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(54) **Titre : ANTICORPS MONOCLONAUX IgE DE LIAISON A UN ALLERGENE ET PROCEDE DE PREPARATION
D'HYPOALLERGENES**

(54) **Title: ALLERGEN-BINDING IgE MONOCLONAL ANTIBODIES AND METHOD FOR PREPARING HYPOALLERGENS**

(57) **Abrégé/Abstract:**

The present invention relates to human IgE antibodies and derivatives thereof, which bind non-continuous planar allergenic epitope, such as in β -lactoglobulin, with high affinity and specificity. The present invention also relates to processes for making and engineering such allergen binding monoclonal antibodies and to methods for using these antibodies and derivatives thereof in the field of immunodiagnostics and immunotherapy.



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(54) Title: ALLERGEN-BINDING IGE MONOCLONAL ANTIBODIES AND METHOD FOR PREPARING HYPOALLERGENS

(57) Abstract: The present invention relates to human IgE antibodies and derivatives thereof, which bind non-continuous planar allergenic epitope, such as in β -lactoglobulin, with high affinity and specificity. The present invention also relates to processes for making and engineering such allergen binding monoclonal antibodies and to methods for using these antibodies and derivatives thereof in the field of immunodiagnostics and immunotherapy.



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Allergen-binding IgE monoclonal antibodies and method for preparing hypoallergens**FIELD OF THE INVENTION**

5 This invention relates to protein engineering technology. More particularly, the present invention relates to human IgE antibodies and derivatives thereof, which bind non-continuous allergenic epitope, a planar surface with the area of 600-900 Å², e.g. IgE antibodies binding to bovine milk β-lactoglobulin with high affinity and specificity. The present invention also relates to processes for making and engineering such allergen-
10 binding monoclonal antibodies with Type I interaction and to methods for using these antibodies and derivatives thereof in the field of immunodiagnostics, enabling qualitative and quantitative determination and removal of allergenic substances in biological and raw material samples, as well as the construction of focused IgE libraries towards allergens, enabling the development of allergen-specific antibodies. In immunotherapy, the present
15 invention enables blocking the Type I surface interaction of allergenic substances by modifying amino acid residues of allergens. Hypoallergen variant can be obtained by mutating some (1-5) amino acid residues on the planar (flat) epitope surface with bulky residues (such as Arg, Tyr, Lys, Trp). The mutated residues are those which side chains are pointing outside towards solvent thus causing minimal change to the basic structure of the
20 allergen. The purpose of the mutagenesis is to modify the flat surface to convex surface which prevent the binding of IgE-antibodies. The resulting modified allergen can be used to evoke tolerance against particular allergens in allergic patients. The present invention allows the development of human IgE VH-region derived antibodies for those therapeutic and diagnostic targets where the binding specificity is towards areas of protein structures
25 that are not located on the protruding regions of the surface. The invention also provides means for screening or molecular modelling of substances capable of blocking the binding of an antibody to the Type I allergenic epitope. In this invention, the development, characterisation and structure determination of the human IgE antibody fragment and derivatives thereof that binds allergenic β-lactoglobulin with affinity and specificity high
30 enough to be utilised as reagents in immunoassays are also described.

BACKGROUND OF THE INVENTION

Almost 20% of the population world-wide are suffering from allergy. Consequently, it is a health problem of increasing seriousness. Allergy is a hypersensitivity reaction against substances in air, food or water, which are normally harmless (Corry and Kheradmand, 1999). A new and foreign external agent triggers an allergic reaction, which aims at disposal of that agent from the body. In IgE-mediated allergic reactions, also called immediate or type I hypersensitivity reactions, under the first exposure of a foreign substance, allergen, to the body, IgE-bearing B-cells begin to produce soluble IgE molecules which will then bind to high-affinity IgE receptors present on the surface of a wide variety of cells, most importantly to mast cells and basophils. If the same foreign substance is encountered again, the cross-linking of the receptor-bound IgE molecules by the allergen occurs, resulting in cellular activation followed by the release of toxic products such as histamine, which will elicit the signs and symptoms of an allergic reaction.

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Cow's milk allergy (CMA) is a most common cause of clinically important adverse food reactions with infants and children during the first 2 years of life (Savilahti, 1981; Host and Halken, 1990; Saarinen et al., 1999). It is characterized by a strong IgE response to milk proteins and clinical symptoms in skin and gastrointestinal tract such as atopic eczema, vomiting and diarrhoea (Vaarala et al., 1995; Saarinen, 2000). Symptoms in respiratory ducts and anaphylactic shock are also possible (Host and Halken, 1990; Schrandt et al., 1993; Hill et al., 1999; Vanto et al., 1999; Saarinen, 2000). CMA is a serious problem with children, because milk is an important source of energy (up to 50%) for young children and is not very easily replaceable with non-dairy products. Nearly 85% of the milk allergic children will outgrow of their allergy by the age of 3, but remission of CMA may occur in up to one-third of older children (Sampson and Scanlon, 1989)

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One of the major allergens in cow's milk is β -lactoglobulin, which belongs to the protein family known as lipocalins. Lipocalins consists a group of a small ligand binding proteins, mostly respiratory allergens such as Mus m1, Rat n1 (mouse and rat urinary proteins) and a German cockroach allergen Bla g4 (Rouvinen et al. 2001). β -lactoglobulin occurs naturally in the form of a 36 kD dimer with each subunit corresponding 162 amino acids. Totally six genetic variants of the β -lactoglobulin has been identified based on the sequence

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differences. The most prevalent variants A and B differ only at the position 64 (Asp → Gly) and 118 (Val → Ala) (Godovac-Zimmermann and Braunitzer, 1987). The 3D-structure of the β -lactoglobulin has been determined by X-ray diffraction (Sawyer L. et al, 1985, Brownlow, S. et al, 1997)

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IgE antibodies distinctively recognise allergenic epitopes, which would be useful in clinics and immunodiagnostics for detecting and determining allergen concentrations of complex materials. Further, according to this invention, allergenic epitopes are usually different from the immunogenic epitopes of proteins. This fact has hampered the production of monoclonal antibodies capable of specific binding of allergenic epitopes by conventional methodology such as hybridoma technology. It has been recently shown that the development of allergen-specific IgE antibodies is possible by the phage display technology (Steinberger *et al.*, 1996). This methodology is giving new tools to produce allergen-specific recombinant antibodies that can be produced in consistent quality for clinical and diagnostic applications.

The technical problem to which the present invention is related is the detection of actual binding sites of IgE antibodies in allergenic polypeptides and use of this information, e.g., to modify these polypeptides to decrease their allergenicity. Previous solutions for this problem are disclosed in U.S. Patent Application No. 2003/0175312 (Holm et al.), WO 03/096869 (Alk Abello A/S) and Jenkins et al. 2005 (J. Allergy Clin. Immunol. 115:163-170). In these documents, it is described that the putative IgE binding sites in allergenic polypeptides may be detected by sequence analysis of conserved surface structures of allergenic polypeptides. Further, in US 2005/0181446 (Roggen et al.) and Hantusch et al. 2004 (J. Allergy Clin. Immunol.) a peptide-scan approach is used to find IgE binding epitopes. However, none of these documents discloses the method of the present invention wherein an IgE binding site on an allergenic polypeptide is found based on the experimental 3D and molecular modelling data of a novel type of IgE epitope having essentially planar or flat nature. MacCallum et al. 1996 (J. Mol. Biol. 262:732-745) disclose the presence of planar surfaces on antibodies, but teach only modification of antibody structures not antigen structures. Further, the disclosure of MacCallum et al. is directed to antibodies and different kinds of antigens, such as carbohydrates and peptides, in general and does not teach anything particular on the binding between IgE antibodies and allergenic polypeptides or the surface structures of these polypeptides.

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SUMMARY OF THE INVENTION

The present invention relates to human IgE antibodies and derivatives thereof, which bind
5 to non-continuous allergenic epitope, a planar Type I surface with the area of 600-900 Å²,
e.g. to IgE antibodies binding to bovine milk β-lactoglobulin with high affinity and
specificity. The present invention also enables blocking the Type I surface interaction of
allergenic substances by modifying amino acid residues of said surface structure or by
producing a mimetope binding said surface.

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We also describe in this application the development, characterisation and structure
determination of the human IgE antibody fragment and derivatives thereof that binds
allergenic β-lactoglobulin with affinity and specificity high enough to be utilised as
reagents in immunoassays designed for the qualitative and quantitative measurement of β-
15 lactoglobulin in biological samples, in removal of the β-lactoglobulin, in immunotherapy
of allergic patients and in the construction of focused antibody libraries based on the
structural data. Specifically, the present invention describes selection of human IgE
antibodies specific to β-lactoglobulin by the phage display technique, the characterisation
of the binding properties of the engineered antibody fragments produced in *E.coli*, and
20 structure determination of the antibody-allergen immunocomplex.

This invention thus provides new reagents to be utilised in different kinds of immunoassay
protocols, as well as in human immunotherapy and construction of focused antibody
libraries. The invention also permits guaranteed continuous supply of these specific
25 reagents of uniform quality, eliminating inherent batch-to-batch variation of polyclonal
antisera. These advantageous effects permit the manufacture of new, specific and
economical immunodiagnostic assays of uniform quality.

Consequently, one specific object of the present invention is to provide human IgE mono-
30 clonal antibodies, fragments thereof, or other derivatives of such antibodies, which bind β-
lactoglobulin with affinity and specificity high enough to allow qualitative and quantitative
measurement of β-lactoglobulin in biological samples, as well as their use in

immunotherapy. The monovalent antibodies of the present invention demonstrate a specific binding to allergenic β -lactoglobulin.

Another object of the present invention is to provide cDNA clones encoding β -lactoglobulin -specific antibody chains, as well as constructs and methods for expression of such clones to produce β -lactoglobulin -binding antibodies, fragments thereof or other derivatives of such antibodies.

A further object of this invention is to provide methods of using such β -lactoglobulin -binding antibodies, fragments thereof or other derivatives of such antibodies, or combinations of them for qualitative and quantitative measurement of β -lactoglobulin in biological samples. Additionally, this invention provides β -lactoglobulin -binding antibodies, fragments thereof or other derivatives of such antibodies, or combinations of them for immunotherapy in allergic patients.

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A further object of this invention is to provide methods of using structural data obtained for constructing focused IgE antibody libraries towards allergens for diagnostics and human IgE VH-region derived antibody libraries for therapeutic and diagnostic targets where the binding specificity is towards areas of protein structures that are not located on the protruding regions of the surface.

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According to one aspect of the invention there is provided a method for producing a modified allergenic polypeptide, the method comprising the steps of:

(a) modifying nucleic acid sequence encoding an allergenic polypeptide comprising a planar surface so that in the polypeptide expressed from the modified nucleic acid the structure of the planar surface of said polypeptide is altered;

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(b) expressing or producing the modified allergenic polypeptide from the modified nucleic acid; and

(c) selecting those modified allergenic polypeptides towards which an IgE-antibody specific to said allergenic polypeptide shows at least tenfold lower affinity;

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wherein said planar surface has an area of 600-900 Å² and is determined by computational analysis to be as the allergenic epitope of β -lactoglobulin defined by the structure or 3D-coordinates of β -lactoglobulin amino acids Trp19-Tyr20, Val43-Lys47, Leu57-Gln59, Cys66-Gln68, Pro126-Glu127, and Thr154-Glu157 of SEQ ID NO:8 in an antibody- β -lactoglobulin immunocomplex.

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According to a further aspect of the invention there is provided a method for identifying a molecule binding to the planar surface structure of an allergenic polypeptide, said molecule being capable to inhibit or hinder the binding of a specific IgE-antibody to said allergenic polypeptide; comprising the steps of: (a) contacting a particle comprising the allergenic epitope and a candidate binder molecule; and (b) isolating those candidate binder molecules which are able to bind to the planar surface of said allergen;

wherein said planar surface has an area of 600-900 Å² and is determined by computational analysis to be as the allergenic epitope of β-lactoglobulin defined by the structure or 3D-coordinates of β-lactoglobulin amino acids Trp19-Tyr20, Val43-Lys47, Leu57-Gln59, Cys66-Gln68, Pro126-Glu127, and Thr154-Glu157 of SEQ ID NO:8 in an antibody-β-lactoglobulin immunocomplex.

According to another aspect of the invention there is provided a method for identifying a molecule binding to the allergenic epitope of β-lactoglobulin defined by structure coordinates of β-lactoglobulin amino acids Trp19 and Tyr20 of SEQ ID NO:8 from beta-strand A and Glu44 of SEQ ID NO:8 from beta-strand B in an antibody-β-lactoglobulin immunocomplex; comprising the steps of:

(a) contacting a molecule comprising the allergenic epitope of β-lactoglobulin and a candidate binder molecule; and

(b) isolating those candidate binder molecules which were able to bind to said allergenic epitope of β-lactoglobulin.

According to yet another aspect of the invention there is provided a method for identifying a molecule binding to the allergenic epitope of β-lactoglobulin defined by structure coordinates of β-lactoglobulin amino acids Val43-Lys47 and Leu57-Gln59 of SEQ ID NO:8 in an antibody-β-lactoglobulin immunocomplex; comprising the steps of:

(a) contacting a molecule comprising the allergenic epitope of β-lactoglobulin and a candidate binder molecule; and

(b) isolating those candidate binder molecules which were able to bind to said allergenic epitope of β-lactoglobulin.

According to still another aspect of the invention there is provided a method for identifying a modulator of binding between the allergenic epitope of β-lactoglobulin and its ligand, said allergenic epitope of β-lactoglobulin being defined by structure coordinates of β-lactoglobulin amino acids Trp19 and Tyr20 of SEQ ID NO:8 from beta-strand A and Glu44 of SEQ ID

5b

NO:8 from beta-strand B in an antibody- β -lactoglobulin immunocomplex; comprising the steps of:

- (a) contacting a molecule comprising the allergenic epitope of β -lactoglobulin and its ligand in the presence and in the absence of a putative modulator compound;
- 5 (b) detecting binding between the allergenic epitope of β -lactoglobulin and its ligand in the presence and absence of the putative modulator; and
- (c) identifying a modulator compound in view of decreased or increased binding between the allergenic epitope of β -lactoglobulin and its ligand in the presence of the putative modulator, as compared to binding in the absence of the putative modulator.

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According to a further aspect of the invention there is provided a method for identifying a modulator of binding between the allergenic epitope of β -lactoglobulin and its ligand, said allergenic epitope of β -lactoglobulin being defined by structure coordinates of β -lactoglobulin amino acids Val43-Lys47 and Leu57-Gln59 of SEQ ID NO:8 in an antibody- β -lactoglobulin immunocomplex; comprising the steps of:

- (a) contacting a molecule comprising the allergenic epitope of β -lactoglobulin and its ligand in the presence and in the absence of a putative modulator compound;
- (b) detecting binding between the allergenic epitope of β -lactoglobulin and its ligand in the presence and absence of the putative modulator; and
- 20 (c) identifying a modulator compound in view of decreased or increased binding between the allergenic epitope of β -lactoglobulin and its ligand in the presence of the putative modulator, as compared to binding in the absence of the putative modulator.

According to another aspect of the invention there is provided a method for producing a modified allergenic polypeptide, the method comprising the steps of:

- (a) detecting by structural analysis or molecular modelling techniques a potential IgE binding site in an allergenic polypeptide;
- (b) determining by computational analysis of a three-dimensional structure of said allergenic polypeptide whether said potential IgE binding site contains a planar or flat surface area of 600-900 Å² as the planar surface as defined by the 3D-coordinates of β -lactoglobulin amino acids Val43-Lys47 and Leu57-Gln59 of SEQ ID NO:8 in an antibody- β -lactoglobulin immunocomplex, if a planar or flat surface as the one in β -lactoglobulin is found, the method is continued by
- 30 (c) modifying a nucleic acid sequence encoding said polypeptide so that in the polypeptide expressed from the modified nucleic acid the structure of the planar or flat surface of said polypeptide is altered; and

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5c

(d) expressing or producing a modified allergenic polypeptide from the modified nucleic acid obtained from step c).

5 Other objects, features and advantages of the present invention will become apparent from the following drawings and detailed description. It should be understood, however, that the detailed description and the specific examples, while indicating preferred embodiments of the invention, are given for illustration only.

BRIEF DESCRIPTION OF THE DRAWINGS

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Figure 1 shows a schematic presentation of an intact human IgE subclass antibody, Fab fragment and single-chain antibody (scFv). The antigen-binding site is indicated by a triangle.

Figure 2 shows schematically the panning procedure.

Figure 3 shows a schematic presentation of the scFv phage display vector used for the
5 construction of scFv phage libraries.

Figure 4 shows the deduced amino acid and nucleotide sequence of the heavy chain variable region of the D1 IgE Fab. The Complementarity Determining Regions (CDRs) are underlined. Numbering is according to Kabat (Kabat *et al.*, 1991).

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Figure 5 shows the deduced amino acid and nucleotide sequence of the light chain variable region of the D1 IgE Fab. CDRs are underlined. Numbering is according to Kabat (Kabat *et al.*, 1991).

15 **Figure 6** shows the curve obtained from the competitive ELISA of D1 IgE Fab fragment with human IgG1 subtype whose binding to immobilized, biotinylated β -lactoglobulin has been inhibited by soluble native β -lactoglobulin .

Figure 7 shows the result from immunoprecipitation assay. The D1 IgE Fab binds the
20 native β -lactoglobulin from cow milk. 1=Low molecular weight marker, 2-5 = D1 IgE fab immobilized in proteinL beads + untreated milk sample, milk sample, heated 15 min +95 °C, 30 min +95 °C, 60 min +95 °C 6-7 = negative controls (= empty proteinL beads + untreated milk sample or heated 60 min +95 °C) 8 = purified β -lactoglobulin from Sigma 0,5 9 = purified D1 IgE Fab 0,5 μ g.

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Figure 8 shows the result of the competitive ELISA. The binding of D1 IgE Fab fragments with human IgG1 subtype to β -lactoglobulin is inhibited by patient sera.

Figure 9 shows the binding of the D1 IgE Fab -antibody to the β -lactoglobulin. (a), A
30 schematic view of binding an allergen (grey) to two IgE molecules (light chain L, heavy chain H)

Figure 10 shows the different segments of the β -lactoglobulin epitope which are numbered 1-6.

Figure 11 shows the binding of the D1 IgE Fab to β -lactoglobulin with the side view on the surface of D1/IgE-Fab fragment.

Figure 12 shows the surface of β -lactoglobulin epitope with the CDR loops of the D1 IgE Fab and the residues of the D1 IgE Fab which make contacts with β -lactoglobulin.

Figure 13 shows the binding of the D1 IgE Fab to β -lactoglobulin (left), the IgG antibody-antigen type binding IgG Fab 2JEL to phosphocarrier protein (middle) and IgG-allergen type binding of the BV16/Fab to the pollen allergen Bet v 1 (right).

Figure 14 shows the potential IgE epitope from different allergens: Equ c 1, horse skin (Lascombe et al., 2000, J. Biol. Chem. 275(28):21572-21577); Bos d 5, Beta-lactoglobulin; Bet v 1, birch pollen (Spangfort et al. 2003, J. Immunol. 171(6):3084-3090); Bos d 2, bovine dander (Rautiainen et al., 1998, Biochem. Biophys. Res. Commun. 247:746-750); Cyp c 1, carp parvalbumin (Swoboda et al., 2002, J. Immunol. 168(9):4576-4584); and Hev b 6, latex (see WO02094878). The planar (flat) surfaces are indicated with thick lines/bars.

Figure 15 shows the result of competition ELISA. The binding of the D1 IgE Fab to BLG is inhibited by a short peptide, KRVG. Ctr 1 and ctr2 are the background controls where ctr1 is the result obtained after incubation without D1 IgE Fab and ctr2 without the BLG (see Example 4).

Figure 16 shows the surface of D1/Fab antibody and ribbon model of allergen BLG. In this figure identical residues of the D1/Fab with hevein-binding IgE-antibody (clone IC2) are shown in light grey, different residues are in dark grey; a) front view, b) side view showing extensive similarity between the light chains of two IgE antibodies binding structurally very different allergens.

Figure 17. Antibody binding to flat, convex and concave epitopes. In the first row the solvent excluded surface (probe radius 10 Å) is shown. Because of a large probe sphere the surface show more large scale features. The surface is coloured according to the Gaussian curvature. Flat areas are in white. Antibody is shown as a ribbon model. The second row shows similar structures but now the surfaces represent interaction surface which corresponds epitope.

Figure 18. The molecular surfaces (probe radius 10 Å) of five different allergens in two orientations. The surface is coloured according to the curvature, flat areas are in white. The putative flat area for IgE-binding are shown as a rectangle on the left. The side view is on the right and the position of the same area are shown as a line.

Figure 19. Purification of the rBLG-His6 and its mutants. After the second IMAC-purification the protein samples were analysed on the Coomassie-stained 15% SDS-PAGE gels (with β-mercaptoethanol). The pooled fractions are shown by arrows.

Figure 20. The purified rBLG-His6 and its mutants were analysed by western blotting followed by the detection with the rabbit anti-BLG antibody and goat AFOS-conjugated anti-rabbit antibody. 3 µg protein were subjected into the well. Lane 1=LMW, lane 2= native BLG(Sigma), lane 3=rBLG-His6, lane 4=rBLG-His6 T18Y, and lane 5=rBLG-His6 T18Y/E45Y/L57Y.

Figure 21. CD-spectra of the nBLG, rBLG-His6 and its mutants are shown.

Figure 22. The binding properties of the D1 IgE Fab to different BLGs were analysed by ELISA. Biotinylated nBLG, rBLG-His6 or its mutants were immobilised on to the SA-microtitre wells. Bound D1 IgE Fab was detected using AFOS-conjugated goat anti-kappa antibody. Triple = rBLG-His6 T18Y/E45Y/L57Y mutant, Bsa = bovine serum albumin, and control-sample shows the background obtained from anti kappa-AFOS conjugate when the BLGs are immobilised but no D1 IgE Fab used.

Figure 23. The binding properties of the IgE serum samples from allergic and non-allergic donor to different BLGs were analysed by ELISA. Biotinylated nBLG, rBLG-His6 or its

mutants were immobilised on to the SA-microtitre wells. The bound IgE was detected using AFOS-conjugated goat anti-human IgE.

Figure 24. BIAcore analysis of the nBLG, rBLG-His6 and its mutants. Binding curves of the 69.6 nM D1 IgE Fab solution for binding to different BLGs are shown. The association and dissociation constants of the D1 IgE Fab to nBLG, rBLG-His6 and its mutants are calculated and shown in Table XI.

The figures of the constructions are not in scale.

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ABBREVIATIONS

	cDNA	complementary deoxyribonucleic acid
	CDR	complementarity determining region
15	DNA	deoxyribonucleic acid
	<i>E. coli</i>	<i>Escherichia coli</i>
	ELISA	enzyme-linked immunosorbent assay
	Fab	fragment with specific antigen binding
	Fd	variable and first constant domain of a heavy chain
20	Fv	variable regions of an antibody with specific antigen binding
	IgE	immunoglobulin E
	mRNA	messenger ribonucleic acid
	NMR	nuclear magnetic resonance
	PCR	polymerase chain reaction
25	RNA	ribonucleic acid
	scFv	single-chain antibody
	<i>supE</i>	a genotype of bacterial strain carrying a glutamine-inserting amber suppressor tRNA
	V _H	variable region of a heavy chain
30	V _L	variable region of a light chain

DETAILED DESCRIPTION OF THE INVENTION

The following definitions are provided for some terms used in this specification. The terms, "immunoglobulin", "heavy chain", "light chain" and "Fab" are used in the same way
5 as in the European Patent Application No. 0125023.

"Antibody" in its various grammatical forms is used herein as a collective noun that refers to a population of immunoglobulin molecules and/or immunologically active portions of immunoglobulin molecules, i.e., molecules that contain an antigen binding site or a
10 paratope.

An "antigen-binding site", a "paratope", is the structural portion of an antibody molecule that specifically binds an antigen.

15 Exemplary antibodies are those portions of an immunoglobulin molecule that contain the paratope, including those portions known as Fab and Fv.

"Fab" (fragment with specific antigen binding), a portion of antibodies can be prepared by the proteolytic reaction of papain on substantially intact antibodies by methods that are
20 well known. See for example, U.S. Patent No. 4,342,566. Fab fragments can also be produced by recombinant methods, which are well known to those skilled in the art. See, for example, U.S. Patent 4,949,778.

"Domain" is used to describe an independently folding part of a protein. General structural
25 definitions for domain borders in natural proteins are given in Argos, 1988.

A "variable domain" or "Fv" is used to describe those regions of the immunoglobulin molecule, which are responsible for antigen or hapten binding. Usually these consist of approximately the first 100 amino acids of the N-termini of the light and the heavy chain of
30 the immunoglobulin molecule.

"Single-chain antibody" (scFv) is used to define a molecule in which the variable domains of the heavy and light chain of an antibody are joined together via a linker peptide to form a continuous amino acid chain synthesised from a single mRNA molecule (transcript).

"Linker" or "linker peptide" is used to describe an amino acid sequence that extends between adjacent domains in a natural or engineered protein.

5 A " β -lactoglobulin -binding antibody" is an antibody, which specifically recognises β -lactoglobulin and binds to it, due to interaction mediated by its variable domains. As used herein, the term "specifically binding" or "specifically recognizing" or the expression "having binding specificity to an allergenic epitope of β -lactoglobulin" refers to a low background and high affinity binding between an antibody or a fragment or derivative
10 thereof and its target molecule (i.e. lack of non-specific binding). One of the embodiments of the present invention is a monoclonal antibody having binding specificity to an allergenic epitope of β -lactoglobulin (SEQ ID NO:8), or a functional fragment or derivative thereof having said specificity.

15 The term "planar (or flat) surface" refers to the surface structure as defined in Example 8.

As examples of fragments of such antibodies falling within the scope of the invention we disclose here scFv fragments of D1 IgE fab as shown in Figures 4 and 5. In one preferred embodiment, the present invention thus provides derivatives of β -lactoglobulin -binding
20 antibodies, e.g. Fab fragments or scFv fragments. It will be appreciated that mutant versions of the CDR sequences or complete V_L and V_H sequences having one or more conservative substitutions which do not substantially affect binding capability, may alternatively be employed and are included into the scope of the invention.

25 For use in immunoassay, e.g. for qualitative or quantitative determination of β -lactoglobulin in biological samples, antibodies and antibody derivatives of the invention may be labelled. For these purposes, any type of label conventionally employed for antibody labelling is acceptable.

30 For use in immunotherapy, e.g. for blocking allergenic β -lactoglobulin in allergic patients, antibodies and antibody derivatives of the invention may be labelled. For these purposes, any pharmaceutically acceptable label conventionally employed for antibody labelling is appropriate (see, e.g., US 2007/0003579).

In another aspect, the present invention also provides DNA molecules encoding an antibody or antibody derivative of the invention, and fragments of such DNAs, which encode the CDRs of the V_L and/or V_H region. Such a DNA may be cloned in a vector, more particularly, for example, an expression vector which is capable of directing expression of antibody derivatives of the invention, or at least one antibody chain or a part of one antibody chain.

In a further aspect of the invention, host cells are provided, selected from bacterial cells, yeast cells, fungal cells, insect cells, plant cells and mammalian cells, containing a DNA molecule of the invention, including host cells capable of expressing an antibody or antibody derivative of the invention. Thus, antibody derivatives of the invention may be prepared by culturing host cells of the invention expressing the required antibody chain(s), and either directly recovering the desired protein or, if necessary, initially recovering and combining individual chains.

The above-indicated scFv fragments were obtained by biopanning of a human IgE scFv-phage library using allergenic recombinant β -lactoglobulin. The human IgE scFv-phage library was constructed from mRNAs isolated from lymphocytes of a milk-allergic patient. The variable region of the light and heavy chain cDNAs were synthesised using human IgE-specific primers for Fd cDNAs and human kappa (κ) and lambda (λ) light chains using human κ and λ chain specific primers. The variable regions of the light and heavy chains were amplified by PCR using human κ and λ chain specific primers for V κ and V λ cDNAs and human IgE specific primers for V_H cDNAs, respectively. The human IgE scFv library was constructed by cloning the variable region cDNAs into a scFv phage display vector using restriction sites introduced into the PCR primers.

The human IgE scFv library was selected by phage display using a panning procedure. The human IgE scFv phage library was screened by a biotinylated allergenic native β -lactoglobulin in solution and the binders were captured on streptavidin. The elution of phages was done with 100 μ M non biotinylated native β -lactoglobulin AB dimer. The phage eluate was amplified in *E. coli* cells. After 2 rounds of biopanning, soluble scFv fragments were produced from isolated phages. The binding specificity of the selected

scFv fragments was analysed by ELISA. Several β -lactoglobulin -specific scFv fragment clones were obtained.

As described herein, the phage display technique is an efficient and feasible approach to
5 develop human IgE recombinant anti- β -lactoglobulin antibodies for diagnostic and therapeutic applications.

While one successful selection strategy for obtaining antibody fragments of the invention has been described, numerous variations, by which antibody fragments of the invention
10 may be obtained, will be apparent to those skilled in the art. It may prove possible to select scFv fragments of the invention directly from a phage or microbial display library of scFv fragment or its derivatives. A phage or microbial cell, which presents a scFv fragment or other antibody fragment of the invention as a fusion protein with a surface protein, represents a still further aspect of the invention.

15

While microbial expression of antibodies and antibody derivatives of the invention offers means for efficient and economical production of highly specific reagents of uniform quality suitable for use in immunodiagnostic assays and immunotherapy, alternatively it may prove possible to produce such a reagent, or at least a portion thereof, synthetically.
20 By applying conventional genetic engineering techniques, initially obtained antibody fragments of the invention may be altered, e.g. new sequences linked, without substantially altering the binding characteristics. Such techniques may be employed to produce novel β -lactoglobulin -binding hybrid proteins, which retain both affinity and specificity for β -lactoglobulin as defined hereinbefore.

25

Planar surface of allergens and production and use of hypoallergens

The present invention enables blocking the Type I surface interaction of allergenic substances by modifying amino acid residues on non-continuous allergenic epitope, i.e. a
30 planar surface with the area of 600-900 Å² on the allergenic substance (see Figs. 14 and 16). The planar (flat) surface may contain a β -sheet on the surface of the protein such as in β -lactoglobulin and Bet v 1, or α -helixes packed near to each other such as in Fel d 1.

Other allergens with the planar structure are Equ c 1 (horse skin), Bos d 2 (bovine dander), Cyp c 1 (carp parvalbumin), and Hev b 6 (latex).

Hypoallergen variant can be obtained by mutating some (1-5) amino acid residues on the planar (flat) epitope surface with bulky residues (e.g. Arg, Tyr, Lys, Trp can be mutated to Ala). The mutated residues are those which side chains are pointing outside towards solvent thus causing minimal change to the basic structure of the allergen. The purpose of the mutagenesis is to modify the flat surface to convex surface which prevent the binding of IgE-antibodies. The effect of the mutation on the planar surface can be seen as lower affinity of the allergen specific IgE-antibody towards the modified allergen, preferably the mutation decreases the affinity of the specific antibody at least tenfold, more preferably more than tenfold. The resulting modified allergen can be used to evoke tolerance against particular allergens in allergic patients. Thus, the present invention provides a modified allergen carrying the type I planar epitope which has been distorted by the directed introduction of one or several mutations thereby decreasing the affinity towards the recombinant IgE molecule at least tenfold, preferably more than tenfold.

The present invention also provides a method to create tolerance in a patient for a specific allergen with a planar allergenic epitope comprising the steps of

- a) disrupting the planar surface of the allergen with a mutation decreasing the affinity of the IgE towards the epitope more than ten folds;
- b) producing the mutated allergen (i.e. hypoallergen);
- c) administering, preferably parentally, the mutated allergen into the patient one or several times.

The present invention also provides a method for the isolation of recombinant IgE monoclonal antibodies comprising the steps of

- a) isolating mRNA from IgE producing cells from a human derived sample;
- b) synthesizing of the cDNAs encoding the IgE Fd gene region and kappa/lambda light chain genes to create an IgE expression library;
- c) screening the expressed library against a polypeptide or protein carrying the planar (flat) type I surface typical for allergens and isolating clones showing medium or high affinity (over $10^7 M^{-1}$) towards the planar surface;
- d) isolating the DNA encoding the IgE antibody obtained from step c).

Preferably said polypeptide is β -lactoglobulin and said planar surface is defined by the structure or 3D-coordinates of β -lactoglobulin amino acids Val43-Lys47 and Leu57-Gln59 and/or amino acids around these amino acids in an antibody- β -lactoglobulin immunocomplex (see Table VIII).

The present invention further provides a method for producing a modified allergenic polypeptide, the method comprising the steps of (a) modifying nucleic acid sequence encoding said polypeptide so that in the polypeptide expressed from the modified nucleic acid the structure of allergenic epitope of said polypeptide is altered, and (b) expressing or producing the modified allergenic polypeptide from the modified nucleic acid. Preferably step (b) comprises the steps of expressing said modified nucleic acid in a suitable host in a culture system and isolating said modified polypeptide from the culture, or producing synthetically of said modified polypeptide. Preferably said modified allergenic polypeptide is β -lactoglobulin, and/or said allergenic epitope is the planar surface as defined above, more preferably planar surface is defined by the structure or 3D-coordinates of β -lactoglobulin amino acids Val43-Lys47 and Leu57-Gln59 and/or amino acids around these amino acids, in an antibody- β -lactoglobulin immunocomplex. Said allergenic epitope can also be the epitope defined by structure coordinates of β -lactoglobulin amino acids Trp19 and Tyr20 from beta-strand A and Glu44 from beta-strand B in an antibody- β -lactoglobulin immunocomplex.

The present invention further provides a method for identifying a molecule binding to an allergenic epitope of an allergen; comprising the steps of: (a) contacting a particle, such as a virus particle, comprising the allergenic epitope and a candidate binder molecule; (b) isolating those candidate binder molecules which were able to bind to said allergenic epitope. Preferably said allergen is β -lactoglobulin, said molecule is a peptide, and said allergenic epitope is the planar surface as defined above; more preferably planar surface is defined by the structure or 3D-coordinates of β -lactoglobulin amino acids Val43-Lys47, and Leu57-Gln59 and/or amino acids around these amino acids in an antibody- β -lactoglobulin immunocomplex. A good approach in this method is the use of affinity chromatography.

Crystallographic and *in Silico* Screening

The three-dimensional structure of the allergenic epitope of β -lactoglobulin is defined by a set of structure coordinates as set forth below. The term "structure coordinates" refers to Cartesian coordinates derived from mathematical equations related to the patterns obtained on diffraction of a monochromatic beam of X-rays by the atoms (scattering centers) of the allergenic epitope of β -lactoglobulin in crystal form of an antibody-allergen immunocomplex. The diffraction data are used to calculate an electron density map of the repeating unit of the crystal. The electron density maps are then used to establish the positions of the individual atoms of the allergenic epitope of β -lactoglobulin.

Those of skill in the art will understand that a set of structure coordinates for a protein or a protein-complex or a portion thereof, is a relative set of points that define a shape in three dimensions. Thus, it is possible that an entirely different set of coordinates could define a similar or identical shape. Moreover, slight variations in the individual coordinates will have little effect on overall shape.

The variations in coordinates discussed above may be generated because of mathematical manipulations of the structure coordinates. For example, the structure coordinates set forth below could be manipulated by crystallographic permutations of the structure coordinates, fractionalization of the structure coordinates, integer additions or subtractions to sets of the structure coordinates, inversion of the structure coordinates or any combination of the above.

Alternatively, modifications in the crystal structure due to mutations, additions, substitutions, and/or deletions of amino acids, or other changes in any of the components that make up the crystal could also account for variations in structure coordinates. If such variations are within an acceptable standard error as compared to the original coordinates, the resulting three-dimensional shape is considered to be the same.

30

Various computational analyses are therefore necessary to determine whether a molecule or molecular complex or a portion thereof is sufficiently similar to all or parts of the allergenic epitope of β -lactoglobulin described herein as to be considered the same. Such

analyses may be carried out in current software applications, such as the Molecular Similarity application of QUANTA (Molecular Simulations Inc., San Diego, CA) version 4.1, and as described in the accompanying User's Guide.

- 5 Once the structure coordinates of a protein crystal have been determined they are useful in solving the structures of other crystals, especially crystals of other similar proteins.

Thus, in accordance with the present invention, the structure coordinates of the allergenic epitope of β -lactoglobulin, and portions thereof is stored in a machine-readable storage
10 medium. Such data may be used for a variety of purposes, such as drug discovery and x-ray crystallographic analysis or protein crystal.

Accordingly, in one embodiment of this invention is provided a machine-readable data storage medium comprising a data storage material encoded with the structure coordinates
15 set forth below.

For the first time, the present invention permits the use of structure-based or rational drug design techniques to design, select, and synthesize chemical entities, including inhibitory compounds that are capable of binding to the allergenic epitope of β -lactoglobulin, or any
20 portion thereof.

Those of skill in the art will realize that association of natural ligands or substrates with the binding pockets of their corresponding receptors or enzymes is the basis of many biological mechanisms of action. The term "binding site", as used herein, refers to a region
25 of a molecule or molecular complex that, as a result of its shape, favourably associates with another chemical entity or compound. Similarly, many drugs exert their biological effects through association with the binding pockets of receptors and enzymes. Such associations may occur with all or any parts of the binding pockets. An understanding of such associations will help lead to the design of molecules such as drugs having more
30 favourable associations with their target receptor or enzyme, and thus, improved biological effects. Therefore, this information is valuable in designing potential ligands or inhibitors of receptors or enzymes.

The term "associating with" or "interacting with" refers to a condition of proximity between chemical entities or compounds, or portions thereof. The association or interaction may be non-covalent, wherein the juxtaposition is energetically favoured by hydrogen bonding or van der Waals or electrostatic interactions, or it may be covalent.

5

In iterative molecular design, crystals of a series of protein/compound complexes are obtained and then the three-dimensional structures of each complex are solved. Such an approach provides insight into the association between the proteins and compounds of each complex. This is accomplished by selecting compounds with inhibitory activity, obtaining
10 crystals of this new protein/compound complex, solving the three-dimensional structure of the complex, and comparing the associations between the new protein/compound complex and previously solved protein/compound complexes. By observing how changes in the compound affected the protein/compound associations, these associations may be optimized.

15

In some cases, iterative molecular design is carried out by forming successive protein-compound complexes and then crystallizing each new complex. Alternatively, a pre-formed protein crystal is soaked in the presence of an inhibitor, thereby forming a protein/compound complex and obviating the need to crystallize each individual
20 protein/compound complex. Advantageously, the allergenic epitope of β -lactoglobulin crystals, may be soaked in the presence of a compound or compounds, such as antibodies, to provide β -lactoglobulin /antibody crystal complexes.

As used herein, the term "soaked" refers to a process in which the crystal is transferred to a
25 solution containing the compound of interest.

The storage medium

The storage medium in which the atomic co-ordinates are provided is preferably random access memory (RAM), but may also be read-only memory (ROM e. g. CDROM), or a
30 diskette. The storage medium may be local to the computer, or may be remote (e. g. a networked storage medium, including the internet).

The invention also provides a computer-readable medium for a computer, characterised in that the medium contains atomic co-ordinates of the allergenic epitope of β -lactoglobulin.

- 5 The atomic co-ordinates are preferably those set forth below, or variants thereof.

Any suitable computer can be used in the present invention.

Molecular modelling techniques

- 10 Molecular modelling techniques can be applied to the atomic co-ordinates of the allergenic epitope of β -lactoglobulin to derive a range of 3D models and to investigate the structure of ligand binding sites. A variety of molecular modelling methods are available to the skilled person for use according to the invention.

- 15 At the simplest level, visual inspection of a computer model of the allergenic epitope of β -lactoglobulin can be used, in association with manual docking of models of functional groups into its binding sites.

- Software for implementing molecular modelling techniques may also be used. These
20 molecular modelling techniques allow the construction of structural models that can be used for in silico drug design and modelling.

De novo compound design

- The molecular modelling steps used in the methods of the invention may use the atomic
25 co-ordinates of the allergenic epitope of β -lactoglobulin, and models derived therefrom, to determine binding surfaces.

This preferably reveals van der Waals contacts, electrostatic interactions, and/or hydrogen bonding opportunities.

30

These binding surfaces will typically be used by grid-based techniques (e. g. GRID

[Goodford (1985) J. Med. Chem. 28: 849-857], CERIUS2) and/or multiple copy simultaneous search (MCSS) techniques to map favourable interaction positions for functional groups. This preferably reveals positions in the allergenic epitope of β -lactoglobulin for interactions such as, but not limited to, those with protons, hydroxyl groups, amine groups, hydrophobic groups (e. g. methyl, ethyl, benzyl) and/or divalent cations.

Once functional groups or small molecule fragments which can interact with specific sites in the binding surface of the allergenic epitope of β -lactoglobulin have been identified, they can be linked in a single compound using either bridging fragments with the correct size and geometry or frameworks which can support the functional groups at favourable orientations, thereby providing a compound according to the invention. Whilst linking of functional groups in this way can be done manually, perhaps with the help of software such as QUANTA or SYBYL, the following software may be used for assistance: HOOK [Available from Molecular Simulations Inc], which links multiple functional groups with molecular templates taken from a database, and/or CAVEAT [Lauri & Bartlett (1994) Comp. Aided Mol. Design 8: 51-66], which designs linking units to constrain acyclic molecules.

Docking

Compounds in known in silico libraries can also be screened for their ability to interact with the allergenic epitope of β -lactoglobulin by using their respective atomic co-ordinates in automated docking algorithms.

Suitable docking algorithms include: DOCK [Kuntz et al. (1982) J. Mol. Biol. 161: 269-288], AUTODOCK [Available from Oxford Molecular], MOE-DOCK [Available from Chemical Computing Group Inc.] or FLEXX [Available from Tripos Inc.]. Docking algorithms can also be used to verify interactions with ligands designed *de novo*.

Focused IgE-antibody library towards allergens

The amino acid sequence comparison of published IgE sequences reveals that the light chains of the known IgE antibodies binding to diverse groups of allergens are strikingly

conserved (see Table VII). This gives tools to construct focused allergen specific libraries that can be utilised for the isolation of allergen specific antibodies applicable in the diagnosis of allergens. The conserved light chain sequence information is used to construct a limited pool of light chains or a single light chain with the characteristic amino acid sequences identified in the IgE antibodies. This light chain sequence information is combined with a diverse pool of IgE heavy chain genes isolated from lymphocytes of several allergic patients. The resulting antibody phage display library, in either scFv or Fab display format, is used to select allergen specific IgE antibodies essentially as described in Example 1/II and Hoogenboom *et al.* (1998).

Human antibody (scFv, Fab or whole antibody) libraries containing the human IgE VH-regions

The IgE VH-region of the D1 IgE Fab and especially the HCDR3 loop are structurally different when compared to IgG antibodies. It is forming a loop structure that is recognizing a cleft on the BLG-allergen structure. Based on this observation it should be possible to develop human IgE VH-region containing antibodies for those therapeutic targets where the binding specificity is required towards protein structures that are not exposed on the surface, e.g., substrate binding sites of enzymes and drug resistance pumps (De Genst *et al.* 2006). A diverse IgE VH-pool from human lymphocytes is used as a building block to construct a functional human antibody library in a scFv, Fab or whole antibody format. Resulting libraries are selected against therapeutic targets requiring specific recognition of cleft structures.

The development and characterisation of the human β -lactoglobulin -binding recombinant antibodies and their usefulness in immunoassays is now described in more detail in the following examples.

EXAMPLE 1

The recombinant β -lactoglobulin-specific scfv fragment by phage display selection

5 In this example the human IgE scFv library was constructed and selected by allergenic β -lactoglobulin in order to isolate scFv fragments with affinity and specificity to β -lactoglobulin (BLG). Construction of human IgE scFv phage library was prepared indirectly by constructing IgE Fab- κ and Fab- λ libraries first, and then the particular library DNAs were used for PCR amplification of variable domains of heavy and light
10 chains.

I. Construction of the human IgE scFv phage libraries

50 ml of heparinised blood was obtained from a milk-allergic patient. Lymphocytes were
15 isolated according to an Ig-Prime kit protocol (Novagen). Per 10 ml of blood 30 ml of lysis buffer (155 mM NH_4Cl , 10 mM NH_4HCO_3 , 0.1 mM EDTA, pH 7.4) was added and incubated on ice for 15 min with shaking occasionally. After centrifugation at 450 g for 10 min the lymphocytes, i.e. the white blood cell pellet, were collected. The pellet was washed twice with lysis buffer and after the final centrifugation the lymphocyte pellet was resus-
20 pended in D-solution. Lymphocyte RNAs were isolated using Promega's RNeasy Total RNA Isolation kit according to the manufacturer's protocol. The first strand cDNA synthesis was carried out using Promega's Reverse Transcription system kit. For the synthesis of Fd-fragment cDNA and light chain cDNAs the primers of the constant region of the epsilon (ϵ) chain (C ϵ 1) and the primer of the kappa (C κ 1) and lambda (C λ 1) chain were
25 used, respectively. Primers used for the cDNA synthesis and PCR amplifications of human IgE Fd region and light chains are showed in Table I and Table II.

