



INTERNATIONAL APPLICATION PUBLISHED UNDER THE PATENT COOPERATION TREATY (PCT)

(51) International Patent Classification ⁵ : C12P 21/08, C07K 15/00, 3/00 C07K 13/00	A1	(11) International Publication Number: WO 93/22450 (43) International Publication Date: 11 November 1993 (11.11.93)
(21) International Application Number: PCT/US93/04335 (22) International Filing Date: 7 May 1993 (07.05.93) (30) Priority data: 07/879,630 7 May 1992 (07.05.92) US (71) Applicants: THE REGENTS OF THE UNIVERSITY OF CALIFORNIA [US/US]; 300 Lakeside Drive, 22nd Floor, Oakland, CA 94612-3550 (US). SERAGEN, INC. [US/US]; 97 South Street, Hopkinton, MA 01748 (US). (72) Inventors: CHOE, Seunghyon ; 7311 Darby Place, Reseda, CA 01335 (US). EISENBERG, David ; 342 Comstock Avenue, Los Angeles, CA 90024 (US). GENBAUFFE, Francis, S., Jr. ; 4 Briarwood Lane, Upton, MA 01568 (US).		(74) Agent: CLARK, Paul, T.; Fish & Richardson, 225 Franklin Street, Boston, MA 02110 (US). (81) Designated States: AT, AU, BB, BG, BR, CA, CH, CZ, DE, DK, ES, FI, GB, HU, JP, KP, KR, LK, LU, MG, MN, MW, NL, NO, NZ, PL, PT, RO, RU, SD, SE, SK, UA, VN, European patent (AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE), OAPI patent (BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG). Published <i>With international search report.</i>
(54) Title: NOVEL DIPHTHERIA TOXIN-BASED MOLECULES (57) Abstract The invention features a chimeric diphtheria toxin molecule wherein all or part of a complementarity determining region of an antibody is inserted into a loop region of the Diphtheria toxin receptor binding-domain.		

FOR THE PURPOSES OF INFORMATION ONLY

Codes used to identify States party to the PCT on the front pages of pamphlets publishing international applications under the PCT.

AT	Austria	FR	France	MR	Mauritania
AU	Australia	GA	Gabon	MW	Malawi
BB	Barbados	GB	United Kingdom	NL	Netherlands
BE	Belgium	GN	Guinea	NO	Norway
BF	Burkina Faso	GR	Greece	NZ	New Zealand
BG	Bulgaria	HU	Hungary	PL	Poland
BJ	Benin	IE	Ireland	PT	Portugal
BR	Brazil	IT	Italy	RO	Romania
CA	Canada	JP	Japan	RU	Russian Federation
CF	Central African Republic	KP	Democratic People's Republic of Korea	SD	Sudan
CG	Congo	KR	Republic of Korea	SE	Sweden
CH	Switzerland	KZ	Kazakhstan	SK	Slovak Republic
CI	Côte d'Ivoire	LJ	Liechtenstein	SN	Senegal
CM	Cameroon	LK	Sri Lanka	SU	Soviet Union
CS	Czechoslovakia	LU	Luxembourg	TD	Chad
CZ	Czech Republic	MC	Monaco	TG	Togo
DE	Germany	MG	Madagascar	UA	Ukraine
DK	Denmark	ML	Mali	US	United States of America
ES	Spain	MN	Mongolia	VN	Viet Nam
FI	Finland				

- 1 -

NOVEL DIPHTHERIA TOXIN-BASED MOLECULES

Background of the Invention

The field of the invention is chimeric molecules.

5 Hybrid molecules in which all or part of an antibody is fused to another molecule have been suggested as a means for targeting molecules to particular sites. Diphtheria toxin (DT) is an extremely potent cytotoxin which is secreted by *Corynebacterium diphtheriae* that has
10 been lysogenized by a bacteriophage carrying the Diphtheria toxin gene. Naturally occurring Diphtheria toxin is a single polypeptide chain of 535 residues. Mild trypsinization and reduction of Diphtheria toxin *in vitro* generates two fragments, Fragment A (amino-terminal, ~21K) and Fragment B (carboxy-terminal, ~37K), as a
15 result of cleavage at residue 190, 192, or 193. A similar proteolytic cleavage ('nicking') occurs *in vivo* before or soon after the toxin binds to a sensitive cell. Fragment B of the toxin binds the protein to receptors on
20 the cell surface and promotes transfer of the Fragment A to the cytoplasm. Fragment A in the cytoplasm catalyzes the transfer of the ADP-ribosyl group of NAD⁺ to elongation factor 2 (EF-2). This inactivates EF-2, stopping protein synthesis and killing the target cell.
25 Introduction of a single molecule of Fragment A into the cytoplasm can kill a cell. While the exact mechanism by which Diphtheria toxin enters a cell is not completely understood, it is known that Diphtheria toxin binds a receptor and is endocytosed and delivered to endosomes
30 where it encounters acidic conditions. At a threshold pH of ~5.0 the toxin undergoes a conformational change, which promotes insertion and formation of an ion-selective channel in the membrane, and Fragment A is translocated and released into the cytoplasm.

- 2 -

Summary of the Invention

In general, the invention features a chimeric diphtheria toxin molecule wherein all or part of a complementarity determining region (CDR) of an antibody
5 is inserted into a loop region of the Diphtheria toxin receptor binding-domain. By "loop region" is meant any of the portions of the Diphtheria toxin receptor binding domain lying between β strands as delimited herein. The term encompasses single amino acids. By "Diphtheria
10 toxin receptor binding domain" is meant the portion of Diphtheria toxin lying from amino acids 386 to amino acid 535, inclusive. By "CDR" is meant a portion of a complementarity determining region of an antibody as defined by sequence heterogeneity, e.g., according to
15 Kabat et al (in *Sequences of Proteins of Immunological Interest*, U.S. Dept. of Health and Human Services, U.S. Government Printing Office, 1987). In a preferred embodiment, the antibody is capable of specifically binding a cell surface antigen expressed on a cell, the
20 chimeric diphtheria toxin molecule is capable of specifically binding the same cell surface antigen and is substantially incapable of binding to the diphtheria toxin receptor. By "cell surface antigen" is meant any cell surface marker, e.g., a protein or a carbohydrate.
25 By "specifically binding" is meant does not substantially bind to other molecules. By "diphtheria toxin receptor" is meant the receptor for naturally-occurring Diphtheria toxin. In a more preferred embodiment, the molecule is capable of decreasing the viability of the cell. In an
30 even more preferred embodiment the molecule kills the cell.

In another preferred embodiment, all or part of a first CDR is inserted into a first loop region, all or part of a second CDR is inserted into a second loop
35 region, and the first and the second CDR are of a single

- 3 -

antibody chain. By "of a single antibody chain" is meant CDR sequences found within a single heavy or light chain. In a preferred embodiment, the molecule lacks diphtheria toxin catalytic activity. By "diphtheria toxin catalytic
5 activity" is meant the ability to inhibit translation. In a yet more preferred embodiment, the molecule lacks all or part of the catalytic domain of diphtheria toxin.

In other preferred embodiments, the loop region is RL3 and the CDR is a CDR1; and the loop region is RL9 and
10 the CDR is a CDR3.

In a related aspect, the invention features a hybrid molecule which includes a first and a second portion joined together covalently, the first portion includes a chimeric diphtheria toxin molecule wherein all
15 or part of a CDR of an antibody is inserted into a loop region of the receptor binding-domain of diphtheria toxin, the antibody being capable of specifically binding a cell surface antigen expressed on a cell, the chimeric diphtheria toxin molecule being capable of specifically
20 binding the cell surface antigen, being substantially incapable of binding to the diphtheria toxin receptor, and lacking Diphtheria toxin catalytic activity; and the second portion includes a molecule to be delivered to the cell. In various preferred embodiments, the molecule to
25 be delivered to the cell is a protein; is an enzyme; is a protein which modulates transcription; is a nucleic acid binding protein; is a nucleic acid-binding protein capable of binding a single-stranded nucleic acid; and is a nucleic acid.

30 In a related aspect, the invention features a hybrid molecule which includes a first and a second portion joined together covalently, the first portion includes a chimeric diphtheria toxin molecule wherein all or part of a CDR of an antibody is inserted into a loop

- 4 -

region of a first diphtheria toxin receptor binding-domain, the antibody being capable of specifically binding a cell surface antigen expressed on a cell, the chimeric diphtheria toxin molecule being capable of specifically binding the same cell surface antigen and being substantially incapable of binding to the diphtheria toxin receptor, wherein the amino-terminus of a second diphtheria toxin receptor-binding domain is connected to the carboxy-terminus of the first diphtheria toxin receptor-binding domain, the second diphtheria toxin receptor-binding domain being substantially incapable of binding to the diphtheria toxin receptor. In preferred embodiments, the carboxy terminus is connected to the amino terminus through a polypeptide chain; and all or part of a CDR of an antibody is inserted into a loop region of the second diphtheria toxin receptor-binding domain. By "connected" is meant linked via one or a series of covalent bonds, e.g., by a polypeptide chain. In a more preferred embodiment, all or part of a first the CDR is inserted into a first loop region of the first diphtheria toxin receptor-binding domain and all or part of a second the CDR is inserted into a second the loop region of the first diphtheria toxin receptor-binding domain. In an even more preferred embodiment, all or part of a third CDR is inserted into a first loop region of the second diphtheria toxin receptor-binding domain and all or part of a fourth CDR is inserted into a second the loop region of the second diphtheria toxin receptor-binding domain. In a yet more preferred embodiment, the first and the second CDR are of a first antibody chain and the third and the fourth the CDR are of a second antibody chain. In still more preferred embodiments, the first and the second antibody chains are from antibodies recognizing the same antigen; the first and second antibody chains are from the same

- 5 -

antibody molecule; and the first antibody chain is the light chain of an antibody and the second antibody chain is the heavy chain of the same antibody.

In a related aspect, the invention features a
5 chimeric diphtheria toxin molecule wherein all or part of a CDR-like sequence of a ligand binding protein having an antibody variable domain-like ligand binding-domain is inserted into a loop region of the receptor binding domain of diphtheria toxin. By "CDR-like sequence" is
10 meant a sequence which is responsible for ligand binding and which has the same relationship to overall structure of a protein as does the CDR of an antibody variable domain. By "an antibody variable domain-like ligand binding domain" is meant a ligand binding domain which
15 has structural homology to an immunoglobulin variable domain. For example tumor necrosis factor includes an antibody variable domain-like ligand binding domain.

The chimeric molecules of the invention bind specifically to the same epitope (antigen) as the
20 antibody from which the inserted CDR sequences are derived. Thus it is possible to generate a molecule targeted to any antigen. Because these chimeric molecules can enter cells to which they bind, they can be used to introduce any molecule into a specific class of
25 cells.

Other features and advantages of the invention will be apparent from the following description of the preferred embodiments thereof, and from the claims.

Detailed Description

30 The drawings are first briefly described.

Figure 1 is a schematic drawing of Diphtheria toxin in which each secondary structural segment is identified. The first letter denotes the domain: C for catalytic, T for transmembrane, and R for receptor-
35 binding domains. The second letter denotes the secondary

- 6 -

structure class: H for helix, B for β strand, L for loop.

The third symbol is the sequential number of each secondary segment from the N-terminus of each domain.

The residue numbers in each segment are as follows:

- 5 CH1:2-7, CB1:11-14, CB2:16-24, CH2:28-34, CB3:52-57,
CH3:58-66, CB4:76-86, CB5:88-96, CH4:99-106, CH5:120-126,
CB6:130-136, CB7:147-152, CB8:159-166, CH6:168-173,
CH7:176-186; TH1:205-221, TH2:225-231, TH3:238-257,
TH4:258-269, TH5:274-288, TH6:297-307, TH7:310-315,
10 TH8:326-346, TH9:356-378; RB1:386-390, RB2:393-399,
RB3:412-424, RB4:428-438, RB5:447-453, RB6:455-465,
RB7:467-480, RB8:483-495, RB9:513-520, and RB10:525-534.

Figure 2 is a representation of the α skeleton of Diphtheria toxin from the same viewpoint as that of Fig.

- 15 1. An ApUp molecule occupies the active site of Diphtheria toxin.

Figure 3 is a stereo pair representation of the electron density maps calculated at 2.5Å from $(2F_{\text{obs}} - F_c)$ and the refined model phases. Maps are superimposed on
20 the corresponding region of the refined model.

Figure 4 is a representation of the Diphtheria toxin dimer observed within the Form4 crystal. The two monomers are related by a crystallographic 2-fold rotation axis, which is vertical. The molecule at the
25 left (in thick line) has the same orientation as that in Fig. 1.

Figure 5 is a stereo pair representation of the α skeleton of the C domain. The entrance to the active site is at the lower right. The four loops, CL1 to CL4,
30 are highlighted. Notice that they form a hinge which may permit the C domain to form a more elongated structure.

Figure 6 is a stereo pair representation of the α skeleton of the T domain, with the direction of view from the right side of Diphtheria toxin in Fig. 1. Helix TH1
35 lies in back, starting at residue 205. Helix TH2 runs to

- 7 -

the left at the bottom, followed by a turn and helix TH3 running to the right. In front center is TH5 (running to the left) and above it are helices TH6 and TH7. Behind these pairs of antiparallel helices is another pair of
5 antiparallel helices, TH8 and TH9, with TH9 running upwards and ending at residue 378. The Asp and Glu side chains are shown. Notice the tips of two helix layers, TL3 and TL5 contain a total of six acidic groups (on the left).

10 Figure 7 is a stereo pair representation of the T domain as in Fig. 6 except that the Lys, Arg and His side chains are shown. Notice the positive charge asymmetry, with all charges at the bottom and back of the domain, with an exception Lys₂₉₉ near the loop TL3 between TH5 and
15 TH6.

Figure 8 is a schematic representation of the R domain of Diphtheria toxin (panel A), an Ig variable domain (panel B) and tumor necrosis factor (panel C). R domain is viewed in the direction from the back side of
20 Diphtheria toxin in Fig. 1. Numbers from 2 to 10 of the R domain represent the strands RB2 through RB10 of Diphtheria toxin. Notice that strands 2, 3, 4, 8, 9, and 10 of the R domain correspond well to strands A, B, C, E, F, and G of the Ig variable domain. Also strands 3, 4,
25 5, 6, 7, 8, and 9 correspond well to strands C, D, E, F, G, H, and I of tumor necrosis factor, a classical jellyroll.

Figure 9 is a schematic drawing of a rearranged Diphtheria toxin receptor-binding domain. Each
30 structural segment is identified.

Figure 10, panel A is a schematic representation of the receptor-binding domain of diphtheria toxin with each β strand labeled (RB1-RB10) and each loop region labeled (RL1-RL9). The amino acid end points refer to
35 the β sheets, e.g., RB3 consists of residues 412-424

- 8 -

inclusive and RL3 consists of residues 425-427 inclusive. Panel B is a schematic representation of a Diphtheria toxin molecule which has undergone segment rearrangement. The notation for the regions is a in panel A except that
5 447, 483, 467, and 455 indicate the amino acid residues of immediately adjacent to residues 407, 455, 445, and 483 respectively.

Chimeric Diphtheria Toxin Molecules

Described below is the structure of diphtheria
10 toxin as determined by x-ray crystallography. As will be discussed more fully below, the receptor-binding domain of diphtheria toxin has a structure similar to the variable domain of an antibody. Because of this similarity, Diphtheria toxin can be modified so that
15 certain portions of its receptor-binding domain are replaced by, or modified to include, antigen-binding portions (complementarity determining regions) of an antibody of choice. Such modification results in the creation of a chimeric diphtheria molecule which
20 recognizes and binds the same antigen as the selected antibody. If a chimeric molecule is modified so as to substantially eliminate binding to the diphtheria toxin receptor, it will selectively bind only to cells bearing the antigen recognized by the antibody from which the
25 complementarity determining regions were derived.

Chimeric molecules of the type described above can be targeted to selected cell types. For example, portions of an antibody directed against the interleukin-2 (IL-2) receptor can be used to make a chimeric
30 diphtheria toxin molecule which binds to cells bearing the IL-2 receptor. If the chimeric molecule is designed so as to retain the translocation and catalytic functions normally associated with diphtheria toxin, the chimeric molecule will enter and kill cells bearing the IL-2
35 receptor. If in the course of creating this chimeric

- 9 -

diphtheria toxin molecules the receptor binding domain is altered so that the chimeric molecule does not bind to the diphtheria toxin receptor, this chimeric molecule will bind and kill cells bearing the IL-2 receptor while
5 leaving all other cells unharmed.

Alternatively, chimeric diphtheria toxin molecules can be used to introduce any molecule into a selected group of cells. For example, if a chimeric diphtheria toxin molecule capable of binding to cells bearing the
10 IL-2 receptor is modified so that the catalytic domain of diphtheria toxin is replaced by an enzyme, that enzyme can be selectively introduced into cells bearing the IL-2 receptor. Similar modifications would permit an antisense RNA molecule capable of blocking translation of
15 selected RNA to be introduced into cells bearing the IL-2 receptor. Alternatively, the catalytic domain may be substantially inactivated by mutation rather than deletion.

The approaches used to create chimeric diphtheria
20 toxin molecules are completely general. Once the target antigen, e.g., a cell surface protein or carbohydrate, has been selected, a chimeric diphtheria toxin molecule is created by: (1) generating (or selecting) an antibody which recognizes the antigen; (2) cloning and sequencing
25 at least the variable domain of a heavy or light chain of the antibody; (3) identifying the complementarity determining regions within the antibody variable domain; (4) modifying diphtheria toxin to insert all or part of a complementarity determining region(s) into a loop
30 region(s) of the diphtheria toxin receptor binding domain; and (5) testing the ability of the chimeric molecule to bind to the selected antigen.

The molecules of the invention can be more completely understood by first detailing the structure of
35 Diphtheria toxin itself. Accordingly, the overall

- 10 -

structure of Diphtheria toxin is discussed below followed by a detailed discussion of the structure of its receptor-binding domain. The relationship between the diphtheria toxin receptor-binding domain and an antibody variable domain is then described. This is followed by a discussion of methods for generating and screening chimeric molecules. This discussion is followed by a description of the structure of other parts of Diphtheria toxin including the catalytic domain, the translocation domain and the domain junctions. Lastly, details of the structure determination are presented.

Structure of Diphtheria toxin

Diphtheria toxin consists of three abutting domains that are connected by interdomain linkers. The amino-terminal domain (residues 1-193) is the catalytic (C) domain. The middle domain (residues 205-378) is the transmembrane (T) domain, and the carboxy-terminal domain (residues 386-535) is the receptor binding (R) domain. Schematically, Diphtheria toxin is Y-shaped with the base formed by the T domain, one arm of the Y formed by the C domain, and the other arm formed by the R domain. The Y is about 90Å high, 50Å across the top of the Y, but only 30Å thick (Figure 1).

Each of the three domains has a distinctive fold. The C domain is a mixed structure of eight β strands (CB1-CB8) and seven α -helices (CH1-CH7). The eight β strands form two β sheets of 3 and 5 strands each. These β sheets form a core that is surrounded by 7 short helices. The overall folding of the C domain is similar to that of *Pseudomonas aeruginosa* exotoxin A (ETA) especially near the active site (Allured et al., *Proc. Natl. Acad. Sci USA* 83:1320, 1986), a result that had been foreshadowed by a weak similarity in amino acid sequences (Carroll et al., *Mol. Microbiol.* 2:293, 1988; Brandhuber et al., *Proteins* 3:146, 1988). Sixma et al.

- 11 -

(*Nature* 351:371, 1991) recently demonstrated that the folding of the active site region of *E. coli* heat labile enterotoxin also closely resembles that of ETA. The T domain contains nine helices (TH1-TH9) that are folded into three helix layers, each of which is formed by two or more antiparallel helices. A similar feature was observed in the structure of the channel-forming domain of colicin A (Parker et al., *Nature* 337:93, 1989). The R domain contains ten β strands (RB1-RB10), nine of which (RB2-RB10) build two β sheets. These two β sheets form a β sandwich with a topology similar to a jellyroll fold (Richardson, *Adv. Protein Chem.* 34:167, 1981). The three-domain organization of Diphtheria toxin is shared by two other bacterial toxins, ETA and δ -endotoxin from *Bacillus thuringiensis* (Carroll, et al., *Nature* 353:815, 1991). The catalytic domains of Diphtheria toxin and ETA are the closest among all these domains in their structures and functions.

Receptor-binding domain

Referring to Fig. 8 (panel A) and Fig. 10 (panel A), the receptor-binding (R) domain is formed from two β sheets. β strands RB2 (residues 393-399), RB3 (residues 412-424), RB5 (residues 445-453), and RB8 (residues 483-495) form a four-stranded β sheet that faces a five-stranded β sheet containing β strands RB4 (residues 428-438), RB6 (residues 455-465), RB7 (residues 467-480), RB9 (residues 513-520), and RB10 (residues 525-534). RB6 interacts with both β sheets through hydrogen bonds. The connection of the strands is such that the R domain is similar to the jellyroll topology found in many proteins that are exclusively formed from antiparallel β strands (Richardson, *J. Adv. Protein Chem.* 34:167, 1981). Jellyroll domains include viral coat proteins, tumor necrosis factor, and the receptor-binding domain of ETA. The R domain differs somewhat from a strict jellyroll

- 12 -

topology (Fig. 9) in having strand 2 in the "front" sheet, and having a strand 10 in the "back".

The R domain is also similar in structure to an immunoglobulin (Ig) variable domain (Fig. 9, panel B), but differs from the Ig fold in having an "insert" of strands 5 and 6 between 4 and 7, and also in lacking two short strands (C' and C" in Fig. 9, panel B) between 4 and 5. The portion of the R domain that resembles a strict jellyroll in topology is the right side as viewed in Fig. 9; and the portion that resembles the Ig variable domain is the left side, the side that is away from the rest of the Diphtheria toxin monomer.

Chimeric Diphtheria Toxin Molecules

In chimeric diphtheria toxin molecules all or part of one or more complementarity determining regions derived from an antibody are inserted into one or more loop regions of the Diphtheria toxin receptor-binding domain. Generally, only one CDR sequence is inserted into each loop and the insertion may or may not be accompanied by deletion of all or a portion of the loop region.

The design of chimeric diphtheria toxin molecules can be more readily understood by first considering certain aspects of antibody structure. An antibody consists of two identical light chains (L) and two identical heavy chains (H). Each light chain is attached to a heavy chain by one or more disulfide bonds. Likewise, the two heavy chains are attached to each other by one or more disulfide bonds. Overall, a single antibody forms a "Y" shaped structure in which the carboxy-terminal portion of the heavy chains forms the base of the Y and the amino-terminal portion of a single heavy chain and the amino-terminal portion of a single light chain together form each arm. Each chain, heavy or light, is composed of structurally similar domains. The

- 13 -

domains are referred to as constant or variable based on sequence heterogeneity. Proceeding from the carboxy-terminus, a heavy chain is composed of the CH₃ constant domain, the CH₂ constant domain, the CH₁ constant domain, and the V_H variable domain. Proceeding from the carboxy-terminus, a light chain is composed of a C_L constant domain followed by a V_L variable domain.

The variable domains (V_L and V_H) are of particular interest since together they form the antigen binding site. Each variable domain is approximately 110 amino acids long and is composed of three hypervariable or complementarity-determining regions (CDR1, CDR2, and CDR3) interspersed with four less-variable framework regions (FR1, FR2, FR3, and FR4). The complementarity-determining regions (collectively, CDR's) are responsible for antigen recognition.

Structurally, each variable domain consists of two β sheets which together form a structural motif often referred to as the immunoglobulin fold. (Constant regions, with a slight variation, also form an immunoglobulin fold.) One β sheet is composed of four β strands (A, B, D and E) the other sheet is composed of five β strands (C, C', C'', F and G). There are loops between each β strand. Three of these loops, to a first approximation, correspond roughly to the three CDR's. However, as will be discussed below, the identification of a CDR or a framework region is based primarily on sequence heterogeneity rather than secondary structure. Thus, the identification of these regions within a given antibody molecule requires analysis of the amino acid sequence of the antibody. This caveat notwithstanding, the loop between B and C often includes all or part of CDR1; the loop between C' and C'' often includes all or part of CDR2; and the loop between F and G often includes all or part of CDR3.

- 14 -

A comparison between the structure of the receptor binding domain of Diphtheria toxin and immunoglobulin V domain illustrates the structural similarities (Fig. 9). There is a correspondence, not identity, between the β strands of the Diphtheria toxin receptor domain (described above) and the β strands of an immunoglobulin variable domain as follows: RB2 \equiv A, RB3 \equiv B, RB4 \equiv C, RB5 \equiv D, RB6 \equiv C", RB7 \equiv C', RB8 \equiv E, RB9 \equiv F, RB10 \equiv G. Two of the Diphtheria toxin receptor binding domain loops, RL3 and RL9 thus correspond to CDR1, and CDR3, respectively.

Given this understanding, it can be seen that the receptor domain can be engineered to more closely resemble a variable domain. In particular, CDR sequences can be inserted into RL3 and RL9 in a process referred to herein as 'loop grafting' to yield a chimeric molecule which includes a CDR1 sequence or a CDR3 sequence or both. In the course of grafting all or part of either or both loop regions may be deleted. Further, the region of Diphtheria toxin from RB5 to RB8 can be rearranged so that it more closely resembles the region of a variable domain extending from strand C through strand E. This process, referred to herein as 'segment rearrangement', can provide a framework for the grafting of a CDR2 sequence into Diphtheria toxin. In combination, these two approaches can be used to create a chimeric molecule into which three CDR's (CDR1, CDR3, CDR3) have been introduced. It may also be possible to insert a CDR2 sequence into RL5 without segment rearrangement.

30 Loop Grafting

Loop grafting is similar to CDR grafting in which the CDR of a first antibody are exchanged for those of a second antibody, and the techniques employed in CDR grafting will, in general, be useful for loop grafting. Jones et al. (Nature 321:522, 1986), Riechmann et al.

- 15 -

(*Nature* 322:323, 1988), Winter et al. (PCT/GB89/00113), Winter (EPA 0 239 400), and Clackson et al. (*Nucl. Acids Res.* 17:10163, 1989) describe CDR grafting techniques which can be applied to loop grafting.

5 It should be understood that the precise limits of the regions to be grafted are a matter of experimental choice. All or part of RL3 (residues 425-427) could be replaced by all or part of the CDR1 of an antibody heavy or light chain of choice. All or part of RL9 (residues
10 521-524) could be replaced by all or part of the CDR2 of the same antibody heavy or light chain (or, less preferably, an antibody heavy or light chain of an antibody recognizing the same epitope). Of course, the above boundaries of RL3 and RL9, while precise in terms
15 of structure, represent only approximate limits to the region which might be replaced by all or part of a CDR. Further insertion of a CDR can take place without the deletion of any loop region sequence. Thus, a CDR may replace a few residues of RB3 and a few residues of RB4
20 as well as all of RL3 (e.g., residues 422-429). Alternatively, a CDR might replace only a part of RL3 (e.g., residues 426 and 427). Alternatively, no residues are deleted.

 In identifying a CDR to graft into Diphtheria
25 toxin, it should be understood that CDR's are identified by sequence hypervariability (Kabat et al., in *Sequences of Proteins of Immunological Interest*, U.S. Dept. of Health and Human Services, U.S. Government Printing Office, 1987) and/or structural hypervariability (Chothia
30 et al. *J. Mol. Biol.* 196:901, 1987) rather than by secondary structure (e.g., a loop). Thus, a CDR so-defined may include only a portion of the loop between two β -strands and likewise may include part or all of one or both β -strands flanking the loop. Nevertheless, it
35 should be understood that in many antibodies CDR's are

- 16 -

found at similar positions. Thus, within a variable domain CDR1 is commonly located near amino acid 30, CDR2 is commonly located near amino acid 50 and CDR3 is commonly located near amino acid 95 (Roitt et al.,
5 *Immunology* Gower Medical Publishing, London, 1985).

Useful CDR's may be derived from either immunoglobulin H or L chains. Further, antibodies derived from any species may be used as a source of CDR's. Because CDR's appear not to contain species
10 specific motifs, CDR's from a first species can be used without substantially increasing the immunogenicity of the chimeric molecule in a second species.

Segment Rearrangement

Segment rearrangement essentially consists of
15 reorganizing the portion of Diphtheria toxin from the beginning of RB5 to the end of RL7. This reorganization results in the formation of a rearranged R domain which more closely resembles an antibody variable domain than does the native R domain. This rearrangement in
20 combination with loop grafting of all or part of RL3 and/or RL9 can provide a molecule with improved antigen binding characteristics compared to a molecule which has undergone grafting of the same loops but has not undergone segment rearrangement. Domain rearrangement
25 can also provide a location, between rearranged RB7 and rearranged RB6, for the addition of a CDR2.

In detail domain rearrangement entails constructing a molecule in which the R domain has the following sequence of elements (beginning at its amino-
30 terminus): RB1-RL1-RB2-RL2-RB3-RL3-RB4-RL4-RB7-RL7-RB6-RL6-RB5-RL5-RB8-RL8-RB9-RL9-RB10 (Fig. 10, panel B). All or part of a CDR2 sequence can be introduced by replacing all, part, or none of RL7 (in the rearranged molecule located between RB7 and RB6). Referring to Fig. 9, panel
35 A, this rearranged receptor-binding domain more closely

- 17 -

resembles an immunoglobulin variable domain (Fig. 9, panel B) than does the naturally occurring Diphtheria toxin receptor-binding domain (Fig. 8, panel A).

Eliminating Binding to the Diphtheria Toxin Receptor

5 The diphtheria toxin receptor binding ability of Diphtheria toxin receptor domain must be substantially reduced in chimeric molecules compared to native Diphtheria toxin so that the chimeric molecules do not substantially bind to or enter non-targeted cells (i.e.,
10 cells not bearing the antigen recognized by the CDR's). This can be accomplished by incorporating into the chimeric molecules certain mutations which reduce binding of Diphtheria toxin to its natural receptor. CRM9 (Hu et al., *Biochim. Biophys. Acta* 902:24, 1987) CRM107 and
15 CRM103 (Greenfield et al., *Science* 238:536, 1987) are mutant Diphtheria toxin molecules with reduced receptor binding. The sequences changes in these mutants can be incorporated into chimeric diphtheria toxin molecules. It should also be recognized that replacing all or part
20 of RL3 and/or all or part of RL9 with a CDR may essentially eliminate binding of the chimeric molecule to the diphtheria toxin receptor. Further, the insertion of a CDR sequence into a loop of the R domain in the absence of any deletion may, in and of itself, substantially
25 eliminate binding to the diphtheria toxin receptor. While the diphtheria toxin receptor has not been positively identified (Naglich et al., *Proc. Nat'l Acad. Sci. USA.* 89:2170, 1992), the diphtheria toxin receptor-binding ability of chimeric diphtheria toxin molecules
30 can be assessed by standard techniques (Middlebrook et al., *Can. J. Microbiol.* 23:183, 1978; Middlebrook et al., *J. Biol. Chem.* 253:7325, 1978) using Vero cells or other cell lines.

Chimeric Diphtheria Toxin Molecules Having Two R Domains

- 18 -

In naturally occurring antibodies the antigen binding site is formed by a V_H domain and a V_L domain, and structural studies suggest that antigen binding is mediated by contacts with both domains. Fv fragments, which are non-covalently associated heterodimers of V_H and V_L domains, have been developed to provide small, engineered molecules with antigen binding activity similar to the intact antibody from which the domains were derived (Glockshuber et al., *Biochemistry* 29:1362, 1990). Because Fv molecules are prone to dissociation, single-chain Fv molecules (sFv) have been developed by linking the domains with a flexible hydrophilic polypeptide (Bird et al., *Science* 423:423, 1988; Huston et al., *Proc. Nat'l. Acad. Sci. USA* 85:5879, 1988). As an alternative, the domains can be linked by disulfide bonds (Glockshuber et al., *Biochemistry* 29:1362, 1990). In a similar fashion it is possible to generate chimeric diphtheria toxin molecules having two R domains. When properly constructed the R domains of such molecules resemble a single-chain Fv fragment. Loops within one or both R domains can be modified to include CDR sequences. These changes, in combination with modifications which prevent either receptor binding domain from recognizing the diphtheria toxin receptor, result in the creation of a molecule which will specifically recognize the same antigen as the antibody from which the CDR sequences were derived.

To generate chimeric diphtheria toxin molecules having two R domains, the carboxy-terminus of RB10 of a diphtheria toxin molecule is fused to the amino-terminus of RB1 or RB2 of an R domain portion of diphtheria toxin. CDR sequences can be introduced into these molecules in manner described above by modifying the loop regions of one or both of the R domains. The result is a molecule which has a domain ($R+R'$) resembling an sFv molecule

- 19 -

fused to the diphtheria toxin translocation and catalytic domains. In certain circumstances it may be possible to generate antigen binding molecules by introducing CDR sequences into only one of the two R domains. This is
5 because the mere existence of an unmodified R domain may improve contacts between the CDR sequences in the other modified R domain and the antigen. In any case, if the chimeric molecule is to be specifically targeted, both receptor binding domains must be modified to essentially
10 eliminate recognition of the diphtheria toxin receptor. If both R domains have been engineered to introduce CDR sequences, it is preferred all of the CDR sequences be derived from the same antibody (or at least antibodies recognizing the same epitope), and that the CDR sequences
15 of one R domain be derived from a V_H domain, and the that the CDR sequences of the other R domain be derived from a V_L domain. This creates a molecule which more closely resembles an Fv fragment.

In general, methods used for the generation of
20 sFv molecules (Bird et al., *Science* 423:423, 1988; Huston et al., *Proc. Nat'l. Acad. Sci. USA* 85:5879, 1988) can be used to generate chimeric diphtheria toxin molecules having two R domains. In designing chimeric diphtheria toxin molecules in which the two R domains are linked by
25 a polypeptide chain it is important that the linking polypeptide chain be selected so as to hold the two R domains in a configuration that resembles an Fv molecule. Lardner et al. (US Patent 4,946,778 and US Patent 4,704,692) describe techniques for selecting polypeptides
30 to link V_H and V_L domains to form sFv. The same techniques can be used to generate chimeric diphtheria toxin molecules having two R domains. As an alternative, the two domains can be linked by disulfide bonds as described by Glockshuber et al. (*Biochemistry* 29:1362,
35 1990) for single-chain Fv molecules.

- 20 -

As discussed above for simple chimeric diphtheria toxin molecules, chimeric diphtheria toxin molecules having two R domains and CDR sequences can be modified to act as delivery vehicles rather than cytotoxins. This is accomplished by replacing the catalytic domain with a molecule to be introduced into cells thus creating a hybrid molecule. The R domains will then target the hybrid molecule to a selected class of cells and the translocation domain will mediate entry.

10 Generation of Antibodies and Identification of CDR's

In order to create a chimeric diphtheria toxin molecule directed against a selected antigen, it is first necessary to identify an antibody directed against that antigen. In many instances appropriate antibodies will already be available (see Kabat et al., *supra*; *Catalogue of Cell Lines and Hybridomas*, American Type Culture Collection, Rockville, MD). Alternatively, antibodies (polyclonal or monoclonal) directed against the selected antigen can be generated and screened by standard methods (*Current Protocols in Immunology*, Wiley-Interscience, New York, 1991). Once a hybridoma secreting an antibody with the desired specificity has been isolated there are several approaches which can be used to sequence the variable domain for the purpose of identifying CDR sequences. The heavy and/or light chains can be cloned and sequenced. Alternatively, variable domains can be amplified for cloning using the polymerase chain reaction and oligonucleotide primers which recognize conserved sequences at each end of the heavy or light chain variable region (Orlandi et al., *Proc. Nat'l. Acad. Sci. USA* 86:3833, 1989; Larrick et al., *Biochem. Biophys. Res. Comm.* 160:1250, 1989; Sastry et al., *Proc. Nat'l Acad. Sci. USA* 86:5728, 1989). This approach allows the cloning of the variable regions of human antibody genes

- 21 -

from unstable human-mouse hybridomas as well as the cloning of variable regions from other unstable hybridomas, single hybridoma cells, and single B lymphocytes. These techniques permit the expression of antibody fragments in bacteria (Skerra et al., Science 240:1038, 1988; Better et al., Science 240:1041, 1988) or on the surface of phage (McCafferty et al., Nature 348:552, 1990). Expression in one or another of these systems permits the use of a number of efficient screening methods (Skerra et al., Analytical Biochem. 196:151, 1991; Huse et al., Science 246:1275, 1989) which can be used to identify antibodies fragments that bind the selected antigen with the desired affinity.

In addition various non-immunization techniques (Marks et al., J. Mol. Biol. 222:581, 1991; Persson et al., Proc. Nat'l Acad. Sci. USA 88:2432, 1991. Huse et al., *supra*) can be used to generate antibodies which can serve as a source of CDR sequences.

Once the variable regions are sequenced CDR's are identified according to Kabat et al. (*supra*).

Generation and Screening of Chimeric Diphtheria Toxin Molecules

The chimeric molecules are generated using the standard techniques of molecular biology (*Current Protocols in Molecular Biology*, Wiley-Interscience, New York, 1991). The primary approach involves the generation of nucleic acids encoding the chimeric molecules. The chimeric molecules themselves can be produced in bacterial cells, mammalian cells, or insect cells by standard techniques. In designing chimeric molecules the techniques of computer-based molecular modeling may be useful. The coordinates of the solved diphtheria toxin structure are included (appendix) to aid in this process. It should be understood that changes in

- 22 -

the amino acid sequence may be introduced at any position to generate more stable molecules or molecules with higher binding specificity.

Once the chimeric molecules have been produced,
5 they can be screened for antigen binding ability using any of the approaches described above for antibodies and antibody fragments. The binding specificity of a cytotoxic chimeric molecules targeted to a particular antigen can be determined by comparing the toxicity of
10 the molecule toward cells bearing the antigen to its toxicity towards cells not bearing the antigen. For non-toxic chimeric molecules, a detectable label may be covalently linked to the chimeric molecule to facilitate comparison of binding to antigen-bearing cells and cells
15 not bearing antigen.

Examples

A chimeric diphtheria toxin molecule capable of recognizing cells bearing the Campath-1 antigen can be constructed by replacing all of RL3 with the CDR1
20 sequence identified by Waldman et al. (PCT/GB89/00113, hereby incorporated by reference) and replacing all of RL9 with the CDR3 sequence identified by Waldman et al. (*supra*).

A chimeric diphtheria toxin molecule capable of
25 recognizing cells bearing the interleukin-1 receptor can be constructed by replacing all of RL3 with residues 26-33 of the anti-tac antibody light chain and replacing all of RL9 with residues 99-107 of the anti-tac antibody light chain. (*supra*).

30 Structure determination

The structure is based on analyses of Form1, Form3, and Form4 crystals. Form1 crystals of Diphtheria toxin complexed with adenylyl-3',5'-uridine monophosphate (ApUp) belong to triclinic space group P1 with unit cell

- 23 -

dimensions of $a=70.4\text{\AA}$, $b=70.6\text{\AA}$, $c=65.4\text{\AA}$, $\alpha=94.9^\circ$, $\beta=91.0^\circ$, and $\gamma=99.6^\circ$ with two chains per asymmetric unit. This dimeric asymmetric unit is consistent with the fact that a dimeric form of Diphtheria toxin is sometimes
5 found in crude or purified preparations of the protein (Collier et al., *J. Biol. Chem.* 257:5283, 1982). Dimeric Diphtheria toxin itself is not toxic, presumably because it does not bind to receptors, but it slowly dissociates to fully toxic monomers (Carroll et al., *Biochem.*
10 25:2425, 1986). The dimer may represent a conformationally altered form of the biologically active monomeric toxin. Irreproducible crystallization conditions for obtaining Form1 crystals hampered crystallographic studies of structure determination until
15 three new crystal forms were obtained (Fujii et al., *J. Mol. Biol.* 222:861, 1991). Form3 and Form4 belong to monoclinic space group C2 with unit cell dimensions for Form3 of $a=107.3\text{\AA}$, $b=91.7\text{\AA}$, $c=66.3\text{\AA}$, and $\beta=94.7^\circ$, and for Form4 of $a=108.3\text{\AA}$, $b=92.3\text{\AA}$, $c=66.1\text{\AA}$, and $\beta=90.4^\circ$. In
20 both of these forms there is one Diphtheria toxin chain per asymmetric unit and pairs of Diphtheria toxin chains are related by a 2-fold rotation axis.

The initial model was based on the structure determination of Form4 crystals at 3.0\AA resolution, using
25 the multiple isomorphous replacement (MIR) method followed by solvent flattening (Wang, *Methods in Enzymol.* 115:90, 1985). With the initial model, the structures of Form1 and Form3 were readily solved by molecular replacement (Brünger, *Acta Cryst.*, A47:195, 1991; Rossman
30 et al., *Acta Cryst.*, 15:24, 1962). Single isomorphous replacement (SIR) phases were also obtained for Form3. Native data were then collected to 2.5\AA resolution, and the model was rebuilt into 2.5\AA maps with Form3 (SIR) and Form4 (MIR) after the phases had been extended and

- 24 -

- modified by the method of Zhang et al. *Acta Cryst.* A46:377, 1991. This was followed by real-space density averaging between two forms. Sequence fitting was difficult in the ~120 C-terminal residues (part of
- 5 receptor-binding or R domain) where the most ambiguous regions were near residues 408 and 510. Some of the useful markers in the density maps were W_{50} , W_{153} , W_{281} , W_{398} , a 5-residue segment of M_{178} , Y_{179} , E_{180} , Y_{181} , M_{182} , a 4-residue segment of F_{355} , Y_{358} , H_{372} , Y_{375} , a cluster of
- 10 Y_{514} , F_{530} , F_{531} , with big side chains near the carboxy terminus (Fig. 3), and two disulfide bonds between C_{186} and C_{201} and C_{461} and C_{471} . An initial improper fitting in the R domain was detected by profile window plots (Lüthy et al., *Nature* 355:xxx, 1992) and then corrected.
- 15 Iterative cycles of refinement were carried out independently at 2.5Å for each data set. The atomic model for each form is essentially identical except for crystal packing. Assessment of the accuracy of the model rests on the fit of the model to the MIR and density-
- 20 modified maps, crystallographic R-factors, real-space R-factors, (Jones et al., *Acta Cryst.* A47:110, 1991), the free R-value (Brünger *Nature* 355:472, 1992), which is only 4% higher than the crystallographic R factor, and profile window plots (Lüthy, *supra*). At the present
- 25 stage of refinement, the agreement of the atomic models to crystallographic data is characterized by R factors of 21.1, 21.6 and 21.9%, respectively, for Form1, Form3, and Form4 for all observed data having F_{ob} greater than 1σ (F_{ob}) between 6 and 2.5Å resolution.
- 30 The final model consists of 4137 non-hydrogen atoms with individual isotropic temperature factors. The model also includes ApUp in the active site cleft of the catalytic (C) domain, but no solvent atoms. There are poorly-defined regions in the electron density maps where

- 25 -

main chain densities for residues 170-172, 190-195, 389-390, 500-503, are not well defined. Residues 190-195 are part of the protease-sensitive region of the first disulfide loop, where nicking occurs; this region may be intrinsically flexible. So may be the loop between the transmembrane (T) and R domains, which includes residues 389-390. Aspects of data collection, phase determination and refinement are presented below and in Table 1.

Data Collection, Phase Determination and Refinement

- 10 Statistics for X-ray data collection, phase determination and refinement. Crystal Forms, 1, 3 and 4 were used for the current study (Fuji, *supra*). Diffraction data were collected on a Rigaku AFC-6 diffractometer operating at 8.5 kW, equipped with a two-panel area detector of Xuong-Hamlin design (San Diego Multiwire Systems). Images were recorded as 0.1° oscillation frames, integrated and merged into batches of 50 frames (5°). Integrated intensities were scaled and merged for FOURIER scaling method (Weissman, *Thesis*, Univ. California, LA, 1979).
- 20 Form4 native and derivative data were later collected to 2.5 °Å with a RAXIS imaging plate system.

Heavy atom derivatives

- KOS: K_2OsO_4 , soaked for 3 days at the concentration saturated in artificial mother liquor (12% PEG8000, 0.43M NaCl, 43mM Tris-HCl, pH 7.8); CNP: 4-chloro-2-nitro-mercury phenol, soaked for 5 days at the concentration saturated in artificial mother liquor; KNP: 1 to 1 mixture of KOS and CNP; CAP, trans-dichlorodiamine Platinum (II), soaked for 3 days at 2 mg/ml in artificial mother liquor; KAP: 1 to 1 mixture of KOS and CAP; GCL, $HgCl_2$, soaked for 3 days at 2 mg/ml in artificial mother liquor.

