experimentally determining the interaction of the agent with the progesterone receptor polypeptide.

45. The method of claim 44, further comprising comparing the interaction of the agent with the progesterone receptor polypeptide to an interaction of a second agent with the progesterone receptor polypeptide.

46. A method, comprising:
selecting an agent by performing rational drug design with a three-dimensional structure of a complex according to any one of claims 1 to 24
contacting the agent with a progesterone receptor polypeptide; and
detecting the ability of the agent to bind the progesterone receptor polypeptide.

47. The method of claim 46, wherein the agent is selected via computer modeling.

48. The method of claim 46 or 47, further comprising synthesizing the agent.

49. The method of any one of claims 46 to 48, further comprising:
obtaining a supplemental crystalline complex comprising the progesterone polypeptide receptor and the agent;
determining the three-dimensional structure of the supplemental crystalline complex;
selecting a second agent by performing rational drug design with the three-dimensional structure of the supplemental crystalline complex;
contacting the second agent with the progesterone polypeptide receptor; and
detecting the ability of the second agent to bind the progesterone receptor polypeptide.

50. The method of claim 49, wherein the second agent is selected via computer modeling.

51. The method of claim 49 or 50, further comprising synthesizing the second agent.

52. A method, comprising:
5 contacting a polypeptide with a non-steroidal ligand to grow a crystal of a complex according to any one of claims 1 to 24.

53. The method of claim 52, wherein the method includes using hanging drop vapor diffusion.

10 54. A software system, comprising instructions for causing a computer system to:
accept information relating to the structure of a progesterone receptor polypeptide bound to a non-steroidal ligand that is an agonist of the progesterone receptor polypeptide or an antagonist of the progesterone receptor polypeptide;

15 accept information relating to a candidate agent; and
determine binding characteristics of the candidate agent to the progesterone receptor polypeptide,

wherein the determination is based on the information relating to the structure of the progesterone receptor polypeptide and the information relating to the candidate agent.

20 55. The software system of claim 54, wherein the structure of the progesterone receptor polypeptide bound to the non-steroidal ligand is a crystal structure.

25 56. The software system of claim 55, wherein the crystal structure comprises the structural coordinates of Table 2, $\pm$ a root mean square deviation for alpha carbon atoms of not more than 1.5 Å.

57. The software system of any one of claims 54 to 56, further comprising instructions for causing the computer system to:

30 apply information from a database, the information relating to candidate agents; and

identify a candidate agent in the database that can bind the progesterone receptor polypeptide,

wherein the identification is based on the information relating to the structure of the progesterone receptor polypeptide and information relating to the candidate agent.

5

58. The software system of claim 57, further comprising instructions for causing the computer system to model the binding characteristics of the candidate agent with the progesterone receptor polypeptide.

10

59. A computer program residing on a computer readable medium having a plurality of instructions stored thereon, which, when executed by one or more processors, cause the one or more processors to:

15

accept information relating to the structure of a progesterone receptor polypeptide bound to a non-steroidal ligand that is an agonist of the progesterone receptor polypeptide or an antagonist of the progesterone receptor polypeptide;

accept information relating to a candidate agent; and

determine binding characteristics of the candidate agent to the progesterone receptor polypeptide,

20

wherein the determination is based on the information relating to the structure of the progesterone receptor polypeptide and the information relating to the candidate agent.

60. A method, comprising:

25

accepting information relating to the structure of a progesterone receptor polypeptide bound to a non-steroidal ligand that is an agonist of the progesterone receptor polypeptide or an antagonist of the progesterone receptor polypeptide; and

modeling the binding characteristics of the progesterone receptor polypeptide with a candidate agent,

wherein the method is implemented by a software system.

61. The method of claim 60, further comprising applying information from a database of candidate agents to identify a candidate agent that can bind the progesterone receptor polypeptide,

wherein the identification is based on the information relating to the structure of the progesterone receptor polypeptide and information relating to the candidate agent.

62. A computer program residing on a computer readable medium having a plurality of instructions stored thereon, which, when executed by one or more processors, cause the one or more processors to:

accept information relating to the structure of a progesterone receptor polypeptide bound to a non-steroidal ligand that is an agonist of the progesterone receptor polypeptide or an antagonist of the progesterone receptor polypeptide; and

model the binding characteristics of the progesterone receptor polypeptide with a candidate agent.