PCR amplifications were carried out in two steps: a primary PCR for amplifying Fd and light chains from cDNA templates and a secondary PCR for adding restriction sites to the
30 5'-end of the DNA fragments obtained after a primary PCR. First the Fd region was amplified by PCR using the primers specific for the variable region of the heavy chains (VH1a-VH7a) and C ϵ 1 primer. Accordingly, the kappa and lambda light chains were amplified using specific primers for variable region of the light chains (V κ 1a-V κ 6b and

V λ 1a-V λ 10) and C κ / λ 1 primer, respectively. Primers for the secondary PCR were C κ 1 and V κ / λ 1 and C κ for the kappa light region, V κ / λ 1 and C λ 1 for the kappa light chain and V λ 1A and C κ / λ 1 for the lambda light chain. The primary PCR amplification was done at the following conditions: 1 cycle of 3 min at 93°C for denaturation, 7 cycles of 1 min at 93°C, 30 s at 63°C and 50 s at 58°C for annealing and 1 min at 72°C for elongation, 23 cycles of 1 min at 93°C, 30 s at 63°C and 1 min at 72°C followed by 1 cycle of 10 min at 72°C. For the secondary PCR the amplification conditions were as follows: 1 cycle of 3 min at 95°C for denaturation, 25 cycles of 1.5 min at 94°C, 1 min at 65°C for annealing and 1.5 min at 72°C for elongation followed by 1 cycle of 10 min at 72°C. Between the primary and the secondary PCR and after the secondary PCR the amplified DNA fragments were purified.

The final PCR products of the different antibody fragments were pooled and digested with appropriate restriction enzymes. Digested DNA fragments, encoding IgE Fd region and κ and λ light chains, were ligated into a phagemid vector and transformed into *E. coli* XL-1 Blue cells to yield an Fab- κ and Fab- λ libraries of 10^6 independent clones. To avoid possible problems on the expression of Fab fragments on a phage particle an antibody library in scFv format was constructed. Phagemid DNAs from different libraries were isolated and used as template DNAs for amplifying the variable regions of the human IgE heavy and human light chains in order to construct human IgE scFv- κ and scFv- λ libraries.

PCR amplification of the variable region of the heavy chain was carried out using human V_H specific primers (VH1-VH4 and VH1A). Amplification of the variable region of the light chains was done using the following primer pairs: V κ 1-V κ 7, V κ 2-V κ 8, V κ 3-V κ 9, V κ 4-V κ 10, V κ 5-V κ 11 and V κ 6-V κ 11 for human kappa chain and V λ 1-V λ 8, V λ 2-V λ 9, V λ 3-V λ 9, V λ 4-V λ 9, V λ 5-V λ 10, V λ 6-V λ 10 and V λ 7-V λ 10 for human lambda chain (see Tables III and IV). The amplified DNA fragments were purified and digested in order to ligate into a scFv phage display vector (Fig.3). Ligation mixtures were transformed into *E. coli* XL-1 Blue cells resulting in the human IgE scFv- κ and scFv- λ libraries with approximately 10^5 independent clones.

II. Selection of the human scFv-libraries

The human scFv- κ and scFv- λ libraries were selected by the phage display technique (McCafferty *et al.*, 1990, Barbas *et al.*, 1991). To isolate β -lactoglobulin -binding antibody fragments, the human IgE scFv- κ and scFv- λ libraries displayed on the surface of the bacteriophage were panned using an affinity panning procedure (Fig.2). First the phage pools were allowed to react either with biotinylated, immunoreactive β -lactoglobulin or as a negative control, without antigen for 1.5 h. Thereafter, the phage pools were transferred to microtitre plate wells coated with biotin binding streptavidin. After a 30-min incubation, the wells were washed 3 times with PBS + 0,05% Tween20 and the binders were eluted with soluble antigen (100 μ M nonbiotinylated β -lactoglobulin AB dimer). For the next panning round the eluted phage pools were amplified by infecting *E. coli* XL-1 Blue cells. Two rounds of panning were performed.

III. Characterisation of the β -lactoglobulin -binders

After the last panning cycle scFv phage display DNA was isolated and transformed into *E. coli* HB2151 (*supE*⁻) cells in order to express soluble scFv fragments. Between the scFv sequence and the phage gene III sequence the scFv phage display vector contains TAG-amber stop codon which will be translated as glutamate in *E. coli* strains with *supE*⁺ genotype but as a stop codon in *E. coli* strains with *supE*⁻ genotype. Sixty-two individual clones were grown in a small scale to produce soluble scFv fragments for preliminary characterisation. Clones were analysed on ELISA test using β -lactoglobulin -coated wells to catch the β -lactoglobulin -specific binders and control protein wells to see non-specific binding (data not shown). Most of the clones bound with high affinity to β -lactoglobulin. Clones were analyzed first by DNA-fingerprinting and six of the clones were sequenced (Sanger *et al.*, 1977). Finally, one of the clones was selected for further characterisation (Figures 4 and 5).

EXAMPLE 2

Cloning and characterisation of human Fab fragment with β -lactoglobulin-binding specificity

In this example the human IgE scFvs with β -lactoglobulin-binding specificity was converted to human Fab fragments with IgG1 subtype. Due to known difficulties in forming multimers, the D1 scFv, obtained from the scFv antibody library, was cloned and bacterially expressed as Fab fragments (Holliger *et al.*, 1993, Desplancq *et al.*, 1994). The resulting antibody fragments were further characterised by a competitive ELISA.

I. Cloning of the human Fab fragments with β -lactoglobulin -binding specificity

The Fd regions were amplified by overlapping PCR. The primers used for the PCR are given in Table V.

The resulting cDNAs of the Fd region and light chains were cloned into the bacterial expression vector, pKKtac and then transformed into *E. coli* RV308. Soluble Fab fragment designated to D1 IgE Fab was produced by fermentation (Nevanen *et al.*, 2001) and the Fab fragment was purified by an introduced C-terminal hexahistidiny tag on a Sepharose column with immobilised nickel to a substantial purity (data not shown).

II. Characterisation of the human IgE Fab fragments

The characterisation of the purified D1 IgE Fab was performed by competitive ELISA. First, increasing amounts of the soluble, non-biotinylated β -lactoglobulin was incubated with the D1 IgE Fab, and then the reaction mixtures were applied onto Streptavidin microtitre plate wells coated with allergenic, biotinylated β -lactoglobulin. Figure 6 shows the result of the competitive ELISA. The binding of the D1 IgE Fab (Figure 6) to biotinylated β -lactoglobulin could be inhibited by adding increasing amounts of native β -lactoglobulin.

To study if the D1 IgE Fab is able to bind β -lactoglobulin from milk samples, the immunoprecipitation assay was performed (Figure 7). The D1 IgE Fab was immobilized via kappa light chain to protein L beads and this complex was introduced to milk samples, which were heated for various times (0, 15, 30 and 60min). The D1 IgE Fab bound to the protein L beads was incubated with milk samples 1 hour at room temperature and after

this, the beads were washed several times with PBS+0,05% Tween20 to remove unspecific binding of the milk proteins to protein L beads. The D1 IgE Fab β -lactoglobulin complex was eluted from protein L-beads with low pH (0,1 M Glycine, pH 2.1) and the eluted fraction was neutralized with 3 M Tris, pH 8.8. A small portion of the elution fraction was
5 analyzed with 15% SDS-PAGE followed by silver staining. The correct size bands were cut out from the SDS-PAGE gel and further analyzed by mass spectrometry to confirm that the protein, which D1 IgE Fab recognised from cow milk was β -lactoglobulin.

To study if the D1 IgE Fab recognizes the same allergenic epitope as the IgE antibodies
10 from patient serum, the biotinylated β -lactoglobulin was first immobilised to a microtitre plate wells coated with streptavidin. The patient serum samples were incubated in the wells together with increasing concentrations of D1 IgE Fab and the amount of the bound patient serum IgE was detected with alkaline phosphatase labelled secondary antibody, which specifically recognizes the human IgE isotype. A slight inhibition can be seen in the case
15 of each patient tested, suggesting that the epitope which D1 IgE Fab recognizes is the same as the IgE from the patient serum. The reason why the binding of the patient serum IgE is not totally blocked, might be that the β -lactoglobulin harbours a multiple IgE-epitopes.

EXAMPLE 3

20

I. Crystallisation of the antibody-allergen immunocomplex

Crystallization and data collection Microcrystals (about 70 x 50 x 50 μ m) of BLG-D1 IgE Fab were obtained with vapour diffusion method by mixing 2 μ l of D1/Fab solution (concentration 1.4 mg/ml in 20 mM phosphate buffer, pH 7.0), 1 μ l BLG solution (2
25 mg/ml in pure water), 0,5 μ l of n-dodecyl- β -D-maltoside solution, and 2.5 μ l of reservoir solution (14 % (w/v) polyethylene glycol 3350, 0.1 M BTP (1,3-bis[tris(hydroxymethyl)methylamino] propane-hydrochloric acid) buffer, pH 5.5). The diffraction data set was collected from single crystal at the beamline ID29 in ESRF (wavelength 1.000 $\text{\AA}$) at 100 K. The crystal belonged to the space group $P2_12_12_1$ with unit-
30 cell dimensions $a=67.0$, $b=100.6$, $c=168.1$ $\text{\AA}$. The data set was collected at 2.8 $\text{\AA}$ resolution.

II. Structure determination of antibody-allergen immunocomplex

The structure was solved with the molecular replacement method using Molrep program implemented in CCP4 program package. BLG monomer (PDB code 1B8E) and Fab fragment of IgG antibody against GP41 of HIV virus (1DFB) (identity 92 % for light and 79 % for heavy chain) were used as search models. The final structure contained one dimer of BLG complexed with two Fab fragments. Model building and refinement were done with the programs O and CNS. Because of low number of reflections restraints were used to keep both Fab/D1 fragments and BLG monomers similar. BLG exist in two isomers, the electron density suggested that we have glycine at position 64 and alanine at position 118. No water molecules were added but the elongated electron density in the lipid binding cavity of BLG was modelled as an n-dodecyl- β -D-maltoside. The final structure has an R value 24.5 % and an R_{free} value of 29.9%. 83.5 % of the residues are in the most favoured regions and 0.6 % of the residues in the disallowed regions in the Ramachandran plot. All figures were generated with Pymol (Delano, W. L. The PyMol Molecular Graphics System.

EXAMPLE 4

Inhibition of the D1 IgE Fab binding to BLG was carried out using a short peptide, KRVG that is the longest linear BLG binding peptide in the HCDR3. In competitive ELISA the biotinylated AB dimer of BLG was immobilised onto streptavidin-coated microtitre wells. First the peptide (an inhibitor) was dissolved into 0.5%BSA-PBS and then different amounts of it were incubated with the immobilised BLG. After that the wells were either washed trice with PBS or not. D1 IgE Fab was added and followed by the washings with PBS. The bound antibody was detected with AFOS-conjugated goat anti-human kappa antibody. After addition of the substrate, *p*-nitrophenylphosphatase, the absorbance values were read at 405 nm. The results are shown in Figure 15.

EXAMPLE 5

30

The identification of a flat epitope by calculation of molecular surface and curvature

In this example we have used commercial AMIRA program (with AmiraMol module) to calculate the solvent excluded surface (probe radius 10 Å). The surfaces are coloured according to the Gaussian curvature which is the product of the two principal curvatures. It is negative in surface areas with hyperbolic geometry (convex-concave, like near saddle points) and positive in areas with elliptic geometry (strictly convex or strictly concave). We have also used AMIRA program to calculate molecular interface area (cutoff 3 Å). The program shows a surface which is located exactly in the middle between two proteins. In Figure 17 examples for antibody binding to flat (BLG D1(IgE/Fab)), convex (Bet v 1 – IgG/Fab; 1BV1) and concave (lysozyme-single chain camel antibody; 1MEL) epitopes are shown.

It is thus possible to calculate the molecular surface by using a large probe value (preferably 8-12 Å) for allergens if their three-dimensional structure is available. Such molecular surfaces can be rotated and looked in all directions and with the aid of curvature coloured surfaces a large flat area (600-900 Å²) can be identified. In Figure 18 we represent molecular surfaces for five allergens. The first one is BLG (Bos d 5) and the flat epitope is shown in two orientations. In the following pictures similar flat areas from four other allergens, Bet v 1, Bos d 2, Phl p 7, and Hev b 6 are identified. These are suggested flat epitopes for IgE binding. The four allergens represent structurally very different classes. Bos d 5 and Bos d 2 are β-proteins (consisting mainly of β-strands). Bet v 1 has both β-strands and α-helices. Phl p 7 has only α-helices and Hev b 6 is a small protein with low secondary structure content.

EXAMPLE 6

25

Characterisation of recombinant β-lactoglobulin and its mutants

Based on the D1 IgE and the BLG immunocomplex structure, mutations were designed to the flat surface epitope on the BLG in order to produce hypoallergenic variants. Two different recombinant BLG (rBLG) mutants, T18Y and T18Y/E45Y/L57Y, were constructed (Table IX). The cDNAs encoding the rBLG and its mutants were cloned into bacterial expression vector, produced in *Escherichia coli* cells, chromatographically purified to a substantial purity and finally their properties were characterised.

I. Cloning of the recombinant BLGs

The bovine recombinant BLG (rBLG) cDNA was purchased from GenScript Corporation
5 (USA) in vector pUC57 and it contained the restriction sites of *SfiI*/*NcoI* at the 5' end and
HindIII at the 3' end (Table X). The rBLG cDNA was cloned into pKKTac bacterial
expression vector with the fusion of the *Erwinia carotovora*'s pectate lyase (pelB) signal
sequence (Takkinen *et al.*, 1991) as an *SfiI* – *HindIII* fragment. The hexa histidiny (His6)
tag was introduced into 3' end of the rBLG cDNA by PCR amplification using primers 1
10 and 2 (Table X). Phusion DNA polymerase (Finnzymes) was used in all PCR
amplifications. The amplified cDNA of rBLG-His6 was digested with *SfiI* and *HindIII*
(New England Biolabs) and cloned into pKKTac expression vector. *Escherichia coli* XL-1
Blue was used as a host strain to construct the recombinant BLG (rBLG) and its mutants.

15 Two different rBLG mutants, T18Y and T18Y/E45Y/L57Y (Table IX), were cloned into
pKKTac vector. The cDNAs of the rBLG-His6 T18Y and T18Y/E45Y/L57Y mutant were
amplified with PCR using mismatch primers 2, 3, 4 and 5 (Table X) and the original rBLG
cDNA in pUC57 vector as a template. The cDNA encoding the T18Y mutant was
amplified using primers 2 and 3 and the amplified cDNA was digested with *StuI* and
20 *HindIII* (New England Biolabs) and cloned into the pKKTac/rBLG-His6 vector (see above).
The cDNA encoding the T18Y/E45Y/L57Y mutant was amplified in two steps using
overlapping primers. First, the cDNA fragment of 27-165 bp was amplified using primers
3 and 4 and the cDNA fragment of 147-530 bp with the 2 and 5. Then the resulting DNA
fragments were combined by overlapping PCR amplification. The primer 4 and 5 have an
25 overlapping sequence. Finally the cDNA encoding the T18Y/E45Y/L57Y mutant was
digested with *StuI* and *HindIII* and cloned into pKKTac/rBLGHis expression vector.

The DNA sequences of the rBLG-His6 and its mutants were verified by DNA sequencing
(ABI 3100 Genetic Analyzer, Applied Biosystems).

30

II. Production of the recombinant BLGs

The rBLG-His6 and its mutants were transformed into *E. coli* RV308 (ATCC 31608) strain for the bacterial expression of the rBLGs. Single colonies of each clone were inoculated into 3 ml LB, 100µg/ml ampicillin and 1% glucose and cultivated for 16 h at +37°C with 220 rpm shaking. Then the cultivations were 1:50 diluted into 3 ml LB with ampicillin and
5 cultivated 3 hours at +37°C. After that the protein expression was induced by the addition of IPTG to a final concentration of 1mM and cells were cultivated for 16 h at +30°C with 220 rpm shaking. Then the cells were harvested and the supernatants were stored for later use. The periplasmic fraction of the cells was isolated by a freeze-thaw method (Boer *et al.*, 2007). Briefly, cells were resuspended in 20% sucrose, 30 mM Tris, 1 mM EDTA (pH
10 8.0) and then incubated 5 min in dry ice-ethanol bath followed by the resuspension in 5 mM MgSO₄ and incubation for 5 min at +37°C, and this freezing and thawing step was repeated trice. The supernatant and the periplasmic fractions were analysed by western blotting. First the samples were run on a 15% SDS-PAGE gel (with β-mercaptoethanol) and then the proteins were transferred onto the nitrocellulose filter. The rBLGs were
15 detected using rabbit anti-BLG antibody (Mäkinen-Kiljunen and Palosuo, 1992) followed by AFOS-conjugated goat anti-rabbit antibody (Bio-Rad).

During the bacterial production the recombinant BLGs were secreted into the periplasmic space with almost no leakage into culture medium. For the large scale production of the
20 rBLGs the cells containing the rBLG-His6 and its mutants in pKKTac vector in *E. coli* RV308 strain were inoculated TB medium containing 100 µg/ml ampicillin, 1% glucose. The cells were cultivated for 16 h at +37°C with 220 rpm shaking. Then the cell cultures were 1:50 diluted into TB medium with 100 µg/ml ampicillin. The cells were grown at +37°C with 220 rpm shaking until the OD₆₀₀ was 4 and IPTG was added to a final
25 concentration of 0.1mM. The induction of the cells was carried out for 6 h at +28°C with 220rpm shaking. Then the cells were harvested by centrifugation with 4000 x g for 15 min at +4°C. The periplasmic fractions containing the recombinant BLGs were isolated by freeze-thaw method as above.

30 III. Purification of the rBLGs

The purification of recombinant BLGs was performed using immobilised metal affinity chromatography (IMAC) as described earlier (Porath and Olin, 1983). Briefly, periplasmic

fractions containing the rBLGs were 1:2 diluted with the binding buffer (10mM Hepes, 1M NaCl, 10% Glycerol, 1mM imidazole, pH 7.4) and incubated with Ni²⁺-loaded Chelating Sepharose (Pharmacia) for 16 h at +4°C. The column matrix with bound rBLGs was loaded into the column with gravity flow and washed stepwise with 1mM, 10mM, 20mM and 50mM imidazole in the binding buffer. Finally, the rBLGs were eluted with 75mM, 100mM, 200mM and 5 x 500 mM imidazole in the binding buffer and 2 ml fractions were collected. The eluted fractions were analysed on 15% SDS-PAGE gel (with β -mercaptoethanol). The fractions containing the desired proteins were pooled and the IMAC-purification was repeated in a smaller scale. After the second IMAC-purification the fractions were analysed again on a SDS-PAGE gel (Fig. 19). As a result the fractions containing the particular purified BLG were pooled, dialysed against 10mM HEPES, 0.9% NaCl, pH 7.4 for 16 h at +4°C. The purified proteins were analysed by western blotting using rabbit anti-BLG antibody and AFOS-conjugated goat anti-rabbit antibody detection (Fig. 20).

15

IV. Circular dichroism measurements

For circular dichroism (CD) measurements the buffer of all rBLGs was exchanged into 5mM Hepes (pH 7.4) using Econo Pac 10DG desalting columns (Bio-Rad) with the cut of 6000 Da. Far-UV spectrum of the native BLG (nBLG, Sigma), rBLG-His6 and the rBLG-His6 mutants was measured with Jasco J-715 spectropolarimeter at +20°C controlled with a Peltier thermostat (Jasco PTC-348WI) using a 1-mm quartz cell. The concentrations of the proteins were 1mg/ml for nBLG, 0.25mg/ml for rBLG-His6, 1.3mg/ml for rBLG-His6 T18Y and 0.93mg/ml for rBLG-His6 T18Y/E45Y/L57Y mutant. The CD-spectra shown are averages of three measurements (Fig. 21).

25

V. Characterisation of the D1 IgE Fab binding to rBLGs by ELISA

First the rBLGs were biotinylated. The biotinylation of the rBLGs was performed with Sulfo-NHS-LC-biotin (Pierce) in a molar ratio of 2 mol biotin : 1mol protein in 10mM Hepes, 0.9% NaCl for 30 min at RT with a gentle shaking. The unreacted biotin was removed using Econo Pac 10 DG desalting columns (Bio-Rad). The incorporation of the biotin to the rBLGs was analysed by western blotting using SA-AFOS detection.

30

Then 1 μ g biotinylated nBLG, rBLG-His6, rBLG-His6 T18Y mutants in 110 μ l 0.5% BSA/PBS were immobilised onto the streptavidin microtitre wells (Roche) for 1h at RT. After that 100 μ l 1:15000 diluted anti-BLG D1 Fab (1.6mg/ml) in 0.5% BSA, PBS was
5 added to the washed wells. After a 1-h incubation the wells were washed three times with PBS. The detection of the BLGs was carried out using AFOS-conjugated goat anti-human kappa antibody (Southern Biotech). Then p-nitrophenylphosphate substrate (Sigma) was added to the wells (2mg/ml in diethanolamine buffer). The absorbance at the wavelength 405 nm was measured after 20 minutes of adding the substrate (Fig. 22).

10

The ELISA analysis with the serum samples (1:8 dilution in 0.5% BSA, PBS) was performed as above except the bound IgE from allergic patient serum was detected with AFOS-conjugated goat anti-human IgE (Southern Biotech). The absorbances were measured at 405nm after a 2-h incubation of adding the substrate (Fig. 23).

15

VI. Analysis of the binding kinetics

The association and dissociation constants of the D1 IgE Fab to nBLG, rBLG-His6 and its mutants were measured by BIAcore. The biotinylated BLGs were immobilised in HBS
20 buffer (10mM Hepes, 0.15M NaCl, 3.4mM EDTA, 0.005% BIAcore P20 surfactant, pH 7.4) and at a concentration of 1 μ g/ml onto the streptavidin biosensor chip resulting in a surface of approximately 400-500 RU. The biotinylated nBLG was immobilised only with 200 RU onto the surface of the SA-chip. The binding kinetics of the purified D1 IgE Fab was analysed at a flow rate of 30 μ l/min with the concentrations 138.9nM, 69.6nM,
25 34.8nM, 17.4nM, 8.7nM, 4.3nM, 2.2 and 1.1 nM. Regeneration of the BLG surface was performed with 100 μ M nBLG (Sigma). Binding curves of the 69.6 nM D1 IgE Fab solution are shown in Figure 24.

TABLE I: Primers used for cDNA synthesis and PCR amplification of the human IgE Fd region.

	Cε1: 5'- GCTGAAGGTTTTGTTGTCGACCCAGTC -3'
5	CεNotI: 5'- GAATGGTGCGGCCCGCGCTGAAGGTTTTGTTGTCG -3'
	VH1a: 5'- ATGGCCGCAGCTCAGGTCAGCTGGTGCAG -3'
	VH1b: 5'- ATGGCCGCAGCTCAGGTCCAGCTTGTGCAG -3'
	VH1c: 5'- ATGGCCGCAGCTSAGGTCCAGCTGGTACAG -3'
	VH1d: 5'- ATGGCCGCAGCTCARATGCAGCTGGTGCAG -3'
10	VH2a: 5'- ATGGCCGCAGCTCAGATCACCTTGAAGGAG -3'
	VH2b: 5'- ATGGCCGCAGCTCAGGTTCACCTTGARGGAG -3'
	VH3a: 5'- ATGGCCGCAGCTGARGTGCAGCTGGTGGAG -3'
	VH3b: 5'- ATGGCCGCAGCTCAGGTGCAGCTGGTGGAG -3'
	VH3c: 5'- ATGGCCGCAGCTGAGGTGCAGCTGTTGGAG -3'
15	VH4a: 5'- ATGGCCGCAGCTCAGSTGCAGCTGCAGGAG -3'
	VH4b: 5'- ATGGCCGCAGCTCAGGTGCAGCTACAGCAG -3'
	VH5a: 5'- ATGGCCGCAGCTGARGTGCAGCTGGTGCAG -3'
	VH6a: 5'- ATGGCCGCAGCTCAGGTACAGCTGCAGCAG -3'
	VH7a: 5'- ATGGCCGCAGCTCAGGTSCAGCTGGTGCAA -3'
20	VH1A: 5'- TTA CTCGCGGCCCGAGCCGGCCATGGCCGCAGCT -3'

TABLE II: Primers used for cDNA synthesis and PCR amplification of human kappa and lambda chains.

	Cκ1: 5'- AGGTAGGGCGCGCCTTAACACTCTCCCCTGTTGAAGC -3'
5	Vκ1a: 5'- ATGGCAGCGGCTRACATCCAGATGACCCAG -3'
	Vκ1b: 5'- ATGGCAGCGGCTGMCATCCAGTTGACCCAG -3'
	Vκ1c: 5'- ATGGCAGCGGCTGCCATCCRGATGACCCAG -3'
	Vκ1d: 5'- ATGGCAGCGGCTGTCATCTGGATGACCCAG -3'
	Vκ2a: 5'- ATGGCAGCGGCTGATATTGTGATGACCCAG -3'
10	Vκ2b: 5'- ATGGCAGCGGCTGATRITTGTGATGACTCAG -3'
	Vκ3a: 5'- ATGGCAGCGGCTGAAATTGTGTTGACRCAG -3'
	Vκ3b: 5'- ATGGCAGCGGCTGAAATAGTGATGACGCAG -3'
	Vκ3c: 5'- ATGGCAGCGGCTGAAATTGTAATGACACAG -3'
	Vκ4a: 5'- ATGGCAGCGGCTGACATCGTGATGACCCAG -3'
15	Vκ5a: 5'- ATGGCAGCGGCTGAAACGACACTCACGCAG -3'
	Vκ6a: 5'- ATGGCAGCGGCTGAAATTGTGCTGACTCAG -3'
	Vκ6b: 5'- ATGGCAGCGGCTGATGTTGTGATGACACAG -3'
	Vκ/λ1: 5'- TTGTTATTGCTAGCTGCACAACCAGCAATGGCAGCGGCT -3'
	Cλ1: 5'- AGGTAGGGCGCGCCTTATGAACATTCTYGYAGGGGC -3'
20	Vλ1a: 5'- ATGGCAGCGGCTCAGTCTGTGCTGACTCAG -3'
	Vλ1b: 5'- ATGGCAGCGGCTCAGTCTGTGYTGACGCAG -3'
	Vλ1c: 5'- ATGGCAGCGGCTCAGTCTGTCTGTGACGCAG -3'
	Vλ2 : 5'- ATGGCAGCGGCTCAGTCTGCCCTGACTCAG -3'
	Vλ3a: 5'- ATGGCAGCGGCTTCCTATGWGCTGACTCAG -3'
25	Vλ3b: 5'- ATGGCAGCGGCTTCCTATGAGCTGACACAG -3'
	Vλ3c: 5'- ATGGCAGCGGCTTCTTCTGAGCTGACTCAG -3'
	Vλ3d: 5'- ATGGCAGCGGCTTCCTATGAGCTGATGCAG -3'
	Vλ4 : 5'- ATGGCAGCGGCTCAGCYTGTGCTGACTCAA -3'
	Vλ5 : 5'- ATGGCAGCGGCTCAGSCTGTGCTGACTCAG -3'
30	Vλ6 : 5'- ATGGCAGCGGCTAATTTTATGCTGACTCAG -3'
	Vλ7 : 5'- ATGGCAGCGGCTCAGRCTGTGGTGACTCAG -3'
	Vλ8 : 5'- ATGGCAGCGGCTCAGACTGTGGTGACCCAG -3'

V λ 4/9: 5'- ATGGCAGCGGCTCWGCCTGTGCTGACTCAG -3'

V λ 10: 5'- ATGGCAGCGGCTCAGGCAGGGCTGACTCAG -3'

- 5 TABLE III: Primers used for PCR amplification of the human variable regions of the heavy chain.

VH1: 5'- ATTTACTCGAGTGAGGAGACGGTGACCAGGGTGCC -3'

VH2: 5'- ATTTACTCGAGTGAAGAGACGGTGACCATTGTCCC -3'

- 10 VH3: 5'- ATTTACTCGAGTGAGGAGACGGTGACCAGGGTTCC -3'

VH4: 5'- ATTTACTCGAGTGAGGAGACGGTGACCGTGGTCCC -3'

VH1A: 5'- TTTACTCGCGGCCAGCCGGCCATGGCCGCAGCT -3'

- 15 TABLE IV: Primers used for PCR amplification of the human variable regions of the light chains.

V κ 1: 5'- TTATAGAGCTCGACATCCAGATGACCCAGTCTCC -3'

V κ 2: 5'- TTATAGAGCTCGATGTTGTGATGACTCAGTCTCC -3'

- 20 V κ 3: 5'- TTATAGAGCTCGAAATTGTGTTGACGCAGTCTCC -3'

V κ 4: 5'- TTATAGAGCTCGACATCGTGATGACCCAGTCTCC -3'

V κ 5: 5'- TTATAGAGCTCGAAACGACACTCACGCAGTCTCC -3'

V κ 6: 5'- TTATAGAGCTCGAAATTGTGCTGACTCAGTCTCC -3'

V κ 7: 5'- TATAAGCGGCCCGCACGTTTGATTTCCACCTTGGTCCC -3'

- 25 V κ 8: 5'- TATAAGCGGCCCGCACGTTTGATCTCCAGCTTGGTCCC -3'

V κ 9: 5'- TATAAGCGGCCCGCACGTTTGATATCCACTTTGGTCCC -3'

V κ 10: 5'- TATAAGCGGCCCGCACGTTTGATCTCCACCTTGGTCCC -3'

V κ 11: 5'- TATAAGCGGCCCGCACGTTTAATCTCCAGTCGTGTCCC -3'

V λ 1: 5'- ATTTAGAGCTCCAGTCTGTGTTGACGCAGCCGCC -3'

- 30 V λ 2: 5'- ATTTAGAGCTCCAGTCTGCCCTGACTCAGCCTGC -3'

V λ 3: 5'- ATTTAGAGCTCTCCTATGTGCTGACTCAGCCACC -3'

V λ 4: 5'- ATTTAGAGCTCTCTTCTGAGCTGACTCAGGACCC -3'

V λ 5: 5'- ATTTAGAGCTCCACGTTATACTGACTCAACCGCC -3'

Vλ6: 5'- ATTTAGAGCTCCAGGCTGTGCTCACTCAGCCGTC -3'
Vλ7: 5'- ATTTAGAGCTCAATTTTATGCTGACTCAGCCCCA -3'
Vλ8: 5'- ATATTGCGGCCCGCACCTAGGACGGTGACCTTGGTCCC -3'
Vλ9: 5'- ATATTGCGGCCCGCACCTAGGACGGTCAGCTTGGTCCC -3'
5 Vλ10:5'-ATATTGCGGCCCGCACCTAAAACGGTGAGCTGGGTCCC-3'

TABLE V: Primers used for PCR amplification of the human Fd regions with IgE and IgG1 subtype.

10

5'Cε: 5'-GCTCACCGTCTCCTCAGCCTCCACACAGAGCCCATCCG-3'
3'Cε: 5'-GCATTGCATTGCGGCCGCTTAATGGTGATGGTGATGATGGCTGAAGGT
TTTGTTGTCGACCC-3'
5'Cγ: 5'-GGTCACCGTCTCCTCAGCCTCCACCAAGGGCCC-3'
15 3'Cγ: 5'-TTTAGTTTATGCGGCCGCTTAATGGTGATGATGATGGTGACAAGATTG
GGCTCTGC-3'
5'Ve: 5'-ACTCATTAGGCACCCCAGGC-3'
3'Ve: 5'-TGAGGAGACGGTGACC-3'
5'Cκ: 5'-CGAACTGTGGCTGCACC-3'
20 3'Cκ: 5'-AGGTAGGGCGCGCCTTAACACTCTCCCCTGTTGAAGC-3'
5'Vk: 5'-TTGTTATTGCTAGCTGCACAACCAGCAATGGCAGACATCGTGATGACC
CAGTCTCC-3'
3'Vk: 5'-GGTGCAGCCACAGTTCGTTTGATYTCASCTTGGTCCC-3'.

TABLE VI. The D1 IgE Fab binding epitopes of β -lactoglobulin. Core epitope: residues which are making direct contacts with D1 IgE Fab. Extended epitope: includes also residues which mutation may affect binding of D1 IgE Fab. The segments are as shown in Fig. 9d.

5

Segment	Core epitope	Extended epitope
1	W19-Y20	T18-Y20
2	V43-K47	Y42-K47
3	L57-Q59	E55-Q59
4	C66-Q68	E65-K70
5	P126-E127	T125-E127
6	T154-E157	T154-H161

TABLE VII. The amino acid sequence comparison of published IgE sequences reveals that the light chains of the known IgE antibodies binding to diverse groups of allergens are strikingly conserved. Conserved amino acids are shown in bold.

antigen	Ig	clone	PDB	CDR-L1	CDR-L2	CDR-L3
CDR				XXXXXXXXXXXXXXXXXX..	XXXXXXXXXX	XXXXXXXXXXXXXXXXX.
Bet v 1	IgE	C-H1				QQSYSTP -- RT
		C-H2				AAWDDSLSGRVV
		C-H3				QQRSNWP -- PLT
Phl p 1	IgE	25		SQSIGN ----- YLNWY	LLIYAASSLQS	QQSNRTP -- ITF
		10		SQTFNN ----- YLNWY	LLIYAASTLRR	QQSYSTP -- LTF
		43		SRTIYN ----- YLNWY	LLIHAASTLQD	QQSHGTP -- LTF
Phl p 2						
Phl p 5	IgE	31		SQSISS ----- YLNWY	LLIYAASSLQS	QQSHSTP -- YTF
		14		SHSISN ----- YLNWY	LLIYAASSLQS	QESFPS -- GTF
		28		SQSILG ----- YLNWY	LLIYAASTLQS	QQSYITP -- RTE
		5		SQGISS ----- WLAWY	LLIYSASSLQS	QQANSEP -- YTF
		1A4		SQSVSS ----- SYLAWY	LLIYGASSRAT	QQYGSSP -- LTF
hevein						
hevein						
Bos d 5	IgE	1C2		SQSISS ----- YLNWY	LLIYAASSLQS	QQSYSTP -- RTE
		D1		SQGISS ----- RLAWY	LLIYAASSLQS	QQYHSYP -- WTF

TABLE VIII. Structure coordinates of the epitopes of allergenic beta-lactoglobulin in an antibody-beta-lactoglobulin immunocomplex; REMARK A = monomer A of allergen; REMARK L = light chain of antibody, variable domain; REMARK H = heavy chain of antibody, variable domain

	<u>Atom</u>	<u>type</u>	<u>Resid</u>	<u>#</u>	<u>X</u>	<u>Y</u>	<u>Z</u>	<u>OCC</u>	<u>B</u>	
ATOM	1	CB	THR A	4	-23.309	-4.747	-0.142	1.00	69.95	A
ATOM	2	OG1	THR A	4	-22.553	-4.413	-1.318	1.00	70.24	A
ATOM	3	CG2	THR A	4	-22.399	-5.463	0.852	1.00	69.08	A
ATOM	4	C	THR A	4	-25.438	-4.928	-1.503	1.00	69.21	A
ATOM	5	O	THR A	4	-25.191	-3.780	-1.887	1.00	68.89	A
ATOM	6	N	THR A	4	-24.039	-6.943	-1.113	1.00	69.41	A
ATOM	7	CA	THR A	4	-24.516	-5.659	-0.519	1.00	69.43	A
ATOM	8	N	GLN A	5	-26.503	-5.615	-1.909	1.00	68.87	A
ATOM	9	CA	GLN A	5	-27.482	-5.071	-2.843	1.00	68.15	A
ATOM	10	CB	GLN A	5	-28.213	-3.889	-2.204	1.00	69.22	A
ATOM	11	CG	GLN A	5	-29.389	-3.378	-3.017	1.00	71.17	A
ATOM	12	CD	GLN A	5	-30.366	-4.488	-3.374	1.00	72.36	A
ATOM	13	OE1	GLN A	5	-30.836	-5.225	-2.499	1.00	73.05	A
ATOM	14	NE2	GLN A	5	-30.683	-4.610	-4.664	1.00	71.92	A
ATOM	15	C	GLN A	5	-26.828	-4.630	-4.150	1.00	67.11	A
ATOM	16	O	GLN A	5	-26.732	-3.435	-4.438	1.00	66.95	A
ATOM	17	N	THR A	6	-26.374	-5.604	-4.934	1.00	66.26	A
ATOM	18	CA	THR A	6	-25.732	-5.328	-6.216	1.00	64.71	A
ATOM	19	CB	THR A	6	-24.481	-6.213	-6.444	1.00	64.50	A
ATOM	20	OG1	THR A	6	-24.887	-7.549	-6.765	1.00	63.11	A
ATOM	21	CG2	THR A	6	-23.607	-6.239	-5.198	1.00	64.44	A
ATOM	22	C	THR A	6	-26.711	-5.608	-7.348	1.00	63.92	A
ATOM	23	O	THR A	6	-27.769	-6.205	-7.141	1.00	63.78	A
ATOM	24	N	MET A	7	-26.341	-5.182	-8.549	1.00	63.06	A
ATOM	25	CA	MET A	7	-27.172	-5.377	-9.728	1.00	61.96	A
ATOM	26	CB	MET A	7	-26.431	-4.865	-10.959	1.00	60.12	A
ATOM	27	CG	MET A	7	-27.207	-4.975	-12.239	1.00	58.56	A
ATOM	28	SD	MET A	7	-26.235	-4.362	-13.595	1.00	56.18	A
ATOM	29	CE	MET A	7	-27.117	-2.858	-14.005	1.00	57.10	A
ATOM	30	C	MET A	7	-27.521	-6.852	-9.911	1.00	62.21	A
ATOM	31	O	MET A	7	-26.792	-7.730	-9.448	1.00	63.03	A
ATOM	32	N	LYS A	8	-28.637	-7.121	-10.583	1.00	61.64	A
ATOM	33	CA	LYS A	8	-29.054	-8.496	-10.821	1.00	61.39	A
ATOM	34	CB	LYS A	8	-30.516	-8.542	-11.274	1.00	62.21	A
ATOM	35	CG	LYS A	8	-31.481	-7.995	-10.222	1.00	64.73	A
ATOM	36	CD	LYS A	8	-32.952	-8.076	-10.648	1.00	65.77	A
ATOM	37	CE	LYS A	8	-33.470	-9.511	-10.688	1.00	66.53	A
ATOM	38	NZ	LYS A	8	-32.973	-10.272	-11.870	1.00	67.48	A
ATOM	39	C	LYS A	8	-28.147	-9.139	-11.864	1.00	60.59	A
ATOM	40	O	LYS A	8	-26.924	-9.122	-11.720	1.00	61.07	A
ATOM	41	N	GLY A	9	-28.729	-9.717	-12.906	1.00	59.03	A
ATOM	42	CA	GLY A	9	-27.899	-10.326	-13.932	1.00	56.96	A
ATOM	43	C	GLY A	9	-27.156	-9.276	-14.746	1.00	54.94	A
ATOM	44	O	GLY A	9	-27.725	-8.245	-15.097	1.00	55.67	A
ATOM	45	N	LEU A	10	-25.889	-9.531	-15.049	1.00	52.32	A
ATOM	46	CA	LEU A	10	-25.090	-8.591	-15.834	1.00	50.35	A
ATOM	47	CB	LEU A	10	-23.875	-8.150	-15.029	1.00	49.63	A
ATOM	48	CG	LEU A	10	-22.872	-7.298	-15.807	1.00	49.13	A
ATOM	49	CD1	LEU A	10	-23.483	-5.950	-16.144	1.00	48.82	A
ATOM	50	CD2	LEU A	10	-21.620	-7.119	-14.984	1.00	49.11	A
ATOM	51	C	LEU A	10	-24.619	-9.172	-17.177	1.00	49.26	A
ATOM	52	O	LEU A	10	-24.125	-10.298	-17.231	1.00	48.64	A

ATOM	53	N	ASP	A	11	-24.755	-8.393	-18.253	1.00	48.28	A
ATOM	54	CA	ASP	A	11	-24.353	-8.835	-19.593	1.00	47.09	A
ATOM	55	CB	ASP	A	11	-25.218	-8.166	-20.666	1.00	47.90	A
ATOM	56	CG	ASP	A	11	-24.959	-8.721	-22.072	1.00	48.81	A
ATOM	57	OD1	ASP	A	11	-25.713	-8.359	-22.999	1.00	49.16	A
ATOM	58	OD2	ASP	A	11	-24.011	-9.513	-22.260	1.00	49.60	A
ATOM	59	C	ASP	A	11	-22.887	-8.534	-19.863	1.00	45.64	A
ATOM	60	O	ASP	A	11	-22.542	-7.556	-20.525	1.00	45.05	A
ATOM	61	N	ILE	A	12	-22.033	-9.405	-19.348	1.00	44.43	A
ATOM	62	CA	ILE	A	12	-20.590	-9.279	-19.493	1.00	43.31	A
ATOM	63	CB	ILE	A	12	-19.911	-10.595	-19.096	1.00	43.33	A
ATOM	64	CG2	ILE	A	12	-18.408	-10.420	-19.082	1.00	43.02	A
ATOM	65	CG1	ILE	A	12	-20.418	-11.030	-17.719	1.00	45.17	A
ATOM	66	CD1	ILE	A	12	-20.114	-12.483	-17.357	1.00	46.47	A
ATOM	67	C	ILE	A	12	-20.135	-8.893	-20.907	1.00	42.33	A
ATOM	68	O	ILE	A	12	-19.201	-8.111	-21.082	1.00	42.79	A
ATOM	69	N	GLN	A	13	-20.797	-9.433	-21.918	1.00	40.46	A
ATOM	70	CA	GLN	A	13	-20.413	-9.131	-23.286	1.00	38.91	A
ATOM	71	CB	GLN	A	13	-21.223	-9.984	-24.266	1.00	40.33	A
ATOM	72	CG	GLN	A	13	-21.016	-11.479	-24.112	1.00	41.54	A
ATOM	73	CD	GLN	A	13	-19.554	-11.868	-24.138	1.00	42.01	A
ATOM	74	OE1	GLN	A	13	-18.858	-11.822	-23.114	1.00	40.76	A
ATOM	75	NE2	GLN	A	13	-19.070	-12.230	-25.321	1.00	42.60	A
ATOM	76	C	GLN	A	13	-20.551	-7.659	-23.672	1.00	37.09	A
ATOM	77	O	GLN	A	13	-19.874	-7.181	-24.584	1.00	37.01	A
ATOM	78	N	LYS	A	14	-21.410	-6.923	-22.980	1.00	34.35	A
ATOM	79	CA	LYS	A	14	-21.611	-5.527	-23.340	1.00	30.28	A
ATOM	80	CB	LYS	A	14	-23.098	-5.198	-23.253	1.00	30.76	A
ATOM	81	CG	LYS	A	14	-23.960	-5.988	-24.226	1.00	30.07	A
ATOM	82	CD	LYS	A	14	-25.398	-5.510	-24.182	1.00	31.58	A
ATOM	83	CE	LYS	A	14	-26.266	-6.180	-25.243	1.00	33.34	A
ATOM	84	NZ	LYS	A	14	-27.727	-5.841	-25.086	1.00	33.49	A
ATOM	85	C	LYS	A	14	-20.804	-4.474	-22.596	1.00	28.04	A
ATOM	86	O	LYS	A	14	-20.754	-3.332	-23.028	1.00	27.31	A
ATOM	87	N	VAL	A	15	-20.178	-4.837	-21.486	1.00	25.96	A
ATOM	88	CA	VAL	A	15	-19.381	-3.861	-20.752	1.00	23.39	A
ATOM	89	CB	VAL	A	15	-19.232	-4.270	-19.276	1.00	23.10	A
ATOM	90	CG1	VAL	A	15	-20.589	-4.329	-18.632	1.00	23.40	A
ATOM	91	CG2	VAL	A	15	-18.528	-5.624	-19.171	1.00	23.09	A
ATOM	92	C	VAL	A	15	-17.995	-3.739	-21.396	1.00	22.23	A
ATOM	93	O	VAL	A	15	-17.168	-2.929	-20.991	1.00	20.60	A
ATOM	94	N	ALA	A	16	-17.754	-4.557	-22.411	1.00	21.06	A
ATOM	95	CA	ALA	A	16	-16.475	-4.547	-23.095	1.00	20.08	A
ATOM	96	CB	ALA	A	16	-16.431	-5.661	-24.133	1.00	18.43	A
ATOM	97	C	ALA	A	16	-16.181	-3.204	-23.757	1.00	19.05	A
ATOM	98	O	ALA	A	16	-17.085	-2.469	-24.176	1.00	18.34	A
ATOM	99	N	GLY	A	17	-14.892	-2.913	-23.867	1.00	16.89	A
ATOM	100	CA	GLY	A	17	-14.470	-1.684	-24.480	1.00	13.91	A
ATOM	101	C	GLY	A	17	-13.760	-0.779	-23.512	1.00	14.13	A
ATOM	102	O	GLY	A	17	-13.420	-1.165	-22.389	1.00	13.58	A
ATOM	103	N	THR	A	18	-13.558	0.449	-23.980	1.00	14.39	A
ATOM	104	CA	THR	A	18	-12.888	1.508	-23.251	1.00	12.62	A
ATOM	105	CB	THR	A	18	-12.402	2.559	-24.231	1.00	12.52	A
ATOM	106	OG1	THR	A	18	-11.264	2.046	-24.934	1.00	15.36	A
ATOM	107	CG2	THR	A	18	-12.035	3.850	-23.508	1.00	13.69	A
ATOM	108	C	THR	A	18	-13.764	2.168	-22.206	1.00	12.74	A
ATOM	109	O	THR	A	18	-14.978	2.296	-22.382	1.00	13.81	A
ATOM	110	N	TRP	A	19	-13.128	2.570	-21.111	1.00	10.41	A
ATOM	111	CA	TRP	A	19	-13.806	3.231	-20.014	1.00	8.52	A
ATOM	112	CB	TRP	A	19	-14.211	2.235	-18.930	1.00	7.65	A
ATOM	113	CG	TRP	A	19	-15.284	1.302	-19.337	1.00	7.67	A