- 26 -

Heavy Atom Parameters

Heavy atom parameters were refined and MIR phases calculated using the program HEAVY (Terwilliger et al., *Acta Cryst. A*43:1, 1987). We initially obtained the Os derivative for Form3 crystals. From electron density maps based on the single isomorphous replacement (SIR) phases after solvent flattening at 3.5Å resolution, the shape of the molecule was interpreted to have three domains. However, secondary structures were not easily interpretable and the course of the polypeptide chain was difficult to determine. A search for additional heavy atom derivatives was hampered by the lack of good quality crystals of Form3. We, therefore, shifted our efforts to Form4 crystals. MIR phases for Form4 were obtained from six heavy atom derivatives using isomorphous differences and anomalous differences. The Os and Pt derivatives were solved by isomorphous difference Patterson functions, and the Hg derivative by a difference Fourier synthesis. Os derivatives of Form4 and Form3 have the same single site binding.

Solvent Flattening

Initial electron density maps of Form4 were calculated at 3.0Å resolution, with phases modified using an iterative solvent flattening procedure (Wang, *Methods in Enzymol.* 115:90, 1985) including phases extended to 3.0Å from 3.2Å by the Wang phase extension algorithm (Wang, *supra*). A solvent volume of 45% was used to ensure that all protein density was included in the protein mask, somewhat smaller than the 57% estimated from the molecular weight. From these maps, all secondary structures were identified and an initial model was built using a polyalanine chain.

- 27 -

Model Building

Model building was expedited with the program FRODO (Jones *Methods in Enzymol.* 115:157, 1985) and the fragment-fitting routines of the program O (Jones, *Acta Cryst.* A47:110, 1991). Starting with α carbon coordinates that were manually built, main chain atoms were added using the database of 34 well-refined protein structures. Then side chains were added using the rotamer database (Ponder, *J. Mol. Biol.* 193:775, 1987).

10 Refinement

This initial model was adjusted by visual inspection of density maps before it was refined by the simulated annealing protocol of the program XPLOR (Brünger et al. *Acta Cryst.* A46:585, 1990). The relative orientations of Diphtheria toxin in Forms 1, 3, and 4 were determined by a Patterson-space rotation and translation search of the refined Form4 model against Form1 and Form3 data. Two top solutions (9σ) for Form1 data correspond to two Diphtheria toxin chains related by a noncrystallographic symmetry in asymmetric unit. The transformation from Form4 to Form1 is essentially a change of coordinate system from C2 to P1, where the crystallographic rotation axis of C2 becomes a noncrystallographic rotation symmetry axis of P1 that is nearly parallel with (110) axis of P1. One top solution (7σ) for Form3 corresponds to a rotation of less than 0.5° in any direction. The transformation from Form4 to Form3 is essentially a 5\AA translation along the a axis. This result is consistent with the observation that the average absolute difference of the amplitudes of structure factors of 0kl reflections between Form3 and Form4 is 15%, whereas those between h0l or hk0 reflections between Form3 and Form4 are almost random ($R=48\%$). Also, when the model was superimposed on the

- 28 -

solvent-flattened electron density maps of Form3 based on the SIR phases, most of the secondary structures were recognized with the model as a guide. Real-space averaging of densities between Form4 and Form3 with MIR
5 and SIR phases at 3.0Å improved the density maps at this stage. Subsequently, experimental phases were extended to 2.5Å by the algorithm based on solvent flattening, histogram matching, and Sayre's equation (Brünger, *supra*) for Form3 and Form4. Form3 maps at 2.5Å were again
10 skewed and averaged with Form4 maps. These were the most interpretable maps. Refinement of the atomic model was carried out independently for Form1, Form3, and Form4 with all observed data having F_{ob} greater than $1\sigma(F_{ob})$ between 6 and 2.5Å.

- 29 -

TABLE 1

<u>Native Data</u>		Overall (R^{\dagger}_{scale})	10-4.0	4.0-3.0	3.5-3.0	3.0-2.5A
5	Form4 Total	36758(11.9)	26897	4977	4884	
	Unique (% complete)	10875(83)	5190(99)	2414(92)	3271(63)	
10	Form4(new) Total	35897(6.1)				
	Unique (% complete)	18665(84)	5195(99)	2673(98)		4268(82)
15	Form3 Total	61009(7.6)	21984	15368	105573	13084
	Unique (% complete)	19912(90)	5231(100)	2682(98)	4603(88)	
20	Form1 Total	66464(7.5)	22245	21118	15277	7824
	Unique (% complete)	25854(68)	6523(96)	7665(92)	7102(76)	
<u>Derivatives</u>						
25	Form4	Overall	10-4.6	4.6-3.6	3.6-3.0	3.0-2.8A
	KOS Unique (R^{\dagger}_{scale})	11765 (9.16)				
30	$R^{\dagger}_{C}(fh/e\$)$	0.66(1.23)	0.66(1.29)	0.62(1.18)	0.75(1.28)	0.80(1.06)
	CNP Unique (R^{\dagger}_{scale})	12255 (12.0)				
35	$R^{\dagger}_{C}(fh/e\$)$	0.70(1.06)	0.68(1.33)	0.72(0.93)	0.72(0.97)	0.66(1.11)
	KNP Unique (R^{\dagger}_{scale})	8164(8.32)				
30	$R^{\dagger}_{C}(fh/e\$)$	0.71(1.00)	0.72(0.87)	0.67(1.18)	0.75(1.33)	
	CAP Unique (R^{\dagger}_{scale})	7552(15.3)				
30	$R^{\dagger}_{C}(fh/e\$)$	0.71(1.28)	0.70(1.54)	0.72(1.12)	0.88(1.20)	
	KAP Unique (R^{\dagger}_{scale})	10152 (12.26)				
30	$R^{\dagger}_{C}(fh/e\$)$	0.81(1.26)	0.81(1.43)	0.71(1.19)	0.75(0.89)	
	GCL Unique (R^{\dagger}_{scale})	6595 (11.90)				
35	$R^{\dagger}_{C}(fh/e\$)$	0.70(1.10)	0.69(1.13)	0.66(1.09)	0.50(1.05)	
	Form3					
35	KOS Unique (R^{\dagger}_{scale})	11435 (13.57)				
	$R^{\dagger}_{C}(fh/e\$)$	0.54(1.10)	0.56(1.32)	0.60(0.74)		

- 30 -

Refinement	Form1	Form3	Form4
R factor $\Psi(6-2.5\text{\AA})$	0.211	0.216	0.219
r.m.s. bond (Å)	0.021	0.021	0.021
r.m.s. angle (°)	4.54	4.40	4.48
5 r.m.s. dihedral (°)	26.4	25.9	26.1

- 10 $R_{\text{scale}} = \Sigma(|I_i - I_j|) / \Sigma(I_{\text{av}})$ where I_i and I_j are the i th and j th measurements of the equivalent reflections (Weissman, Thesis, Univ. California, LA, 1979). R_c is Cullis R factor for centric reflections. Φ_{h}/e is the phasing power, Φ_{h} , the mean amplitude of heavy atom structure factors divided by e , the r.m.s. lack-of-closure error. Ψ R factor = $\Sigma(|F_{\text{ob}} - F_c|) / \Sigma(F_{\text{ob}})$ where F_{ob} and F_c are the structure factors observed and calculated from the model, respectively. The R-factors for all forms increased by about 1.9% when a single temperature factor was used for all atoms.

15 Catalytic domain

- 20 The C domain is formed from two β sheet subdomains, which subtend the active site cleft (Fig. 5). These β sheets are oriented roughly perpendicular to each other and form the core of the domain. One subdomain consists of β strands CB2, CB4, and CB8, surrounded by α -helices, CH2, CH3, CH6, and CH7. The other subdomain consists of β strands CB1, CB3, CB5, CB6, and CB7 surrounded by helices, CH1, CH4, and CH5. The two subdomains are
- 25 connected by extended loops, CL1 through CL4, which link the two subdomains. These four loops appear to suggest potential for flexibility or even extension to a longer and narrower shape. Conceivably the C domain can assume this partially unfolded structure
- 30 during membrane translocation.

- The active site cleft of the C domain, identified by the binding of the dinucleotide ApUp, is formed primarily by β strands, CB2, CB3, CH3, CB7 and the loop, CL2 and is also bounded by β strand
- 35 RB6 of the R domain. Located within the active site cleft are the following residues: Glu₁₄₈ which is

- 31 -

believed to play a key role in catalysis (Carroll et al., *Proc. Natl. Acad. Sci USA* 81:3307, 1984), His₂₁ (Papini et al., *J. Biol. Chem.* 264:12385, 1989) and Tyr₆₅ (Papini et al., *J. Biol. Chem.* 266:2494, 1991),
5 both of which have been implicated in NAD⁺ binding, and various other residues suggested to be at or near the active site (Gly₅₂ (Carroll, *supra* and Giannini et al., *Nuc. Acid Res.* 12:4063, 1984), Trp₅₀ (Collins et al., *Biochim. Biophys. Acta* 828:138,
10 1985), Lys₄₇₄ (Proia, *J. Biol. Chem.* 255:12025, 1980). Least squares superposition of the α carbon coordinates of the C domains of Diphtheria toxin and ETA yields an r.m.s. difference of 1.44Å between 85
15 residues (16-33, 34-38, 49-66, 75-90, 91-96, 131-136, 147-164 of Diphtheria toxin and 437-452, 454-458, 465-482, 493-508, 511-516, 540-545, 552-569 of ETA).

The approximate position of the substance NAD⁺ in the active site can be inferred, because the
20 dinucleotide, ApUp, binds competitively with NAD⁺. The high affinity of ApUp (~0.3nM as compared with ~8-16μM for NAD⁺; (Carroll et al., *Biochem.* 25:2425, 1986) may be a consequence of multiple contacts with the C domain and of salt bridges between the 3'-
25 terminal phosphate of ApUp and the side chains of Thr₄₂ and Arg₄₅₈, the latter of which is a residue of the R domain. Although the structure of bound ApUp resembles that of NAD⁺ and ApUp to make difficult the prediction of the conformation of NAD⁺ in the
30 cleft. However, assuming that the adenine phosphate portion of NAD⁺ binds in the same conformation as that of ApUp, the nicotinamide ring will be positioned close to the site of the uridine ring.

- 32 -

This places the nicotinamide ring adjacent to side chains of His₂₁, Tyr₆₅, and Glu₁₄₈.

Domain junctions

One of the two intramolecular disulfide bonds of Diphtheria toxin bridges a handle-like loop TL1 on the molecular surface (Fig. 1). This 14 residue loop (187-200) connects Fragment A to Fragment B; it is rich in Arg and known to be easily nicked by proteases (Moskaug et al., *J. Biol. Chem.* 264:15709, 1989; Collier, *J. Biol. Chem.* 246:1496, 1971). Once this loop is nicked, Fragment A and Fragment B are covalently linked only by the disulfide bond. There is evidence that nicking plays a role in the cytotoxic action of Diphtheria toxin (4), and it is generally believed that nicked Diphtheria toxin separates into free Fragment A and Fragment B when this disulfide bond is exposed to the reducing environment of the cytoplasm during membrane translocation of the toxin. The second disulfide bond makes a 9 residue loop between residues 461 and 471 within Fragment B. Residues near this loop (456, 458, 460, 472, 474) are also rich in positive charges and face the active site cleft, probably forming the so-called phosphate-binding or P-site (Lory et al., *Proc. Natl. Acad. Sci. USA* 77:267, 1980).

The structure suggests why whole Diphtheria toxin is inactive in catalyzing the ADP-ribosylation of EF-2 until the C domain dissociates, in the form of Fragment A, from Fragment B. As shown in Fig. 2, the active site is shielded by the 18-residue loop CL2 and the R domain. Thus, in whole Diphtheria toxin, the approach of EF-2 ($M_r \sim 100K$) to the active site is blocked. The active site of whole

- 33 -

Diphtheria toxin remains accessible to NAD⁺, however and catalyzes the NAD-glycohydrolysis (a slow side reaction that is probably physiologically insignificant). The lack of secondary structural elements within loop CL2 may allow a substantial movement of main chain atoms of the loop, permitting substrate entry to the active site.

Transmembrane domain

The structure of the T domain exhibits two features that suggest how it might experience pH-triggered insertion into the membrane. The first is that the T domain is entirely α -helical, similar to the known and proposed transmembrane proteins, and that some of the helices have hydrophobic characteristics more typical of transmembrane helices than of globular proteins (Rees, *Science* 245:510, 1989). The nine helices are arranged more or less in three layers, each layer consisting of an antiparallel pair of helices. The two long, carboxy terminal helices, TH8 and TH9, are unusually apolar and constitute the central core layer. One flanking layer, made up of helices TH5-TH7, also contains hydrophobic helices, TH6 and TH7. The other layer made up of helices TH1-TH3, is, in contrast, very hydrophilic even compared to globular proteins. The second noteworthy feature of the T domain is the acidic composition of the loops that connect pairs of these helices. Both loop TL3 between helices TH5 and TH6, and loop TL5 between hydrophobic helices TH8 and TH9 contain a total of six Asp and Glu residues (Fig. 6). At neutral pH, these loops are highly charged and water soluble. But at acidic pH, these residues would be at least partially protonated, and hence more nearly neutral and

- 34 -

membrane-soluble, especially near the surface of the membrane that has even higher concentration of protons due to the surface potential (McLaughlin, *Curr. Topics Memb. Transport* 9:71, 1977). Thus, the lower pH inside the endosome would tend to render these tip-shaped loops into membrane-soluble "daggers" that would lead the two apolar helix pairs into the membrane.

Other structural characteristics of the T domain suggest that it has the capacity to insert into the membrane and can assist the translocation of the C domain. The first is that the nearly parallel packing of the three helix layers would permit spreading on the membrane surface of the first helix layer (TH1-TH3) if other layers were inserted. This insertion would require local conformational changes in loops, but no alteration of the helices themselves. Also the pronounced hydrophobic asymmetry is compatible with the proposed rearrangement: 15 of 16 Lys and Arg residues and all 6 His residues of the T domain are located on the opposite side from the "dagger" tips (Fig. 8), making the whole domain a hydrophobic dipole, once the Asp and Glu residues are neutralized. It is possible that the hairpin loop TL5 and probably TL3 cross the membrane, where the Asp and Glu residues will once again be charged in the neutral pH of the cytoplasm.

The Diphtheria toxin dimer

Two monomers associate tightly to form a dimer with an interface between RB1/RB2 of one Diphtheria toxin molecule and RB2/RB1 of the other Diphtheria toxin molecule related by 2-fold rotation symmetry (Fig. 4). This interface is one of three major

- 35 -

protein-protein contacts in crystal packing and involves 3 hydrogen bonds per monomer. These hydrogen bonds are well defined since they are formed between main chain N and C atoms of RB1 and RB2. The other interfaces are not common among three different crystal forms. The inability of the dimer to bind to the Diphtheria toxin receptor (Carroll et al., *Biochem.* 25:2425, 1986) suggests that the dimer interaction sterically blocks the receptor binding domains of each monomer from the receptors on the surface of a target cell. The conformational differences between the monomer within the dimer and the native monomeric Diphtheria toxin remain uncertain, but biochemical evidence suggests they are not large. Binding data show that the affinity constant of the dimer for ApUp is the same as that of the monomer, and that the dimer binds 2 ApUp's (Carroll, *supra*). In addition, comparable specific activities of NAD-glucohydrolase activity and affinities for NAD⁺ were found in the monomer and dimer. Further, the specific ADP-ribosyltransferase activity of Fragment A released from the dimer after reduction was the same as that from the monomer (Carroll, *supra*). These findings show that the conformations of the C domain, and of the portion of the R domain interfacing the C domain, are relatively unperturbed in the dimer.

Use

The chimeric molecules of the invention can be used, for example, to kill particular classes of cells. As one example a chimeric diphtheria toxin molecule which binds specifically to cells bearing the interleukin-2 receptor can be used in treatment of various autoimmune diseases, e.g., arthritis.

- 36 -

Non-cytotoxic hybrid molecules in which a chimeric diphtheria toxin molecule is linked to a second molecule can be used to introduce the second molecule into selected cells, e.g., to correct an enzyme deficiency caused by a genetic disease. For example Tay-Sachs may be treated by introducing hexosaminidase A into appropriate cells.

Other Embodiments

The diphtheria toxin catalytic domain of chimeric diphtheria toxin molecules can be replaced by the catalytic domain of other toxin molecules to generate other targeted cytotoxins. Peptide toxins are preferred, but others are also useful. Many peptide toxins have a generalized eukaryotic receptor binding domain; in these instances the toxin must be modified to prevent intoxication of non-targeted cells. Any such modifications must be made in a manner which preserves the cytotoxic functions of the molecule. Potentially useful toxins include, but are not limited to: cholera toxin, ricin, 0-Shiga-like toxin (SLT-I, SLT-II, SLT II_v), LT toxin, C3 toxin, Shiga toxin, pertussis toxin, tetanus toxin, *Pseudomonas* exotoxin, alorin, saporin, modeccin, and gelanin.

If the catalytic domain is to be removed for the purpose of creating a hybrid molecule which includes a molecule to be introduced into a selected class of cells, it is preferred that the molecule to be introduced be fused to the chimeric diphtheria toxin molecule just to the amino-terminal side of the junction of Fragment A and Fragment B, i.e., to the amino-terminal side of residue 190.

What is claimed is:

- 37 -

EMARK Crystal structure of diphtheria toxin at 2. A resolution				created by user: Choe at UCLA		
EMARK	DATE:	09:1	54			
TOM	1	N	GLY	1	2.945	55.968
TOM	2	CA	GLY	1	3.593	56.074
TOM	3	C	GLY	1	5.077	55.817
TOM	4	O	GLY	1	5.462	56.232
TOM	5	N	ALA	2	5.943	55.211
TOM	6	CA	ALA	2	7.365	54.864
TOM	7	CB	ALA	2	8.258	56.056
TOM	8	C	ALA	2	7.744	54.396
TOM	9	O	ALA	2	8.358	53.330
TOM	10	N	ASP	3	7.527	55.014
TOM	11	CA	ASP	3	7.607	54.330
TOM	12	CB	ASP	3	7.513	55.308
TOM	13	CG	ASP	3	7.010	54.776
TOM	14	OD1	ASP	3	5.799	54.716
TOM	15	OD2	ASP	3	7.809	54.443
TOM	16	C	ASP	3	6.354	53.474
TOM	17	O	ASP	3	5.247	53.926
TOM	18	N	ASP	4	6.563	52.344
TOM	19	CA	ASP	4	5.653	51.225
TOM	20	CB	ASP	4	4.113	51.597
TOM	21	CG	ASP	4	3.362	52.232
TOM	22	OD1	ASP	4	3.933	53.012
TOM	23	OD2	ASP	4	2.168	51.934
TOM	24	C	ASP	4	6.020	50.536
TOM	25	O	ASP	4	5.301	49.689
TOM	26	N	VAL	5	7.130	50.877
TOM	27	CA	VAL	5	7.699	50.091
TOM	28	CB	VAL	5	7.302	50.613
TOM	29	CG1	VAL	5	8.058	49.880
TOM	30	CG2	VAL	5	5.862	50.266
TOM	31	C	VAL	5	9.229	50.095
TOM	32	O	VAL	5	9.916	49.115
TOM	33	N	VAL	6	9.839	51.206
TOM	34	CA	VAL	6	11.282	51.239
TOM	35	CB	VAL	6	12.008	52.585
TOM	36	CG1	VAL	6	13.387	52.794
TOM	37	CG2	VAL	6	12.268	52.498
TOM	38	C	VAL	6	11.391	51.124
TOM	39	O	VAL	6	11.670	50.023
TOM	40	N	ASP	7	10.931	52.175
TOM	41	CA	ASP	7	11.328	52.417
TOM	42	CB	ASP	7	10.865	53.871
TOM	43	CG	ASP	7	11.499	54.960
TOM	44	OD1	ASP	7	12.703	54.917
TOM	45	OD2	ASP	7	10.785	55.863
TOM	46	C	ASP	7	11.107	51.486
TOM	47	O	ASP	7	10.227	51.429
TOM	48	N	SER	8	12.079	50.645
TOM	49	CA	SER	8	12.908	49.603
TOM	50	CB	SER	8	13.087	48.329
TOM	51	OG	SER	8	14.149	47.478
TOM	52	C	SER	8	14.046	50.516
TOM	53	O	SER	8	14.388	50.716
TOM	54	N	SER	9	14.326	51.327
TOM	55	CA	SER	9	15.299	52.400
TOM	56	CB	SER	9	15.361	53.238
TOM	57	OG	SER	9	14.155	53.366
TOM	58	C	SER	9	16.666	51.806
TOM	59	O	SER	9	17.598	52.461
TOM	60	N	LYS	10	16.783	50.520
TOM	61	CA	LYS	10	18.006	49.741
TOM	62	CB	LYS	10	17.672	48.623
TOM	63	CG	LYS	10	17.340	49.250
TOM	64	CD	LYS	10	15.872	49.271

APPENDIX

0001

- 38 -

TOM	65	CE	L	10	15.584	50.400	61.90
TOM	66	NZ	LYS	10	16.412	50.536	68.402
TOM	67	C	LYS	10	18.558	49.339	61.982
TOM	68	O	LYS	10	18.790	48.201	61.491
TOM	69	N	SER	11	18.861	50.516	61.401
TOM	70	CA	SER	11	19.499	50.763	60.118
TOM	71	CB	SER	11	18.671	51.617	59.194
TOM	72	OG	SER	11	17.361	51.194	58.912
TOM	73	C	SER	11	20.734	51.646	60.378
TOM	74	O	SER	11	20.813	52.332	61.394
TOM	75	N	PHE	12	21.748	51.644	59.506
TOM	76	CA	PHE	12	22.734	52.717	59.465
TOM	77	CB	PHE	12	23.566	52.812	60.707
TOM	78	CG	PHE	12	23.630	54.323	60.927
TOM	79	CD1	PHE	12	22.480	55.107	60.739
TOM	80	CD2	PHE	12	24.836	54.943	61.193
TOM	81	CE1	PHE	12	22.555	56.481	60.802
TOM	82	CE2	PHE	12	24.887	56.321	61.252
TOM	83	CZ	PHE	12	23.766	57.089	61.057
TOM	84	C	PHE	12	23.717	52.798	58.330
TOM	85	O	PHE	12	23.521	52.157	57.293
TOM	86	N	VAL	13	24.633	53.752	58.333
TOM	87	CA	VAL	13	25.655	53.685	57.315
TOM	88	CB	VAL	13	25.807	55.201	56.807
TOM	89	CG1	VAL	13	26.437	56.194	57.788
TOM	90	CG2	VAL	13	26.500	55.045	55.433
TOM	91	C	VAL	13	26.871	52.949	57.933
TOM	92	O	VAL	13	27.246	53.100	59.111
TOM	93	N	MET	14	27.345	51.927	57.211
TOM	94	CA	MET	14	28.456	51.149	57.704
TOM	95	CB	MET	14	28.121	49.646	57.580
TOM	96	CG	MET	14	28.858	48.700	58.560
TOM	97	SD	MET	14	29.861	47.422	57.770
TOM	98	CE	MET	14	31.292	47.220	58.807
TOM	99	C	MET	14	29.680	51.510	56.893
TOM	100	O	MET	14	29.551	51.799	55.698
TOM	101	N	GLU	15	30.867	51.596	57.516
TOM	102	CA	GLU	15	32.118	51.785	56.752
TOM	103	CB	GLU	15	33.257	52.069	57.707
TOM	104	CG	GLU	15	34.585	52.387	56.959
TOM	105	CD	GLU	15	34.718	53.750	56.290
TOM	106	OE1	GLU	15	35.660	54.432	56.621
TOM	107	OE2	GLU	15	33.927	54.143	55.451
TOM	108	C	GLU	15	32.498	50.556	55.913
TOM	109	O	GLU	15	32.261	49.494	56.462
TOM	110	N	ASN	16	32.995	50.479	54.677
TOM	111	CA	ASN	16	33.279	49.180	54.025
TOM	112	CB	ASN	16	34.574	48.559	54.524
TOM	113	CG	ASN	16	35.764	49.448	54.430
TOM	114	OD1	ASN	16	36.298	49.792	55.476
TOM	115	ND2	ASN	16	36.304	49.908	53.322
TOM	116	C	ASN	16	32.236	48.031	54.135
TOM	117	O	ASN	16	32.637	46.858	54.177
TOM	118	N	PHE	17	30.912	48.268	54.228
TOM	119	CA	PHE	17	29.908	47.218	54.351
TOM	120	CB	PHE	17	28.594	47.708	53.932
TOM	121	CG	PHE	17	27.442	46.709	54.013
TOM	122	CD1	PHE	17	26.850	46.258	52.852
TOM	123	CD2	PHE	17	26.987	46.272	55.244
TOM	124	CE1	PHE	17	25.809	45.370	52.950
TOM	125	CE2	PHE	17	25.939	45.381	55.325
TOM	126	CZ	PHE	17	25.356	44.936	54.174
TOM	127	C	PHE	17	30.170	45.965	53.535
TOM	128	O	PHE	17	30.463	46.068	52.333
TOM	129	N	SER	18	30.026	44.804	54.170
TOM	130	CA	SER	18	30.325	43.590	53.487

0002

- 39 -

TOM	131	CB	SER	18	31.748	43.199	53.8
TOM	132	OG	SER	18	32.177	42.152	52.941
TOM	133	C	SER	18	29.430	42.382	53.716
TOM	134	O	SER	18	29.095	41.871	54.791
TOM	135	N	SER	19	29.075	41.865	52.564
TOM	136	CA	SER	19	28.158	40.731	52.508
TOM	137	CB	SER	19	26.977	41.066	51.626
TOM	138	OG	SER	19	25.838	41.501	52.334
TOM	139	C	SER	19	28.706	39.404	52.001
TOM	140	O	SER	19	29.688	39.287	51.251
TOM	141	N	TYR	20	27.974	38.360	52.350
TOM	142	CA	TYR	20	28.263	37.047	51.823
TOM	143	CB	TYR	20	28.176	36.103	52.973
TOM	144	CG	TYR	20	29.315	36.384	53.944
TOM	145	CD1	TYR	20	30.612	36.097	53.557
TOM	146	CE1	TYR	20	31.651	36.378	54.400
TOM	147	CD2	TYR	20	29.057	36.952	55.177
TOM	148	CE2	TYR	20	30.096	37.240	56.040
TOM	149	CZ	TYR	20	31.387	36.941	55.627
TOM	150	OH	TYR	20	32.462	37.208	56.447
TOM	151	C	TYR	20	27.363	36.649	50.675
TOM	152	O	TYR	20	26.208	37.053	50.621
TOM	153	N	HIS	21	27.836	35.977	49.642
TOM	154	CA	HIS	21	26.980	35.525	48.554
TOM	155	CB	HIS	21	27.008	36.472	47.349
TOM	156	CG	HIS	21	26.162	36.068	46.132
TOM	157	CD2	HIS	21	24.797	35.902	46.170
TOM	158	ND1	HIS	21	26.544	35.855	44.859
TOM	159	CE1	HIS	21	25.489	35.584	44.126
TOM	160	NE2	HIS	21	24.454	35.615	44.936
TOM	161	C	HIS	21	27.546	34.195	48.099
TOM	162	O	HIS	21	28.754	34.150	47.856
TOM	163	N	GLY	22	26.781	33.110	47.927
TOM	164	CA	GLY	22	27.383	31.844	47.519
TOM	165	C	GLY	22	27.230	31.512	46.074
TOM	166	O	GLY	22	26.157	31.781	45.574
TOM	167	N	THR	23	28.200	30.991	45.341
TOM	168	CA	THR	23	27.931	30.734	43.936
TOM	169	CB	THR	23	28.506	31.940	43.179
TOM	170	OG1	THR	23	28.578	31.657	41.772
TOM	171	CG2	THR	23	29.888	32.282	43.693
TOM	172	C	THR	23	28.307	29.412	43.215
TOM	173	O	THR	23	29.213	28.627	43.507
TOM	174	N	LYS	24	27.484	29.164	42.217
TOM	175	CA	LYS	24	27.472	28.024	41.351
TOM	176	CB	LYS	24	26.540	28.257	40.186
TOM	177	CG	LYS	24	25.128	27.778	40.388
TOM	178	CD	LYS	24	24.496	28.078	41.743
TOM	179	CE	LYS	24	22.979	27.943	41.636
TOM	180	NZ	LYS	24	22.374	27.962	42.952
TOM	181	C	LYS	24	28.770	27.574	40.765
TOM	182	O	LYS	24	29.630	28.421	40.451
TOM	183	N	PRO	25	28.879	26.224	40.564
TOM	184	CD	PRO	25	28.040	25.185	41.195
TOM	185	CA	PRO	25	29.866	25.638	39.663
TOM	186	CB	PRO	25	29.711	24.167	40.071
TOM	187	CG	PRO	25	28.244	24.001	40.329
TOM	188	C	PRO	25	29.738	26.032	38.135
TOM	189	O	PRO	25	28.763	25.923	37.368
TOM	190	N	GLY	26	30.870	26.578	37.691
TOM	191	CA	GLY	26	30.964	27.240	36.404
TOM	192	C	GLY	26	30.951	28.777	36.578
TOM	193	O	GLY	26	31.346	29.549	35.706
TOM	194	N	TYR	27	30.553	29.274	37.761
TOM	195	CA	TYR	27	30.394	30.705	38.000
TOM	196	CB	TYR	27	28.870	30.940	38.035

0003

- 40 -

TOM	197	CG	TYR	27	28.287	30.777	36.6
TOM	198	CD1	TYR	27	28.923	31.380	35.577
TOM	199	CE1	TYR	27	28.442	31.335	34.290
TOM	200	CD2	TYR	27	27.141	30.080	36.401
TOM	201	CE2	TYR	27	26.631	30.032	35.105
TOM	202	CZ	TYR	27	27.284	30.657	34.054
TOM	203	OH	TYR	27	26.761	30.685	32.769
TOM	204	C	TYR	27	31.101	31.345	39.190
TOM	205	O	TYR	27	30.928	32.515	39.489
TOM	206	N	VAL	28	31.941	30.610	39.910
TOM	207	CA	VAL	28	32.762	31.165	41.008
TOM	208	CB	VAL	28	32.957	30.000	42.053
TOM	209	CG1	VAL	28	33.336	28.694	41.382
TOM	210	CG2	VAL	28	34.024	30.391	43.042
TOM	211	C	VAL	28	34.094	31.823	40.557
TOM	212	O	VAL	28	34.653	32.766	41.128
TOM	213	N	ASP	29	34.603	31.394	39.415
TOM	214	CA	ASP	29	35.809	31.961	38.805
TOM	215	CB	ASP	29	36.236	31.027	37.616
TOM	216	CG	ASP	29	36.712	29.615	38.012
TOM	217	OD1	ASP	29	35.923	28.652	37.930
TOM	218	OD2	ASP	29	37.875	29.500	38.412
TOM	219	C	ASP	29	35.666	33.410	38.322
TOM	220	O	ASP	29	36.454	34.301	38.615
TOM	221	N	SER	30	34.551	33.582	37.620
TOM	222	CA	SER	30	34.090	34.792	36.918
TOM	223	CB	SER	30	33.062	34.346	35.868
TOM	224	OG	SER	30	31.907	33.764	36.493
TOM	225	C	SER	30	33.493	35.979	37.706
TOM	226	O	SER	30	33.805	37.149	37.457
TOM	227	N	ILE	31	32.533	35.634	38.586
TOM	228	CA	ILE	31	31.885	36.467	39.617
TOM	229	CB	ILE	31	31.005	35.422	40.487
TOM	230	CG2	ILE	31	31.876	34.674	41.519
TOM	231	CG1	ILE	31	29.949	36.097	41.310
TOM	232	CD	ILE	31	28.833	35.108	41.633
TOM	233	C	ILE	31	32.844	37.349	40.471
TOM	234	O	ILE	31	32.466	38.415	40.972
TOM	235	N	GLN	32	34.115	36.960	40.650
TOM	236	CA	GLN	32	35.080	37.760	41.407
TOM	237	CB	GLN	32	36.319	36.965	41.784
TOM	238	CG	GLN	32	36.415	35.805	42.771
TOM	239	CD	GLN	32	37.902	35.412	42.827
TOM	240	OE1	GLN	32	38.539	35.557	43.855
TOM	241	NE2	GLN	32	38.735	34.988	41.889
TOM	242	C	GLN	32	35.565	38.964	40.579
TOM	243	O	GLN	32	35.836	40.080	41.040
TOM	244	N	LYS	33	35.644	38.756	39.277
TOM	245	CA	LYS	33	35.979	39.843	38.365
TOM	246	CB	LYS	33	36.463	39.052	37.143
TOM	247	CG	LYS	33	37.742	38.280	37.509
TOM	248	CD	LYS	33	37.884	36.949	36.797
TOM	249	CE	LYS	33	38.226	37.057	35.325
TOM	250	NZ	LYS	33	38.021	35.774	34.652
TOM	251	C	LYS	33	34.861	40.927	38.090
TOM	252	O	LYS	33	35.111	41.962	37.457
TOM	253	N	GLY	34	33.572	40.799	38.501
TOM	254	CA	GLY	34	32.569	41.853	38.236
TOM	255	C	GLY	34	31.071	41.609	38.415
TOM	256	O	GLY	34	30.462	40.933	37.592
TOM	257	N	ILE	35	30.376	42.145	39.424
TOM	258	CA	ILE	35	28.916	41.899	39.609
TOM	259	CB	ILE	35	28.538	42.183	41.119
TOM	260	CG2	ILE	35	27.071	41.886	41.386
TOM	261	CG1	ILE	35	29.346	41.265	42.060
TOM	262	CD	ILE	35	29.174	39.720	41.924

0004

- 41 -

TOM	263	C	ILE	35	27.915	42.626	38.105
TOM	264	O	ILE	35	27.386	43.705	38.104
TOM	265	N	GLN	36	27.643	41.957	37.552
TOM	266	CA	GLN	36	26.760	42.434	36.493
TOM	267	CB	GLN	36	27.609	42.270	35.184
TOM	268	CG	GLN	36	26.960	42.647	33.803
TOM	269	CD	GLN	36	26.645	44.123	33.464
TOM	270	OE1	GLN	36	27.297	45.067	33.907
TOM	271	NE2	GLN	36	25.663	44.487	32.655
TOM	272	C	GLN	36	25.307	41.855	36.338
TOM	273	O	GLN	36	25.069	40.662	36.474
TOM	274	N	LYS	37	24.239	42.606	36.024
TOM	275	CA	LYS	37	22.876	42.075	35.815
TOM	276	CB	LYS	37	21.915	43.244	35.573
TOM	277	CG	LYS	37	20.455	42.867	35.393
TOM	278	CD	LYS	37	19.625	44.130	35.475
TOM	279	CE	LYS	37	18.178	43.734	35.749
TOM	280	NZ	LYS	37	17.314	44.901	35.850
TOM	281	C	LYS	37	22.630	41.049	34.712
TOM	282	O	LYS	37	22.845	41.343	33.526
TOM	283	N	PRO	38	22.163	39.841	35.017
TOM	284	CD	PRO	38	22.310	39.199	36.307
TOM	285	CA	PRO	38	21.741	38.841	34.031
TOM	286	CB	PRO	38	21.143	37.746	34.900
TOM	287	CG	PRO	38	22.184	37.707	35.970
TOM	288	C	PRO	38	20.847	39.193	32.828
TOM	289	O	PRO	38	19.690	39.617	32.924
TOM	290	N	LYS	39	21.421	38.932	31.652
TOM	291	CA	LYS	39	20.771	39.107	30.363
TOM	292	CB	LYS	39	21.814	38.749	29.300
TOM	293	CG	LYS	39	22.625	37.446	29.505
TOM	294	CD	LYS	39	23.929	37.396	28.665
TOM	295	CE	LYS	39	23.871	37.042	27.154
TOM	296	NZ	LYS	39	23.200	38.004	26.271
TOM	297	C	LYS	39	19.472	38.313	30.140
TOM	298	O	LYS	39	18.623	38.584	29.285
TOM	299	N	SER	40	19.287	37.269	30.926
TOM	300	CA	SER	40	18.184	36.330	30.738
TOM	301	CB	SER	40	18.613	35.085	29.961
TOM	302	OG	SER	40	19.269	34.046	30.703
TOM	303	C	SER	40	17.666	35.813	32.051
TOM	304	O	SER	40	18.493	35.596	32.942
TOM	305	N	GLY	41	16.372	35.617	32.230
TOM	306	CA	GLY	41	15.960	34.930	33.440
TOM	307	C	GLY	41	15.204	35.647	34.544
TOM	308	O	GLY	41	13.987	35.790	34.419
TOM	309	N	THR	42	15.814	36.110	35.631
TOM	310	CA	THR	42	14.995	36.522	36.773
TOM	311	CB	THR	42	14.689	35.384	37.749
TOM	312	OG1	THR	42	15.983	35.049	38.265
TOM	313	CG2	THR	42	13.992	34.168	37.166
TOM	314	C	THR	42	15.355	37.630	37.744
TOM	315	O	THR	42	14.489	38.474	38.005
TOM	316	N	GLN	43	16.574	37.602	38.360
TOM	317	CA	GLN	43	17.037	38.422	39.507
TOM	318	CB	GLN	43	17.187	39.905	39.086
TOM	319	CG	GLN	43	17.998	40.223	37.828
TOM	320	CD	GLN	43	17.370	39.854	36.472
TOM	321	OE1	GLN	43	17.360	38.693	36.056
TOM	322	NE2	GLN	43	16.779	40.750	35.697
TOM	323	C	GLN	43	16.032	38.295	40.725
TOM	324	O	GLN	43	16.420	38.030	41.880
TOM	325	N	GLY	44	14.703	38.466	40.504
TOM	326	CA	GLY	44	13.682	38.172	41.461
TOM	327	C	GLY	44	12.222	38.079	40.993
TOM	328	O	GLY	44	11.432	37.917	41.909

0005

- 42 -

TOM	329	N	ASN	45	11.678	38.053	39.70
TOM	330	CA	ASN	45	10.183	38.225	39.485
TOM	331	CB	ASN	45	9.421	36.861	39.595
TOM	332	CG	ASN	45	7.885	36.881	39.357
TOM	333	OD1	ASN	45	7.097	36.349	40.129
TOM	334	ND2	ASN	45	7.288	37.481	38.340
TOM	335	C	ASN	45	9.275	39.292	40.242
TOM	336	O	ASN	45	8.688	39.137	41.314
TOM	337	N	TYR	46	9.089	40.469	39.622
TOM	338	CA	TYR	46	8.353	41.636	40.132
TOM	339	CB	TYR	46	7.869	42.521	38.949
TOM	340	CG	TYR	46	8.387	42.216	37.547
TOM	341	CD1	TYR	46	7.980	41.037	36.920
TOM	342	CE1	TYR	46	8.447	40.689	35.665
TOM	343	CD2	TYR	46	9.266	43.065	36.903
TOM	344	CE2	TYR	46	9.725	42.721	35.645
TOM	345	CZ	TYR	46	9.318	41.541	35.043
TOM	346	OH	TYR	46	9.780	41.201	33.799
TOM	347	C	TYR	46	7.154	41.580	41.114
TOM	348	O	TYR	46	5.988	41.709	40.759
TOM	349	N	ASP	47	7.286	41.391	42.408
TOM	350	CA	ASP	47	6.175	41.556	43.335
TOM	351	CB	ASP	47	6.536	40.671	44.551
TOM	352	CG	ASP	47	5.580	40.696	45.739
TOM	353	OD1	ASP	47	5.991	40.948	46.878
TOM	354	OD2	ASP	47	4.398	40.457	45.502
TOM	355	C	ASP	47	6.024	43.071	43.649
TOM	356	O	ASP	47	5.946	43.495	44.813
TOM	357	N	ASP	48	5.931	43.856	42.545
TOM	358	CA	ASP	48	6.107	45.324	42.417
TOM	359	CB	ASP	48	5.312	46.106	43.508
TOM	360	CG	ASP	48	3.789	46.170	43.368
TOM	361	OD1	ASP	48	3.264	45.563	42.436
TOM	362	OD2	ASP	48	3.116	46.824	44.180
TOM	363	C	ASP	48	7.617	45.741	42.468
TOM	364	O	ASP	48	8.023	46.903	42.508
TOM	365	N	ASP	49	8.493	44.711	42.473
TOM	366	CA	ASP	49	9.948	44.690	42.302
TOM	367	CB	ASP	49	10.387	45.685	41.245
TOM	368	CG	ASP	49	9.901	45.386	39.853
TOM	369	OD1	ASP	49	8.954	46.049	39.423
TOM	370	OD2	ASP	49	10.477	44.512	39.199
TOM	371	C	ASP	49	11.130	44.779	43.255
TOM	372	O	ASP	49	11.669	45.834	43.608
TOM	373	N	TRP	50	11.612	43.585	43.606
TOM	374	CA	TRP	50	12.985	43.477	44.139
TOM	375	CB	TRP	50	13.143	42.845	45.615
TOM	376	CG	TRP	50	12.258	43.341	46.804
TOM	377	CD2	TRP	50	10.913	43.123	46.891
TOM	378	CE2	TRP	50	10.578	43.645	48.151
TOM	379	CE3	TRP	50	10.004	42.522	46.029
TOM	380	CD1	TRP	50	12.682	43.978	47.971
TOM	381	NE1	TRP	50	11.637	44.143	48.780
TOM	382	CZ2	TRP	50	9.288	43.543	48.562
TOM	383	CZ3	TRP	50	8.712	42.441	46.469
TOM	384	CH2	TRP	50	8.367	42.936	47.712
TOM	385	C	TRP	50	13.536	42.494	43.077
TOM	386	O	TRP	50	13.092	41.365	42.907
TOM	387	N	LYS	51	14.224	43.080	42.119
TOM	388	CA	LYS	51	15.009	42.444	41.083
TOM	389	CB	LYS	51	14.557	42.845	39.683
TOM	390	CG	LYS	51	13.937	41.731	38.842
TOM	391	CD	LYS	51	13.738	42.142	37.377
TOM	392	CE	LYS	51	13.214	40.951	36.564
TOM	393	NZ	LYS	51	12.040	40.325	37.159
TOM	394	C	LYS	51	16.394	43.050	41.328

0006

TOM	395	O	LYS	51	16.694	44.209	41.0
TOM	396	N	GLY	52	17.328	42.355	41.930
TOM	397	CA	GLY	52	18.578	42.993	42.292
TOM	398	C	GLY	52	19.460	41.928	42.898
TOM	399	O	GLY	52	18.941	40.851	43.227
TOM	400	N	PHE	53	20.777	42.194	42.979
TOM	401	CA	PHE	53	21.707	41.208	43.495
TOM	402	CB	PHE	53	23.079	41.752	43.287
TOM	403	CG	PHE	53	24.254	40.896	43.775
TOM	404	CD1	PHE	53	24.697	39.822	43.010
TOM	405	CD2	PHE	53	24.891	41.230	44.988
TOM	406	CE1	PHE	53	25.765	39.113	43.486
TOM	407	CE2	PHE	53	25.965	40.503	45.443
TOM	408	CZ	PHE	53	26.390	39.446	44.681
TOM	409	C	PHE	53	21.397	40.945	44.953
TOM	410	O	PHE	53	21.167	41.848	45.754
TOM	411	N	TYR	54	21.218	39.671	45.266
TOM	412	CA	TYR	54	20.878	39.302	46.629
TOM	413	CB	TYR	54	19.785	38.278	46.645
TOM	414	CG	TYR	54	18.375	38.737	46.416
TOM	415	CD1	TYR	54	18.027	39.265	45.188
TOM	416	CE1	TYR	54	16.763	39.764	44.977
TOM	417	CD2	TYR	54	17.479	38.668	47.459
TOM	418	CE2	TYR	54	16.199	39.154	47.249
TOM	419	CZ	TYR	54	15.862	39.702	46.016
TOM	420	OH	TYR	54	14.609	40.227	45.833
TOM	421	C	TYR	54	22.037	38.719	47.410
TOM	422	O	TYR	54	22.865	37.954	46.875
TOM	423	N	SER	55	22.119	39.016	48.698
TOM	424	CA	SER	55	23.211	38.427	49.453
TOM	425	CB	SER	55	24.461	39.339	49.409
TOM	426	OG	SER	55	24.329	40.704	49.842
TOM	427	C	SER	55	22.794	38.177	50.884
TOM	428	O	SER	55	21.605	38.341	51.203
TOM	429	N	THR	56	23.681	37.674	51.747
TOM	430	CA	THR	56	23.290	37.532	53.158
TOM	431	CB	THR	56	22.716	36.107	53.472
TOM	432	OG1	THR	56	22.330	36.231	54.840
TOM	433	CG2	THR	56	23.632	34.926	53.289
TOM	434	C	THR	56	24.457	37.831	54.089
TOM	435	O	THR	56	25.554	37.978	53.575
TOM	436	N	ASP	57	24.322	37.977	55.406
TOM	437	CA	ASP	57	25.460	38.221	56.285
TOM	438	CB	ASP	57	24.997	39.021	57.467
TOM	439	CG	ASP	57	24.035	38.299	58.403
TOM	440	OD1	ASP	57	24.332	38.137	59.585
TOM	441	OD2	ASP	57	22.988	37.879	57.940
TOM	442	C	ASP	57	26.107	36.927	56.790
TOM	443	O	ASP	57	26.970	36.868	57.674
TOM	444	N	ASN	58	25.660	35.816	56.200
TOM	445	CA	ASN	58	25.994	34.474	56.636
TOM	446	CB	ASN	58	24.648	33.894	57.054
TOM	447	CG	ASN	58	24.562	32.852	58.141
TOM	448	OD1	ASN	58	25.161	31.802	58.072
TOM	449	ND2	ASN	58	23.746	33.062	59.142
TOM	450	C	ASN	58	26.686	33.678	55.543
TOM	451	O	ASN	58	26.010	33.308	54.586
TOM	452	N	LYS	59	28.015	33.498	55.563
TOM	453	CA	LYS	59	28.707	32.528	54.679
TOM	454	CB	LYS	59	30.207	32.549	54.910
TOM	455	CG	LYS	59	30.664	32.277	56.328
TOM	456	CD	LYS	59	32.032	32.822	56.156
TOM	457	CE	LYS	59	32.461	33.455	57.438
TOM	458	NZ	LYS	59	33.336	34.546	57.033
TOM	459	C	LYS	59	28.280	31.045	54.735
TOM	460	O	LYS	59	28.420	30.295	53.770