63. The computer program of claim 62, further comprising instructions which cause the one or more processors to:

apply information from a database, the information relating to candidate agents; and identify a candidate agent in the database that can bind the progesterone receptor polypeptide,

wherein the identification is based on the information relating to the structure of the progesterone receptor polypeptide.

64. The computer program of claim 63, further comprising instructions which cause the one or more processors to model the binding characteristics of the candidate agent with the progesterone receptor polypeptide.

65. A software system, comprising instructions for causing a computer system to: accept information relating to the structure of a progesterone receptor polypeptide bound to a non-steroidal ligand that is an agonist of the progesterone receptor polypeptide or an antagonist of the progesterone receptor polypeptide; and

model the binding characteristics of the progesterone receptor polypeptide with a candidate agent.

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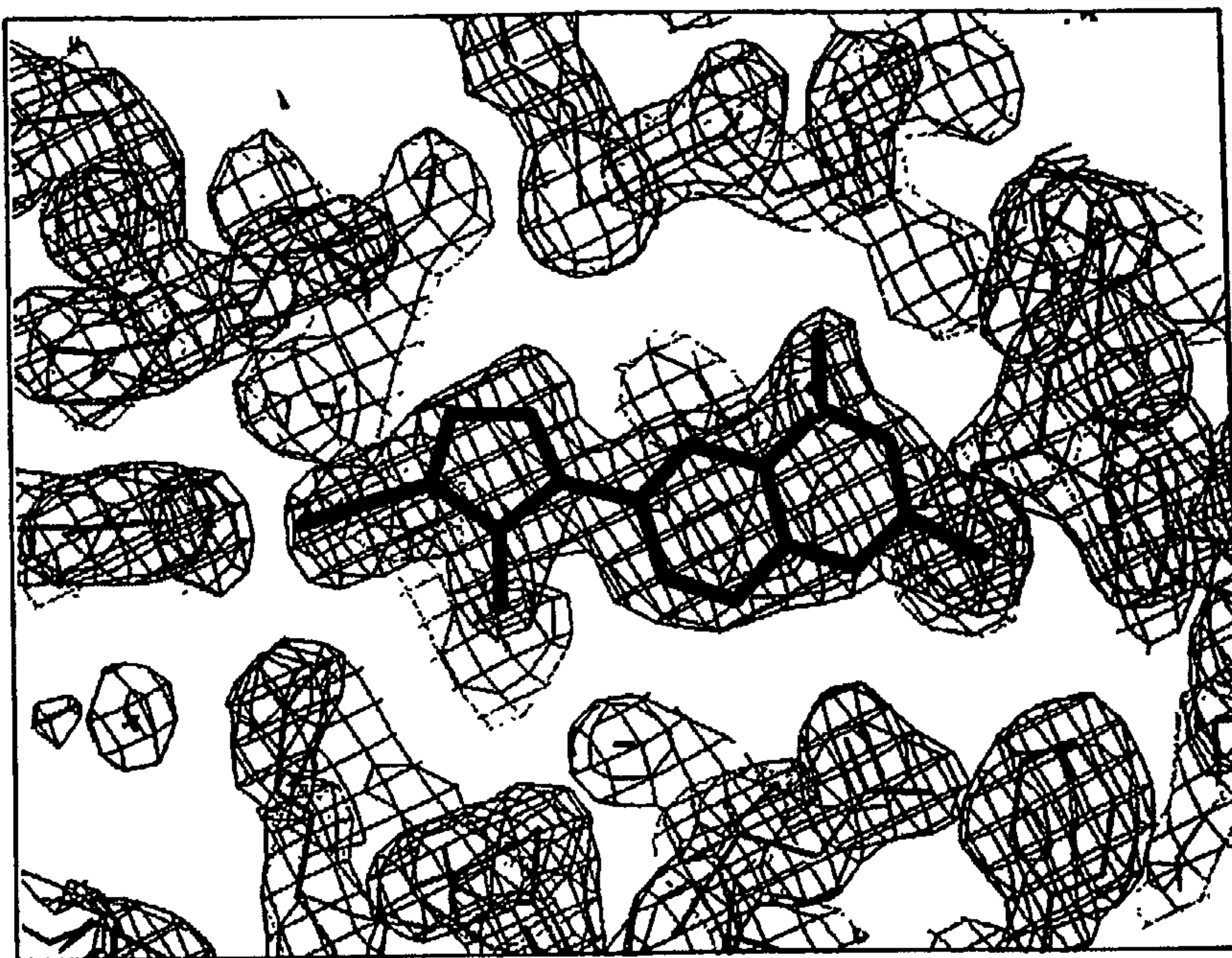