ATOM	114	CD2	TRP	A	19	-16.693	1.564	-19.329	1.00	6.14	A
ATOM	115	CE2	TRP	A	19	-17.338	0.392	-19.761	1.00	6.23	A
ATOM	116	CE3	TRP	A	19	-17.470	2.677	-18.995	1.00	4.83	A
ATOM	117	CD1	TRP	A	19	-15.135	0.022	-19.770	1.00	7.58	A
ATOM	118	NE1	TRP	A	19	-16.367	-0.534	-20.027	1.00	7.80	A
ATOM	119	CZ2	TRP	A	19	-18.721	0.298	-19.861	1.00	5.58	A
ATOM	120	CZ3	TRP	A	19	-18.844	2.583	-19.095	1.00	4.02	A
ATOM	121	CH2	TRP	A	19	-19.457	1.403	-19.523	1.00	3.57	A
ATOM	122	C	TRP	A	19	-12.860	4.233	-19.391	1.00	8.93	A
ATOM	123	O	TRP	A	19	-11.666	4.215	-19.651	1.00	10.27	A
ATOM	124	N	TYR	A	20	-13.408	5.089	-18.542	1.00	9.09	A
ATOM	125	CA	TYR	A	20	-12.628	6.076	-17.841	1.00	8.07	A
ATOM	126	CB	TYR	A	20	-12.812	7.460	-18.464	1.00	9.62	A
ATOM	127	CG	TYR	A	20	-12.102	7.654	-19.781	1.00	10.80	A
ATOM	128	CD1	TYR	A	20	-12.788	7.510	-21.004	1.00	9.64	A
ATOM	129	CE1	TYR	A	20	-12.127	7.683	-22.222	1.00	9.99	A
ATOM	130	CD2	TYR	A	20	-10.739	7.976	-19.813	1.00	7.81	A
ATOM	131	CE2	TYR	A	20	-10.076	8.146	-21.028	1.00	9.67	A
ATOM	132	CZ	TYR	A	20	-10.771	7.999	-22.226	1.00	9.03	A
ATOM	133	OH	TYR	A	20	-10.102	8.158	-23.420	1.00	7.27	A
ATOM	134	C	TYR	A	20	-13.138	6.087	-16.419	1.00	8.31	A
ATOM	135	O	TYR	A	20	-14.338	5.909	-16.185	1.00	9.09	A
ATOM	136	N	SER	A	21	-12.227	6.279	-15.470	1.00	7.65	A
ATOM	137	CA	SER	A	21	-12.604	6.334	-14.059	1.00	7.21	A
ATOM	138	CB	SER	A	21	-11.463	5.836	-13.169	1.00	7.63	A
ATOM	139	OG	SER	A	21	-11.239	4.436	-13.360	1.00	8.81	A
ATOM	140	C	SER	A	21	-12.891	7.792	-13.745	1.00	7.24	A
ATOM	141	O	SER	A	21	-11.968	8.573	-13.525	1.00	7.82	A
ATOM	142	N	LEU	A	22	-14.173	8.151	-13.722	1.00	7.35	A
ATOM	143	CA	LEU	A	22	-14.608	9.525	-13.458	1.00	6.56	A
ATOM	144	CB	LEU	A	22	-16.067	9.703	-13.891	1.00	6.94	A
ATOM	145	CG	LEU	A	22	-16.419	10.956	-14.702	1.00	8.26	A
ATOM	146	CD1	LEU	A	22	-17.899	11.308	-14.465	1.00	10.43	A
ATOM	147	CD2	LEU	A	22	-15.548	12.118	-14.299	1.00	6.27	A
ATOM	148	C	LEU	A	22	-14.500	9.946	-12.003	1.00	6.17	A
ATOM	149	O	LEU	A	22	-14.001	11.027	-11.707	1.00	6.09	A
ATOM	150	N	ALA	A	23	-14.981	9.081	-11.112	1.00	5.52	A
ATOM	151	CA	ALA	A	23	-15.002	9.366	-9.686	1.00	5.14	A
ATOM	152	CB	ALA	A	23	-16.360	9.993	-9.308	1.00	1.05	A
ATOM	153	C	ALA	A	23	-14.780	8.092	-8.884	1.00	6.08	A
ATOM	154	O	ALA	A	23	-15.039	6.983	-9.372	1.00	5.25	A
ATOM	155	N	MET	A	24	-14.293	8.244	-7.654	1.00	6.12	A
ATOM	156	CA	MET	A	24	-14.073	7.086	-6.810	1.00	7.92	A
ATOM	157	CB	MET	A	24	-12.682	6.499	-7.065	1.00	10.53	A
ATOM	158	CG	MET	A	24	-11.538	7.490	-6.968	1.00	13.91	A
ATOM	159	SD	MET	A	24	-9.954	6.748	-7.475	1.00	19.85	A
ATOM	160	CE	MET	A	24	-10.155	6.742	-9.241	1.00	16.62	A
ATOM	161	C	MET	A	24	-14.258	7.449	-5.347	1.00	7.96	A
ATOM	162	O	MET	A	24	-14.166	8.621	-4.975	1.00	7.86	A
ATOM	163	N	ALA	A	25	-14.543	6.440	-4.525	1.00	6.87	A
ATOM	164	CA	ALA	A	25	-14.753	6.647	-3.098	1.00	5.96	A
ATOM	165	CB	ALA	A	25	-16.233	6.907	-2.810	1.00	5.94	A
ATOM	166	C	ALA	A	25	-14.286	5.410	-2.362	1.00	5.84	A
ATOM	167	O	ALA	A	25	-14.196	4.337	-2.949	1.00	6.04	A
ATOM	168	N	ALA	A	26	-13.973	5.568	-1.081	1.00	5.75	A
ATOM	169	CA	ALA	A	26	-13.513	4.456	-0.264	1.00	6.01	A
ATOM	170	CB	ALA	A	26	-12.011	4.329	-0.363	1.00	3.18	A
ATOM	171	C	ALA	A	26	-13.927	4.664	1.185	1.00	7.89	A
ATOM	172	O	ALA	A	26	-14.186	5.795	1.612	1.00	4.99	A
ATOM	173	N	SER	A	27	-13.982	3.567	1.938	1.00	10.42	A
ATOM	174	CA	SER	A	27	-14.376	3.623	3.336	1.00	12.99	A

ATOM	175	CB	SER	A	27	-14.720	2.216	3.850	1.00	13.33	A
ATOM	176	OG	SER	A	27	-13.559	1.482	4.189	1.00	16.45	A
ATOM	177	C	SER	A	27	-13.286	4.252	4.205	1.00	14.05	A
ATOM	178	O	SER	A	27	-13.582	4.820	5.249	1.00	13.73	A
ATOM	179	N	ASP	A	28	-12.033	4.148	3.772	1.00	16.92	A
ATOM	180	CA	ASP	A	28	-10.907	4.709	4.515	1.00	19.69	A
ATOM	181	CB	ASP	A	28	-9.980	3.601	5.011	1.00	22.47	A
ATOM	182	CG	ASP	A	28	-10.467	2.984	6.309	1.00	27.75	A
ATOM	183	OD1	ASP	A	28	-11.704	3.020	6.564	1.00	28.49	A
ATOM	184	OD2	ASP	A	28	-9.616	2.448	7.069	1.00	31.52	A
ATOM	185	C	ASP	A	28	-10.124	5.674	3.652	1.00	19.92	A
ATOM	186	O	ASP	A	28	-9.742	5.342	2.531	1.00	20.07	A
ATOM	187	N	ILE	A	29	-9.873	6.866	4.188	1.00	19.78	A
ATOM	188	CA	ILE	A	29	-9.152	7.909	3.468	1.00	19.41	A
ATOM	189	CB	ILE	A	29	-8.901	9.120	4.384	1.00	18.35	A
ATOM	190	CG2	ILE	A	29	-8.030	10.140	3.671	1.00	16.12	A
ATOM	191	CG1	ILE	A	29	-10.244	9.747	4.787	1.00	16.69	A
ATOM	192	CD1	ILE	A	29	-10.131	10.862	5.803	1.00	13.07	A
ATOM	193	C	ILE	A	29	-7.820	7.431	2.901	1.00	20.55	A
ATOM	194	O	ILE	A	29	-7.491	7.716	1.752	1.00	20.09	A
ATOM	195	N	SER	A	30	-7.065	6.702	3.714	1.00	21.94	A
ATOM	196	CA	SER	A	30	-5.754	6.183	3.329	1.00	23.62	A
ATOM	197	CB	SER	A	30	-5.203	5.341	4.461	1.00	24.48	A
ATOM	198	OG	SER	A	30	-6.132	4.313	4.756	1.00	28.16	A
ATOM	199	C	SER	A	30	-5.794	5.331	2.068	1.00	24.82	A
ATOM	200	O	SER	A	30	-4.777	5.153	1.385	1.00	23.69	A
ATOM	201	N	LEU	A	31	-6.974	4.794	1.774	1.00	26.67	A
ATOM	202	CA	LEU	A	31	-7.169	3.943	0.602	1.00	27.64	A
ATOM	203	CB	LEU	A	31	-8.567	3.303	0.645	1.00	26.50	A
ATOM	204	CG	LEU	A	31	-8.795	2.278	1.757	1.00	26.16	A
ATOM	205	CD1	LEU	A	31	-10.266	1.929	1.859	1.00	25.35	A
ATOM	206	CD2	LEU	A	31	-7.943	1.063	1.483	1.00	25.12	A
ATOM	207	C	LEU	A	31	-6.988	4.697	-0.711	1.00	28.40	A
ATOM	208	O	LEU	A	31	-6.503	4.136	-1.696	1.00	28.86	A
ATOM	209	N	LEU	A	32	-7.374	5.969	-0.715	1.00	29.73	A
ATOM	210	CA	LEU	A	32	-7.286	6.821	-1.907	1.00	30.99	A
ATOM	211	CB	LEU	A	32	-8.691	7.246	-2.360	1.00	30.24	A
ATOM	212	CG	LEU	A	32	-9.505	6.344	-3.285	1.00	29.74	A
ATOM	213	CD1	LEU	A	32	-9.570	4.958	-2.695	1.00	30.44	A
ATOM	214	CD2	LEU	A	32	-10.907	6.919	-3.502	1.00	27.92	A
ATOM	215	C	LEU	A	32	-6.459	8.081	-1.670	1.00	32.27	A
ATOM	216	O	LEU	A	32	-6.026	8.719	-2.623	1.00	31.51	A
ATOM	217	N	ASP	A	33	-6.275	8.447	-0.403	1.00	34.56	A
ATOM	218	CA	ASP	A	33	-5.508	9.636	-0.026	1.00	37.18	A
ATOM	219	CB	ASP	A	33	-5.508	9.788	1.504	1.00	38.37	A
ATOM	220	CG	ASP	A	33	-5.076	11.178	1.973	1.00	38.48	A
ATOM	221	OD1	ASP	A	33	-5.360	12.175	1.270	1.00	37.67	A
ATOM	222	OD2	ASP	A	33	-4.472	11.271	3.067	1.00	38.63	A
ATOM	223	C	ASP	A	33	-4.086	9.502	-0.553	1.00	38.68	A
ATOM	224	O	ASP	A	33	-3.396	8.516	-0.267	1.00	39.31	A
ATOM	225	N	ALA	A	34	-3.660	10.504	-1.318	1.00	40.30	A
ATOM	226	CA	ALA	A	34	-2.340	10.522	-1.937	1.00	42.39	A
ATOM	227	CB	ALA	A	34	-1.280	9.999	-0.971	1.00	42.13	A
ATOM	228	C	ALA	A	34	-2.400	9.648	-3.190	1.00	43.89	A
ATOM	229	O	ALA	A	34	-2.869	8.507	-3.141	1.00	43.68	A
ATOM	230	N	GLN	A	35	-1.927	10.193	-4.309	1.00	46.04	A
ATOM	231	CA	GLN	A	35	-1.932	9.494	-5.597	1.00	47.75	A
ATOM	232	CB	GLN	A	35	-1.183	10.333	-6.632	1.00	49.01	A
ATOM	233	CG	GLN	A	35	-1.860	10.368	-7.996	1.00	51.86	A
ATOM	234	CD	GLN	A	35	-1.440	11.582	-8.833	1.00	53.04	A
ATOM	235	OE1	GLN	A	35	-0.302	11.662	-9.323	1.00	53.42	A

ATOM	236	NE2	GLN	A	35	-2.361	12.540	-8.988	1.00	52.30	A
ATOM	237	C	GLN	A	35	-1.361	8.068	-5.563	1.00	48.50	A
ATOM	238	O	GLN	A	35	-1.853	7.183	-6.278	1.00	49.53	A
ATOM	239	N	SER	A	36	-0.342	7.847	-4.732	1.00	47.82	A
ATOM	240	CA	SER	A	36	0.282	6.533	-4.604	1.00	47.78	A
ATOM	241	CB	SER	A	36	1.714	6.688	-4.076	1.00	49.93	A
ATOM	242	OG	SER	A	36	2.479	5.493	-4.271	1.00	51.54	A
ATOM	243	C	SER	A	36	-0.535	5.662	-3.644	1.00	46.74	A
ATOM	244	O	SER	A	36	0.005	5.062	-2.717	1.00	47.36	A
ATOM	245	N	ALA	A	37	-1.839	5.597	-3.875	1.00	45.30	A
ATOM	246	CA	ALA	A	37	-2.715	4.820	-3.022	1.00	44.15	A
ATOM	247	CB	ALA	A	37	-4.078	5.486	-2.940	1.00	45.03	A
ATOM	248	C	ALA	A	37	-2.855	3.373	-3.492	1.00	43.52	A
ATOM	249	O	ALA	A	37	-2.697	3.059	-4.679	1.00	43.45	A
ATOM	250	N	PRO	A	38	-3.155	2.466	-2.548	1.00	42.24	A
ATOM	251	CD	PRO	A	38	-3.315	2.745	-1.106	1.00	41.30	A
ATOM	252	CA	PRO	A	38	-3.322	1.038	-2.821	1.00	40.88	A
ATOM	253	CB	PRO	A	38	-3.259	0.426	-1.425	1.00	41.84	A
ATOM	254	CG	PRO	A	38	-3.924	1.471	-0.588	1.00	41.59	A
ATOM	255	C	PRO	A	38	-4.609	0.669	-3.562	1.00	39.03	A
ATOM	256	O	PRO	A	38	-4.761	-0.460	-4.028	1.00	39.26	A
ATOM	257	N	LEU	A	39	-5.539	1.611	-3.666	1.00	36.16	A
ATOM	258	CA	LEU	A	39	-6.793	1.334	-4.357	1.00	32.67	A
ATOM	259	CB	LEU	A	39	-7.947	1.214	-3.366	1.00	34.76	A
ATOM	260	CG	LEU	A	39	-7.972	-0.013	-2.458	1.00	36.49	A
ATOM	261	CD1	LEU	A	39	-9.296	0.006	-1.684	1.00	39.85	A
ATOM	262	CD2	LEU	A	39	-7.859	-1.289	-3.285	1.00	37.68	A
ATOM	263	C	LEU	A	39	-7.105	2.420	-5.344	1.00	28.83	A
ATOM	264	O	LEU	A	39	-8.216	2.498	-5.854	1.00	28.46	A
ATOM	265	N	ARG	A	40	-6.116	3.262	-5.615	1.00	25.66	A
ATOM	266	CA	ARG	A	40	-6.307	4.351	-6.560	1.00	22.85	A
ATOM	267	CB	ARG	A	40	-5.431	5.533	-6.175	1.00	21.75	A
ATOM	268	CG	ARG	A	40	-5.740	6.803	-6.931	1.00	21.09	A
ATOM	269	CD	ARG	A	40	-5.789	7.968	-5.960	1.00	22.80	A
ATOM	270	NE	ARG	A	40	-5.618	9.265	-6.616	1.00	22.93	A
ATOM	271	CZ	ARG	A	40	-5.550	10.426	-5.965	1.00	22.37	A
ATOM	272	NH1	ARG	A	40	-5.643	10.462	-4.645	1.00	19.87	A
ATOM	273	NH2	ARG	A	40	-5.373	11.551	-6.634	1.00	25.01	A
ATOM	274	C	ARG	A	40	-5.945	3.844	-7.943	1.00	21.35	A
ATOM	275	O	ARG	A	40	-4.907	4.184	-8.503	1.00	21.42	A
ATOM	276	N	VAL	A	41	-6.822	3.016	-8.489	1.00	19.98	A
ATOM	277	CA	VAL	A	41	-6.593	2.442	-9.796	1.00	17.66	A
ATOM	278	CB	VAL	A	41	-6.881	0.953	-9.765	1.00	16.68	A
ATOM	279	CG1	VAL	A	41	-6.242	0.349	-8.540	1.00	16.35	A
ATOM	280	CG2	VAL	A	41	-8.355	0.716	-9.769	1.00	17.46	A
ATOM	281	C	VAL	A	41	-7.491	3.113	-10.816	1.00	16.54	A
ATOM	282	O	VAL	A	41	-8.517	3.686	-10.458	1.00	17.39	A
ATOM	283	N	TYR	A	42	-7.092	3.049	-12.081	1.00	16.55	A
ATOM	284	CA	TYR	A	42	-7.859	3.634	-13.173	1.00	15.47	A
ATOM	285	CB	TYR	A	42	-7.104	4.815	-13.788	1.00	13.88	A
ATOM	286	CG	TYR	A	42	-6.574	5.785	-12.751	1.00	12.95	A
ATOM	287	CD1	TYR	A	42	-5.266	5.683	-12.281	1.00	12.86	A
ATOM	288	CE1	TYR	A	42	-4.791	6.520	-11.269	1.00	11.80	A
ATOM	289	CD2	TYR	A	42	-7.400	6.756	-12.183	1.00	12.39	A
ATOM	290	CE2	TYR	A	42	-6.927	7.597	-11.166	1.00	12.09	A
ATOM	291	CZ	TYR	A	42	-5.623	7.458	-10.720	1.00	10.82	A
ATOM	292	OH	TYR	A	42	-5.168	8.232	-9.694	1.00	12.77	A
ATOM	293	C	TYR	A	42	-8.124	2.586	-14.236	1.00	15.00	A
ATOM	294	O	TYR	A	42	-7.191	2.015	-14.797	1.00	13.20	A
ATOM	295	N	VAL	A	43	-9.407	2.329	-14.480	1.00	15.77	A
ATOM	296	CA	VAL	A	43	-9.858	1.367	-15.478	1.00	16.87	A

ATOM	297	CB	VAL	A	43	-11.367	1.045	-15.294	1.00	18.26	A
ATOM	298	CG1	VAL	A	43	-11.814	-0.036	-16.278	1.00	18.05	A
ATOM	299	CG2	VAL	A	43	-11.628	0.610	-13.866	1.00	19.17	A
ATOM	300	C	VAL	A	43	-9.661	1.967	-16.869	1.00	17.12	A
ATOM	301	O	VAL	A	43	-9.888	3.162	-17.081	1.00	18.44	A
ATOM	302	N	GLU	A	44	-9.233	1.144	-17.817	1.00	17.63	A
ATOM	303	CA	GLU	A	44	-9.023	1.628	-19.175	1.00	18.37	A
ATOM	304	CB	GLU	A	44	-7.540	1.600	-19.526	1.00	17.78	A
ATOM	305	CG	GLU	A	44	-6.700	2.474	-18.632	1.00	19.02	A
ATOM	306	CD	GLU	A	44	-5.327	2.720	-19.212	1.00	22.11	A
ATOM	307	OE1	GLU	A	44	-4.657	1.733	-19.630	1.00	22.53	A
ATOM	308	OE2	GLU	A	44	-4.912	3.905	-19.239	1.00	22.89	A
ATOM	309	C	GLU	A	44	-9.776	0.792	-20.180	1.00	17.64	A
ATOM	310	O	GLU	A	44	-10.422	1.325	-21.078	1.00	16.88	A
ATOM	311	N	GLU	A	45	-9.704	-0.519	-19.994	1.00	18.74	A
ATOM	312	CA	GLU	A	45	-10.335	-1.452	-20.898	1.00	20.81	A
ATOM	313	CB	GLU	A	45	-9.283	-1.935	-21.902	1.00	21.48	A
ATOM	314	CG	GLU	A	45	-9.777	-2.219	-23.312	1.00	25.33	A
ATOM	315	CD	GLU	A	45	-9.527	-1.059	-24.264	1.00	27.54	A
ATOM	316	OE1	GLU	A	45	-8.411	-0.490	-24.239	1.00	27.39	A
ATOM	317	OE2	GLU	A	45	-10.440	-0.720	-25.050	1.00	29.46	A
ATOM	318	C	GLU	A	45	-10.932	-2.658	-20.163	1.00	21.59	A
ATOM	319	O	GLU	A	45	-10.384	-3.141	-19.163	1.00	20.49	A
ATOM	320	N	LEU	A	46	-12.065	-3.129	-20.673	1.00	23.36	A
ATOM	321	CA	LEU	A	46	-12.732	-4.308	-20.138	1.00	25.89	A
ATOM	322	CB	LEU	A	46	-14.129	-3.968	-19.595	1.00	24.67	A
ATOM	323	CG	LEU	A	46	-14.163	-3.256	-18.243	1.00	22.90	A
ATOM	324	CD1	LEU	A	46	-15.589	-3.016	-17.823	1.00	22.10	A
ATOM	325	CD2	LEU	A	46	-13.418	-4.094	-17.209	1.00	23.07	A
ATOM	326	C	LEU	A	46	-12.831	-5.297	-21.301	1.00	27.65	A
ATOM	327	O	LEU	A	46	-13.572	-5.079	-22.255	1.00	27.18	A
ATOM	328	N	LYS	A	47	-12.058	-6.373	-21.213	1.00	31.02	A
ATOM	329	CA	LYS	A	47	-12.015	-7.396	-22.240	1.00	34.48	A
ATOM	330	CB	LYS	A	47	-10.571	-7.543	-22.731	1.00	35.53	A
ATOM	331	CG	LYS	A	47	-10.313	-8.672	-23.702	1.00	37.60	A
ATOM	332	CD	LYS	A	47	-8.938	-8.510	-24.347	1.00	38.84	A
ATOM	333	CE	LYS	A	47	-8.324	-9.851	-24.708	1.00	39.57	A
ATOM	334	NZ	LYS	A	47	-6.998	-9.685	-25.365	1.00	40.23	A
ATOM	335	C	LYS	A	47	-12.529	-8.730	-21.701	1.00	36.80	A
ATOM	336	O	LYS	A	47	-11.854	-9.400	-20.910	1.00	36.52	A
ATOM	337	N	PRO	A	48	-13.743	-9.122	-22.117	1.00	38.18	A
ATOM	338	CD	PRO	A	48	-14.620	-8.395	-23.048	1.00	38.61	A
ATOM	339	CA	PRO	A	48	-14.376	-10.372	-21.701	1.00	39.51	A
ATOM	340	CB	PRO	A	48	-15.811	-10.197	-22.178	1.00	39.56	A
ATOM	341	CG	PRO	A	48	-15.619	-9.461	-23.448	1.00	38.54	A
ATOM	342	C	PRO	A	48	-13.698	-11.561	-22.361	1.00	40.34	A
ATOM	343	O	PRO	A	48	-13.371	-11.511	-23.541	1.00	39.26	A
ATOM	344	N	THR	A	49	-13.491	-12.622	-21.588	1.00	42.45	A
ATOM	345	CA	THR	A	49	-12.851	-13.831	-22.088	1.00	43.91	A
ATOM	346	CB	THR	A	49	-11.982	-14.493	-21.028	1.00	43.45	A
ATOM	347	OG1	THR	A	49	-12.820	-14.990	-19.981	1.00	43.90	A
ATOM	348	CG2	THR	A	49	-10.988	-13.510	-20.461	1.00	43.33	A
ATOM	349	C	THR	A	49	-13.923	-14.839	-22.466	1.00	45.42	A
ATOM	350	O	THR	A	49	-15.070	-14.753	-22.012	1.00	45.06	A
ATOM	351	N	PRO	A	50	-13.555	-15.825	-23.290	1.00	46.42	A
ATOM	352	CD	PRO	A	50	-12.200	-16.122	-23.785	1.00	46.56	A
ATOM	353	CA	PRO	A	50	-14.503	-16.851	-23.721	1.00	47.28	A
ATOM	354	CB	PRO	A	50	-13.664	-17.721	-24.651	1.00	46.60	A
ATOM	355	CG	PRO	A	50	-12.292	-17.599	-24.079	1.00	46.90	A
ATOM	356	C	PRO	A	50	-15.078	-17.634	-22.539	1.00	48.52	A
ATOM	357	O	PRO	A	50	-16.274	-17.939	-22.506	1.00	48.29	A

ATOM	358	N	GLU	A	51	-14.233	-17.944	-21.559	1.00	49.18	A
ATOM	359	CA	GLU	A	51	-14.702	-18.694	-20.400	1.00	49.93	A
ATOM	360	CB	GLU	A	51	-13.520	-19.151	-19.542	1.00	50.20	A
ATOM	361	CG	GLU	A	51	-12.405	-18.147	-19.450	1.00	52.19	A
ATOM	362	CD	GLU	A	51	-11.193	-18.543	-20.287	1.00	54.81	A
ATOM	363	OE1	GLU	A	51	-10.460	-19.478	-19.886	1.00	55.81	A
ATOM	364	OE2	GLU	A	51	-10.972	-17.930	-21.355	1.00	54.93	A
ATOM	365	C	GLU	A	51	-15.698	-17.910	-19.541	1.00	50.04	A
ATOM	366	O	GLU	A	51	-16.178	-18.410	-18.521	1.00	51.24	A
ATOM	367	N	GLY	A	52	-16.017	-16.685	-19.952	1.00	48.90	A
ATOM	368	CA	GLY	A	52	-16.967	-15.882	-19.192	1.00	46.90	A
ATOM	369	C	GLY	A	52	-16.353	-14.928	-18.179	1.00	45.73	A
ATOM	370	O	GLY	A	52	-17.063	-14.220	-17.454	1.00	44.51	A
ATOM	371	N	ASP	A	53	-15.024	-14.912	-18.119	1.00	44.59	A
ATOM	372	CA	ASP	A	53	-14.325	-14.026	-17.198	1.00	42.64	A
ATOM	373	CB	ASP	A	53	-12.937	-14.574	-16.846	1.00	43.41	A
ATOM	374	CG	ASP	A	53	-12.996	-15.915	-16.139	1.00	44.82	A
ATOM	375	OD1	ASP	A	53	-13.850	-16.091	-15.237	1.00	44.78	A
ATOM	376	OD2	ASP	A	53	-12.168	-16.794	-16.477	1.00	46.39	A
ATOM	377	C	ASP	A	53	-14.172	-12.653	-17.833	1.00	40.68	A
ATOM	378	O	ASP	A	53	-14.540	-12.445	-18.988	1.00	39.21	A
ATOM	379	N	LEU	A	54	-13.612	-11.721	-17.073	1.00	39.63	A
ATOM	380	CA	LEU	A	54	-13.411	-10.364	-17.555	1.00	37.71	A
ATOM	381	CB	LEU	A	54	-14.402	-9.437	-16.858	1.00	37.78	A
ATOM	382	CG	LEU	A	54	-14.543	-8.033	-17.426	1.00	38.04	A
ATOM	383	CD1	LEU	A	54	-14.949	-8.112	-18.888	1.00	38.98	A
ATOM	384	CD2	LEU	A	54	-15.575	-7.277	-16.618	1.00	38.45	A
ATOM	385	C	LEU	A	54	-11.980	-9.874	-17.314	1.00	36.15	A
ATOM	386	O	LEU	A	54	-11.547	-9.725	-16.170	1.00	35.39	A
ATOM	387	N	GLU	A	55	-11.241	-9.639	-18.395	1.00	33.89	A
ATOM	388	CA	GLU	A	55	-9.880	-9.144	-18.267	1.00	31.45	A
ATOM	389	CB	GLU	A	55	-9.063	-9.455	-19.513	1.00	33.59	A
ATOM	390	CG	GLU	A	55	-7.566	-9.428	-19.278	1.00	36.34	A
ATOM	391	CD	GLU	A	55	-6.790	-9.078	-20.532	1.00	39.61	A
ATOM	392	OE1	GLU	A	55	-7.034	-9.707	-21.586	1.00	41.88	A
ATOM	393	OE2	GLU	A	55	-5.930	-8.169	-20.470	1.00	41.11	A
ATOM	394	C	GLU	A	55	-9.993	-7.636	-18.096	1.00	28.49	A
ATOM	395	O	GLU	A	55	-10.872	-7.001	-18.677	1.00	27.60	A
ATOM	396	N	ILE	A	56	-9.108	-7.064	-17.295	1.00	25.67	A
ATOM	397	CA	ILE	A	56	-9.154	-5.639	-17.045	1.00	22.66	A
ATOM	398	CB	ILE	A	56	-9.662	-5.362	-15.632	1.00	21.92	A
ATOM	399	CG2	ILE	A	56	-9.571	-3.875	-15.312	1.00	20.65	A
ATOM	400	CG1	ILE	A	56	-11.087	-5.857	-15.508	1.00	20.67	A
ATOM	401	CD1	ILE	A	56	-11.338	-6.533	-14.224	1.00	20.88	A
ATOM	402	C	ILE	A	56	-7.812	-4.976	-17.202	1.00	21.00	A
ATOM	403	O	ILE	A	56	-6.832	-5.376	-16.579	1.00	19.63	A
ATOM	404	N	LEU	A	57	-7.783	-3.945	-18.038	1.00	20.06	A
ATOM	405	CA	LEU	A	57	-6.563	-3.191	-18.266	1.00	19.69	A
ATOM	406	CB	LEU	A	57	-6.454	-2.789	-19.733	1.00	16.44	A
ATOM	407	CG	LEU	A	57	-5.166	-2.067	-20.075	1.00	14.61	A
ATOM	408	CD1	LEU	A	57	-4.000	-2.961	-19.751	1.00	12.30	A
ATOM	409	CD2	LEU	A	57	-5.170	-1.661	-21.537	1.00	13.35	A
ATOM	410	C	LEU	A	57	-6.667	-1.948	-17.396	1.00	20.13	A
ATOM	411	O	LEU	A	57	-7.624	-1.187	-17.529	1.00	19.45	A
ATOM	412	N	LEU	A	58	-5.702	-1.742	-16.502	1.00	20.63	A
ATOM	413	CA	LEU	A	58	-5.752	-0.578	-15.632	1.00	22.21	A
ATOM	414	CB	LEU	A	58	-6.504	-0.928	-14.350	1.00	21.17	A
ATOM	415	CG	LEU	A	58	-5.911	-2.034	-13.479	1.00	20.12	A
ATOM	416	CD1	LEU	A	58	-4.774	-1.473	-12.644	1.00	20.35	A
ATOM	417	CD2	LEU	A	58	-6.988	-2.595	-12.557	1.00	20.30	A
ATOM	418	C	LEU	A	58	-4.398	0.017	-15.285	1.00	24.46	A

ATOM	419	O	LEU	A	58	-3.354	-0.557	-15.597	1.00	22.97	A
ATOM	420	N	GLN	A	59	-4.435	1.179	-14.632	1.00	27.45	A
ATOM	421	CA	GLN	A	59	-3.225	1.893	-14.215	1.00	29.95	A
ATOM	422	CB	GLN	A	59	-3.066	3.199	-15.014	1.00	30.32	A
ATOM	423	CG	GLN	A	59	-3.110	3.066	-16.533	1.00	29.93	A
ATOM	424	CD	GLN	A	59	-1.849	2.471	-17.121	1.00	31.13	A
ATOM	425	OE1	GLN	A	59	-1.779	2.205	-18.322	1.00	31.40	A
ATOM	426	NE2	GLN	A	59	-0.839	2.265	-16.283	1.00	30.58	A
ATOM	427	C	GLN	A	59	-3.297	2.234	-12.723	1.00	31.07	A
ATOM	428	O	GLN	A	59	-4.370	2.495	-12.190	1.00	29.29	A
ATOM	429	N	LYS	A	60	-2.146	2.228	-12.063	1.00	35.25	A
ATOM	430	CA	LYS	A	60	-2.064	2.563	-10.648	1.00	40.05	A
ATOM	431	CB	LYS	A	60	-2.547	1.406	-9.772	1.00	41.46	A
ATOM	432	CG	LYS	A	60	-1.838	0.098	-10.010	1.00	44.79	A
ATOM	433	CD	LYS	A	60	-2.453	-1.010	-9.156	1.00	47.46	A
ATOM	434	CE	LYS	A	60	-1.904	-2.379	-9.554	1.00	49.65	A
ATOM	435	NZ	LYS	A	60	-2.316	-3.473	-8.616	1.00	51.45	A
ATOM	436	C	LYS	A	60	-0.633	2.919	-10.297	1.00	42.65	A
ATOM	437	O	LYS	A	60	0.304	2.379	-10.884	1.00	42.07	A
ATOM	438	N	TRP	A	61	-0.471	3.837	-9.347	1.00	46.96	A
ATOM	439	CA	TRP	A	61	0.852	4.285	-8.938	1.00	51.03	A
ATOM	440	CB	TRP	A	61	0.742	5.554	-8.081	1.00	53.76	A
ATOM	441	CG	TRP	A	61	1.987	6.403	-8.115	1.00	57.70	A
ATOM	442	CD2	TRP	A	61	2.192	7.602	-8.887	1.00	59.81	A
ATOM	443	CE2	TRP	A	61	3.526	8.021	-8.660	1.00	60.30	A
ATOM	444	CE3	TRP	A	61	1.380	8.357	-9.752	1.00	61.20	A
ATOM	445	CD1	TRP	A	61	3.169	6.160	-7.467	1.00	57.99	A
ATOM	446	NE1	TRP	A	61	4.095	7.127	-7.790	1.00	59.69	A
ATOM	447	CZ2	TRP	A	61	4.069	9.170	-9.267	1.00	61.29	A
ATOM	448	CZ3	TRP	A	61	1.921	9.503	-10.359	1.00	62.02	A
ATOM	449	CH2	TRP	A	61	3.254	9.892	-10.112	1.00	61.97	A
ATOM	450	C	TRP	A	61	1.588	3.181	-8.192	1.00	52.67	A
ATOM	451	O	TRP	A	61	0.991	2.420	-7.428	1.00	52.42	A
ATOM	452	N	GLU	A	62	2.892	3.093	-8.438	1.00	55.20	A
ATOM	453	CA	GLU	A	62	3.733	2.075	-7.817	1.00	57.16	A
ATOM	454	CB	GLU	A	62	3.580	0.762	-8.579	1.00	57.04	A
ATOM	455	CG	GLU	A	62	3.574	-0.464	-7.708	1.00	58.73	A
ATOM	456	CD	GLU	A	62	3.273	-1.727	-8.494	1.00	60.57	A
ATOM	457	OE1	GLU	A	62	4.126	-2.144	-9.315	1.00	61.75	A
ATOM	458	OE2	GLU	A	62	2.179	-2.305	-8.296	1.00	60.52	A
ATOM	459	C	GLU	A	62	5.205	2.506	-7.812	1.00	58.20	A
ATOM	460	O	GLU	A	62	5.873	2.520	-8.851	1.00	58.37	A
ATOM	461	N	ASN	A	63	5.695	2.856	-6.625	1.00	59.00	A
ATOM	462	CA	ASN	A	63	7.072	3.309	-6.426	1.00	59.09	A
ATOM	463	CB	ASN	A	63	8.057	2.146	-6.601	1.00	60.08	A
ATOM	464	CG	ASN	A	63	9.464	2.490	-6.111	1.00	61.16	A
ATOM	465	OD1	ASN	A	63	10.420	1.746	-6.347	1.00	62.06	A
ATOM	466	ND2	ASN	A	63	9.591	3.620	-5.416	1.00	60.90	A
ATOM	467	C	ASN	A	63	7.468	4.452	-7.366	1.00	58.34	A
ATOM	468	O	ASN	A	63	8.341	4.293	-8.216	1.00	58.61	A
ATOM	469	N	GLY	A	64	6.824	5.601	-7.206	1.00	57.66	A
ATOM	470	CA	GLY	A	64	7.147	6.745	-8.035	1.00	57.23	A
ATOM	471	C	GLY	A	64	7.081	6.503	-9.532	1.00	56.69	A
ATOM	472	O	GLY	A	64	7.988	6.892	-10.271	1.00	57.24	A
ATOM	473	N	GLU	A	65	6.014	5.852	-9.982	1.00	55.45	A
ATOM	474	CA	GLU	A	65	5.816	5.581	-11.407	1.00	53.27	A
ATOM	475	CB	GLU	A	65	6.940	4.700	-11.956	1.00	54.85	A
ATOM	476	CG	GLU	A	65	6.771	4.365	-13.442	1.00	57.62	A
ATOM	477	CD	GLU	A	65	7.591	3.152	-13.876	1.00	59.68	A
ATOM	478	OE1	GLU	A	65	8.808	3.316	-14.166	1.00	60.24	A
ATOM	479	OE2	GLU	A	65	7.012	2.032	-13.913	1.00	59.19	A

ATOM	480	C	GLU	A	65	4.473	4.904	-11.675	1.00	50.57	A
ATOM	481	O	GLU	A	65	4.070	3.987	-10.961	1.00	48.97	A
ATOM	482	N	CYS	A	66	3.787	5.367	-12.714	1.00	47.19	A
ATOM	483	CA	CYS	A	66	2.503	4.803	-13.084	1.00	43.59	A
ATOM	484	C	CYS	A	66	2.756	3.455	-13.762	1.00	40.51	A
ATOM	485	O	CYS	A	66	3.625	3.345	-14.632	1.00	40.39	A
ATOM	486	CB	CYS	A	66	1.767	5.752	-14.033	1.00	44.83	A
ATOM	487	SG	CYS	A	66	-0.027	5.451	-14.082	1.00	47.82	A
ATOM	488	N	ALA	A	67	2.022	2.424	-13.346	1.00	36.07	A
ATOM	489	CA	ALA	A	67	2.194	1.093	-13.927	1.00	32.69	A
ATOM	490	CB	ALA	A	67	2.661	0.127	-12.860	1.00	31.43	A
ATOM	491	C	ALA	A	67	0.930	0.550	-14.599	1.00	30.95	A
ATOM	492	O	ALA	A	67	-0.175	0.772	-14.116	1.00	30.29	A
ATOM	493	N	GLN	A	68	1.096	-0.160	-15.714	1.00	29.19	A
ATOM	494	CA	GLN	A	68	-0.039	-0.736	-16.433	1.00	28.43	A
ATOM	495	CB	GLN	A	68	0.202	-0.729	-17.954	1.00	27.45	A
ATOM	496	CG	GLN	A	68	-1.040	-1.062	-18.789	1.00	26.69	A
ATOM	497	CD	GLN	A	68	-0.746	-1.378	-20.248	1.00	26.54	A
ATOM	498	OE1	GLN	A	68	-0.308	-2.480	-20.575	1.00	25.60	A
ATOM	499	NE2	GLN	A	68	-0.986	-0.410	-21.131	1.00	25.13	A
ATOM	500	C	GLN	A	68	-0.198	-2.170	-15.960	1.00	28.78	A
ATOM	501	O	GLN	A	68	0.779	-2.908	-15.856	1.00	30.77	A
ATOM	502	N	LYS	A	69	-1.424	-2.575	-15.668	1.00	28.41	A
ATOM	503	CA	LYS	A	69	-1.637	-3.932	-15.211	1.00	27.79	A
ATOM	504	CB	LYS	A	69	-1.709	-3.942	-13.680	1.00	29.08	A
ATOM	505	CG	LYS	A	69	-0.407	-3.533	-12.974	1.00	29.62	A
ATOM	506	CD	LYS	A	69	-0.279	-4.243	-11.611	1.00	32.13	A
ATOM	507	CE	LYS	A	69	0.997	-3.868	-10.829	1.00	32.54	A
ATOM	508	NZ	LYS	A	69	0.984	-4.540	-9.486	1.00	33.14	A
ATOM	509	C	LYS	A	69	-2.883	-4.575	-15.832	1.00	27.00	A
ATOM	510	O	LYS	A	69	-3.878	-3.904	-16.121	1.00	26.83	A
ATOM	511	N	LYS	A	70	-2.801	-5.877	-16.068	1.00	26.65	A
ATOM	512	CA	LYS	A	70	-3.911	-6.629	-16.644	1.00	27.65	A
ATOM	513	CB	LYS	A	70	-3.465	-7.395	-17.883	1.00	28.88	A
ATOM	514	CG	LYS	A	70	-3.161	-6.516	-19.080	1.00	29.87	A
ATOM	515	CD	LYS	A	70	-2.682	-7.330	-20.275	1.00	31.48	A
ATOM	516	CE	LYS	A	70	-1.275	-7.868	-20.062	1.00	33.90	A
ATOM	517	NZ	LYS	A	70	-0.764	-8.550	-21.295	1.00	34.28	A
ATOM	518	C	LYS	A	70	-4.412	-7.608	-15.599	1.00	28.24	A
ATOM	519	O	LYS	A	70	-3.702	-8.539	-15.206	1.00	28.11	A
ATOM	520	N	ILE	A	71	-5.646	-7.393	-15.163	1.00	28.75	A
ATOM	521	CA	ILE	A	71	-6.256	-8.217	-14.139	1.00	29.38	A
ATOM	522	CB	ILE	A	71	-6.784	-7.342	-12.995	1.00	29.74	A
ATOM	523	CG2	ILE	A	71	-7.449	-8.201	-11.945	1.00	29.87	A
ATOM	524	CG1	ILE	A	71	-5.634	-6.519	-12.406	1.00	31.07	A
ATOM	525	CD1	ILE	A	71	-4.411	-7.320	-12.037	1.00	29.99	A
ATOM	526	C	ILE	A	71	-7.402	-9.028	-14.688	1.00	30.07	A
ATOM	527	O	ILE	A	71	-8.092	-8.594	-15.601	1.00	30.69	A
ATOM	528	N	ILE	A	72	-7.598	-10.215	-14.126	1.00	31.03	A
ATOM	529	CA	ILE	A	72	-8.684	-11.094	-14.543	1.00	31.39	A
ATOM	530	CB	ILE	A	72	-8.157	-12.481	-15.016	1.00	30.67	A
ATOM	531	CG2	ILE	A	72	-7.592	-12.374	-16.420	1.00	29.84	A
ATOM	532	CG1	ILE	A	72	-7.117	-13.031	-14.025	1.00	31.46	A
ATOM	533	CD1	ILE	A	72	-5.791	-12.272	-13.964	1.00	30.80	A
ATOM	534	C	ILE	A	72	-9.681	-11.297	-13.395	1.00	31.89	A
ATOM	535	O	ILE	A	72	-9.339	-11.822	-12.344	1.00	31.15	A
ATOM	536	N	ALA	A	73	-10.911	-10.843	-13.601	1.00	33.09	A
ATOM	537	CA	ALA	A	73	-11.961	-10.990	-12.608	1.00	34.36	A
ATOM	538	CB	ALA	A	73	-12.854	-9.756	-12.592	1.00	32.94	A
ATOM	539	C	ALA	A	73	-12.763	-12.218	-13.018	1.00	36.37	A
ATOM	540	O	ALA	A	73	-13.492	-12.180	-14.012	1.00	35.78	A