- 44 -

TOM	461	N	TY	60	27.641	30.651	55	36
TOM	462	CA	TYR	60	27.029	29.318	56.007	
TOM	463	CB	TYR	60	26.670	29.033	57.526	
TOM	464	CG	TYR	60	27.984	29.057	58.296	
TOM	465	CD1	TYR	60	28.894	28.026	58.133	
TOM	466	CE1	TYR	60	30.173	28.086	58.622	
TOM	467	CD2	TYR	60	28.361	30.161	59.010	
TOM	468	CE2	TYR	60	29.652	30.215	59.498	
TOM	469	CZ	TYR	60	30.544	29.191	59.290	
TOM	470	OH	TYR	60	31.867	29.336	59.622	
TOM	471	C	TYR	60	25.776	29.157	55.159	
TOM	472	O	TYR	60	25.728	28.208	54.396	
TOM	473	N	ASP	61	24.775	30.052	55.257	
TOM	474	CA	ASP	61	23.584	30.165	54.366	
TOM	475	CB	ASP	61	22.654	31.174	54.961	
TOM	476	CG	ASP	61	22.048	30.478	56.158	
TOM	477	OD1	ASP	61	21.044	29.817	55.944	
TOM	478	OD2	ASP	61	22.588	30.517	57.264	
TOM	479	C	ASP	61	23.741	30.501	52.881	
TOM	480	O	ASP	61	23.076	29.897	52.043	
TOM	481	N	ALA	62	24.606	31.468	52.502	
TOM	482	CA	ALA	62	25.072	31.701	51.122	
TOM	483	CB	ALA	62	26.252	32.665	51.198	
TOM	484	C	ALA	62	25.500	30.430	50.334	
TOM	485	O	ALA	62	25.098	30.152	49.207	
TOM	486	N	ALA	63	26.359	29.624	50.985	
TOM	487	CA	ALA	63	26.799	28.281	50.566	
TOM	488	CB	ALA	63	27.711	27.765	51.635	
TOM	489	C	ALA	63	25.714	27.210	50.310	
TOM	490	O	ALA	63	25.915	26.154	49.688	
TOM	491	N	GLY	64	24.568	27.529	50.931	
TOM	492	CA	GLY	64	23.294	26.882	50.743	
TOM	493	C	GLY	64	22.878	26.962	49.304	
TOM	494	O	GLY	64	22.708	25.980	48.616	
TOM	495	N	TYR	65	22.864	28.136	48.745	
TOM	496	CA	TYR	65	22.512	28.325	47.352	
TOM	497	CB	TYR	65	21.681	29.611	47.318	
TOM	498	CG	TYR	65	22.250	30.901	47.893	
TOM	499	CD1	TYR	65	23.146	31.610	47.101	
TOM	500	CE1	TYR	65	23.652	32.826	47.494	
TOM	501	CD2	TYR	65	21.837	31.391	49.124	
TOM	502	CE2	TYR	65	22.347	32.617	49.521	
TOM	503	CZ	TYR	65	23.240	33.307	48.694	
TOM	504	OH	TYR	65	23.713	34.534	49.024	
TOM	505	C	TYR	65	23.684	28.330	46.339	
TOM	506	O	TYR	65	23.952	29.257	45.560	
TOM	507	N	SER	66	24.373	27.176	46.328	
TOM	508	CA	SER	66	25.520	26.973	45.435	
TOM	509	CB	SER	66	26.833	27.005	46.251	
TOM	510	OG	SER	66	27.102	25.934	47.170	
TOM	511	C	SER	66	25.556	25.717	44.544	
TOM	512	O	SER	66	26.634	25.322	44.117	
TOM	513	N	VAL	67	24.406	25.133	44.134	
TOM	514	CA	VAL	67	24.237	23.874	43.346	
TOM	515	CB	VAL	67	23.721	22.828	44.351	
TOM	516	CG1	VAL	67	23.726	21.466	43.675	
TOM	517	CG2	VAL	67	24.574	22.801	45.627	
TOM	518	C	VAL	67	23.237	24.050	42.146	
TOM	519	O	VAL	67	22.520	25.029	42.361	
TOM	520	N	ASP	68	22.947	23.411	40.946	
TOM	521	CA	ASP	68	21.767	23.875	40.099	
TOM	522	CB	ASP	68	22.306	24.933	39.128	
TOM	523	CG	ASP	68	21.221	25.808	38.465	
TOM	524	OD1	ASP	68	20.185	26.101	39.092	
TOM	525	OD2	ASP	68	21.415	26.182	37.297	
TOM	526	C	ASP	68	20.624	23.178	39.261	

0008

TOM	527	O	ASN	68	19.435	23.396	39.556
TOM	528	N	ASN	69	20.805	22.436	38.154
TOM	529	CA	ASN	69	19.721	21.867	37.279
TOM	530	CB	ASN	69	19.353	22.817	36.062
TOM	531	CG	ASN	69	18.728	22.229	34.771
TOM	532	OD1	ASN	69	19.330	22.112	33.685
TOM	533	ND2	ASN	69	17.462	21.831	34.788
TOM	534	C	ASN	69	20.320	20.578	36.741
TOM	535	O	ASN	69	21.301	20.610	35.998
TOM	536	N	GLU	70	19.638	19.493	37.135
TOM	537	CA	GLU	70	20.142	18.118	37.104
TOM	538	CB	GLU	70	20.577	17.660	35.648
TOM	539	CG	GLU	70	19.352	17.122	34.833
TOM	540	CD	GLU	70	19.555	16.630	33.384
TOM	541	OE1	GLU	70	18.879	15.673	32.947
TOM	542	OE2	GLU	70	20.366	17.238	32.666
TOM	543	C	GLU	70	21.315	17.965	38.121
TOM	544	O	GLU	70	22.360	17.298	37.948
TOM	545	N	ASN	71	20.906	18.653	39.245
TOM	546	CA	ASN	71	21.528	18.711	40.575
TOM	547	CB	ASN	71	21.295	20.066	41.268
TOM	548	CG	ASN	71	19.892	20.478	41.797
TOM	549	OD1	ASN	71	18.979	20.687	41.014
TOM	550	ND2	ASN	71	19.507	20.705	43.041
TOM	551	C	ASN	71	21.087	17.645	41.621
TOM	552	O	ASN	71	21.933	17.146	42.377
TOM	553	N	PRO	72	19.814	17.212	41.804
TOM	554	CD	PRO	72	19.135	16.344	40.839
TOM	555	CA	PRO	72	19.123	17.192	43.134
TOM	556	CB	PRO	72	18.615	15.789	43.079
TOM	557	CG	PRO	72	18.031	15.779	41.661
TOM	558	C	PRO	72	19.921	17.620	44.399
TOM	559	O	PRO	72	20.525	18.709	44.334
TOM	560	N	LEU	73	20.012	17.026	45.600
TOM	561	CA	LEU	73	21.165	17.451	46.443
TOM	562	CB	LEU	73	21.072	17.453	48.054
TOM	563	CG	LEU	73	22.195	18.004	49.082
TOM	564	CD1	LEU	73	23.636	17.879	48.470
TOM	565	CD2	LEU	73	21.931	19.463	49.433
TOM	566	C	LEU	73	22.018	16.260	46.099
TOM	567	O	LEU	73	21.949	15.206	46.737
TOM	568	N	SER	74	22.701	16.359	44.966
TOM	569	CA	SER	74	23.676	15.306	44.643
TOM	570	CB	SER	74	22.956	14.207	43.824
TOM	571	OG	SER	74	22.346	14.732	42.658
TOM	572	C	SER	74	24.926	15.803	43.912
TOM	573	O	SER	74	26.061	15.614	44.348
TOM	574	N	GLY	75	24.711	16.566	42.846
TOM	575	CA	GLY	75	25.782	17.088	42.009
TOM	576	C	GLY	75	26.340	18.479	42.346
TOM	577	O	GLY	75	25.772	19.480	41.922
TOM	578	N	LYS	76	27.406	18.523	43.170
TOM	579	CA	LYS	76	28.267	19.675	43.526
TOM	580	CB	LYS	76	29.565	19.468	42.677
TOM	581	CG	LYS	76	29.518	19.183	41.185
TOM	582	CD	LYS	76	29.684	20.466	40.353
TOM	583	CE	LYS	76	29.489	20.133	38.846
TOM	584	NZ	LYS	76	29.721	21.205	37.876
TOM	585	C	LYS	76	28.025	21.210	43.628
TOM	586	O	LYS	76	27.653	21.985	42.754
TOM	587	N	ALA	77	28.293	21.646	44.846
TOM	588	CA	ALA	77	28.317	23.047	42.294
TOM	589	CB	ALA	77	28.393	23.136	42.826
TOM	590	C	ALA	77	29.538	23.785	44.753
TOM	591	O	ALA	77	30.605	23.165	44.741
TOM	592	N	GLY	78	29.446	25.047	44.306

- 46 -

TOM	593	CA	GL	78	30.572	25.800	43.12
TOM	594	C	GLY	78	31.414	26.711	44.635
TOM	595	O	GLY	78	32.644	26.770	44.512
TOM	596	N	GLY	79	30.850	27.452	45.578
TOM	597	CA	GLY	79	31.649	28.302	46.425
TOM	598	C	GLY	79	30.945	29.468	47.112
TOM	599	O	GLY	79	29.734	29.662	47.082
TOM	600	N	VAL	80	31.669	30.291	47.830
TOM	601	CA	VAL	80	31.087	31.484	48.405
TOM	602	CB	VAL	80	30.866	31.227	49.902
TOM	603	CG1	VAL	80	30.294	32.483	50.505
TOM	604	CG2	VAL	80	29.901	30.079	50.151
TOM	605	C	VAL	80	32.009	32.694	48.136
TOM	606	O	VAL	80	33.211	32.575	47.926
TOM	607	N	VAL	81	31.477	33.895	48.061
TOM	608	CA	VAL	81	32.228	35.104	47.801
TOM	609	CB	VAL	81	32.127	35.578	46.335
TOM	610	CG1	VAL	81	33.328	35.026	45.612
TOM	611	CG2	VAL	81	30.833	35.163	45.663
TOM	612	C	VAL	81	31.770	36.269	48.669
TOM	613	O	VAL	81	30.567	36.506	48.761
TOM	614	N	LYS	82	32.745	36.932	49.322
TOM	615	CA	LYS	82	32.560	38.100	50.201
TOM	616	CB	LYS	82	33.617	38.074	51.277
TOM	617	CG	LYS	82	33.628	39.308	52.109
TOM	618	CD	LYS	82	33.938	38.925	53.506
TOM	619	CE	LYS	82	35.046	39.760	54.073
TOM	620	NZ	LYS	82	36.312	39.259	53.594
TOM	621	C	LYS	82	32.611	39.446	49.459
TOM	622	O	LYS	82	33.670	40.027	49.181
TOM	623	N	VAL	83	31.417	39.953	49.138
TOM	624	CA	VAL	83	31.319	41.159	48.322
TOM	625	CB	VAL	83	30.027	41.022	47.464
TOM	626	CG1	VAL	83	29.901	39.614	46.891
TOM	627	CG2	VAL	83	28.809	41.193	48.318
TOM	628	C	VAL	83	31.354	42.442	49.188
TOM	629	O	VAL	83	30.819	42.508	50.297
TOM	630	N	THR	84	32.028	43.489	48.741
TOM	631	CA	THR	84	32.196	44.700	49.542
TOM	632	CB	THR	84	33.687	44.893	50.026
TOM	633	OG1	THR	84	33.895	43.790	50.869
TOM	634	CG2	THR	84	34.022	46.056	50.940
TOM	635	C	THR	84	31.788	45.983	48.853
TOM	636	O	THR	84	31.881	46.243	47.638
TOM	637	N	TYR	85	31.190	46.784	49.708
TOM	638	CA	TYR	85	30.967	48.177	49.352
TOM	639	CB	TYR	85	29.585	48.531	49.894
TOM	640	CG	TYR	85	28.505	48.261	48.879
TOM	641	CD1	TYR	85	28.738	48.604	47.575
TOM	642	CE1	TYR	85	27.738	48.461	46.653
TOM	643	CD2	TYR	85	27.276	47.757	49.262
TOM	644	CE2	TYR	85	26.266	47.614	48.323
TOM	645	CZ	TYR	85	26.512	47.981	47.025
TOM	646	OH	TYR	85	25.531	47.950	46.069
TOM	647	C	TYR	85	32.087	49.175	49.804
TOM	648	O	TYR	85	32.156	49.735	50.906
TOM	649	N	PRO	86	33.024	49.413	48.882
TOM	650	CD	PRO	86	32.986	49.011	47.469
TOM	651	CA	PRO	86	34.237	50.157	49.136
TOM	652	CB	PRO	86	34.839	50.322	47.725
TOM	653	CG	PRO	86	34.463	49.003	47.079
TOM	654	C	PRO	86	34.142	51.455	49.928
TOM	655	O	PRO	86	35.127	51.758	50.617
TOM	656	N	GLY	87	33.025	52.212	49.930
TOM	657	CA	GLY	87	33.024	53.417	50.781
TOM	658	C	GLY	87	32.117	53.453	52.032

0010

TOM	659	O	GLY	87	32.160	52.600	52.9
TOM	660	N	LEU	88	31.314	54.516	52.140
TOM	661	CA	LEU	88	30.315	54.628	53.187
TOM	662	CB	LEU	88	29.880	56.039	53.442
TOM	663	CG	LEU	88	29.832	56.665	54.825
TOM	664	CD1	LEU	88	30.997	56.182	55.680
TOM	665	CD2	LEU	88	29.863	58.186	54.652
TOM	666	C	LEU	88	29.173	53.982	52.482
TOM	667	O	LEU	88	29.049	54.215	51.277
TOM	668	N	THR	89	28.381	53.139	53.149
TOM	669	CA	THR	89	27.204	52.514	52.501
TOM	670	CB	THR	89	27.629	51.220	51.737
TOM	671	OG1	THR	89	26.527	50.324	51.751
TOM	672	CG2	THR	89	28.908	50.620	52.325
TOM	673	C	THR	89	26.138	52.210	53.523
TOM	674	O	THR	89	26.357	51.804	54.659
TOM	675	N	LYS	90	24.953	52.502	53.115
TOM	676	CA	LYS	90	23.778	52.531	53.975
TOM	677	CB	LYS	90	23.021	53.856	53.690
TOM	678	CG	LYS	90	21.547	54.041	54.169
TOM	679	CD	LYS	90	21.423	54.553	55.563
TOM	680	CE	LYS	90	20.008	54.405	56.045
TOM	681	NZ	LYS	90	19.987	54.767	57.450
TOM	682	C	LYS	90	22.842	51.334	53.827
TOM	683	O	LYS	90	22.398	50.862	52.759
TOM	684	N	VAL	91	22.511	50.890	55.022
TOM	685	CA	VAL	91	21.686	49.721	55.174
TOM	686	CB	VAL	91	22.538	48.777	56.111
TOM	687	CG1	VAL	91	21.648	47.659	56.634
TOM	688	CG2	VAL	91	23.724	48.157	55.372
TOM	689	C	VAL	91	20.288	50.064	55.705
TOM	690	O	VAL	91	20.234	50.617	56.810
TOM	691	N	LEU	92	19.179	49.707	55.032
TOM	692	CA	LEU	92	17.798	49.949	55.527
TOM	693	CB	LEU	92	16.897	50.561	54.451
TOM	694	CG	LEU	92	16.570	52.053	54.135
TOM	695	CD1	LEU	92	15.859	52.040	52.770
TOM	696	CD2	LEU	92	15.700	52.762	55.202
TOM	697	C	LEU	92	16.983	48.762	56.070
TOM	698	O	LEU	92	16.429	47.966	55.291
TOM	699	N	ALA	93	16.787	48.607	57.382
TOM	700	CA	ALA	93	16.004	47.470	57.885
TOM	701	CB	ALA	93	16.272	47.205	59.330
TOM	702	C	ALA	93	14.481	47.553	57.787
TOM	703	O	ALA	93	13.756	47.978	58.710
TOM	704	N	LEU	94	13.951	47.101	56.650
TOM	705	CA	LEU	94	12.487	47.076	56.456
TOM	706	CB	LEU	94	12.099	46.962	55.019
TOM	707	CG	LEU	94	13.136	46.930	53.976
TOM	708	CD1	LEU	94	12.673	46.244	52.693
TOM	709	CD2	LEU	94	13.556	48.340	53.842
TOM	710	C	LEU	94	11.664	45.983	57.160
TOM	711	O	LEU	94	11.798	44.754	56.997
TOM	712	N	LYS	95	10.754	46.523	57.973
TOM	713	CA	LYS	95	9.820	45.746	58.802
TOM	714	CB	LYS	95	9.570	46.578	60.088
TOM	715	CG	LYS	95	9.082	47.960	59.816
TOM	716	CD	LYS	95	9.074	48.874	60.996
TOM	717	CE	LYS	95	8.246	48.437	62.151
TOM	718	NZ	LYS	95	8.080	49.625	62.959
TOM	719	C	LYS	95	8.478	45.274	58.175
TOM	720	O	LYS	95	7.492	44.837	58.788
TOM	721	N	VAL	96	8.450	45.358	56.866
TOM	722	CA	VAL	96	7.324	44.903	56.101
TOM	723	CB	VAL	96	6.289	46.061	55.909
TOM	724	CG1	VAL	96	5.298	45.645	54.831

- 48 -

TOM	725	CG2	VAL	96	5.439	46.324	57.1
TOM	726	C	VAL	96	7.891	44.460	54.758
TOM	727	O	VAL	96	8.903	44.985	54.302
TOM	728	N	ASP	97	7.333	43.450	54.128
TOM	729	CA	ASP	97	7.686	43.181	52.754
TOM	730	CB	ASP	97	8.444	41.837	52.704
TOM	731	CG	ASP	97	7.836	40.760	51.818
TOM	732	OD1	ASP	97	7.614	39.676	52.367
TOM	733	OD2	ASP	97	7.587	41.009	50.620
TOM	734	C	ASP	97	6.389	43.204	51.912
TOM	735	O	ASP	97	5.386	42.566	52.232
TOM	736	N	ASN	98	6.510	43.745	50.707
TOM	737	CA	ASN	98	5.389	44.161	49.850
TOM	738	CB	ASN	98	4.297	44.844	50.742
TOM	739	CG	ASN	98	2.801	44.711	50.443
TOM	740	OD1	ASN	98	2.309	44.803	49.327
TOM	741	ND2	ASN	98	1.954	44.517	51.426
TOM	742	C	ASN	98	6.021	45.219	48.901
TOM	743	O	ASN	98	6.261	46.260	49.531
TOM	744	N	ALA	99	6.370	45.248	47.588
TOM	745	CA	ALA	99	6.989	46.536	47.122
TOM	746	CB	ALA	99	7.816	46.410	45.834
TOM	747	C	ALA	99	5.964	47.645	46.828
TOM	748	O	ALA	99	5.973	48.246	45.761
TOM	749	N	GLU	100	5.198	48.038	47.863
TOM	750	CA	GLU	100	3.917	48.714	47.683
TOM	751	CB	GLU	100	2.821	47.745	47.132
TOM	752	CG	GLU	100	1.300	48.055	47.313
TOM	753	CD	GLU	100	0.534	48.684	46.135
TOM	754	OE1	GLU	100	-0.695	48.868	46.282
TOM	755	OE2	GLU	100	1.156	48.962	45.090
TOM	756	C	GLU	100	3.451	49.203	49.018
TOM	757	O	GLU	100	2.703	50.158	49.082
TOM	758	N	THR	101	3.717	48.529	50.121
TOM	759	CA	THR	101	3.540	49.209	51.406
TOM	760	CB	THR	101	3.516	48.219	52.600
TOM	761	OG1	THR	101	2.878	47.076	52.055
TOM	762	CG2	THR	101	2.699	48.646	53.839
TOM	763	C	THR	101	4.816	50.075	51.449
TOM	764	O	THR	101	4.797	51.232	51.832
TOM	765	N	ILE	102	5.944	49.554	50.918
TOM	766	CA	ILE	102	7.211	50.293	50.754
TOM	767	CB	ILE	102	8.380	49.399	50.122
TOM	768	CG2	ILE	102	9.667	50.052	50.596
TOM	769	CG1	ILE	102	8.449	47.907	50.571
TOM	770	CD	ILE	102	8.421	47.541	52.066
TOM	771	C	ILE	102	6.879	51.451	49.827
TOM	772	O	ILE	102	6.643	52.512	50.386
TOM	773	N	LYS	103	6.776	51.343	48.497
TOM	774	CA	LYS	103	6.209	52.433	47.642
TOM	775	CB	LYS	103	5.649	51.922	46.309
TOM	776	CG	LYS	103	6.674	51.389	45.331
TOM	777	CD	LYS	103	5.909	51.285	44.025
TOM	778	CE	LYS	103	6.628	50.576	42.927
TOM	779	NZ	LYS	103	6.841	49.195	43.297
TOM	780	C	LYS	103	5.055	53.353	48.156
TOM	781	O	LYS	103	5.164	54.587	48.151
TOM	782	N	LYS	104	3.921	52.806	48.611
TOM	783	CA	LYS	104	2.880	53.657	49.137
TOM	784	CB	LYS	104	1.609	52.874	49.418
TOM	785	CG	LYS	104	0.297	53.668	49.259
TOM	786	CD	LYS	104	-0.440	53.700	50.577
TOM	787	CE	LYS	104	-0.248	55.030	51.241
TOM	788	NZ	LYS	104	-0.765	54.886	52.585
TOM	789	C	LYS	104	3.255	54.373	50.412
TOM	790	O	LYS	104	2.878	55.525	50.522

0012

- 49 -

TOM	791	N	GLU	105	3.971	53.877	51. J
TOM	792	CA	GLU	105	4.155	54.728	52.591
TOM	793	CB	GLU	105	3.621	54.011	53.837
TOM	794	CG	GLU	105	2.141	54.399	53.965
TOM	795	CD	GLU	105	1.349	53.890	55.162
TOM	796	OE1	GLU	105	0.129	54.035	55.149
TOM	797	OE2	GLU	105	1.932	53.354	56.106
TOM	798	C	GLU	105	5.542	55.255	52.878
TOM	799	O	GLU	105	5.881	55.685	53.992
TOM	800	N	LEU	106	6.240	55.293	51.744
TOM	801	CA	LEU	106	7.629	55.701	51.672
TOM	802	CB	LEU	106	8.489	54.482	52.116
TOM	803	CG	LEU	106	9.943	54.889	52.303
TOM	804	CD1	LEU	106	10.195	55.056	53.796
TOM	805	CD2	LEU	106	10.850	53.917	51.564
TOM	806	C	LEU	106	8.184	56.281	50.337
TOM	807	O	LEU	106	8.130	57.480	50.042
TOM	808	N	GLY	107	8.731	55.394	49.487
TOM	809	CA	GLY	107	9.487	55.713	48.260
TOM	810	C	GLY	107	8.638	55.741	47.010
TOM	811	O	GLY	107	8.724	54.898	46.124
TOM	812	N	LEU	108	7.815	56.774	47.070
TOM	813	CA	LEU	108	6.741	57.067	46.145
TOM	814	CB	LEU	108	6.422	58.567	46.262
TOM	815	CG	LEU	108	5.440	59.168	47.312
TOM	816	CD1	LEU	108	6.054	59.143	48.707
TOM	817	CD2	LEU	108	5.148	60.643	46.966
TOM	818	C	LEU	108	6.583	56.747	44.666
TOM	819	O	LEU	108	5.426	56.862	44.317
TOM	820	N	SER	109	7.397	56.307	43.692
TOM	821	CA	SER	109	6.951	56.222	42.264
TOM	822	CB	SER	109	7.940	55.500	41.370
TOM	823	OG	SER	109	7.940	54.104	41.697
TOM	824	C	SER	109	5.621	55.554	41.865
TOM	825	O	SER	109	5.018	55.836	40.816
TOM	826	N	LEU	110	5.198	54.602	42.709
TOM	827	CA	LEU	110	3.991	53.782	42.533
TOM	828	CB	LEU	110	2.787	54.643	42.946
TOM	829	CG	LEU	110	2.764	54.963	44.467
TOM	830	CD1	LEU	110	2.351	56.418	44.674
TOM	831	CD2	LEU	110	1.868	53.977	45.201
TOM	832	C	LEU	110	3.727	53.058	41.200
TOM	833	O	LEU	110	2.979	52.098	41.266
TOM	834	N	THR	111	4.178	53.378	39.972
TOM	835	CA	THR	111	4.235	52.379	38.859
TOM	836	CB	THR	111	3.047	52.479	37.851
TOM	837	OG1	THR	111	3.190	53.661	37.063
TOM	838	CG2	THR	111	1.730	52.410	38.593
TOM	839	C	THR	111	5.548	52.415	38.004
TOM	840	O	THR	111	5.711	52.672	36.801
TOM	841	N	GLU	112	6.588	52.133	38.755
TOM	842	CA	GLU	112	7.971	52.078	38.289
TOM	843	CB	GLU	112	8.539	53.544	38.187
TOM	844	CG	GLU	112	9.950	53.922	37.601
TOM	845	CD	GLU	112	10.212	53.905	36.071
TOM	846	OE1	GLU	112	10.333	52.812	35.507
TOM	847	OE2	GLU	112	10.333	54.973	35.445
TOM	848	C	GLU	112	8.656	51.247	39.411
TOM	849	O	GLU	112	8.394	51.499	40.596
TOM	850	N	PRO	113	9.503	50.246	39.141
TOM	851	CD	PRO	113	10.102	50.060	37.822
TOM	852	CA	PRO	113	10.173	49.407	40.135
TOM	853	CB	PRO	113	11.353	48.857	39.392
TOM	854	CG	PRO	113	10.846	48.776	37.960
TOM	855	C	PRO	113	10.629	49.878	41.499
TOM	856	O	PRO	113	11.296	50.885	41.510

0013

TOM	857	N	LEU	114	10.410	49.303	42.6
TOM	858	CA	LEU	114	11.148	49.680	43.901
TOM	859	CB	LEU	114	10.581	48.868	45.062
TOM	860	CG	LEU	114	11.216	48.810	46.467
TOM	861	CD1	LEU	114	10.830	49.978	47.382
TOM	862	CD2	LEU	114	10.751	47.510	47.057
TOM	863	C	LEU	114	12.697	49.472	43.852
TOM	864	O	LEU	114	13.497	50.379	44.133
TOM	865	N	MET	115	13.270	48.303	43.499
TOM	866	CA	MET	115	14.748	48.225	43.434
TOM	867	CB	MET	115	15.294	46.843	43.111
TOM	868	CG	MET	115	16.188	46.408	44.261
TOM	869	SD	MET	115	15.328	45.758	45.704
TOM	870	CE	MET	115	15.501	46.905	47.031
TOM	871	C	MET	115	15.390	49.148	42.420
TOM	872	O	MET	115	16.502	49.574	42.643
TOM	873	N	GLU	116	14.738	49.547	41.327
TOM	874	CA	GLU	116	15.288	50.541	40.397
TOM	875	CB	GLU	116	14.398	50.699	39.211
TOM	876	CG	GLU	116	15.106	50.252	37.948
TOM	877	CD	GLU	116	14.314	50.486	36.663
TOM	878	OE1	GLU	116	14.719	49.911	35.636
TOM	879	OE2	GLU	116	13.313	51.235	36.690
TOM	880	C	GLU	116	15.363	51.870	41.125
TOM	881	O	GLU	116	16.395	52.540	41.290
TOM	882	N	GLN	117	14.197	52.141	41.679
TOM	883	CA	GLN	117	14.060	53.246	42.599
TOM	884	CB	GLN	117	12.643	53.180	43.129
TOM	885	CG	GLN	117	11.652	53.843	42.221
TOM	886	CD	GLN	117	10.825	54.682	43.150
TOM	887	OE1	GLN	117	11.148	55.815	43.485
TOM	888	NE2	GLN	117	9.729	54.167	43.643
TOM	889	C	GLN	117	15.082	53.325	43.768
TOM	890	O	GLN	117	15.599	54.404	44.110
TOM	891	N	VAL	118	15.503	52.197	44.353
TOM	892	CA	VAL	118	16.411	52.331	45.473
TOM	893	CB	VAL	118	16.246	51.054	46.396
TOM	894	CG1	VAL	118	14.797	50.912	46.827
TOM	895	CG2	VAL	118	16.706	49.829	45.707
TOM	896	C	VAL	118	17.865	52.606	45.036
TOM	897	O	VAL	118	18.799	52.863	45.818
TOM	898	N	GLY	119	18.032	52.660	43.710
TOM	899	CA	GLY	119	19.298	53.124	43.159
TOM	900	C	GLY	119	19.320	54.535	42.542
TOM	901	O	GLY	119	20.188	54.797	41.719
TOM	902	N	THR	120	18.408	55.465	42.854
TOM	903	CA	THR	120	18.358	56.845	42.309
TOM	904	CB	THR	120	16.872	57.388	42.095
TOM	905	OG1	THR	120	16.106	57.268	43.311
TOM	906	CG2	THR	120	16.218	56.678	40.935
TOM	907	C	THR	120	19.057	57.904	43.177
TOM	908	O	THR	120	18.986	57.798	44.391
TOM	909	N	GLU	121	19.750	58.957	42.701
TOM	910	CA	GLU	121	20.308	59.999	43.593
TOM	911	CB	GLU	121	20.897	61.146	42.769
TOM	912	CG	GLU	121	22.188	60.948	41.899
TOM	913	CD	GLU	121	22.553	62.129	40.968
TOM	914	OE1	GLU	121	22.755	61.910	39.760
TOM	915	OE2	GLU	121	22.629	63.268	41.450
TOM	916	C	GLU	121	19.274	60.601	44.560
TOM	917	O	GLU	121	19.510	60.843	45.752
TOM	918	N	GLU	122	18.058	60.721	44.000
TOM	919	CA	GLU	122	16.841	61.180	44.693
TOM	920	CB	GLU	122	15.614	61.044	43.798
TOM	921	CG	GLU	122	15.480	61.661	42.378
TOM	922	CD	GLU	122	16.208	61.047	41.169

- 51 -

TOM	923	OE1	GLU	122	17.439	60.943	41.21
TOM	924	OE2	GLU	122	15.545	60.715	40.171
TOM	925	C	GLU	122	16.576	60.342	45.955
TOM	926	O	GLU	122	16.443	60.832	47.063
TOM	927	N	PHE	123	16.524	59.020	45.789
TOM	928	CA	PHE	123	16.393	58.019	46.862
TOM	929	CB	PHE	123	16.062	56.635	46.168
TOM	930	CG	PHE	123	15.390	55.617	47.059
TOM	931	CD1	PHE	123	14.020	55.482	47.002
TOM	932	CD2	PHE	123	16.119	54.916	48.002
TOM	933	CE1	PHE	123	13.388	54.657	47.903
TOM	934	CE2	PHE	123	15.463	54.089	48.904
TOM	935	CZ	PHE	123	14.099	53.957	48.863
TOM	936	C	PHE	123	17.666	57.904	47.762
TOM	937	O	PHE	123	17.701	58.127	48.984
TOM	938	N	ILE	124	18.774	57.534	47.101
TOM	939	CA	ILE	124	20.071	57.233	47.692
TOM	940	CB	ILE	124	20.980	57.016	46.449
TOM	941	CG2	ILE	124	22.431	57.100	46.864
TOM	942	CG1	ILE	124	20.682	55.664	45.765
TOM	943	CD	ILE	124	21.601	54.404	45.948
TOM	944	C	ILE	124	20.606	58.251	48.720
TOM	945	O	ILE	124	21.471	57.914	49.548
TOM	946	N	LYS	125	19.999	59.459	48.722
TOM	947	CA	LYS	125	20.293	60.562	49.618
TOM	948	CB	LYS	125	19.197	61.606	49.358
TOM	949	CG	LYS	125	19.236	62.955	50.115
TOM	950	CD	LYS	125	20.440	63.872	49.769
TOM	951	CE	LYS	125	20.570	65.239	50.498
TOM	952	NZ	LYS	125	19.592	66.238	50.083
TOM	953	C	LYS	125	20.436	60.222	51.117
TOM	954	O	LYS	125	20.973	61.031	51.905
TOM	955	N	ARG	126	20.000	58.986	51.507
TOM	956	CA	ARG	126	20.066	58.426	52.877
TOM	957	CB	ARG	126	19.350	57.063	52.922
TOM	958	CG	ARG	126	17.886	56.959	52.508
TOM	959	CD	ARG	126	17.052	58.168	52.840
TOM	960	NE	ARG	126	16.982	59.017	51.659
TOM	961	CZ	ARG	126	16.625	60.313	51.685
TOM	962	NH1	ARG	126	16.514	61.026	50.544
TOM	963	NH2	ARG	126	16.369	60.892	52.852
TOM	964	C	ARG	126	21.443	58.266	53.566
TOM	965	O	ARG	126	22.122	57.242	53.807
TOM	966	N	PHE	127	21.748	59.509	53.984
TOM	967	CA	PHE	127	22.945	59.877	54.738
TOM	968	CB	PHE	127	22.934	58.906	55.983
TOM	969	CG	PHE	127	21.673	59.016	56.863
TOM	970	CD1	PHE	127	20.411	59.305	56.346
TOM	971	CD2	PHE	127	21.832	58.884	58.217
TOM	972	CE1	PHE	127	19.321	59.466	57.148
TOM	973	CE2	PHE	127	20.740	59.046	59.028
TOM	974	CZ	PHE	127	19.493	59.333	58.507
TOM	975	C	PHE	127	24.179	59.804	53.804
TOM	976	O	PHE	127	24.053	60.221	52.645
TOM	977	N	GLY	128	25.388	59.362	54.148
TOM	978	CA	GLY	128	26.421	59.184	53.146
TOM	979	C	GLY	128	26.154	58.041	52.139
TOM	980	O	GLY	128	26.616	56.933	52.366
TOM	981	N	ASP	129	25.359	58.248	51.082
TOM	982	CA	ASP	129	25.163	57.381	49.905
TOM	983	CB	ASP	129	25.858	58.151	48.807
TOM	984	CG	ASP	129	27.125	57.495	48.258
TOM	985	OD1	ASP	129	27.097	57.180	47.064
TOM	986	OD2	ASP	129	28.079	57.251	49.018
TOM	987	C	ASP	129	25.378	55.844	49.632
TOM	988	O	ASP	129	26.427	55.210	49.784

0015

- 52 -

TOM	989	N	GLY	130	24.361	55.250	48.994
TOM	990	CA	GLY	130	24.316	53.831	48.645
TOM	991	C	GLY	130	23.385	53.204	49.645
TOM	992	O	GLY	130	23.696	53.246	50.814
TOM	993	N	ALA	131	22.177	52.760	49.315
TOM	994	CA	ALA	131	21.280	52.079	50.263
TOM	995	CB	ALA	131	20.073	53.010	50.595
TOM	996	C	ALA	131	20.752	50.672	49.832
TOM	997	O	ALA	131	19.887	50.430	48.991
TOM	998	N	SER	132	21.399	49.691	50.445
TOM	999	CA	SER	132	21.086	48.256	50.378
TOM	1000	CB	SER	132	22.308	47.428	50.886
TOM	1001	OG	SER	132	22.287	46.002	50.963
TOM	1002	C	SER	132	19.875	47.994	51.304
TOM	1003	O	SER	132	19.805	48.544	52.427
TOM	1004	N	ARG	133	18.866	47.199	50.902
TOM	1005	CA	ARG	133	17.767	46.889	51.835
TOM	1006	CB	ARG	133	16.489	46.823	51.049
TOM	1007	CG	ARG	133	16.434	48.088	50.195
TOM	1008	CD	ARG	133	15.108	48.765	50.115
TOM	1009	NE	ARG	133	14.023	47.908	49.674
TOM	1010	CZ	ARG	133	12.791	48.190	50.120
TOM	1011	NH1	ARG	133	11.734	47.428	49.798
TOM	1012	NH2	ARG	133	12.583	49.232	50.952
TOM	1013	C	ARG	133	17.904	45.640	52.712
TOM	1014	O	ARG	133	18.632	44.687	52.434
TOM	1015	N	VAL	134	17.284	45.636	53.869
TOM	1016	CA	VAL	134	17.473	44.543	54.794
TOM	1017	CB	VAL	134	18.233	44.992	56.110
TOM	1018	CG1	VAL	134	18.476	43.876	57.102
TOM	1019	CG2	VAL	134	19.670	45.195	55.843
TOM	1020	C	VAL	134	16.111	44.008	55.166
TOM	1021	O	VAL	134	15.459	44.628	55.994
TOM	1022	N	VAL	135	15.594	42.919	54.578
TOM	1023	CA	VAL	135	14.352	42.328	55.101
TOM	1024	CB	VAL	135	13.477	41.746	53.982
TOM	1025	CG1	VAL	135	12.045	41.997	54.412
TOM	1026	CG2	VAL	135	13.582	42.465	52.674
TOM	1027	C	VAL	135	14.614	41.226	56.174
TOM	1028	O	VAL	135	15.481	40.343	56.159
TOM	1029	N	LEU	136	13.922	41.576	57.250
TOM	1030	CA	LEU	136	14.115	40.999	58.562
TOM	1031	CB	LEU	136	13.231	41.742	59.627
TOM	1032	CG	LEU	136	13.882	42.931	60.395
TOM	1033	CD1	LEU	136	13.227	44.216	59.916
TOM	1034	CD2	LEU	136	13.746	42.771	61.919
TOM	1035	C	LEU	136	13.923	39.528	58.684
TOM	1036	O	LEU	136	12.979	38.905	59.145
TOM	1037	N	SER	137	15.162	39.172	58.530
TOM	1038	CA	SER	137	15.666	37.823	58.513
TOM	1039	CB	SER	137	15.108	36.992	59.759
TOM	1040	OG	SER	137	15.806	35.786	60.173
TOM	1041	C	SER	137	15.417	37.075	57.201
TOM	1042	O	SER	137	14.897	37.604	56.221
TOM	1043	N	LEU	138	15.943	35.861	57.135
TOM	1044	CA	LEU	138	15.738	34.963	55.997
TOM	1045	CB	LEU	138	17.087	34.149	55.733
TOM	1046	CG	LEU	138	18.493	34.217	55.148
TOM	1047	CD1	LEU	138	18.877	32.727	54.932
TOM	1048	CD2	LEU	138	18.638	34.559	53.677
TOM	1049	C	LEU	138	14.567	33.917	56.087
TOM	1050	O	LEU	138	14.558	33.055	55.188
TOM	1051	N	PRO	139	13.629	33.763	57.076
TOM	1052	CD	PRO	139	13.704	34.316	58.388
TOM	1053	CA	PRO	139	13.097	32.474	57.530
TOM	1054	CB	PRO	139	14.293	31.972	58.125

0016

- 53 -

TOM	1055	CG	PRO	139	14.544	33.205	58.96
TOM	1056	C	PRO	139	11.831	32.231	58.405
TOM	1057	O	PRO	139	10.793	32.117	57.759
TOM	1058	N	PHE	140	11.723	32.070	59.779
TOM	1059	CA	PHE	140	10.440	31.775	60.586
TOM	1060	CB	PHE	140	10.785	31.459	62.003
TOM	1061	CG	PHE	140	10.539	30.124	62.700
TOM	1062	CD1	PHE	140	9.903	30.136	63.934
TOM	1063	CD2	PHE	140	11.058	28.928	62.189
TOM	1064	CE1	PHE	140	9.812	28.952	64.641
TOM	1065	CE2	PHE	140	10.960	27.752	62.902
TOM	1066	CZ	PHE	140	10.339	27.775	64.137
TOM	1067	C	PHE	140	9.258	32.798	60.736
TOM	1068	O	PHE	140	8.517	32.926	61.724
TOM	1069	N	ALA	141	9.240	33.509	59.606
TOM	1070	CA	ALA	141	8.778	34.846	59.263
TOM	1071	CB	ALA	141	7.783	35.396	60.287
TOM	1072	C	ALA	141	10.169	35.551	59.412
TOM	1073	O	ALA	141	10.969	35.700	58.486
TOM	1074	N	GLU	142	10.529	35.538	60.715
TOM	1075	CA	GLU	142	11.690	36.089	61.403
TOM	1076	CB	GLU	142	11.082	37.163	62.288
TOM	1077	CG	GLU	142	12.051	38.067	63.025
TOM	1078	CD	GLU	142	12.514	39.205	62.137
TOM	1079	OE1	GLU	142	11.661	40.029	61.775
TOM	1080	OE2	GLU	142	13.708	39.252	61.807
TOM	1081	C	GLU	142	12.557	35.055	62.213
TOM	1082	O	GLU	142	13.719	34.852	61.850
TOM	1083	N	GLY	143	12.052	34.351	63.284
TOM	1084	CA	GLY	143	12.705	33.357	64.228
TOM	1085	C	GLY	143	13.481	32.052	63.766
TOM	1086	O	GLY	143	13.101	30.892	63.971
TOM	1087	N	SER	144	14.580	32.290	63.009
TOM	1088	CA	SER	144	15.637	31.427	62.402
TOM	1089	CB	SER	144	14.964	30.505	61.382
TOM	1090	OG	SER	144	13.530	30.644	61.229
TOM	1091	C	SER	144	16.633	32.492	61.758
TOM	1092	O	SER	144	17.090	32.595	60.623
TOM	1093	N	SER	145	16.974	33.323	62.751
TOM	1094	CA	SER	145	17.703	34.585	62.900
TOM	1095	CB	SER	145	17.767	34.727	64.453
TOM	1096	OG	SER	145	16.606	34.355	65.253
TOM	1097	C	SER	145	19.025	35.088	62.265
TOM	1098	O	SER	145	20.127	35.015	62.825
TOM	1099	N	SER	146	18.947	35.680	61.075
TOM	1100	CA	SER	146	20.046	36.259	60.285
TOM	1101	CB	SER	146	21.028	35.184	59.744
TOM	1102	OG	SER	146	20.833	34.482	58.521
TOM	1103	C	SER	146	19.479	37.048	59.091
TOM	1104	O	SER	146	18.312	36.870	58.831
TOM	1105	N	VAL	147	20.058	37.912	58.241
TOM	1106	CA	VAL	147	19.256	38.745	57.338
TOM	1107	CB	VAL	147	19.264	40.240	57.903
TOM	1108	CG1	VAL	147	18.835	40.247	59.324
TOM	1109	CG2	VAL	147	20.619	40.835	57.996
TOM	1110	C	VAL	147	19.460	38.809	55.810
TOM	1111	O	VAL	147	20.509	38.500	55.216
TOM	1112	N	GLU	148	18.390	39.237	55.133
TOM	1113	CA	GLU	148	18.464	39.312	53.676
TOM	1114	CB	GLU	148	17.044	39.147	53.006
TOM	1115	CG	GLU	148	17.010	38.886	51.469
TOM	1116	CD	GLU	148	17.141	37.457	50.885
TOM	1117	OE1	GLU	148	16.377	37.143	49.975
TOM	1118	OE2	GLU	148	17.998	36.659	51.271
TOM	1119	C	GLU	148	19.058	40.638	53.230
TOM	1120	O	GLU	148	18.669	41.716	53.706