FIG. 1A

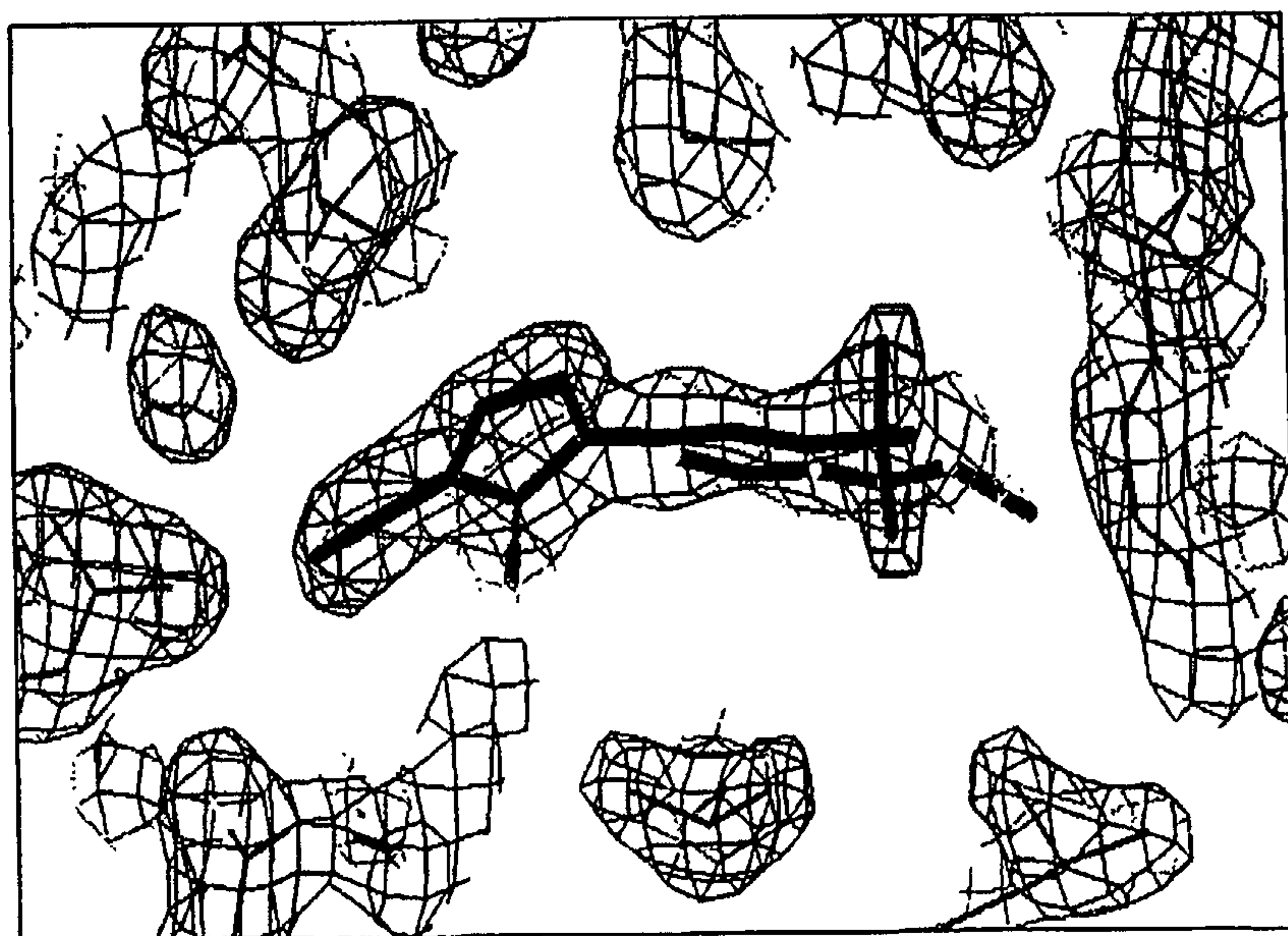


FIG. 1B

GST:PR-LBD fusion protein

MSPILGYWKI	KGLVQPTRL	LEYLEEKYEE	HLYERDEGDK	WRNKKFELGL	EFNLPYYID
GDKLTQSM	IIRYIADKHN	MLGGCPKERA	EISMLEGAVL	DIRYGVSR	IA YSKDFETLKV
DFLSKLPEML	KMFEDRLCHK	TYLNGDHVTH	PDFMLYDALD	VVLYMDPMCL	DAFPKLVCFK
KRIEAIQID	KYLKSSKYIA	WPLQGQATF	GGGDHPPKSD	LVPRGSPGQD	IQLIPPLINL
LMSIEPDVIY	AGHDNTKPD	TSSLLTSLNQ	LGERQLLSV	KWSKSLPGFR	NLHIDDQITL
IQYSWMSLMV	FGLGWR	SYKH VSGQMLYFAP	DLILNEQRMK	ESSFYSLCLT	MWQIPQEFVK
LQVSQEEFLC	MKVLLLLNTI	PLEGLRSQTQ	FEEMRSSYIR	ELIKAIGLRQ	KGVVSSSQRF
YQLTKLLDNL	HDLVKQLHLY	CLNTFIQSRA	LSVEFFPEMMS	EVIAAQLPKI	LAGMVKPLLF
HKK	(SEQ ID NO:1)				

FIG. 2A

PR-LBD (PR numbering)

671	----	GSPGQD	IQLIPPLINL	LMSIEPDVIY	AGHDNTKPD	TSSLLTSLNQ	LGERQLLSV
731	KWSKSLPGFR	NLHIDDQITL	IQYSWMSLMV	FGLGWR	SYKH VSGQMLYFAP	DLILNEQRMK	
791	ESSFYSLCLT	MWQIPQEFVK	LQVSQEEFLC	MKVLLLLNTI	PLEGLRSQTQ	FEEMRSSYIR	
851	ELIKAIGLRQ	KGVVSSSQRF	YQLTKLLDNL	HDLVKQLHLY	CLNTFIQSRA	LSVEFFPEMMS	
911	EVIAAQLPKI	LAGMVKPLLF	HKK	(SEQ ID NO:2)			

FIG. 2B