ATOM	541	N	GLU	A	74	-12.612	-13.307	-12.264	1.00	38.55	A
ATOM	542	CA	GLU	A	74	-13.311	-14.559	-12.554	1.00	40.60	A
ATOM	543	CB	GLU	A	74	-12.599	-15.720	-11.853	1.00	42.50	A
ATOM	544	CG	GLU	A	74	-11.126	-15.861	-12.232	1.00	46.59	A
ATOM	545	CD	GLU	A	74	-10.349	-16.791	-11.301	1.00	48.06	A
ATOM	546	OE1	GLU	A	74	-10.349	-16.548	-10.074	1.00	49.47	A
ATOM	547	OE2	GLU	A	74	-9.732	-17.754	-11.803	1.00	48.88	A
ATOM	548	C	GLU	A	74	-14.765	-14.505	-12.106	1.00	41.17	A
ATOM	549	O	GLU	A	74	-15.062	-14.102	-10.983	1.00	40.92	A
ATOM	550	N	LYS	A	75	-15.676	-14.910	-12.983	1.00	42.54	A
ATOM	551	CA	LYS	A	75	-17.086	-14.895	-12.630	1.00	43.98	A
ATOM	552	CB	LYS	A	75	-17.962	-15.093	-13.872	1.00	44.43	A
ATOM	553	CG	LYS	A	75	-17.430	-16.091	-14.874	1.00	45.71	A
ATOM	554	CD	LYS	A	75	-18.037	-17.459	-14.685	1.00	46.72	A
ATOM	555	CE	LYS	A	75	-17.517	-18.420	-15.743	1.00	48.20	A
ATOM	556	NZ	LYS	A	75	-16.030	-18.585	-15.686	1.00	48.26	A
ATOM	557	C	LYS	A	75	-17.373	-15.962	-11.589	1.00	44.70	A
ATOM	558	O	LYS	A	75	-16.731	-17.012	-11.561	1.00	45.03	A
ATOM	559	N	THR	A	76	-18.335	-15.673	-10.720	1.00	45.79	A
ATOM	560	CA	THR	A	76	-18.704	-16.594	-9.656	1.00	46.49	A
ATOM	561	CB	THR	A	76	-18.482	-15.931	-8.265	1.00	46.29	A
ATOM	562	OG1	THR	A	76	-19.386	-14.829	-8.099	1.00	44.95	A
ATOM	563	CG2	THR	A	76	-17.043	-15.425	-8.139	1.00	44.80	A
ATOM	564	C	THR	A	76	-20.163	-17.048	-9.784	1.00	47.70	A
ATOM	565	O	THR	A	76	-20.834	-16.742	-10.771	1.00	48.25	A
ATOM	566	N	LYS	A	77	-20.638	-17.777	-8.775	1.00	48.61	A
ATOM	567	CA	LYS	A	77	-22.004	-18.290	-8.735	1.00	49.17	A
ATOM	568	CB	LYS	A	77	-22.063	-19.543	-7.853	1.00	49.66	A
ATOM	569	CG	LYS	A	77	-21.293	-20.737	-8.418	1.00	50.61	A
ATOM	570	CD	LYS	A	77	-21.051	-21.797	-7.360	1.00	51.96	A
ATOM	571	CE	LYS	A	77	-20.127	-22.895	-7.867	1.00	52.72	A
ATOM	572	NZ	LYS	A	77	-19.518	-23.679	-6.741	1.00	52.80	A
ATOM	573	C	LYS	A	77	-22.947	-17.220	-8.201	1.00	49.74	A
ATOM	574	O	LYS	A	77	-24.022	-17.513	-7.675	1.00	50.02	A
ATOM	575	N	ILE	A	78	-22.516	-15.971	-8.333	1.00	50.28	A
ATOM	576	CA	ILE	A	78	-23.296	-14.818	-7.895	1.00	50.17	A
ATOM	577	CB	ILE	A	78	-22.618	-14.092	-6.746	1.00	51.47	A
ATOM	578	CG2	ILE	A	78	-23.550	-13.013	-6.193	1.00	50.83	A
ATOM	579	CG1	ILE	A	78	-22.241	-15.099	-5.659	1.00	51.83	A
ATOM	580	CD1	ILE	A	78	-21.526	-14.477	-4.487	1.00	53.00	A
ATOM	581	C	ILE	A	78	-23.394	-13.860	-9.072	1.00	49.78	A
ATOM	582	O	ILE	A	78	-22.386	-13.481	-9.656	1.00	50.43	A
ATOM	583	N	PRO	A	79	-24.613	-13.438	-9.416	1.00	49.21	A
ATOM	584	CD	PRO	A	79	-25.782	-13.560	-8.530	1.00	48.92	A
ATOM	585	CA	PRO	A	79	-24.913	-12.530	-10.524	1.00	48.42	A
ATOM	586	CB	PRO	A	79	-26.114	-11.762	-10.004	1.00	48.75	A
ATOM	587	CG	PRO	A	79	-26.860	-12.841	-9.308	1.00	49.27	A
ATOM	588	C	PRO	A	79	-23.803	-11.611	-11.039	1.00	47.58	A
ATOM	589	O	PRO	A	79	-23.015	-11.999	-11.917	1.00	48.27	A
ATOM	590	N	ALA	A	80	-23.751	-10.394	-10.504	1.00	44.81	A
ATOM	591	CA	ALA	A	80	-22.765	-9.417	-10.938	1.00	41.38	A
ATOM	592	CB	ALA	A	80	-23.427	-8.058	-11.109	1.00	40.61	A
ATOM	593	C	ALA	A	80	-21.599	-9.312	-9.978	1.00	39.63	A
ATOM	594	O	ALA	A	80	-21.166	-8.219	-9.625	1.00	39.74	A
ATOM	595	N	VAL	A	81	-21.076	-10.457	-9.567	1.00	37.52	A
ATOM	596	CA	VAL	A	81	-19.950	-10.479	-8.646	1.00	35.26	A
ATOM	597	CB	VAL	A	81	-20.380	-11.038	-7.276	1.00	34.98	A
ATOM	598	CG1	VAL	A	81	-19.193	-11.110	-6.337	1.00	32.95	A
ATOM	599	CG2	VAL	A	81	-21.473	-10.175	-6.692	1.00	34.19	A
ATOM	600	C	VAL	A	81	-18.815	-11.328	-9.204	1.00	34.49	A
ATOM	601	O	VAL	A	81	-19.012	-12.490	-9.559	1.00	34.64	A

ATOM	602	N	PHE	A	82	-17.628	-10.742	-9.286	1.00	33.80	A
ATOM	603	CA	PHE	A	82	-16.471	-11.457	-9.805	1.00	34.10	A
ATOM	604	CB	PHE	A	82	-15.909	-10.758	-11.049	1.00	32.25	A
ATOM	605	CG	PHE	A	82	-16.919	-10.533	-12.134	1.00	30.18	A
ATOM	606	CD1	PHE	A	82	-17.829	-9.492	-12.048	1.00	28.63	A
ATOM	607	CD2	PHE	A	82	-16.967	-11.367	-13.245	1.00	29.67	A
ATOM	608	CE1	PHE	A	82	-18.764	-9.286	-13.051	1.00	28.96	A
ATOM	609	CE2	PHE	A	82	-17.903	-11.162	-14.248	1.00	29.77	A
ATOM	610	CZ	PHE	A	82	-18.803	-10.121	-14.151	1.00	29.10	A
ATOM	611	C	PHE	A	82	-15.401	-11.508	-8.735	1.00	35.20	A
ATOM	612	O	PHE	A	82	-15.527	-10.872	-7.695	1.00	35.28	A
ATOM	613	N	LYS	A	83	-14.344	-12.261	-8.988	1.00	37.28	A
ATOM	614	CA	LYS	A	83	-13.281	-12.354	-8.014	1.00	40.61	A
ATOM	615	CB	LYS	A	83	-13.354	-13.689	-7.282	1.00	41.61	A
ATOM	616	CG	LYS	A	83	-12.383	-13.787	-6.118	1.00	44.64	A
ATOM	617	CD	LYS	A	83	-12.342	-15.182	-5.500	1.00	45.25	A
ATOM	618	CE	LYS	A	83	-11.773	-16.211	-6.467	1.00	46.11	A
ATOM	619	NZ	LYS	A	83	-11.737	-17.558	-5.854	1.00	45.81	A
ATOM	620	C	LYS	A	83	-11.917	-12.198	-8.667	1.00	42.61	A
ATOM	621	O	LYS	A	83	-11.716	-12.622	-9.801	1.00	41.97	A
ATOM	622	N	ILE	A	84	-10.989	-11.582	-7.941	1.00	45.99	A
ATOM	623	CA	ILE	A	84	-9.634	-11.357	-8.422	1.00	50.16	A
ATOM	624	CB	ILE	A	84	-9.173	-9.929	-8.133	1.00	50.06	A
ATOM	625	CG2	ILE	A	84	-7.789	-9.706	-8.719	1.00	50.61	A
ATOM	626	CG1	ILE	A	84	-10.159	-8.929	-8.724	1.00	49.73	A
ATOM	627	CD1	ILE	A	84	-10.097	-7.572	-8.059	1.00	50.68	A
ATOM	628	C	ILE	A	84	-8.713	-12.309	-7.682	1.00	53.84	A
ATOM	629	O	ILE	A	84	-8.653	-12.295	-6.453	1.00	54.52	A
ATOM	630	N	ASP	A	85	-7.989	-13.127	-8.437	1.00	58.42	A
ATOM	631	CA	ASP	A	85	-7.077	-14.110	-7.855	1.00	62.83	A
ATOM	632	CB	ASP	A	85	-6.543	-15.030	-8.960	1.00	64.60	A
ATOM	633	CG	ASP	A	85	-6.508	-16.494	-8.540	1.00	66.46	A
ATOM	634	OD1	ASP	A	85	-6.292	-17.364	-9.421	1.00	67.24	A
ATOM	635	OD2	ASP	A	85	-6.695	-16.771	-7.330	1.00	67.13	A
ATOM	636	C	ASP	A	85	-5.909	-13.512	-7.052	1.00	64.82	A
ATOM	637	O	ASP	A	85	-5.184	-14.243	-6.373	1.00	65.69	A
ATOM	638	N	ALA	A	86	-5.725	-12.195	-7.129	1.00	66.46	A
ATOM	639	CA	ALA	A	86	-4.655	-11.533	-6.386	1.00	68.14	A
ATOM	640	CB	ALA	A	86	-4.686	-10.028	-6.644	1.00	67.64	A
ATOM	641	C	ALA	A	86	-4.843	-11.817	-4.896	1.00	69.84	A
ATOM	642	O	ALA	A	86	-5.910	-12.273	-4.477	1.00	71.12	A
ATOM	643	N	LEU	A	87	-3.814	-11.551	-4.097	1.00	71.20	A
ATOM	644	CA	LEU	A	87	-3.893	-11.792	-2.655	1.00	71.87	A
ATOM	645	CB	LEU	A	87	-2.572	-11.406	-1.967	1.00	72.10	A
ATOM	646	CG	LEU	A	87	-2.329	-11.877	-0.520	1.00	72.35	A
ATOM	647	CD1	LEU	A	87	-2.150	-13.388	-0.499	1.00	71.46	A
ATOM	648	CD2	LEU	A	87	-1.084	-11.201	0.051	1.00	72.25	A
ATOM	649	C	LEU	A	87	-5.043	-10.989	-2.045	1.00	72.03	A
ATOM	650	O	LEU	A	87	-5.599	-10.086	-2.683	1.00	71.30	A
ATOM	651	N	ASN	A	88	-5.383	-11.326	-0.802	1.00	71.95	A
ATOM	652	CA	ASN	A	88	-6.457	-10.664	-0.064	1.00	71.65	A
ATOM	653	CB	ASN	A	88	-6.299	-9.132	-0.143	1.00	73.05	A
ATOM	654	CG	ASN	A	88	-4.849	-8.670	0.032	1.00	73.75	A
ATOM	655	OD1	ASN	A	88	-4.164	-9.051	0.989	1.00	74.21	A
ATOM	656	ND2	ASN	A	88	-4.387	-7.831	-0.891	1.00	73.03	A
ATOM	657	C	ASN	A	88	-7.838	-11.067	-0.606	1.00	70.43	A
ATOM	658	O	ASN	A	88	-8.851	-10.913	0.084	1.00	70.57	A
ATOM	659	N	GLU	A	89	-7.863	-11.582	-1.839	1.00	68.18	A
ATOM	660	CA	GLU	A	89	-9.100	-11.997	-2.511	1.00	65.08	A
ATOM	661	CB	GLU	A	89	-9.798	-13.114	-1.728	1.00	67.04	A
ATOM	662	CG	GLU	A	89	-9.172	-14.497	-1.905	1.00	69.48	A

ATOM	663	CD	GLU	A	89	-9.208	-14.972	-3.357	1.00	70.72	A
ATOM	664	OE1	GLU	A	89	-8.437	-14.439	-4.191	1.00	71.05	A
ATOM	665	OE2	GLU	A	89	-10.024	-15.869	-3.664	1.00	71.34	A
ATOM	666	C	GLU	A	89	-10.076	-10.844	-2.719	1.00	61.80	A
ATOM	667	O	GLU	A	89	-11.203	-10.870	-2.224	1.00	62.02	A
ATOM	668	N	ASN	A	90	-9.630	-9.829	-3.448	1.00	57.36	A
ATOM	669	CA	ASN	A	90	-10.460	-8.671	-3.727	1.00	52.67	A
ATOM	670	CB	ASN	A	90	-9.647	-7.646	-4.533	1.00	52.48	A
ATOM	671	CG	ASN	A	90	-8.928	-6.634	-3.646	1.00	52.32	A
ATOM	672	OD1	ASN	A	90	-9.508	-5.631	-3.216	1.00	53.38	A
ATOM	673	ND2	ASN	A	90	-7.663	-6.899	-3.364	1.00	52.47	A
ATOM	674	C	ASN	A	90	-11.715	-9.096	-4.501	1.00	49.56	A
ATOM	675	O	ASN	A	90	-11.625	-9.859	-5.458	1.00	48.05	A
ATOM	676	N	LYS	A	91	-12.886	-8.639	-4.061	1.00	46.27	A
ATOM	677	CA	LYS	A	91	-14.127	-8.960	-4.756	1.00	42.55	A
ATOM	678	CB	LYS	A	91	-15.196	-9.528	-3.816	1.00	43.88	A
ATOM	679	CG	LYS	A	91	-15.043	-11.009	-3.467	1.00	46.95	A
ATOM	680	CD	LYS	A	91	-16.307	-11.537	-2.772	1.00	49.01	A
ATOM	681	CE	LYS	A	91	-16.120	-12.957	-2.226	1.00	48.98	A
ATOM	682	NZ	LYS	A	91	-17.356	-13.517	-1.586	1.00	47.83	A
ATOM	683	C	LYS	A	91	-14.667	-7.697	-5.394	1.00	39.10	A
ATOM	684	O	LYS	A	91	-14.642	-6.621	-4.797	1.00	38.37	A
ATOM	685	N	VAL	A	92	-15.150	-7.839	-6.619	1.00	35.12	A
ATOM	686	CA	VAL	A	92	-15.703	-6.721	-7.356	1.00	31.05	A
ATOM	687	CB	VAL	A	92	-15.035	-6.638	-8.732	1.00	30.40	A
ATOM	688	CG1	VAL	A	92	-15.487	-5.402	-9.460	1.00	30.11	A
ATOM	689	CG2	VAL	A	92	-13.526	-6.647	-8.558	1.00	29.54	A
ATOM	690	C	VAL	A	92	-17.210	-6.939	-7.502	1.00	28.12	A
ATOM	691	O	VAL	A	92	-17.658	-8.058	-7.731	1.00	27.38	A
ATOM	692	N	LEU	A	93	-17.991	-5.875	-7.348	1.00	25.32	A
ATOM	693	CA	LEU	A	93	-19.442	-5.972	-7.470	1.00	23.52	A
ATOM	694	CB	LEU	A	93	-20.109	-5.806	-6.107	1.00	24.09	A
ATOM	695	CG	LEU	A	93	-19.510	-6.500	-4.880	1.00	22.89	A
ATOM	696	CD1	LEU	A	93	-19.306	-7.960	-5.154	1.00	23.08	A
ATOM	697	CD2	LEU	A	93	-18.197	-5.831	-4.513	1.00	24.87	A
ATOM	698	C	LEU	A	93	-19.955	-4.875	-8.392	1.00	22.06	A
ATOM	699	O	LEU	A	93	-19.679	-3.699	-8.169	1.00	22.62	A
ATOM	700	N	VAL	A	94	-20.700	-5.250	-9.423	1.00	20.24	A
ATOM	701	CA	VAL	A	94	-21.234	-4.262	-10.359	1.00	19.43	A
ATOM	702	CB	VAL	A	94	-21.402	-4.869	-11.785	1.00	18.31	A
ATOM	703	CG1	VAL	A	94	-21.967	-3.841	-12.735	1.00	16.47	A
ATOM	704	CG2	VAL	A	94	-20.072	-5.368	-12.291	1.00	14.46	A
ATOM	705	C	VAL	A	94	-22.582	-3.795	-9.823	1.00	19.37	A
ATOM	706	O	VAL	A	94	-23.565	-4.536	-9.843	1.00	19.85	A
ATOM	707	N	LEU	A	95	-22.618	-2.563	-9.333	1.00	18.93	A
ATOM	708	CA	LEU	A	95	-23.838	-2.009	-8.766	1.00	18.77	A
ATOM	709	CB	LEU	A	95	-23.502	-0.785	-7.915	1.00	20.01	A
ATOM	710	CG	LEU	A	95	-22.774	-1.051	-6.591	1.00	20.85	A
ATOM	711	CD1	LEU	A	95	-22.627	0.263	-5.844	1.00	20.24	A
ATOM	712	CD2	LEU	A	95	-23.576	-2.041	-5.738	1.00	21.51	A
ATOM	713	C	LEU	A	95	-24.898	-1.639	-9.793	1.00	18.28	A
ATOM	714	O	LEU	A	95	-26.080	-1.907	-9.591	1.00	16.17	A
ATOM	715	N	ASP	A	96	-24.477	-1.024	-10.889	1.00	19.53	A
ATOM	716	CA	ASP	A	96	-25.413	-0.623	-11.926	1.00	21.52	A
ATOM	717	CB	ASP	A	96	-26.225	0.582	-11.460	1.00	21.47	A
ATOM	718	CG	ASP	A	96	-27.412	0.850	-12.350	1.00	22.85	A
ATOM	719	OD1	ASP	A	96	-28.132	-0.126	-12.655	1.00	25.16	A
ATOM	720	OD2	ASP	A	96	-27.635	2.020	-12.733	1.00	23.28	A
ATOM	721	C	ASP	A	96	-24.667	-0.269	-13.204	1.00	22.80	A
ATOM	722	O	ASP	A	96	-23.461	-0.023	-13.169	1.00	24.06	A
ATOM	723	N	THR	A	97	-25.383	-0.247	-14.326	1.00	22.38	A

ATOM	724	CA	THR	A	97	-24.776	0.095	-15.600	1.00	22.34	A
ATOM	725	CB	THR	A	97	-23.696	-0.931	-16.006	1.00	22.56	A
ATOM	726	OG1	THR	A	97	-23.116	-0.553	-17.264	1.00	22.90	A
ATOM	727	CG2	THR	A	97	-24.303	-2.319	-16.139	1.00	20.01	A
ATOM	728	C	THR	A	97	-25.803	0.143	-16.707	1.00	22.52	A
ATOM	729	O	THR	A	97	-26.726	-0.659	-16.711	1.00	23.66	A
ATOM	730	N	ASP	A	98	-25.642	1.083	-17.637	1.00	22.22	A
ATOM	731	CA	ASP	A	98	-26.544	1.203	-18.780	1.00	21.65	A
ATOM	732	CB	ASP	A	98	-26.949	2.671	-19.004	1.00	22.77	A
ATOM	733	CG	ASP	A	98	-25.814	3.527	-19.532	1.00	24.72	A
ATOM	734	OD1	ASP	A	98	-24.658	3.311	-19.127	1.00	27.27	A
ATOM	735	OD2	ASP	A	98	-26.075	4.434	-20.347	1.00	26.48	A
ATOM	736	C	ASP	A	98	-25.819	0.635	-20.007	1.00	21.37	A
ATOM	737	O	ASP	A	98	-26.393	0.538	-21.086	1.00	20.79	A
ATOM	738	N	TYR	A	99	-24.555	0.252	-19.815	1.00	20.65	A
ATOM	739	CA	TYR	A	99	-23.708	-0.330	-20.864	1.00	19.29	A
ATOM	740	CB	TYR	A	99	-24.451	-1.454	-21.601	1.00	16.84	A
ATOM	741	CG	TYR	A	99	-24.856	-2.627	-20.750	1.00	14.61	A
ATOM	742	CD1	TYR	A	99	-23.946	-3.617	-20.406	1.00	12.54	A
ATOM	743	CE1	TYR	A	99	-24.328	-4.698	-19.614	1.00	12.07	A
ATOM	744	CD2	TYR	A	99	-26.156	-2.742	-20.280	1.00	13.65	A
ATOM	745	CE2	TYR	A	99	-26.547	-3.814	-19.492	1.00	13.03	A
ATOM	746	CZ	TYR	A	99	-25.631	-4.792	-19.157	1.00	13.13	A
ATOM	747	OH	TYR	A	99	-26.036	-5.856	-18.365	1.00	12.49	A
ATOM	748	C	TYR	A	99	-23.194	0.667	-21.902	1.00	20.53	A
ATOM	749	O	TYR	A	99	-22.073	0.530	-22.379	1.00	20.58	A
ATOM	750	N	LYS	A	100	-24.005	1.670	-22.238	1.00	21.61	A
ATOM	751	CA	LYS	A	100	-23.649	2.654	-23.258	1.00	21.03	A
ATOM	752	CB	LYS	A	100	-24.891	3.004	-24.085	1.00	23.12	A
ATOM	753	CG	LYS	A	100	-25.705	1.800	-24.531	1.00	26.96	A
ATOM	754	CD	LYS	A	100	-24.896	0.871	-25.424	1.00	29.57	A
ATOM	755	CE	LYS	A	100	-25.436	-0.584	-25.398	1.00	33.09	A
ATOM	756	NZ	LYS	A	100	-26.875	-0.751	-25.800	1.00	33.75	A
ATOM	757	C	LYS	A	100	-23.046	3.946	-22.718	1.00	20.25	A
ATOM	758	O	LYS	A	100	-22.413	4.689	-23.461	1.00	20.17	A
ATOM	759	N	LYS	A	101	-23.236	4.228	-21.435	1.00	19.04	A
ATOM	760	CA	LYS	A	101	-22.701	5.467	-20.874	1.00	17.66	A
ATOM	761	CB	LYS	A	101	-23.837	6.492	-20.704	1.00	17.25	A
ATOM	762	CG	LYS	A	101	-24.408	7.018	-22.017	1.00	18.59	A
ATOM	763	CD	LYS	A	101	-25.507	8.052	-21.803	1.00	21.15	A
ATOM	764	CE	LYS	A	101	-26.614	7.492	-20.892	1.00	25.51	A
ATOM	765	NZ	LYS	A	101	-27.841	8.354	-20.716	1.00	25.35	A
ATOM	766	C	LYS	A	101	-21.927	5.328	-19.552	1.00	16.29	A
ATOM	767	O	LYS	A	101	-20.783	5.767	-19.457	1.00	16.64	A
ATOM	768	N	TYR	A	102	-22.541	4.723	-18.539	1.00	13.96	A
ATOM	769	CA	TYR	A	102	-21.884	4.579	-17.250	1.00	12.20	A
ATOM	770	CB	TYR	A	102	-22.552	5.485	-16.221	1.00	13.37	A
ATOM	771	CG	TYR	A	102	-23.967	5.074	-15.913	1.00	14.80	A
ATOM	772	CD1	TYR	A	102	-25.026	5.452	-16.743	1.00	15.56	A
ATOM	773	CE1	TYR	A	102	-26.332	5.040	-16.473	1.00	16.40	A
ATOM	774	CD2	TYR	A	102	-24.245	4.275	-14.810	1.00	14.91	A
ATOM	775	CE2	TYR	A	102	-25.537	3.852	-14.533	1.00	16.83	A
ATOM	776	CZ	TYR	A	102	-26.574	4.231	-15.362	1.00	17.72	A
ATOM	777	OH	TYR	A	102	-27.843	3.776	-15.086	1.00	19.73	A
ATOM	778	C	TYR	A	102	-21.870	3.163	-16.691	1.00	11.60	A
ATOM	779	O	TYR	A	102	-22.555	2.272	-17.194	1.00	11.84	A
ATOM	780	N	LEU	A	103	-21.081	2.973	-15.636	1.00	9.56	A
ATOM	781	CA	LEU	A	103	-20.979	1.690	-14.954	1.00	8.12	A
ATOM	782	CB	LEU	A	103	-20.022	0.743	-15.694	1.00	8.06	A
ATOM	783	CG	LEU	A	103	-19.983	-0.682	-15.115	1.00	7.72	A
ATOM	784	CD1	LEU	A	103	-19.586	-1.676	-16.152	1.00	8.20	A

ATOM	785	CD2	LEU	A	103	-19.049	-0.720	-13.930	1.00	7.20	A
ATOM	786	C	LEU	A	103	-20.488	1.948	-13.526	1.00	9.01	A
ATOM	787	O	LEU	A	103	-19.541	2.692	-13.313	1.00	8.51	A
ATOM	788	N	LEU	A	104	-21.136	1.319	-12.551	1.00	9.89	A
ATOM	789	CA	LEU	A	104	-20.773	1.513	-11.158	1.00	10.66	A
ATOM	790	CB	LEU	A	104	-21.958	2.088	-10.398	1.00	10.47	A
ATOM	791	CG	LEU	A	104	-22.586	3.339	-11.002	1.00	9.11	A
ATOM	792	CD1	LEU	A	104	-23.833	3.732	-10.219	1.00	8.12	A
ATOM	793	CD2	LEU	A	104	-21.576	4.465	-10.984	1.00	8.64	A
ATOM	794	C	LEU	A	104	-20.354	0.225	-10.485	1.00	11.23	A
ATOM	795	O	LEU	A	104	-21.083	-0.758	-10.534	1.00	13.70	A
ATOM	796	N	PHE	A	105	-19.202	0.232	-9.829	1.00	10.76	A
ATOM	797	CA	PHE	A	105	-18.748	-0.969	-9.153	1.00	11.87	A
ATOM	798	CB	PHE	A	105	-17.829	-1.782	-10.068	1.00	10.16	A
ATOM	799	CG	PHE	A	105	-16.489	-1.140	-10.292	1.00	9.81	A
ATOM	800	CD1	PHE	A	105	-16.337	-0.129	-11.249	1.00	8.87	A
ATOM	801	CD2	PHE	A	105	-15.391	-1.494	-9.482	1.00	8.20	A
ATOM	802	CE1	PHE	A	105	-15.118	0.521	-11.394	1.00	9.90	A
ATOM	803	CE2	PHE	A	105	-14.164	-0.857	-9.606	1.00	6.67	A
ATOM	804	CZ	PHE	A	105	-14.016	0.156	-10.563	1.00	9.33	A
ATOM	805	C	PHE	A	105	-17.996	-0.615	-7.877	1.00	14.65	A
ATOM	806	O	PHE	A	105	-17.598	0.535	-7.675	1.00	13.84	A
ATOM	807	N	CYS	A	106	-17.809	-1.620	-7.028	1.00	17.88	A
ATOM	808	CA	CYS	A	106	-17.085	-1.469	-5.774	1.00	21.18	A
ATOM	809	C	CYS	A	106	-16.159	-2.660	-5.649	1.00	24.19	A
ATOM	810	O	CYS	A	106	-16.388	-3.698	-6.272	1.00	24.79	A
ATOM	811	CB	CYS	A	106	-18.026	-1.484	-4.571	1.00	20.47	A
ATOM	812	SG	CYS	A	106	-19.182	-0.095	-4.399	1.00	22.55	A
ATOM	813	N	MET	A	107	-15.115	-2.521	-4.846	1.00	27.17	A
ATOM	814	CA	MET	A	107	-14.205	-3.625	-4.652	1.00	32.34	A
ATOM	815	CB	MET	A	107	-12.999	-3.483	-5.575	1.00	31.11	A
ATOM	816	CG	MET	A	107	-12.201	-2.228	-5.382	1.00	30.90	A
ATOM	817	SD	MET	A	107	-11.147	-1.907	-6.805	1.00	30.75	A
ATOM	818	CE	MET	A	107	-11.313	-0.129	-6.939	1.00	30.73	A
ATOM	819	C	MET	A	107	-13.779	-3.692	-3.202	1.00	36.20	A
ATOM	820	O	MET	A	107	-13.458	-2.670	-2.606	1.00	36.17	A
ATOM	821	N	GLU	A	108	-13.806	-4.894	-2.625	1.00	41.42	A
ATOM	822	CA	GLU	A	108	-13.416	-5.086	-1.225	1.00	45.26	A
ATOM	823	CB	GLU	A	108	-14.655	-5.281	-0.344	1.00	45.70	A
ATOM	824	CG	GLU	A	108	-15.475	-6.512	-0.691	1.00	47.75	A
ATOM	825	CD	GLU	A	108	-16.441	-6.901	0.412	1.00	48.53	A
ATOM	826	OE1	GLU	A	108	-17.331	-6.087	0.742	1.00	48.20	A
ATOM	827	OE2	GLU	A	108	-16.303	-8.024	0.948	1.00	50.31	A
ATOM	828	C	GLU	A	108	-12.500	-6.287	-1.055	1.00	47.65	A
ATOM	829	O	GLU	A	108	-12.474	-7.181	-1.894	1.00	47.55	A
ATOM	830	N	ASN	A	109	-11.744	-6.297	0.034	1.00	51.81	A
ATOM	831	CA	ASN	A	109	-10.852	-7.408	0.310	1.00	56.91	A
ATOM	832	CB	ASN	A	109	-9.469	-6.900	0.729	1.00	58.54	A
ATOM	833	CG	ASN	A	109	-8.779	-6.089	-0.373	1.00	60.68	A
ATOM	834	OD1	ASN	A	109	-9.271	-5.030	-0.790	1.00	61.57	A
ATOM	835	ND2	ASN	A	109	-7.636	-6.590	-0.853	1.00	60.43	A
ATOM	836	C	ASN	A	109	-11.451	-8.258	1.415	1.00	59.35	A
ATOM	837	O	ASN	A	109	-11.616	-7.800	2.544	1.00	59.16	A
ATOM	838	N	SER	A	110	-11.789	-9.494	1.072	1.00	63.16	A
ATOM	839	CA	SER	A	110	-12.367	-10.425	2.034	1.00	66.90	A
ATOM	840	CB	SER	A	110	-12.335	-11.850	1.471	1.00	66.79	A
ATOM	841	OG	SER	A	110	-12.800	-12.790	2.426	0.00	67.03	A
ATOM	842	C	SER	A	110	-11.629	-10.390	3.378	1.00	68.96	A
ATOM	843	O	SER	A	110	-12.247	-10.508	4.442	1.00	69.21	A
ATOM	844	N	ALA	A	111	-10.309	-10.228	3.324	1.00	70.87	A
ATOM	845	CA	ALA	A	111	-9.497	-10.182	4.534	1.00	73.10	A

ATOM	846	CB	ALA	A	111	-8.041	-9.886	4.178	1.00	74.11	A
ATOM	847	C	ALA	A	111	-10.027	-9.127	5.502	1.00	74.80	A
ATOM	848	O	ALA	A	111	-10.281	-9.414	6.672	1.00	75.12	A
ATOM	849	N	GLU	A	112	-10.191	-7.904	5.010	1.00	76.54	A
ATOM	850	CA	GLU	A	112	-10.699	-6.812	5.832	1.00	77.67	A
ATOM	851	CB	GLU	A	112	-9.578	-5.812	6.142	1.00	78.60	A
ATOM	852	CG	GLU	A	112	-8.796	-6.095	7.440	1.00	79.84	A
ATOM	853	CD	GLU	A	112	-8.054	-7.425	7.433	1.00	80.21	A
ATOM	854	OE1	GLU	A	112	-7.213	-7.638	6.529	1.00	80.30	A
ATOM	855	OE2	GLU	A	112	-8.305	-8.248	8.344	1.00	79.95	A
ATOM	856	C	GLU	A	112	-11.858	-6.105	5.130	1.00	77.80	A
ATOM	857	O	GLU	A	112	-11.687	-5.032	4.555	1.00	77.90	A
ATOM	858	N	PRO	A	113	-13.060	-6.710	5.164	1.00	77.88	A
ATOM	859	CD	PRO	A	113	-13.373	-8.027	5.750	1.00	77.78	A
ATOM	860	CA	PRO	A	113	-14.248	-6.130	4.527	1.00	77.56	A
ATOM	861	CB	PRO	A	113	-15.233	-7.294	4.526	1.00	77.90	A
ATOM	862	CG	PRO	A	113	-14.885	-8.010	5.793	1.00	78.21	A
ATOM	863	C	PRO	A	113	-14.791	-4.909	5.275	1.00	76.94	A
ATOM	864	O	PRO	A	113	-15.998	-4.664	5.290	1.00	77.05	A
ATOM	865	N	GLU	A	114	-13.888	-4.151	5.893	1.00	75.57	A
ATOM	866	CA	GLU	A	114	-14.258	-2.954	6.646	1.00	73.78	A
ATOM	867	CB	GLU	A	114	-14.203	-3.244	8.151	1.00	75.45	A
ATOM	868	CG	GLU	A	114	-15.247	-4.243	8.650	1.00	78.06	A
ATOM	869	CD	GLU	A	114	-15.136	-4.521	10.149	1.00	79.68	A
ATOM	870	OE1	GLU	A	114	-15.184	-3.554	10.947	1.00	80.23	A
ATOM	871	OE2	GLU	A	114	-15.006	-5.709	10.529	1.00	80.56	A
ATOM	872	C	GLU	A	114	-13.327	-1.785	6.314	1.00	71.15	A
ATOM	873	O	GLU	A	114	-13.738	-0.620	6.330	1.00	70.50	A
ATOM	874	N	GLN	A	115	-12.071	-2.110	6.017	1.00	68.29	A
ATOM	875	CA	GLN	A	115	-11.057	-1.110	5.681	1.00	64.44	A
ATOM	876	CB	GLN	A	115	-9.952	-1.083	6.757	1.00	66.01	A
ATOM	877	CG	GLN	A	115	-9.552	-2.450	7.325	1.00	66.72	A
ATOM	878	CD	GLN	A	115	-10.479	-2.918	8.444	1.00	67.94	A
ATOM	879	OE1	GLN	A	115	-10.572	-2.282	9.497	1.00	68.73	A
ATOM	880	NE2	GLN	A	115	-11.166	-4.035	8.220	1.00	68.36	A
ATOM	881	C	GLN	A	115	-10.436	-1.334	4.297	1.00	59.98	A
ATOM	882	O	GLN	A	115	-9.217	-1.230	4.120	1.00	59.29	A
ATOM	883	N	SER	A	116	-11.289	-1.638	3.322	1.00	54.28	A
ATOM	884	CA	SER	A	116	-10.852	-1.868	1.956	1.00	48.50	A
ATOM	885	CB	SER	A	116	-10.068	-3.177	1.847	1.00	49.02	A
ATOM	886	OG	SER	A	116	-10.929	-4.299	1.952	1.00	48.61	A
ATOM	887	C	SER	A	116	-12.041	-1.914	1.009	1.00	44.48	A
ATOM	888	O	SER	A	116	-12.159	-2.826	0.200	1.00	45.41	A
ATOM	889	N	LEU	A	117	-12.939	-0.946	1.123	1.00	39.02	A
ATOM	890	CA	LEU	A	117	-14.085	-0.894	0.233	1.00	33.21	A
ATOM	891	CB	LEU	A	117	-15.398	-0.842	1.023	1.00	32.48	A
ATOM	892	CG	LEU	A	117	-16.677	-0.687	0.179	1.00	32.08	A
ATOM	893	CD1	LEU	A	117	-16.989	-1.984	-0.551	1.00	32.14	A
ATOM	894	CD2	LEU	A	117	-17.843	-0.320	1.073	1.00	32.82	A
ATOM	895	C	LEU	A	117	-13.965	0.348	-0.643	1.00	29.70	A
ATOM	896	O	LEU	A	117	-14.139	1.469	-0.164	1.00	29.28	A
ATOM	897	N	ALA	A	118	-13.640	0.152	-1.917	1.00	25.59	A
ATOM	898	CA	ALA	A	118	-13.524	1.268	-2.854	1.00	21.14	A
ATOM	899	CB	ALA	A	118	-12.120	1.322	-3.465	1.00	19.41	A
ATOM	900	C	ALA	A	118	-14.566	1.083	-3.942	1.00	17.56	A
ATOM	901	O	ALA	A	118	-14.859	-0.038	-4.351	1.00	17.34	A
ATOM	902	N	CYS	A	119	-15.133	2.185	-4.402	1.00	15.41	A
ATOM	903	CA	CYS	A	119	-16.147	2.127	-5.447	1.00	14.62	A
ATOM	904	C	CYS	A	119	-15.805	3.145	-6.520	1.00	12.55	A
ATOM	905	O	CYS	A	119	-15.160	4.150	-6.239	1.00	12.39	A
ATOM	906	CB	CYS	A	119	-17.527	2.449	-4.881	1.00	16.58	A

ATOM	907	SG	CYS	A	119	-18.118	1.399	-3.507	1.00	19.89	A
ATOM	908	N	GLN	A	120	-16.242	2.902	-7.751	1.00	11.31	A
ATOM	909	CA	GLN	A	120	-15.931	3.837	-8.826	1.00	9.34	A
ATOM	910	CB	GLN	A	120	-14.691	3.382	-9.600	1.00	8.23	A
ATOM	911	CG	GLN	A	120	-13.408	3.510	-8.824	1.00	9.44	A
ATOM	912	CD	GLN	A	120	-12.192	3.228	-9.666	1.00	10.28	A
ATOM	913	OE1	GLN	A	120	-12.276	3.187	-10.895	1.00	9.16	A
ATOM	914	NE2	GLN	A	120	-11.042	3.044	-9.011	1.00	11.24	A
ATOM	915	C	GLN	A	120	-17.055	4.029	-9.808	1.00	7.85	A
ATOM	916	O	GLN	A	120	-17.935	3.191	-9.936	1.00	8.44	A
ATOM	917	N	CYS	A	121	-17.015	5.160	-10.491	1.00	6.54	A
ATOM	918	CA	CYS	A	121	-17.985	5.467	-11.505	1.00	5.28	A
ATOM	919	CB	CYS	A	121	-18.684	6.774	-11.200	1.00	3.98	A
ATOM	920	SG	CYS	A	121	-19.807	7.249	-12.559	1.00	6.72	A
ATOM	921	C	CYS	A	121	-17.230	5.594	-12.829	1.00	5.88	A
ATOM	922	O	CYS	A	121	-16.462	6.539	-13.035	1.00	6.74	A
ATOM	923	N	LEU	A	122	-17.439	4.621	-13.711	1.00	4.93	A
ATOM	924	CA	LEU	A	122	-16.796	4.583	-15.016	1.00	4.70	A
ATOM	925	CB	LEU	A	122	-16.472	3.133	-15.390	1.00	2.79	A
ATOM	926	CG	LEU	A	122	-15.544	2.308	-14.507	1.00	3.05	A
ATOM	927	CD1	LEU	A	122	-15.272	0.946	-15.164	1.00	1.00	A
ATOM	928	CD2	LEU	A	122	-14.247	3.051	-14.288	1.00	2.57	A
ATOM	929	C	LEU	A	122	-17.708	5.192	-16.085	1.00	4.56	A
ATOM	930	O	LEU	A	122	-18.909	5.334	-15.871	1.00	3.87	A
ATOM	931	N	VAL	A	123	-17.130	5.577	-17.221	1.00	5.28	A
ATOM	932	CA	VAL	A	123	-17.908	6.131	-18.327	1.00	7.18	A
ATOM	933	CB	VAL	A	123	-18.066	7.656	-18.252	1.00	5.88	A
ATOM	934	CG1	VAL	A	123	-19.103	8.011	-17.226	1.00	4.32	A
ATOM	935	CG2	VAL	A	123	-16.727	8.304	-17.961	1.00	5.09	A
ATOM	936	C	VAL	A	123	-17.262	5.806	-19.655	1.00	8.00	A
ATOM	937	O	VAL	A	123	-16.063	5.591	-19.731	1.00	9.15	A
ATOM	938	N	ARG	A	124	-18.061	5.783	-20.708	1.00	9.32	A
ATOM	939	CA	ARG	A	124	-17.546	5.467	-22.024	1.00	11.59	A
ATOM	940	CB	ARG	A	124	-18.701	5.084	-22.931	1.00	10.68	A
ATOM	941	CG	ARG	A	124	-19.397	3.813	-22.512	1.00	9.01	A
ATOM	942	CD	ARG	A	124	-18.512	2.641	-22.744	1.00	10.13	A
ATOM	943	NE	ARG	A	124	-19.251	1.379	-22.807	1.00	10.56	A
ATOM	944	CZ	ARG	A	124	-18.684	0.222	-23.122	1.00	10.23	A
ATOM	945	NH1	ARG	A	124	-17.387	0.172	-23.399	1.00	11.34	A
ATOM	946	NH2	ARG	A	124	-19.401	-0.878	-23.151	1.00	9.22	A
ATOM	947	C	ARG	A	124	-16.742	6.600	-22.646	1.00	12.71	A
ATOM	948	O	ARG	A	124	-15.653	6.378	-23.172	1.00	11.93	A
ATOM	949	N	THR	A	125	-17.265	7.817	-22.598	1.00	13.65	A
ATOM	950	CA	THR	A	125	-16.533	8.934	-23.177	1.00	14.62	A
ATOM	951	CB	THR	A	125	-17.445	9.802	-24.041	1.00	14.21	A
ATOM	952	OG1	THR	A	125	-18.544	10.273	-23.253	1.00	13.29	A
ATOM	953	CG2	THR	A	125	-17.951	8.995	-25.232	1.00	12.45	A
ATOM	954	C	THR	A	125	-15.885	9.784	-22.098	1.00	15.60	A
ATOM	955	O	THR	A	125	-16.376	9.859	-20.977	1.00	17.35	A
ATOM	956	N	PRO	A	126	-14.757	10.427	-22.422	1.00	15.78	A
ATOM	957	CD	PRO	A	126	-14.037	10.316	-23.700	1.00	16.42	A
ATOM	958	CA	PRO	A	126	-14.019	11.274	-21.488	1.00	16.99	A
ATOM	959	CB	PRO	A	126	-12.689	11.472	-22.203	1.00	17.41	A
ATOM	960	CG	PRO	A	126	-13.083	11.474	-23.641	1.00	15.72	A
ATOM	961	C	PRO	A	126	-14.717	12.596	-21.183	1.00	18.38	A
ATOM	962	O	PRO	A	126	-14.110	13.671	-21.247	1.00	18.55	A
ATOM	963	N	GLU	A	127	-15.995	12.508	-20.844	1.00	19.23	A
ATOM	964	CA	GLU	A	127	-16.789	13.686	-20.562	1.00	19.40	A
ATOM	965	CB	GLU	A	127	-17.916	13.797	-21.595	1.00	21.19	A
ATOM	966	CG	GLU	A	127	-18.145	15.195	-22.115	1.00	25.72	A
ATOM	967	CD	GLU	A	127	-17.240	15.548	-23.277	1.00	28.77	A

ATOM	968	OE1	GLU	A	127	-16.003	15.421	-23.156	1.00	31.16	A
ATOM	969	OE2	GLU	A	127	-17.774	15.970	-24.319	1.00	30.40	A
ATOM	970	C	GLU	A	127	-17.362	13.511	-19.176	1.00	18.77	A
ATOM	971	O	GLU	A	127	-17.372	12.399	-18.644	1.00	17.85	A
ATOM	972	N	VAL	A	128	-17.816	14.609	-18.581	1.00	18.87	A
ATOM	973	CA	VAL	A	128	-18.422	14.551	-17.259	1.00	19.36	A
ATOM	974	CB	VAL	A	128	-18.215	15.865	-16.488	1.00	19.07	A
ATOM	975	CG1	VAL	A	128	-18.943	15.808	-15.150	1.00	16.94	A
ATOM	976	CG2	VAL	A	128	-16.731	16.100	-16.285	1.00	19.94	A
ATOM	977	C	VAL	A	128	-19.925	14.274	-17.392	1.00	19.92	A
ATOM	978	O	VAL	A	128	-20.694	15.098	-17.885	1.00	18.96	A
ATOM	979	N	ASP	A	129	-20.335	13.095	-16.952	1.00	21.31	A
ATOM	980	CA	ASP	A	129	-21.735	12.708	-17.018	1.00	22.53	A
ATOM	981	CB	ASP	A	129	-21.839	11.213	-17.310	1.00	22.60	A
ATOM	982	CG	ASP	A	129	-23.247	10.784	-17.628	1.00	24.84	A
ATOM	983	OD1	ASP	A	129	-24.172	11.273	-16.931	1.00	25.94	A
ATOM	984	OD2	ASP	A	129	-23.428	9.955	-18.563	1.00	24.73	A
ATOM	985	C	ASP	A	129	-22.402	13.026	-15.681	1.00	23.04	A
ATOM	986	O	ASP	A	129	-22.375	12.214	-14.767	1.00	22.72	A
ATOM	987	N	ASP	A	130	-23.007	14.203	-15.568	1.00	25.17	A
ATOM	988	CA	ASP	A	130	-23.652	14.599	-14.324	1.00	27.39	A
ATOM	989	CB	ASP	A	130	-24.307	15.967	-14.483	1.00	28.36	A
ATOM	990	CG	ASP	A	130	-23.295	17.080	-14.682	1.00	30.38	A
ATOM	991	OD1	ASP	A	130	-22.407	17.253	-13.811	1.00	30.27	A
ATOM	992	OD2	ASP	A	130	-23.402	17.791	-15.707	1.00	31.41	A
ATOM	993	C	ASP	A	130	-24.689	13.589	-13.829	1.00	28.10	A
ATOM	994	O	ASP	A	130	-24.758	13.288	-12.629	1.00	27.21	A
ATOM	995	N	GLU	A	131	-25.497	13.073	-14.749	1.00	28.87	A
ATOM	996	CA	GLU	A	131	-26.528	12.098	-14.396	1.00	30.34	A
ATOM	997	CB	GLU	A	131	-27.415	11.780	-15.608	1.00	32.40	A
ATOM	998	CG	GLU	A	131	-28.620	10.891	-15.283	1.00	36.77	A
ATOM	999	CD	GLU	A	131	-29.516	10.597	-16.495	1.00	39.79	A
ATOM	1000	OE1	GLU	A	131	-29.391	9.498	-17.097	1.00	39.74	A
ATOM	1001	OE2	GLU	A	131	-30.347	11.473	-16.842	1.00	41.54	A
ATOM	1002	C	GLU	A	131	-25.902	10.804	-13.871	1.00	29.77	A
ATOM	1003	O	GLU	A	131	-26.481	10.124	-13.013	1.00	30.31	A
ATOM	1004	N	ALA	A	132	-24.724	10.462	-14.390	1.00	27.73	A
ATOM	1005	CA	ALA	A	132	-24.022	9.261	-13.961	1.00	24.94	A
ATOM	1006	CB	ALA	A	132	-22.890	8.951	-14.917	1.00	25.43	A
ATOM	1007	C	ALA	A	132	-23.485	9.459	-12.547	1.00	24.00	A
ATOM	1008	O	ALA	A	132	-23.628	8.584	-11.690	1.00	22.89	A
ATOM	1009	N	LEU	A	133	-22.875	10.613	-12.301	1.00	22.77	A
ATOM	1010	CA	LEU	A	133	-22.346	10.916	-10.978	1.00	23.19	A
ATOM	1011	CB	LEU	A	133	-21.685	12.293	-10.977	1.00	21.08	A
ATOM	1012	CG	LEU	A	133	-20.298	12.301	-11.606	1.00	20.59	A
ATOM	1013	CD1	LEU	A	133	-19.737	13.703	-11.645	1.00	20.36	A
ATOM	1014	CD2	LEU	A	133	-19.398	11.374	-10.808	1.00	20.36	A
ATOM	1015	C	LEU	A	133	-23.490	10.889	-9.976	1.00	23.95	A
ATOM	1016	O	LEU	A	133	-23.321	10.464	-8.835	1.00	24.50	A
ATOM	1017	N	GLU	A	134	-24.653	11.349	-10.428	1.00	24.99	A
ATOM	1018	CA	GLU	A	134	-25.855	11.383	-9.619	1.00	25.76	A
ATOM	1019	CB	GLU	A	134	-27.027	11.882	-10.457	1.00	28.60	A
ATOM	1020	CG	GLU	A	134	-27.242	13.373	-10.379	1.00	34.21	A
ATOM	1021	CD	GLU	A	134	-27.894	13.791	-9.068	1.00	38.01	A
ATOM	1022	OE1	GLU	A	134	-29.127	13.596	-8.931	1.00	40.41	A
ATOM	1023	OE2	GLU	A	134	-27.175	14.300	-8.173	1.00	39.41	A
ATOM	1024	C	GLU	A	134	-26.169	10.002	-9.081	1.00	25.10	A
ATOM	1025	O	GLU	A	134	-26.307	9.797	-7.877	1.00	25.75	A
ATOM	1026	N	LYS	A	135	-26.286	9.042	-9.980	1.00	23.93	A
ATOM	1027	CA	LYS	A	135	-26.581	7.696	-9.550	1.00	22.05	A
ATOM	1028	CB	LYS	A	135	-26.738	6.789	-10.767	1.00	21.87	A