0017

TOM	1121	N	TYR	149	20.025	40.605	52.341
TOM	1122	CA	TYR	149	20.420	41.870	51.742
TOM	1123	CB	TYR	149	21.954	42.051	51.864
TOM	1124	CG	TYR	149	22.474	42.236	53.289
TOM	1125	CD1	TYR	149	22.027	43.239	54.104
TOM	1126	CE1	TYR	149	22.498	43.338	55.396
TOM	1127	CD2	TYR	149	23.373	41.350	53.748
TOM	1128	CE2	TYR	149	23.858	41.435	55.025
TOM	1129	CZ	TYR	149	23.427	42.428	55.867
TOM	1130	OH	TYR	149	23.956	42.512	57.159
TOM	1131	C	TYR	149	20.002	41.958	50.275
TOM	1132	O	TYR	149	20.538	41.229	49.418
TOM	1133	N	ILE	150	19.033	42.811	49.955
TOM	1134	CA	ILE	150	18.669	43.086	48.555
TOM	1135	CB	ILE	150	17.222	43.280	48.453
TOM	1136	CG2	ILE	150	16.908	43.153	46.997
TOM	1137	CG1	ILE	150	16.454	42.291	49.261
TOM	1138	CD	ILE	150	15.093	42.797	49.705
TOM	1139	C	ILE	150	19.344	44.347	47.940
TOM	1140	O	ILE	150	19.139	45.503	48.378
TOM	1141	N	ASN	151	20.115	44.138	46.856
TOM	1142	CA	ASN	151	20.973	45.184	46.264
TOM	1143	CB	ASN	151	22.416	44.835	46.127
TOM	1144	CG	ASN	151	23.074	44.388	47.381
TOM	1145	OD1	ASN	151	22.696	44.790	48.477
TOM	1146	ND2	ASN	151	24.060	43.508	47.266
TOM	1147	C	ASN	151	20.664	45.588	44.849
TOM	1148	O	ASN	151	20.592	44.730	43.980
TOM	1149	N	ASN	152	20.564	46.877	44.553
TOM	1150	CA	ASN	152	20.301	47.293	43.176
TOM	1151	CB	ASN	152	19.784	48.751	43.273
TOM	1152	CG	ASN	152	19.613	49.481	41.948
TOM	1153	OD1	ASN	152	20.178	49.135	40.927
TOM	1154	ND2	ASN	152	18.855	50.522	41.775
TOM	1155	C	ASN	152	21.544	47.118	42.245
TOM	1156	O	ASN	152	22.698	47.496	42.537
TOM	1157	N	TRP	153	21.245	46.582	41.056
TOM	1158	CA	TRP	153	22.234	46.266	40.024
TOM	1159	CB	TRP	153	21.466	45.795	38.800
TOM	1160	CG	TRP	153	20.957	44.376	38.972
TOM	1161	CD2	TRP	153	21.713	43.243	39.139
TOM	1162	CE2	TRP	153	20.731	42.273	39.314
TOM	1163	CE3	TRP	153	23.046	42.915	39.266
TOM	1164	CD1	TRP	153	19.617	44.109	39.036
TOM	1165	NE1	TRP	153	19.504	42.816	39.248
TOM	1166	CZ2	TRP	153	21.066	40.978	39.623
TOM	1167	CZ3	TRP	153	23.363	41.615	39.572
TOM	1168	CH2	TRP	153	22.388	40.661	39.751
TOM	1169	C	TRP	153	23.238	47.356	39.632
TOM	1170	O	TRP	153	24.349	47.070	39.200
TOM	1171	N	GLU	154	22.912	48.637	39.811
TOM	1172	CA	GLU	154	23.867	49.677	39.514
TOM	1173	CB	GLU	154	23.151	51.006	39.357
TOM	1174	CG	GLU	154	23.539	51.694	38.049
TOM	1175	CD	GLU	154	25.030	51.839	37.681
TOM	1176	OE1	GLU	154	25.865	52.128	38.550
TOM	1177	OE2	GLU	154	25.348	51.663	36.495
TOM	1178	C	GLU	154	24.978	49.834	40.563
TOM	1179	O	GLU	154	26.138	49.544	40.261
TOM	1180	N	GLN	155	24.751	50.273	41.817
TOM	1181	CA	GLN	155	25.891	50.433	42.730
TOM	1182	CB	GLN	155	25.626	51.298	44.006
TOM	1183	CG	GLN	155	26.968	51.908	44.547
TOM	1184	CD	GLN	155	27.182	52.136	46.050
TOM	1185	OE1	GLN	155	28.302	52.405	46.469
TOM	1186	NE2	GLN	155	26.257	52.008	46.993

TOM	1187	C	GLN	155	26.329	49.066	43.20
TOM	1188	O	GLN	155	27.331	48.923	43.898
TOM	1189	N	ALA	156	25.590	47.998	42.904
TOM	1190	CA	ALA	156	26.201	46.677	43.015
TOM	1191	CB	ALA	156	25.189	45.613	42.561
TOM	1192	C	ALA	156	27.469	46.659	42.111
TOM	1193	O	ALA	156	28.495	46.180	42.562
TOM	1194	N	LYS	157	27.542	47.276	40.914
TOM	1195	CA	LYS	157	28.761	47.322	40.106
TOM	1196	CB	LYS	157	28.468	48.179	38.889
TOM	1197	CG	LYS	157	27.642	47.520	37.774
TOM	1198	CD	LYS	157	27.362	48.469	36.570
TOM	1199	CE	LYS	157	28.654	49.076	35.931
TOM	1200	NZ	LYS	157	28.416	50.175	35.005
TOM	1201	C	LYS	157	30.037	47.847	40.828
TOM	1202	O	LYS	157	31.207	47.522	40.507
TOM	1203	N	ALA	158	29.737	48.701	41.847
TOM	1204	CA	ALA	158	30.689	49.301	42.811
TOM	1205	CB	ALA	158	29.985	50.354	43.626
TOM	1206	C	ALA	158	31.344	48.320	43.811
TOM	1207	O	ALA	158	32.428	48.587	44.363
TOM	1208	N	LEU	159	30.616	47.186	44.018
TOM	1209	CA	LEU	159	30.983	46.004	44.808
TOM	1210	CB	LEU	159	29.967	44.888	44.720
TOM	1211	CG	LEU	159	28.631	44.905	45.386
TOM	1212	CD1	LEU	159	27.954	43.627	45.061
TOM	1213	CD2	LEU	159	28.762	45.024	46.893
TOM	1214	C	LEU	159	32.292	45.289	44.459
TOM	1215	O	LEU	159	32.455	44.675	43.379
TOM	1216	N	SER	160	33.243	45.304	45.409
TOM	1217	CA	SER	160	34.503	44.592	45.184
TOM	1218	CB	SER	160	35.639	45.258	45.902
TOM	1219	OG	SER	160	35.576	45.000	47.296
TOM	1220	C	SER	160	34.393	43.162	45.676
TOM	1221	O	SER	160	33.731	42.910	46.673
TOM	1222	N	VAL	161	34.948	42.167	44.994
TOM	1223	CA	VAL	161	34.793	40.749	45.389
TOM	1224	CB	VAL	161	33.855	40.007	44.350
TOM	1225	CG1	VAL	161	32.746	39.470	45.186
TOM	1226	CG2	VAL	161	33.230	40.844	43.231
TOM	1227	C	VAL	161	36.048	39.851	45.607
TOM	1228	O	VAL	161	36.851	39.651	44.701
TOM	1229	N	GLU	162	36.314	39.352	46.816
TOM	1230	CA	GLU	162	37.376	38.351	47.020
TOM	1231	CB	GLU	162	38.069	38.392	48.472
TOM	1232	CG	GLU	162	37.256	37.931	49.726
TOM	1233	CD	GLU	162	37.930	37.214	50.926
TOM	1234	OE1	GLU	162	38.164	37.785	51.998
TOM	1235	OE2	GLU	162	38.186	36.021	50.821
TOM	1236	C	GLU	162	36.757	36.957	46.866
TOM	1237	O	GLU	162	35.538	36.826	46.739
TOM	1238	N	LEU	163	37.504	35.858	46.908
TOM	1239	CA	LEU	163	36.892	34.517	46.961
TOM	1240	CB	LEU	163	37.653	33.594	46.123
TOM	1241	CG	LEU	163	37.086	32.293	45.645
TOM	1242	CD1	LEU	163	38.265	31.344	45.947
TOM	1243	CD2	LEU	163	35.679	31.904	46.214
TOM	1244	C	LEU	163	36.933	33.982	48.383
TOM	1245	O	LEU	163	38.058	33.877	48.866
TOM	1246	N	GLU	164	35.842	33.611	49.083
TOM	1247	CA	GLU	164	35.962	33.175	50.475
TOM	1248	CB	GLU	164	34.793	33.702	51.262
TOM	1249	CG	GLU	164	35.377	33.713	52.673
TOM	1250	CD	GLU	164	34.876	34.777	53.643
TOM	1251	OE1	GLU	164	35.391	35.907	53.646
TOM	1252	OE2	GLU	164	33.968	34.454	54.411

- 56 -

TOM	1253	C	GLU	164	36.101	31.666	50.754
TOM	1254	O	GLU	164	36.728	31.238	51.733
TOM	1255	N	ILE	165	35.454	30.810	49.949
TOM	1256	CA	ILE	165	35.695	29.361	49.949
TOM	1257	CB	ILE	165	34.928	28.572	51.017
TOM	1258	CG2	ILE	165	33.449	28.693	50.853
TOM	1259	CG1	ILE	165	35.443	27.139	50.953
TOM	1260	CD	ILE	165	34.631	25.990	51.574
TOM	1261	C	ILE	165	35.244	28.871	48.593
TOM	1262	O	ILE	165	34.318	29.423	48.013
TOM	1263	N	ASN	166	35.956	27.910	48.020
TOM	1264	CA	ASN	166	35.711	27.380	46.693
TOM	1265	CB	ASN	166	36.689	28.035	45.770
TOM	1266	CG	ASN	166	36.667	27.472	44.374
TOM	1267	OD1	ASN	166	37.486	26.664	44.002
TOM	1268	ND2	ASN	166	35.692	27.596	43.535
TOM	1269	C	ASN	166	35.865	25.870	46.613
TOM	1270	O	ASN	166	36.418	25.254	47.530
TOM	1271	N	PHE	167	35.316	25.325	45.514
TOM	1272	CA	PHE	167	35.543	23.972	44.931
TOM	1273	CB	PHE	167	35.566	24.212	43.442
TOM	1274	CG	PHE	167	34.576	23.361	42.679
TOM	1275	CD1	PHE	167	34.429	22.017	42.991
TOM	1276	CD2	PHE	167	33.909	23.959	41.627
TOM	1277	CE1	PHE	167	33.624	21.260	42.233
TOM	1278	CE2	PHE	167	33.095	23.190	40.863
TOM	1279	CZ	PHE	167	32.974	21.857	41.179
TOM	1280	C	PHE	167	36.616	22.876	45.234
TOM	1281	O	PHE	167	36.272	21.690	45.239
TOM	1282	N	GLU	168	37.900	23.189	45.448
TOM	1283	CA	GLU	168	39.000	22.261	45.811
TOM	1284	CB	GLU	168	40.204	23.038	46.352
TOM	1285	CG	GLU	168	40.961	23.873	45.309
TOM	1286	CD	GLU	168	40.127	24.945	44.630
TOM	1287	OE1	GLU	168	39.605	24.666	43.546
TOM	1288	OE2	GLU	168	39.984	26.029	45.202
TOM	1289	C	GLU	168	38.646	21.206	46.848
TOM	1290	O	GLU	168	38.458	20.020	46.569
TOM	1291	N	THR	169	38.510	21.638	48.076
TOM	1292	CA	THR	169	37.818	20.757	48.973
TOM	1293	CB	THR	169	38.389	20.936	50.344
TOM	1294	OG1	THR	169	38.422	22.344	50.576
TOM	1295	CG2	THR	169	39.732	20.220	50.484
TOM	1296	C	THR	169	36.298	21.010	48.968
TOM	1297	O	THR	169	35.680	21.376	49.965
TOM	1298	N	ARG	170	35.636	20.896	47.805
TOM	1299	CA	ARG	170	34.155	20.921	47.709
TOM	1300	CB	ARG	170	33.632	22.224	46.982
TOM	1301	CG	ARG	170	33.682	23.516	47.788
TOM	1302	CD	ARG	170	32.358	24.240	48.004
TOM	1303	NE	ARG	170	32.431	24.907	49.303
TOM	1304	CZ	ARG	170	31.366	25.486	49.886
TOM	1305	NH1	ARG	170	31.472	26.065	51.088
TOM	1306	NH2	ARG	170	30.166	25.501	49.297
TOM	1307	C	ARG	170	33.573	19.677	46.972
TOM	1308	O	ARG	170	32.878	18.787	47.511
TOM	1309	N	GLY	171	33.974	19.665	45.690
TOM	1310	CA	GLY	171	33.663	18.591	44.753
TOM	1311	C	GLY	171	34.626	17.427	44.985
TOM	1312	O	GLY	171	34.247	16.368	45.521
TOM	1313	N	LYS	172	35.925	17.580	44.669
TOM	1314	CA	LYS	172	36.851	16.528	45.072
TOM	1315	CB	LYS	172	37.830	16.192	43.961
TOM	1316	CG	LYS	172	36.984	15.356	43.012
TOM	1317	CD	LYS	172	36.371	14.144	43.745
TOM	1318	CE	LYS	172	35.186	13.608	42.959

0020

TOM	1319	NZ	LYS	172	34.969	12.203	43.200
TOM	1320	C	LYS	172	37.607	16.739	46.357
TOM	1321	O	LYS	172	38.605	17.427	46.533
TOM	1322	N	ARG	173	36.585	16.382	47.164
TOM	1323	CA	ARG	173	36.546	16.064	48.587
TOM	1324	CB	ARG	173	36.145	17.253	49.461
TOM	1325	CG	ARG	173	36.916	17.379	50.797
TOM	1326	CD	ARG	173	36.417	16.334	51.767
TOM	1327	NE	ARG	173	37.270	16.051	52.900
TOM	1328	CZ	ARG	173	36.855	15.244	53.885
TOM	1329	NH1	ARG	173	37.734	14.986	54.837
TOM	1330	NH2	ARG	173	35.608	14.730	53.992
TOM	1331	C	ARG	173	35.426	15.014	48.685
TOM	1332	O	ARG	173	35.115	14.555	49.767
TOM	1333	N	GLY	174	34.729	14.568	47.624
TOM	1334	CA	GLY	174	33.712	13.502	47.771
TOM	1335	C	GLY	174	32.305	13.893	47.333
TOM	1336	O	GLY	174	31.389	13.087	47.364
TOM	1337	N	GLN	175	32.171	15.130	46.822
TOM	1338	CA	GLN	175	30.961	15.853	46.421
TOM	1339	CB	GLN	175	30.037	14.973	45.553
TOM	1340	CG	GLN	175	30.652	14.024	44.478
TOM	1341	CD	GLN	175	31.397	14.534	43.242
TOM	1342	OE1	GLN	175	31.523	15.712	42.907
TOM	1343	NE2	GLN	175	31.893	13.601	42.449
TOM	1344	C	GLN	175	30.148	16.370	47.623
TOM	1345	O	GLN	175	29.112	16.998	47.466
TOM	1346	N	ASP	176	30.588	16.181	48.882
TOM	1347	CA	ASP	176	29.871	16.577	50.114
TOM	1348	CB	ASP	176	29.768	15.327	50.990
TOM	1349	CG	ASP	176	30.954	14.993	51.879
TOM	1350	OD1	ASP	176	31.872	14.290	51.466
TOM	1351	OD2	ASP	176	30.916	15.425	53.017
TOM	1352	C	ASP	176	30.355	17.756	50.983
TOM	1353	O	ASP	176	29.537	18.432	51.602
TOM	1354	N	ALA	177	31.681	17.975	51.120
TOM	1355	CA	ALA	177	32.377	19.153	51.730
TOM	1356	CB	ALA	177	33.545	19.548	50.868
TOM	1357	C	ALA	177	31.759	20.509	52.126
TOM	1358	O	ALA	177	32.190	21.133	53.106
TOM	1359	N	MET	178	30.748	20.980	51.375
TOM	1360	CA	MET	178	29.816	22.058	51.766
TOM	1361	CB	MET	178	28.710	22.113	50.742
TOM	1362	CG	MET	178	27.655	23.194	50.799
TOM	1363	SD	MET	178	26.236	22.731	49.752
TOM	1364	CE	MET	178	25.004	22.764	51.028
TOM	1365	C	MET	178	29.208	21.789	53.144
TOM	1366	O	MET	178	28.993	22.673	53.957
TOM	1367	N	TYR	179	28.956	20.544	53.518
TOM	1368	CA	TYR	179	28.360	20.280	54.798
TOM	1369	CB	TYR	179	27.633	18.964	54.745
TOM	1370	CG	TYR	179	26.279	19.187	54.115
TOM	1371	CD1	TYR	179	25.230	19.771	54.823
TOM	1372	CE1	TYR	179	23.985	19.981	54.250
TOM	1373	CD2	TYR	179	26.097	18.800	52.819
TOM	1374	CE2	TYR	179	24.855	18.985	52.236
TOM	1375	CZ	TYR	179	23.819	19.564	52.949
TOM	1376	OH	TYR	179	22.609	19.656	52.304
TOM	1377	C	TYR	179	29.338	20.317	55.933
TOM	1378	O	TYR	179	29.011	20.775	57.027
TOM	1379	N	GLU	180	30.577	19.935	55.685
TOM	1380	CA	GLU	180	31.640	20.135	56.671
TOM	1381	CB	GLU	180	32.930	19.696	56.134
TOM	1382	CG	GLU	180	33.195	18.320	55.591
TOM	1383	CD	GLU	180	34.655	18.300	55.170
TOM	1384	OE1	GLU	180	35.539	18.715	55.956

TOM	1385	OE2	GLU	180	34.894	17.868	54.26
TOM	1386	C	GLU	180	31.753	21.655	56.879
TOM	1387	O	GLU	180	31.851	22.137	57.990
TOM	1388	N	TYR	181	31.723	22.444	55.803
TOM	1389	CA	TYR	181	31.577	23.904	55.871
TOM	1390	CB	TYR	181	31.278	24.431	54.505
TOM	1391	CG	TYR	181	31.229	25.920	54.413
TOM	1392	CD1	TYR	181	32.462	26.528	54.337
TOM	1393	CE1	TYR	181	32.569	27.876	54.244
TOM	1394	CD2	TYR	181	30.043	26.633	54.414
TOM	1395	CE2	TYR	181	30.139	28.001	54.323
TOM	1396	CZ	TYR	181	31.408	28.585	54.236
TOM	1397	OH	TYR	181	31.581	29.935	54.073
TOM	1398	C	TYR	181	30.442	24.374	56.804
TOM	1399	O	TYR	181	30.679	25.061	57.813
TOM	1400	N	MET	182	29.196	23.934	56.514
TOM	1401	CA	MET	182	28.020	24.387	57.299
TOM	1402	CB	MET	182	26.681	23.768	56.673
TOM	1403	CG	MET	182	26.540	24.060	55.160
TOM	1404	SD	MET	182	25.017	24.041	54.156
TOM	1405	CE	MET	182	24.083	25.419	54.725
TOM	1406	C	MET	182	28.207	24.029	58.766
TOM	1407	O	MET	182	27.893	24.790	59.676
TOM	1408	N	ALA	183	28.931	22.933	58.983
TOM	1409	CA	ALA	183	29.250	22.438	60.312
TOM	1410	CB	ALA	183	29.876	21.042	60.248
TOM	1411	C	ALA	183	30.201	23.304	61.099
TOM	1412	O	ALA	183	30.276	23.210	62.317
TOM	1413	N	GLN	184	30.954	24.165	60.413
TOM	1414	CA	GLN	184	31.887	25.081	61.059
TOM	1415	CB	GLN	184	32.623	25.698	59.898
TOM	1416	CG	GLN	184	33.831	26.550	60.150
TOM	1417	CD	GLN	184	34.479	26.883	58.820
TOM	1418	OE1	GLN	184	35.552	26.412	58.463
TOM	1419	NE2	GLN	184	33.908	27.682	57.944
TOM	1420	C	GLN	184	31.183	26.098	61.997
TOM	1421	O	GLN	184	31.701	26.601	62.996
TOM	1422	N	ALA	185	29.899	26.360	61.752
TOM	1423	CA	ALA	185	29.068	27.233	62.567
TOM	1424	CB	ALA	185	27.769	27.272	61.819
TOM	1425	C	ALA	185	28.854	26.877	64.058
TOM	1426	O	ALA	185	28.515	27.652	64.961
TOM	1427	N	CYS	186	29.090	25.624	64.355
TOM	1428	CA	CYS	186	28.864	25.071	65.665
TOM	1429	CB	CYS	186	27.791	24.022	65.395
TOM	1430	SG	CYS	186	27.273	22.875	66.687
TOM	1431	C	CYS	186	30.225	24.584	66.201
TOM	1432	O	CYS	186	31.150	24.059	65.542
TOM	1433	N	ALA	187	30.423	24.951	67.466
TOM	1434	CA	ALA	187	31.677	24.629	68.145
TOM	1435	CB	ALA	187	31.694	25.304	69.525
TOM	1436	C	ALA	187	31.958	23.136	68.318
TOM	1437	O	ALA	187	31.113	22.370	68.779
TOM	1438	N	GLY	188	33.131	22.779	67.783
TOM	1439	CA	GLY	188	33.722	21.426	67.880
TOM	1440	C	GLY	188	35.271	21.285	67.736
TOM	1441	O	GLY	188	36.030	20.860	68.633
TOM	1442	N	ASN	189	35.722	21.654	66.520
TOM	1443	CA	ASN	189	37.107	21.587	66.002
TOM	1444	CB	ASN	189	38.107	22.302	66.943
TOM	1445	CG	ASN	189	37.693	23.721	67.298
TOM	1446	OD1	ASN	189	36.668	23.963	67.927
TOM	1447	ND2	ASN	189	38.430	24.747	66.931
TOM	1448	C	ASN	189	37.695	20.186	65.714
TOM	1449	O	ASN	189	37.906	19.805	64.562
TOM	1450	N	ALA	190	37.935	19.370	66.747

TOM	1451	CA	ALA	190	38.529	18.030	66.55
TOM	1452	CB	ALA	190	40.002	18.168	66.205
TOM	1453	C	ALA	190	38.451	17.085	67.826
TOM	1454	O	ALA	190	39.293	17.136	68.746
TOM	1455	N	VAL	191	37.374	16.228	67.744
TOM	1456	CA	VAL	191	36.868	15.162	68.677
TOM	1457	CB	VAL	191	37.744	13.803	68.451
TOM	1458	CG1	VAL	191	37.797	12.791	69.600
TOM	1459	CG2	VAL	191	37.056	13.049	67.332
TOM	1460	C	VAL	191	36.802	15.552	70.155
TOM	1461	O	VAL	191	35.738	15.533	70.754
TOM	1462	N	ALA	192	37.947	15.998	70.653
TOM	1463	CA	ALA	192	38.288	16.448	72.001
TOM	1464	CB	ALA	192	39.666	17.109	71.955
TOM	1465	C	ALA	192	37.432	17.351	72.869
TOM	1466	O	ALA	192	37.634	17.298	74.082
TOM	1467	N	ALA	193	36.605	18.256	72.291
TOM	1468	CA	ALA	193	35.621	19.028	73.075
TOM	1469	CB	ALA	193	35.322	20.420	72.479
TOM	1470	C	ALA	193	34.281	18.271	73.133
TOM	1471	O	ALA	193	34.013	17.647	74.161
TOM	1472	N	SER	194	33.505	18.247	72.031
TOM	1473	CA	SER	194	32.166	17.667	71.864
TOM	1474	CB	SER	194	31.706	16.715	72.974
TOM	1475	OG	SER	194	31.548	17.415	74.210
TOM	1476	C	SER	194	30.965	18.612	71.749
TOM	1477	O	SER	194	30.293	18.595	70.720
TOM	1478	N	VAL	195	30.566	19.449	72.714
TOM	1479	CA	VAL	195	29.302	20.216	72.586
TOM	1480	CB	VAL	195	28.914	20.810	74.019
TOM	1481	CG1	VAL	195	27.433	21.224	74.073
TOM	1482	CG2	VAL	195	29.141	19.769	75.113
TOM	1483	C	VAL	195	29.305	21.344	71.516
TOM	1484	O	VAL	195	30.340	21.980	71.325
TOM	1485	N	GLY	196	28.216	21.669	70.795
TOM	1486	CA	GLY	196	28.272	22.777	69.832
TOM	1487	C	GLY	196	27.066	23.697	69.549
TOM	1488	O	GLY	196	25.998	23.306	69.084
TOM	1489	N	SER	197	27.329	24.995	69.790
TOM	1490	CA	SER	197	26.505	26.219	69.518
TOM	1491	CB	SER	197	27.324	27.024	68.482
TOM	1492	OG	SER	197	28.605	27.345	69.022
TOM	1493	C	SER	197	24.990	26.308	69.138
TOM	1494	O	SER	197	24.487	27.120	68.341
TOM	1495	N	SER	198	24.301	25.482	69.946
TOM	1496	CA	SER	198	22.862	25.164	70.035
TOM	1497	CB	SER	198	21.954	26.259	69.436
TOM	1498	OG	SER	198	20.582	25.901	69.486
TOM	1499	C	SER	198	22.456	23.816	69.383
TOM	1500	O	SER	198	22.882	23.368	68.297
TOM	1501	N	LEU	199	21.628	23.211	70.274
TOM	1502	CA	LEU	199	21.110	21.832	70.317
TOM	1503	CB	LEU	199	20.498	21.527	68.955
TOM	1504	CG	LEU	199	19.014	21.957	68.715
TOM	1505	CD1	LEU	199	18.518	23.177	69.556
TOM	1506	CD2	LEU	199	18.938	22.165	67.212
TOM	1507	C	LEU	199	22.244	20.887	70.731
TOM	1508	O	LEU	199	22.328	20.683	71.945
TOM	1509	N	SER	200	23.126	20.294	69.905
TOM	1510	CA	SER	200	24.394	19.602	70.327
TOM	1511	CB	SER	200	24.185	18.289	71.145
TOM	1512	OG	SER	200	25.359	17.832	71.840
TOM	1513	C	SER	200	25.206	19.219	69.067
TOM	1514	O	SER	200	24.546	18.989	68.045
TOM	1515	N	CYS	201	26.557	19.076	69.008
TOM	1516	CA	CYS	201	27.175	19.055	67.667

TOM	1517	CB	CYS	201	28.349	20.051	67.67
TOM	1518	SG	CYS	201	28.260	21.138	66.204
TOM	1519	C	CYS	201	27.631	17.806	66.866
TOM	1520	O	CYS	201	28.106	16.768	67.335
TOM	1521	N	ILE	202	27.435	17.884	65.556
TOM	1522	CA	ILE	202	27.679	16.794	64.637
TOM	1523	CB	ILE	202	26.343	16.152	64.153
TOM	1524	CG2	ILE	202	26.534	15.106	63.103
TOM	1525	CG1	ILE	202	25.736	15.505	65.324
TOM	1526	CD	ILE	202	25.115	14.102	65.148
TOM	1527	C	ILE	202	28.447	17.238	63.424
TOM	1528	O	ILE	202	27.808	17.802	62.544
TOM	1529	N	ASN	203	29.791	17.069	63.340
TOM	1530	CA	ASN	203	30.534	17.370	62.087
TOM	1531	CB	ASN	203	31.912	17.973	62.301
TOM	1532	CG	ASN	203	31.876	19.181	63.186
TOM	1533	OD1	ASN	203	31.827	19.083	64.408
TOM	1534	ND2	ASN	203	31.898	20.367	62.630
TOM	1535	C	ASN	203	30.801	16.137	61.230
TOM	1536	O	ASN	203	30.433	16.140	60.052
TOM	1537	N	LEU	204	31.399	15.102	61.879
TOM	1538	CA	LEU	204	31.854	13.812	61.297
TOM	1539	CB	LEU	204	30.660	12.868	61.052
TOM	1540	CG	LEU	204	30.148	12.082	62.242
TOM	1541	CD1	LEU	204	29.765	12.962	63.408
TOM	1542	CD2	LEU	204	28.896	11.383	61.804
TOM	1543	C	LEU	204	32.711	13.721	60.022
TOM	1544	O	LEU	204	32.406	14.266	58.956
TOM	1545	N	ASP	205	33.817	12.991	60.047
TOM	1546	CA	ASP	205	34.630	12.948	58.840
TOM	1547	CB	ASP	205	36.100	12.451	59.163
TOM	1548	CG	ASP	205	37.164	12.771	58.109
TOM	1549	OD1	ASP	205	38.005	13.635	58.317
TOM	1550	OD2	ASP	205	37.154	12.153	57.052
TOM	1551	C	ASP	205	33.950	12.036	57.827
TOM	1552	O	ASP	205	34.060	10.822	57.977
TOM	1553	N	TRP	206	33.188	12.541	56.840
TOM	1554	CA	TRP	206	32.664	11.664	55.781
TOM	1555	CB	TRP	206	31.726	12.352	54.744
TOM	1556	CG	TRP	206	30.417	12.659	55.441
TOM	1557	CD2	TRP	206	29.404	11.778	55.789
TOM	1558	CE2	TRP	206	28.605	12.597	56.589
TOM	1559	CE3	TRP	206	29.127	10.437	55.732
TOM	1560	CD1	TRP	206	30.230	13.918	55.950
TOM	1561	NE1	TRP	206	29.128	13.840	56.656
TOM	1562	CZ2	TRP	206	27.544	12.125	57.331
TOM	1563	CZ3	TRP	206	28.063	9.965	56.476
TOM	1564	CH2	TRP	206	27.279	10.786	57.265
TOM	1565	C	TRP	206	33.738	10.996	54.953
TOM	1566	O	TRP	206	33.497	9.850	54.581
TOM	1567	N	ASP	207	34.941	11.569	54.701
TOM	1568	CA	ASP	207	35.938	10.789	53.955
TOM	1569	CB	ASP	207	36.972	11.737	53.330
TOM	1570	CG	ASP	207	36.446	12.194	51.962
TOM	1571	OD1	ASP	207	35.544	13.014	51.932
TOM	1572	OD2	ASP	207	36.878	11.715	50.916
TOM	1573	C	ASP	207	36.651	9.633	54.652
TOM	1574	O	ASP	207	37.415	8.893	54.030
TOM	1575	N	VAL	208	36.333	9.432	55.942
TOM	1576	CA	VAL	208	36.656	8.174	56.629
TOM	1577	CB	VAL	208	36.798	8.311	58.136
TOM	1578	CG1	VAL	208	37.255	6.972	58.669
TOM	1579	CG2	VAL	208	37.854	9.269	58.532
TOM	1580	C	VAL	208	35.484	7.197	56.399
TOM	1581	O	VAL	208	35.676	6.145	55.784
TOM	1582	N	ILE	209	34.254	7.517	56.868

- 61 -

TOM	1583	CA	ILE	209	32.992	6.758	56.6.
TOM	1584	CB	ILE	209	31.792	7.657	57.025
TOM	1585	CG2	ILE	209	30.472	6.881	56.963
TOM	1586	CG1	ILE	209	31.940	8.161	58.429
TOM	1587	CD	ILE	209	31.034	9.345	58.700
TOM	1588	C	ILE	209	32.678	6.110	55.353
TOM	1589	O	ILE	209	32.281	4.953	55.242
TOM	1590	N	ARG	210	32.778	6.817	54.261
TOM	1591	CA	ARG	210	32.631	6.179	52.951
TOM	1592	CB	ARG	210	32.770	7.243	51.910
TOM	1593	CG	ARG	210	31.770	8.358	52.155
TOM	1594	CD	ARG	210	32.348	9.581	51.504
TOM	1595	NE	ARG	210	31.332	10.187	50.716
TOM	1596	CZ	ARG	210	30.925	9.669	49.565
TOM	1597	NH1	ARG	210	29.918	10.254	48.902
TOM	1598	NH2	ARG	210	31.556	8.613	49.049
TOM	1599	C	ARG	210	33.645	5.044	52.700
TOM	1600	O	ARG	210	33.310	4.059	52.029
TOM	1601	N	ASP	211	34.872	5.110	53.263
TOM	1602	CA	ASP	211	35.833	4.000	53.150
TOM	1603	CB	ASP	211	37.288	4.401	53.394
TOM	1604	CG	ASP	211	38.028	4.572	52.052
TOM	1605	OD1	ASP	211	38.027	3.649	51.205
TOM	1606	OD2	ASP	211	38.588	5.660	51.849
TOM	1607	C	ASP	211	35.532	2.914	54.144
TOM	1608	O	ASP	211	35.320	1.751	53.780
TOM	1609	N	LYS	212	35.416	3.301	55.409
TOM	1610	CA	LYS	212	35.014	2.373	56.454
TOM	1611	CB	LYS	212	34.737	3.264	57.604
TOM	1612	CG	LYS	212	34.295	2.715	58.938
TOM	1613	CD	LYS	212	34.505	3.887	59.885
TOM	1614	CE	LYS	212	35.989	4.218	60.059
TOM	1615	NZ	LYS	212	36.535	3.885	61.369
TOM	1616	C	LYS	212	33.825	1.478	56.056
TOM	1617	O	LYS	212	33.904	0.248	56.079
TOM	1618	N	THR	213	32.776	2.083	55.495
TOM	1619	CA	THR	213	31.583	1.333	55.128
TOM	1620	CB	THR	213	30.427	2.362	54.684
TOM	1621	OG1	THR	213	29.275	1.578	54.415
TOM	1622	CG2	THR	213	30.681	3.153	53.423
TOM	1623	C	THR	213	31.876	0.279	54.052
TOM	1624	O	THR	213	31.480	-0.883	54.188
TOM	1625	N	LYS	214	32.745	0.618	53.084
TOM	1626	CA	LYS	214	33.124	-0.212	51.914
TOM	1627	CB	LYS	214	34.071	0.603	51.004
TOM	1628	CG	LYS	214	34.146	0.160	49.553
TOM	1629	CD	LYS	214	32.821	0.289	48.760
TOM	1630	CE	LYS	214	32.271	1.702	48.464
TOM	1631	NZ	LYS	214	31.997	2.459	49.680
TOM	1632	C	LYS	214	33.803	-1.528	52.312
TOM	1633	O	LYS	214	33.398	-2.627	51.918
TOM	1634	N	THR	215	34.817	-1.376	53.174
TOM	1635	CA	THR	215	35.525	-2.470	53.830
TOM	1636	CB	THR	215	36.611	-1.825	54.769
TOM	1637	OG1	THR	215	37.792	-2.157	54.060
TOM	1638	CG2	THR	215	36.725	-2.271	56.247
TOM	1639	C	THR	215	34.519	-3.336	54.584
TOM	1640	O	THR	215	34.552	-4.565	54.535
TOM	1641	N	LYS	216	33.546	-2.744	55.273
TOM	1642	CA	LYS	216	32.543	-3.584	55.892
TOM	1643	CB	LYS	216	31.789	-2.826	56.977
TOM	1644	CG	LYS	216	32.684	-2.868	58.190
TOM	1645	CD	LYS	216	32.115	-2.146	59.375
TOM	1646	CE	LYS	216	33.263	-1.479	60.082
TOM	1647	NZ	LYS	216	33.840	-0.433	59.253
TOM	1648	C	LYS	216	31.542	-4.182	54.930

- 62 -

TOM	1649	O	LYS	216	31.119	-5.280	55.25
TOM	1650	N	ILE	217	31.116	-3.627	53.76
TOM	1651	CA	ILE	217	30.218	-4.384	52.905
TOM	1652	CB	ILE	217	29.658	-3.561	51.617
TOM	1653	CG2	ILE	217	28.142	-3.778	51.714
TOM	1654	CG1	ILE	217	29.928	-2.022	51.535
TOM	1655	CD	ILE	217	29.138	-1.105	50.522
TOM	1656	C	ILE	217	31.071	-5.579	52.430
TOM	1657	O	ILE	217	30.745	-6.727	52.761
TOM	1658	N	GLU	218	32.255	-5.318	51.834
TOM	1659	CA	GLU	218	33.243	-6.331	51.379
TOM	1660	CB	GLU	218	34.522	-5.482	51.163
TOM	1661	CG	GLU	218	35.769	-5.957	50.421
TOM	1662	CD	GLU	218	37.199	-5.814	51.047
TOM	1663	OE1	GLU	218	38.123	-6.208	50.311
TOM	1664	OE2	GLU	218	37.414	-5.365	52.205
TOM	1665	C	GLU	218	33.418	-7.563	52.349
TOM	1666	O	GLU	218	33.003	-8.694	52.084
TOM	1667	N	SER	219	33.902	-7.315	53.569
TOM	1668	CA	SER	219	34.098	-8.248	54.685
TOM	1669	CB	SER	219	34.996	-7.522	55.704
TOM	1670	OG	SER	219	36.217	-7.054	55.103
TOM	1671	C	SER	219	32.866	-8.832	55.403
TOM	1672	O	SER	219	32.905	-9.670	56.325
TOM	1673	N	LEU	220	31.733	-8.214	55.085
TOM	1674	CA	LEU	220	30.399	-8.577	55.558
TOM	1675	CB	LEU	220	29.378	-7.436	55.374
TOM	1676	CG	LEU	220	28.608	-6.662	56.431
TOM	1677	CD1	LEU	220	27.222	-7.259	56.599
TOM	1678	CD2	LEU	220	29.467	-6.584	57.666
TOM	1679	C	LEU	220	29.896	-9.743	54.709
TOM	1680	O	LEU	220	29.191	-10.616	55.204
TOM	1681	N	LYS	221	30.193	-9.793	53.405
TOM	1682	CA	LYS	221	29.823	-10.941	52.563
TOM	1683	CB	LYS	221	30.019	-10.533	51.113
TOM	1684	CG	LYS	221	29.148	-9.499	50.407
TOM	1685	CD	LYS	221	29.634	-9.517	48.942
TOM	1686	CE	LYS	221	29.593	-10.939	48.299
TOM	1687	NZ	LYS	221	30.150	-10.995	46.956
TOM	1688	C	LYS	221	30.683	-12.201	52.872
TOM	1689	O	LYS	221	30.975	-13.011	51.996
TOM	1690	N	GLU	222	31.061	-12.466	54.131
TOM	1691	CA	GLU	222	32.125	-13.421	54.410
TOM	1692	CB	GLU	222	33.198	-12.678	55.185
TOM	1693	CG	GLU	222	34.485	-12.684	54.360
TOM	1694	CD	GLU	222	34.463	-11.831	53.090
TOM	1695	OE1	GLU	222	33.842	-12.196	52.090
TOM	1696	OE2	GLU	222	35.120	-10.798	53.085
TOM	1697	C	GLU	222	32.006	-14.801	55.028
TOM	1698	O	GLU	222	31.010	-15.159	55.669
TOM	1699	N	HIS	223	33.119	-15.538	54.718
TOM	1700	CA	HIS	223	33.331	-16.991	54.937
TOM	1701	CB	HIS	223	34.828	-17.354	55.040
TOM	1702	CG	HIS	223	35.696	-16.987	53.838
TOM	1703	CD2	HIS	223	35.274	-16.873	52.532
TOM	1704	ND1	HIS	223	37.011	-16.702	53.860
TOM	1705	CE1	HIS	223	37.420	-16.416	52.646
TOM	1706	NE2	HIS	223	36.363	-16.523	51.863
TOM	1707	C	HIS	223	32.668	-17.757	56.080
TOM	1708	O	HIS	223	33.256	-18.213	57.061
TOM	1709	N	GLY	224	31.363	-17.838	55.829
TOM	1710	CA	GLY	224	30.448	-18.611	56.607
TOM	1711	C	GLY	224	29.114	-17.897	56.689
TOM	1712	O	GLY	224	28.464	-17.628	55.679
TOM	1713	N	PRO	225	28.751	-17.553	57.930
TOM	1714	CD	PRO	225	29.714	-17.535	59.033

0026

- 63 -

TOM	1715	CA	PRO	225	27.456	-17.070	58.406
TOM	1716	CB	PRO	225	27.885	-16.226	59.552
TOM	1717	CG	PRO	225	28.860	-17.159	60.191
TOM	1718	C	PRO	225	26.387	-16.387	57.561
TOM	1719	O	PRO	225	25.177	-16.584	57.713
TOM	1720	N	ILE	226	26.842	-15.521	56.684
TOM	1721	CA	ILE	226	25.954	-14.786	55.802
TOM	1722	CB	ILE	226	26.658	-13.503	55.161
TOM	1723	CG2	ILE	226	25.681	-12.736	54.280
TOM	1724	CG1	ILE	226	27.144	-12.539	56.232
TOM	1725	CD	ILE	226	28.511	-12.940	56.856
TOM	1726	C	ILE	226	25.558	-15.743	54.694
TOM	1727	O	ILE	226	24.385	-16.041	54.464
TOM	1728	N	LYS	227	26.618	-16.288	54.074
TOM	1729	CA	LYS	227	26.554	-17.109	52.855
TOM	1730	CB	LYS	227	27.922	-17.820	52.692
TOM	1731	CG	LYS	227	28.512	-17.988	51.281
TOM	1732	CD	LYS	227	28.595	-19.498	50.912
TOM	1733	CE	LYS	227	29.298	-19.836	49.579
TOM	1734	NZ	LYS	227	28.816	-19.104	48.414
TOM	1735	C	LYS	227	25.380	-18.081	52.992
TOM	1736	O	LYS	227	24.433	-17.999	52.208
TOM	1737	N	ASN	228	25.303	-18.849	54.086
TOM	1738	CA	ASN	228	24.111	-19.648	54.334
TOM	1739	CB	ASN	228	24.450	-20.759	55.380
TOM	1740	CG	ASN	228	24.911	-20.387	56.816
TOM	1741	OD1	ASN	228	26.037	-20.692	57.251
TOM	1742	ND2	ASN	228	24.126	-19.785	57.693
TOM	1743	C	ASN	228	22.870	-18.834	54.780
TOM	1744	O	ASN	228	22.316	-19.117	55.858
TOM	1745	N	LYS	229	22.403	-17.776	54.068
TOM	1746	CA	LYS	229	21.124	-17.131	54.415
TOM	1747	CB	LYS	229	21.290	-16.124	55.558
TOM	1748	CG	LYS	229	20.444	-16.432	56.811
TOM	1749	CD	LYS	229	18.925	-16.454	56.601
TOM	1750	CE	LYS	229	18.298	-17.090	57.840
TOM	1751	NZ	LYS	229	16.943	-17.559	57.588
TOM	1752	C	LYS	229	20.335	-16.398	53.331
TOM	1753	O	LYS	229	19.173	-16.056	53.526
TOM	1754	N	MET	230	20.837	-16.165	52.129
TOM	1755	CA	MET	230	20.075	-15.474	51.055
TOM	1756	CB	MET	230	21.041	-14.764	50.095
TOM	1757	CG	MET	230	22.466	-15.249	50.078
TOM	1758	SD	MET	230	23.176	-14.733	51.654
TOM	1759	CE	MET	230	24.272	-13.526	50.939
TOM	1760	C	MET	230	19.109	-16.315	50.185
TOM	1761	O	MET	230	18.808	-16.050	49.014
TOM	1762	N	SER	231	18.566	-17.375	50.777
TOM	1763	CA	SER	231	17.804	-18.366	50.005
TOM	1764	CB	SER	231	18.400	-19.836	50.173
TOM	1765	OG	SER	231	19.753	-20.138	49.739
TOM	1766	C	SER	231	16.320	-18.417	50.352
TOM	1767	O	SER	231	15.905	-18.315	51.514
TOM	1768	N	GLU	232	15.646	-18.595	49.198
TOM	1769	CA	GLU	232	14.198	-18.667	48.922
TOM	1770	CB	GLU	232	13.475	-19.298	50.140
TOM	1771	CG	GLU	232	13.092	-20.773	49.887
TOM	1772	CD	GLU	232	14.229	-21.777	49.656
TOM	1773	OE1	GLU	232	15.113	-21.571	48.807
TOM	1774	OE2	GLU	232	14.209	-22.800	50.342
TOM	1775	C	GLU	232	13.483	-17.359	48.471
TOM	1776	O	GLU	232	12.797	-16.588	49.151
TOM	1777	N	SER	233	13.820	-17.260	47.166
TOM	1778	CA	SER	233	13.579	-16.233	46.124
TOM	1779	CB	SER	233	13.437	-14.837	46.695
TOM	1780	OG	SER	233	13.235	-13.844	45.695