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MTELKAKGPRAPHVAGGPPSPEVGSPLLCRPAAGPFPQSQTSDTLPEVSAI
PISLDGLLFPRPCQGQDPSDEKTQDQQSLSDVEGAYSRAEATRGAGGSSSS
PPEKDSGLLDVLDITLLAPSGPGQSQPSPPEACEVTSSWCLFGPELPEDPFA
APATQORVLSPLMSRSGCKVGDSSGTAAAHKVLPRGLSPARQLLLPASESH
WSGAPVKPSPQAAAVEVEEEDSSESEESAGPLLKGKPRALGGAAAGGGAAA
CPPGAAAGGVALVPKEDSRFSAPRVALVEQDAPMAPGRSPLATTVMDFIHW
PILPLNHALLAARTRQLEDESVDGGAGAASAFAPPRTPSPCASSTPVAVGD
FPDCAYPPDAEPKDDAYPLYSDFFQPPALKIKEEEEGAEASARSPRSYLVAG
ANPAAFPDFPLGPPPPLPPRATPSRPGEAAVTAAPASASVSSASSSGSTIE
CILYKAEGAPPQOGPFAPPCKAPGASGCLPRDGLPSTSASAAAAGAAFA
LYPALGLNGLPQLGYQAAVLKEGLPQVYPYLYLNRPDSEASQSPQYSFES
LPQKICLICGDEASGCHYGVLTGSGCKVFVKRAMEGQHNYLCAGRNDICVD
KIRRKNCPCRLRKCCQAGMVLGGRKFKKENKVRVVRALDAVALPQPLGVF
NESQALSQRFTFSPGQDIQLIPPLINLLMSIEPDVIYAGHDNTKPDTSSSL
LTSLNQLGERQLLSVVKWSKSLPGFRNLHIDDQITLIQYSWMSLMVFGLGW
RSYKHVSGQMLYFAPDLILNEQRMKESSFYSCLTMWQIPQEFVKLQVSQE
EFLCMKVLLLLNTIPLEGLRSQTQFEEMRSSYIRELIKAIGLRQKGVVSSS
QRFYQLTKLLDNLHDLVKQLHLYCLNTFIQSRALSVEFPPEMMSEVIAAQIP
KILAGMVKPLL FHKK (SEQ ID NO:4)

FIG. 2C