ATOM	1029	CG	LYS	A	135	-27.675	7.367	-11.806	1.00	22.27	A
ATOM	1030	CD	LYS	A	135	-28.199	6.301	-12.732	1.00	23.04	A
ATOM	1031	CE	LYS	A	135	-29.081	6.926	-13.792	1.00	24.13	A
ATOM	1032	NZ	LYS	A	135	-29.705	5.909	-14.672	1.00	25.19	A
ATOM	1033	C	LYS	A	135	-25.470	7.187	-8.645	1.00	20.93	A
ATOM	1034	O	LYS	A	135	-25.715	6.338	-7.810	1.00	22.80	A
ATOM	1035	N	PHE	A	136	-24.256	7.712	-8.800	1.00	19.44	A
ATOM	1036	CA	PHE	A	136	-23.123	7.276	-7.986	1.00	17.59	A
ATOM	1037	CB	PHE	A	136	-21.804	7.753	-8.623	1.00	16.15	A
ATOM	1038	CG	PHE	A	136	-20.553	7.155	-8.008	1.00	12.06	A
ATOM	1039	CD1	PHE	A	136	-20.380	5.777	-7.924	1.00	10.59	A
ATOM	1040	CD2	PHE	A	136	-19.523	7.986	-7.562	1.00	10.64	A
ATOM	1041	CE1	PHE	A	136	-19.194	5.235	-7.408	1.00	8.70	A
ATOM	1042	CE2	PHE	A	136	-18.333	7.461	-7.045	1.00	8.38	A
ATOM	1043	CZ	PHE	A	136	-18.170	6.080	-6.970	1.00	8.38	A
ATOM	1044	C	PHE	A	136	-23.263	7.820	-6.575	1.00	17.94	A
ATOM	1045	O	PHE	A	136	-23.060	7.094	-5.610	1.00	18.11	A
ATOM	1046	N	ASP	A	137	-23.608	9.097	-6.454	1.00	18.56	A
ATOM	1047	CA	ASP	A	137	-23.777	9.705	-5.140	1.00	20.78	A
ATOM	1048	CB	ASP	A	137	-24.020	11.199	-5.283	1.00	21.98	A
ATOM	1049	CG	ASP	A	137	-22.761	11.933	-5.650	1.00	26.64	A
ATOM	1050	OD1	ASP	A	137	-22.791	13.172	-5.803	1.00	28.97	A
ATOM	1051	OD2	ASP	A	137	-21.715	11.255	-5.780	1.00	29.46	A
ATOM	1052	C	ASP	A	137	-24.916	9.055	-4.381	1.00	21.56	A
ATOM	1053	O	ASP	A	137	-24.829	8.823	-3.180	1.00	20.68	A
ATOM	1054	N	LYS	A	138	-25.978	8.757	-5.114	1.00	23.89	A
ATOM	1055	CA	LYS	A	138	-27.163	8.119	-4.575	1.00	24.77	A
ATOM	1056	CB	LYS	A	138	-28.201	7.983	-5.685	1.00	26.49	A
ATOM	1057	CG	LYS	A	138	-29.590	8.464	-5.311	1.00	29.38	A
ATOM	1058	CD	LYS	A	138	-30.440	8.746	-6.551	1.00	31.73	A
ATOM	1059	CE	LYS	A	138	-30.787	7.464	-7.309	1.00	33.18	A
ATOM	1060	NZ	LYS	A	138	-31.684	6.561	-6.512	1.00	32.38	A
ATOM	1061	C	LYS	A	138	-26.834	6.738	-4.020	1.00	24.53	A
ATOM	1062	O	LYS	A	138	-27.283	6.368	-2.933	1.00	25.44	A
ATOM	1063	N	ALA	A	139	-26.047	5.981	-4.771	1.00	23.16	A
ATOM	1064	CA	ALA	A	139	-25.684	4.640	-4.365	1.00	22.42	A
ATOM	1065	CB	ALA	A	139	-25.192	3.859	-5.557	1.00	22.54	A
ATOM	1066	C	ALA	A	139	-24.631	4.653	-3.296	1.00	22.29	A
ATOM	1067	O	ALA	A	139	-24.315	3.619	-2.725	1.00	23.95	A
ATOM	1068	N	LEU	A	140	-24.091	5.823	-3.007	1.00	22.46	A
ATOM	1069	CA	LEU	A	140	-23.050	5.906	-2.002	1.00	22.59	A
ATOM	1070	CB	LEU	A	140	-21.923	6.819	-2.494	1.00	21.49	A
ATOM	1071	CG	LEU	A	140	-20.640	6.154	-2.992	1.00	20.22	A
ATOM	1072	CD1	LEU	A	140	-20.962	5.055	-3.974	1.00	20.98	A
ATOM	1073	CD2	LEU	A	140	-19.746	7.196	-3.618	1.00	19.16	A
ATOM	1074	C	LEU	A	140	-23.552	6.400	-0.661	1.00	23.85	A
ATOM	1075	O	LEU	A	140	-22.930	6.131	0.362	1.00	24.84	A
ATOM	1076	N	LYS	A	141	-24.684	7.098	-0.660	1.00	23.81	A
ATOM	1077	CA	LYS	A	141	-25.221	7.650	0.572	1.00	23.95	A
ATOM	1078	CB	LYS	A	141	-26.479	8.488	0.275	1.00	27.33	A
ATOM	1079	CG	LYS	A	141	-27.732	7.679	-0.062	1.00	31.67	A
ATOM	1080	CD	LYS	A	141	-28.961	8.581	-0.222	1.00	34.16	A
ATOM	1081	CE	LYS	A	141	-30.252	7.750	-0.167	1.00	35.86	A
ATOM	1082	NZ	LYS	A	141	-31.508	8.520	-0.454	1.00	34.90	A
ATOM	1083	C	LYS	A	141	-25.521	6.577	1.620	1.00	22.86	A
ATOM	1084	O	LYS	A	141	-25.814	6.886	2.776	1.00	23.16	A
ATOM	1085	N	ALA	A	142	-25.425	5.320	1.202	1.00	21.93	A
ATOM	1086	CA	ALA	A	142	-25.673	4.164	2.058	1.00	20.55	A
ATOM	1087	CB	ALA	A	142	-26.646	3.227	1.371	1.00	20.26	A
ATOM	1088	C	ALA	A	142	-24.373	3.399	2.385	1.00	20.23	A
ATOM	1089	O	ALA	A	142	-24.393	2.329	2.994	1.00	20.08	A

ATOM	1090	N	LEU	A	143	-23.241	3.928	1.957	1.00	19.08	A
ATOM	1091	CA	LEU	A	143	-21.983	3.284	2.249	1.00	16.71	A
ATOM	1092	CB	LEU	A	143	-21.222	2.995	0.957	1.00	16.66	A
ATOM	1093	CG	LEU	A	143	-21.938	2.027	0.009	1.00	14.82	A
ATOM	1094	CD1	LEU	A	143	-21.160	1.904	-1.280	1.00	11.61	A
ATOM	1095	CD2	LEU	A	143	-22.080	0.661	0.683	1.00	14.87	A
ATOM	1096	C	LEU	A	143	-21.186	4.210	3.152	1.00	16.35	A
ATOM	1097	O	LEU	A	143	-21.389	5.427	3.138	1.00	16.52	A
ATOM	1098	N	PRO	A	144	-20.266	3.639	3.954	1.00	16.35	A
ATOM	1099	CD	PRO	A	144	-20.060	2.183	4.085	1.00	15.80	A
ATOM	1100	CA	PRO	A	144	-19.410	4.356	4.896	1.00	14.08	A
ATOM	1101	CB	PRO	A	144	-19.073	3.278	5.904	1.00	15.09	A
ATOM	1102	CG	PRO	A	144	-18.889	2.090	5.023	1.00	14.40	A
ATOM	1103	C	PRO	A	144	-18.185	4.926	4.221	1.00	12.91	A
ATOM	1104	O	PRO	A	144	-17.054	4.622	4.612	1.00	11.28	A
ATOM	1105	N	MET	A	145	-18.419	5.753	3.204	1.00	11.90	A
ATOM	1106	CA	MET	A	145	-17.332	6.378	2.456	1.00	10.38	A
ATOM	1107	CB	MET	A	145	-17.820	6.851	1.083	1.00	10.21	A
ATOM	1108	CG	MET	A	145	-18.395	5.753	0.207	1.00	12.43	A
ATOM	1109	SD	MET	A	145	-17.224	4.412	-0.200	1.00	13.28	A
ATOM	1110	CE	MET	A	145	-17.618	3.241	1.092	1.00	14.67	A
ATOM	1111	C	MET	A	145	-16.819	7.566	3.229	1.00	9.66	A
ATOM	1112	O	MET	A	145	-17.605	8.384	3.689	1.00	11.74	A
ATOM	1113	N	HIS	A	146	-15.506	7.663	3.388	1.00	9.91	A
ATOM	1114	CA	HIS	A	146	-14.936	8.807	4.098	1.00	9.87	A
ATOM	1115	CB	HIS	A	146	-14.282	8.358	5.403	1.00	8.49	A
ATOM	1116	CG	HIS	A	146	-15.269	7.866	6.418	1.00	9.17	A
ATOM	1117	CD2	HIS	A	146	-15.920	8.512	7.415	1.00	8.75	A
ATOM	1118	ND1	HIS	A	146	-15.717	6.565	6.448	1.00	8.57	A
ATOM	1119	CE1	HIS	A	146	-16.599	6.427	7.422	1.00	7.28	A
ATOM	1120	NE2	HIS	A	146	-16.738	7.592	8.024	1.00	8.13	A
ATOM	1121	C	HIS	A	146	-13.946	9.581	3.233	1.00	8.88	A
ATOM	1122	O	HIS	A	146	-13.035	10.211	3.741	1.00	9.73	A
ATOM	1123	N	ILE	A	147	-14.158	9.542	1.923	1.00	10.01	A
ATOM	1124	CA	ILE	A	147	-13.315	10.234	0.954	1.00	9.28	A
ATOM	1125	CB	ILE	A	147	-11.833	9.773	1.028	1.00	9.29	A
ATOM	1126	CG2	ILE	A	147	-11.765	8.271	1.046	1.00	10.92	A
ATOM	1127	CG1	ILE	A	147	-11.054	10.332	-0.163	1.00	8.05	A
ATOM	1128	CD1	ILE	A	147	-9.542	10.152	-0.042	1.00	8.07	A
ATOM	1129	C	ILE	A	147	-13.862	9.957	-0.439	1.00	9.12	A
ATOM	1130	O	ILE	A	147	-14.181	8.812	-0.772	1.00	8.68	A
ATOM	1131	N	ARG	A	148	-13.993	11.011	-1.239	1.00	8.42	A
ATOM	1132	CA	ARG	A	148	-14.501	10.878	-2.607	1.00	10.40	A
ATOM	1133	CB	ARG	A	148	-15.975	11.295	-2.724	1.00	13.43	A
ATOM	1134	CG	ARG	A	148	-16.996	10.452	-1.996	1.00	19.51	A
ATOM	1135	CD	ARG	A	148	-17.301	10.971	-0.586	1.00	23.86	A
ATOM	1136	NE	ARG	A	148	-18.387	10.192	-0.002	1.00	27.00	A
ATOM	1137	CZ	ARG	A	148	-19.646	10.211	-0.439	1.00	29.04	A
ATOM	1138	NH1	ARG	A	148	-19.986	10.987	-1.461	1.00	29.76	A
ATOM	1139	NH2	ARG	A	148	-20.561	9.416	0.115	1.00	30.58	A
ATOM	1140	C	ARG	A	148	-13.729	11.790	-3.537	1.00	9.25	A
ATOM	1141	O	ARG	A	148	-13.368	12.896	-3.151	1.00	8.09	A
ATOM	1142	N	LEU	A	149	-13.497	11.346	-4.767	1.00	8.09	A
ATOM	1143	CA	LEU	A	149	-12.792	12.171	-5.741	1.00	8.72	A
ATOM	1144	CB	LEU	A	149	-11.347	11.686	-5.954	1.00	9.94	A
ATOM	1145	CG	LEU	A	149	-10.315	11.644	-4.821	1.00	11.17	A
ATOM	1146	CD1	LEU	A	149	-10.696	10.566	-3.809	1.00	13.78	A
ATOM	1147	CD2	LEU	A	149	-8.959	11.343	-5.398	1.00	11.11	A
ATOM	1148	C	LEU	A	149	-13.520	12.142	-7.088	1.00	9.46	A
ATOM	1149	O	LEU	A	149	-14.094	11.120	-7.486	1.00	8.08	A
ATOM	1150	N	SER	A	150	-13.491	13.272	-7.785	1.00	10.68	A

ATOM	1151	CA	SER	A	150	-14.108	13.391	-9.111	1.00	12.68	A
ATOM	1152	CB	SER	A	150	-15.379	14.239	-9.041	1.00	13.11	A
ATOM	1153	OG	SER	A	150	-15.921	14.443	-10.333	1.00	15.87	A
ATOM	1154	C	SER	A	150	-13.117	14.052	-10.076	1.00	12.26	A
ATOM	1155	O	SER	A	150	-12.519	15.077	-9.746	1.00	11.98	A
ATOM	1156	N	PHE	A	151	-12.979	13.506	-11.278	1.00	12.33	A
ATOM	1157	CA	PHE	A	151	-12.035	14.073	-12.231	1.00	14.30	A
ATOM	1158	CB	PHE	A	151	-11.174	12.934	-12.804	1.00	13.88	A
ATOM	1159	CG	PHE	A	151	-10.390	12.186	-11.754	1.00	14.26	A
ATOM	1160	CD1	PHE	A	151	-9.346	12.800	-11.068	1.00	13.10	A
ATOM	1161	CD2	PHE	A	151	-10.731	10.882	-11.413	1.00	14.46	A
ATOM	1162	CE1	PHE	A	151	-8.661	12.123	-10.055	1.00	12.62	A
ATOM	1163	CE2	PHE	A	151	-10.049	10.203	-10.402	1.00	14.91	A
ATOM	1164	CZ	PHE	A	151	-9.017	10.824	-9.723	1.00	13.40	A
ATOM	1165	C	PHE	A	151	-12.621	14.952	-13.361	1.00	14.36	A
ATOM	1166	O	PHE	A	151	-13.833	14.987	-13.570	1.00	13.80	A
ATOM	1167	N	ASN	A	152	-11.736	15.671	-14.053	1.00	15.86	A
ATOM	1168	CA	ASN	A	152	-12.095	16.544	-15.164	1.00	16.02	A
ATOM	1169	CB	ASN	A	152	-11.376	17.890	-15.097	1.00	18.74	A
ATOM	1170	CG	ASN	A	152	-11.397	18.498	-13.740	1.00	23.20	A
ATOM	1171	OD1	ASN	A	152	-10.753	19.522	-13.506	1.00	22.52	A
ATOM	1172	ND2	ASN	A	152	-12.145	17.877	-12.815	1.00	27.59	A
ATOM	1173	C	ASN	A	152	-11.596	15.925	-16.447	1.00	15.17	A
ATOM	1174	O	ASN	A	152	-10.651	15.141	-16.445	1.00	14.04	A
ATOM	1175	N	PRO	A	153	-12.199	16.315	-17.574	1.00	15.08	A
ATOM	1176	CD	PRO	A	153	-13.352	17.224	-17.726	1.00	15.27	A
ATOM	1177	CA	PRO	A	153	-11.778	15.791	-18.864	1.00	13.73	A
ATOM	1178	CB	PRO	A	153	-12.503	16.701	-19.839	1.00	12.37	A
ATOM	1179	CG	PRO	A	153	-13.791	16.948	-19.133	1.00	13.31	A
ATOM	1180	C	PRO	A	153	-10.259	15.885	-18.988	1.00	13.52	A
ATOM	1181	O	PRO	A	153	-9.603	14.920	-19.377	1.00	14.15	A
ATOM	1182	N	THR	A	154	-9.684	17.029	-18.629	1.00	12.52	A
ATOM	1183	CA	THR	A	154	-8.231	17.177	-18.747	1.00	11.18	A
ATOM	1184	CB	THR	A	154	-7.763	18.587	-18.357	1.00	9.17	A
ATOM	1185	OG1	THR	A	154	-8.404	19.554	-19.196	1.00	12.66	A
ATOM	1186	CG2	THR	A	154	-6.264	18.704	-18.522	1.00	6.13	A
ATOM	1187	C	THR	A	154	-7.477	16.194	-17.883	1.00	9.97	A
ATOM	1188	O	THR	A	154	-6.415	15.722	-18.263	1.00	9.78	A
ATOM	1189	N	GLN	A	155	-8.015	15.900	-16.709	1.00	10.79	A
ATOM	1190	CA	GLN	A	155	-7.342	14.980	-15.811	1.00	11.97	A
ATOM	1191	CB	GLN	A	155	-7.960	15.067	-14.435	1.00	10.76	A
ATOM	1192	CG	GLN	A	155	-7.894	16.455	-13.894	1.00	11.68	A
ATOM	1193	CD	GLN	A	155	-8.361	16.542	-12.473	1.00	11.87	A
ATOM	1194	OE1	GLN	A	155	-9.539	16.324	-12.169	1.00	9.48	A
ATOM	1195	NE2	GLN	A	155	-7.434	16.859	-11.579	1.00	12.87	A
ATOM	1196	C	GLN	A	155	-7.391	13.550	-16.312	1.00	13.34	A
ATOM	1197	O	GLN	A	155	-6.529	12.742	-15.978	1.00	15.38	A
ATOM	1198	N	LEU	A	156	-8.403	13.235	-17.112	1.00	13.70	A
ATOM	1199	CA	LEU	A	156	-8.532	11.904	-17.662	1.00	13.24	A
ATOM	1200	CB	LEU	A	156	-9.929	11.720	-18.238	1.00	10.39	A
ATOM	1201	CG	LEU	A	156	-11.052	11.820	-17.229	1.00	11.34	A
ATOM	1202	CD1	LEU	A	156	-12.388	11.688	-17.961	1.00	11.83	A
ATOM	1203	CD2	LEU	A	156	-10.913	10.747	-16.157	1.00	9.95	A
ATOM	1204	C	LEU	A	156	-7.490	11.667	-18.752	1.00	15.89	A
ATOM	1205	O	LEU	A	156	-7.306	10.543	-19.194	1.00	16.59	A
ATOM	1206	N	GLU	A	157	-6.824	12.733	-19.184	1.00	19.18	A
ATOM	1207	CA	GLU	A	157	-5.822	12.626	-20.225	1.00	23.89	A
ATOM	1208	CB	GLU	A	157	-5.570	13.984	-20.878	1.00	21.16	A
ATOM	1209	CG	GLU	A	157	-6.829	14.699	-21.299	1.00	21.05	A
ATOM	1210	CD	GLU	A	157	-6.534	15.965	-22.071	1.00	20.58	A
ATOM	1211	OE1	GLU	A	157	-5.525	16.629	-21.756	1.00	20.06	A

ATOM	1212	OE2	GLU	A	157	-7.311	16.302	-22.983	1.00	21.31	A
ATOM	1213	C	GLU	A	157	-4.522	12.088	-19.646	1.00	28.18	A
ATOM	1214	O	GLU	A	157	-3.538	11.905	-20.362	1.00	29.82	A
ATOM	1215	N	GLU	A	158	-4.517	11.835	-18.345	1.00	32.98	A
ATOM	1216	CA	GLU	A	158	-3.330	11.319	-17.681	1.00	38.78	A
ATOM	1217	CB	GLU	A	158	-2.996	12.164	-16.458	1.00	39.64	A
ATOM	1218	CG	GLU	A	158	-2.128	13.371	-16.796	1.00	44.59	A
ATOM	1219	CD	GLU	A	158	-0.665	13.000	-17.086	1.00	46.03	A
ATOM	1220	OE1	GLU	A	158	-0.419	11.941	-17.718	1.00	47.74	A
ATOM	1221	OE2	GLU	A	158	0.236	13.780	-16.692	1.00	45.88	A
ATOM	1222	C	GLU	A	158	-3.413	9.858	-17.275	1.00	42.20	A
ATOM	1223	O	GLU	A	158	-4.325	9.435	-16.551	1.00	42.84	A
ATOM	1224	N	GLN	A	159	-2.436	9.090	-17.750	1.00	45.59	A
ATOM	1225	CA	GLN	A	159	-2.349	7.664	-17.463	1.00	47.67	A
ATOM	1226	CB	GLN	A	159	-0.942	7.158	-17.786	1.00	48.76	A
ATOM	1227	CG	GLN	A	159	0.128	8.223	-17.656	1.00	50.01	A
ATOM	1228	CD	GLN	A	159	1.465	7.645	-17.258	1.00	51.72	A
ATOM	1229	OE1	GLN	A	159	1.926	6.648	-17.829	1.00	51.63	A
ATOM	1230	NE2	GLN	A	159	2.107	8.275	-16.275	1.00	52.16	A
ATOM	1231	C	GLN	A	159	-2.664	7.412	-16.001	1.00	48.11	A
ATOM	1232	O	GLN	A	159	-3.296	6.416	-15.659	1.00	48.73	A
ATOM	1233	N	CYS	A	160	-2.224	8.329	-15.144	1.00	48.60	A
ATOM	1234	CA	CYS	A	160	-2.454	8.209	-13.709	1.00	49.21	A
ATOM	1235	C	CYS	A	160	-3.262	9.371	-13.146	1.00	50.25	A
ATOM	1236	O	CYS	A	160	-3.207	9.640	-11.947	1.00	50.25	A
ATOM	1237	CB	CYS	A	160	-1.111	8.090	-12.970	1.00	48.31	A
ATOM	1238	SG	CYS	A	160	-0.706	6.398	-12.410	1.00	47.53	A
ATOM	1239	N	HIS	A	161	-4.010	10.052	-14.017	1.00	52.12	A
ATOM	1240	CA	HIS	A	161	-4.855	11.199	-13.631	1.00	53.87	A
ATOM	1241	CB	HIS	A	161	-6.062	10.722	-12.801	1.00	51.81	A
ATOM	1242	CG	HIS	A	161	-7.069	9.939	-13.586	1.00	50.36	A
ATOM	1243	CD2	HIS	A	161	-8.422	9.928	-13.542	1.00	49.28	A
ATOM	1244	ND1	HIS	A	161	-6.712	8.997	-14.530	1.00	50.71	A
ATOM	1245	CE1	HIS	A	161	-7.802	8.440	-15.030	1.00	49.63	A
ATOM	1246	NE2	HIS	A	161	-8.853	8.987	-14.446	1.00	49.13	A
ATOM	1247	C	HIS	A	161	-4.105	12.295	-12.856	1.00	55.61	A
ATOM	1248	O	HIS	A	161	-3.703	12.089	-11.701	1.00	55.42	A
ATOM	1249	N	ILE	A	162	-3.938	13.455	-13.504	1.00	57.43	A
ATOM	1250	CA	ILE	A	162	-3.253	14.631	-12.936	1.00	58.86	A
ATOM	1251	CB	ILE	A	162	-3.873	15.962	-13.480	1.00	58.80	A
ATOM	1252	CG2	ILE	A	162	-3.183	17.170	-12.812	1.00	58.56	A
ATOM	1253	CG1	ILE	A	162	-3.750	16.023	-15.012	1.00	57.83	A
ATOM	1254	CD1	ILE	A	162	-4.369	17.271	-15.642	1.00	55.94	A
ATOM	1255	C	ILE	A	162	-3.272	14.695	-11.400	1.00	59.78	A
ATOM	1256	OT1	ILE	A	162	-2.170	14.685	-10.788	1.00	59.36	A
ATOM	1257	OT2	ILE	A	162	-4.394	14.754	-10.837	1.00	60.08	A
ATOM	1258	CB	ASP	L	1	16.550	5.554	-25.535	1.00	16.37	L
ATOM	1259	CG	ASP	L	1	16.503	7.069	-25.599	1.00	19.69	L
ATOM	1260	OD1	ASP	L	1	16.752	7.733	-24.551	1.00	21.13	L
ATOM	1261	OD2	ASP	L	1	16.236	7.600	-26.702	1.00	18.80	L
ATOM	1262	C	ASP	L	1	15.914	3.511	-24.259	1.00	13.85	L
ATOM	1263	O	ASP	L	1	16.895	2.773	-24.238	1.00	15.08	L
ATOM	1264	N	ASP	L	1	17.141	5.276	-23.136	1.00	16.84	L
ATOM	1265	CA	ASP	L	1	16.101	5.010	-24.177	1.00	15.47	L
ATOM	1266	N	ILE	L	2	14.669	3.052	-24.335	1.00	11.38	L
ATOM	1267	CA	ILE	L	2	14.423	1.626	-24.435	1.00	8.80	L
ATOM	1268	CB	ILE	L	2	12.995	1.271	-23.982	1.00	8.68	L
ATOM	1269	CG2	ILE	L	2	12.795	-0.225	-24.067	1.00	6.83	L
ATOM	1270	CG1	ILE	L	2	12.771	1.771	-22.551	1.00	9.62	L
ATOM	1271	CD1	ILE	L	2	11.413	1.456	-21.968	1.00	8.82	L
ATOM	1272	C	ILE	L	2	14.643	1.214	-25.886	1.00	8.52	L

ATOM	1273	O	ILE	L	2	14.104	1.824	-26.816	1.00	4.81	L
ATOM	1274	N	VAL	L	3	15.474	0.195	-26.078	1.00	8.21	L
ATOM	1275	CA	VAL	L	3	15.778	-0.278	-27.422	1.00	7.79	L
ATOM	1276	CB	VAL	L	3	17.284	-0.578	-27.549	1.00	5.49	L
ATOM	1277	CG1	VAL	L	3	17.627	-0.990	-28.958	1.00	1.00	L
ATOM	1278	CG2	VAL	L	3	18.072	0.648	-27.135	1.00	5.03	L
ATOM	1279	C	VAL	L	3	14.959	-1.520	-27.769	1.00	9.17	L
ATOM	1280	O	VAL	L	3	15.054	-2.547	-27.098	1.00	11.84	L
ATOM	1281	N	MET	L	4	14.133	-1.417	-28.802	1.00	8.22	L
ATOM	1282	CA	MET	L	4	13.304	-2.543	-29.202	1.00	7.73	L
ATOM	1283	CB	MET	L	4	11.923	-2.055	-29.655	1.00	9.47	L
ATOM	1284	CG	MET	L	4	11.149	-1.225	-28.653	1.00	5.71	L
ATOM	1285	SD	MET	L	4	10.934	-2.041	-27.095	1.00	9.24	L
ATOM	1286	CE	MET	L	4	9.556	-3.115	-27.385	1.00	4.45	L
ATOM	1287	C	MET	L	4	13.978	-3.286	-30.350	1.00	8.02	L
ATOM	1288	O	MET	L	4	14.298	-2.685	-31.382	1.00	6.96	L
ATOM	1289	N	THR	L	5	14.196	-4.586	-30.173	1.00	8.30	L
ATOM	1290	CA	THR	L	5	14.835	-5.392	-31.210	1.00	8.27	L
ATOM	1291	CB	THR	L	5	16.100	-6.107	-30.656	1.00	8.90	L
ATOM	1292	OG1	THR	L	5	16.842	-5.200	-29.822	1.00	10.13	L
ATOM	1293	CG2	THR	L	5	16.993	-6.557	-31.794	1.00	7.36	L
ATOM	1294	C	THR	L	5	13.831	-6.423	-31.706	1.00	8.20	L
ATOM	1295	O	THR	L	5	13.344	-7.256	-30.940	1.00	7.90	L
ATOM	1296	N	GLN	L	6	13.484	-6.333	-32.984	1.00	9.47	L
ATOM	1297	CA	GLN	L	6	12.533	-7.268	-33.580	1.00	9.71	L
ATOM	1298	CB	GLN	L	6	11.683	-6.576	-34.635	1.00	9.96	L
ATOM	1299	CG	GLN	L	6	10.217	-6.389	-34.283	1.00	10.83	L
ATOM	1300	CD	GLN	L	6	9.560	-5.379	-35.227	1.00	12.71	L
ATOM	1301	OE1	GLN	L	6	9.754	-4.156	-35.100	1.00	11.89	L
ATOM	1302	NE2	GLN	L	6	8.812	-5.888	-36.204	1.00	11.00	L
ATOM	1303	C	GLN	L	6	13.283	-8.409	-34.223	1.00	9.95	L
ATOM	1304	O	GLN	L	6	14.476	-8.311	-34.513	1.00	9.91	L
ATOM	1305	N	SER	L	7	12.580	-9.501	-34.460	1.00	10.84	L
ATOM	1306	CA	SER	L	7	13.234	-10.652	-35.045	1.00	10.80	L
ATOM	1307	CB	SER	L	7	14.081	-11.315	-33.982	1.00	9.99	L
ATOM	1308	OG	SER	L	7	15.047	-12.144	-34.575	1.00	16.72	L
ATOM	1309	C	SER	L	7	12.191	-11.624	-35.554	1.00	10.08	L
ATOM	1310	O	SER	L	7	11.206	-11.886	-34.876	1.00	12.81	L
ATOM	1311	N	PRO	L	8	12.365	-12.131	-36.779	1.00	9.04	L
ATOM	1312	CD	PRO	L	8	11.571	-13.254	-37.308	1.00	7.85	L
ATOM	1313	CA	PRO	L	8	13.490	-11.816	-37.668	1.00	9.77	L
ATOM	1314	CB	PRO	L	8	13.490	-12.991	-38.640	1.00	8.02	L
ATOM	1315	CG	PRO	L	8	12.033	-13.328	-38.732	1.00	8.29	L
ATOM	1316	C	PRO	L	8	13.241	-10.474	-38.377	1.00	10.57	L
ATOM	1317	O	PRO	L	8	12.140	-9.923	-38.302	1.00	10.48	L
ATOM	1318	N	SER	L	9	14.251	-9.939	-39.052	1.00	11.09	L
ATOM	1319	CA	SER	L	9	14.070	-8.667	-39.757	1.00	13.69	L
ATOM	1320	CB	SER	L	9	15.426	-8.033	-40.090	1.00	15.41	L
ATOM	1321	OG	SER	L	9	16.465	-9.001	-40.081	1.00	20.93	L
ATOM	1322	C	SER	L	9	13.231	-8.841	-41.031	1.00	13.61	L
ATOM	1323	O	SER	L	9	12.517	-7.923	-41.456	1.00	11.42	L
ATOM	1324	N	SER	L	10	13.316	-10.024	-41.636	1.00	14.50	L
ATOM	1325	CA	SER	L	10	12.531	-10.330	-42.833	1.00	16.25	L
ATOM	1326	CB	SER	L	10	13.280	-9.938	-44.104	1.00	16.02	L
ATOM	1327	OG	SER	L	10	14.253	-10.900	-44.437	1.00	19.67	L
ATOM	1328	C	SER	L	10	12.202	-11.817	-42.850	1.00	15.53	L
ATOM	1329	O	SER	L	10	13.002	-12.648	-42.426	1.00	15.73	L
ATOM	1330	N	LEU	L	11	11.011	-12.143	-43.329	1.00	15.59	L
ATOM	1331	CA	LEU	L	11	10.571	-13.524	-43.361	1.00	16.29	L
ATOM	1332	CB	LEU	L	11	9.730	-13.789	-42.120	1.00	16.99	L
ATOM	1333	CG	LEU	L	11	9.261	-15.225	-41.963	1.00	18.29	L

ATOM	1334	CD1	LEU	L	11	10.338	-15.994	-41.199	1.00	19.78	L
ATOM	1335	CD2	LEU	L	11	7.929	-15.276	-41.212	1.00	17.06	L
ATOM	1336	C	LEU	L	11	9.748	-13.852	-44.609	1.00	17.00	L
ATOM	1337	O	LEU	L	11	9.089	-12.978	-45.171	1.00	19.02	L
ATOM	1338	N	SER	L	12	9.786	-15.109	-45.043	1.00	17.38	L
ATOM	1339	CA	SER	L	12	8.999	-15.533	-46.200	1.00	16.83	L
ATOM	1340	CB	SER	L	12	9.893	-15.852	-47.395	1.00	16.19	L
ATOM	1341	OG	SER	L	12	10.483	-14.670	-47.897	1.00	18.96	L
ATOM	1342	C	SER	L	12	8.229	-16.772	-45.792	1.00	15.74	L
ATOM	1343	O	SER	L	12	8.820	-17.778	-45.395	1.00	16.18	L
ATOM	1344	N	ALA	L	13	6.907	-16.689	-45.893	1.00	14.50	L
ATOM	1345	CA	ALA	L	13	6.040	-17.790	-45.510	1.00	13.88	L
ATOM	1346	CB	ALA	L	13	5.435	-17.524	-44.142	1.00	11.70	L
ATOM	1347	C	ALA	L	13	4.941	-18.025	-46.520	1.00	14.84	L
ATOM	1348	O	ALA	L	13	4.414	-17.080	-47.098	1.00	15.89	L
ATOM	1349	N	SER	L	14	4.590	-19.289	-46.726	1.00	16.55	L
ATOM	1350	CA	SER	L	14	3.548	-19.653	-47.686	1.00	18.52	L
ATOM	1351	CB	SER	L	14	3.584	-21.161	-47.953	1.00	21.34	L
ATOM	1352	OG	SER	L	14	4.906	-21.598	-48.266	1.00	25.96	L
ATOM	1353	C	SER	L	14	2.187	-19.280	-47.146	1.00	17.08	L
ATOM	1354	O	SER	L	14	1.926	-19.420	-45.954	1.00	15.37	L
ATOM	1355	N	VAL	L	15	1.321	-18.795	-48.025	1.00	18.37	L
ATOM	1356	CA	VAL	L	15	-0.022	-18.426	-47.602	1.00	20.11	L
ATOM	1357	CB	VAL	L	15	-0.895	-17.953	-48.814	1.00	19.65	L
ATOM	1358	CG1	VAL	L	15	-0.468	-18.683	-50.077	1.00	21.07	L
ATOM	1359	CG2	VAL	L	15	-2.386	-18.191	-48.526	1.00	16.68	L
ATOM	1360	C	VAL	L	15	-0.660	-19.631	-46.912	1.00	20.75	L
ATOM	1361	O	VAL	L	15	-0.853	-20.677	-47.520	1.00	21.60	L
ATOM	1362	N	GLY	L	16	-0.957	-19.483	-45.628	1.00	21.09	L
ATOM	1363	CA	GLY	L	16	-1.554	-20.579	-44.901	1.00	22.33	L
ATOM	1364	C	GLY	L	16	-0.814	-20.944	-43.632	1.00	23.59	L
ATOM	1365	O	GLY	L	16	-1.451	-21.194	-42.616	1.00	25.28	L
ATOM	1366	N	ASP	L	17	0.514	-20.979	-43.657	1.00	24.99	L
ATOM	1367	CA	ASP	L	17	1.230	-21.341	-42.436	1.00	27.99	L
ATOM	1368	CB	ASP	L	17	2.693	-21.717	-42.723	1.00	28.83	L
ATOM	1369	CG	ASP	L	17	3.458	-20.625	-43.424	1.00	29.50	L
ATOM	1370	OD1	ASP	L	17	3.262	-19.441	-43.048	1.00	31.11	L
ATOM	1371	OD2	ASP	L	17	4.271	-20.954	-44.329	1.00	27.86	L
ATOM	1372	C	ASP	L	17	1.160	-20.221	-41.407	1.00	29.07	L
ATOM	1373	O	ASP	L	17	0.811	-19.091	-41.747	1.00	30.22	L
ATOM	1374	N	ARG	L	18	1.473	-20.540	-40.150	1.00	29.29	L
ATOM	1375	CA	ARG	L	18	1.428	-19.550	-39.085	1.00	28.54	L
ATOM	1376	CB	ARG	L	18	0.964	-20.185	-37.758	1.00	30.31	L
ATOM	1377	CG	ARG	L	18	2.046	-20.954	-36.997	1.00	33.86	L
ATOM	1378	CD	ARG	L	18	1.515	-21.703	-35.764	1.00	35.75	L
ATOM	1379	NE	ARG	L	18	0.691	-20.880	-34.879	1.00	38.27	L
ATOM	1380	CZ	ARG	L	18	-0.645	-20.869	-34.882	1.00	39.93	L
ATOM	1381	NH1	ARG	L	18	-1.317	-21.642	-35.726	1.00	39.27	L
ATOM	1382	NH2	ARG	L	18	-1.316	-20.085	-34.037	1.00	40.51	L
ATOM	1383	C	ARG	L	18	2.814	-18.946	-38.934	1.00	27.76	L
ATOM	1384	O	ARG	L	18	3.829	-19.658	-38.958	1.00	27.29	L
ATOM	1385	N	VAL	L	19	2.858	-17.623	-38.810	1.00	26.27	L
ATOM	1386	CA	VAL	L	19	4.124	-16.924	-38.655	1.00	24.20	L
ATOM	1387	CB	VAL	L	19	4.290	-15.843	-39.743	1.00	24.36	L
ATOM	1388	CG1	VAL	L	19	3.975	-16.440	-41.112	1.00	25.14	L
ATOM	1389	CG2	VAL	L	19	3.387	-14.671	-39.464	1.00	26.02	L
ATOM	1390	C	VAL	L	19	4.209	-16.292	-37.278	1.00	22.08	L
ATOM	1391	O	VAL	L	19	3.190	-15.978	-36.676	1.00	20.97	L
ATOM	1392	N	THR	L	20	5.432	-16.132	-36.782	1.00	21.47	L
ATOM	1393	CA	THR	L	20	5.671	-15.541	-35.469	1.00	19.88	L
ATOM	1394	CB	THR	L	20	5.991	-16.619	-34.422	1.00	17.86	L

ATOM	1395	OG1	THR	L	20	4.866	-17.480	-34.259	1.00	18.26	L
ATOM	1396	CG2	THR	L	20	6.324	-15.994	-33.100	1.00	16.28	L
ATOM	1397	C	THR	L	20	6.847	-14.575	-35.499	1.00	20.30	L
ATOM	1398	O	THR	L	20	7.946	-14.931	-35.918	1.00	20.29	L
ATOM	1399	N	ILE	L	21	6.610	-13.351	-35.055	1.00	20.44	L
ATOM	1400	CA	ILE	L	21	7.658	-12.349	-35.000	1.00	20.12	L
ATOM	1401	CB	ILE	L	21	7.236	-11.072	-35.736	1.00	20.69	L
ATOM	1402	CG2	ILE	L	21	8.406	-10.088	-35.799	1.00	18.90	L
ATOM	1403	CG1	ILE	L	21	6.759	-11.441	-37.142	1.00	21.95	L
ATOM	1404	CD1	ILE	L	21	6.285	-10.252	-37.972	1.00	22.52	L
ATOM	1405	C	ILE	L	21	7.904	-12.024	-33.528	1.00	20.23	L
ATOM	1406	O	ILE	L	21	6.961	-11.872	-32.735	1.00	19.59	L
ATOM	1407	N	THR	L	22	9.174	-11.915	-33.169	1.00	19.11	L
ATOM	1408	CA	THR	L	22	9.534	-11.605	-31.801	1.00	19.72	L
ATOM	1409	CB	THR	L	22	10.651	-12.529	-31.291	1.00	19.77	L
ATOM	1410	OG1	THR	L	22	10.343	-13.878	-31.647	1.00	20.92	L
ATOM	1411	CG2	THR	L	22	10.773	-12.442	-29.770	1.00	17.04	L
ATOM	1412	C	THR	L	22	10.009	-10.172	-31.690	1.00	20.10	L
ATOM	1413	O	THR	L	22	10.498	-9.590	-32.660	1.00	19.87	L
ATOM	1414	N	CYS	L	23	9.848	-9.617	-30.493	1.00	20.03	L
ATOM	1415	CA	CYS	L	23	10.255	-8.257	-30.192	1.00	20.14	L
ATOM	1416	C	CYS	L	23	10.753	-8.272	-28.748	1.00	20.68	L
ATOM	1417	O	CYS	L	23	10.063	-8.777	-27.861	1.00	20.07	L
ATOM	1418	CB	CYS	L	23	9.050	-7.327	-30.361	1.00	19.95	L
ATOM	1419	SG	CYS	L	23	9.273	-5.579	-29.906	1.00	24.16	L
ATOM	1420	N	ARG	L	24	11.972	-7.776	-28.521	1.00	20.89	L
ATOM	1421	CA	ARG	L	24	12.538	-7.736	-27.172	1.00	19.57	L
ATOM	1422	CB	ARG	L	24	13.771	-8.629	-27.042	1.00	21.13	L
ATOM	1423	CG	ARG	L	24	13.464	-10.092	-27.137	1.00	23.44	L
ATOM	1424	CD	ARG	L	24	14.727	-10.917	-27.090	1.00	26.37	L
ATOM	1425	NE	ARG	L	24	14.457	-12.270	-27.558	1.00	30.08	L
ATOM	1426	CZ	ARG	L	24	14.080	-12.559	-28.794	1.00	32.01	L
ATOM	1427	NH1	ARG	L	24	13.935	-11.583	-29.695	1.00	34.19	L
ATOM	1428	NH2	ARG	L	24	13.831	-13.819	-29.112	1.00	32.69	L
ATOM	1429	C	ARG	L	24	12.927	-6.335	-26.809	1.00	18.40	L
ATOM	1430	O	ARG	L	24	13.490	-5.615	-27.629	1.00	18.93	L
ATOM	1431	N	ALA	L	25	12.628	-5.958	-25.568	1.00	17.14	L
ATOM	1432	CA	ALA	L	25	12.925	-4.624	-25.063	1.00	16.03	L
ATOM	1433	CB	ALA	L	25	11.804	-4.169	-24.158	1.00	16.46	L
ATOM	1434	C	ALA	L	25	14.249	-4.594	-24.317	1.00	15.36	L
ATOM	1435	O	ALA	L	25	14.662	-5.597	-23.742	1.00	14.07	L
ATOM	1436	N	SER	L	26	14.913	-3.442	-24.343	1.00	16.19	L
ATOM	1437	CA	SER	L	26	16.195	-3.277	-23.668	1.00	16.76	L
ATOM	1438	CB	SER	L	26	16.888	-1.996	-24.132	1.00	17.23	L
ATOM	1439	OG	SER	L	26	16.373	-0.865	-23.464	1.00	20.63	L
ATOM	1440	C	SER	L	26	16.003	-3.246	-22.149	1.00	16.15	L
ATOM	1441	O	SER	L	26	16.967	-3.188	-21.394	1.00	15.95	L
ATOM	1442	N	GLN	L	27	14.749	-3.260	-21.711	1.00	15.84	L
ATOM	1443	CA	GLN	L	27	14.416	-3.291	-20.289	1.00	14.82	L
ATOM	1444	CB	GLN	L	27	14.690	-1.950	-19.615	1.00	15.42	L
ATOM	1445	CG	GLN	L	27	13.719	-0.864	-19.989	1.00	17.28	L
ATOM	1446	CD	GLN	L	27	13.715	0.267	-18.991	1.00	19.54	L
ATOM	1447	OE1	GLN	L	27	14.671	1.046	-18.916	1.00	19.13	L
ATOM	1448	NE2	GLN	L	27	12.647	0.345	-18.184	1.00	21.52	L
ATOM	1449	C	GLN	L	27	12.933	-3.625	-20.170	1.00	13.71	L
ATOM	1450	O	GLN	L	27	12.190	-3.547	-21.152	1.00	11.47	L
ATOM	1451	N	GLY	L	28	12.507	-3.998	-18.970	1.00	12.79	L
ATOM	1452	CA	GLY	L	28	11.116	-4.345	-18.765	1.00	11.73	L
ATOM	1453	C	GLY	L	28	10.230	-3.167	-19.092	1.00	12.33	L
ATOM	1454	O	GLY	L	28	10.534	-2.029	-18.728	1.00	12.44	L
ATOM	1455	N	ILE	L	29	9.136	-3.437	-19.792	1.00	11.90	L