0027

- 64 -

TOM	1781	C	SER	233	14.837	-16.216	45.2
TOM	1782	O	SER	233	15.834	-16.746	45.734
TOM	1783	N	PRO	234	15.070	-15.739	44.011
TOM	1784	CD	PRO	234	16.308	-16.076	43.285
TOM	1785	CA	PRO	234	14.274	-14.821	43.200
TOM	1786	CB	PRO	234	14.932	-14.921	41.810
TOM	1787	CG	PRO	234	15.886	-16.102	41.812
TOM	1788	C	PRO	234	12.763	-14.816	43.089
TOM	1789	O	PRO	234	12.077	-15.732	43.506
TOM	1790	N	ASN	235	12.244	-13.708	42.552
TOM	1791	CA	ASN	235	10.817	-13.375	42.365
TOM	1792	CB	ASN	235	10.122	-14.487	41.472
TOM	1793	CG	ASN	235	10.310	-14.427	39.928
TOM	1794	OD1	ASN	235	9.384	-14.269	39.125
TOM	1795	ND2	ASN	235	11.493	-14.568	39.358
TOM	1796	C	ASN	235	9.931	-13.108	43.619
TOM	1797	O	ASN	235	8.715	-12.898	43.508
TOM	1798	N	LYS	236	10.396	-12.992	44.858
TOM	1799	CA	LYS	236	9.468	-12.805	45.981
TOM	1800	CB	LYS	236	10.238	-13.151	47.250
TOM	1801	CG	LYS	236	9.286	-13.440	48.428
TOM	1802	CD	LYS	236	8.169	-14.420	48.072
TOM	1803	CE	LYS	236	7.396	-14.627	49.357
TOM	1804	NZ	LYS	236	6.458	-15.739	49.250
TOM	1805	C	LYS	236	8.631	-11.529	46.245
TOM	1806	O	LYS	236	8.782	-10.823	47.244
TOM	1807	N	THR	237	7.633	-11.175	45.447
TOM	1808	CA	THR	237	6.782	-10.000	45.785
TOM	1809	CB	THR	237	5.791	-9.709	44.630
TOM	1810	OG1	THR	237	4.826	-8.698	45.019
TOM	1811	CG2	THR	237	5.177	-11.063	44.198
TOM	1812	C	THR	237	5.948	-10.015	47.091
TOM	1813	O	THR	237	5.482	-8.967	47.550
TOM	1814	N	VAL	238	5.706	-11.145	47.771
TOM	1815	CA	VAL	238	4.842	-11.168	48.951
TOM	1816	CB	VAL	238	4.409	-12.625	49.294
TOM	1817	CG1	VAL	238	3.296	-12.611	50.331
TOM	1818	CG2	VAL	238	3.856	-13.335	48.061
TOM	1819	C	VAL	238	5.547	-10.546	50.152
TOM	1820	O	VAL	238	6.172	-11.220	50.983
TOM	1821	N	SER	239	5.363	-9.215	50.187
TOM	1822	CA	SER	239	5.905	-8.242	51.164
TOM	1823	CB	SER	239	5.035	-6.955	51.237
TOM	1824	OG	SER	239	5.683	-5.730	51.580
TOM	1825	C	SER	239	6.070	-8.754	52.574
TOM	1826	O	SER	239	7.137	-8.562	53.146
TOM	1827	N	GLU	240	5.094	-9.487	53.113
TOM	1828	CA	GLU	240	5.300	-10.158	54.383
TOM	1829	CB	GLU	240	4.093	-10.958	54.857
TOM	1830	CG	GLU	240	3.466	-11.857	53.788
TOM	1831	CD	GLU	240	2.868	-13.188	54.238
TOM	1832	OE1	GLU	240	3.164	-14.193	53.574
TOM	1833	OE2	GLU	240	2.105	-13.211	55.217
TOM	1834	C	GLU	240	6.443	-11.149	54.363
TOM	1835	O	GLU	240	7.412	-10.919	55.083
TOM	1836	N	GLU	241	6.484	-12.186	53.517
TOM	1837	CA	GLU	241	7.537	-13.184	53.704
TOM	1838	CB	GLU	241	7.198	-14.479	53.003
TOM	1839	CG	GLU	241	6.132	-15.241	53.834
TOM	1840	CD	GLU	241	6.312	-15.346	55.368
TOM	1841	OE1	GLU	241	5.351	-15.045	56.089
TOM	1842	OE2	GLU	241	7.386	-15.739	55.847
TOM	1843	C	GLU	241	8.951	-12.834	53.355
TOM	1844	O	GLU	241	9.810	-13.158	54.161
TOM	1845	N	LYS	242	9.266	-12.113	52.278
TOM	1846	CA	LYS	242	10.632	-11.550	52.089

0028

- 65 -

TOM	1847	CB	LYS	242	10.689	-10.683	50.847
TOM	1848	CG	LYS	242	9.734	-9.509	50.842
TOM	1849	CD	LYS	242	10.154	-8.492	49.844
TOM	1850	CE	LYS	242	8.888	-7.776	49.467
TOM	1851	NZ	LYS	242	8.023	-8.675	48.725
TOM	1852	C	LYS	242	11.109	-10.679	53.273
TOM	1853	O	LYS	242	12.220	-10.828	53.800
TOM	1854	N	ALA	243	10.205	-9.807	53.745
TOM	1855	CA	ALA	243	10.436	-8.964	54.872
TOM	1856	CB	ALA	243	9.274	-8.061	55.115
TOM	1857	C	ALA	243	10.606	-9.809	56.086
TOM	1858	O	ALA	243	11.229	-9.348	57.037
TOM	1859	N	LYS	244	10.058	-11.032	56.125
TOM	1860	CA	LYS	244	10.411	-11.968	57.205
TOM	1861	CB	LYS	244	9.445	-13.119	57.236
TOM	1862	CG	LYS	244	8.757	-13.200	58.581
TOM	1863	CD	LYS	244	7.377	-13.829	58.419
TOM	1864	CE	LYS	244	6.270	-12.785	58.548
TOM	1865	NZ	LYS	244	6.300	-11.746	57.529
TOM	1866	C	LYS	244	11.824	-12.508	56.989
TOM	1867	O	LYS	244	12.640	-12.354	57.889
TOM	1868	N	GLN	245	12.201	-13.052	55.818
TOM	1869	CA	GLN	245	13.531	-13.553	55.514
TOM	1870	CB	GLN	245	13.678	-13.694	54.013
TOM	1871	CG	GLN	245	15.050	-14.259	53.589
TOM	1872	CD	GLN	245	15.856	-13.343	52.657
TOM	1873	OE1	GLN	245	15.361	-12.399	52.025
TOM	1874	NE2	GLN	245	17.156	-13.530	52.525
TOM	1875	C	GLN	245	14.609	-12.615	56.061
TOM	1876	O	GLN	245	15.365	-12.995	56.966
TOM	1877	N	TYR	246	14.718	-11.356	55.638
TOM	1878	CA	TYR	246	15.647	-10.480	56.361
TOM	1879	CB	TYR	246	16.279	-9.431	55.386
TOM	1880	CG	TYR	246	15.457	-8.681	54.359
TOM	1881	CD1	TYR	246	15.884	-8.737	53.068
TOM	1882	CE1	TYR	246	15.207	-8.026	52.116
TOM	1883	CD2	TYR	246	14.363	-7.936	54.712
TOM	1884	CE2	TYR	246	13.674	-7.227	53.771
TOM	1885	CZ	TYR	246	14.102	-7.274	52.469
TOM	1886	OH	TYR	246	13.400	-6.591	51.473
TOM	1887	C	TYR	246	15.178	-9.783	57.660
TOM	1888	O	TYR	246	15.888	-8.909	58.131
TOM	1889	N	LEU	247	14.056	-10.036	58.357
TOM	1890	CA	LEU	247	14.108	-9.734	59.784
TOM	1891	CB	LEU	247	12.743	-9.729	60.568
TOM	1892	CG	LEU	247	12.617	-9.840	62.190
TOM	1893	CD1	LEU	247	13.417	-8.839	62.986
TOM	1894	CD2	LEU	247	11.228	-9.445	62.628
TOM	1895	C	LEU	247	14.933	-10.924	60.233
TOM	1896	O	LEU	247	15.469	-10.842	61.320
TOM	1897	N	GLU	248	15.161	-12.064	59.517
TOM	1898	CA	GLU	248	16.170	-13.074	59.948
TOM	1899	CB	GLU	248	15.812	-14.510	59.574
TOM	1900	CG	GLU	248	14.392	-15.109	59.770
TOM	1901	CD	GLU	248	14.289	-16.331	58.846
TOM	1902	OE1	GLU	248	13.970	-16.153	57.665
TOM	1903	OE2	GLU	248	14.598	-17.455	59.270
TOM	1904	C	GLU	248	17.551	-12.808	59.327
TOM	1905	O	GLU	248	18.444	-12.541	60.156
TOM	1906	N	GLU	249	17.860	-12.804	57.995
TOM	1907	CA	GLU	249	19.193	-12.337	57.452
TOM	1908	CB	GLU	249	18.974	-11.913	55.966
TOM	1909	CG	GLU	249	19.777	-10.800	55.266
TOM	1910	CD	GLU	249	21.276	-10.943	55.034
TOM	1911	OE1	GLU	249	21.722	-11.789	54.272
TOM	1912	OE2	GLU	249	22.024	-10.170	55.596

0029

- 66 -

TOM	1913	C	GLU	249	19.994	-11.221	58.2
TOM	1914	O	GLU	249	21.090	-11.437	58.747
TOM	1915	N	PHE	250	19.442	-10.025	58.281
TOM	1916	CA	PHE	250	19.824	-8.992	59.205
TOM	1917	CB	PHE	250	18.586	-8.029	59.396
TOM	1918	CG	PHE	250	18.633	-7.035	60.569
TOM	1919	CD1	PHE	250	19.577	-6.020	60.596
TOM	1920	CD2	PHE	250	17.865	-7.277	61.669
TOM	1921	CE1	PHE	250	19.784	-5.273	61.722
TOM	1922	CE2	PHE	250	18.095	-6.516	62.787
TOM	1923	CZ	PHE	250	19.046	-5.521	62.834
TOM	1924	C	PHE	250	20.340	-9.448	60.571
TOM	1925	O	PHE	250	21.516	-9.200	60.837
TOM	1926	N	HIS	251	19.630	-10.119	61.486
TOM	1927	CA	HIS	251	20.179	-10.366	62.834
TOM	1928	CB	HIS	251	19.069	-10.666	63.884
TOM	1929	CG	HIS	251	19.113	-9.876	65.233
TOM	1930	CD2	HIS	251	17.956	-9.459	65.911
TOM	1931	ND1	HIS	251	20.150	-9.473	66.004
TOM	1932	CE1	HIS	251	19.697	-8.851	67.085
TOM	1933	NE2	HIS	251	18.375	-8.855	67.011
TOM	1934	C	HIS	251	21.168	-11.526	62.869
TOM	1935	O	HIS	251	21.869	-11.685	63.875
TOM	1936	N	GLN	252	21.208	-12.302	61.754
TOM	1937	CA	GLN	252	22.204	-13.351	61.529
TOM	1938	CB	GLN	252	21.957	-14.179	60.268
TOM	1939	CG	GLN	252	20.551	-14.709	59.982
TOM	1940	CD	GLN	252	19.913	-15.766	60.897
TOM	1941	OE1	GLN	252	20.052	-16.957	60.692
TOM	1942	NE2	GLN	252	19.101	-15.543	61.910
TOM	1943	C	GLN	252	23.482	-12.567	61.304
TOM	1944	O	GLN	252	24.202	-12.385	62.290
TOM	1945	N	THR	253	23.719	-11.926	60.132
TOM	1946	CA	THR	253	24.967	-11.135	59.905
TOM	1947	CB	THR	253	25.088	-10.636	58.479
TOM	1948	OG1	THR	253	26.484	-10.365	58.270
TOM	1949	CG2	THR	253	24.219	-9.393	58.230
TOM	1950	C	THR	253	25.279	-9.884	60.760
TOM	1951	O	THR	253	26.396	-9.378	60.739
TOM	1952	N	ALA	254	24.326	-9.245	61.440
TOM	1953	CA	ALA	254	24.602	-8.230	62.481
TOM	1954	CB	ALA	254	23.407	-7.278	62.624
TOM	1955	C	ALA	254	24.891	-8.808	63.883
TOM	1956	O	ALA	254	24.651	-8.201	64.924
TOM	1957	N	LEU	255	25.314	-10.062	63.970
TOM	1958	CA	LEU	255	25.652	-10.739	65.231
TOM	1959	CB	LEU	255	24.452	-11.450	65.896
TOM	1960	CG	LEU	255	23.365	-10.785	66.777
TOM	1961	CD1	LEU	255	22.193	-11.761	66.994
TOM	1962	CD2	LEU	255	23.956	-10.415	68.128
TOM	1963	C	LEU	255	26.629	-11.796	64.776
TOM	1964	O	LEU	255	27.812	-11.716	65.105
TOM	1965	N	GLU	256	26.185	-12.775	63.972
TOM	1966	CA	GLU	256	27.140	-13.616	63.249
TOM	1967	CB	GLU	256	26.548	-14.882	62.649
TOM	1968	CG	GLU	256	27.299	-16.065	63.268
TOM	1969	CD	GLU	256	28.806	-15.965	63.692
TOM	1970	OE1	GLU	256	29.085	-16.240	64.869
TOM	1971	OE2	GLU	256	29.703	-15.632	62.891
TOM	1972	C	GLU	256	27.850	-12.894	62.077
TOM	1973	O	GLU	256	27.911	-13.257	60.903
TOM	1974	N	HIS	257	28.627	-11.991	62.689
TOM	1975	CA	HIS	257	29.559	-10.967	62.216
TOM	1976	CB	HIS	257	29.086	-9.986	61.086
TOM	1977	CG	HIS	257	30.270	-9.241	60.457
TOM	1978	CD2	HIS	257	31.272	-9.891	59.751

0030

- 67 -

TOM	1979	ND1	HIS	257	30.558	-7.941	60.401
TOM	1980	CE1	HIS	257	31.652	-7.794	59.701
TOM	1981	NE2	HIS	257	32.078	-8.980	59.305
TOM	1982	C	HIS	257	29.812	-10.056	63.426
TOM	1983	O	HIS	257	28.967	-9.233	63.758
TOM	1984	N	PRO	258	30.980	-10.083	64.077
TOM	1985	CD	PRO	258	31.843	-11.248	64.174
TOM	1986	CA	PRO	258	31.642	-8.906	64.665
TOM	1987	CB	PRO	258	33.058	-9.360	64.887
TOM	1988	CG	PRO	258	33.184	-10.543	63.967
TOM	1989	C	PRO	258	31.592	-7.625	63.836
TOM	1990	O	PRO	258	30.717	-7.488	62.983
TOM	1991	N	GLU	259	32.459	-6.619	64.018
TOM	1992	CA	GLU	259	32.569	-5.456	63.092
TOM	1993	CB	GLU	259	33.606	-5.878	62.025
TOM	1994	CG	GLU	259	34.072	-4.737	61.157
TOM	1995	CD	GLU	259	35.000	-5.087	60.024
TOM	1996	OE1	GLU	259	34.684	-5.951	59.210
TOM	1997	OE2	GLU	259	36.033	-4.437	59.942
TOM	1998	C	GLU	259	31.287	-4.901	62.431
TOM	1999	O	GLU	259	31.171	-4.765	61.216
TOM	2000	N	LEU	260	30.317	-4.716	63.340
TOM	2001	CA	LEU	260	28.892	-4.452	63.042
TOM	2002	CB	LEU	260	28.282	-5.196	61.880
TOM	2003	CG	LEU	260	27.195	-4.608	61.101
TOM	2004	CD1	LEU	260	27.803	-3.763	59.977
TOM	2005	CD2	LEU	260	26.429	-5.703	60.433
TOM	2006	C	LEU	260	28.065	-5.007	64.194
TOM	2007	O	LEU	260	27.177	-4.351	64.720
TOM	2008	N	SER	261	28.276	-6.268	64.578
TOM	2009	CA	SER	261	27.651	-6.690	65.827
TOM	2010	CB	SER	261	27.906	-8.168	66.232
TOM	2011	OG	SER	261	27.683	-8.554	67.592
TOM	2012	C	SER	261	28.291	-5.826	66.902
TOM	2013	O	SER	261	27.561	-5.254	67.685
TOM	2014	N	GLU	262	29.608	-5.548	66.826
TOM	2015	CA	GLU	262	30.272	-4.812	67.888
TOM	2016	CB	GLU	262	31.651	-4.302	67.413
TOM	2017	CG	GLU	262	32.837	-4.590	68.358
TOM	2018	CD	GLU	262	32.856	-4.035	69.786
TOM	2019	OE1	GLU	262	33.792	-3.316	70.106
TOM	2020	OE2	GLU	262	31.984	-4.340	70.605
TOM	2021	C	GLU	262	29.467	-3.635	68.438
TOM	2022	O	GLU	262	28.635	-3.734	69.353
TOM	2023	N	LEU	263	29.508	-2.581	67.668
TOM	2024	CA	LEU	263	28.880	-1.390	68.144
TOM	2025	CB	LEU	263	29.621	-0.237	67.482
TOM	2026	CG	LEU	263	31.106	-0.014	67.842
TOM	2027	CD1	LEU	263	31.457	-0.716	69.155
TOM	2028	CD2	LEU	263	31.971	-0.606	66.788
TOM	2029	C	LEU	263	27.398	-1.433	67.856
TOM	2030	O	LEU	263	26.570	-1.338	68.755
TOM	2031	N	LYS	264	27.030	-1.698	66.623
TOM	2032	CA	LYS	264	25.648	-1.679	66.276
TOM	2033	CB	LYS	264	25.645	-1.519	64.806
TOM	2034	CG	LYS	264	24.683	-0.442	64.336
TOM	2035	CD	LYS	264	24.023	-1.038	63.080
TOM	2036	CE	LYS	264	23.295	-2.377	63.376
TOM	2037	NZ	LYS	264	22.125	-2.235	64.259
TOM	2038	C	LYS	264	24.828	-2.848	66.778
TOM	2039	O	LYS	264	23.631	-2.712	66.795
TOM	2040	N	THR	265	25.277	-4.014	67.221
TOM	2041	CA	THR	265	24.405	-4.988	67.929
TOM	2042	CB	THR	265	25.102	-6.486	68.207
TOM	2043	OG1	THR	265	24.330	-7.473	67.527
TOM	2044	CG2	THR	265	25.203	-6.945	69.666

0031

- 68 -

TOM	2045	C	THR	265	24.216	-4.241	69.245
TOM	2046	O	THR	265	23.080	-3.918	69.573
TOM	2047	N	VAL	266	25.266	-3.793	69.973
TOM	2048	CA	VAL	266	25.053	-3.254	71.322
TOM	2049	CB	VAL	266	26.408	-2.955	71.977
TOM	2050	CG1	VAL	266	26.295	-2.259	73.367
TOM	2051	CG2	VAL	266	27.081	-4.300	72.170
TOM	2052	C	VAL	266	24.169	-2.019	71.419
TOM	2053	O	VAL	266	23.375	-1.850	72.341
TOM	2054	N	THR	267	24.322	-1.158	70.414
TOM	2055	CA	THR	267	23.547	0.071	70.315
TOM	2056	CB	THR	267	24.401	1.213	69.733
TOM	2057	OG1	THR	267	24.481	0.963	68.358
TOM	2058	CG2	THR	267	25.795	1.320	70.352
TOM	2059	C	THR	267	22.253	-0.020	69.519
TOM	2060	O	THR	267	21.330	0.738	69.800
TOM	2061	N	GLY	268	22.059	-0.966	68.600
TOM	2062	CA	GLY	268	20.767	-1.214	67.940
TOM	2063	C	GLY	268	19.757	-1.671	69.017
TOM	2064	O	GLY	268	18.651	-2.115	68.696
TOM	2065	N	THR	269	19.971	-1.615	70.341
TOM	2066	CA	THR	269	18.846	-1.923	71.239
TOM	2067	CB	THR	269	19.366	-3.137	72.119
TOM	2068	OG1	THR	269	19.953	-4.132	71.233
TOM	2069	CG2	THR	269	18.220	-3.797	72.901
TOM	2070	C	THR	269	18.117	-0.786	72.079
TOM	2071	O	THR	269	18.377	-0.350	73.224
TOM	2072	N	ASN	270	17.135	-0.299	71.270
TOM	2073	CA	ASN	270	16.002	0.618	71.529
TOM	2074	CB	ASN	270	16.391	2.070	71.817
TOM	2075	CG	ASN	270	16.648	2.539	73.281
TOM	2076	OD1	ASN	270	17.690	3.127	73.615
TOM	2077	ND2	ASN	270	15.723	2.493	74.230
TOM	2078	C	ASN	270	15.165	0.626	70.225
TOM	2079	O	ASN	270	15.689	0.680	69.105
TOM	2080	N	PRO	271	13.823	0.547	70.275
TOM	2081	CD	PRO	271	13.007	0.982	71.406
TOM	2082	CA	PRO	271	12.957	-0.118	69.298
TOM	2083	CB	PRO	271	11.706	-0.464	70.082
TOM	2084	CG	PRO	271	11.561	0.763	70.927
TOM	2085	C	PRO	271	12.580	0.504	67.965
TOM	2086	O	PRO	271	11.703	-0.013	67.275
TOM	2087	N	VAL	272	13.172	1.670	67.715
TOM	2088	CA	VAL	272	13.053	2.416	66.468
TOM	2089	CB	VAL	272	13.247	3.977	66.737
TOM	2090	CG1	VAL	272	13.925	4.722	65.574
TOM	2091	CG2	VAL	272	11.884	4.633	66.892
TOM	2092	C	VAL	272	14.144	1.888	65.554
TOM	2093	O	VAL	272	13.967	1.985	64.343
TOM	2094	N	PHE	273	15.255	1.329	66.069
TOM	2095	CA	PHE	273	16.363	0.852	65.225
TOM	2096	CB	PHE	273	17.722	1.279	65.835
TOM	2097	CG	PHE	273	17.785	2.697	66.447
TOM	2098	CD1	PHE	273	18.172	2.835	67.755
TOM	2099	CD2	PHE	273	17.354	3.812	65.723
TOM	2100	CE1	PHE	273	18.108	4.057	68.335
TOM	2101	CE2	PHE	273	17.296	5.042	66.329
TOM	2102	CZ	PHE	273	17.670	5.154	67.638
TOM	2103	C	PHE	273	16.395	-0.669	65.001
TOM	2104	O	PHE	273	17.348	-1.256	64.501
TOM	2105	N	ALA	274	15.333	-1.393	65.316
TOM	2106	CA	ALA	274	15.309	-2.844	65.182
TOM	2107	CB	ALA	274	14.136	-3.376	65.914
TOM	2108	C	ALA	274	15.239	-3.413	63.782
TOM	2109	O	ALA	274	15.147	-2.683	62.806
TOM	2110	N	GLY	275	15.209	-4.733	63.604

0032

- 69 -

TOM	2111	CA	GLY	75	15.197	-5.352	62.28
TOM	2112	C	GLY	275	13.984	-5.004	61.474
TOM	2113	O	GLY	275	14.048	-4.656	60.291
TOM	2114	N	ALA	276	12.853	-5.028	62.178
TOM	2115	CA	ALA	276	11.584	-4.736	61.520
TOM	2116	CB	ALA	276	10.551	-4.716	62.627
TOM	2117	C	ALA	276	11.615	-3.412	60.705
TOM	2118	O	ALA	276	11.174	-3.278	59.562
TOM	2119	N	ASN	277	12.334	-2.466	61.318
TOM	2120	CA	ASN	277	12.632	-1.153	60.784
TOM	2121	CB	ASN	277	13.011	-0.316	61.979
TOM	2122	CG	ASN	277	11.806	-0.163	62.924
TOM	2123	OD1	ASN	277	11.830	-0.489	64.116
TOM	2124	ND2	ASN	277	10.648	0.270	62.450
TOM	2125	C	ASN	277	13.715	-1.213	59.715
TOM	2126	O	ASN	277	13.445	-0.800	58.586
TOM	2127	N	TYR	278	14.931	-1.725	59.923
TOM	2128	CA	TYR	278	15.882	-1.858	58.820
TOM	2129	CB	TYR	278	17.057	-2.498	59.328
TOM	2130	CG	TYR	278	18.034	-1.666	60.095
TOM	2131	CD1	TYR	278	19.030	-1.073	59.356
TOM	2132	CE1	TYR	278	20.047	-0.412	60.010
TOM	2133	CD2	TYR	278	18.040	-1.591	61.489
TOM	2134	CE2	TYR	278	19.070	-0.920	62.142
TOM	2135	CZ	TYR	278	20.062	-0.343	61.380
TOM	2136	OH	TYR	278	21.105	0.334	61.936
TOM	2137	C	TYR	278	15.404	-2.670	57.581
TOM	2138	O	TYR	278	15.795	-2.354	56.437
TOM	2139	N	ALA	279	14.591	-3.753	57.812
TOM	2140	CA	ALA	279	13.907	-4.610	56.800
TOM	2141	CB	ALA	279	13.447	-5.896	57.452
TOM	2142	C	ALA	279	12.689	-3.997	56.072
TOM	2143	O	ALA	279	12.562	-3.992	54.847
TOM	2144	N	ALA	280	11.766	-3.398	56.807
TOM	2145	CA	ALA	280	10.775	-2.504	56.214
TOM	2146	CB	ALA	280	9.994	-1.826	57.309
TOM	2147	C	ALA	280	11.454	-1.429	55.360
TOM	2148	O	ALA	280	11.090	-1.249	54.200
TOM	2149	N	TRP	281	12.509	-0.742	55.858
TOM	2150	CA	TRP	281	13.280	0.227	55.067
TOM	2151	CB	TRP	281	14.424	0.791	55.908
TOM	2152	CG	TRP	281	15.344	1.737	55.150
TOM	2153	CD2	TRP	281	14.987	2.988	54.712
TOM	2154	CE2	TRP	281	16.111	3.372	53.997
TOM	2155	CE3	TRP	281	13.809	3.735	54.704
TOM	2156	CD1	TRP	281	16.612	1.388	54.751
TOM	2157	NE1	TRP	281	17.050	2.399	54.040
TOM	2158	CZ2	TRP	281	16.032	4.534	53.262
TOM	2159	CZ3	TRP	281	13.739	4.884	53.974
TOM	2160	CH2	TRP	281	14.849	5.268	53.264
TOM	2161	C	TRP	281	13.843	-0.395	53.790
TOM	2162	O	TRP	281	13.702	0.149	52.690
TOM	2163	N	ALA	282	14.400	-1.619	53.945
TOM	2164	CA	ALA	282	15.070	-2.421	52.888
TOM	2165	CB	ALA	282	15.544	-3.731	53.463
TOM	2166	C	ALA	282	14.204	-2.744	51.703
TOM	2167	O	ALA	282	14.557	-2.629	50.531
TOM	2168	N	VAL	283	13.010	-3.174	52.086
TOM	2169	CA	VAL	283	11.981	-3.427	51.109
TOM	2170	CB	VAL	283	10.692	-4.054	51.819
TOM	2171	CG1	VAL	283	9.502	-4.193	50.882
TOM	2172	CG2	VAL	283	10.900	-5.505	52.129
TOM	2173	C	VAL	283	11.697	-2.049	50.479
TOM	2174	O	VAL	283	12.052	-1.877	49.303
TOM	2175	N	ASN	284	11.225	-1.052	51.289
TOM	2176	CA	ASN	284	10.829	0.278	50.835

0033

TOM	2177	CB	ASN	284	10.827	1.285	51.96
TOM	2178	CG	ASN	284	9.710	1.166	53.002
TOM	2179	OD1	ASN	284	8.668	0.572	52.788
TOM	2180	ND2	ASN	284	9.780	1.712	54.210
TOM	2181	C	ASN	284	11.715	0.851	49.753
TOM	2182	O	ASN	284	11.177	1.323	48.763
TOM	2183	N	VAL	285	13.060	0.768	49.837
TOM	2184	CA	VAL	285	13.950	1.266	48.754
TOM	2185	CB	VAL	285	15.502	1.133	49.164
TOM	2186	CG1	VAL	285	16.362	1.627	48.037
TOM	2187	CG2	VAL	285	15.895	1.964	50.359
TOM	2188	C	VAL	285	13.679	0.435	47.473
TOM	2189	O	VAL	285	13.258	0.851	46.382
TOM	2190	N	ALA	286	13.827	-0.859	47.689
TOM	2191	CA	ALA	286	13.766	-1.837	46.622
TOM	2192	CB	ALA	286	14.313	-3.066	47.285
TOM	2193	C	ALA	286	12.400	-2.033	45.925
TOM	2194	O	ALA	286	12.274	-2.437	44.756
TOM	2195	N	GLN	287	11.326	-1.629	46.592
TOM	2196	CA	GLN	287	9.978	-1.651	46.008
TOM	2197	CB	GLN	287	9.084	-1.945	47.125
TOM	2198	CG	GLN	287	7.889	-2.549	46.539
TOM	2199	CD	GLN	287	6.927	-2.885	47.633
TOM	2200	OE1	GLN	287	7.247	-3.270	48.775
TOM	2201	NE2	GLN	287	5.683	-2.745	47.220
TOM	2202	C	GLN	287	9.570	-0.328	45.310
TOM	2203	O	GLN	287	8.392	0.051	45.165
TOM	2204	N	VAL	288	10.628	0.403	44.910
TOM	2205	CA	VAL	288	10.559	1.778	44.430
TOM	2206	CB	VAL	288	10.940	2.744	45.604
TOM	2207	CG1	VAL	288	11.096	4.166	45.141
TOM	2208	CG2	VAL	288	9.822	2.728	46.638
TOM	2209	C	VAL	288	11.461	2.017	43.247
TOM	2210	O	VAL	288	10.985	2.425	42.193
TOM	2211	N	ILE	289	12.764	1.766	43.387
TOM	2212	CA	ILE	289	13.689	2.105	42.282
TOM	2213	CB	ILE	289	15.167	2.490	42.903
TOM	2214	CG2	ILE	289	15.079	3.445	44.084
TOM	2215	CG1	ILE	289	15.884	1.265	43.380
TOM	2216	CD	ILE	289	16.961	0.881	42.353
TOM	2217	C	ILE	289	13.866	1.120	41.069
TOM	2218	O	ILE	289	13.776	-0.111	41.198
TOM	2219	N	ASP	290	14.073	1.696	39.866
TOM	2220	CA	ASP	290	14.410	0.993	38.628
TOM	2221	CB	ASP	290	13.277	0.982	37.639
TOM	2222	CG	ASP	290	11.937	0.339	37.993
TOM	2223	OD1	ASP	290	11.933	-0.752	38.579
TOM	2224	OD2	ASP	290	10.902	0.928	37.643
TOM	2225	C	ASP	290	15.605	1.635	37.894
TOM	2226	O	ASP	290	16.439	2.204	38.603
TOM	2227	N	SER	291	15.824	1.616	36.543
TOM	2228	CA	SER	291	16.948	2.316	35.818
TOM	2229	CB	SER	291	16.887	2.094	34.332
TOM	2230	OG	SER	291	15.597	2.542	33.909
TOM	2231	C	SER	291	17.058	3.864	35.960
TOM	2232	O	SER	291	17.981	4.624	35.596
TOM	2233	N	GLU	292	15.993	4.335	36.593
TOM	2234	CA	GLU	292	15.829	5.671	37.143
TOM	2235	CB	GLU	292	14.340	5.909	37.412
TOM	2236	CG	GLU	292	13.373	5.248	36.390
TOM	2237	CD	GLU	292	12.473	4.120	36.909
TOM	2238	OE1	GLU	292	11.969	3.350	36.084
TOM	2239	OE2	GLU	292	12.247	4.008	38.116
TOM	2240	C	GLU	292	16.621	5.623	38.459
TOM	2241	O	GLU	292	16.063	5.770	39.548
TOM	2242	N	THR	293	17.920	5.356	38.233

- 71 -

TOM	2243	CA	THR	293	19.071	5.133	39.14
TOM	2244	CB	THR	293	19.019	3.918	40.100
TOM	2245	OG1	THR	293	18.923	2.735	39.341
TOM	2246	CG2	THR	293	17.859	3.963	41.011
TOM	2247	C	THR	293	20.345	4.834	38.320
TOM	2248	O	THR	293	21.443	5.247	38.661
TOM	2249	N	ALA	294	20.280	4.178	37.159
TOM	2250	CA	ALA	294	21.395	3.787	36.254
TOM	2251	CB	ALA	294	20.906	3.941	34.820
TOM	2252	C	ALA	294	22.838	4.337	36.264
TOM	2253	O	ALA	294	23.810	3.615	36.064
TOM	2254	N	ASP	295	22.941	5.659	36.418
TOM	2255	CA	ASP	295	24.182	6.449	36.635
TOM	2256	CB	ASP	295	24.580	7.310	35.416
TOM	2257	CG	ASP	295	25.439	6.608	34.379
TOM	2258	OD1	ASP	295	26.349	5.873	34.782
TOM	2259	OD2	ASP	295	25.196	6.805	33.182
TOM	2260	C	ASP	295	24.056	7.466	37.792
TOM	2261	O	ASP	295	24.994	8.134	38.264
TOM	2262	N	ASN	296	22.796	7.562	38.240
TOM	2263	CA	ASN	296	22.415	8.686	39.042
TOM	2264	CB	ASN	296	22.060	9.846	38.107
TOM	2265	CG	ASN	296	20.894	9.620	37.182
TOM	2266	OD1	ASN	296	19.924	10.373	37.176
TOM	2267	ND2	ASN	296	20.940	8.607	36.342
TOM	2268	C	ASN	296	21.407	8.747	40.139
TOM	2269	O	ASN	296	20.194	8.593	40.053
TOM	2270	N	LEU	297	22.106	9.401	41.040
TOM	2271	CA	LEU	297	21.541	9.873	42.288
TOM	2272	CB	LEU	297	22.692	10.253	43.289
TOM	2273	CG	LEU	297	24.161	10.458	42.815
TOM	2274	CD1	LEU	297	24.249	11.668	41.870
TOM	2275	CD2	LEU	297	25.076	10.688	44.003
TOM	2276	C	LEU	297	20.599	11.060	42.035
TOM	2277	O	LEU	297	19.884	11.461	42.936
TOM	2278	N	GLU	298	20.489	11.656	40.840
TOM	2279	CA	GLU	298	19.488	12.696	40.534
TOM	2280	CB	GLU	298	19.554	13.052	39.020
TOM	2281	CG	GLU	298	18.565	14.088	38.422
TOM	2282	CD	GLU	298	18.534	14.308	36.897
TOM	2283	OE1	GLU	298	17.530	14.834	36.403
TOM	2284	OE2	GLU	298	19.499	13.971	36.198
TOM	2285	C	GLU	298	18.099	12.158	40.893
TOM	2286	O	GLU	298	17.441	12.598	41.848
TOM	2287	N	LYS	299	17.731	11.111	40.158
TOM	2288	CA	LYS	299	16.533	10.414	40.497
TOM	2289	CB	LYS	299	16.046	9.781	39.189
TOM	2290	CG	LYS	299	14.588	9.261	39.137
TOM	2291	CD	LYS	299	13.417	10.273	39.233
TOM	2292	CE	LYS	299	13.158	10.996	40.588
TOM	2293	NZ	LYS	299	13.349	10.137	41.768
TOM	2294	C	LYS	299	16.760	9.426	41.663
TOM	2295	O	LYS	299	15.852	9.370	42.479
TOM	2296	N	THR	300	17.806	8.624	41.938
TOM	2297	CA	THR	300	17.873	7.923	43.241
TOM	2298	CB	THR	300	19.166	7.170	43.579
TOM	2299	OG1	THR	300	19.670	6.576	42.410
TOM	2300	CG2	THR	300	18.916	6.129	44.661
TOM	2301	C	THR	300	17.752	8.766	44.535
TOM	2302	O	THR	300	16.850	8.543	45.354
TOM	2303	N	THR	301	18.658	9.749	44.770
TOM	2304	CA	THR	301	18.787	10.580	46.000
TOM	2305	CB	THR	301	19.581	11.935	45.723
TOM	2306	OG1	THR	301	20.966	11.552	45.754
TOM	2307	CG2	THR	301	19.260	13.119	46.663
TOM	2308	C	THR	301	17.466	10.950	46.601

- 72 -

TOM	2309	O	THR	301	17.234	10.717	47.719
TOM	2310	N	ALA	302	16.709	11.427	45.592
TOM	2311	CA	ALA	302	15.367	11.966	45.584
TOM	2312	CB	ALA	302	15.318	12.838	44.373
TOM	2313	C	ALA	302	14.164	11.015	45.616
TOM	2314	O	ALA	302	13.172	11.308	46.308
TOM	2315	N	ALA	303	14.164	9.868	44.898
TOM	2316	CA	ALA	303	13.104	8.882	45.127
TOM	2317	CB	ALA	303	13.226	7.754	44.152
TOM	2318	C	ALA	303	13.266	8.339	46.559
TOM	2319	O	ALA	303	12.331	8.345	47.359
TOM	2320	N	LEU	304	14.491	8.007	46.988
TOM	2321	CA	LEU	304	14.825	7.609	48.383
TOM	2322	CB	LEU	304	16.345	7.305	48.432
TOM	2323	CG	LEU	304	17.024	6.378	49.444
TOM	2324	CD1	LEU	304	18.432	6.089	48.964
TOM	2325	CD2	LEU	304	17.199	7.012	50.794
TOM	2326	C	LEU	304	14.435	8.640	49.467
TOM	2327	O	LEU	304	14.028	8.262	50.562
TOM	2328	N	SER	305	14.533	9.961	49.192
TOM	2329	CA	SER	305	14.093	11.079	50.067
TOM	2330	CB	SER	305	14.507	12.441	49.538
TOM	2331	OG	SER	305	14.107	12.780	48.199
TOM	2332	C	SER	305	12.605	11.223	50.346
TOM	2333	O	SER	305	12.184	12.017	51.179
TOM	2334	N	ILE	306	11.688	10.520	49.667
TOM	2335	CA	ILE	306	10.270	10.625	50.065
TOM	2336	CB	ILE	306	9.287	10.811	48.904
TOM	2337	CG2	ILE	306	9.103	12.310	48.778
TOM	2338	CG1	ILE	306	9.721	10.098	47.642
TOM	2339	CD	ILE	306	8.627	10.252	46.551
TOM	2340	C	ILE	306	9.756	9.426	50.830
TOM	2341	O	ILE	306	8.612	9.408	51.307
TOM	2342	N	LEU	307	10.648	8.436	50.977
TOM	2343	CA	LEU	307	10.313	7.222	51.687
TOM	2344	CB	LEU	307	11.397	6.155	51.476
TOM	2345	CG	LEU	307	11.398	5.400	50.166
TOM	2346	CD1	LEU	307	12.729	4.785	49.875
TOM	2347	CD2	LEU	307	10.306	4.366	50.271
TOM	2348	C	LEU	307	10.113	7.395	53.157
TOM	2349	O	LEU	307	10.795	8.155	53.843
TOM	2350	N	PRO	308	9.159	6.628	53.674
TOM	2351	CD	PRO	308	8.348	5.661	52.945
TOM	2352	CA	PRO	308	8.644	6.769	55.006
TOM	2353	CB	PRO	308	7.512	5.750	55.039
TOM	2354	CG	PRO	308	7.017	5.709	53.639
TOM	2355	C	PRO	308	9.397	6.728	56.328
TOM	2356	O	PRO	308	8.941	7.542	57.150
TOM	2357	N	GLY	309	10.412	5.872	56.647
TOM	2358	CA	GLY	309	10.982	5.798	58.016
TOM	2359	C	GLY	309	12.503	5.652	58.222
TOM	2360	O	GLY	309	12.956	4.622	58.689
TOM	2361	N	ILE	310	13.370	6.638	57.955
TOM	2362	CA	ILE	310	14.849	6.611	58.066
TOM	2363	CB	ILE	310	15.531	7.782	57.197
TOM	2364	CG2	ILE	310	16.979	7.389	56.935
TOM	2365	CG1	ILE	310	14.940	7.959	55.769
TOM	2366	CD	ILE	310	15.840	8.577	54.695
TOM	2367	C	ILE	310	15.448	6.694	59.481
TOM	2368	O	ILE	310	16.579	6.243	59.677
TOM	2369	N	GLY	311	14.825	7.277	60.520
TOM	2370	CA	GLY	311	15.382	7.283	61.885
TOM	2371	C	GLY	311	15.836	5.906	62.416
TOM	2372	O	GLY	311	16.678	5.771	63.305
TOM	2373	N	SER	312	15.280	4.823	61.892
TOM	2374	CA	SER	312	15.750	3.461	62.193

- 73 -

TOM	2375	CB	SER	312	14.880	2.450	61.51
TOM	2376	OG	SER	312	13.538	2.737	61.884
TOM	2377	C	SER	312	17.173	3.250	61.706
TOM	2378	O	SER	312	18.045	2.884	62.487
TOM	2379	N	VAL	313	17.405	3.565	60.430
TOM	2380	CA	VAL	313	18.739	3.646	59.793
TOM	2381	CB	VAL	313	18.501	3.809	58.258
TOM	2382	CG1	VAL	313	19.758	4.032	57.426
TOM	2383	CG2	VAL	313	17.895	2.494	57.820
TOM	2384	C	VAL	313	19.663	4.775	60.330
TOM	2385	O	VAL	313	20.721	4.538	60.920
TOM	2386	N	MET	314	19.256	6.058	60.182
TOM	2387	CA	MET	314	20.007	7.252	60.613
TOM	2388	CB	MET	314	19.322	8.542	60.231
TOM	2389	CG	MET	314	19.782	8.925	58.837
TOM	2390	SD	MET	314	19.185	10.510	58.210
TOM	2391	CE	MET	314	20.130	11.291	59.476
TOM	2392	C	MET	314	20.303	7.403	62.065
TOM	2393	O	MET	314	21.104	8.269	62.417
TOM	2394	N	GLY	315	19.644	6.588	62.907
TOM	2395	CA	GLY	315	19.859	6.578	64.351
TOM	2396	C	GLY	315	19.227	7.662	65.216
TOM	2397	O	GLY	315	19.562	7.813	66.409
TOM	2398	N	ILE	316	18.250	8.370	64.648
TOM	2399	CA	ILE	316	17.554	9.451	65.327
TOM	2400	CB	ILE	316	17.377	10.615	64.271
TOM	2401	CG2	ILE	316	16.938	11.885	64.976
TOM	2402	CG1	ILE	316	18.667	10.997	63.580
TOM	2403	CD	ILE	316	18.470	12.097	62.514
TOM	2404	C	ILE	316	16.209	9.032	65.981
TOM	2405	O	ILE	316	15.362	8.313	65.475
TOM	2406	N	ALA	317	15.929	9.482	67.177
TOM	2407	CA	ALA	317	14.670	9.170	67.827
TOM	2408	CB	ALA	317	14.641	7.712	68.275
TOM	2409	C	ALA	317	14.453	10.041	69.074
TOM	2410	O	ALA	317	15.412	10.358	69.804
TOM	2411	N	ASP	318	13.178	10.385	69.331
TOM	2412	CA	ASP	318	12.715	11.143	70.504
TOM	2413	CB	ASP	318	13.040	10.387	71.838
TOM	2414	CG	ASP	318	12.733	8.884	72.058
TOM	2415	OD1	ASP	318	12.861	8.407	73.201
TOM	2416	OD2	ASP	318	12.402	8.172	71.107
TOM	2417	C	ASP	318	13.495	12.467	70.406
TOM	2418	O	ASP	318	13.286	13.129	69.404
TOM	2419	N	GLY	319	14.424	12.950	71.237
TOM	2420	CA	GLY	319	15.137	14.205	70.926
TOM	2421	C	GLY	319	16.223	14.267	69.813
TOM	2422	O	GLY	319	16.169	15.056	68.880
TOM	2423	N	ALA	320	17.247	13.398	69.827
TOM	2424	CA	ALA	320	18.423	13.598	68.991
TOM	2425	CB	ALA	320	19.530	14.178	69.891
TOM	2426	C	ALA	320	19.047	12.515	68.142
TOM	2427	O	ALA	320	18.426	11.499	67.871
TOM	2428	N	VAL	321	20.286	12.734	67.684
TOM	2429	CA	VAL	321	21.054	11.815	66.838
TOM	2430	CB	VAL	321	22.039	12.714	65.875
TOM	2431	CG1	VAL	321	22.739	11.785	64.928
TOM	2432	CG2	VAL	321	21.327	13.711	64.935
TOM	2433	C	VAL	321	21.822	10.794	67.718
TOM	2434	O	VAL	321	22.814	11.055	68.365
TOM	2435	N	HIS	322	21.388	9.560	67.866
TOM	2436	CA	HIS	322	22.097	8.586	68.684
TOM	2437	CB	HIS	322	21.136	7.517	69.054
TOM	2438	CG	HIS	322	19.907	8.043	69.769
TOM	2439	CD2	HIS	322	19.835	8.458	71.098
TOM	2440	ND1	HIS	322	18.709	8.121	69.254