ATOM	1456	CA	ILE	L	29	8.206	-2.389	-20.166	1.00	12.68	L
ATOM	1457	CB	ILE	L	29	8.252	-2.078	-21.664	1.00	11.70	L
ATOM	1458	CG2	ILE	L	29	9.607	-1.483	-22.023	1.00	12.24	L
ATOM	1459	CG1	ILE	L	29	7.948	-3.348	-22.465	1.00	12.26	L
ATOM	1460	CD1	ILE	L	29	7.626	-3.110	-23.937	1.00	10.24	L
ATOM	1461	C	ILE	L	29	6.800	-2.808	-19.828	1.00	14.29	L
ATOM	1462	O	ILE	L	29	5.833	-2.365	-20.458	1.00	14.88	L
ATOM	1463	N	SER	L	30	6.686	-3.681	-18.839	1.00	15.26	L
ATOM	1464	CA	SER	L	30	5.373	-4.129	-18.422	1.00	16.96	L
ATOM	1465	CB	SER	L	30	4.545	-2.903	-18.005	1.00	17.33	L
ATOM	1466	OG	SER	L	30	3.175	-3.203	-17.824	1.00	18.85	L
ATOM	1467	C	SER	L	30	4.721	-4.845	-19.600	1.00	17.57	L
ATOM	1468	O	SER	L	30	5.328	-5.689	-20.258	1.00	18.80	L
ATOM	1469	N	SER	L	31	3.476	-4.492	-19.862	1.00	16.56	L
ATOM	1470	CA	SER	L	31	2.737	-5.081	-20.956	1.00	16.37	L
ATOM	1471	CB	SER	L	31	1.472	-5.751	-20.415	1.00	16.56	L
ATOM	1472	OG	SER	L	31	0.798	-4.889	-19.505	1.00	17.23	L
ATOM	1473	C	SER	L	31	2.375	-3.971	-21.939	1.00	15.72	L
ATOM	1474	O	SER	L	31	1.424	-4.085	-22.727	1.00	14.38	L
ATOM	1475	N	ARG	L	32	3.137	-2.886	-21.882	1.00	14.57	L
ATOM	1476	CA	ARG	L	32	2.869	-1.761	-22.763	1.00	12.87	L
ATOM	1477	CB	ARG	L	32	3.232	-0.432	-22.077	1.00	12.78	L
ATOM	1478	CG	ARG	L	32	2.545	-0.190	-20.731	1.00	13.17	L
ATOM	1479	CD	ARG	L	32	2.896	1.199	-20.286	1.00	16.26	L
ATOM	1480	NE	ARG	L	32	2.682	1.484	-18.877	1.00	20.43	L
ATOM	1481	CZ	ARG	L	32	1.751	2.314	-18.409	1.00	24.20	L
ATOM	1482	NH1	ARG	L	32	0.931	2.937	-19.255	1.00	23.63	L
ATOM	1483	NH2	ARG	L	32	1.669	2.550	-17.095	1.00	21.89	L
ATOM	1484	C	ARG	L	32	3.624	-1.888	-24.086	1.00	10.58	L
ATOM	1485	O	ARG	L	32	4.626	-1.222	-24.312	1.00	11.04	L
ATOM	1486	N	LEU	L	33	3.135	-2.759	-24.950	1.00	7.55	L
ATOM	1487	CA	LEU	L	33	3.728	-2.953	-26.243	1.00	5.79	L
ATOM	1488	CB	LEU	L	33	4.558	-4.233	-26.293	1.00	6.51	L
ATOM	1489	CG	LEU	L	33	5.261	-4.460	-27.669	1.00	6.68	L
ATOM	1490	CD1	LEU	L	33	6.728	-4.722	-27.445	1.00	5.42	L
ATOM	1491	CD2	LEU	L	33	4.616	-5.605	-28.430	1.00	3.57	L
ATOM	1492	C	LEU	L	33	2.613	-3.045	-27.273	1.00	4.13	L
ATOM	1493	O	LEU	L	33	1.559	-3.640	-27.011	1.00	3.72	L
ATOM	1494	N	ALA	L	34	2.857	-2.480	-28.454	1.00	3.03	L
ATOM	1495	CA	ALA	L	34	1.857	-2.507	-29.521	1.00	3.10	L
ATOM	1496	CB	ALA	L	34	1.245	-1.114	-29.712	1.00	3.61	L
ATOM	1497	C	ALA	L	34	2.455	-2.991	-30.820	1.00	2.38	L
ATOM	1498	O	ALA	L	34	3.662	-2.950	-31.000	1.00	2.65	L
ATOM	1499	N	TRP	L	35	1.594	-3.455	-31.715	1.00	3.03	L
ATOM	1500	CA	TRP	L	35	2.016	-3.967	-33.007	1.00	4.01	L
ATOM	1501	CB	TRP	L	35	1.714	-5.459	-33.112	1.00	5.67	L
ATOM	1502	CG	TRP	L	35	2.557	-6.314	-32.225	1.00	7.10	L
ATOM	1503	CD2	TRP	L	35	3.882	-6.790	-32.507	1.00	6.96	L
ATOM	1504	CE2	TRP	L	35	4.308	-7.525	-31.380	1.00	7.48	L
ATOM	1505	CE3	TRP	L	35	4.751	-6.663	-33.604	1.00	6.37	L
ATOM	1506	CD1	TRP	L	35	2.242	-6.768	-30.973	1.00	5.81	L
ATOM	1507	NE1	TRP	L	35	3.287	-7.493	-30.459	1.00	7.49	L
ATOM	1508	CZ2	TRP	L	35	5.581	-8.140	-31.318	1.00	6.10	L
ATOM	1509	CZ3	TRP	L	35	6.012	-7.271	-33.541	1.00	5.88	L
ATOM	1510	CH2	TRP	L	35	6.411	-8.002	-32.403	1.00	5.71	L
ATOM	1511	C	TRP	L	35	1.310	-3.251	-34.147	1.00	4.05	L
ATOM	1512	O	TRP	L	35	0.074	-3.220	-34.209	1.00	2.57	L
ATOM	1513	N	TYR	L	36	2.099	-2.693	-35.055	1.00	2.93	L
ATOM	1514	CA	TYR	L	36	1.522	-1.981	-36.169	1.00	3.86	L
ATOM	1515	CB	TYR	L	36	2.035	-0.544	-36.209	1.00	1.42	L
ATOM	1516	CG	TYR	L	36	1.701	0.264	-34.970	1.00	2.49	L

ATOM	1517	CD1	TYR	L	36	0.469	0.885	-34.829	1.00	1.00	L
ATOM	1518	CE1	TYR	L	36	0.178	1.650	-33.715	1.00	1.00	L
ATOM	1519	CD2	TYR	L	36	2.635	0.427	-33.944	1.00	2.52	L
ATOM	1520	CE2	TYR	L	36	2.342	1.196	-32.819	1.00	1.93	L
ATOM	1521	CZ	TYR	L	36	1.109	1.807	-32.722	1.00	1.00	L
ATOM	1522	OH	TYR	L	36	0.838	2.597	-31.632	1.00	1.00	L
ATOM	1523	C	TYR	L	36	1.851	-2.671	-37.464	1.00	5.39	L
ATOM	1524	O	TYR	L	36	2.844	-3.388	-37.575	1.00	5.41	L
ATOM	1525	N	GLN	L	37	1.002	-2.455	-38.453	1.00	7.83	L
ATOM	1526	CA	GLN	L	37	1.207	-3.054	-39.754	1.00	9.39	L
ATOM	1527	CB	GLN	L	37	0.046	-3.980	-40.097	1.00	11.00	L
ATOM	1528	CG	GLN	L	37	0.086	-4.527	-41.501	1.00	9.81	L
ATOM	1529	CD	GLN	L	37	-1.129	-5.339	-41.803	1.00	10.26	L
ATOM	1530	OE1	GLN	L	37	-2.238	-4.815	-41.847	1.00	12.94	L
ATOM	1531	NE2	GLN	L	37	-0.941	-6.637	-41.983	1.00	13.63	L
ATOM	1532	C	GLN	L	37	1.274	-1.933	-40.766	1.00	10.97	L
ATOM	1533	O	GLN	L	37	0.415	-1.056	-40.787	1.00	11.76	L
ATOM	1534	N	GLN	L	38	2.296	-1.966	-41.609	1.00	13.25	L
ATOM	1535	CA	GLN	L	38	2.443	-0.946	-42.622	1.00	15.72	L
ATOM	1536	CB	GLN	L	38	3.562	0.023	-42.258	1.00	16.17	L
ATOM	1537	CG	GLN	L	38	3.619	1.227	-43.194	1.00	17.87	L
ATOM	1538	CD	GLN	L	38	4.854	2.054	-43.000	1.00	18.58	L
ATOM	1539	OE1	GLN	L	38	4.887	3.241	-43.360	1.00	18.70	L
ATOM	1540	NE2	GLN	L	38	5.896	1.436	-42.437	1.00	18.33	L
ATOM	1541	C	GLN	L	38	2.739	-1.530	-43.991	1.00	17.75	L
ATOM	1542	O	GLN	L	38	3.618	-2.372	-44.144	1.00	17.47	L
ATOM	1543	N	LYS	L	39	2.003	-1.051	-44.984	1.00	19.94	L
ATOM	1544	CA	LYS	L	39	2.172	-1.466	-46.360	1.00	20.60	L
ATOM	1545	CB	LYS	L	39	0.843	-1.990	-46.911	1.00	19.44	L
ATOM	1546	CG	LYS	L	39	0.372	-3.242	-46.214	1.00	18.77	L
ATOM	1547	CD	LYS	L	39	-1.043	-3.641	-46.559	1.00	18.38	L
ATOM	1548	CE	LYS	L	39	-1.314	-5.039	-45.989	1.00	19.75	L
ATOM	1549	NZ	LYS	L	39	-2.760	-5.437	-45.970	1.00	19.42	L
ATOM	1550	C	LYS	L	39	2.615	-0.225	-47.142	1.00	23.17	L
ATOM	1551	O	LYS	L	39	2.320	0.916	-46.762	1.00	22.18	L
ATOM	1552	N	PRO	L	40	3.319	-0.440	-48.258	1.00	25.17	L
ATOM	1553	CD	PRO	L	40	3.543	-1.778	-48.829	1.00	25.97	L
ATOM	1554	CA	PRO	L	40	3.846	0.591	-49.157	1.00	25.55	L
ATOM	1555	CB	PRO	L	40	4.172	-0.194	-50.417	1.00	25.75	L
ATOM	1556	CG	PRO	L	40	4.583	-1.491	-49.863	1.00	26.38	L
ATOM	1557	C	PRO	L	40	2.863	1.705	-49.444	1.00	25.25	L
ATOM	1558	O	PRO	L	40	1.775	1.467	-49.973	1.00	25.17	L
ATOM	1559	N	GLY	L	41	3.262	2.923	-49.101	1.00	24.69	L
ATOM	1560	CA	GLY	L	41	2.419	4.082	-49.343	1.00	23.52	L
ATOM	1561	C	GLY	L	41	1.056	4.091	-48.665	1.00	21.83	L
ATOM	1562	O	GLY	L	41	0.195	4.900	-49.004	1.00	20.85	L
ATOM	1563	N	LYS	L	42	0.848	3.200	-47.708	1.00	21.05	L
ATOM	1564	CA	LYS	L	42	-0.418	3.159	-47.017	1.00	20.64	L
ATOM	1565	CB	LYS	L	42	-1.022	1.758	-47.112	1.00	23.78	L
ATOM	1566	CG	LYS	L	42	-1.251	1.276	-48.549	1.00	27.37	L
ATOM	1567	CD	LYS	L	42	-1.686	-0.178	-48.582	1.00	29.55	L
ATOM	1568	CE	LYS	L	42	-1.463	-0.807	-49.960	1.00	31.53	L
ATOM	1569	NZ	LYS	L	42	-1.924	-2.247	-50.023	1.00	30.21	L
ATOM	1570	C	LYS	L	42	-0.235	3.567	-45.561	1.00	19.67	L
ATOM	1571	O	LYS	L	42	0.888	3.642	-45.057	1.00	22.24	L
ATOM	1572	N	ALA	L	43	-1.353	3.831	-44.895	1.00	17.35	L
ATOM	1573	CA	ALA	L	43	-1.379	4.238	-43.500	1.00	14.73	L
ATOM	1574	CB	ALA	L	43	-2.707	4.896	-43.197	1.00	13.07	L
ATOM	1575	C	ALA	L	43	-1.166	3.061	-42.561	1.00	13.46	L
ATOM	1576	O	ALA	L	43	-1.844	2.044	-42.655	1.00	13.73	L
ATOM	1577	N	PRO	L	44	-0.206	3.177	-41.639	1.00	11.50	L

ATOM	1578	CD	PRO	L	44	0.860	4.180	-41.480	1.00	9.68	L
ATOM	1579	CA	PRO	L	44	-0.007	2.050	-40.730	1.00	11.04	L
ATOM	1580	CB	PRO	L	44	1.101	2.552	-39.805	1.00	10.36	L
ATOM	1581	CG	PRO	L	44	1.920	3.409	-40.739	1.00	9.88	L
ATOM	1582	C	PRO	L	44	-1.307	1.721	-39.975	1.00	10.49	L
ATOM	1583	O	PRO	L	44	-2.161	2.583	-39.759	1.00	9.88	L
ATOM	1584	N	LYS	L	45	-1.453	0.459	-39.599	1.00	11.44	L
ATOM	1585	CA	LYS	L	45	-2.631	-0.005	-38.881	1.00	12.22	L
ATOM	1586	CB	LYS	L	45	-3.368	-1.063	-39.698	1.00	15.28	L
ATOM	1587	CG	LYS	L	45	-4.045	-0.532	-40.955	1.00	18.72	L
ATOM	1588	CD	LYS	L	45	-4.689	-1.651	-41.789	1.00	23.99	L
ATOM	1589	CE	LYS	L	45	-5.758	-2.410	-40.990	1.00	28.70	L
ATOM	1590	NZ	LYS	L	45	-6.539	-3.436	-41.781	1.00	30.44	L
ATOM	1591	C	LYS	L	45	-2.243	-0.599	-37.542	1.00	10.66	L
ATOM	1592	O	LYS	L	45	-1.270	-1.343	-37.433	1.00	11.06	L
ATOM	1593	N	LEU	L	46	-3.011	-0.271	-36.517	1.00	9.86	L
ATOM	1594	CA	LEU	L	46	-2.738	-0.780	-35.185	1.00	8.87	L
ATOM	1595	CB	LEU	L	46	-3.336	0.180	-34.147	1.00	9.27	L
ATOM	1596	CG	LEU	L	46	-3.140	0.020	-32.631	1.00	9.63	L
ATOM	1597	CD1	LEU	L	46	-4.354	-0.644	-32.037	1.00	9.45	L
ATOM	1598	CD2	LEU	L	46	-1.857	-0.768	-32.330	1.00	10.10	L
ATOM	1599	C	LEU	L	46	-3.382	-2.150	-35.103	1.00	8.10	L
ATOM	1600	O	LEU	L	46	-4.573	-2.287	-35.357	1.00	8.98	L
ATOM	1601	N	LEU	L	47	-2.593	-3.160	-34.757	1.00	7.67	L
ATOM	1602	CA	LEU	L	47	-3.109	-4.525	-34.662	1.00	6.84	L
ATOM	1603	CB	LEU	L	47	-2.148	-5.527	-35.320	1.00	5.42	L
ATOM	1604	CG	LEU	L	47	-1.750	-5.328	-36.793	1.00	6.34	L
ATOM	1605	CD1	LEU	L	47	-0.631	-6.286	-37.139	1.00	3.93	L
ATOM	1606	CD2	LEU	L	47	-2.960	-5.530	-37.695	1.00	5.28	L
ATOM	1607	C	LEU	L	47	-3.298	-4.949	-33.224	1.00	6.82	L
ATOM	1608	O	LEU	L	47	-4.347	-5.457	-32.860	1.00	6.11	L
ATOM	1609	N	ILE	L	48	-2.263	-4.732	-32.417	1.00	7.58	L
ATOM	1610	CA	ILE	L	48	-2.261	-5.145	-31.015	1.00	7.30	L
ATOM	1611	CB	ILE	L	48	-1.351	-6.420	-30.815	1.00	6.26	L
ATOM	1612	CG2	ILE	L	48	-1.227	-6.758	-29.342	1.00	2.73	L
ATOM	1613	CG1	ILE	L	48	-1.879	-7.611	-31.641	1.00	3.91	L
ATOM	1614	CD1	ILE	L	48	-3.265	-8.085	-31.244	1.00	5.88	L
ATOM	1615	C	ILE	L	48	-1.709	-4.047	-30.119	1.00	9.05	L
ATOM	1616	O	ILE	L	48	-0.800	-3.313	-30.513	1.00	9.25	L
ATOM	1617	N	TYR	L	49	-2.267	-3.930	-28.918	1.00	9.07	L
ATOM	1618	CA	TYR	L	49	-1.796	-2.955	-27.936	1.00	7.79	L
ATOM	1619	CB	TYR	L	49	-2.663	-1.698	-27.928	1.00	8.17	L
ATOM	1620	CG	TYR	L	49	-4.122	-1.920	-27.631	1.00	8.50	L
ATOM	1621	CD1	TYR	L	49	-4.986	-2.388	-28.610	1.00	8.58	L
ATOM	1622	CE1	TYR	L	49	-6.343	-2.525	-28.351	1.00	9.02	L
ATOM	1623	CD2	TYR	L	49	-4.650	-1.604	-26.383	1.00	6.91	L
ATOM	1624	CE2	TYR	L	49	-6.000	-1.739	-26.117	1.00	5.94	L
ATOM	1625	CZ	TYR	L	49	-6.843	-2.194	-27.102	1.00	7.73	L
ATOM	1626	OH	TYR	L	49	-8.196	-2.299	-26.855	1.00	8.78	L
ATOM	1627	C	TYR	L	49	-1.884	-3.647	-26.586	1.00	8.45	L
ATOM	1628	O	TYR	L	49	-2.469	-4.723	-26.476	1.00	7.21	L
ATOM	1629	N	ALA	L	50	-1.306	-3.042	-25.556	1.00	8.94	L
ATOM	1630	CA	ALA	L	50	-1.332	-3.661	-24.243	1.00	10.42	L
ATOM	1631	CB	ALA	L	50	-2.751	-3.633	-23.674	1.00	10.58	L
ATOM	1632	C	ALA	L	50	-0.837	-5.114	-24.366	1.00	11.72	L
ATOM	1633	O	ALA	L	50	-1.317	-6.023	-23.677	1.00	12.15	L
ATOM	1634	N	ALA	L	51	0.117	-5.322	-25.273	1.00	11.70	L
ATOM	1635	CA	ALA	L	51	0.727	-6.631	-25.523	1.00	9.42	L
ATOM	1636	CB	ALA	L	51	1.330	-7.173	-24.234	1.00	7.05	L
ATOM	1637	C	ALA	L	51	-0.173	-7.694	-26.159	1.00	9.55	L
ATOM	1638	O	ALA	L	51	0.275	-8.458	-27.015	1.00	8.26	L

ATOM	1639	N	SER	L	52	-1.439	-7.753	-25.763	1.00	9.60	L
ATOM	1640	CA	SER	L	52	-2.315	-8.771	-26.328	1.00	10.62	L
ATOM	1641	CB	SER	L	52	-2.398	-9.948	-25.363	1.00	10.40	L
ATOM	1642	OG	SER	L	52	-2.708	-9.513	-24.050	1.00	10.76	L
ATOM	1643	C	SER	L	52	-3.735	-8.345	-26.704	1.00	11.70	L
ATOM	1644	O	SER	L	52	-4.538	-9.179	-27.112	1.00	12.32	L
ATOM	1645	N	SER	L	53	-4.063	-7.070	-26.542	1.00	12.45	L
ATOM	1646	CA	SER	L	53	-5.392	-6.620	-26.887	1.00	12.61	L
ATOM	1647	CB	SER	L	53	-5.735	-5.353	-26.127	1.00	12.98	L
ATOM	1648	OG	SER	L	53	-6.024	-5.669	-24.770	1.00	11.76	L
ATOM	1649	C	SER	L	53	-5.434	-6.384	-28.380	1.00	14.27	L
ATOM	1650	O	SER	L	53	-4.563	-5.711	-28.961	1.00	16.33	L
ATOM	1651	N	LEU	L	54	-6.448	-6.972	-28.998	1.00	12.16	L
ATOM	1652	CA	LEU	L	54	-6.631	-6.882	-30.426	1.00	12.45	L
ATOM	1653	CB	LEU	L	54	-7.256	-8.181	-30.925	1.00	12.18	L
ATOM	1654	CG	LEU	L	54	-7.643	-8.244	-32.395	1.00	11.41	L
ATOM	1655	CD1	LEU	L	54	-6.376	-8.187	-33.226	1.00	14.26	L
ATOM	1656	CD2	LEU	L	54	-8.408	-9.519	-32.662	1.00	10.12	L
ATOM	1657	C	LEU	L	54	-7.505	-5.699	-30.821	1.00	13.60	L
ATOM	1658	O	LEU	L	54	-8.662	-5.606	-30.419	1.00	16.51	L
ATOM	1659	N	GLN	L	55	-6.944	-4.798	-31.616	1.00	13.48	L
ATOM	1660	CA	GLN	L	55	-7.668	-3.627	-32.096	1.00	14.51	L
ATOM	1661	CB	GLN	L	55	-6.766	-2.832	-33.036	1.00	14.61	L
ATOM	1662	CG	GLN	L	55	-7.487	-1.838	-33.930	1.00	14.24	L
ATOM	1663	CD	GLN	L	55	-8.269	-0.805	-33.149	1.00	12.97	L
ATOM	1664	OE1	GLN	L	55	-7.943	-0.504	-32.002	1.00	11.02	L
ATOM	1665	NE2	GLN	L	55	-9.292	-0.236	-33.777	1.00	13.96	L
ATOM	1666	C	GLN	L	55	-8.942	-4.053	-32.829	1.00	15.51	L
ATOM	1667	O	GLN	L	55	-8.971	-5.097	-33.496	1.00	16.22	L
ATOM	1668	N	SER	L	56	-9.994	-3.254	-32.714	1.00	15.89	L
ATOM	1669	CA	SER	L	56	-11.232	-3.609	-33.386	1.00	17.33	L
ATOM	1670	CB	SER	L	56	-12.354	-2.646	-33.030	1.00	17.45	L
ATOM	1671	OG	SER	L	56	-13.505	-2.971	-33.799	1.00	20.41	L
ATOM	1672	C	SER	L	56	-11.052	-3.599	-34.889	1.00	17.72	L
ATOM	1673	O	SER	L	56	-10.285	-2.807	-35.428	1.00	18.29	L
ATOM	1674	N	GLY	L	57	-11.779	-4.477	-35.566	1.00	19.09	L
ATOM	1675	CA	GLY	L	57	-11.685	-4.542	-37.011	1.00	19.73	L
ATOM	1676	C	GLY	L	57	-10.493	-5.311	-37.551	1.00	20.28	L
ATOM	1677	O	GLY	L	57	-10.216	-5.259	-38.749	1.00	22.53	L
ATOM	1678	N	VAL	L	58	-9.779	-6.001	-36.672	1.00	20.10	L
ATOM	1679	CA	VAL	L	58	-8.639	-6.796	-37.080	1.00	20.30	L
ATOM	1680	CB	VAL	L	58	-7.386	-6.488	-36.211	1.00	21.32	L
ATOM	1681	CG1	VAL	L	58	-6.265	-7.495	-36.511	1.00	19.34	L
ATOM	1682	CG2	VAL	L	58	-6.904	-5.074	-36.495	1.00	19.12	L
ATOM	1683	C	VAL	L	58	-9.009	-8.264	-36.925	1.00	19.94	L
ATOM	1684	O	VAL	L	58	-9.526	-8.678	-35.889	1.00	18.67	L
ATOM	1685	N	PRO	L	59	-8.757	-9.065	-37.966	1.00	21.08	L
ATOM	1686	CD	PRO	L	59	-8.083	-8.678	-39.214	1.00	20.13	L
ATOM	1687	CA	PRO	L	59	-9.054	-10.500	-37.963	1.00	21.74	L
ATOM	1688	CB	PRO	L	59	-8.499	-10.964	-39.306	1.00	21.19	L
ATOM	1689	CG	PRO	L	59	-7.436	-9.961	-39.603	1.00	21.70	L
ATOM	1690	C	PRO	L	59	-8.437	-11.242	-36.770	1.00	22.49	L
ATOM	1691	O	PRO	L	59	-7.299	-10.991	-36.380	1.00	22.11	L
ATOM	1692	N	SER	L	60	-9.207	-12.164	-36.207	1.00	22.49	L
ATOM	1693	CA	SER	L	60	-8.785	-12.928	-35.048	1.00	22.80	L
ATOM	1694	CB	SER	L	60	-9.923	-13.845	-34.621	1.00	25.54	L
ATOM	1695	OG	SER	L	60	-11.097	-13.085	-34.367	1.00	28.03	L
ATOM	1696	C	SER	L	60	-7.510	-13.747	-35.223	1.00	22.02	L
ATOM	1697	O	SER	L	60	-6.896	-14.162	-34.227	1.00	20.07	L
ATOM	1698	N	ARG	L	61	-7.108	-13.982	-36.475	1.00	20.14	L
ATOM	1699	CA	ARG	L	61	-5.897	-14.768	-36.735	1.00	19.34	L

ATOM	1700	CB	ARG	L	61	-5.785	-15.149	-38.216	1.00	19.85	L
ATOM	1701	CG	ARG	L	61	-5.642	-14.011	-39.193	1.00	19.55	L
ATOM	1702	CD	ARG	L	61	-5.201	-14.557	-40.548	1.00	18.85	L
ATOM	1703	NE	ARG	L	61	-4.882	-13.496	-41.510	1.00	18.60	L
ATOM	1704	CZ	ARG	L	61	-5.791	-12.698	-42.066	1.00	18.92	L
ATOM	1705	NH1	ARG	L	61	-7.071	-12.843	-41.760	1.00	19.33	L
ATOM	1706	NH2	ARG	L	61	-5.429	-11.749	-42.918	1.00	17.42	L
ATOM	1707	C	ARG	L	61	-4.611	-14.073	-36.265	1.00	18.31	L
ATOM	1708	O	ARG	L	61	-3.560	-14.716	-36.123	1.00	17.76	L
ATOM	1709	N	PHE	L	62	-4.711	-12.768	-36.014	1.00	16.50	L
ATOM	1710	CA	PHE	L	62	-3.591	-11.994	-35.502	1.00	14.82	L
ATOM	1711	CB	PHE	L	62	-3.683	-10.521	-35.896	1.00	13.22	L
ATOM	1712	CG	PHE	L	62	-3.259	-10.232	-37.296	1.00	11.96	L
ATOM	1713	CD1	PHE	L	62	-4.194	-10.132	-38.318	1.00	11.33	L
ATOM	1714	CD2	PHE	L	62	-1.914	-10.060	-37.597	1.00	12.51	L
ATOM	1715	CE1	PHE	L	62	-3.789	-9.860	-39.635	1.00	12.01	L
ATOM	1716	CE2	PHE	L	62	-1.494	-9.789	-38.906	1.00	12.70	L
ATOM	1717	CZ	PHE	L	62	-2.433	-9.688	-39.929	1.00	11.60	L
ATOM	1718	C	PHE	L	62	-3.708	-12.094	-33.996	1.00	15.02	L
ATOM	1719	O	PHE	L	62	-4.782	-11.897	-33.425	1.00	14.54	L
ATOM	1720	N	SER	L	63	-2.603	-12.404	-33.345	1.00	14.08	L
ATOM	1721	CA	SER	L	63	-2.637	-12.535	-31.907	1.00	13.29	L
ATOM	1722	CB	SER	L	63	-2.785	-14.020	-31.547	1.00	13.93	L
ATOM	1723	OG	SER	L	63	-2.372	-14.294	-30.217	1.00	19.30	L
ATOM	1724	C	SER	L	63	-1.341	-11.975	-31.373	1.00	12.67	L
ATOM	1725	O	SER	L	63	-0.377	-11.831	-32.122	1.00	12.77	L
ATOM	1726	N	GLY	L	64	-1.313	-11.666	-30.082	1.00	11.59	L
ATOM	1727	CA	GLY	L	64	-0.103	-11.137	-29.493	1.00	11.87	L
ATOM	1728	C	GLY	L	64	0.019	-11.587	-28.068	1.00	12.34	L
ATOM	1729	O	GLY	L	64	-0.988	-11.691	-27.376	1.00	12.02	L
ATOM	1730	N	SER	L	65	1.242	-11.885	-27.638	1.00	14.21	L
ATOM	1731	CA	SER	L	65	1.481	-12.309	-26.263	1.00	15.67	L
ATOM	1732	CB	SER	L	65	1.411	-13.821	-26.144	1.00	17.02	L
ATOM	1733	OG	SER	L	65	2.436	-14.431	-26.905	1.00	21.04	L
ATOM	1734	C	SER	L	65	2.855	-11.853	-25.844	1.00	15.90	L
ATOM	1735	O	SER	L	65	3.612	-11.325	-26.653	1.00	17.42	L
ATOM	1736	N	GLY	L	66	3.173	-12.074	-24.576	1.00	15.84	L
ATOM	1737	CA	GLY	L	66	4.464	-11.678	-24.061	1.00	15.61	L
ATOM	1738	C	GLY	L	66	4.338	-10.874	-22.793	1.00	16.12	L
ATOM	1739	O	GLY	L	66	3.241	-10.464	-22.407	1.00	16.35	L
ATOM	1740	N	SER	L	67	5.467	-10.649	-22.134	1.00	17.61	L
ATOM	1741	CA	SER	L	67	5.458	-9.888	-20.898	1.00	18.73	L
ATOM	1742	CB	SER	L	67	4.733	-10.686	-19.817	1.00	19.61	L
ATOM	1743	OG	SER	L	67	4.853	-10.060	-18.555	1.00	24.17	L
ATOM	1744	C	SER	L	67	6.866	-9.572	-20.441	1.00	18.10	L
ATOM	1745	O	SER	L	67	7.790	-10.352	-20.666	1.00	19.07	L
ATOM	1746	N	GLY	L	68	7.023	-8.430	-19.786	1.00	16.86	L
ATOM	1747	CA	GLY	L	68	8.331	-8.055	-19.293	1.00	15.58	L
ATOM	1748	C	GLY	L	68	9.251	-7.559	-20.389	1.00	14.93	L
ATOM	1749	O	GLY	L	68	9.273	-6.371	-20.712	1.00	15.09	L
ATOM	1750	N	THR	L	69	10.003	-8.474	-20.983	1.00	14.58	L
ATOM	1751	CA	THR	L	69	10.932	-8.101	-22.042	1.00	13.89	L
ATOM	1752	CB	THR	L	69	12.358	-8.443	-21.664	1.00	12.62	L
ATOM	1753	OG1	THR	L	69	12.695	-7.784	-20.444	1.00	11.61	L
ATOM	1754	CG2	THR	L	69	13.309	-7.978	-22.739	1.00	14.73	L
ATOM	1755	C	THR	L	69	10.695	-8.740	-23.398	1.00	14.85	L
ATOM	1756	O	THR	L	69	11.043	-8.165	-24.421	1.00	15.44	L
ATOM	1757	N	GLU	L	70	10.142	-9.941	-23.419	1.00	15.79	L
ATOM	1758	CA	GLU	L	70	9.921	-10.589	-24.698	1.00	17.69	L
ATOM	1759	CB	GLU	L	70	10.551	-11.987	-24.706	1.00	19.10	L
ATOM	1760	CG	GLU	L	70	10.379	-12.728	-26.021	1.00	22.22	L

ATOM	1761	CD	GLU	L	70	10.928	-14.127	-25.957	1.00	24.82	L
ATOM	1762	OE1	GLU	L	70	10.358	-14.952	-25.217	1.00	27.80	L
ATOM	1763	OE2	GLU	L	70	11.933	-14.412	-26.643	1.00	27.03	L
ATOM	1764	C	GLU	L	70	8.435	-10.656	-25.035	1.00	17.15	L
ATOM	1765	O	GLU	L	70	7.623	-11.105	-24.218	1.00	16.60	L
ATOM	1766	N	PHE	L	71	8.105	-10.191	-26.245	1.00	15.52	L
ATOM	1767	CA	PHE	L	71	6.739	-10.141	-26.776	1.00	12.84	L
ATOM	1768	CB	PHE	L	71	6.292	-8.694	-26.866	1.00	9.40	L
ATOM	1769	CG	PHE	L	71	6.236	-8.024	-25.544	1.00	9.01	L
ATOM	1770	CD1	PHE	L	71	5.043	-7.994	-24.816	1.00	6.35	L
ATOM	1771	CD2	PHE	L	71	7.395	-7.470	-24.988	1.00	7.48	L
ATOM	1772	CE1	PHE	L	71	5.002	-7.423	-23.552	1.00	7.02	L
ATOM	1773	CE2	PHE	L	71	7.368	-6.895	-23.721	1.00	8.02	L
ATOM	1774	CZ	PHE	L	71	6.168	-6.867	-22.990	1.00	7.39	L
ATOM	1775	C	PHE	L	71	6.688	-10.771	-28.153	1.00	13.30	L
ATOM	1776	O	PHE	L	71	7.689	-10.812	-28.857	1.00	14.78	L
ATOM	1777	N	THR	L	72	5.522	-11.252	-28.552	1.00	11.72	L
ATOM	1778	CA	THR	L	72	5.449	-11.884	-29.837	1.00	12.93	L
ATOM	1779	CB	THR	L	72	5.851	-13.382	-29.677	1.00	13.79	L
ATOM	1780	OG1	THR	L	72	5.871	-14.029	-30.955	1.00	16.29	L
ATOM	1781	CG2	THR	L	72	4.884	-14.093	-28.750	1.00	14.12	L
ATOM	1782	C	THR	L	72	4.112	-11.732	-30.578	1.00	14.12	L
ATOM	1783	O	THR	L	72	3.017	-11.877	-30.004	1.00	13.32	L
ATOM	1784	N	LEU	L	73	4.223	-11.418	-31.868	1.00	13.71	L
ATOM	1785	CA	LEU	L	73	3.068	-11.240	-32.746	1.00	13.61	L
ATOM	1786	CB	LEU	L	73	3.288	-10.048	-33.681	1.00	13.61	L
ATOM	1787	CG	LEU	L	73	2.285	-9.831	-34.820	1.00	12.11	L
ATOM	1788	CD1	LEU	L	73	0.937	-9.387	-34.247	1.00	11.81	L
ATOM	1789	CD2	LEU	L	73	2.831	-8.780	-35.766	1.00	11.75	L
ATOM	1790	C	LEU	L	73	2.940	-12.500	-33.577	1.00	13.74	L
ATOM	1791	O	LEU	L	73	3.887	-12.902	-34.252	1.00	14.87	L
ATOM	1792	N	THR	L	74	1.773	-13.124	-33.531	1.00	13.00	L
ATOM	1793	CA	THR	L	74	1.554	-14.347	-34.285	1.00	12.76	L
ATOM	1794	CB	THR	L	74	1.182	-15.517	-33.337	1.00	11.52	L
ATOM	1795	OG1	THR	L	74	2.251	-15.739	-32.410	1.00	9.59	L
ATOM	1796	CG2	THR	L	74	0.942	-16.779	-34.112	1.00	11.42	L
ATOM	1797	C	THR	L	74	0.431	-14.157	-35.302	1.00	14.52	L
ATOM	1798	O	THR	L	74	-0.611	-13.566	-34.999	1.00	13.39	L
ATOM	1799	N	ILE	L	75	0.655	-14.664	-36.507	1.00	16.24	L
ATOM	1800	CA	ILE	L	75	-0.324	-14.575	-37.575	1.00	19.83	L
ATOM	1801	CB	ILE	L	75	0.263	-13.885	-38.825	1.00	19.67	L
ATOM	1802	CG2	ILE	L	75	-0.818	-13.745	-39.902	1.00	18.59	L
ATOM	1803	CG1	ILE	L	75	0.850	-12.533	-38.437	1.00	19.11	L
ATOM	1804	CD1	ILE	L	75	1.501	-11.807	-39.572	1.00	17.61	L
ATOM	1805	C	ILE	L	75	-0.678	-16.002	-37.944	1.00	21.94	L
ATOM	1806	O	ILE	L	75	0.164	-16.729	-38.452	1.00	24.70	L
ATOM	1807	N	SER	L	76	-1.914	-16.408	-37.713	1.00	23.66	L
ATOM	1808	CA	SER	L	76	-2.287	-17.778	-38.016	1.00	26.41	L
ATOM	1809	CB	SER	L	76	-3.609	-18.105	-37.334	1.00	26.86	L
ATOM	1810	OG	SER	L	76	-3.430	-18.113	-35.939	1.00	28.66	L
ATOM	1811	C	SER	L	76	-2.358	-18.135	-39.491	1.00	27.72	L
ATOM	1812	O	SER	L	76	-1.348	-18.468	-40.109	1.00	26.56	L
ATOM	1813	N	SER	L	77	-3.563	-18.071	-40.048	1.00	29.97	L
ATOM	1814	CA	SER	L	77	-3.790	-18.392	-41.458	1.00	31.58	L
ATOM	1815	CB	SER	L	77	-5.293	-18.554	-41.711	1.00	33.53	L
ATOM	1816	OG	SER	L	77	-5.886	-19.442	-40.766	1.00	35.88	L
ATOM	1817	C	SER	L	77	-3.240	-17.287	-42.368	1.00	30.85	L
ATOM	1818	O	SER	L	77	-3.999	-16.466	-42.864	1.00	30.63	L
ATOM	1819	N	LEU	L	78	-1.928	-17.278	-42.596	1.00	30.53	L
ATOM	1820	CA	LEU	L	78	-1.301	-16.258	-43.429	1.00	30.15	L
ATOM	1821	CB	LEU	L	78	0.170	-16.605	-43.668	1.00	28.83	L

ATOM	1822	CG	LEU	L	78	1.088	-15.437	-44.047	1.00	28.76	L
ATOM	1823	CD1	LEU	L	78	1.268	-14.518	-42.853	1.00	28.55	L
ATOM	1824	CD2	LEU	L	78	2.440	-15.956	-44.511	1.00	28.72	L
ATOM	1825	C	LEU	L	78	-2.015	-16.083	-44.765	1.00	31.57	L
ATOM	1826	O	LEU	L	78	-2.232	-17.044	-45.496	1.00	32.52	L
ATOM	1827	N	GLN	L	79	-2.393	-14.850	-45.079	1.00	32.63	L
ATOM	1828	CA	GLN	L	79	-3.073	-14.576	-46.335	1.00	33.55	L
ATOM	1829	CB	GLN	L	79	-4.296	-13.709	-46.086	1.00	33.63	L
ATOM	1830	CG	GLN	L	79	-5.243	-14.244	-45.029	1.00	35.38	L
ATOM	1831	CD	GLN	L	79	-5.963	-15.507	-45.450	1.00	36.55	L
ATOM	1832	OE1	GLN	L	79	-6.674	-15.531	-46.457	1.00	38.30	L
ATOM	1833	NE2	GLN	L	79	-5.796	-16.564	-44.668	1.00	37.18	L
ATOM	1834	C	GLN	L	79	-2.125	-13.863	-47.304	1.00	34.40	L
ATOM	1835	O	GLN	L	79	-1.092	-13.315	-46.905	1.00	33.83	L
ATOM	1836	N	PRO	L	80	-2.473	-13.850	-48.596	1.00	34.60	L
ATOM	1837	CD	PRO	L	80	-3.736	-14.323	-49.186	1.00	34.49	L
ATOM	1838	CA	PRO	L	80	-1.641	-13.202	-49.611	1.00	34.81	L
ATOM	1839	CB	PRO	L	80	-2.377	-13.516	-50.901	1.00	35.12	L
ATOM	1840	CG	PRO	L	80	-3.816	-13.495	-50.448	1.00	35.60	L
ATOM	1841	C	PRO	L	80	-1.511	-11.705	-49.383	1.00	34.93	L
ATOM	1842	O	PRO	L	80	-0.559	-11.091	-49.858	1.00	36.49	L
ATOM	1843	N	GLU	L	81	-2.466	-11.119	-48.663	1.00	34.01	L
ATOM	1844	CA	GLU	L	81	-2.442	-9.687	-48.386	1.00	32.18	L
ATOM	1845	CB	GLU	L	81	-3.841	-9.089	-48.569	1.00	33.65	L
ATOM	1846	CG	GLU	L	81	-4.969	-10.115	-48.665	1.00	36.06	L
ATOM	1847	CD	GLU	L	81	-5.402	-10.622	-47.322	1.00	36.33	L
ATOM	1848	OE1	GLU	L	81	-6.230	-11.567	-47.274	1.00	35.64	L
ATOM	1849	OE2	GLU	L	81	-4.908	-10.059	-46.320	1.00	37.30	L
ATOM	1850	C	GLU	L	81	-1.885	-9.342	-47.007	1.00	30.05	L
ATOM	1851	O	GLU	L	81	-1.886	-8.182	-46.611	1.00	30.43	L
ATOM	1852	N	ASP	L	82	-1.403	-10.354	-46.291	1.00	27.93	L
ATOM	1853	CA	ASP	L	82	-0.807	-10.142	-44.985	1.00	26.19	L
ATOM	1854	CB	ASP	L	82	-0.855	-11.425	-44.150	1.00	26.09	L
ATOM	1855	CG	ASP	L	82	-2.219	-11.665	-43.540	1.00	26.98	L
ATOM	1856	OD1	ASP	L	82	-3.016	-10.704	-43.500	1.00	27.12	L
ATOM	1857	OD2	ASP	L	82	-2.498	-12.799	-43.086	1.00	26.87	L
ATOM	1858	C	ASP	L	82	0.639	-9.684	-45.164	1.00	25.38	L
ATOM	1859	O	ASP	L	82	1.377	-9.507	-44.191	1.00	25.53	L
ATOM	1860	N	PHE	L	83	1.034	-9.513	-46.423	1.00	24.11	L
ATOM	1861	CA	PHE	L	83	2.373	-9.055	-46.791	1.00	22.21	L
ATOM	1862	CB	PHE	L	83	2.555	-9.135	-48.304	1.00	24.70	L
ATOM	1863	CG	PHE	L	83	3.496	-8.112	-48.854	1.00	27.07	L
ATOM	1864	CD1	PHE	L	83	4.852	-8.143	-48.535	1.00	29.04	L
ATOM	1865	CD2	PHE	L	83	3.021	-7.095	-49.676	1.00	27.98	L
ATOM	1866	CE1	PHE	L	83	5.729	-7.169	-49.031	1.00	29.51	L
ATOM	1867	CE2	PHE	L	83	3.885	-6.115	-50.179	1.00	28.81	L
ATOM	1868	CZ	PHE	L	83	5.245	-6.150	-49.856	1.00	28.92	L
ATOM	1869	C	PHE	L	83	2.539	-7.611	-46.345	1.00	19.13	L
ATOM	1870	O	PHE	L	83	1.738	-6.748	-46.694	1.00	17.37	L
ATOM	1871	N	ALA	L	84	3.586	-7.348	-45.577	1.00	17.11	L
ATOM	1872	CA	ALA	L	84	3.829	-5.998	-45.083	1.00	14.54	L
ATOM	1873	CB	ALA	L	84	2.576	-5.475	-44.393	1.00	14.75	L
ATOM	1874	C	ALA	L	84	4.990	-5.969	-44.109	1.00	12.00	L
ATOM	1875	O	ALA	L	84	5.614	-6.993	-43.853	1.00	11.20	L
ATOM	1876	N	THR	L	85	5.287	-4.787	-43.580	1.00	10.99	L
ATOM	1877	CA	THR	L	85	6.343	-4.662	-42.576	1.00	9.98	L
ATOM	1878	CB	THR	L	85	7.239	-3.431	-42.768	1.00	10.55	L
ATOM	1879	OG1	THR	L	85	7.894	-3.485	-44.042	1.00	12.19	L
ATOM	1880	CG2	THR	L	85	8.290	-3.401	-41.656	1.00	9.30	L
ATOM	1881	C	THR	L	85	5.623	-4.495	-41.241	1.00	8.43	L
ATOM	1882	O	THR	L	85	4.729	-3.673	-41.120	1.00	6.48	L

ATOM	1883	N	TYR	L	86	5.997	-5.306	-40.259	1.00	8.48	L
ATOM	1884	CA	TYR	L	86	5.391	-5.245	-38.949	1.00	7.21	L
ATOM	1885	CB	TYR	L	86	5.028	-6.649	-38.460	1.00	6.82	L
ATOM	1886	CG	TYR	L	86	3.949	-7.290	-39.306	1.00	6.34	L
ATOM	1887	CD1	TYR	L	86	4.243	-7.762	-40.588	1.00	6.20	L
ATOM	1888	CE1	TYR	L	86	3.253	-8.227	-41.429	1.00	6.26	L
ATOM	1889	CD2	TYR	L	86	2.617	-7.319	-38.877	1.00	4.76	L
ATOM	1890	CE2	TYR	L	86	1.602	-7.785	-39.714	1.00	5.10	L
ATOM	1891	CZ	TYR	L	86	1.929	-8.236	-40.996	1.00	7.14	L
ATOM	1892	OH	TYR	L	86	0.941	-8.659	-41.866	1.00	6.72	L
ATOM	1893	C	TYR	L	86	6.373	-4.579	-37.995	1.00	7.26	L
ATOM	1894	O	TYR	L	86	7.579	-4.870	-38.005	1.00	4.91	L
ATOM	1895	N	TYR	L	87	5.845	-3.677	-37.174	1.00	6.41	L
ATOM	1896	CA	TYR	L	87	6.652	-2.933	-36.225	1.00	7.18	L
ATOM	1897	CB	TYR	L	87	6.676	-1.444	-36.575	1.00	8.52	L
ATOM	1898	CG	TYR	L	87	7.429	-1.033	-37.814	1.00	8.46	L
ATOM	1899	CD1	TYR	L	87	6.774	-0.864	-39.030	1.00	9.06	L
ATOM	1900	CE1	TYR	L	87	7.469	-0.430	-40.166	1.00	9.29	L
ATOM	1901	CD2	TYR	L	87	8.800	-0.765	-37.761	1.00	8.75	L
ATOM	1902	CE2	TYR	L	87	9.497	-0.336	-38.887	1.00	8.41	L
ATOM	1903	CZ	TYR	L	87	8.831	-0.172	-40.080	1.00	8.83	L
ATOM	1904	OH	TYR	L	87	9.539	0.236	-41.185	1.00	11.80	L
ATOM	1905	C	TYR	L	87	6.099	-3.031	-34.825	1.00	7.93	L
ATOM	1906	O	TYR	L	87	4.885	-2.992	-34.632	1.00	7.55	L
ATOM	1907	N	CYS	L	88	6.977	-3.152	-33.840	1.00	8.98	L
ATOM	1908	CA	CYS	L	88	6.499	-3.166	-32.469	1.00	11.08	L
ATOM	1909	C	CYS	L	88	6.912	-1.822	-31.879	1.00	9.49	L
ATOM	1910	O	CYS	L	88	7.922	-1.246	-32.288	1.00	8.19	L
ATOM	1911	CB	CYS	L	88	7.086	-4.336	-31.669	1.00	13.87	L
ATOM	1912	SG	CYS	L	88	8.894	-4.471	-31.607	1.00	20.10	L
ATOM	1913	N	GLN	L	89	6.116	-1.308	-30.948	1.00	7.20	L
ATOM	1914	CA	GLN	L	89	6.407	-0.018	-30.327	1.00	6.74	L
ATOM	1915	CB	GLN	L	89	5.560	1.069	-31.001	1.00	6.69	L
ATOM	1916	CG	GLN	L	89	5.789	2.460	-30.496	1.00	6.01	L
ATOM	1917	CD	GLN	L	89	4.544	3.052	-29.902	1.00	6.62	L
ATOM	1918	OE1	GLN	L	89	3.475	3.034	-30.516	1.00	7.04	L
ATOM	1919	NE2	GLN	L	89	4.669	3.591	-28.699	1.00	6.50	L
ATOM	1920	C	GLN	L	89	6.122	-0.056	-28.827	1.00	6.25	L
ATOM	1921	O	GLN	L	89	5.090	-0.584	-28.414	1.00	6.91	L
ATOM	1922	N	GLN	L	90	7.033	0.467	-28.002	1.00	4.40	L
ATOM	1923	CA	GLN	L	90	6.784	0.480	-26.556	1.00	2.66	L
ATOM	1924	CB	GLN	L	90	8.018	0.016	-25.758	1.00	2.41	L
ATOM	1925	CG	GLN	L	90	9.279	0.918	-25.727	1.00	1.00	L
ATOM	1926	CD	GLN	L	90	9.148	2.183	-24.860	1.00	1.97	L
ATOM	1927	OE1	GLN	L	90	8.495	2.190	-23.802	1.00	1.00	L
ATOM	1928	NE2	GLN	L	90	9.788	3.262	-25.311	1.00	1.00	L
ATOM	1929	C	GLN	L	90	6.359	1.865	-26.082	1.00	3.53	L
ATOM	1930	O	GLN	L	90	6.774	2.889	-26.635	1.00	1.89	L
ATOM	1931	N	TYR	L	91	5.507	1.893	-25.068	1.00	4.57	L
ATOM	1932	CA	TYR	L	91	5.053	3.153	-24.516	1.00	5.80	L
ATOM	1933	CB	TYR	L	91	3.646	3.498	-25.013	1.00	5.04	L
ATOM	1934	CG	TYR	L	91	2.594	2.439	-24.830	1.00	3.81	L
ATOM	1935	CD1	TYR	L	91	1.726	2.476	-23.745	1.00	2.40	L
ATOM	1936	CE1	TYR	L	91	0.722	1.522	-23.601	1.00	3.37	L
ATOM	1937	CD2	TYR	L	91	2.438	1.418	-25.774	1.00	4.35	L
ATOM	1938	CE2	TYR	L	91	1.433	0.450	-25.643	1.00	4.21	L
ATOM	1939	CZ	TYR	L	91	0.576	0.512	-24.548	1.00	4.57	L
ATOM	1940	OH	TYR	L	91	-0.437	-0.423	-24.391	1.00	5.24	L
ATOM	1941	C	TYR	L	91	5.106	3.122	-23.001	1.00	6.62	L
ATOM	1942	O	TYR	L	91	4.224	3.610	-22.314	1.00	6.77	L
ATOM	1943	N	HIS	L	92	6.187	2.565	-22.486	1.00	8.26	L

ATOM	1944	CA	HIS	L	92	6.379	2.482	-21.055	1.00	9.83	L
ATOM	1945	CB	HIS	L	92	7.304	1.307	-20.732	1.00	10.19	L
ATOM	1946	CG	HIS	L	92	7.597	1.157	-19.277	1.00	13.25	L
ATOM	1947	CD2	HIS	L	92	8.751	1.290	-18.579	1.00	14.04	L
ATOM	1948	ND1	HIS	L	92	6.617	0.877	-18.351	1.00	15.26	L
ATOM	1949	CE1	HIS	L	92	7.153	0.846	-17.143	1.00	15.88	L
ATOM	1950	NE2	HIS	L	92	8.446	1.095	-17.254	1.00	14.69	L
ATOM	1951	C	HIS	L	92	6.992	3.797	-20.592	1.00	9.20	L
ATOM	1952	O	HIS	L	92	6.559	4.372	-19.608	1.00	10.88	L
ATOM	1953	N	SER	L	93	8.020	4.257	-21.291	1.00	9.19	L
ATOM	1954	CA	SER	L	93	8.664	5.515	-20.936	1.00	10.15	L
ATOM	1955	CB	SER	L	93	9.917	5.274	-20.075	1.00	9.91	L
ATOM	1956	OG	SER	L	93	10.867	4.497	-20.754	1.00	9.93	L
ATOM	1957	C	SER	L	93	9.037	6.274	-22.212	1.00	11.08	L
ATOM	1958	O	SER	L	93	9.094	5.699	-23.300	1.00	13.59	L
ATOM	1959	N	TYR	L	94	9.258	7.575	-22.080	1.00	11.16	L
ATOM	1960	CA	TYR	L	94	9.645	8.405	-23.207	1.00	10.67	L
ATOM	1961	CB	TYR	L	94	9.220	9.831	-22.952	1.00	10.20	L
ATOM	1962	CG	TYR	L	94	7.750	10.031	-23.055	1.00	11.98	L
ATOM	1963	CD1	TYR	L	94	7.126	10.063	-24.299	1.00	13.10	L
ATOM	1964	CE1	TYR	L	94	5.764	10.284	-24.409	1.00	12.68	L
ATOM	1965	CD2	TYR	L	94	6.970	10.214	-21.913	1.00	12.34	L
ATOM	1966	CE2	TYR	L	94	5.606	10.434	-22.019	1.00	11.24	L
ATOM	1967	CZ	TYR	L	94	5.017	10.473	-23.272	1.00	10.97	L
ATOM	1968	OH	TYR	L	94	3.683	10.752	-23.393	1.00	12.39	L
ATOM	1969	C	TYR	L	94	11.152	8.359	-23.350	1.00	10.75	L
ATOM	1970	O	TYR	L	94	11.864	8.329	-22.339	1.00	12.12	L
ATOM	1971	N	PRO	L	95	11.659	8.378	-24.599	1.00	10.12	L
ATOM	1972	CD	PRO	L	95	13.096	8.523	-24.881	1.00	10.42	L
ATOM	1973	CA	PRO	L	95	10.891	8.452	-25.845	1.00	9.23	L
ATOM	1974	CB	PRO	L	95	11.939	8.828	-26.890	1.00	10.36	L
ATOM	1975	CG	PRO	L	95	13.074	9.396	-26.088	1.00	11.18	L
ATOM	1976	C	PRO	L	95	10.259	7.125	-26.181	1.00	9.78	L
ATOM	1977	O	PRO	L	95	10.742	6.054	-25.786	1.00	9.82	L
ATOM	1978	N	TRP	L	96	9.171	7.189	-26.926	1.00	9.66	L
ATOM	1979	CA	TRP	L	96	8.516	5.961	-27.329	1.00	8.38	L
ATOM	1980	CB	TRP	L	96	7.080	6.265	-27.733	1.00	6.22	L
ATOM	1981	CG	TRP	L	96	6.222	6.675	-26.553	1.00	6.85	L
ATOM	1982	CD2	TRP	L	96	4.985	7.388	-26.614	1.00	5.61	L
ATOM	1983	CE2	TRP	L	96	4.444	7.404	-25.307	1.00	5.12	L
ATOM	1984	CE3	TRP	L	96	4.276	8.003	-27.649	1.00	5.94	L
ATOM	1985	CD1	TRP	L	96	6.390	6.310	-25.232	1.00	5.28	L
ATOM	1986	NE1	TRP	L	96	5.319	6.743	-24.486	1.00	5.09	L
ATOM	1987	CZ2	TRP	L	96	3.226	8.011	-25.012	1.00	4.95	L
ATOM	1988	CZ3	TRP	L	96	3.063	8.607	-27.360	1.00	6.82	L
ATOM	1989	CH2	TRP	L	96	2.546	8.603	-26.045	1.00	6.87	L
ATOM	1990	C	TRP	L	96	9.331	5.389	-28.481	1.00	7.69	L
ATOM	1991	O	TRP	L	96	9.669	6.098	-29.427	1.00	8.74	L
ATOM	1992	N	THR	L	97	9.648	4.105	-28.400	1.00	6.85	L
ATOM	1993	CA	THR	L	97	10.472	3.511	-29.424	1.00	5.66	L
ATOM	1994	CB	THR	L	97	11.755	2.906	-28.839	1.00	5.83	L
ATOM	1995	OG1	THR	L	97	12.374	3.857	-27.979	1.00	5.11	L
ATOM	1996	CG2	THR	L	97	12.736	2.559	-29.969	1.00	9.74	L
ATOM	1997	C	THR	L	97	9.827	2.448	-30.254	1.00	5.70	L
ATOM	1998	O	THR	L	97	8.964	1.712	-29.784	1.00	5.77	L
ATOM	1999	N	PHE	L	98	10.268	2.377	-31.503	1.00	5.71	L
ATOM	2000	CA	PHE	L	98	9.779	1.385	-32.417	1.00	5.89	L
ATOM	2001	CB	PHE	L	98	9.439	2.032	-33.739	1.00	5.15	L
ATOM	2002	CG	PHE	L	98	8.181	2.801	-33.716	1.00	4.13	L
ATOM	2003	CD1	PHE	L	98	8.177	4.124	-33.316	1.00	5.60	L
ATOM	2004	CD2	PHE	L	98	6.988	2.196	-34.091	1.00	4.22	L

ATOM	2005	CE1	PHE	L	98	6.989	4.857	-33.293	1.00	7.42	L
ATOM	2006	CE2	PHE	L	98	5.793	2.907	-34.075	1.00	6.81	L
ATOM	2007	CZ	PHE	L	98	5.789	4.244	-33.673	1.00	7.48	L
ATOM	2008	C	PHE	L	98	10.838	0.332	-32.625	1.00	7.27	L
ATOM	2009	O	PHE	L	98	11.988	0.502	-32.219	1.00	8.89	L
ATOM	2010	N	GLY	L	99	10.434	-0.780	-33.218	1.00	7.92	L
ATOM	2011	CA	GLY	L	99	11.389	-1.824	-33.490	1.00	9.17	L
ATOM	2012	C	GLY	L	99	11.865	-1.576	-34.911	1.00	9.56	L
ATOM	2013	O	GLY	L	99	11.177	-0.905	-35.682	1.00	10.42	L
ATOM	2014	N	GLN	L	100	13.028	-2.109	-35.267	1.00	9.40	L
ATOM	2015	CA	GLN	L	100	13.551	-1.937	-36.604	1.00	9.59	L
ATOM	2016	CB	GLN	L	100	14.878	-2.691	-36.751	1.00	8.63	L
ATOM	2017	CG	GLN	L	100	14.688	-4.183	-36.949	1.00	13.79	L
ATOM	2018	CD	GLN	L	100	14.906	-4.984	-35.693	1.00	15.52	L
ATOM	2019	OE1	GLN	L	100	14.629	-4.519	-34.583	1.00	16.85	L
ATOM	2020	NE2	GLN	L	100	15.397	-6.213	-35.860	1.00	16.25	L
ATOM	2021	C	GLN	L	100	12.527	-2.468	-37.621	1.00	9.72	L
ATOM	2022	O	GLN	L	100	12.577	-2.128	-38.793	1.00	11.02	L
ATOM	2023	N	GLY	L	101	11.600	-3.308	-37.179	1.00	8.67	L
ATOM	2024	CA	GLY	L	101	10.612	-3.835	-38.108	1.00	10.14	L
ATOM	2025	C	GLY	L	101	10.929	-5.179	-38.768	1.00	10.68	L
ATOM	2026	O	GLY	L	101	12.091	-5.550	-38.941	1.00	10.81	L
ATOM	2027	N	THR	L	102	9.882	-5.907	-39.145	1.00	10.02	L
ATOM	2028	CA	THR	L	102	10.019	-7.212	-39.782	1.00	10.68	L
ATOM	2029	CB	THR	L	102	9.391	-8.306	-38.919	1.00	10.47	L
ATOM	2030	OG1	THR	L	102	10.062	-8.363	-37.657	1.00	12.78	L
ATOM	2031	CG2	THR	L	102	9.482	-9.642	-39.605	1.00	9.34	L
ATOM	2032	C	THR	L	102	9.302	-7.227	-41.125	1.00	12.44	L
ATOM	2033	O	THR	L	102	8.083	-7.049	-41.176	1.00	12.34	L
ATOM	2034	N	LYS	L	103	10.038	-7.460	-42.207	1.00	12.98	L
ATOM	2035	CA	LYS	L	103	9.422	-7.471	-43.528	1.00	14.84	L
ATOM	2036	CB	LYS	L	103	10.385	-6.893	-44.567	1.00	15.63	L
ATOM	2037	CG	LYS	L	103	9.767	-6.747	-45.945	1.00	18.74	L
ATOM	2038	CD	LYS	L	103	10.845	-6.785	-47.009	1.00	21.41	L
ATOM	2039	CE	LYS	L	103	10.264	-6.625	-48.396	1.00	22.44	L
ATOM	2040	NZ	LYS	L	103	9.589	-5.300	-48.528	1.00	23.85	L
ATOM	2041	C	LYS	L	103	8.974	-8.871	-43.943	1.00	14.71	L
ATOM	2042	O	LYS	L	103	9.794	-9.778	-44.132	1.00	15.12	L
ATOM	2043	N	LEU	L	104	7.666	-9.031	-44.112	1.00	14.45	L
ATOM	2044	CA	LEU	L	104	7.091	-10.325	-44.468	1.00	14.60	L
ATOM	2045	CB	LEU	L	104	5.972	-10.670	-43.481	1.00	11.99	L
ATOM	2046	CG	LEU	L	104	5.099	-11.881	-43.764	1.00	11.10	L
ATOM	2047	CD1	LEU	L	104	5.932	-13.135	-43.663	1.00	11.33	L
ATOM	2048	CD2	LEU	L	104	3.942	-11.917	-42.770	1.00	11.59	L
ATOM	2049	C	LEU	L	104	6.562	-10.423	-45.892	1.00	15.97	L
ATOM	2050	O	LEU	L	104	5.579	-9.775	-46.258	1.00	16.90	L
ATOM	2051	N	GLU	L	105	7.223	-11.236	-46.701	1.00	16.86	L
ATOM	2052	CA	GLU	L	105	6.762	-11.411	-48.063	1.00	19.59	L
ATOM	2053	CB	GLU	L	105	7.919	-11.295	-49.046	1.00	20.51	L
ATOM	2054	CG	GLU	L	105	8.883	-12.420	-48.980	1.00	20.99	L
ATOM	2055	CD	GLU	L	105	8.948	-13.134	-50.299	1.00	21.61	L
ATOM	2056	OE1	GLU	L	105	9.142	-12.436	-51.313	1.00	22.37	L
ATOM	2057	OE2	GLU	L	105	8.809	-14.376	-50.328	1.00	21.64	L
ATOM	2058	C	GLU	L	105	6.094	-12.771	-48.168	1.00	20.32	L
ATOM	2059	O	GLU	L	105	6.404	-13.685	-47.398	1.00	20.09	L
ATOM	2060	N	ILE	L	106	5.169	-12.898	-49.111	1.00	21.44	L
ATOM	2061	CA	ILE	L	106	4.446	-14.143	-49.276	1.00	23.43	L
ATOM	2062	CB	ILE	L	106	3.028	-13.889	-49.771	1.00	22.83	L
ATOM	2063	CG2	ILE	L	106	2.236	-15.179	-49.698	1.00	22.89	L
ATOM	2064	CG1	ILE	L	106	2.389	-12.769	-48.945	1.00	20.99	L
ATOM	2065	CD1	ILE	L	106	2.379	-13.024	-47.451	1.00	20.39	L

ATOM	2066	C	ILE	L	106	5.121	-15.103	-50.230	1.00	24.93	L
ATOM	2067	O	ILE	L	106	5.380	-14.771	-51.387	1.00	24.17	L
ATOM	2068	N	LYS	L	107	5.409	-16.296	-49.722	1.00	28.03	L
ATOM	2069	CA	LYS	L	107	6.045	-17.327	-50.515	1.00	30.61	L
ATOM	2070	CB	LYS	L	107	6.328	-18.571	-49.679	1.00	32.10	L
ATOM	2071	CG	LYS	L	107	7.301	-19.534	-50.336	1.00	34.09	L
ATOM	2072	CD	LYS	L	107	8.721	-19.326	-49.823	1.00	36.04	L
ATOM	2073	CE	LYS	L	107	8.846	-19.791	-48.369	1.00	36.60	L
ATOM	2074	NZ	LYS	L	107	10.213	-19.608	-47.801	1.00	37.56	L
ATOM	2075	C	LYS	L	107	5.041	-17.670	-51.579	1.00	31.41	L
ATOM	2076	O	LYS	L	107	3.827	-17.614	-51.373	1.00	31.92	L
ATOM	2077	N	ARG	L	108	5.536	-18.025	-52.734	1.00	31.09	L
ATOM	2078	CA	ARG	L	108	4.608	-18.351	-53.773	1.00	30.67	L
ATOM	2079	CB	ARG	L	108	4.218	-17.065	-54.487	1.00	29.56	L
ATOM	2080	CG	ARG	L	108	2.983	-17.166	-55.316	1.00	29.55	L
ATOM	2081	CD	ARG	L	108	3.044	-16.154	-56.428	1.00	29.00	L
ATOM	2082	NE	ARG	L	108	3.220	-16.825	-57.705	1.00	30.73	L
ATOM	2083	CZ	ARG	L	108	2.221	-17.208	-58.491	1.00	31.28	L
ATOM	2084	NH1	ARG	L	108	0.967	-16.966	-58.125	1.00	32.82	L
ATOM	2085	NH2	ARG	L	108	2.473	-17.856	-59.628	1.00	30.38	L
ATOM	2086	C	ARG	L	108	5.292	-19.314	-54.710	1.00	30.78	L
ATOM	2087	O	ARG	L	108	6.516	-19.477	-54.662	1.00	30.73	L
ATOM	2885	CB	GLN	H	1	-17.228	9.372	-41.991	1.00	38.03	H
ATOM	2886	CG	GLN	H	1	-17.154	10.882	-41.725	1.00	41.63	H
ATOM	2887	CD	GLN	H	1	-18.494	11.453	-41.221	1.00	44.22	H
ATOM	2888	OE1	GLN	H	1	-19.539	11.258	-41.860	1.00	45.30	H
ATOM	2889	NE2	GLN	H	1	-18.464	12.166	-40.083	1.00	44.03	H
ATOM	2890	C	GLN	H	1	-14.757	9.019	-41.817	1.00	31.13	H
ATOM	2891	O	GLN	H	1	-14.172	10.095	-41.886	1.00	31.51	H
ATOM	2892	N	GLN	H	1	-16.184	7.270	-42.783	1.00	34.00	H
ATOM	2893	CA	GLN	H	1	-15.992	8.747	-42.656	1.00	34.12	H
ATOM	2894	N	VAL	H	2	-14.367	8.024	-41.031	1.00	26.54	H
ATOM	2895	CA	VAL	H	2	-13.212	8.138	-40.155	1.00	23.34	H
ATOM	2896	CB	VAL	H	2	-13.245	7.012	-39.131	1.00	22.59	H
ATOM	2897	CG1	VAL	H	2	-13.829	5.784	-39.774	1.00	21.51	H
ATOM	2898	CG2	VAL	H	2	-11.850	6.738	-38.596	1.00	22.41	H
ATOM	2899	C	VAL	H	2	-11.892	8.101	-40.926	1.00	21.85	H
ATOM	2900	O	VAL	H	2	-11.568	7.107	-41.560	1.00	22.10	H
ATOM	2901	N	SER	H	3	-11.121	9.179	-40.868	1.00	20.36	H
ATOM	2902	CA	SER	H	3	-9.858	9.213	-41.596	1.00	18.47	H
ATOM	2903	CB	SER	H	3	-10.141	9.399	-43.095	1.00	18.64	H
ATOM	2904	OG	SER	H	3	-10.823	10.625	-43.336	1.00	18.79	H
ATOM	2905	C	SER	H	3	-8.909	10.315	-41.108	1.00	16.35	H
ATOM	2906	O	SER	H	3	-9.301	11.207	-40.349	1.00	14.67	H
ATOM	2907	N	LEU	H	4	-7.655	10.245	-41.545	1.00	14.24	H
ATOM	2908	CA	LEU	H	4	-6.668	11.258	-41.184	1.00	14.54	H
ATOM	2909	CB	LEU	H	4	-5.672	10.723	-40.157	1.00	13.53	H
ATOM	2910	CG	LEU	H	4	-6.211	10.379	-38.766	1.00	13.76	H
ATOM	2911	CD1	LEU	H	4	-5.092	9.717	-37.965	1.00	12.35	H
ATOM	2912	CD2	LEU	H	4	-6.742	11.635	-38.063	1.00	11.54	H
ATOM	2913	C	LEU	H	4	-5.913	11.687	-42.427	1.00	14.67	H
ATOM	2914	O	LEU	H	4	-5.243	10.867	-43.049	1.00	15.74	H
ATOM	2915	N	ARG	H	5	-6.024	12.964	-42.788	1.00	15.44	H
ATOM	2916	CA	ARG	H	5	-5.350	13.478	-43.975	1.00	17.23	H
ATOM	2917	CB	ARG	H	5	-6.361	14.004	-45.003	1.00	20.91	H
ATOM	2918	CG	ARG	H	5	-7.130	12.917	-45.748	1.00	26.83	H
ATOM	2919	CD	ARG	H	5	-7.934	13.525	-46.904	1.00	34.28	H
ATOM	2920	NE	ARG	H	5	-9.324	13.826	-46.553	1.00	38.31	H
ATOM	2921	CZ	ARG	H	5	-10.294	12.916	-46.470	1.00	41.05	H
ATOM	2922	NH1	ARG	H	5	-10.030	11.638	-46.708	1.00	41.35	H
ATOM	2923	NH2	ARG	H	5	-11.537	13.283	-46.169	1.00	42.82	H

ATOM	2924	C	ARG	H	5	-4.358	14.567	-43.655	1.00	15.33	H
ATOM	2925	O	ARG	H	5	-4.731	15.672	-43.252	1.00	15.11	H
ATOM	2926	N	GLU	H	6	-3.082	14.252	-43.830	1.00	14.48	H
ATOM	2927	CA	GLU	H	6	-2.043	15.240	-43.555	1.00	13.53	H
ATOM	2928	CB	GLU	H	6	-0.837	14.591	-42.848	1.00	10.37	H
ATOM	2929	CG	GLU	H	6	-0.242	13.379	-43.502	1.00	10.69	H
ATOM	2930	CD	GLU	H	6	-0.904	12.053	-43.105	1.00	12.25	H
ATOM	2931	OE1	GLU	H	6	-1.689	11.509	-43.910	1.00	11.59	H
ATOM	2932	OE2	GLU	H	6	-0.622	11.540	-41.999	1.00	11.51	H
ATOM	2933	C	GLU	H	6	-1.595	16.021	-44.790	1.00	11.79	H
ATOM	2934	O	GLU	H	6	-1.707	15.556	-45.914	1.00	11.18	H
ATOM	2935	N	SER	H	7	-1.120	17.236	-44.576	1.00	12.26	H
ATOM	2936	CA	SER	H	7	-0.672	18.049	-45.684	1.00	12.42	H
ATOM	2937	CB	SER	H	7	-1.867	18.735	-46.366	1.00	9.88	H
ATOM	2938	OG	SER	H	7	-2.516	19.601	-45.461	1.00	8.60	H
ATOM	2939	C	SER	H	7	0.302	19.099	-45.169	1.00	13.19	H
ATOM	2940	O	SER	H	7	0.463	19.295	-43.950	1.00	11.90	H
ATOM	2941	N	GLY	H	8	0.934	19.777	-46.120	1.00	13.68	H
ATOM	2942	CA	GLY	H	8	1.892	20.813	-45.801	1.00	13.72	H
ATOM	2943	C	GLY	H	8	3.277	20.422	-46.251	1.00	13.27	H
ATOM	2944	O	GLY	H	8	4.133	21.279	-46.429	1.00	14.46	H
ATOM	2945	N	GLY	H	9	3.493	19.125	-46.446	1.00	13.04	H
ATOM	2946	CA	GLY	H	9	4.802	18.651	-46.855	1.00	13.75	H
ATOM	2947	C	GLY	H	9	5.258	19.190	-48.193	1.00	14.12	H
ATOM	2948	O	GLY	H	9	4.449	19.475	-49.070	1.00	14.64	H
ATOM	2949	N	GLY	H	10	6.569	19.324	-48.335	1.00	12.90	H
ATOM	2950	CA	GLY	H	10	7.147	19.815	-49.562	1.00	11.12	H
ATOM	2951	C	GLY	H	10	8.640	19.951	-49.395	1.00	12.16	H
ATOM	2952	O	GLY	H	10	9.231	19.397	-48.460	1.00	14.47	H
ATOM	2953	N	LEU	H	11	9.254	20.695	-50.301	1.00	11.81	H
ATOM	2954	CA	LEU	H	11	10.695	20.902	-50.264	1.00	11.20	H
ATOM	2955	CB	LEU	H	11	11.194	21.229	-51.666	1.00	11.52	H
ATOM	2956	CG	LEU	H	11	12.655	21.626	-51.772	1.00	9.91	H
ATOM	2957	CD1	LEU	H	11	13.531	20.399	-51.735	1.00	9.46	H
ATOM	2958	CD2	LEU	H	11	12.840	22.394	-53.039	1.00	11.08	H
ATOM	2959	C	LEU	H	11	10.970	22.065	-49.336	1.00	10.64	H
ATOM	2960	O	LEU	H	11	10.341	23.103	-49.445	1.00	11.74	H
ATOM	2961	N	VAL	H	12	11.895	21.898	-48.412	1.00	11.07	H
ATOM	2962	CA	VAL	H	12	12.199	22.984	-47.500	1.00	11.68	H
ATOM	2963	CB	VAL	H	12	11.525	22.744	-46.117	1.00	11.62	H
ATOM	2964	CG1	VAL	H	12	11.994	21.426	-45.533	1.00	11.18	H
ATOM	2965	CG2	VAL	H	12	11.831	23.881	-45.177	1.00	10.48	H
ATOM	2966	C	VAL	H	12	13.714	23.124	-47.362	1.00	11.68	H
ATOM	2967	O	VAL	H	12	14.449	22.135	-47.333	1.00	11.18	H
ATOM	2968	N	GLN	H	13	14.178	24.364	-47.284	1.00	13.31	H
ATOM	2969	CA	GLN	H	13	15.606	24.628	-47.187	1.00	15.00	H
ATOM	2970	CB	GLN	H	13	15.919	26.019	-47.755	1.00	15.90	H
ATOM	2971	CG	GLN	H	13	16.193	26.029	-49.271	1.00	16.90	H
ATOM	2972	CD	GLN	H	13	16.243	27.430	-49.863	1.00	18.00	H
ATOM	2973	OE1	GLN	H	13	16.870	28.332	-49.308	1.00	18.96	H
ATOM	2974	NE2	GLN	H	13	15.597	27.611	-51.009	1.00	18.93	H
ATOM	2975	C	GLN	H	13	16.152	24.501	-45.777	1.00	13.89	H
ATOM	2976	O	GLN	H	13	15.469	24.805	-44.806	1.00	14.83	H
ATOM	2977	N	PRO	H	14	17.402	24.044	-45.647	1.00	13.23	H
ATOM	2978	CD	PRO	H	14	18.348	23.638	-46.699	1.00	13.82	H
ATOM	2979	CA	PRO	H	14	18.001	23.893	-44.319	1.00	12.61	H
ATOM	2980	CB	PRO	H	14	19.445	23.511	-44.630	1.00	11.95	H
ATOM	2981	CG	PRO	H	14	19.321	22.762	-45.916	1.00	13.51	H
ATOM	2982	C	PRO	H	14	17.895	25.206	-43.561	1.00	12.29	H
ATOM	2983	O	PRO	H	14	18.215	26.265	-44.089	1.00	13.56	H
ATOM	2984	N	GLY	H	15	17.415	25.127	-42.329	1.00	11.52	H

ATOM	2985	CA	GLY	H	15	17.278	26.320	-41.529	1.00	10.23	H
ATOM	2986	C	GLY	H	15	15.918	26.977	-41.625	1.00	11.22	H
ATOM	2987	O	GLY	H	15	15.526	27.715	-40.724	1.00	9.73	H
ATOM	2988	N	ARG	H	16	15.186	26.719	-42.702	1.00	12.69	H
ATOM	2989	CA	ARG	H	16	13.877	27.342	-42.854	1.00	14.66	H
ATOM	2990	CB	ARG	H	16	13.435	27.319	-44.314	1.00	18.56	H
ATOM	2991	CG	ARG	H	16	14.241	28.208	-45.227	1.00	21.98	H
ATOM	2992	CD	ARG	H	16	13.934	29.663	-44.974	1.00	25.86	H
ATOM	2993	NE	ARG	H	16	14.396	30.485	-46.095	1.00	32.22	H
ATOM	2994	CZ	ARG	H	16	13.815	30.518	-47.295	1.00	34.94	H
ATOM	2995	NH1	ARG	H	16	12.732	29.783	-47.529	1.00	36.64	H
ATOM	2996	NH2	ARG	H	16	14.333	31.255	-48.274	1.00	36.71	H
ATOM	2997	C	ARG	H	16	12.875	26.594	-42.005	1.00	14.25	H
ATOM	2998	O	ARG	H	16	13.233	25.638	-41.321	1.00	14.28	H
ATOM	2999	N	SER	H	17	11.623	27.037	-42.029	1.00	13.56	H
ATOM	3000	CA	SER	H	17	10.585	26.376	-41.248	1.00	12.76	H
ATOM	3001	CB	SER	H	17	10.251	27.185	-39.976	1.00	10.97	H
ATOM	3002	OG	SER	H	17	9.880	28.517	-40.261	1.00	10.44	H
ATOM	3003	C	SER	H	17	9.338	26.116	-42.083	1.00	12.50	H
ATOM	3004	O	SER	H	17	8.999	26.880	-42.990	1.00	11.82	H
ATOM	3005	N	LEU	H	18	8.672	25.012	-41.763	1.00	12.08	H
ATOM	3006	CA	LEU	H	18	7.480	24.574	-42.471	1.00	12.12	H
ATOM	3007	CB	LEU	H	18	7.854	23.397	-43.366	1.00	12.29	H
ATOM	3008	CG	LEU	H	18	6.806	22.856	-44.314	1.00	15.26	H
ATOM	3009	CD1	LEU	H	18	6.544	23.892	-45.426	1.00	16.99	H
ATOM	3010	CD2	LEU	H	18	7.298	21.565	-44.932	1.00	14.85	H
ATOM	3011	C	LEU	H	18	6.409	24.131	-41.469	1.00	12.46	H
ATOM	3012	O	LEU	H	18	6.740	23.668	-40.376	1.00	13.86	H
ATOM	3013	N	ARG	H	19	5.134	24.269	-41.837	1.00	11.69	H
ATOM	3014	CA	ARG	H	19	4.053	23.858	-40.949	1.00	11.63	H
ATOM	3015	CB	ARG	H	19	3.108	25.010	-40.584	1.00	13.15	H
ATOM	3016	CG	ARG	H	19	2.323	24.705	-39.311	1.00	17.79	H
ATOM	3017	CD	ARG	H	19	1.220	25.700	-39.011	1.00	20.71	H
ATOM	3018	NE	ARG	H	19	0.145	25.586	-39.985	1.00	24.55	H
ATOM	3019	CZ	ARG	H	19	-1.106	25.997	-39.786	1.00	26.15	H
ATOM	3020	NH1	ARG	H	19	-1.453	26.559	-38.629	1.00	27.90	H
ATOM	3021	NH2	ARG	H	19	-2.011	25.833	-40.750	1.00	23.19	H
ATOM	3022	C	ARG	H	19	3.232	22.752	-41.554	1.00	10.59	H
ATOM	3023	O	ARG	H	19	2.636	22.908	-42.622	1.00	11.48	H
ATOM	3024	N	LEU	H	20	3.195	21.625	-40.856	1.00	8.72	H
ATOM	3025	CA	LEU	H	20	2.431	20.459	-41.299	1.00	6.73	H
ATOM	3026	CB	LEU	H	20	3.193	19.198	-40.933	1.00	5.77	H
ATOM	3027	CG	LEU	H	20	3.855	18.376	-42.018	1.00	6.73	H
ATOM	3028	CD1	LEU	H	20	4.504	19.241	-43.114	1.00	5.43	H
ATOM	3029	CD2	LEU	H	20	4.875	17.511	-41.312	1.00	4.29	H
ATOM	3030	C	LEU	H	20	1.076	20.433	-40.599	1.00	5.76	H
ATOM	3031	O	LEU	H	20	0.984	20.689	-39.406	1.00	6.95	H
ATOM	3032	N	SER	H	21	0.026	20.111	-41.329	1.00	5.05	H
ATOM	3033	CA	SER	H	21	-1.271	20.061	-40.691	1.00	5.74	H
ATOM	3034	CB	SER	H	21	-2.160	21.227	-41.124	1.00	5.27	H
ATOM	3035	OG	SER	H	21	-2.582	21.072	-42.462	1.00	8.84	H
ATOM	3036	C	SER	H	21	-1.929	18.744	-41.036	1.00	5.36	H
ATOM	3037	O	SER	H	21	-1.707	18.214	-42.121	1.00	2.68	H
ATOM	3038	N	CYS	H	22	-2.698	18.215	-40.083	1.00	7.14	H
ATOM	3039	CA	CYS	H	22	-3.415	16.950	-40.221	1.00	9.56	H
ATOM	3040	C	CYS	H	22	-4.910	17.166	-39.980	1.00	9.14	H
ATOM	3041	O	CYS	H	22	-5.308	17.596	-38.894	1.00	7.69	H
ATOM	3042	CB	CYS	H	22	-2.922	15.911	-39.204	1.00	11.39	H
ATOM	3043	SG	CYS	H	22	-3.763	14.298	-39.439	1.00	13.19	H
ATOM	3044	N	THR	H	23	-5.731	16.873	-40.989	1.00	8.90	H
ATOM	3045	CA	THR	H	23	-7.184	17.020	-40.872	1.00	9.76	H

ATOM	3046	CB	THR	H	23	-7.819	17.476	-42.177	1.00	10.09	H
ATOM	3047	OG1	THR	H	23	-7.296	18.758	-42.534	1.00	12.65	H
ATOM	3048	CG2	THR	H	23	-9.335	17.552	-42.022	1.00	8.41	H
ATOM	3049	C	THR	H	23	-7.862	15.714	-40.488	1.00	9.51	H
ATOM	3050	O	THR	H	23	-7.682	14.686	-41.152	1.00	9.77	H
ATOM	3051	N	ALA	H	24	-8.664	15.771	-39.430	1.00	7.58	H
ATOM	3052	CA	ALA	H	24	-9.375	14.601	-38.941	1.00	6.53	H
ATOM	3053	CB	ALA	H	24	-9.189	14.512	-37.453	1.00	5.54	H
ATOM	3054	C	ALA	H	24	-10.873	14.590	-39.280	1.00	6.84	H
ATOM	3055	O	ALA	H	24	-11.472	15.630	-39.561	1.00	6.30	H
ATOM	3056	N	SER	H	25	-11.468	13.402	-39.268	1.00	7.53	H
ATOM	3057	CA	SER	H	25	-12.891	13.275	-39.529	1.00	9.12	H
ATOM	3058	CB	SER	H	25	-13.207	13.521	-41.003	1.00	10.49	H
ATOM	3059	OG	SER	H	25	-12.900	12.376	-41.778	1.00	13.85	H
ATOM	3060	C	SER	H	25	-13.392	11.900	-39.138	1.00	8.68	H
ATOM	3061	O	SER	H	25	-12.610	10.959	-39.071	1.00	9.15	H
ATOM	3062	N	GLY	H	26	-14.694	11.803	-38.863	1.00	7.31	H
ATOM	3063	CA	GLY	H	26	-15.294	10.534	-38.512	1.00	5.63	H
ATOM	3064	C	GLY	H	26	-15.259	10.129	-37.052	1.00	6.29	H
ATOM	3065	O	GLY	H	26	-15.746	9.043	-36.718	1.00	6.85	H
ATOM	3066	N	PHE	H	27	-14.676	10.970	-36.195	1.00	5.39	H
ATOM	3067	CA	PHE	H	27	-14.602	10.703	-34.764	1.00	3.21	H
ATOM	3068	CB	PHE	H	27	-13.394	9.836	-34.430	1.00	3.38	H
ATOM	3069	CG	PHE	H	27	-12.069	10.493	-34.681	1.00	6.17	H
ATOM	3070	CD1	PHE	H	27	-11.388	11.128	-33.649	1.00	7.13	H
ATOM	3071	CD2	PHE	H	27	-11.485	10.459	-35.948	1.00	8.80	H
ATOM	3072	CE1	PHE	H	27	-10.129	11.725	-33.872	1.00	8.38	H
ATOM	3073	CE2	PHE	H	27	-10.224	11.053	-36.192	1.00	7.26	H
ATOM	3074	CZ	PHE	H	27	-9.546	11.687	-35.145	1.00	7.99	H
ATOM	3075	C	PHE	H	27	-14.534	12.027	-34.038	1.00	3.40	H
ATOM	3076	O	PHE	H	27	-14.437	13.059	-34.677	1.00	2.87	H
ATOM	3077	N	THR	H	28	-14.622	12.007	-32.710	1.00	5.40	H
ATOM	3078	CA	THR	H	28	-14.601	13.243	-31.932	1.00	6.21	H
ATOM	3079	CB	THR	H	28	-15.466	13.120	-30.668	1.00	6.55	H
ATOM	3080	OG1	THR	H	28	-16.790	12.732	-31.047	1.00	7.06	H
ATOM	3081	CG2	THR	H	28	-15.537	14.448	-29.940	1.00	5.57	H
ATOM	3082	C	THR	H	28	-13.178	13.618	-31.539	1.00	8.34	H
ATOM	3083	O	THR	H	28	-12.650	13.174	-30.513	1.00	7.70	H
ATOM	3084	N	PHE	H	29	-12.586	14.471	-32.366	1.00	9.20	H
ATOM	3085	CA	PHE	H	29	-11.219	14.939	-32.223	1.00	8.64	H
ATOM	3086	CB	PHE	H	29	-11.023	16.179	-33.108	1.00	6.86	H
ATOM	3087	CG	PHE	H	29	-9.588	16.496	-33.401	1.00	5.50	H
ATOM	3088	CD1	PHE	H	29	-8.792	15.590	-34.095	1.00	4.60	H
ATOM	3089	CD2	PHE	H	29	-9.033	17.706	-32.999	1.00	4.43	H
ATOM	3090	CE1	PHE	H	29	-7.466	15.879	-34.382	1.00	5.04	H
ATOM	3091	CE2	PHE	H	29	-7.706	18.005	-33.281	1.00	4.00	H
ATOM	3092	CZ	PHE	H	29	-6.923	17.089	-33.977	1.00	5.16	H
ATOM	3093	C	PHE	H	29	-10.706	15.231	-30.821	1.00	9.74	H
ATOM	3094	O	PHE	H	29	-9.661	14.697	-30.422	1.00	8.35	H
ATOM	3095	N	ARG	H	30	-11.421	16.073	-30.077	1.00	12.71	H
ATOM	3096	CA	ARG	H	30	-10.984	16.465	-28.728	1.00	14.89	H
ATOM	3097	CB	ARG	H	30	-11.880	17.577	-28.172	1.00	18.34	H
ATOM	3098	CG	ARG	H	30	-13.328	17.141	-28.001	1.00	25.22	H
ATOM	3099	CD	ARG	H	30	-14.242	18.281	-27.550	1.00	30.89	H
ATOM	3100	NE	ARG	H	30	-14.174	18.521	-26.112	1.00	34.44	H
ATOM	3101	CZ	ARG	H	30	-14.768	19.538	-25.477	1.00	37.44	H
ATOM	3102	NH1	ARG	H	30	-15.486	20.435	-26.150	1.00	36.31	H
ATOM	3103	NH2	ARG	H	30	-14.647	19.660	-24.153	1.00	37.84	H
ATOM	3104	C	ARG	H	30	-10.960	15.307	-27.739	1.00	14.44	H
ATOM	3105	O	ARG	H	30	-10.426	15.442	-26.641	1.00	14.72	H
ATOM	3106	N	HIS	H	31	-11.522	14.170	-28.134	1.00	13.78	H