0037

- 74 -

TOM	2441	CE1	HIS	322	17.918	8.555	70.211
TOM	2442	NE2	HIS	322	18.586	8.758	71.325
TOM	2443	C	HIS	322	23.296	7.958	67.951
TOM	2444	O	HIS	322	24.298	7.507	68.497
TOM	2445	N	HIS	323	23.206	7.815	66.624
TOM	2446	CA	HIS	323	24.344	7.298	65.871
TOM	2447	CB	HIS	323	23.891	6.657	64.538
TOM	2448	CG	HIS	323	23.004	5.425	64.616
TOM	2449	CD2	HIS	323	22.499	4.872	65.771
TOM	2450	ND1	HIS	323	22.542	4.725	63.575
TOM	2451	CE1	HIS	323	21.777	3.765	64.014
TOM	2452	NE2	HIS	323	21.762	3.880	65.335
TOM	2453	C	HIS	323	25.317	8.459	65.577
TOM	2454	O	HIS	323	25.467	8.931	64.447
TOM	2455	N	ASN	324	25.934	8.995	66.625
TOM	2456	CA	ASN	324	26.954	9.994	66.431
TOM	2457	CB	ASN	324	26.581	11.318	67.155
TOM	2458	CG	ASN	324	26.083	11.284	68.606
TOM	2459	OD1	ASN	324	25.988	10.261	69.262
TOM	2460	ND2	ASN	324	25.698	12.390	69.209
TOM	2461	C	ASN	324	28.293	9.404	66.921
TOM	2462	O	ASN	324	28.541	9.049	68.073
TOM	2463	N	THR	325	28.967	9.045	65.805
TOM	2464	CA	THR	325	30.298	8.455	65.626
TOM	2465	CB	THR	325	30.661	7.222	66.509
TOM	2466	OG1	THR	325	29.452	6.527	66.854
TOM	2467	CG2	THR	325	31.533	7.660	67.702
TOM	2468	C	THR	325	30.460	7.921	64.197
TOM	2469	O	THR	325	29.596	7.280	63.598
TOM	2470	N	GLU	326	31.594	8.149	63.562
TOM	2471	CA	GLU	326	31.827	7.613	62.216
TOM	2472	CB	GLU	326	33.153	8.150	61.613
TOM	2473	CG	GLU	326	33.482	9.652	61.447
TOM	2474	CD	GLU	326	33.743	10.396	62.762
TOM	2475	OE1	GLU	326	34.010	9.775	63.806
TOM	2476	OE2	GLU	326	33.683	11.627	62.744
TOM	2477	C	GLU	326	31.893	6.072	62.165
TOM	2478	O	GLU	326	31.847	5.458	61.107
TOM	2479	N	GLU	327	32.072	5.351	63.264
TOM	2480	CA	GLU	327	32.001	3.890	63.275
TOM	2481	CB	GLU	327	32.730	3.371	64.525
TOM	2482	CG	GLU	327	33.138	1.925	64.487
TOM	2483	CD	GLU	327	34.037	1.676	63.280
TOM	2484	OE1	GLU	327	33.635	0.926	62.384
TOM	2485	OE2	GLU	327	35.122	2.270	63.207
TOM	2486	C	GLU	327	30.550	3.362	63.254
TOM	2487	O	GLU	327	30.209	2.687	62.277
TOM	2488	N	ILE	328	29.590	3.631	64.180
TOM	2489	CA	ILE	328	28.272	3.008	64.068
TOM	2490	CB	ILE	328	27.611	2.820	65.506
TOM	2491	CG2	ILE	328	28.686	2.796	66.567
TOM	2492	CG1	ILE	328	26.692	3.907	65.930
TOM	2493	CD	ILE	328	25.902	3.289	67.151
TOM	2494	C	ILE	328	27.248	3.651	63.079
TOM	2495	O	ILE	328	26.090	3.212	62.907
TOM	2496	N	VAL	329	27.702	4.726	62.417
TOM	2497	CA	VAL	329	27.036	5.268	61.272
TOM	2498	CB	VAL	329	27.479	6.747	61.003
TOM	2499	CG1	VAL	329	27.564	7.239	59.516
TOM	2500	CG2	VAL	329	26.351	7.546	61.639
TOM	2501	C	VAL	329	27.451	4.389	60.105
TOM	2502	O	VAL	329	26.602	3.812	59.422
TOM	2503	N	ALA	330	28.765	4.263	59.859
TOM	2504	CA	ALA	330	29.332	3.450	58.763
TOM	2505	CB	ALA	330	30.834	3.313	58.897
TOM	2506	C	ALA	330	28.771	2.025	58.733

0038

- 75 -

TOM	2507	O	ALA	330	28.317	1.513	57.704
TOM	2508	N	GLN	331	28.696	1.423	59.935
TOM	2509	CA	GLN	331	28.092	0.118	60.059
TOM	2510	CB	GLN	331	28.217	-0.401	61.423
TOM	2511	CG	GLN	331	29.662	-0.473	61.705
TOM	2512	CD	GLN	331	29.795	-0.771	63.163
TOM	2513	OE1	GLN	331	28.826	-0.715	63.910
TOM	2514	NE2	GLN	331	30.924	-1.096	63.754
TOM	2515	C	GLN	331	26.632	0.106	59.708
TOM	2516	O	GLN	331	26.228	-0.760	58.925
TOM	2517	N	SER	332	25.785	1.008	60.197
TOM	2518	CA	SER	332	24.397	0.987	59.739
TOM	2519	CB	SER	332	23.471	2.091	60.228
TOM	2520	OG	SER	332	22.082	1.811	60.013
TOM	2521	C	SER	332	24.395	1.163	58.260
TOM	2522	O	SER	332	23.667	0.414	57.612
TOM	2523	N	ILE	333	25.273	1.971	57.661
TOM	2524	CA	ILE	333	25.211	1.985	56.199
TOM	2525	CB	ILE	333	25.568	3.378	55.676
TOM	2526	CG2	ILE	333	24.831	3.461	54.335
TOM	2527	CG1	ILE	333	25.152	4.530	56.592
TOM	2528	CD	ILE	333	25.792	5.829	56.066
TOM	2529	C	ILE	333	26.058	0.930	55.450
TOM	2530	O	ILE	333	26.297	0.977	54.245
TOM	2531	N	ALA	334	26.596	-0.053	56.152
TOM	2532	CA	ALA	334	27.201	-1.242	55.532
TOM	2533	CB	ALA	334	28.344	-1.735	56.421
TOM	2534	C	ALA	334	26.047	-2.236	55.506
TOM	2535	O	ALA	334	25.504	-2.615	54.464
TOM	2536	N	LEU	335	25.533	-2.509	56.702
TOM	2537	CA	LEU	335	24.338	-3.340	56.914
TOM	2538	CB	LEU	335	24.005	-3.374	58.411
TOM	2539	CG	LEU	335	22.866	-4.252	58.895
TOM	2540	CD1	LEU	335	23.288	-5.662	58.591
TOM	2541	CD2	LEU	335	22.584	-4.108	60.374
TOM	2542	C	LEU	335	23.046	-2.912	56.162
TOM	2543	O	LEU	335	22.159	-3.697	55.802
TOM	2544	N	SER	336	22.837	-1.628	55.936
TOM	2545	CA	SER	336	21.675	-1.205	55.178
TOM	2546	CB	SER	336	21.500	0.285	55.287
TOM	2547	OG	SER	336	21.097	0.588	56.617
TOM	2548	C	SER	336	21.904	-1.586	53.734
TOM	2549	O	SER	336	21.099	-2.285	53.136
TOM	2550	N	SER	337	23.067	-1.265	53.194
TOM	2551	CA	SER	337	23.408	-1.603	51.824
TOM	2552	CB	SER	337	24.816	-1.155	51.427
TOM	2553	OG	SER	337	25.142	-1.321	50.040
TOM	2554	C	SER	337	23.358	-3.088	51.551
TOM	2555	O	SER	337	22.699	-3.468	50.577
TOM	2556	N	LEU	338	23.939	-3.985	52.392
TOM	2557	CA	LEU	338	23.792	-5.410	52.057
TOM	2558	CB	LEU	338	24.660	-6.259	52.984
TOM	2559	CG	LEU	338	25.261	-7.593	52.447
TOM	2560	CD1	LEU	338	24.979	-7.808	50.952
TOM	2561	CD2	LEU	338	26.782	-7.536	52.602
TOM	2562	C	LEU	338	22.339	-5.910	52.094
TOM	2563	O	LEU	338	21.927	-6.665	51.209
TOM	2564	N	MET	339	21.497	-5.416	53.009
TOM	2565	CA	MET	339	20.050	-5.699	53.059
TOM	2566	CB	MET	339	19.440	-4.988	54.265
TOM	2567	CG	MET	339	19.922	-5.684	55.522
TOM	2568	SD	MET	339	18.724	-5.653	56.853
TOM	2569	CE	MET	339	17.347	-6.178	55.910
TOM	2570	C	MET	339	19.241	-5.331	51.820
TOM	2571	O	MET	339	18.486	-6.167	51.336
TOM	2572	N	VAL	340	19.325	-4.130	51.255

- 76 -

TOM	2573	CA	VAL	340	18.736	-3.873	49.931
TOM	2574	CB	VAL	340	18.716	-2.244	49.553
TOM	2575	CG1	VAL	340	19.748	-1.465	50.336
TOM	2576	CG2	VAL	340	19.075	-1.939	48.096
TOM	2577	C	VAL	340	19.446	-4.709	48.851
TOM	2578	O	VAL	340	18.750	-5.128	47.923
TOM	2579	N	ALA	341	20.747	-5.044	48.846
TOM	2580	CA	ALA	341	21.303	-6.034	47.873
TOM	2581	CB	ALA	341	22.786	-6.345	48.164
TOM	2582	C	ALA	341	20.569	-7.410	47.862
TOM	2583	O	ALA	341	20.377	-8.095	46.842
TOM	2584	N	GLN	342	20.122	-7.833	49.055
TOM	2585	CA	GLN	342	19.290	-9.013	49.164
TOM	2586	CB	GLN	342	19.101	-9.373	50.602
TOM	2587	CG	GLN	342	18.746	-10.850	50.669
TOM	2588	CD	GLN	342	19.897	-11.734	51.140
TOM	2589	OE1	GLN	342	19.684	-12.562	52.031
TOM	2590	NE2	GLN	342	21.140	-11.675	50.644
TOM	2591	C	GLN	342	17.925	-8.774	48.534
TOM	2592	O	GLN	342	17.489	-9.506	47.653
TOM	2593	N	ALA	343	17.221	-7.722	48.932
TOM	2594	CA	ALA	343	15.942	-7.354	48.350
TOM	2595	CB	ALA	343	15.431	-6.167	49.112
TOM	2596	C	ALA	343	15.821	-7.037	46.839
TOM	2597	O	ALA	343	14.780	-7.328	46.205
TOM	2598	N	ILE	344	16.825	-6.465	46.161
TOM	2599	CA	ILE	344	16.688	-6.200	44.720
TOM	2600	CB	ILE	344	18.000	-5.564	44.239
TOM	2601	CG2	ILE	344	18.201	-5.662	42.716
TOM	2602	CG1	ILE	344	17.960	-4.139	44.747
TOM	2603	CD	ILE	344	19.222	-3.275	44.485
TOM	2604	C	ILE	344	16.305	-7.425	43.875
TOM	2605	O	ILE	344	15.440	-7.220	43.033
TOM	2606	N	PRO	345	16.756	-8.701	44.059
TOM	2607	CD	PRO	345	18.113	-9.076	44.486
TOM	2608	CA	PRO	345	16.067	-9.907	43.569
TOM	2609	CB	PRO	345	17.131	-10.962	43.683
TOM	2610	CG	PRO	345	17.955	-10.529	44.846
TOM	2611	C	PRO	345	14.732	-10.345	44.201
TOM	2612	O	PRO	345	14.019	-11.253	43.744
TOM	2613	N	LEU	346	14.379	-9.737	45.311
TOM	2614	CA	LEU	346	13.177	-10.129	46.009
TOM	2615	CB	LEU	346	13.301	-10.135	47.516
TOM	2616	CG	LEU	346	13.774	-11.262	48.358
TOM	2617	CD1	LEU	346	15.194	-11.686	48.003
TOM	2618	CD2	LEU	346	13.732	-10.771	49.769
TOM	2619	C	LEU	346	11.966	-9.300	45.804
TOM	2620	O	LEU	346	10.899	-9.880	45.894
TOM	2621	N	VAL	347	12.139	-7.986	45.590
TOM	2622	CA	VAL	347	11.030	-6.986	45.581
TOM	2623	CB	VAL	347	11.369	-5.777	46.461
TOM	2624	CG1	VAL	347	11.647	-6.011	47.927
TOM	2625	CG2	VAL	347	12.661	-5.335	45.878
TOM	2626	C	VAL	347	10.511	-6.365	44.268
TOM	2627	O	VAL	347	9.306	-6.131	44.128
TOM	2628	N	GLY	348	11.388	-6.085	43.292
TOM	2629	CA	GLY	348	11.009	-5.372	42.086
TOM	2630	C	GLY	348	11.884	-5.742	40.886
TOM	2631	O	GLY	348	12.690	-6.685	40.912
TOM	2632	N	GLU	349	11.733	-4.993	39.789
TOM	2633	CA	GLU	349	12.456	-5.296	38.564
TOM	2634	CB	GLU	349	11.395	-5.222	37.406
TOM	2635	CG	GLU	349	10.934	-3.907	36.708
TOM	2636	CD	GLU	349	10.001	-2.908	37.406
TOM	2637	OE1	GLU	349	9.389	-3.253	38.422
TOM	2638	OE2	GLU	349	9.868	-1.781	36.908

0040

- 77 -

TOM	2639	C	GLU	349	13.717	-4.439	38.30
TOM	2640	O	GLU	349	13.824	-3.581	37.411
TOM	2641	N	LEU	350	14.718	-4.626	39.170
TOM	2642	CA	LEU	350	15.989	-3.957	38.924
TOM	2643	CB	LEU	350	16.598	-3.332	40.165
TOM	2644	CG	LEU	350	17.856	-2.533	39.832
TOM	2645	CD1	LEU	350	17.490	-1.308	39.029
TOM	2646	CD2	LEU	350	18.565	-2.115	41.091
TOM	2647	C	LEU	350	17.009	-4.939	38.391
TOM	2648	O	LEU	350	17.055	-6.100	38.796
TOM	2649	N	VAL	351	17.801	-4.503	37.413
TOM	2650	CA	VAL	351	18.939	-5.308	36.889
TOM	2651	CB	VAL	351	19.503	-4.621	35.568
TOM	2652	CG1	VAL	351	20.176	-5.629	34.648
TOM	2653	CG2	VAL	351	18.364	-3.995	34.803
TOM	2654	C	VAL	351	20.094	-5.478	37.953
TOM	2655	O	VAL	351	19.916	-5.247	39.173
TOM	2656	N	ASP	352	21.313	-5.911	37.564
TOM	2657	CA	ASP	352	22.430	-5.989	38.510
TOM	2658	CB	ASP	352	23.802	-6.051	37.759
TOM	2659	CG	ASP	352	25.033	-6.428	38.621
TOM	2660	OD1	ASP	352	25.671	-5.551	39.236
TOM	2661	OD2	ASP	352	25.358	-7.619	38.659
TOM	2662	C	ASP	352	22.486	-4.832	39.530
TOM	2663	O	ASP	352	22.227	-3.640	39.275
TOM	2664	N	ILE	353	22.589	-5.409	40.740
TOM	2665	CA	ILE	353	22.804	-4.713	42.005
TOM	2666	CB	ILE	353	22.839	-5.633	43.220
TOM	2667	CG2	ILE	353	22.542	-4.704	44.367
TOM	2668	CG1	ILE	353	21.882	-6.808	43.180
TOM	2669	CD	ILE	353	22.563	-8.107	42.741
TOM	2670	C	ILE	353	24.147	-4.009	42.021
TOM	2671	O	ILE	353	25.183	-4.540	42.398
TOM	2672	N	GLY	354	24.085	-2.848	41.387
TOM	2673	CA	GLY	354	25.144	-1.837	41.431
TOM	2674	C	GLY	354	24.732	-0.710	42.394
TOM	2675	O	GLY	354	25.298	0.378	42.557
TOM	2676	N	PHE	355	23.627	-1.021	43.059
TOM	2677	CA	PHE	355	22.976	-0.124	43.968
TOM	2678	CB	PHE	355	21.525	-0.458	43.940
TOM	2679	CG	PHE	355	20.680	0.763	44.132
TOM	2680	CD1	PHE	355	20.861	1.851	43.318
TOM	2681	CD2	PHE	355	19.729	0.747	45.119
TOM	2682	CE1	PHE	355	20.057	2.935	43.511
TOM	2683	CE2	PHE	355	18.932	1.842	45.296
TOM	2684	CZ	PHE	355	19.099	2.926	44.491
TOM	2685	C	PHE	355	23.576	-0.316	45.328
TOM	2686	O	PHE	355	24.491	0.413	45.696
TOM	2687	N	ALA	356	23.144	-1.305	46.079
TOM	2688	CA	ALA	356	23.708	-1.568	47.402
TOM	2689	CB	ALA	356	22.811	-2.570	48.032
TOM	2690	C	ALA	356	25.172	-2.073	47.350
TOM	2691	O	ALA	356	25.561	-3.251	47.405
TOM	2692	N	ALA	357	25.949	-1.002	47.188
TOM	2693	CA	ALA	357	27.373	-1.009	46.901
TOM	2694	CB	ALA	357	27.770	-1.931	45.694
TOM	2695	C	ALA	357	27.695	0.425	46.493
TOM	2696	O	ALA	357	28.515	1.086	47.116
TOM	2697	N	TYR	358	27.014	1.016	45.522
TOM	2698	CA	TYR	358	27.451	2.315	45.037
TOM	2699	CB	TYR	358	27.949	2.084	43.584
TOM	2700	CG	TYR	358	28.684	0.777	43.170
TOM	2701	CD1	TYR	358	28.130	-0.005	42.170
TOM	2702	CE1	TYR	358	28.773	-1.099	41.666
TOM	2703	CD2	TYR	358	29.916	0.424	43.683
TOM	2704	CE2	TYR	358	30.575	-0.669	43.190

0041

- 78 -

TOM	2705	CZ	TYR	358	30.010	-1.424	42.1
TOM	2706	OH	TYR	358	30.729	-2.482	41.613
TOM	2707	C	TYR	358	26.473	3.509	45.101
TOM	2708	O	TYR	358	26.300	4.162	46.134
TOM	2709	N	ASN	359	25.703	3.826	44.054
TOM	2710	CA	ASN	359	24.789	4.971	43.979
TOM	2711	CB	ASN	359	24.534	5.194	42.489
TOM	2712	CG	ASN	359	25.785	5.553	41.653
TOM	2713	OD1	ASN	359	26.332	6.667	41.669
TOM	2714	ND2	ASN	359	26.326	4.644	40.848
TOM	2715	C	ASN	359	23.474	4.909	44.770
TOM	2716	O	ASN	359	22.342	5.207	44.375
TOM	2717	N	PHE	360	23.670	4.340	45.932
TOM	2718	CA	PHE	360	22.700	4.208	47.008
TOM	2719	CB	PHE	360	22.204	2.758	47.074
TOM	2720	CG	PHE	360	21.672	2.409	48.428
TOM	2721	CD1	PHE	360	20.445	2.867	48.785
TOM	2722	CD2	PHE	360	22.495	1.717	49.319
TOM	2723	CE1	PHE	360	20.054	2.629	50.089
TOM	2724	CE2	PHE	360	22.103	1.486	50.625
TOM	2725	CZ	PHE	360	20.862	1.954	51.010
TOM	2726	C	PHE	360	23.442	4.610	48.299
TOM	2727	O	PHE	360	22.887	5.329	49.126
TOM	2728	N	VAL	361	24.689	4.127	48.490
TOM	2729	CA	VAL	361	25.532	4.523	49.609
TOM	2730	CB	VAL	361	26.843	3.693	49.698
TOM	2731	CG1	VAL	361	27.837	4.401	50.645
TOM	2732	CG2	VAL	361	26.543	2.283	50.272
TOM	2733	C	VAL	361	25.886	5.981	49.404
TOM	2734	O	VAL	361	25.964	6.741	50.363
TOM	2735	N	GLU	362	26.089	6.373	48.148
TOM	2736	CA	GLU	362	26.202	7.798	47.832
TOM	2737	CB	GLU	362	26.588	7.956	46.359
TOM	2738	CG	GLU	362	27.938	7.373	45.911
TOM	2739	CD	GLU	362	29.138	7.987	46.607
TOM	2740	OE1	GLU	362	29.471	9.146	46.318
TOM	2741	OE2	GLU	362	29.730	7.287	47.429
TOM	2742	C	GLU	362	24.912	8.621	48.113
TOM	2743	O	GLU	362	24.991	9.772	48.544
TOM	2744	N	SER	363	23.696	8.117	47.837
TOM	2745	CA	SER	363	22.491	8.841	48.254
TOM	2746	CB	SER	363	21.178	8.320	47.602
TOM	2747	OG	SER	363	21.260	8.508	46.181
TOM	2748	C	SER	363	22.397	8.671	49.755
TOM	2749	O	SER	363	23.123	9.454	50.328
TOM	2750	N	ILE	364	21.735	7.776	50.506
TOM	2751	CA	ILE	364	21.702	7.752	51.991
TOM	2752	CB	ILE	364	21.654	6.195	52.283
TOM	2753	CG2	ILE	364	22.736	5.792	53.251
TOM	2754	CG1	ILE	364	20.263	5.762	52.781
TOM	2755	CD	ILE	364	19.807	6.156	54.201
TOM	2756	C	ILE	364	22.770	8.570	52.778
TOM	2757	O	ILE	364	22.438	9.261	53.725
TOM	2758	N	ILE	365	24.050	8.640	52.412
TOM	2759	CA	ILE	365	25.016	9.531	53.050
TOM	2760	CB	ILE	365	26.450	9.277	52.523
TOM	2761	CG2	ILE	365	27.376	10.439	52.934
TOM	2762	CG1	ILE	365	26.960	7.952	53.067
TOM	2763	CD	ILE	365	28.343	7.666	52.515
TOM	2764	C	ILE	365	24.637	10.986	52.787
TOM	2765	O	ILE	365	24.657	11.790	53.724
TOM	2766	N	ASN	366	24.331	11.368	51.538
TOM	2767	CA	ASN	366	23.712	12.667	51.228
TOM	2768	CB	ASN	366	22.987	12.653	49.875
TOM	2769	CG	ASN	366	22.167	13.901	49.706
TOM	2770	OD1	ASN	366	20.967	13.970	49.943

0042

- 79 -

TOM	2771	ND2	ASN	366	22.755	15.012	49. .6
TOM	2772	C	ASN	366	22.664	13.054	52.264
TOM	2773	O	ASN	366	22.776	14.117	52.880
TOM	2774	N	LEU	367	21.730	12.097	52.470
TOM	2775	CA	LEU	367	20.601	12.276	53.388
TOM	2776	CB	LEU	367	19.449	11.331	53.083
TOM	2777	CG	LEU	367	19.028	10.923	51.694
TOM	2778	CD1	LEU	367	17.840	10.027	51.962
TOM	2779	CD2	LEU	367	18.673	12.061	50.758
TOM	2780	C	LEU	367	20.893	12.078	54.859
TOM	2781	O	LEU	367	20.002	12.082	55.718
TOM	2782	N	PHE	368	22.155	11.688	55.064
TOM	2783	CA	PHE	368	22.699	11.653	56.398
TOM	2784	CB	PHE	368	23.894	10.611	56.441
TOM	2785	CG	PHE	368	23.512	9.206	56.972
TOM	2786	CD1	PHE	368	22.870	8.255	56.181
TOM	2787	CD2	PHE	368	23.707	8.901	58.314
TOM	2788	CE1	PHE	368	22.418	7.054	56.705
TOM	2789	CE2	PHE	368	23.245	7.681	58.837
TOM	2790	CZ	PHE	368	22.587	6.749	58.040
TOM	2791	C	PHE	368	23.127	13.115	56.685
TOM	2792	O	PHE	368	22.926	13.657	57.778
TOM	2793	N	GLN	369	23.647	13.871	55.716
TOM	2794	CA	GLN	369	24.092	15.257	55.927
TOM	2795	CB	GLN	369	24.955	15.742	54.745
TOM	2796	CG	GLN	369	26.268	15.027	54.738
TOM	2797	CD	GLN	369	26.949	15.171	53.412
TOM	2798	OE1	GLN	369	27.487	16.212	53.092
TOM	2799	NE2	GLN	369	27.035	14.180	52.561
TOM	2800	C	GLN	369	22.901	16.194	56.081
TOM	2801	O	GLN	369	22.670	16.759	57.154
TOM	2802	N	VAL	370	22.061	16.265	55.051
TOM	2803	CA	VAL	370	20.869	17.098	55.029
TOM	2804	CB	VAL	370	19.983	16.477	53.958
TOM	2805	CG1	VAL	370	18.522	16.810	54.040
TOM	2806	CG2	VAL	370	20.464	17.118	52.681
TOM	2807	C	VAL	370	20.183	17.285	56.362
TOM	2808	O	VAL	370	19.933	18.406	56.800
TOM	2809	N	VAL	371	20.087	16.188	57.113
TOM	2810	CA	VAL	371	19.483	16.243	58.455
TOM	2811	CB	VAL	371	18.294	15.131	58.517
TOM	2812	CG1	VAL	371	18.443	14.129	57.409
TOM	2813	CG2	VAL	371	18.232	14.444	59.885
TOM	2814	C	VAL	371	20.475	16.178	59.623
TOM	2815	O	VAL	371	20.173	16.588	60.748
TOM	2816	N	HIS	372	21.706	15.728	59.480
TOM	2817	CA	HIS	372	22.647	16.042	60.561
TOM	2818	CB	HIS	372	24.067	15.416	60.273
TOM	2819	CG	HIS	372	24.376	13.923	60.563
TOM	2820	CD2	HIS	372	23.517	12.977	61.091
TOM	2821	ND1	HIS	372	25.563	13.320	60.445
TOM	2822	CE1	HIS	372	25.457	12.085	60.884
TOM	2823	NE2	HIS	372	24.225	11.897	61.266
TOM	2824	C	HIS	372	22.744	11.620	60.635
TOM	2825	O	HIS	372	22.849	11.224	61.667
TOM	2826	N	ASN	373	22.584	18.371	59.568
TOM	2827	CA	ASN	373	22.641	19.820	59.460
TOM	2828	CB	ASN	373	22.748	19.984	57.961
TOM	2829	CG	ASN	373	22.839	21.367	57.392
TOM	2830	OD1	ASN	373	21.906	22.153	57.347
TOM	2831	ND2	ASN	373	24.006	21.700	56.903
TOM	2832	C	ASN	373	21.456	20.564	60.119
TOM	2833	O	ASN	373	21.563	21.477	60.925
TOM	2834	N	SER	374	20.249	20.143	59.790
TOM	2835	CA	SER	374	19.040	20.639	60.430
TOM	2836	CB	SER	374	17.865	19.920	59.775

- 80 -

TOM	2837	OG	SER	374	17.855	19.956	58.336
TOM	2838	C	SEI	374	19.025	20.422	61.714
TOM	2839	O	SER	374	18.366	21.085	62.761
TOM	2840	N	TYR	375	19.704	19.376	62.401
TOM	2841	CA	TYR	375	19.718	19.083	63.836
TOM	2842	CB	TYR	375	19.815	17.548	64.076
TOM	2843	CG	TYR	375	18.462	16.877	64.232
TOM	2844	CD1	TYR	375	17.902	16.149	63.214
TOM	2845	CE1	TYR	375	16.661	15.579	63.334
TOM	2846	CD2	TYR	375	17.782	17.038	65.411
TOM	2847	CE2	TYR	375	16.541	16.466	65.543
TOM	2848	CZ	TYR	375	15.976	15.750	64.501
TOM	2849	OH	TYR	375	14.680	15.255	64.640
TOM	2850	C	TYR	375	20.825	19.761	64.630
TOM	2851	O	TYR	375	20.686	20.195	65.772
TOM	2852	N	ASN	376	21.977	19.964	64.055
TOM	2853	CA	ASN	376	23.068	20.373	64.909
TOM	2854	CB	ASN	376	24.099	19.268	64.773
TOM	2855	CG	ASN	376	23.433	17.920	65.151
TOM	2856	OD1	ASN	376	22.988	17.609	66.256
TOM	2857	ND2	ASN	376	23.200	16.991	64.254
TOM	2858	C	ASN	376	23.558	21.762	64.557
TOM	2859	O	ASN	376	24.691	21.911	64.053
TOM	2860	N	ARG	377	22.536	22.652	64.823
TOM	2861	CA	ARG	377	22.442	24.143	64.720
TOM	2862	CB	ARG	377	23.611	24.656	63.735
TOM	2863	CG	ARG	377	24.148	26.096	63.583
TOM	2864	CD	ARG	377	23.690	26.759	62.248
TOM	2865	NE	ARG	377	24.418	27.984	61.881
TOM	2866	CZ	ARG	377	24.708	28.408	60.613
TOM	2867	NH1	ARG	377	25.420	29.531	60.482
TOM	2868	NH2	ARG	377	24.350	27.770	59.491
TOM	2869	C	ARG	377	21.017	24.701	64.275
TOM	2870	O	ARG	377	20.429	24.239	63.293
TOM	2871	N	PRO	378	20.288	25.687	64.821
TOM	2872	CD	PRO	378	20.339	26.992	64.205
TOM	2873	CA	PRO	378	20.015	26.047	66.196
TOM	2874	CB	PRO	378	20.728	27.375	66.423
TOM	2875	CG	PRO	378	21.341	27.699	65.103
TOM	2876	C	PRO	378	18.549	26.169	66.596
TOM	2877	O	PRO	378	18.230	27.054	67.391
TOM	2878	N	ALA	379	17.643	25.381	66.011
TOM	2879	CA	ALA	379	16.184	25.238	66.329
TOM	2880	CB	ALA	379	15.601	24.093	65.544
TOM	2881	C	ALA	379	15.418	25.075	67.657
TOM	2882	O	ALA	379	15.840	24.579	68.691
TOM	2883	N	TYR	380	14.139	25.441	67.593
TOM	2884	CA	TYR	380	13.160	25.390	68.701
TOM	2885	CB	TYR	380	12.206	26.579	68.593
TOM	2886	CG	TYR	380	12.312	27.356	69.865
TOM	2887	CD1	TYR	380	12.850	28.636	69.891
TOM	2888	CE1	TYR	380	12.953	29.273	71.121
TOM	2889	CD2	TYR	380	11.893	26.721	71.029
TOM	2890	CE2	TYR	380	12.004	27.348	72.245
TOM	2891	CZ	TYR	380	12.529	28.615	72.281
TOM	2892	OH	TYR	380	12.557	29.204	73.525
TOM	2893	C	TYR	380	12.273	24.159	68.935
TOM	2894	O	TYR	380	11.461	23.843	68.075
TOM	2895	N	SER	381	12.361	23.504	70.091
TOM	2896	CA	SER	381	11.636	22.273	70.421
TOM	2897	CB	SER	381	12.530	21.470	71.406
TOM	2898	OG	SER	381	13.428	22.209	72.244
TOM	2899	C	SER	381	10.185	22.151	70.928
TOM	2900	O	SER	381	9.624	23.032	71.593
TOM	2901	N	PRO	382	9.531	21.015	70.603
TOM	2902	CD	PRO	382	9.871	20.120	69.497

0044

- 81 -

TOM	2903	CA	PRO	382	8.339	20.462	71.232
TOM	2904	CB	PRO	382	8.791	19.029	71.374
TOM	2905	CG	PRO	382	9.374	18.779	70.002
TOM	2906	C	PRO	382	7.731	21.077	72.484
TOM	2907	O	PRO	382	8.172	20.766	73.597
TOM	2908	N	GLY	383	6.772	21.996	72.373
TOM	2909	CA	GLY	383	6.145	22.573	73.562
TOM	2910	C	GLY	383	6.811	23.827	74.154
TOM	2911	O	GLY	383	6.611	24.289	75.295
TOM	2912	N	HIS	384	7.721	24.397	73.406
TOM	2913	CA	HIS	384	8.268	25.695	73.788
TOM	2914	CB	HIS	384	9.747	25.726	73.810
TOM	2915	CG	HIS	384	10.529	24.951	74.835
TOM	2916	CD2	HIS	384	11.136	23.764	74.570
TOM	2917	ND1	HIS	384	10.850	25.302	76.077
TOM	2918	CE1	HIS	384	11.638	24.382	76.564
TOM	2919	NE2	HIS	384	11.800	23.462	75.645
TOM	2920	C	HIS	384	7.880	26.522	72.591
TOM	2921	O	HIS	384	7.896	25.947	71.507
TOM	2922	N	LYS	385	7.563	27.811	72.680
TOM	2923	CA	LYS	385	7.144	28.650	71.552
TOM	2924	CB	LYS	385	8.405	28.960	70.731
TOM	2925	CG	LYS	385	8.157	29.825	69.511
TOM	2926	CD	LYS	385	9.441	30.113	68.725
TOM	2927	CE	LYS	385	9.254	31.142	67.604
TOM	2928	NZ	LYS	385	8.322	30.624	66.607
TOM	2929	C	LYS	385	6.022	28.016	70.709
TOM	2930	O	LYS	385	4.965	28.596	70.771
TOM	2931	N	THR	386	6.105	26.889	69.950
TOM	2932	CA	THR	386	4.990	26.186	69.238
TOM	2933	CB	THR	386	4.793	27.002	67.865
TOM	2934	OG1	THR	386	4.441	28.413	68.091
TOM	2935	CG2	THR	386	3.694	26.347	67.057
TOM	2936	C	THR	386	5.023	24.588	69.023
TOM	2937	O	THR	386	6.067	24.018	68.817
TOM	2938	N	GLN	387	3.965	23.748	69.226
TOM	2939	CA	GLN	387	3.708	22.305	68.917
TOM	2940	CB	GLN	387	4.055	22.228	67.452
TOM	2941	CG	GLN	387	3.192	21.239	66.745
TOM	2942	CD	GLN	387	1.759	21.717	66.585
TOM	2943	OE1	GLN	387	0.930	21.620	67.486
TOM	2944	NE2	GLN	387	1.391	22.264	65.429
TOM	2945	C	GLN	387	4.090	20.912	69.574
TOM	2946	O	GLN	387	4.891	20.129	69.015
TOM	2947	N	PRO	388	3.553	20.525	70.764
TOM	2948	CD	PRO	388	3.338	21.455	71.876
TOM	2949	CA	PRO	388	3.661	19.200	71.382
TOM	2950	CB	PRO	388	3.917	19.418	72.886
TOM	2951	CG	PRO	388	3.076	20.611	73.170
TOM	2952	C	PRO	388	2.562	18.146	71.250
TOM	2953	O	PRO	388	1.375	18.347	71.519
TOM	2954	N	PHE	389	3.078	16.925	71.024
TOM	2955	CA	PHE	389	2.279	15.742	70.781
TOM	2956	CB	PHE	389	1.567	16.004	69.436
TOM	2957	CG	PHE	389	2.351	16.445	68.204
TOM	2958	CD1	PHE	389	3.488	17.180	68.252
TOM	2959	CD2	PHE	389	1.878	16.042	67.001
TOM	2960	CE1	PHE	389	4.131	17.492	67.100
TOM	2961	CE2	PHE	389	2.516	16.354	65.851
TOM	2962	CZ	PHE	389	3.651	17.078	65.893
TOM	2963	C	PHE	389	3.021	14.419	70.815
TOM	2964	O	PHE	389	3.430	13.904	69.803
TOM	2965	N	LEU	390	3.221	13.818	71.975
TOM	2966	CA	LEU	390	4.017	12.572	72.289
TOM	2967	CB	LEU	390	3.145	11.648	73.159
TOM	2968	CG	LEU	390	2.474	12.355	74.286

- 82 -

TOM	2969	CD1	LEU	390	1.085	12.784	73.803
TOM	2970	CD2	LEU	390	2.439	11.470	75.494
TOM	2971	C	LEU	390	4.870	11.505	71.507
TOM	2972	O	LEU	390	5.974	11.120	71.921
TOM	2973	N	HIS	391	4.446	10.923	70.386
TOM	2974	CA	HIS	391	5.070	9.689	69.890
TOM	2975	CB	HIS	391	4.328	8.505	70.580
TOM	2976	CG	HIS	391	5.127	7.472	71.403
TOM	2977	CD2	HIS	391	4.640	6.871	72.561
TOM	2978	ND1	HIS	391	6.315	6.907	71.180
TOM	2979	CE1	HIS	391	6.547	6.012	72.122
TOM	2980	NE2	HIS	391	5.534	5.992	72.953
TOM	2981	C	HIS	391	5.147	9.441	68.376
TOM	2982	O	HIS	391	5.729	8.419	68.003
TOM	2983	N	ASP	392	4.458	10.231	67.526
TOM	2984	CA	ASP	392	4.679	10.308	66.082
TOM	2985	CB	ASP	392	4.562	8.968	65.346
TOM	2986	CG	ASP	392	5.944	8.605	64.764
TOM	2987	OD1	ASP	392	6.398	9.155	63.735
TOM	2988	OD2	ASP	392	6.585	7.749	65.380
TOM	2989	C	ASP	392	3.750	11.276	65.389
TOM	2990	O	ASP	392	3.550	12.339	65.977
TOM	2991	N	GLY	393	3.379	11.106	64.101
TOM	2992	CA	GLY	393	2.406	11.952	63.408
TOM	2993	C	GLY	393	2.655	12.426	61.975
TOM	2994	O	GLY	393	2.659	11.646	61.019
TOM	2995	N	TYR	394	2.601	13.770	62.034
TOM	2996	CA	TYR	394	2.762	14.906	61.102
TOM	2997	CB	TYR	394	2.566	14.699	59.624
TOM	2998	CG	TYR	394	3.540	15.546	58.760
TOM	2999	CD1	TYR	394	3.299	16.902	58.522
TOM	3000	CE1	TYR	394	4.138	17.634	57.672
TOM	3001	CD2	TYR	394	4.635	14.955	58.119
TOM	3002	CE2	TYR	394	5.463	15.676	57.277
TOM	3003	CZ	TYR	394	5.213	17.020	57.029
TOM	3004	OH	TYR	394	5.973	17.719	56.074
TOM	3005	C	TYR	394	1.641	15.863	61.451
TOM	3006	O	TYR	394	0.516	15.460	61.724
TOM	3007	N	ALA	395	2.009	17.126	61.654
TOM	3008	CA	ALA	395	1.077	18.198	62.133
TOM	3009	CB	ALA	395	1.258	18.614	63.635
TOM	3010	C	ALA	395	1.341	19.471	61.355
TOM	3011	O	ALA	395	2.459	20.001	61.468
TOM	3012	N	VAL	396	0.383	19.850	60.479
TOM	3013	CA	VAL	396	0.476	21.101	59.723
TOM	3014	CB	VAL	396	0.361	20.885	58.182
TOM	3015	CG1	VAL	396	1.471	19.948	57.746
TOM	3016	CG2	VAL	396	-0.911	20.240	57.788
TOM	3017	C	VAL	396	-0.572	22.106	60.171
TOM	3018	O	VAL	396	-1.475	21.696	60.871
TOM	3019	N	SER	397	-0.488	23.431	59.964
TOM	3020	CA	SER	397	-1.545	24.417	60.316
TOM	3021	CB	SER	397	-1.824	24.606	61.833
TOM	3022	OG	SER	397	-1.504	25.847	62.506
TOM	3023	C	SER	397	-1.252	25.834	59.863
TOM	3024	O	SER	397	-0.091	26.234	59.786
TOM	3025	N	TRP	398	-2.261	26.652	59.551
TOM	3026	CA	TRP	398	-1.988	28.063	59.259
TOM	3027	CB	TRP	398	-3.238	28.828	58.842
TOM	3028	CG	TRP	398	-3.681	28.443	57.456
TOM	3029	CD2	TRP	398	-3.049	28.726	56.267
TOM	3030	CE2	TRP	398	-3.946	28.214	55.344
TOM	3031	CE3	TRP	398	-1.914	29.378	55.839
TOM	3032	CD1	TRP	398	-4.867	27.781	57.270
TOM	3033	NE1	TRP	398	-4.995	27.663	55.956
TOM	3034	CZ2	TRP	398	-3.744	28.338	53.997

- 83 -

TOM	3035	CZ3	TRP	398	-1.693	29.516	54.475
TOM	3036	CH2	TRP	398	-2.598	28.996	53.565
TOM	3037	C	TRP	398	-1.417	28.752	60.499
TOM	3038	O	TRP	398	-2.030	28.749	61.563
TOM	3039	N	ASN	399	-0.147	29.208	60.369
TOM	3040	CA	ASN	399	0.507	30.031	61.402
TOM	3041	CB	ASN	399	1.839	30.610	60.904
TOM	3042	CG	ASN	399	2.724	31.325	61.939
TOM	3043	OD1	ASN	399	3.730	31.910	61.595
TOM	3044	ND2	ASN	399	2.582	31.399	63.249
TOM	3045	C	ASN	399	-0.473	31.163	61.595
TOM	3046	O	ASN	399	-0.807	31.627	62.682
TOM	3047	N	THR	400	-0.736	31.548	60.324
TOM	3048	CA	THR	400	-1.722	32.442	59.780
TOM	3049	CB	THR	400	-2.257	33.360	60.948
TOM	3050	OG1	THR	400	-3.681	33.224	60.822
TOM	3051	CG2	THR	400	-1.580	34.750	61.018
TOM	3052	C	THR	400	-1.288	33.242	58.502
TOM	3053	O	THR	400	-0.186	33.386	57.927
TOM	3054	N	VAL	401	-2.463	33.104	57.878
TOM	3055	CA	VAL	401	-2.899	33.764	56.648
TOM	3056	CB	VAL	401	-3.377	32.676	55.688
TOM	3057	CG1	VAL	401	-4.738	31.987	55.994
TOM	3058	CG2	VAL	401	-3.345	33.390	54.419
TOM	3059	C	VAL	401	-4.026	34.720	57.081
TOM	3060	O	VAL	401	-4.256	35.814	56.545
TOM	3061	N	GLU	402	-4.730	34.244	58.142
TOM	3062	CA	GLU	402	-5.745	34.985	58.852
TOM	3063	CB	GLU	402	-6.446	34.092	59.858
TOM	3064	CG	GLU	402	-7.621	34.839	60.449
TOM	3065	CD	GLU	402	-8.230	34.122	61.629
TOM	3066	OE1	GLU	402	-9.451	33.927	61.603
TOM	3067	OE2	GLU	402	-7.504	33.760	62.563
TOM	3068	C	GLU	402	-5.056	36.147	59.565
TOM	3069	O	GLU	402	-4.484	36.161	60.648
TOM	3070	N	ASP	403	-4.951	37.055	58.663
TOM	3071	CA	ASP	403	-4.376	38.348	58.875
TOM	3072	CB	ASP	403	-2.844	38.257	58.629
TOM	3073	CG	ASP	403	-1.992	37.986	59.904
TOM	3074	OD1	ASP	403	-2.441	38.214	61.053
TOM	3075	OD2	ASP	403	-0.849	37.544	59.725
TOM	3076	C	ASP	403	-5.206	38.953	57.767
TOM	3077	O	ASP	403	-6.161	39.647	58.051
TOM	3078	N	SER	404	-4.961	38.534	56.538
TOM	3079	CA	SER	404	-5.894	38.790	55.463
TOM	3080	CB	SER	404	-5.638	40.140	54.725
TOM	3081	OG	SER	404	-6.772	40.522	53.908
TOM	3082	C	SER	404	-5.663	37.588	54.526
TOM	3083	O	SER	404	-4.678	37.423	53.778
TOM	3084	N	ILE	405	-6.580	36.638	54.839
TOM	3085	CA	ILE	405	-6.713	35.282	54.222
TOM	3086	CB	ILE	405	-7.764	34.493	55.072
TOM	3087	CG2	ILE	405	-8.928	35.372	55.535
TOM	3088	CG1	ILE	405	-8.182	33.283	54.261
TOM	3089	CD	ILE	405	-7.157	32.187	53.944
TOM	3090	C	ILE	405	-7.054	35.308	52.740
TOM	3091	O	ILE	405	-8.055	35.934	52.403
TOM	3092	N	ILE	406	-6.350	34.554	51.894
TOM	3093	CA	ILE	406	-6.200	34.961	50.475
TOM	3094	CB	ILE	406	-6.222	33.730	49.462
TOM	3095	CG2	ILE	406	-5.449	34.296	48.219
TOM	3096	CG1	ILE	406	-5.542	32.434	49.929
TOM	3097	CD	ILE	406	-5.317	31.436	48.772
TOM	3098	C	ILE	406	-7.135	36.057	49.869
TOM	3099	O	ILE	406	-8.259	35.862	49.416
TOM	3100	N	ARG	407	-6.682	37.313	49.975

- 84 -

TOM	3101	CA	ARG	407	-7.445	38.489	49.546
TOM	3102	CB	ARG	407	-6.792	39.654	50.243
TOM	3103	CG	ARG	407	-7.676	40.815	50.675
TOM	3104	CD	ARG	407	-7.851	42.068	49.726
TOM	3105	NE	ARG	407	-6.790	43.078	49.817
TOM	3106	CZ	ARG	407	-6.470	43.730	50.954
TOM	3107	NH1	ARG	407	-5.424	44.555	50.934
TOM	3108	NH2	ARG	407	-7.182	43.633	52.092
TOM	3109	C	ARG	407	-7.493	38.688	48.023
TOM	3110	O	ARG	407	-6.582	38.222	47.330
TOM	3111	N	THR	408	-8.520	39.278	47.405
TOM	3112	CA	THR	408	-8.386	39.712	45.998
TOM	3113	CB	THR	408	-8.982	38.700	44.997
TOM	3114	OG1	THR	408	-9.792	37.760	45.688
TOM	3115	CG2	THR	408	-7.839	38.072	44.195
TOM	3116	C	THR	408	-8.930	41.120	45.607
TOM	3117	O	THR	408	-9.372	41.924	46.458
TOM	3118	N	GLY	409	-8.841	41.525	44.326
TOM	3119	CA	GLY	409	-9.005	42.960	44.043
TOM	3120	C	GLY	409	-7.731	43.765	44.459
TOM	3121	O	GLY	409	-7.694	44.559	45.402
TOM	3122	N	PHE	410	-6.583	43.602	43.794
TOM	3123	CA	PHE	410	-5.384	44.342	44.184
TOM	3124	CB	PHE	410	-4.320	43.419	44.772
TOM	3125	CG	PHE	410	-4.267	42.988	46.246
TOM	3126	CD1	PHE	410	-5.224	42.178	46.805
TOM	3127	CD2	PHE	410	-3.142	43.285	46.975
TOM	3128	CE1	PHE	410	-5.036	41.663	48.054
TOM	3129	CE2	PHE	410	-2.964	42.768	48.228
TOM	3130	CZ	PHE	410	-3.911	41.948	48.769
TOM	3131	C	PHE	410	-4.643	45.183	43.142
TOM	3132	O	PHE	410	-3.811	44.680	42.369
TOM	3133	N	GLN	411	-4.939	46.494	43.160
TOM	3134	CA	GLN	411	-4.291	47.559	42.356
TOM	3135	CB	GLN	411	-5.202	48.786	42.422
TOM	3136	CG	GLN	411	-5.415	49.541	41.105
TOM	3137	CD	GLN	411	-6.048	48.706	39.990
TOM	3138	OE1	GLN	411	-6.572	47.632	40.247
TOM	3139	NE2	GLN	411	-6.036	49.016	38.703
TOM	3140	C	GLN	411	-2.852	47.915	42.838
TOM	3141	O	GLN	411	-2.408	49.060	43.026
TOM	3142	N	GLY	412	-2.096	46.823	42.952
TOM	3143	CA	GLY	412	-0.805	46.839	43.608
TOM	3144	C	GLY	412	-0.285	45.452	44.012
TOM	3145	O	GLY	412	0.773	45.320	44.638
TOM	3146	N	GLU	413	-1.098	44.423	43.712
TOM	3147	CA	GLU	413	-0.669	43.028	43.716
TOM	3148	CB	GLU	413	-0.386	42.685	42.250
TOM	3149	CG	GLU	413	-0.477	43.759	41.143
TOM	3150	CD	GLU	413	0.641	43.701	40.114
TOM	3151	OE1	GLU	413	0.395	44.002	38.939
TOM	3152	OE2	GLU	413	1.767	43.397	40.514
TOM	3153	C	GLU	413	0.429	42.340	44.552
TOM	3154	O	GLU	413	1.551	42.163	44.057
TOM	3155	N	SER	414	0.182	41.773	45.740
TOM	3156	CA	SER	414	1.243	41.166	46.593
TOM	3157	CB	SER	414	2.204	42.214	47.103
TOM	3158	OG	SER	414	3.335	41.648	47.740
TOM	3159	C	SER	414	0.804	40.410	47.849
TOM	3160	O	SER	414	0.389	41.028	48.840
TOM	3161	N	GLY	415	0.902	39.068	47.883
TOM	3162	CA	GLY	415	0.380	38.297	49.031
TOM	3163	C	GLY	415	1.385	37.423	49.755
TOM	3164	O	GLY	415	2.249	36.754	49.186
TOM	3165	N	HIS	416	1.400	37.354	51.077
TOM	3166	CA	HIS	416	2.467	36.603	51.753

0048

- 85 -

TOM	3167	CB	HIS	416	3.540	37.617	52.309
TOM	3168	CG	HIS	416	3.913	38.680	51.271
TOM	3169	CD2	HIS	416	4.459	38.461	50.010
TOM	3170	ND1	HIS	416	3.606	39.965	51.383
TOM	3171	CE1	HIS	416	3.914	40.530	50.244
TOM	3172	NE2	HIS	416	4.417	39.626	49.432
TOM	3173	C	HIS	416	2.067	35.647	52.862
TOM	3174	O	HIS	416	2.559	35.829	53.977
TOM	3175	N	ASP	417	1.340	34.571	52.534
TOM	3176	CA	ASP	417	0.807	33.596	53.489
TOM	3177	CB	ASP	417	-0.392	32.829	52.889
TOM	3178	CG	ASP	417	-1.159	33.461	51.737
TOM	3179	OD1	ASP	417	-0.893	33.023	50.618
TOM	3180	OD2	ASP	417	-1.976	34.368	51.937
TOM	3181	C	ASP	417	1.787	32.533	54.006
TOM	3182	O	ASP	417	2.560	31.971	53.239
TOM	3183	N	ILE	418	1.714	32.199	55.314
TOM	3184	CA	ILE	418	2.627	31.275	56.057
TOM	3185	CB	ILE	418	3.450	32.225	57.103
TOM	3186	CG2	ILE	418	3.928	31.445	58.254
TOM	3187	CG1	ILE	418	4.749	32.819	56.575
TOM	3188	CD	ILE	418	4.845	34.165	57.343
TOM	3189	C	ILE	418	2.067	29.999	56.775
TOM	3190	O	ILE	418	1.188	30.065	57.646
TOM	3191	N	LYS	419	2.589	28.781	56.473
TOM	3192	CA	LYS	419	2.265	27.555	57.249
TOM	3193	CB	LYS	419	1.669	26.398	56.472
TOM	3194	CG	LYS	419	1.793	26.454	54.992
TOM	3195	CD	LYS	419	0.715	27.376	54.437
TOM	3196	CE	LYS	419	0.954	27.625	52.966
TOM	3197	NZ	LYS	419	2.228	28.271	52.771
TOM	3198	C	LYS	419	3.385	26.855	57.990
TOM	3199	O	LYS	419	4.552	26.919	57.623
TOM	3200	N	ILE	420	2.999	26.248	59.111
TOM	3201	CA	ILE	420	3.869	25.460	59.967
TOM	3202	CB	ILE	420	3.791	25.837	61.526
TOM	3203	CG2	ILE	420	2.667	26.850	61.700
TOM	3204	CG1	ILE	420	3.693	24.567	62.467
TOM	3205	CD	ILE	420	4.151	24.588	63.975
TOM	3206	C	ILE	420	3.576	23.987	59.847
TOM	3207	O	ILE	420	2.408	23.622	59.910
TOM	3208	N	THR	421	4.661	23.225	59.694
TOM	3209	CA	THR	421	4.704	21.758	59.643
TOM	3210	CB	THR	421	4.777	21.214	58.101
TOM	3211	OG1	THR	421	5.706	20.137	58.136
TOM	3212	CG2	THR	421	5.089	22.258	57.008
TOM	3213	C	THR	421	5.818	21.085	60.483
TOM	3214	O	THR	421	6.913	21.620	60.711
TOM	3215	N	ALA	422	5.489	19.895	60.999
TOM	3216	CA	ALA	422	6.414	19.026	61.768
TOM	3217	CB	ALA	422	6.613	19.511	63.235
TOM	3218	C	ALA	422	5.969	17.553	61.845
TOM	3219	O	ALA	422	5.230	17.128	60.948
TOM	3220	N	GLU	423	6.284	16.751	62.889
TOM	3221	CA	GLU	423	6.022	15.299	63.021
TOM	3222	CB	GLU	423	6.980	14.613	62.072
TOM	3223	CG	GLU	423	6.490	13.521	61.169
TOM	3224	CD	GLU	423	6.417	12.100	61.743
TOM	3225	OE1	GLU	423	6.903	11.808	62.836
TOM	3226	OE2	GLU	423	5.893	11.245	61.032
TOM	3227	C	GLU	423	6.306	14.874	64.482
TOM	3228	O	GLU	423	6.956	15.728	65.086
TOM	3229	N	ASN	424	5.972	13.810	65.265
TOM	3230	CA	ASN	424	6.720	13.758	66.532
TOM	3231	CB	ASN	424	5.746	13.908	67.678
TOM	3232	CG	ASN	424	6.279	15.091	68.535

0049

- 86 -

TOM	3233	OD1	ASN	424	6.261	15.164	69.768
TOM	3234	ND2	ASN	424	6.793	16.153	67.950
TOM	3235	C	ASN	424	7.796	12.791	67.042
TOM	3236	O	ASN	424	7.999	12.625	68.244
TOM	3237	N	THR	425	8.619	12.260	66.135
TOM	3238	CA	THR	425	9.882	11.569	66.475
TOM	3239	CB	THR	425	9.611	10.339	67.468
TOM	3240	OG1	THR	425	10.902	9.846	67.786
TOM	3241	CG2	THR	425	8.750	9.221	66.962
TOM	3242	C	THR	425	10.611	11.174	65.177
TOM	3243	O	THR	425	10.840	12.163	64.471
TOM	3244	N	PRO	426	10.993	9.966	64.675
TOM	3245	CD	PRO	426	11.857	8.941	65.258
TOM	3246	CA	PRO	426	11.367	9.638	63.319
TOM	3247	CB	PRO	426	10.707	8.296	63.282
TOM	3248	CG	PRO	426	11.767	7.826	64.222
TOM	3249	C	PRO	426	11.367	10.316	61.974
TOM	3250	O	PRO	426	11.556	9.609	60.976
TOM	3251	N	LEU	427	11.353	11.654	61.910
TOM	3252	CA	LEU	427	11.577	12.476	60.680
TOM	3253	CB	LEU	427	13.020	12.909	60.615
TOM	3254	CG	LEU	427	13.979	11.803	60.608
TOM	3255	CD1	LEU	427	15.040	12.281	59.645
TOM	3256	CD2	LEU	427	14.372	11.366	62.021
TOM	3257	C	LEU	427	11.236	12.155	59.232
TOM	3258	O	LEU	427	12.097	12.038	58.343
TOM	3259	N	PRO	428	9.939	12.042	58.957
TOM	3260	CD	PRO	428	8.909	11.382	59.753
TOM	3261	CA	PRO	428	9.495	11.955	57.618
TOM	3262	CB	PRO	428	8.128	11.228	57.654
TOM	3263	CG	PRO	428	8.187	10.349	58.843
TOM	3264	C	PRO	428	9.436	13.341	57.089
TOM	3265	O	PRO	428	9.361	14.315	57.791
TOM	3266	N	ILE	429	9.876	13.216	55.884
TOM	3267	CA	ILE	429	9.796	14.116	54.793
TOM	3268	CB	ILE	429	10.170	13.426	53.439
TOM	3269	CG2	ILE	429	11.501	14.023	53.007
TOM	3270	CG1	ILE	429	10.210	11.937	53.495
TOM	3271	CD	ILE	429	9.011	11.238	54.146
TOM	3272	C	ILE	429	8.531	14.868	54.446
TOM	3273	O	ILE	429	7.387	14.447	54.641
TOM	3274	N	ALA	430	8.859	15.919	53.693
TOM	3275	CA	ALA	430	7.893	16.769	53.010
TOM	3276	CB	ALA	430	8.016	18.217	53.572
TOM	3277	C	ALA	430	8.168	16.756	51.496
TOM	3278	O	ALA	430	8.987	17.540	51.042
TOM	3279	N	GLY	431	7.501	15.974	50.635
TOM	3280	CA	GLY	431	7.916	15.888	49.244
TOM	3281	C	GLY	431	7.544	17.003	48.270
TOM	3282	O	GLY	431	8.242	17.305	47.294
TOM	3283	N	VAL	432	6.378	17.602	48.424
TOM	3284	CA	VAL	432	5.913	18.609	47.464
TOM	3285	CB	VAL	432	5.530	17.890	46.039
TOM	3286	CG1	VAL	432	4.057	17.683	45.600
TOM	3287	CG2	VAL	432	6.117	18.814	45.071
TOM	3288	C	VAL	432	4.740	19.379	48.078
TOM	3289	O	VAL	432	4.232	19.145	49.188
TOM	3290	N	LEU	433	4.399	20.421	47.341
TOM	3291	CA	LEU	433	3.319	21.290	47.722
TOM	3292	CB	LEU	433	4.062	22.285	48.564
TOM	3293	CG	LEU	433	3.483	23.275	49.519
TOM	3294	CD1	LEU	433	3.741	24.595	48.845
TOM	3295	CD2	LEU	433	2.002	23.093	49.843
TOM	3296	C	LEU	433	2.565	21.801	46.464
TOM	3297	O	LEU	433	3.010	22.278	45.404
TOM	3298	N	LEU	434	1.317	21.417	46.569

- 87 -

TOM	3299	CA	LEU	434	0.320	21.734	45.583
TOM	3300	CB	LEU	434	-0.630	20.518	45.728
TOM	3301	CG	LEU	434	-0.829	19.426	44.686
TOM	3302	CD1	LEU	434	0.455	18.800	44.246
TOM	3303	CD2	LEU	434	-1.613	18.307	45.346
TOM	3304	C	LEU	434	-0.312	23.163	45.791
TOM	3305	O	LEU	434	-1.412	23.297	46.392
TOM	3306	N	PRO	435	0.273	24.332	45.411
TOM	3307	CD	PRO	435	1.681	24.765	45.629
TOM	3308	CA	PRO	435	-0.525	25.565	45.304
TOM	3309	CB	PRO	435	0.554	26.706	45.154
TOM	3310	CG	PRO	435	1.739	26.269	45.993
TOM	3311	C	PRO	435	-1.672	25.762	44.303
TOM	3312	O	PRO	435	-1.652	25.547	43.091
TOM	3313	N	THR	436	-2.762	26.208	44.841
TOM	3314	CA	THR	436	-3.726	26.918	44.014
TOM	3315	CB	THR	436	-4.559	27.767	44.890
TOM	3316	OG1	THR	436	-4.168	27.529	46.251
TOM	3317	CG2	THR	436	-6.017	27.500	44.596
TOM	3318	C	THR	436	-3.218	27.869	42.905
TOM	3319	O	THR	436	-2.123	28.421	43.014
TOM	3320	N	ILE	437	-3.914	28.104	41.789
TOM	3321	CA	ILE	437	-3.615	29.166	40.810
TOM	3322	CB	ILE	437	-2.203	28.846	40.147
TOM	3323	CG2	ILE	437	-2.151	27.440	39.614
TOM	3324	CG1	ILE	437	-1.913	29.861	39.040
TOM	3325	CD	ILE	437	-0.691	29.653	38.087
TOM	3326	C	ILE	437	-4.749	29.411	39.736
TOM	3327	O	ILE	437	-4.961	28.627	38.802
TOM	3328	N	PRO	438	-5.609	30.468	39.829
TOM	3329	CD	PRO	438	-6.472	30.753	40.973
TOM	3330	CA	PRO	438	-6.155	31.189	38.681
TOM	3331	CB	PRO	438	-7.177	32.137	39.241
TOM	3332	CG	PRO	438	-7.751	31.280	40.334
TOM	3333	C	PRO	438	-5.155	31.931	37.809
TOM	3334	O	PRO	438	-4.608	32.989	38.141
TOM	3335	N	GLY	439	-4.923	31.268	36.677
TOM	3336	CA	GLY	439	-4.148	31.680	35.510
TOM	3337	C	GLY	439	-3.626	33.091	35.335
TOM	3338	O	GLY	439	-2.832	33.243	34.436
TOM	3339	N	LYS	440	-4.056	34.183	35.964
TOM	3340	CA	LYS	440	-3.316	35.463	35.975
TOM	3341	CB	LYS	440	-3.509	36.244	34.683
TOM	3342	CG	LYS	440	-2.136	36.446	33.975
TOM	3343	CD	LYS	440	-2.144	37.072	32.548
TOM	3344	CE	LYS	440	-2.769	38.472	32.532
TOM	3345	NZ	LYS	440	-1.971	39.369	33.345
TOM	3346	C	LYS	440	-3.698	36.395	37.124
TOM	3347	O	LYS	440	-3.212	37.515	37.311
TOM	3348	N	LEU	441	-4.530	35.837	37.992
TOM	3349	CA	LEU	441	-5.143	36.506	39.148
TOM	3350	CB	LEU	441	-6.647	36.422	38.981
TOM	3351	CG	LEU	441	-7.215	36.719	37.589
TOM	3352	CD1	LEU	441	-8.623	36.143	37.512
TOM	3353	CD2	LEU	441	-7.105	38.216	37.300
TOM	3354	C	LEU	441	-4.753	35.938	40.521
TOM	3355	O	LEU	441	-5.266	36.338	41.562
TOM	3356	N	ASP	442	-3.936	34.891	40.481
TOM	3357	CA	ASP	442	-3.277	34.288	41.628
TOM	3358	CB	ASP	442	-4.191	33.364	42.516
TOM	3359	CG	ASP	442	-4.760	33.759	43.898
TOM	3360	OD1	ASP	442	-4.260	34.629	44.592
TOM	3361	OD2	ASP	442	-5.728	33.132	44.325
TOM	3362	C	ASP	442	-2.214	33.395	40.963
TOM	3363	O	ASP	442	-2.340	32.164	40.869
TOM	3364	N	VAL	443	-1.170	34.005	40.366

0051

- 88 -

TOM	3365	CA	VAL	443	-0.063	33.232	39.771
TOM	3366	CB	VAL	443	0.546	33.886	38.480
TOM	3367	CG1	VAL	443	0.126	33.147	37.226
TOM	3368	CG2	VAL	443	-0.030	35.252	38.217
TOM	3369	C	VAL	443	0.989	33.184	40.885
TOM	3370	O	VAL	443	0.951	33.979	41.829
TOM	3371	N	ASN	444	2.010	32.331	40.864
TOM	3372	CA	ASN	444	2.837	32.067	42.068
TOM	3373	CB	ASN	444	2.638	30.570	42.249
TOM	3374	CG	ASN	444	3.631	29.773	43.010
TOM	3375	OD1	ASN	444	4.311	30.203	43.904
TOM	3376	ND2	ASN	444	3.776	28.524	42.693
TOM	3377	C	ASN	444	4.287	32.518	42.119
TOM	3378	O	ASN	444	5.042	32.291	41.183
TOM	3379	N	LYS	445	4.728	33.118	43.208
TOM	3380	CA	LYS	445	6.065	33.617	43.223
TOM	3381	CB	LYS	445	5.988	34.955	43.931
TOM	3382	CG	LYS	445	7.167	35.684	43.281
TOM	3383	CD	LYS	445	7.490	37.003	43.858
TOM	3384	CE	LYS	445	8.898	37.049	43.349
TOM	3385	NZ	LYS	445	9.579	38.259	43.776
TOM	3386	C	LYS	445	7.289	32.809	43.712
TOM	3387	O	LYS	445	7.845	32.816	44.831
TOM	3388	N	SER	446	7.763	32.094	42.696
TOM	3389	CA	SER	446	8.961	31.267	42.672
TOM	3390	CB	SER	446	9.313	30.975	41.206
TOM	3391	OG	SER	446	8.246	30.554	40.341
TOM	3392	C	SER	446	10.181	31.866	43.381
TOM	3393	O	SER	446	10.873	31.148	44.092
TOM	3394	N	LYS	447	10.458	33.171	43.319
TOM	3395	CA	LYS	447	11.592	33.720	44.057
TOM	3396	CB	LYS	447	12.004	35.000	43.288
TOM	3397	CG	LYS	447	12.923	36.057	43.992
TOM	3398	CD	LYS	447	12.332	37.196	44.911
TOM	3399	CE	LYS	447	13.032	37.220	46.306
TOM	3400	NZ	LYS	447	12.517	38.250	47.202
TOM	3401	C	LYS	447	11.357	33.982	45.558
TOM	3402	O	LYS	447	12.240	33.851	46.410
TOM	3403	N	THR	448	10.137	34.427	45.895
TOM	3404	CA	THR	448	9.804	34.869	47.255
TOM	3405	CB	THR	448	8.607	35.911	47.227
TOM	3406	OG1	THR	448	9.093	37.176	46.774
TOM	3407	CG2	THR	448	8.022	36.247	48.606
TOM	3408	C	THR	448	9.439	33.696	48.162
TOM	3409	O	THR	448	9.571	33.735	49.407
TOM	3410	N	HIS	449	8.900	32.616	47.557
TOM	3411	CA	HIS	449	8.538	31.486	48.395
TOM	3412	CB	HIS	449	7.136	31.250	48.030
TOM	3413	CG	HIS	449	6.943	30.243	47.002
TOM	3414	CD2	HIS	449	6.192	29.130	47.217
TOM	3415	ND1	HIS	449	7.477	30.272	45.801
TOM	3416	CE1	HIS	449	7.065	29.173	45.222
TOM	3417	NE2	HIS	449	6.300	28.508	46.085
TOM	3418	C	HIS	449	9.398	30.217	48.451
TOM	3419	O	HIS	449	10.008	29.726	47.493
TOM	3420	N	ILE	450	9.298	29.690	49.674
TOM	3421	CA	ILE	450	10.271	28.781	50.310
TOM	3422	CB	ILE	450	11.418	29.697	50.994
TOM	3423	CG2	ILE	450	12.320	30.164	49.846
TOM	3424	CG1	ILE	450	10.920	30.994	51.775
TOM	3425	CD	ILE	450	11.015	31.081	53.305
TOM	3426	C	ILE	450	9.732	27.808	51.377
TOM	3427	O	ILE	450	8.653	28.029	51.939
TOM	3428	N	SER	451	10.428	26.717	51.724
TOM	3429	CA	SER	451	10.187	25.993	53.004
TOM	3430	CB	SER	451	10.093	24.439	52.940

- 89 -

TOM	3431	OG	SER	451	9.604	23.839	54.175
TOM	3432	C	SER	451	11.408	26.243	53.916
TOM	3433	O	SER	451	12.563	26.332	53.429
TOM	3434	N	VAL	452	11.296	26.372	55.241
TOM	3435	CA	VAL	452	12.489	26.585	56.060
TOM	3436	CB	VAL	452	12.720	28.139	56.346
TOM	3437	CG1	VAL	452	11.388	28.859	56.395
TOM	3438	CG2	VAL	452	13.252	28.454	57.736
TOM	3439	C	VAL	452	12.562	25.846	57.365
TOM	3440	O	VAL	452	11.692	26.113	58.191
TOM	3441	N	ASN	453	13.659	25.025	57.424
TOM	3442	CA	ASN	453	14.277	24.350	58.612
TOM	3443	CB	ASN	453	14.878	23.094	58.193
TOM	3444	CG	ASN	453	13.971	22.256	57.320
TOM	3445	OD1	ASN	453	13.520	21.195	57.734
TOM	3446	ND2	ASN	453	13.755	22.681	56.070
TOM	3447	C	ASN	453	15.420	25.087	59.432
TOM	3448	O	ASN	453	15.901	24.748	60.512
TOM	3449	N	GLY	454	15.713	26.308	58.977
TOM	3450	CA	GLY	454	16.703	27.291	59.431
TOM	3451	C	GLY	454	17.209	27.837	58.116
TOM	3452	O	GLY	454	17.272	29.009	57.757
TOM	3453	N	ARG	455	17.463	26.823	57.296
TOM	3454	CA	ARG	455	18.083	26.957	55.989
TOM	3455	CB	ARG	455	18.651	25.620	55.332
TOM	3456	CG	ARG	455	19.365	24.539	56.182
TOM	3457	CD	ARG	455	20.541	25.106	57.098
TOM	3458	NE	ARG	455	20.427	24.705	58.504
TOM	3459	CZ	ARG	455	20.725	25.517	59.528
TOM	3460	NH1	ARG	455	20.536	25.045	60.786
TOM	3461	NH2	ARG	455	21.196	26.762	59.270
TOM	3462	C	ARG	455	16.923	27.365	55.146
TOM	3463	O	ARG	455	15.875	26.730	55.290
TOM	3464	N	LYS	456	17.109	28.428	54.355
TOM	3465	CA	LYS	456	16.065	28.935	53.493
TOM	3466	CB	LYS	456	16.218	30.460	53.360
TOM	3467	CG	LYS	456	14.943	31.127	52.848
TOM	3468	CD	LYS	456	15.238	31.818	51.581
TOM	3469	CE	LYS	456	15.600	33.237	51.972
TOM	3470	NZ	LYS	456	16.683	33.731	51.127
TOM	3471	C	LYS	456	16.326	28.199	52.206
TOM	3472	O	LYS	456	17.376	28.348	51.587
TOM	3473	N	ILE	457	15.373	27.315	51.916
TOM	3474	CA	ILE	457	15.417	26.378	50.778
TOM	3475	CB	ILE	457	14.983	24.892	51.233
TOM	3476	CG2	ILE	457	15.065	24.014	50.075
TOM	3477	CG1	ILE	457	15.955	24.178	52.188
TOM	3478	CD	ILE	457	15.355	22.970	52.898
TOM	3479	C	ILE	457	14.507	26.867	49.667
TOM	3480	O	ILE	457	13.321	27.119	49.803
TOM	3481	N	ARG	458	15.080	27.027	48.513
TOM	3482	CA	ARG	458	14.300	27.520	47.392
TOM	3483	CB	ARG	458	15.236	28.198	46.376
TOM	3484	CG	ARG	458	15.422	29.694	46.651
TOM	3485	CD	ARG	458	14.182	30.389	46.156
TOM	3486	NE	ARG	458	14.442	31.797	46.154
TOM	3487	CZ	ARG	458	15.142	32.355	45.185
TOM	3488	NH1	ARG	458	15.362	33.669	45.220
TOM	3489	NH2	ARG	458	15.524	31.649	44.129
TOM	3490	C	ARG	458	13.497	26.431	46.712
TOM	3491	O	ARG	458	13.830	25.236	46.870
TOM	3492	N	MET	459	12.472	26.836	45.935
TOM	3493	CA	MET	459	11.558	25.876	45.334
TOM	3494	CB	MET	459	10.143	26.329	45.678
TOM	3495	CG	MET	459	9.246	25.209	46.185
TOM	3496	SD	MET	459	9.122	25.357	47.953

0053

-90-

TOM	3497	CE	MET	459	8.168	24.038	48.673
TOM	3498	C	MET	459	11.617	25.561	43.843
TOM	3499	O	MET	459	11.842	26.492	43.050
TOM	3500	N	ARG	460	11.468	24.312	43.338
TOM	3501	CA	ARG	460	11.209	24.225	41.884
TOM	3502	CB	ARG	460	12.055	23.136	41.243
TOM	3503	CG	ARG	460	12.475	23.735	39.862
TOM	3504	CD	ARG	460	13.278	25.070	39.994
TOM	3505	NE	ARG	460	13.849	25.670	38.781
TOM	3506	CZ	ARG	460	15.159	25.592	38.489
TOM	3507	NH1	ARG	460	15.668	26.212	37.418
TOM	3508	NH2	ARG	460	16.000	24.809	39.167
TOM	3509	C	ARG	460	9.716	23.975	41.609
TOM	3510	O	ARG	460	9.085	23.082	42.188
TOM	3511	N	CYS	461	9.070	24.789	40.762
TOM	3512	CA	CYS	461	7.587	24.755	40.595
TOM	3513	CB	CYS	461	6.957	26.043	41.229
TOM	3514	SG	CYS	461	7.198	26.451	42.995
TOM	3515	C	CYS	461	6.885	24.581	39.225
TOM	3516	O	CYS	461	6.457	25.558	38.590
TOM	3517	N	ARG	462	6.661	23.400	38.664
TOM	3518	CA	ARG	462	5.942	23.355	37.373
TOM	3519	CB	ARG	462	6.249	22.098	36.527
TOM	3520	CG	ARG	462	5.859	20.647	36.894
TOM	3521	CD	ARG	462	5.922	19.937	35.528
TOM	3522	NE	ARG	462	6.214	18.514	35.550
TOM	3523	CZ	ARG	462	6.896	17.913	34.544
TOM	3524	NH1	ARG	462	7.012	16.580	34.577
TOM	3525	NH2	ARG	462	7.476	18.575	33.516
TOM	3526	C	ARG	462	4.431	23.382	37.552
TOM	3527	O	ARG	462	3.920	23.128	38.648
TOM	3528	N	ALA	463	3.658	23.748	36.524
TOM	3529	CA	ALA	463	2.203	23.593	36.638
TOM	3530	CB	ALA	463	1.421	24.232	35.487
TOM	3531	C	ALA	463	1.907	22.103	36.579
TOM	3532	O	ALA	463	2.800	21.298	36.304
TOM	3533	N	ILE	464	0.708	21.652	36.888
TOM	3534	CA	ILE	464	0.402	20.233	36.718
TOM	3535	CB	ILE	464	0.590	19.631	38.184
TOM	3536	CG2	ILE	464	-0.547	20.041	39.112
TOM	3537	CG1	ILE	464	0.682	18.125	38.116
TOM	3538	CD	ILE	464	1.190	17.462	39.436
TOM	3539	C	ILE	464	-0.987	20.141	36.045
TOM	3540	O	ILE	464	-1.274	21.000	35.201
TOM	3541	N	ASP	465	-1.932	19.228	36.308
TOM	3542	CA	ASP	465	-3.217	19.225	35.591
TOM	3543	CB	ASP	465	-3.975	17.888	35.868
TOM	3544	CG	ASP	465	-4.413	17.124	34.604
TOM	3545	OD1	ASP	465	-5.004	17.716	33.696
TOM	3546	OD2	ASP	465	-4.164	15.922	34.519
TOM	3547	C	ASP	465	-4.136	20.403	35.936
TOM	3548	O	ASP	465	-4.776	20.324	36.983
TOM	3549	N	GLY	466	-4.104	21.528	35.188
TOM	3550	CA	GLY	466	-5.061	22.645	35.358
TOM	3551	C	GLY	466	-5.558	23.197	36.753
TOM	3552	O	GLY	466	-6.298	22.571	37.524
TOM	3553	N	ASP	467	-5.204	24.485	37.005
TOM	3554	CA	ASP	467	-5.493	25.276	38.212
TOM	3555	CB	ASP	467	-6.975	25.241	38.530
TOM	3556	CG	ASP	467	-7.902	25.781	37.456
TOM	3557	OD1	ASP	467	-8.861	26.434	37.830
TOM	3558	OD2	ASP	467	-7.724	25.539	36.261
TOM	3559	C	ASP	467	-4.744	24.928	39.510
TOM	3560	O	ASP	467	-5.148	25.252	40.640
TOM	3561	N	VAL	468	-3.568	24.319	39.288
TOM	3562	CA	VAL	468	-2.583	23.882	40.289

0054

- 91 -

TOM	3563	CB	VAL	468	-2.776	22.411	40.787
TOM	3564	CG1	VAL	468	-3.642	22.426	42.004
TOM	3565	CG2	VAL	468	-3.405	21.535	39.731
TOM	3566	C	VAL	468	-1.104	23.931	39.856
TOM	3567	O	VAL	468	-0.671	23.579	38.741
TOM	3568	N	THR	469	-0.348	24.439	40.814
TOM	3569	CA	THR	469	1.124	24.449	40.802
TOM	3570	CB	THR	469	1.701	25.781	41.260
TOM	3571	OG1	THR	469	1.478	26.686	40.203
TOM	3572	CG2	THR	469	3.143	25.789	41.487
TOM	3573	C	THR	469	1.627	23.386	41.768
TOM	3574	O	THR	469	1.194	23.168	42.916
TOM	3575	N	PHE	470	2.580	22.695	41.183
TOM	3576	CA	PHE	470	3.283	21.629	41.845
TOM	3577	CB	PHE	470	3.267	20.472	40.826
TOM	3578	CG	PHE	470	4.294	19.407	41.128
TOM	3579	CD1	PHE	470	4.046	18.459	42.098
TOM	3580	CD2	PHE	470	5.507	19.453	40.454
TOM	3581	CE1	PHE	470	5.022	17.551	42.406
TOM	3582	CE2	PHE	470	6.484	18.546	40.769
TOM	3583	CZ	PHE	470	6.226	17.602	41.748
TOM	3584	C	PHE	470	4.669	22.156	42.215
TOM	3585	O	PHE	470	5.467	22.458	41.324
TOM	3586	N	CYS	471	5.038	22.341	43.483
TOM	3587	CA	CYS	471	6.422	22.760	43.863
TOM	3588	CB	CYS	471	6.407	23.991	44.710
TOM	3589	SG	CYS	471	5.708	25.309	43.731
TOM	3590	C	CYS	471	7.368	21.818	44.622
TOM	3591	O	CYS	471	7.141	21.681	45.830
TOM	3592	N	ARG	472	8.404	21.138	44.080
TOM	3593	CA	ARG	472	9.315	20.329	44.944
TOM	3594	CB	ARG	472	10.042	19.166	44.174
TOM	3595	CG	ARG	472	9.119	18.015	43.707
TOM	3596	CD	ARG	472	9.553	16.832	42.736
TOM	3597	NE	ARG	472	10.449	17.159	41.622
TOM	3598	CZ	ARG	472	11.684	16.593	41.545
TOM	3599	NH1	ARG	472	12.529	16.922	40.540
TOM	3600	NH2	ARG	472	12.092	15.680	42.459
TOM	3601	C	ARG	472	10.415	21.184	45.643
TOM	3602	O	ARG	472	11.003	22.136	45.075
TOM	3603	N	PRO	473	10.686	20.999	46.940
TOM	3604	CD	PRO	473	9.904	20.198	47.879
TOM	3605	CA	PRO	473	11.834	21.618	47.542
TOM	3606	CB	PRO	473	11.663	21.200	48.965
TOM	3607	CG	PRO	473	10.911	19.897	48.949
TOM	3608	C	PRO	473	13.070	21.087	46.788
TOM	3609	O	PRO	473	13.188	19.919	46.366
TOM	3610	N	LYS	474	14.024	21.970	46.501
TOM	3611	CA	LYS	474	15.204	21.530	45.763
TOM	3612	CB	LYS	474	15.286	22.548	44.672
TOM	3613	CG	LYS	474	15.631	23.934	45.090
TOM	3614	CD	LYS	474	15.619	24.770	43.876
TOM	3615	CE	LYS	474	16.452	24.137	42.788
TOM	3616	NZ	LYS	474	16.359	24.956	41.610
TOM	3617	C	LYS	474	16.486	21.335	46.617
TOM	3618	O	LYS	474	17.629	21.742	46.394
TOM	3619	N	SER	475	16.171	20.664	47.724
TOM	3620	CA	SER	475	17.070	20.205	48.778
TOM	3621	CB	SER	475	17.878	21.291	49.440
TOM	3622	OG	SER	475	18.662	20.589	50.390
TOM	3623	C	SER	475	16.190	19.614	49.859
TOM	3624	O	SER	475	15.275	20.268	50.341
TOM	3625	N	PRO	476	16.325	18.332	50.138
TOM	3626	CD	PRO	476	17.480	17.551	49.752
TOM	3627	CA	PRO	476	15.321	17.520	50.820
TOM	3628	CB	PRO	476	15.897	16.129	50.747

0055

- 92 -

TOM	3629	CG	PRO	476	17.383	16.391	50.713
TOM	3630	C	PRO	476	14.886	17.897	52.247
TOM	3631	O	PRO	476	15.707	18.058	53.165
TOM	3632	N	VAL	477	13.583	17.998	52.530
TOM	3633	CA	VAL	477	13.216	18.411	53.871
TOM	3634	CB	VAL	477	12.414	19.831	53.706
TOM	3635	CG1	VAL	477	12.268	20.289	52.236
TOM	3636	CG2	VAL	477	11.054	19.742	54.329
TOM	3637	C	VAL	477	12.505	17.343	54.751
TOM	3638	O	VAL	477	11.407	16.807	54.544
TOM	3639	N	TYR	478	13.246	16.928	55.758
TOM	3640	CA	TYR	478	12.768	16.028	56.787
TOM	3641	CB	TYR	478	13.811	15.002	57.219
TOM	3642	CG	TYR	478	14.218	14.089	56.065
TOM	3643	CD1	TYR	478	15.251	14.468	55.236
TOM	3644	CE1	TYR	478	15.652	13.646	54.229
TOM	3645	CD2	TYR	478	13.573	12.885	55.890
TOM	3646	CE2	TYR	478	13.975	12.075	54.871
TOM	3647	CZ	TYR	478	15.009	12.463	54.073
TOM	3648	OH	TYR	478	15.425	11.620	53.084
TOM	3649	C	TYR	478	12.423	16.804	58.035
TOM	3650	O	TYR	478	13.244	17.523	58.603
TOM	3651	N	VAL	479	11.219	16.544	58.506
TOM	3652	CA	VAL	479	10.636	17.235	59.628
TOM	3653	CB	VAL	479	9.434	17.940	58.962
TOM	3654	CG1	VAL	479	8.216	16.988	58.925
TOM	3655	CG2	VAL	479	9.325	19.344	59.598
TOM	3656	C	VAL	479	10.338	16.298	60.804
TOM	3657	O	VAL	479	9.895	15.171	60.628
TOM	3658	N	GLY	480	10.542	16.662	62.043
TOM	3659	CA	GLY	480	10.322	15.743	63.124
TOM	3660	C	GLY	480	10.667	16.359	64.459
TOM	3661	O	GLY	480	10.788	17.567	64.561
TOM	3662	N	ASN	481	10.918	15.590	65.496
TOM	3663	CA	ASN	481	11.124	16.146	66.810
TOM	3664	CB	ASN	481	10.989	14.972	67.760
TOM	3665	CG	ASN	481	11.052	15.359	69.212
TOM	3666	OD1	ASN	481	11.784	16.263	69.617
TOM	3667	ND2	ASN	481	10.248	14.745	70.053
TOM	3668	C	ASN	481	12.439	16.929	66.957
TOM	3669	O	ASN	481	13.527	16.422	67.227
TOM	3670	N	GLY	482	12.288	18.201	66.592
TOM	3671	CA	GLY	482	13.380	19.168	66.635
TOM	3672	C	GLY	482	13.804	19.722	65.281
TOM	3673	O	GLY	482	14.650	20.616	65.202
TOM	3674	N	VAL	483	13.324	19.151	64.178
TOM	3675	CA	VAL	483	13.483	19.881	62.956
TOM	3676	CB	VAL	483	14.333	19.066	61.912
TOM	3677	CG1	VAL	483	14.057	17.582	61.921
TOM	3678	CG2	VAL	483	14.084	19.713	60.536
TOM	3679	C	VAL	483	12.071	20.237	62.494
TOM	3680	O	VAL	483	11.191	19.405	62.286
TOM	3681	N	HIS	484	11.830	21.568	62.498
TOM	3682	CA	HIS	484	10.520	22.165	62.133
TOM	3683	CB	HIS	484	9.941	22.999	63.236
TOM	3684	CG	HIS	484	10.999	23.891	63.840
TOM	3685	CD2	HIS	484	11.122	23.994	65.201
TOM	3686	ND1	HIS	484	11.890	24.734	63.295
TOM	3687	CE1	HIS	484	12.522	25.346	64.260
TOM	3688	NE2	HIS	484	12.042	24.885	65.395
TOM	3689	C	HIS	484	10.457	23.050	60.869
TOM	3690	O	HIS	484	11.490	23.592	60.444
TOM	3691	N	ALA	485	9.263	23.233	60.263
TOM	3692	CA	ALA	485	9.308	23.791	58.967
TOM	3693	CB	ALA	485	9.294	22.629	58.007
TOM	3694	C	ALA	485	8.202	24.785	58.689

0056

- 93 -

TOM	3695	O	ALA	485	7.097	24.666	59.206
TOM	3696	N	ASN	486	8.613	25.874	58.023
TOM	3697	CA	ASN	486	7.724	26.945	57.585
TOM	3698	CB	ASN	486	8.080	28.287	58.273
TOM	3699	CG	ASN	486	6.906	29.261	58.286
TOM	3700	OD1	ASN	486	6.880	30.277	57.613
TOM	3701	ND2	ASN	486	5.838	29.002	59.023
TOM	3702	C	ASN	486	7.807	27.126	56.047
TOM	3703	O	ASN	486	8.820	27.129	55.314
TOM	3704	N	LEU	487	6.583	27.138	55.572
TOM	3705	CA	LEU	487	6.361	27.270	54.165
TOM	3706	CB	LEU	487	5.386	26.201	53.737
TOM	3707	CG	LEU	487	4.907	26.134	52.302
TOM	3708	CD1	LEU	487	6.064	25.836	51.337
TOM	3709	CD2	LEU	487	3.800	25.080	52.267
TOM	3710	C	LEU	487	5.820	28.646	53.943
TOM	3711	O	LEU	487	4.796	29.068	54.472
TOM	3712	N	HIS	488	6.563	29.424	53.233
TOM	3713	CA	HIS	488	5.991	30.691	52.944
TOM	3714	CB	HIS	488	7.027	31.771	53.076
TOM	3715	CG	HIS	488	6.557	33.185	52.835
TOM	3716	CD2	HIS	488	6.757	33.866	51.644
TOM	3717	ND1	HIS	488	6.022	33.984	53.714
TOM	3718	CE1	HIS	488	5.915	35.148	53.118
TOM	3719	NE2	HIS	488	6.352	35.066	51.883
TOM	3720	C	HIS	488	5.515	30.594	51.540
TOM	3721	O	HIS	488	6.360	30.517	50.632
TOM	3722	N	VAL	489	4.190	30.623	51.379
TOM	3723	CA	VAL	489	3.576	30.749	50.039
TOM	3724	CB	VAL	489	2.281	29.837	49.922
TOM	3725	CG1	VAL	489	1.205	30.285	50.875
TOM	3726	CG2	VAL	489	1.736	29.895	48.519
TOM	3727	C	VAL	489	3.248	32.222	49.698
TOM	3728	O	VAL	489	2.668	33.044	50.442
TOM	3729	N	ALA	490	3.684	32.582	48.512
TOM	3730	CA	ALA	490	3.589	33.962	48.146
TOM	3731	CB	ALA	490	4.942	34.633	48.073
TOM	3732	C	ALA	490	3.025	34.018	46.772
TOM	3733	O	ALA	490	3.713	33.651	45.809
TOM	3734	N	PHE	491	1.761	34.430	46.741
TOM	3735	CA	PHE	491	1.100	34.657	45.475
TOM	3736	CB	PHE	491	-0.321	34.389	45.608
TOM	3737	CG	PHE	491	-0.662	33.064	46.202
TOM	3738	CD1	PHE	491	-0.415	31.910	45.495
TOM	3739	CD2	PHE	491	-1.291	33.027	47.425
TOM	3740	CE1	PHE	491	-0.821	30.699	46.029
TOM	3741	CE2	PHE	491	-1.684	31.809	47.931
TOM	3742	CZ	PHE	491	-1.455	30.646	47.244
TOM	3743	C	PHE	491	1.213	36.051	44.834
TOM	3744	O	PHE	491	1.091	37.147	45.400
TOM	3745	N	HIS	492	1.501	36.016	43.554
TOM	3746	CA	HIS	492	1.447	37.217	42.771
TOM	3747	CB	HIS	492	2.749	37.399	42.014
TOM	3748	CG	HIS	492	2.859	38.885	41.665
TOM	3749	CD2	HIS	492	2.317	39.465	40.521
TOM	3750	ND1	HIS	492	3.387	39.860	42.408
TOM	3751	CE1	HIS	492	3.171	40.987	41.769
TOM	3752	NE2	HIS	492	2.533	40.741	40.646
TOM	3753	C	HIS	492	0.253	37.240	41.780
TOM	3754	O	HIS	492	0.224	36.433	40.868
TOM	3755	N	ARG	493	-0.627	38.206	41.971
TOM	3756	CA	ARG	493	-1.704	38.538	41.035
TOM	3757	CB	ARG	493	-2.789	39.159	41.874
TOM	3758	CG	ARG	493	-3.146	38.519	43.237
TOM	3759	CD	ARG	493	-3.562	39.716	44.087
TOM	3760	NE	ARG	493	-4.039	39.477	45.432

0057

- 94 -

TOM	3761	CZ	ARG	493	-3.273	38.896	46.350
TOM	3762	NH1	ARG	493	-3.693	38.815	47.625
TOM	3763	NH2	ARG	493	-2.103	38.348	46.025
TOM	3764	C	ARG	493	-1.235	39.506	39.878
TOM	3765	O	ARG	493	-0.801	40.638	40.088
TOM	3766	N	SER	494	-1.192	39.144	38.598
TOM	3767	CA	SER	494	-0.703	40.032	37.522
TOM	3768	CB	SER	494	-0.429	39.201	36.248
TOM	3769	OG	SER	494	-0.014	39.873	35.065
TOM	3770	C	SER	494	-1.619	41.188	37.132
TOM	3771	O	SER	494	-1.273	42.364	36.949
TOM	3772	N	SER	495	-2.873	40.829	36.957
TOM	3773	CA	SER	495	-3.845	41.818	36.555
TOM	3774	CB	SER	495	-4.943	41.253	35.683
TOM	3775	OG	SER	495	-4.331	40.885	34.463
TOM	3776	C	SER	495	-4.482	42.356	37.787
TOM	3777	O	SER	495	-5.314	41.704	38.434
TOM	3778	N	SER	496	-3.933	43.537	38.107
TOM	3779	CA	SER	496	-4.428	44.386	39.206
TOM	3780	CB	SER	496	-3.906	45.799	39.051
TOM	3781	OG	SER	496	-2.492	45.923	39.150
TOM	3782	C	SER	496	-5.961	44.451	39.281
TOM	3783	O	SER	496	-6.625	44.508	38.251
TOM	3784	N	GLU	497	-6.564	44.391	40.471
TOM	3785	CA	GLU	497	-8.010	44.230	40.731
TOM	3786	CB	GLU	497	-8.654	45.652	40.759
TOM	3787	CG	GLU	497	-8.724	46.031	42.251
TOM	3788	CD	GLU	497	-8.763	47.487	42.718
TOM	3789	OE1	GLU	497	-8.177	47.815	43.759
TOM	3790	OE2	GLU	497	-9.390	48.312	42.063
TOM	3791	C	GLU	497	-8.920	43.264	39.918
TOM	3792	O	GLU	497	-10.018	42.945	40.401
TOM	3793	N	LYS	498	-8.492	42.622	38.803
TOM	3794	CA	LYS	498	-9.348	41.805	37.925
TOM	3795	CB	LYS	498	-8.464	41.579	36.699
TOM	3796	CG	LYS	498	-9.167	41.863	35.355
TOM	3797	CD	LYS	498	-8.353	42.835	34.427
TOM	3798	CE	LYS	498	-8.403	44.346	34.843
TOM	3799	NZ	LYS	498	-7.676	44.779	36.054
TOM	3800	C	LYS	498	-10.108	40.505	38.356
TOM	3801	O	LYS	498	-10.565	39.652	37.572
TOM	3802	N	ILE	499	-10.271	40.321	39.662
TOM	3803	CA	ILE	499	-11.178	39.324	40.222
TOM	3804	CB	ILE	499	-10.560	37.899	40.321
TOM	3805	CG2	ILE	499	-9.129	38.049	40.847
TOM	3806	CG1	ILE	499	-11.483	36.942	41.159
TOM	3807	CD	ILE	499	-10.802	35.791	41.945
TOM	3808	C	ILE	499	-11.555	39.792	41.622
TOM	3809	O	ILE	499	-10.680	40.133	42.417
TOM	3810	N	HIS	500	-12.862	39.923	41.853
TOM	3811	CA	HIS	500	-13.494	40.252	43.129
TOM	3812	CB	HIS	500	-13.475	41.785	43.373
TOM	3813	CG	HIS	500	-14.679	42.341	44.158
TOM	3814	CD2	HIS	500	-15.741	43.041	43.615
TOM	3815	ND1	HIS	500	-15.003	42.188	45.433
TOM	3816	CE1	HIS	500	-16.164	42.716	45.716
TOM	3817	NE2	HIS	500	-16.596	43.229	44.597
TOM	3818	C	HIS	500	-14.956	39.721	43.046
TOM	3819	O	HIS	500	-15.651	39.991	42.066
TOM	3820	N	SER	501	-15.560	39.038	44.033
TOM	3821	CA	SER	501	-16.927	38.432	44.041
TOM	3822	CB	SER	501	-18.100	39.297	43.595
TOM	3823	OG	SER	501	-19.236	38.815	44.280
TOM	3824	C	SER	501	-17.120	37.232	43.155
TOM	3825	O	SER	501	-17.602	36.187	43.588
TOM	3826	N	ASN	502	-16.688	37.399	41.907

0058

- 95 -

TOM	3827	CA	ASN	502	-16.652	36.335	40.897
TOM	3828	CB	ASN	502	-16.213	36.966	39.532
TOM	3829	CG	ASN	502	-14.851	37.661	39.602
TOM	3830	OD1	ASN	502	-14.344	37.979	40.687
TOM	3831	ND2	ASN	502	-14.158	37.902	38.501
TOM	3832	C	ASN	502	-15.712	35.179	41.302
TOM	3833	O	ASN	502	-15.803	34.070	40.784
TOM	3834	N	GLU	503	-14.772	35.494	42.208
TOM	3835	CA	GLU	503	-13.846	34.553	42.830
TOM	3836	CB	GLU	503	-13.585	35.139	44.272
TOM	3837	CG	GLU	503	-14.653	35.958	45.096
TOM	3838	CD	GLU	503	-14.210	37.192	45.934
TOM	3839	OE1	GLU	503	-13.136	37.744	45.679
TOM	3840	OE2	GLU	503	-14.960	37.656	46.812
TOM	3841	C	GLU	503	-14.201	33.045	42.815
TOM	3842	O	GLU	503	-13.652	32.316	41.990
TOM	3843	N	ILE	504	-15.152	32.473	43.567
TOM	3844	CA	ILE	504	-15.535	31.037	43.458
TOM	3845	CB	ILE	504	-16.809	30.790	44.424
TOM	3846	CG2	ILE	504	-17.883	31.853	44.140
TOM	3847	CG1	ILE	504	-17.370	29.367	44.279
TOM	3848	CD	ILE	504	-18.217	28.899	45.479
TOM	3849	C	ILE	504	-15.779	30.440	42.056
TOM	3850	O	ILE	504	-15.605	29.242	41.811
TOM	3851	N	SER	505	-16.064	31.330	41.125
TOM	3852	CA	SER	505	-16.331	30.996	39.729
TOM	3853	CB	SER	505	-17.638	31.605	39.338
TOM	3854	OG	SER	505	-18.559	31.320	40.385
TOM	3855	C	SER	505	-15.258	31.464	38.742
TOM	3856	O	SER	505	-15.300	31.129	37.548
TOM	3857	N	SER	506	-14.274	32.275	39.187
TOM	3858	CA	SER	506	-13.072	32.645	38.401
TOM	3859	CB	SER	506	-12.424	33.915	38.898
TOM	3860	OG	SER	506	-12.147	33.853	40.285
TOM	3861	C	SER	506	-12.018	31.543	38.525
TOM	3862	O	SER	506	-10.842	31.682	38.876
TOM	3863	N	ASP	507	-12.513	30.381	38.161
TOM	3864	CA	ASP	507	-11.864	29.129	38.395
TOM	3865	CB	ASP	507	-10.643	29.034	37.428
TOM	3866	CG	ASP	507	-10.917	28.577	35.968
TOM	3867	OD1	ASP	507	-9.945	28.424	35.220
TOM	3868	OD2	ASP	507	-12.067	28.357	35.560
TOM	3869	C	ASP	507	-11.499	28.871	39.865
TOM	3870	O	ASP	507	-12.411	28.701	40.674
TOM	3871	N	SER	508	-10.293	28.920	40.400
TOM	3872	CA	SER	508	-10.037	28.207	41.673
TOM	3873	CB	SER	508	-8.467	28.073	41.903
TOM	3874	OG	SER	508	-7.616	27.377	40.962
TOM	3875	C	SER	508	-10.623	28.458	43.078
TOM	3876	O	SER	508	-9.922	28.872	44.016
TOM	3877	N	ILE	509	-11.957	28.268	43.215
TOM	3878	CA	ILE	509	-12.503	27.836	44.513
TOM	3879	CB	ILE	509	-13.810	28.545	45.056
TOM	3880	CG2	ILE	509	-14.750	27.644	45.900
TOM	3881	CG1	ILE	509	-13.349	29.616	46.010
TOM	3882	CD	ILE	509	-12.448	29.091	47.169
TOM	3883	C	ILE	509	-12.881	26.385	44.210
TOM	3884	O	ILE	509	-12.079	25.466	44.455
TOM	3885	N	GLY	510	-13.991	26.153	43.489
TOM	3886	CA	GLY	510	-14.466	24.801	43.229
TOM	3887	C	GLY	510	-13.472	23.910	42.500
TOM	3888	O	GLY	510	-13.753	22.727	42.348
TOM	3889	N	VAL	511	-12.323	24.471	42.058
TOM	3890	CA	VAL	511	-11.306	23.730	41.297
TOM	3891	CB	VAL	511	-10.743	24.718	40.264
TOM	3892	CG1	VAL	511	-10.049	23.873	39.214

0059

- 96 -

TOM	3893	CG2	VAL	511	-11.832	25.496	39.502
TOM	3894	C	VAL	511	-10.170	22.997	42.042
TOM	3895	O	VAL	511	-9.464	22.100	41.563
TOM	3896	N	LEU	512	-10.046	23.406	43.295
TOM	3897	CA	LEU	512	-9.128	22.753	44.211
TOM	3898	CB	LEU	512	-7.656	23.298	44.186
TOM	3899	CG	LEU	512	-6.520	22.630	45.055
TOM	3900	CD1	LEU	512	-6.199	21.232	44.567
TOM	3901	CD2	LEU	512	-5.230	23.427	44.938
TOM	3902	C	LEU	512	-9.677	23.004	45.581
TOM	3903	O	LEU	512	-9.976	21.987	46.169
TOM	3904	N	GLY	513	-9.851	24.233	46.111
TOM	3905	CA	GLY	513	-10.337	24.441	47.508
TOM	3906	C	GLY	513	-9.313	24.581	48.692
TOM	3907	O	GLY	513	-9.523	25.242	49.717
TOM	3908	N	TYR	514	-8.118	24.004	48.534
TOM	3909	CA	TYR	514	-7.070	23.942	49.543
TOM	3910	CB	TYR	514	-7.112	22.652	50.413
TOM	3911	CG	TYR	514	-7.236	21.266	49.755
TOM	3912	CD1	TYR	514	-7.611	20.224	50.576
TOM	3913	CE1	TYR	514	-7.790	18.955	50.063
TOM	3914	CD2	TYR	514	-7.039	21.015	48.395
TOM	3915	CE2	TYR	514	-7.214	19.751	47.865
TOM	3916	CZ	TYR	514	-7.592	18.721	48.713
TOM	3917	OH	TYR	514	-7.755	17.424	48.234
TOM	3918	C	TYR	514	-5.685	23.961	48.973
TOM	3919	O	TYR	514	-5.474	23.612	47.816
TOM	3920	N	GLN	515	-4.770	24.354	49.838
TOM	3921	CA	GLN	515	-3.355	24.227	49.535
TOM	3922	CB	GLN	515	-2.538	25.348	50.150
TOM	3923	CG	GLN	515	-3.016	26.626	49.493
TOM	3924	CD	GLN	515	-3.158	27.807	50.424
TOM	3925	OE1	GLN	515	-4.175	28.020	51.060
TOM	3926	NE2	GLN	515	-2.171	28.662	50.595
TOM	3927	C	GLN	515	-2.949	22.916	50.185
TOM	3928	O	GLN	515	-3.320	22.614	51.337
TOM	3929	N	LYS	516	-2.265	22.029	49.463
TOM	3930	CA	LYS	516	-1.832	20.843	50.165
TOM	3931	CB	LYS	516	-2.566	19.569	49.865
TOM	3932	CG	LYS	516	-4.075	19.455	49.936
TOM	3933	CD	LYS	516	-4.434	17.964	49.966
TOM	3934	CE	LYS	516	-4.276	17.238	48.660
TOM	3935	NZ	LYS	516	-2.891	17.090	48.250
TOM	3936	C	LYS	516	-0.430	20.472	49.923
TOM	3937	O	LYS	516	0.197	20.492	48.871
TOM	3938	N	THR	517	-0.038	20.383	51.162
TOM	3939	CA	THR	517	1.246	19.917	51.578
TOM	3940	CB	THR	517	1.480	20.356	53.051
TOM	3941	OG1	THR	517	0.270	20.879	53.557
TOM	3942	CG2	THR	517	2.493	21.465	53.185
TOM	3943	C	THR	517	1.288	18.395	51.436
TOM	3944	O	THR	517	0.596	17.660	52.143
TOM	3945	N	VAL	518	2.006	17.858	50.457
TOM	3946	CA	VAL	518	2.206	16.404	50.310
TOM	3947	CB	VAL	518	2.322	16.262	48.723
TOM	3948	CG1	VAL	518	2.938	14.991	48.154
TOM	3949	CG2	VAL	518	0.885	16.244	48.263
TOM	3950	C	VAL	518	3.385	15.858	51.198
TOM	3951	O	VAL	518	4.478	16.416	51.300
TOM	3952	N	ASP	519	3.122	14.871	52.032
TOM	3953	CA	ASP	519	4.112	14.157	52.853
TOM	3954	CB	ASP	519	3.344	13.860	54.200
TOM	3955	CG	ASP	519	3.950	13.220	55.479
TOM	3956	OD1	ASP	519	3.171	13.004	56.421
TOM	3957	OD2	ASP	519	5.160	12.961	55.556
TOM	3958	C	ASP	519	4.820	12.902	52.247

- 97 -

TOM	3959	O	ASP	519	5.415	12.955	51.152
TOM	3960	N	HIS	520	4.811	11.703	52.854
TOM	3961	CA	HIS	520	5.628	10.577	52.388
TOM	3962	CB	HIS	520	6.282	9.849	53.523
TOM	3963	CG	HIS	520	5.412	9.313	54.628
TOM	3964	CD2	HIS	520	5.272	9.906	55.868
TOM	3965	ND1	HIS	520	4.653	8.223	54.620
TOM	3966	CE1	HIS	520	4.067	8.131	55.799
TOM	3967	NE2	HIS	520	4.447	9.152	56.539
TOM	3968	C	HIS	520	4.979	9.470	51.575
TOM	3969	O	HIS	520	3.845	9.115	51.876
TOM	3970	N	THR	521	5.713	8.772	50.705
TOM	3971	CA	THR	521	5.137	7.687	49.925
TOM	3972	CB	THR	521	5.657	7.770	48.464
TOM	3973	OG1	THR	521	4.472	7.381	47.798
TOM	3974	CG2	THR	521	6.828	6.907	47.981
TOM	3975	C	THR	521	5.289	6.251	50.418
TOM	3976	O	THR	521	6.327	5.633	50.637
TOM	3977	N	GLU	522	4.154	5.824	50.908
TOM	3978	CA	GLU	522	3.877	4.407	51.140
TOM	3979	CB	GLU	522	3.805	4.067	52.656
TOM	3980	CG	GLU	522	3.750	2.537	52.657
TOM	3981	CD	GLU	522	4.008	1.699	53.906
TOM	3982	OE1	GLU	522	3.037	1.396	54.605
TOM	3983	OE2	GLU	522	5.159	1.298	54.140
TOM	3984	C	GLU	522	2.537	4.654	50.462
TOM	3985	O	GLU	522	2.399	4.543	49.241
TOM	3986	N	ILE	523	1.579	5.150	51.240
TOM	3987	CA	ILE	523	0.536	5.974	50.599
TOM	3988	CB	ILE	523	-0.653	6.181	51.658
TOM	3989	CG2	ILE	523	-0.264	7.019	52.877
TOM	3990	CG1	ILE	523	-1.811	6.827	50.934
TOM	3991	CD	ILE	523	-2.737	5.764	50.284
TOM	3992	C	ILE	523	1.238	7.333	50.180
TOM	3993	O	ILE	523	2.004	7.750	51.058
TOM	3994	N	LYS	524	1.295	8.058	49.017
TOM	3995	CA	LYS	524	1.768	9.479	49.072
TOM	3996	CB	LYS	524	2.052	9.933	47.664
TOM	3997	CG	LYS	524	2.777	11.297	47.487
TOM	3998	CD	LYS	524	3.230	11.388	46.001
TOM	3999	CE	LYS	524	2.216	10.818	44.923
TOM	4000	NZ	LYS	524	2.766	10.509	43.604
TOM	4001	C	LYS	524	0.803	10.509	49.815
TOM	4002	O	LYS	524	-0.060	11.275	49.383
TOM	4003	N	SER	525	0.921	10.327	51.113
TOM	4004	CA	SER	525	0.254	11.025	52.175
TOM	4005	CB	SER	525	0.828	10.689	53.533
TOM	4006	OG	SER	525	0.605	11.735	54.456
TOM	4007	C	SER	525	0.348	12.491	52.051
TOM	4008	O	SER	525	1.443	13.037	52.069
TOM	4009	N	LYS	526	-0.878	12.959	51.923
TOM	4010	CA	LYS	526	-1.306	14.319	51.798
TOM	4011	CB	LYS	526	-2.276	14.376	50.639
TOM	4012	CG	LYS	526	-1.685	13.941	49.310
TOM	4013	CD	LYS	526	-2.791	14.112	48.250
TOM	4014	CE	LYS	526	-2.134	14.448	46.901
TOM	4015	NZ	LYS	526	-2.987	15.233	46.007
TOM	4016	C	LYS	526	-1.932	15.034	52.998
TOM	4017	O	LYS	526	-2.925	14.608	53.592
TOM	4018	N	LEU	527	-1.357	16.193	53.314
TOM	4019	CA	LEU	527	-1.867	17.113	54.307
TOM	4020	CB	LEU	527	-0.794	17.650	55.191
TOM	4021	CG	LEU	527	0.030	16.853	56.187
TOM	4022	CD1	LEU	527	-0.728	15.630	56.590
TOM	4023	CD2	LEU	527	1.377	16.503	55.572
TOM	4024	C	LEU	527	-2.546	18.336	53.696

0061

- 98 -

TOM	4025	O	LEU	527	-1.932	19.201	53.076
TOM	4026	N	SER	528	-3.837	18.468	53.969
TOM	4027	CA	SER	528	-4.730	19.520	53.458
TOM	4028	CB	SER	528	-6.108	18.875	53.280
TOM	4029	OG	SER	528	-6.102	17.614	52.578
TOM	4030	C	SER	528	-4.916	20.859	54.199
TOM	4031	O	SER	528	-5.715	20.927	55.145
TOM	4032	N	LEU	529	-4.220	21.958	53.894
TOM	4033	CA	LEU	529	-4.581	23.267	54.490
TOM	4034	CB	LEU	529	-3.331	24.198	54.549
TOM	4035	CG	LEU	529	-2.540	24.439	55.842
TOM	4036	CD1	LEU	529	-3.440	24.181	57.042
TOM	4037	CD2	LEU	529	-1.316	23.572	55.876
TOM	4038	C	LEU	529	-5.733	24.078	53.813
TOM	4039	O	LEU	529	-5.559	24.547	52.674
TOM	4040	N	PHE	530	-6.952	24.300	54.350
TOM	4041	CA	PHE	530	-7.968	25.129	53.634
TOM	4042	CB	PHE	530	-9.392	24.694	53.828
TOM	4043	CG	PHE	530	-9.762	23.269	53.576
TOM	4044	CD1	PHE	530	-10.182	22.898	52.321
TOM	4045	CD2	PHE	530	-9.734	22.393	54.625
TOM	4046	CE1	PHE	530	-10.604	21.607	52.088
TOM	4047	CE2	PHE	530	-10.162	21.103	54.391
TOM	4048	CZ	PHE	530	-10.594	20.705	53.134
TOM	4049	C	PHE	530	-8.150	26.634	53.813
TOM	4050	O	PHE	530	-8.552	27.157	54.867
TOM	4051	N	PHE	531	-8.062	27.269	52.653
TOM	4052	CA	PHE	531	-8.173	28.720	52.481
TOM	4053	CB	PHE	531	-7.366	29.099	51.248
TOM	4054	CG	PHE	531	-7.685	28.542	49.846
TOM	4055	CD1	PHE	531	-8.610	29.174	49.037
TOM	4056	CD2	PHE	531	-6.956	27.493	49.327
TOM	4057	CE1	PHE	531	-8.799	28.774	47.727
TOM	4058	CE2	PHE	531	-7.152	27.108	48.025
TOM	4059	CZ	PHE	531	-8.070	27.740	47.214
TOM	4060	C	PHE	531	-9.530	29.402	52.406
TOM	4061	O	PHE	531	-10.563	28.846	52.769
TOM	4062	N	GLU	532	-9.563	30.636	51.936
TOM	4063	CA	GLU	532	-10.743	31.498	51.883
TOM	4064	CB	GLU	532	-11.081	31.901	53.266
TOM	4065	CG	GLU	532	-12.539	31.927	53.432
TOM	4066	CD	GLU	532	-12.892	31.794	54.867
TOM	4067	OE1	GLU	532	-12.466	32.646	55.647
TOM	4068	OE2	GLU	532	-13.579	30.828	55.172
TOM	4069	C	GLU	532	-10.446	32.759	51.076
TOM	4070	O	GLU	532	-9.580	33.486	51.535
TOM	4071	N	ILE	533	-11.047	33.122	49.931
TOM	4072	CA	ILE	533	-10.674	34.331	49.131
TOM	4073	CB	ILE	533	-10.766	33.950	47.635
TOM	4074	CG2	ILE	533	-9.703	34.768	46.934
TOM	4075	CG1	ILE	533	-10.512	32.470	47.373
TOM	4076	CD	ILE	533	-10.994	32.039	46.003
TOM	4077	C	ILE	533	-11.419	35.694	49.351
TOM	4078	O	ILE	533	-12.366	36.004	48.625
TOM	4079	N	LYS	534	-11.048	36.582	50.289
TOM	4080	CA	LYS	534	-11.858	37.772	50.596
TOM	4081	CB	LYS	534	-11.587	38.197	52.012
TOM	4082	CG	LYS	534	-12.566	37.632	53.000
TOM	4083	CD	LYS	534	-12.402	36.141	53.314
TOM	4084	CE	LYS	534	-13.673	35.777	54.044
TOM	4085	NZ	LYS	534	-13.703	36.545	55.271
TOM	4086	C	LYS	534	-11.828	39.058	49.753
TOM	4087	O	LYS	534	-10.888	39.279	48.972
TOM	4088	N	SER	535	-12.802	39.966	50.068
TOM	4089	CA	SER	535	-13.199	41.192	49.328
TOM	4090	CB	SER	535	-12.117	42.240	49.369

0062

- 9.9 -

TOM	4091	OG	SER	535	-11.539	42.176	50.65
TOM	4092	C	SER	535	-13.561	40.901	47.844
TOM	4093	OT1	SER	535	-14.672	40.373	47.615
TOM	4094	OT2	SER	535	-12.817	41.184	46.880
ND							

- 100 -

Claims

1. A chimeric diphtheria toxin molecule
wherein all or part of a CDR of an antibody is
inserted into a loop region of the diphtheria toxin
5 receptor binding-domain.

2. The molecule of claim 1, said antibody being
capable of specifically binding a cell surface
antigen expressed on a cell, said chimeric
diphtheria toxin molecule being capable of
10 specifically binding said cell surface antigen and
being substantially incapable of binding to the
diphtheria toxin receptor.

3. The molecule of claim 1 wherein all or part
of a first said CDR is inserted into a first said
15 loop region, all or part of a second said CDR is
inserted into a second said loop region, and said
first and second CDR are of a single antibody chain.

4. The molecule of claim 2 said molecule being
capable of decreasing the viability of said cell.

20 5. The molecule of claim 4 wherein said
molecule kills said cell.

6. The molecule of claim 1 wherein said loop
region is RL3 and said CDR is a CDR1.

25 7. The molecule of claim 1 wherein said loop
region is RL9 and said CDR is a CDR3.

8. The molecule of claim 2 wherein said
molecule lacks diphtheria toxin catalytic activity.

- 101 -

9. The molecule of claim 8 wherein said molecule lacks all or part of the catalytic domain of diphtheria toxin.

5 10. A hybrid molecule comprising a first and a second portion joined together covalently, said first portion comprising the molecule of claim 8 and said second portion comprising a molecule to be delivered to said cell.

10 11. The hybrid molecule of claim 10 wherein said molecule to be delivered to said cell is a protein.

12. The hybrid molecule of claim 11 wherein said protein is an enzyme.

15 13. The hybrid molecule of claim 11 wherein said protein modulates transcription.

14. The hybrid molecule of claim 11 wherein said protein is a nucleic acid-binding protein.

20 15. The hybrid molecule of claim 14 wherein said nucleic acid binding protein is capable of binding a single-stranded nucleic acid.

16. The hybrid molecule of claim 10 wherein said molecule to be delivered to said cell is a nucleic acid.

- 102 -

17. The molecule of claim 2 wherein the amino-terminus of a second diphtheria toxin receptor-binding domain is connected to the carboxy-terminus of said first diphtheria toxin receptor-binding domain, said diphtheria toxin second receptor-binding domain being substantially incapable of binding to the diphtheria toxin receptor.

18. The molecule of claim 17 wherein said carboxy terminus is connected to said amino terminus through a polypeptide chain.

19. The molecule of claim 17 wherein all or part of a CDR of an antibody is inserted into a loop region of said second diphtheria toxin receptor-binding domain.

20. The molecule of claim 19 wherein all or part of a first said CDR is inserted into a first said loop region of said first diphtheria toxin receptor-binding domain and all or part of a second said CDR is inserted into a second said loop region of said first diphtheria toxin receptor-binding domain.

21. The molecule of claim 20 wherein all or part of a third said CDR is inserted into a first loop region of said second diphtheria toxin receptor-binding domain and all or part of a fourth said CDR is inserted into a second said loop region of said second receptor-binding domain.

22. The molecule of claim 21 wherein said first and said second CDR are of a first antibody

- 103 -

chain and said third and said fourth said CDR are of a second antibody chain.

23. The molecule of claim 22 wherein said first and said second antibody chains are from antibodies recognizing the same antigen.

24. The molecule of claim 24 wherein said first and second antibody chains are from the same antibody molecule.

25. The molecule of claim 23 wherein said first antibody chain is the light chain of an antibody and said second antibody chain is the heavy chain of said same antibody.

26. A chimeric diphtheria toxin molecule wherein all or part of a CDR-like sequence of a ligand binding protein having an antibody variable domain-like ligand binding-domain is inserted into a loop region of the receptor binding domain of diphtheria toxin.

27. The chimeric diphtheria toxin molecule of claim 26 wherein said ligand binding protein having an antibody variable domain-like ligand binding-domain is tumor necrosis factor.

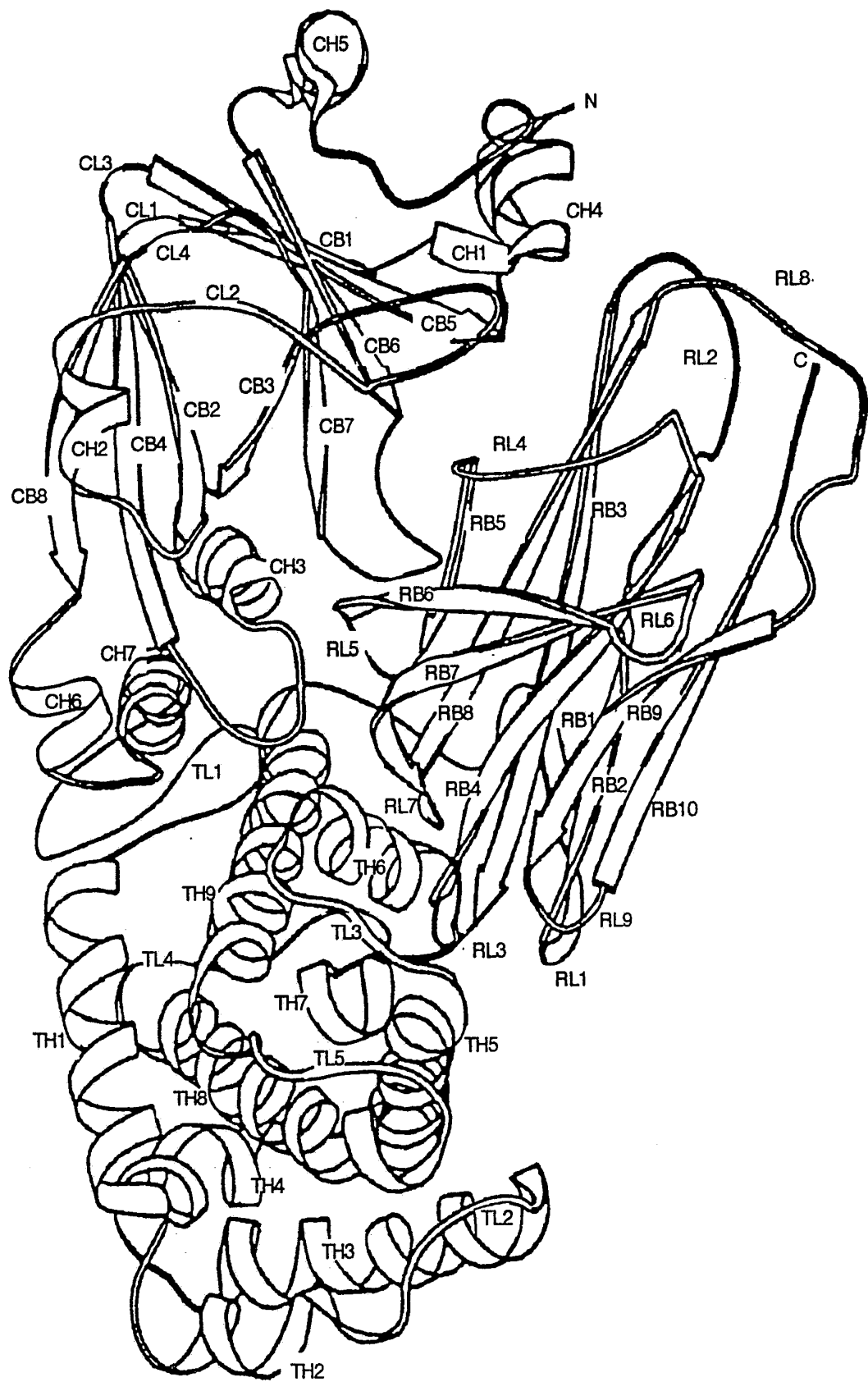


FIG. 1



FIG. 2



FIG. 3

4/10



FIG. 4

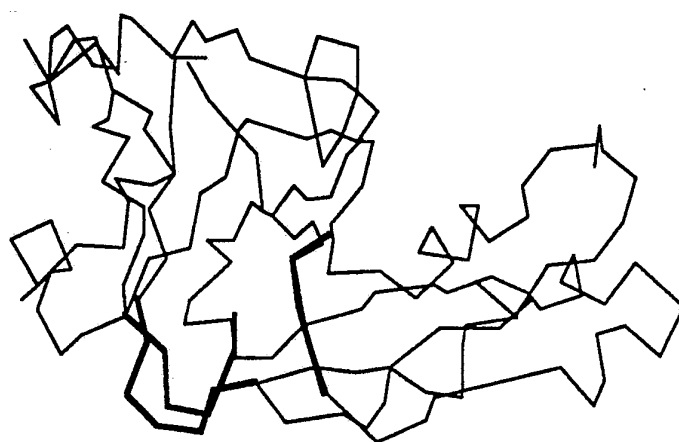
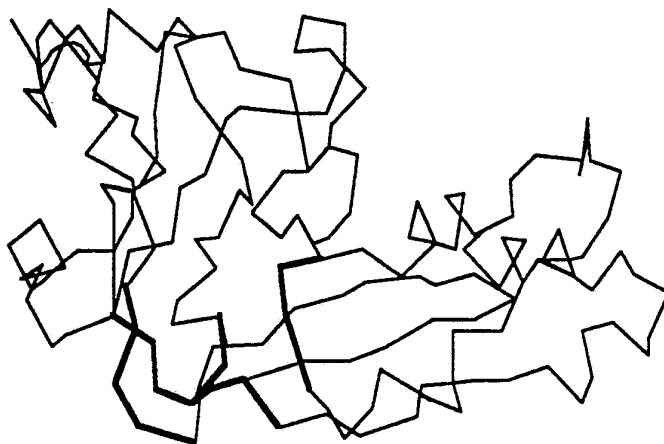


FIG. 5

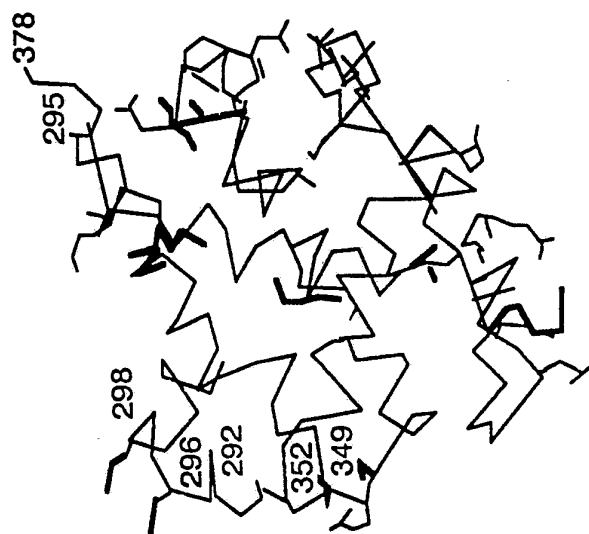
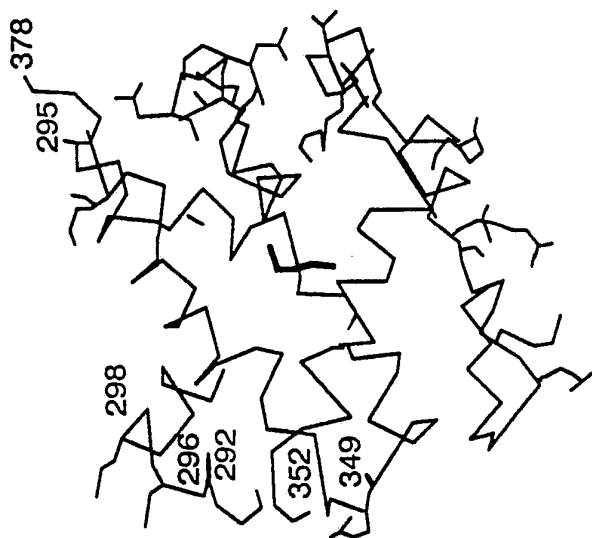


FIG. 6

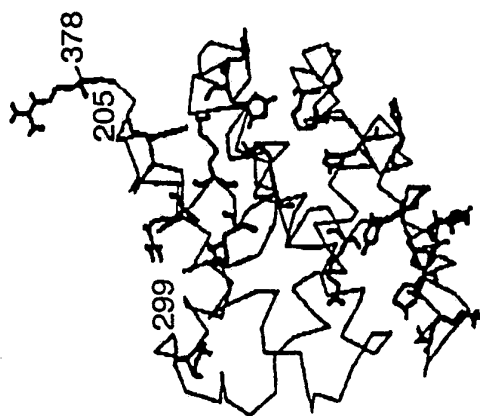
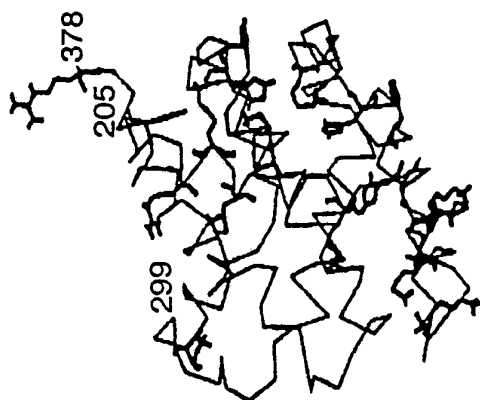


FIG. 7

FIG. 8C

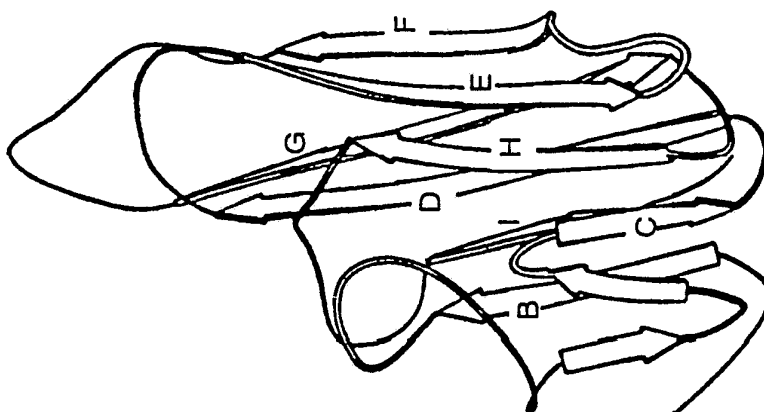


FIG. 8B

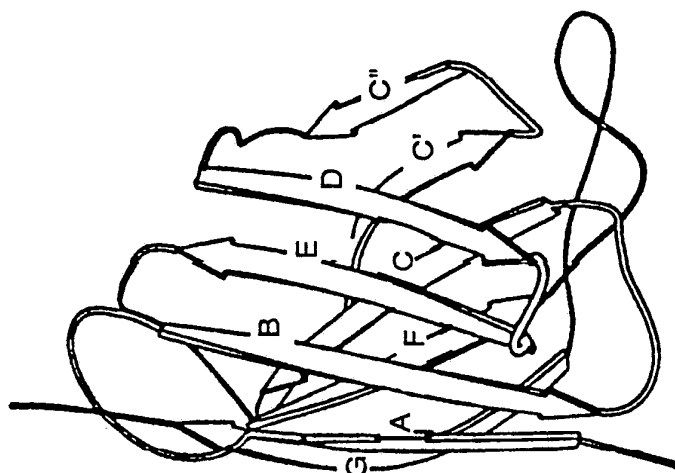
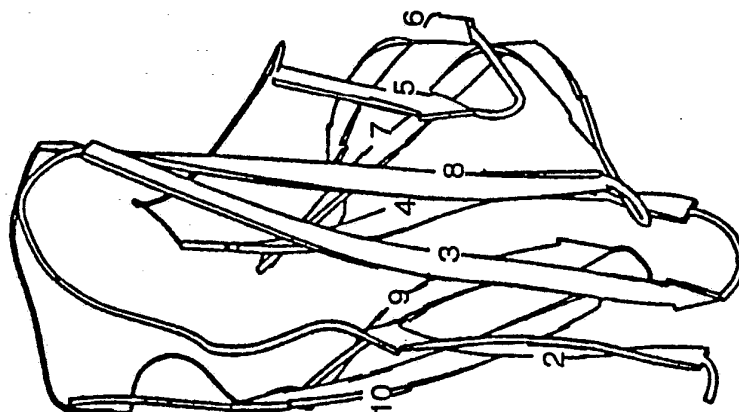


FIG. 8A



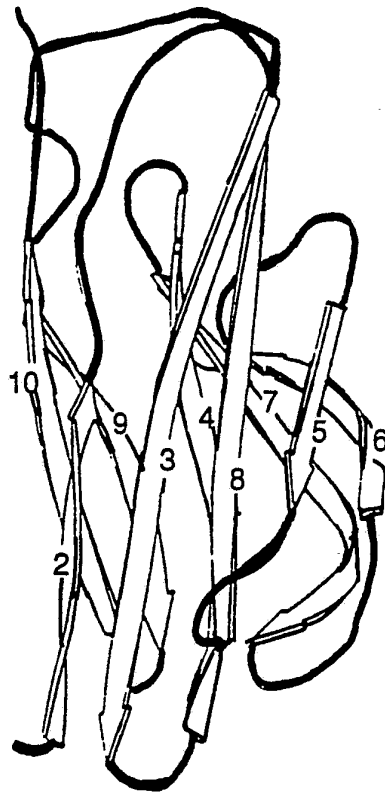


FIG. 9A

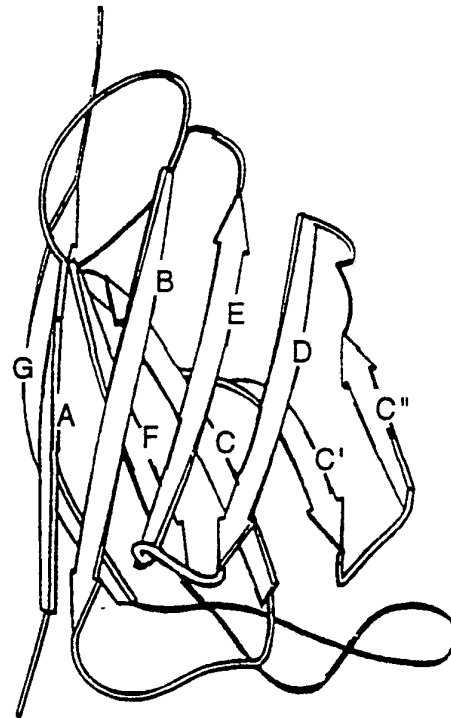


FIG. 9B

10/10

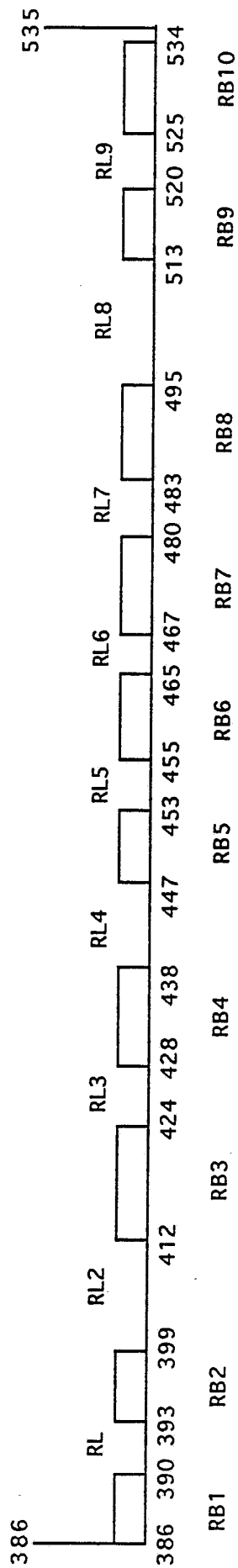


FIG. 10A

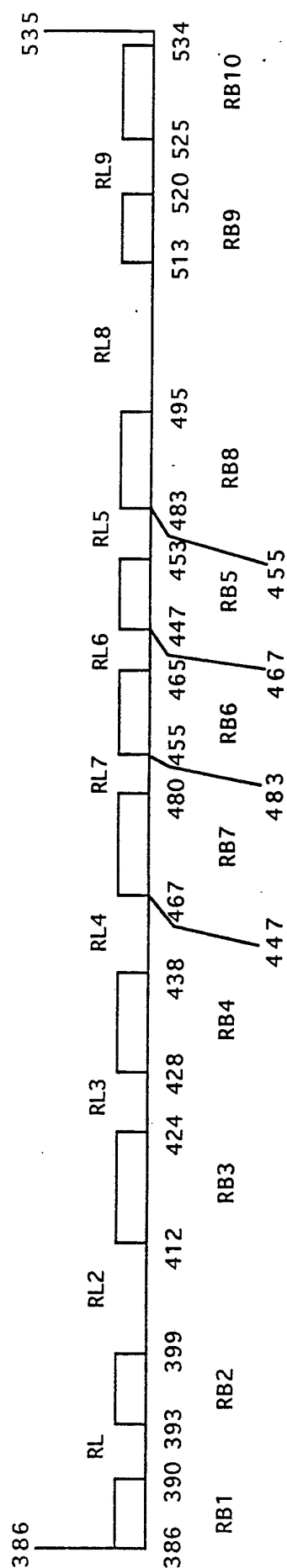


FIG. 10B

INTERNATIONAL SEARCH REPORT

International application No.
PCT/US93/04335**A. CLASSIFICATION OF SUBJECT MATTER**

IPC(5) :C12P 21/08; C07K 15/00, 3/00, 13/00.

US CL :530/387.1, 387.3, 350.

According to International Patent Classification (IPC) or to both national classification and IPC

B. FIELDS SEARCHED

Minimum documentation searched (classification system followed by classification symbols)

U.S. : 530/387.1, 387.3, 350.

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

Electronic data base consulted during the international search (name of data base and, where practicable, search terms used)
Dialog, APS**C. DOCUMENTS CONSIDERED TO BE RELEVANT**

Category*	Citation of document, with indication, where appropriate, of the relevant passages	Relevant to claim No.
A	Science Volume 238, issued 20 November 1987, Vitetta et. al., "Redesigning Nature's Poisons to Create Anti-Tumor Reagents", pages 1098-1104, see entire article.	1-27
A	US, A, 4,946,778 (Ladner et. al.) 07 August 1990, cols. 29-32.	1-27

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

* Special categories of cited documents:	*T later document published after the international filing date or priority date and not in conflict with the application but cited to understand the principle or theory underlying the invention
*A document defining the general state of the art which is not considered to be part of particular relevance	*X document of particular relevance; the claimed invention cannot be considered novel or cannot be considered to involve an inventive step when the document is taken alone
*E earlier document published on or after the international filing date	*Y document of particular relevance; the claimed invention cannot be considered to involve an inventive step when the document is combined with one or more other such documents, such combination being obvious to a person skilled in the art
*L document which may throw doubts on priority claim(s) or which is cited to establish the publication date of another citation or other special reason (as specified)	*Z document member of the same patent family
*O document referring to an oral disclosure, use, exhibition or other means	
*P document published prior to the international filing date but later than the priority date claimed	

Date of the actual completion of the international search
06 August 1993Date of mailing of the international search report
16 AUG 1993Name and mailing address of the ISA/US
Commissioner of Patents and Trademarks
Box PCT
Washington, D.C. 20231

Authorized officer

DAVID LACEY

Facsimile No. NOT APPLICABLE

Telephone No. (703) 308-0196