ATOM	3107	CA	HIS	H	31	-11.580	13.006	-27.263	1.00	13.18	H
ATOM	3108	CB	HIS	H	31	-12.850	12.186	-27.530	1.00	14.12	H
ATOM	3109	CG	HIS	H	31	-14.089	12.735	-26.899	1.00	14.52	H
ATOM	3110	CD2	HIS	H	31	-14.314	13.900	-26.247	1.00	14.13	H
ATOM	3111	ND1	HIS	H	31	-15.279	12.046	-26.883	1.00	13.70	H
ATOM	3112	CE1	HIS	H	31	-16.190	12.761	-26.244	1.00	15.24	H
ATOM	3113	NE2	HIS	H	31	-15.628	13.888	-25.850	1.00	14.50	H
ATOM	3114	C	HIS	H	31	-10.408	12.073	-27.426	1.00	12.58	H
ATOM	3115	O	HIS	H	31	-10.392	10.995	-26.834	1.00	14.16	H
ATOM	3116	N	HIS	H	32	-9.434	12.467	-28.229	1.00	12.49	H
ATOM	3117	CA	HIS	H	32	-8.304	11.585	-28.478	1.00	12.89	H
ATOM	3118	CB	HIS	H	32	-8.545	10.851	-29.808	1.00	13.05	H
ATOM	3119	CG	HIS	H	32	-9.697	9.889	-29.761	1.00	12.70	H
ATOM	3120	CD2	HIS	H	32	-10.988	10.023	-30.149	1.00	12.40	H
ATOM	3121	ND1	HIS	H	32	-9.592	8.631	-29.209	1.00	12.19	H
ATOM	3122	CE1	HIS	H	32	-10.768	8.029	-29.258	1.00	13.35	H
ATOM	3123	NE2	HIS	H	32	-11.633	8.852	-29.822	1.00	12.35	H
ATOM	3124	C	HIS	H	32	-6.976	12.326	-28.504	1.00	12.49	H
ATOM	3125	O	HIS	H	32	-6.920	13.476	-28.918	1.00	14.67	H
ATOM	3126	N	GLY	H	33	-5.914	11.687	-28.026	1.00	11.48	H
ATOM	3127	CA	GLY	H	33	-4.611	12.327	-28.063	1.00	10.32	H
ATOM	3128	C	GLY	H	33	-4.052	12.137	-29.461	1.00	8.82	H
ATOM	3129	O	GLY	H	33	-4.339	11.127	-30.101	1.00	10.42	H
ATOM	3130	N	MET	H	34	-3.276	13.086	-29.965	1.00	7.85	H
ATOM	3131	CA	MET	H	34	-2.721	12.935	-31.320	1.00	6.64	H
ATOM	3132	CB	MET	H	34	-3.173	14.090	-32.218	1.00	4.40	H
ATOM	3133	CG	MET	H	34	-4.710	14.204	-32.374	1.00	4.44	H
ATOM	3134	SD	MET	H	34	-5.426	12.756	-33.283	1.00	3.13	H
ATOM	3135	CE	MET	H	34	-4.669	12.931	-34.869	1.00	3.16	H
ATOM	3136	C	MET	H	34	-1.201	12.896	-31.281	1.00	6.08	H
ATOM	3137	O	MET	H	34	-0.575	13.439	-30.381	1.00	5.25	H
ATOM	3138	N	THR	H	35	-0.607	12.267	-32.274	1.00	6.01	H
ATOM	3139	CA	THR	H	35	0.828	12.175	-32.290	1.00	7.01	H
ATOM	3140	CB	THR	H	35	1.292	10.851	-31.608	1.00	9.35	H
ATOM	3141	OG1	THR	H	35	2.719	10.707	-31.709	1.00	10.60	H
ATOM	3142	CG2	THR	H	35	0.633	9.661	-32.289	1.00	10.35	H
ATOM	3143	C	THR	H	35	1.383	12.231	-33.710	1.00	5.93	H
ATOM	3144	O	THR	H	35	0.672	11.965	-34.690	1.00	4.87	H
ATOM	3145	N	TRP	H	36	2.659	12.591	-33.812	1.00	5.33	H
ATOM	3146	CA	TRP	H	36	3.335	12.655	-35.097	1.00	3.82	H
ATOM	3147	CB	TRP	H	36	4.005	14.005	-35.327	1.00	1.93	H
ATOM	3148	CG	TRP	H	36	3.059	15.064	-35.776	1.00	3.01	H
ATOM	3149	CD2	TRP	H	36	2.500	15.209	-37.090	1.00	2.59	H
ATOM	3150	CE2	TRP	H	36	1.656	16.338	-37.063	1.00	1.00	H
ATOM	3151	CE3	TRP	H	36	2.632	14.491	-38.285	1.00	2.19	H
ATOM	3152	CD1	TRP	H	36	2.540	16.079	-35.029	1.00	1.86	H
ATOM	3153	NE1	TRP	H	36	1.699	16.849	-35.796	1.00	1.16	H
ATOM	3154	CZ2	TRP	H	36	0.953	16.773	-38.178	1.00	1.00	H
ATOM	3155	CZ3	TRP	H	36	1.930	14.923	-39.395	1.00	1.00	H
ATOM	3156	CH2	TRP	H	36	1.100	16.057	-39.334	1.00	1.00	H
ATOM	3157	C	TRP	H	36	4.406	11.617	-35.091	1.00	3.68	H
ATOM	3158	O	TRP	H	36	5.195	11.544	-34.152	1.00	4.93	H
ATOM	3159	N	VAL	H	37	4.429	10.803	-36.130	1.00	3.07	H
ATOM	3160	CA	VAL	H	37	5.465	9.794	-36.254	1.00	4.69	H
ATOM	3161	CB	VAL	H	37	4.895	8.340	-36.114	1.00	5.17	H
ATOM	3162	CG1	VAL	H	37	5.994	7.335	-36.345	1.00	4.96	H
ATOM	3163	CG2	VAL	H	37	4.315	8.126	-34.732	1.00	4.23	H
ATOM	3164	C	VAL	H	37	6.075	10.005	-37.645	1.00	4.66	H
ATOM	3165	O	VAL	H	37	5.371	10.340	-38.593	1.00	5.19	H
ATOM	3166	N	ARG	H	38	7.383	9.846	-37.776	1.00	5.35	H
ATOM	3167	CA	ARG	H	38	8.000	10.039	-39.082	1.00	5.57	H

ATOM	3168	CB	ARG	H	38	8.897	11.272	-39.068	1.00	7.67	H
ATOM	3169	CG	ARG	H	38	10.129	11.136	-38.196	1.00	6.25	H
ATOM	3170	CD	ARG	H	38	10.940	12.385	-38.305	1.00	6.36	H
ATOM	3171	NE	ARG	H	38	12.058	12.368	-37.388	1.00	9.42	H
ATOM	3172	CZ	ARG	H	38	12.969	13.319	-37.330	1.00	8.80	H
ATOM	3173	NH1	ARG	H	38	12.879	14.351	-38.151	1.00	9.68	H
ATOM	3174	NH2	ARG	H	38	13.947	13.249	-36.439	1.00	9.99	H
ATOM	3175	C	ARG	H	38	8.822	8.842	-39.497	1.00	4.93	H
ATOM	3176	O	ARG	H	38	9.135	7.964	-38.693	1.00	4.06	H
ATOM	3177	N	GLN	H	39	9.203	8.840	-40.759	1.00	5.54	H
ATOM	3178	CA	GLN	H	39	9.986	7.751	-41.295	1.00	7.45	H
ATOM	3179	CB	GLN	H	39	9.056	6.716	-41.914	1.00	6.58	H
ATOM	3180	CG	GLN	H	39	9.751	5.495	-42.440	1.00	6.23	H
ATOM	3181	CD	GLN	H	39	8.780	4.490	-42.991	1.00	7.57	H
ATOM	3182	OE1	GLN	H	39	8.002	4.790	-43.895	1.00	9.72	H
ATOM	3183	NE2	GLN	H	39	8.809	3.288	-42.446	1.00	7.92	H
ATOM	3184	C	GLN	H	39	10.949	8.280	-42.342	1.00	8.66	H
ATOM	3185	O	GLN	H	39	10.532	8.690	-43.433	1.00	9.98	H
ATOM	3186	N	ALA	H	40	12.237	8.275	-42.001	1.00	10.55	H
ATOM	3187	CA	ALA	H	40	13.281	8.761	-42.901	1.00	11.32	H
ATOM	3188	CB	ALA	H	40	14.598	8.882	-42.161	1.00	9.49	H
ATOM	3189	C	ALA	H	40	13.412	7.792	-44.062	1.00	12.45	H
ATOM	3190	O	ALA	H	40	13.185	6.595	-43.904	1.00	12.06	H
ATOM	3191	N	PRO	H	41	13.774	8.298	-45.250	1.00	14.18	H
ATOM	3192	CD	PRO	H	41	14.084	9.704	-45.562	1.00	13.94	H
ATOM	3193	CA	PRO	H	41	13.926	7.458	-46.440	1.00	14.90	H
ATOM	3194	CB	PRO	H	41	14.757	8.333	-47.364	1.00	13.64	H
ATOM	3195	CG	PRO	H	41	14.172	9.691	-47.081	1.00	13.81	H
ATOM	3196	C	PRO	H	41	14.565	6.108	-46.165	1.00	16.86	H
ATOM	3197	O	PRO	H	41	15.683	6.018	-45.644	1.00	16.32	H
ATOM	3198	N	GLY	H	42	13.830	5.053	-46.508	1.00	18.46	H
ATOM	3199	CA	GLY	H	42	14.317	3.699	-46.294	1.00	19.28	H
ATOM	3200	C	GLY	H	42	14.764	3.427	-44.863	1.00	20.26	H
ATOM	3201	O	GLY	H	42	15.795	2.798	-44.637	1.00	21.03	H
ATOM	3202	N	LYS	H	43	14.000	3.899	-43.884	1.00	20.62	H
ATOM	3203	CA	LYS	H	43	14.351	3.665	-42.487	1.00	19.70	H
ATOM	3204	CB	LYS	H	43	14.981	4.923	-41.890	1.00	20.93	H
ATOM	3205	CG	LYS	H	43	16.185	5.411	-42.686	1.00	22.44	H
ATOM	3206	CD	LYS	H	43	17.345	4.434	-42.632	1.00	23.53	H
ATOM	3207	CE	LYS	H	43	17.977	4.468	-41.247	1.00	27.18	H
ATOM	3208	NZ	LYS	H	43	19.111	3.504	-41.050	1.00	28.98	H
ATOM	3209	C	LYS	H	43	13.071	3.280	-41.758	1.00	17.81	H
ATOM	3210	O	LYS	H	43	11.991	3.297	-42.361	1.00	17.97	H
ATOM	3211	N	GLY	H	44	13.189	2.923	-40.483	1.00	15.15	H
ATOM	3212	CA	GLY	H	44	12.023	2.520	-39.718	1.00	13.55	H
ATOM	3213	C	GLY	H	44	11.220	3.666	-39.138	1.00	12.70	H
ATOM	3214	O	GLY	H	44	11.564	4.831	-39.331	1.00	13.60	H
ATOM	3215	N	LEU	H	45	10.150	3.342	-38.418	1.00	10.34	H
ATOM	3216	CA	LEU	H	45	9.312	4.371	-37.823	1.00	8.11	H
ATOM	3217	CB	LEU	H	45	8.006	3.765	-37.319	1.00	6.67	H
ATOM	3218	CG	LEU	H	45	7.016	3.285	-38.384	1.00	6.00	H
ATOM	3219	CD1	LEU	H	45	5.807	2.634	-37.700	1.00	6.82	H
ATOM	3220	CD2	LEU	H	45	6.567	4.447	-39.220	1.00	4.53	H
ATOM	3221	C	LEU	H	45	10.010	5.088	-36.680	1.00	8.20	H
ATOM	3222	O	LEU	H	45	10.840	4.514	-35.975	1.00	8.35	H
ATOM	3223	N	GLU	H	46	9.683	6.361	-36.516	1.00	6.89	H
ATOM	3224	CA	GLU	H	46	10.261	7.134	-35.440	1.00	5.45	H
ATOM	3225	CB	GLU	H	46	11.459	7.906	-35.946	1.00	6.53	H
ATOM	3226	CG	GLU	H	46	12.370	8.384	-34.853	1.00	8.96	H
ATOM	3227	CD	GLU	H	46	13.090	9.655	-35.223	1.00	11.41	H
ATOM	3228	OE1	GLU	H	46	13.534	9.759	-36.407	1.00	7.77	H

ATOM	3229	OE2	GLU	H	46	13.211	10.539	-34.320	1.00	13.45	H
ATOM	3230	C	GLU	H	46	9.241	8.109	-34.864	1.00	5.60	H
ATOM	3231	O	GLU	H	46	8.712	8.967	-35.575	1.00	6.68	H
ATOM	3232	N	TRP	H	47	8.978	7.981	-33.571	1.00	4.36	H
ATOM	3233	CA	TRP	H	47	8.028	8.841	-32.886	1.00	3.67	H
ATOM	3234	CB	TRP	H	47	7.788	8.320	-31.481	1.00	4.95	H
ATOM	3235	CG	TRP	H	47	6.989	9.246	-30.659	1.00	4.60	H
ATOM	3236	CD2	TRP	H	47	7.482	10.057	-29.587	1.00	4.44	H
ATOM	3237	CE2	TRP	H	47	6.387	10.818	-29.102	1.00	4.11	H
ATOM	3238	CE3	TRP	H	47	8.748	10.217	-28.989	1.00	2.69	H
ATOM	3239	CD1	TRP	H	47	5.649	9.529	-30.784	1.00	3.52	H
ATOM	3240	NE1	TRP	H	47	5.285	10.475	-29.846	1.00	5.11	H
ATOM	3241	CZ2	TRP	H	47	6.520	11.730	-28.042	1.00	1.81	H
ATOM	3242	CZ3	TRP	H	47	8.883	11.122	-27.938	1.00	1.00	H
ATOM	3243	CH2	TRP	H	47	7.770	11.869	-27.475	1.00	1.00	H
ATOM	3244	C	TRP	H	47	8.579	10.237	-32.816	1.00	2.64	H
ATOM	3245	O	TRP	H	47	9.745	10.425	-32.486	1.00	5.55	H
ATOM	3246	N	VAL	H	48	7.744	11.227	-33.084	1.00	2.44	H
ATOM	3247	CA	VAL	H	48	8.222	12.605	-33.075	1.00	1.81	H
ATOM	3248	CB	VAL	H	48	7.825	13.292	-34.408	1.00	1.31	H
ATOM	3249	CG1	VAL	H	48	8.401	14.689	-34.498	1.00	1.00	H
ATOM	3250	CG2	VAL	H	48	8.286	12.444	-35.562	1.00	1.00	H
ATOM	3251	C	VAL	H	48	7.708	13.413	-31.883	1.00	3.22	H
ATOM	3252	O	VAL	H	48	8.488	13.833	-31.032	1.00	2.46	H
ATOM	3253	N	ALA	H	49	6.398	13.621	-31.823	1.00	3.27	H
ATOM	3254	CA	ALA	H	49	5.802	14.384	-30.745	1.00	4.78	H
ATOM	3255	CB	ALA	H	49	5.819	15.866	-31.110	1.00	3.76	H
ATOM	3256	C	ALA	H	49	4.356	13.912	-30.505	1.00	5.83	H
ATOM	3257	O	ALA	H	49	3.700	13.365	-31.406	1.00	4.82	H
ATOM	3258	N	SER	H	50	3.874	14.135	-29.285	1.00	4.82	H
ATOM	3259	CA	SER	H	50	2.526	13.768	-28.922	1.00	4.97	H
ATOM	3260	CB	SER	H	50	2.516	12.512	-28.059	1.00	5.14	H
ATOM	3261	OG	SER	H	50	2.568	11.365	-28.878	1.00	6.92	H
ATOM	3262	C	SER	H	50	1.815	14.898	-28.220	1.00	5.98	H
ATOM	3263	O	SER	H	50	2.435	15.801	-27.670	1.00	5.57	H
ATOM	3264	N	LEU	H	51	0.495	14.816	-28.224	1.00	7.39	H
ATOM	3265	CA	LEU	H	51	-0.340	15.847	-27.652	1.00	8.22	H
ATOM	3266	CB	LEU	H	51	-0.651	16.828	-28.769	1.00	9.05	H
ATOM	3267	CG	LEU	H	51	-1.506	18.005	-28.376	1.00	10.34	H
ATOM	3268	CD1	LEU	H	51	-0.678	18.875	-27.452	1.00	11.80	H
ATOM	3269	CD2	LEU	H	51	-1.934	18.776	-29.592	1.00	10.62	H
ATOM	3270	C	LEU	H	51	-1.646	15.252	-27.116	1.00	9.09	H
ATOM	3271	O	LEU	H	51	-2.244	14.386	-27.757	1.00	11.36	H
ATOM	3272	N	SER	H	52	-2.112	15.730	-25.970	1.00	7.37	H
ATOM	3273	CA	SER	H	52	-3.364	15.220	-25.428	1.00	7.34	H
ATOM	3274	CB	SER	H	52	-3.453	15.487	-23.920	1.00	6.67	H
ATOM	3275	OG	SER	H	52	-3.234	16.851	-23.580	1.00	6.96	H
ATOM	3276	C	SER	H	52	-4.573	15.823	-26.142	1.00	8.92	H
ATOM	3277	O	SER	H	52	-4.423	16.691	-27.009	1.00	9.13	H
ATOM	3278	N	GLY	H	53	-5.769	15.369	-25.764	1.00	8.62	H
ATOM	3279	CA	GLY	H	53	-6.986	15.856	-26.388	1.00	6.90	H
ATOM	3280	C	GLY	H	53	-7.165	17.339	-26.198	1.00	5.00	H
ATOM	3281	O	GLY	H	53	-7.542	18.062	-27.120	1.00	4.67	H
ATOM	3282	N	SER	H	54	-6.900	17.800	-24.990	1.00	4.14	H
ATOM	3283	CA	SER	H	54	-7.025	19.224	-24.690	1.00	6.17	H
ATOM	3284	CB	SER	H	54	-7.028	19.434	-23.173	1.00	6.62	H
ATOM	3285	OG	SER	H	54	-5.841	18.929	-22.561	1.00	4.64	H
ATOM	3286	C	SER	H	54	-5.842	19.957	-25.320	1.00	7.53	H
ATOM	3287	O	SER	H	54	-5.965	21.101	-25.751	1.00	6.08	H
ATOM	3288	N	GLY	H	55	-4.697	19.277	-25.368	1.00	8.59	H
ATOM	3289	CA	GLY	H	55	-3.516	19.868	-25.956	1.00	9.92	H

ATOM	3290	C	GLY	H	55	-2.648	20.537	-24.916	1.00	10.79	H
ATOM	3291	O	GLY	H	55	-1.634	21.174	-25.232	1.00	8.31	H
ATOM	3292	N	THR	H	56	-3.050	20.398	-23.659	1.00	12.24	H
ATOM	3293	CA	THR	H	56	-2.303	20.999	-22.558	1.00	12.50	H
ATOM	3294	CB	THR	H	56	-3.195	21.164	-21.302	1.00	11.85	H
ATOM	3295	OG1	THR	H	56	-3.497	19.879	-20.739	1.00	11.11	H
ATOM	3296	CG2	THR	H	56	-4.483	21.866	-21.670	1.00	11.04	H
ATOM	3297	C	THR	H	56	-1.089	20.152	-22.191	1.00	11.96	H
ATOM	3298	O	THR	H	56	-0.203	20.601	-21.466	1.00	11.88	H
ATOM	3299	N	LYS	H	57	-1.052	18.924	-22.695	1.00	11.02	H
ATOM	3300	CA	LYS	H	57	0.062	18.047	-22.407	1.00	9.97	H
ATOM	3301	CB	LYS	H	57	-0.400	16.818	-21.626	1.00	8.17	H
ATOM	3302	CG	LYS	H	57	-1.011	17.145	-20.277	1.00	9.71	H
ATOM	3303	CD	LYS	H	57	-1.297	15.893	-19.467	1.00	10.00	H
ATOM	3304	CE	LYS	H	57	-2.760	15.785	-19.084	1.00	11.05	H
ATOM	3305	NZ	LYS	H	57	-3.188	16.841	-18.138	1.00	12.83	H
ATOM	3306	C	LYS	H	57	0.698	17.628	-23.707	1.00	9.96	H
ATOM	3307	O	LYS	H	57	0.085	16.933	-24.507	1.00	11.40	H
ATOM	3308	N	THR	H	58	1.930	18.069	-23.929	1.00	9.40	H
ATOM	3309	CA	THR	H	58	2.626	17.714	-25.154	1.00	8.99	H
ATOM	3310	CB	THR	H	58	2.922	18.939	-26.023	1.00	8.49	H
ATOM	3311	OG1	THR	H	58	4.147	19.530	-25.596	1.00	9.58	H
ATOM	3312	CG2	THR	H	58	1.826	19.960	-25.889	1.00	6.38	H
ATOM	3313	C	THR	H	58	3.938	17.060	-24.777	1.00	9.30	H
ATOM	3314	O	THR	H	58	4.415	17.236	-23.663	1.00	8.22	H
ATOM	3315	N	HIS	H	59	4.508	16.305	-25.717	1.00	9.24	H
ATOM	3316	CA	HIS	H	59	5.769	15.595	-25.519	1.00	8.03	H
ATOM	3317	CB	HIS	H	59	5.499	14.189	-24.981	1.00	11.10	H
ATOM	3318	CG	HIS	H	59	5.068	14.158	-23.547	1.00	14.76	H
ATOM	3319	CD2	HIS	H	59	3.838	14.042	-22.991	1.00	16.75	H
ATOM	3320	ND1	HIS	H	59	5.960	14.219	-22.500	1.00	15.55	H
ATOM	3321	CE1	HIS	H	59	5.300	14.135	-21.355	1.00	16.99	H
ATOM	3322	NE2	HIS	H	59	4.012	14.026	-21.626	1.00	16.44	H
ATOM	3323	C	HIS	H	59	6.534	15.505	-26.841	1.00	6.73	H
ATOM	3324	O	HIS	H	59	5.947	15.238	-27.892	1.00	4.86	H
ATOM	3325	N	PHE	H	60	7.844	15.735	-26.776	1.00	6.24	H
ATOM	3326	CA	PHE	H	60	8.691	15.707	-27.963	1.00	6.73	H
ATOM	3327	CB	PHE	H	60	9.258	17.098	-28.259	1.00	6.25	H
ATOM	3328	CG	PHE	H	60	8.223	18.165	-28.368	1.00	8.88	H
ATOM	3329	CD1	PHE	H	60	7.732	18.795	-27.226	1.00	10.51	H
ATOM	3330	CD2	PHE	H	60	7.700	18.516	-29.604	1.00	10.03	H
ATOM	3331	CE1	PHE	H	60	6.724	19.760	-27.311	1.00	9.17	H
ATOM	3332	CE2	PHE	H	60	6.697	19.474	-29.701	1.00	10.91	H
ATOM	3333	CZ	PHE	H	60	6.207	20.099	-28.543	1.00	11.27	H
ATOM	3334	C	PHE	H	60	9.851	14.743	-27.810	1.00	6.57	H
ATOM	3335	O	PHE	H	60	10.119	14.263	-26.720	1.00	6.46	H
ATOM	3336	N	ALA	H	61	10.524	14.469	-28.922	1.00	8.14	H
ATOM	3337	CA	ALA	H	61	11.684	13.589	-28.956	1.00	10.25	H
ATOM	3338	CB	ALA	H	61	11.711	12.818	-30.262	1.00	9.23	H
ATOM	3339	C	ALA	H	61	12.891	14.521	-28.863	1.00	11.89	H
ATOM	3340	O	ALA	H	61	12.857	15.623	-29.413	1.00	13.75	H
ATOM	3341	N	ASP	H	62	13.953	14.094	-28.188	1.00	13.51	H
ATOM	3342	CA	ASP	H	62	15.124	14.953	-28.047	1.00	15.64	H
ATOM	3343	CB	ASP	H	62	16.236	14.230	-27.277	1.00	18.66	H
ATOM	3344	CG	ASP	H	62	16.077	14.365	-25.771	1.00	23.55	H
ATOM	3345	OD1	ASP	H	62	16.797	13.650	-25.022	1.00	26.30	H
ATOM	3346	OD2	ASP	H	62	15.234	15.197	-25.333	1.00	25.44	H
ATOM	3347	C	ASP	H	62	15.657	15.493	-29.364	1.00	14.78	H
ATOM	3348	O	ASP	H	62	15.992	16.672	-29.464	1.00	16.08	H
ATOM	3349	N	SER	H	63	15.706	14.648	-30.379	1.00	13.12	H
ATOM	3350	CA	SER	H	63	16.222	15.072	-31.667	1.00	13.50	H

ATOM	3351	CB	SER	H	63	16.283	13.885	-32.615	1.00	14.56	H
ATOM	3352	OG	SER	H	63	14.980	13.365	-32.822	1.00	18.30	H
ATOM	3353	C	SER	H	63	15.397	16.165	-32.326	1.00	13.14	H
ATOM	3354	O	SER	H	63	15.734	16.635	-33.411	1.00	12.97	H
ATOM	3355	N	VAL	H	64	14.325	16.594	-31.686	1.00	12.76	H
ATOM	3356	CA	VAL	H	64	13.498	17.595	-32.324	1.00	13.21	H
ATOM	3357	CB	VAL	H	64	12.316	16.857	-33.044	1.00	12.72	H
ATOM	3358	CG1	VAL	H	64	10.991	17.103	-32.335	1.00	13.63	H
ATOM	3359	CG2	VAL	H	64	12.269	17.237	-34.479	1.00	10.90	H
ATOM	3360	C	VAL	H	64	13.021	18.673	-31.340	1.00	13.76	H
ATOM	3361	O	VAL	H	64	12.543	19.749	-31.732	1.00	11.87	H
ATOM	3362	N	LYS	H	65	13.172	18.384	-30.052	1.00	16.05	H
ATOM	3363	CA	LYS	H	65	12.772	19.323	-29.013	1.00	17.75	H
ATOM	3364	CB	LYS	H	65	13.103	18.787	-27.617	1.00	20.48	H
ATOM	3365	CG	LYS	H	65	12.768	19.806	-26.531	1.00	24.24	H
ATOM	3366	CD	LYS	H	65	12.539	19.177	-25.177	1.00	26.75	H
ATOM	3367	CE	LYS	H	65	12.065	20.228	-24.186	1.00	29.20	H
ATOM	3368	NZ	LYS	H	65	11.806	19.649	-22.835	1.00	30.30	H
ATOM	3369	C	LYS	H	65	13.467	20.654	-29.196	1.00	16.93	H
ATOM	3370	O	LYS	H	65	14.672	20.707	-29.452	1.00	17.42	H
ATOM	3371	N	GLY	H	66	12.701	21.725	-29.040	1.00	15.98	H
ATOM	3372	CA	GLY	H	66	13.255	23.047	-29.210	1.00	15.03	H
ATOM	3373	C	GLY	H	66	13.106	23.481	-30.652	1.00	15.31	H
ATOM	3374	O	GLY	H	66	13.118	24.669	-30.945	1.00	17.76	H
ATOM	3375	N	ARG	H	67	12.972	22.540	-31.574	1.00	12.33	H
ATOM	3376	CA	ARG	H	67	12.823	22.955	-32.950	1.00	11.57	H
ATOM	3377	CB	ARG	H	67	13.784	22.198	-33.856	1.00	11.70	H
ATOM	3378	CG	ARG	H	67	15.254	22.497	-33.600	1.00	9.21	H
ATOM	3379	CD	ARG	H	67	16.113	21.818	-34.641	1.00	6.92	H
ATOM	3380	NE	ARG	H	67	15.869	20.379	-34.681	1.00	6.37	H
ATOM	3381	CZ	ARG	H	67	15.526	19.713	-35.778	1.00	7.25	H
ATOM	3382	NH1	ARG	H	67	15.386	20.350	-36.934	1.00	9.14	H
ATOM	3383	NH2	ARG	H	67	15.300	18.413	-35.719	1.00	6.47	H
ATOM	3384	C	ARG	H	67	11.402	22.732	-33.415	1.00	12.38	H
ATOM	3385	O	ARG	H	67	10.849	23.543	-34.143	1.00	13.55	H
ATOM	3386	N	PHE	H	68	10.804	21.632	-32.983	1.00	12.18	H
ATOM	3387	CA	PHE	H	68	9.448	21.319	-33.381	1.00	11.31	H
ATOM	3388	CB	PHE	H	68	9.351	19.850	-33.769	1.00	11.86	H
ATOM	3389	CG	PHE	H	68	9.971	19.516	-35.099	1.00	12.06	H
ATOM	3390	CD1	PHE	H	68	10.973	20.313	-35.653	1.00	11.71	H
ATOM	3391	CD2	PHE	H	68	9.583	18.351	-35.776	1.00	11.05	H
ATOM	3392	CE1	PHE	H	68	11.584	19.953	-36.859	1.00	11.42	H
ATOM	3393	CE2	PHE	H	68	10.186	17.981	-36.980	1.00	9.57	H
ATOM	3394	CZ	PHE	H	68	11.188	18.779	-37.527	1.00	9.82	H
ATOM	3395	C	PHE	H	68	8.436	21.611	-32.291	1.00	12.02	H
ATOM	3396	O	PHE	H	68	8.684	21.376	-31.110	1.00	12.67	H
ATOM	3397	N	THR	H	69	7.283	22.127	-32.693	1.00	11.69	H
ATOM	3398	CA	THR	H	69	6.233	22.416	-31.735	1.00	10.64	H
ATOM	3399	CB	THR	H	69	6.103	23.948	-31.456	1.00	10.59	H
ATOM	3400	OG1	THR	H	69	4.719	24.297	-31.351	1.00	14.40	H
ATOM	3401	CG2	THR	H	69	6.737	24.771	-32.569	1.00	11.79	H
ATOM	3402	C	THR	H	69	4.910	21.841	-32.244	1.00	9.62	H
ATOM	3403	O	THR	H	69	4.450	22.170	-33.337	1.00	9.39	H
ATOM	3404	N	ILE	H	70	4.316	20.962	-31.440	1.00	7.95	H
ATOM	3405	CA	ILE	H	70	3.044	20.325	-31.773	1.00	6.64	H
ATOM	3406	CB	ILE	H	70	2.937	18.914	-31.124	1.00	5.97	H
ATOM	3407	CG2	ILE	H	70	2.930	19.046	-29.621	1.00	3.75	H
ATOM	3408	CG1	ILE	H	70	1.667	18.200	-31.605	1.00	5.93	H
ATOM	3409	CD1	ILE	H	70	1.677	16.710	-31.399	1.00	5.04	H
ATOM	3410	C	ILE	H	70	1.897	21.189	-31.254	1.00	5.92	H
ATOM	3411	O	ILE	H	70	2.041	21.831	-30.219	1.00	7.78	H

ATOM	3412	N	SER	H	71	0.775	21.205	-31.970	1.00	4.08	H
ATOM	3413	CA	SER	H	71	-0.408	21.972	-31.570	1.00	3.29	H
ATOM	3414	CB	SER	H	71	-0.267	23.449	-31.943	1.00	1.76	H
ATOM	3415	OG	SER	H	71	0.300	23.593	-33.232	1.00	5.75	H
ATOM	3416	C	SER	H	71	-1.645	21.384	-32.230	1.00	2.94	H
ATOM	3417	O	SER	H	71	-1.545	20.614	-33.185	1.00	1.59	H
ATOM	3418	N	ARG	H	72	-2.812	21.764	-31.728	1.00	3.54	H
ATOM	3419	CA	ARG	H	72	-4.081	21.231	-32.216	1.00	4.48	H
ATOM	3420	CB	ARG	H	72	-4.441	20.016	-31.343	1.00	4.63	H
ATOM	3421	CG	ARG	H	72	-5.849	19.970	-30.810	1.00	5.35	H
ATOM	3422	CD	ARG	H	72	-5.940	19.277	-29.466	1.00	4.98	H
ATOM	3423	NE	ARG	H	72	-5.546	17.865	-29.437	1.00	6.58	H
ATOM	3424	CZ	ARG	H	72	-6.289	16.841	-29.867	1.00	7.67	H
ATOM	3425	NH1	ARG	H	72	-7.484	17.035	-30.386	1.00	7.98	H
ATOM	3426	NH2	ARG	H	72	-5.854	15.598	-29.742	1.00	9.34	H
ATOM	3427	C	ARG	H	72	-5.167	22.289	-32.161	1.00	5.09	H
ATOM	3428	O	ARG	H	72	-5.086	23.194	-31.351	1.00	5.98	H
ATOM	3429	N	ASP	H	73	-6.164	22.196	-33.036	1.00	7.54	H
ATOM	3430	CA	ASP	H	73	-7.261	23.166	-33.032	1.00	10.50	H
ATOM	3431	CB	ASP	H	73	-7.214	24.030	-34.297	1.00	12.67	H
ATOM	3432	CG	ASP	H	73	-8.309	25.111	-34.327	1.00	13.54	H
ATOM	3433	OD1	ASP	H	73	-9.429	24.831	-33.863	1.00	12.69	H
ATOM	3434	OD2	ASP	H	73	-8.049	26.231	-34.832	1.00	14.66	H
ATOM	3435	C	ASP	H	73	-8.613	22.447	-32.957	1.00	11.07	H
ATOM	3436	O	ASP	H	73	-9.191	22.093	-33.983	1.00	11.19	H
ATOM	3437	N	ASN	H	74	-9.122	22.262	-31.748	1.00	11.92	H
ATOM	3438	CA	ASN	H	74	-10.390	21.589	-31.565	1.00	13.93	H
ATOM	3439	CB	ASN	H	74	-10.538	21.139	-30.115	1.00	13.39	H
ATOM	3440	CG	ASN	H	74	-9.502	20.112	-29.727	1.00	15.07	H
ATOM	3441	OD1	ASN	H	74	-9.020	19.368	-30.581	1.00	15.70	H
ATOM	3442	ND2	ASN	H	74	-9.163	20.045	-28.444	1.00	14.48	H
ATOM	3443	C	ASN	H	74	-11.579	22.456	-31.962	1.00	16.05	H
ATOM	3444	O	ASN	H	74	-12.340	22.924	-31.116	1.00	18.94	H
ATOM	3445	N	SER	H	75	-11.727	22.683	-33.257	1.00	16.45	H
ATOM	3446	CA	SER	H	75	-12.820	23.484	-33.786	1.00	16.17	H
ATOM	3447	CB	SER	H	75	-12.491	24.974	-33.745	1.00	17.32	H
ATOM	3448	OG	SER	H	75	-11.878	25.333	-32.521	1.00	20.43	H
ATOM	3449	C	SER	H	75	-12.884	23.070	-35.223	1.00	17.41	H
ATOM	3450	O	SER	H	75	-13.954	22.830	-35.774	1.00	19.91	H
ATOM	3451	N	ASN	H	76	-11.703	22.992	-35.825	1.00	16.64	H
ATOM	3452	CA	ASN	H	76	-11.568	22.611	-37.217	1.00	15.45	H
ATOM	3453	CB	ASN	H	76	-10.637	23.590	-37.947	1.00	17.04	H
ATOM	3454	CG	ASN	H	76	-9.302	23.775	-37.232	1.00	20.41	H
ATOM	3455	OD1	ASN	H	76	-8.938	23.003	-36.336	1.00	21.95	H
ATOM	3456	ND2	ASN	H	76	-8.558	24.796	-37.636	1.00	21.39	H
ATOM	3457	C	ASN	H	76	-11.019	21.196	-37.340	1.00	13.63	H
ATOM	3458	O	ASN	H	76	-10.672	20.771	-38.436	1.00	11.77	H
ATOM	3459	N	ASN	H	77	-10.934	20.479	-36.222	1.00	11.14	H
ATOM	3460	CA	ASN	H	77	-10.419	19.112	-36.239	1.00	11.22	H
ATOM	3461	CB	ASN	H	77	-11.383	18.193	-36.977	1.00	12.73	H
ATOM	3462	CG	ASN	H	77	-12.674	17.980	-36.224	1.00	16.20	H
ATOM	3463	OD1	ASN	H	77	-13.517	17.176	-36.630	1.00	17.08	H
ATOM	3464	ND2	ASN	H	77	-12.840	18.702	-35.109	1.00	18.52	H
ATOM	3465	C	ASN	H	77	-9.064	19.001	-36.919	1.00	11.03	H
ATOM	3466	O	ASN	H	77	-8.846	18.114	-37.748	1.00	10.80	H
ATOM	3467	N	THR	H	78	-8.157	19.900	-36.565	1.00	8.71	H
ATOM	3468	CA	THR	H	78	-6.852	19.919	-37.178	1.00	7.47	H
ATOM	3469	CB	THR	H	78	-6.651	21.223	-37.953	1.00	9.54	H
ATOM	3470	OG1	THR	H	78	-7.779	21.447	-38.801	1.00	11.42	H
ATOM	3471	CG2	THR	H	78	-5.401	21.149	-38.813	1.00	9.06	H
ATOM	3472	C	THR	H	78	-5.704	19.757	-36.208	1.00	7.12	H

ATOM	3473	O	THR	H	78	-5.692	20.332	-35.119	1.00	4.88	H
ATOM	3474	N	LEU	H	79	-4.728	18.959	-36.626	1.00	6.47	H
ATOM	3475	CA	LEU	H	79	-3.548	18.700	-35.823	1.00	6.13	H
ATOM	3476	CB	LEU	H	79	-3.339	17.188	-35.672	1.00	3.73	H
ATOM	3477	CG	LEU	H	79	-2.217	16.691	-34.754	1.00	2.93	H
ATOM	3478	CD1	LEU	H	79	-0.978	16.427	-35.533	1.00	1.00	H
ATOM	3479	CD2	LEU	H	79	-1.970	17.684	-33.647	1.00	2.62	H
ATOM	3480	C	LEU	H	79	-2.385	19.345	-36.562	1.00	6.55	H
ATOM	3481	O	LEU	H	79	-2.199	19.119	-37.743	1.00	6.69	H
ATOM	3482	N	TYR	H	80	-1.621	20.167	-35.863	1.00	6.40	H
ATOM	3483	CA	TYR	H	80	-0.495	20.836	-36.469	1.00	7.17	H
ATOM	3484	CB	TYR	H	80	-0.607	22.341	-36.206	1.00	6.40	H
ATOM	3485	CG	TYR	H	80	-1.840	22.956	-36.818	1.00	7.53	H
ATOM	3486	CD1	TYR	H	80	-1.955	23.089	-38.195	1.00	7.52	H
ATOM	3487	CE1	TYR	H	80	-3.110	23.592	-38.784	1.00	7.14	H
ATOM	3488	CD2	TYR	H	80	-2.920	23.351	-36.028	1.00	7.68	H
ATOM	3489	CE2	TYR	H	80	-4.083	23.855	-36.607	1.00	8.61	H
ATOM	3490	CZ	TYR	H	80	-4.169	23.970	-37.994	1.00	8.93	H
ATOM	3491	OH	TYR	H	80	-5.332	24.446	-38.576	1.00	10.76	H
ATOM	3492	C	TYR	H	80	0.859	20.317	-35.945	1.00	9.01	H
ATOM	3493	O	TYR	H	80	0.945	19.633	-34.909	1.00	7.86	H
ATOM	3494	N	LEU	H	81	1.906	20.667	-36.691	1.00	9.72	H
ATOM	3495	CA	LEU	H	81	3.289	20.356	-36.370	1.00	9.06	H
ATOM	3496	CB	LEU	H	81	3.706	18.993	-36.914	1.00	8.70	H
ATOM	3497	CG	LEU	H	81	5.192	18.669	-36.656	1.00	7.92	H
ATOM	3498	CD1	LEU	H	81	5.449	18.645	-35.145	1.00	7.49	H
ATOM	3499	CD2	LEU	H	81	5.574	17.343	-37.284	1.00	3.90	H
ATOM	3500	C	LEU	H	81	4.127	21.444	-37.021	1.00	10.37	H
ATOM	3501	O	LEU	H	81	4.178	21.552	-38.256	1.00	9.62	H
ATOM	3502	N	GLN	H	82	4.756	22.259	-36.172	1.00	11.89	H
ATOM	3503	CA	GLN	H	82	5.627	23.362	-36.590	1.00	12.40	H
ATOM	3504	CB	GLN	H	82	5.477	24.554	-35.643	1.00	11.73	H
ATOM	3505	CG	GLN	H	82	6.116	25.822	-36.160	1.00	13.56	H
ATOM	3506	CD	GLN	H	82	5.432	26.305	-37.406	1.00	13.55	H
ATOM	3507	OE1	GLN	H	82	4.204	26.380	-37.451	1.00	13.14	H
ATOM	3508	NE2	GLN	H	82	6.214	26.645	-38.426	1.00	12.96	H
ATOM	3509	C	GLN	H	82	7.081	22.901	-36.562	1.00	12.65	H
ATOM	3510	O	GLN	H	82	7.633	22.606	-35.497	1.00	11.89	H
ATOM	3511	N	MET	H	83	7.685	22.850	-37.742	1.00	13.04	H
ATOM	3512	CA	MET	H	83	9.072	22.442	-37.893	1.00	13.26	H
ATOM	3513	CB	MET	H	83	9.203	21.476	-39.076	1.00	13.61	H
ATOM	3514	CG	MET	H	83	8.251	20.267	-39.014	1.00	13.89	H
ATOM	3515	SD	MET	H	83	8.630	18.987	-40.303	1.00	10.43	H
ATOM	3516	CE	MET	H	83	7.431	19.442	-41.574	1.00	10.13	H
ATOM	3517	C	MET	H	83	9.944	23.664	-38.135	1.00	12.74	H
ATOM	3518	O	MET	H	83	9.885	24.244	-39.221	1.00	12.35	H
ATOM	3519	N	ASP	H	84	10.726	24.064	-37.129	1.00	12.16	H
ATOM	3520	CA	ASP	H	84	11.614	25.219	-37.276	1.00	13.74	H
ATOM	3521	CB	ASP	H	84	11.416	26.247	-36.155	1.00	15.64	H
ATOM	3522	CG	ASP	H	84	9.972	26.738	-36.035	1.00	19.86	H
ATOM	3523	OD1	ASP	H	84	9.331	27.059	-37.079	1.00	19.64	H
ATOM	3524	OD2	ASP	H	84	9.480	26.817	-34.875	1.00	22.08	H
ATOM	3525	C	ASP	H	84	13.066	24.762	-37.284	1.00	14.11	H
ATOM	3526	O	ASP	H	84	13.414	23.741	-36.691	1.00	13.48	H
ATOM	3527	N	ASN	H	85	13.907	25.541	-37.956	1.00	14.96	H
ATOM	3528	CA	ASN	H	85	15.328	25.250	-38.101	1.00	14.80	H
ATOM	3529	CB	ASN	H	85	16.078	25.539	-36.798	1.00	16.03	H
ATOM	3530	CG	ASN	H	85	17.589	25.441	-36.957	1.00	17.56	H
ATOM	3531	OD1	ASN	H	85	18.199	26.153	-37.758	1.00	20.22	H
ATOM	3532	ND2	ASN	H	85	18.199	24.552	-36.196	1.00	20.29	H
ATOM	3533	C	ASN	H	85	15.508	23.795	-38.510	1.00	14.22	H

ATOM	3534	O	ASN	H	85	16.154	23.012	-37.800	1.00	15.62	H
ATOM	3535	N	VAL	H	86	14.941	23.442	-39.666	1.00	12.38	H
ATOM	3536	CA	VAL	H	86	15.013	22.073	-40.172	1.00	10.44	H
ATOM	3537	CB	VAL	H	86	14.026	21.831	-41.351	1.00	8.45	H
ATOM	3538	CG1	VAL	H	86	12.606	22.045	-40.891	1.00	3.18	H
ATOM	3539	CG2	VAL	H	86	14.357	22.741	-42.521	1.00	8.04	H
ATOM	3540	C	VAL	H	86	16.388	21.635	-40.632	1.00	10.36	H
ATOM	3541	O	VAL	H	86	17.037	22.310	-41.426	1.00	10.28	H
ATOM	3542	N	ARG	H	87	16.819	20.493	-40.116	1.00	11.49	H
ATOM	3543	CA	ARG	H	87	18.094	19.917	-40.487	1.00	13.66	H
ATOM	3544	CB	ARG	H	87	18.714	19.147	-39.319	1.00	14.95	H
ATOM	3545	CG	ARG	H	87	18.626	19.789	-37.937	1.00	17.51	H
ATOM	3546	CD	ARG	H	87	19.444	18.934	-36.976	1.00	19.96	H
ATOM	3547	NE	ARG	H	87	19.129	19.055	-35.552	1.00	22.00	H
ATOM	3548	CZ	ARG	H	87	19.207	20.173	-34.840	1.00	24.13	H
ATOM	3549	NH1	ARG	H	87	19.579	21.315	-35.415	1.00	26.64	H
ATOM	3550	NH2	ARG	H	87	18.951	20.135	-33.537	1.00	23.82	H
ATOM	3551	C	ARG	H	87	17.815	18.929	-41.619	1.00	15.16	H
ATOM	3552	O	ARG	H	87	16.659	18.641	-41.938	1.00	15.01	H
ATOM	3553	N	ASP	H	88	18.881	18.392	-42.201	1.00	17.98	H
ATOM	3554	CA	ASP	H	88	18.781	17.421	-43.289	1.00	20.08	H
ATOM	3555	CB	ASP	H	88	20.197	17.139	-43.812	1.00	23.69	H
ATOM	3556	CG	ASP	H	88	21.061	18.413	-43.875	1.00	29.04	H
ATOM	3557	OD1	ASP	H	88	20.911	19.212	-44.842	1.00	30.25	H
ATOM	3558	OD2	ASP	H	88	21.887	18.620	-42.944	1.00	31.49	H
ATOM	3559	C	ASP	H	88	18.110	16.141	-42.770	1.00	19.34	H
ATOM	3560	O	ASP	H	88	17.316	15.507	-43.471	1.00	17.14	H
ATOM	3561	N	GLU	H	89	18.435	15.802	-41.524	1.00	20.05	H
ATOM	3562	CA	GLU	H	89	17.928	14.626	-40.835	1.00	20.41	H
ATOM	3563	CB	GLU	H	89	18.623	14.491	-39.484	1.00	23.61	H
ATOM	3564	CG	GLU	H	89	20.141	14.591	-39.567	1.00	30.26	H
ATOM	3565	CD	GLU	H	89	20.637	16.031	-39.604	1.00	33.35	H
ATOM	3566	OE1	GLU	H	89	20.360	16.764	-38.625	1.00	36.26	H
ATOM	3567	OE2	GLU	H	89	21.304	16.423	-40.595	1.00	34.20	H
ATOM	3568	C	GLU	H	89	16.415	14.647	-40.636	1.00	18.53	H
ATOM	3569	O	GLU	H	89	15.821	13.677	-40.171	1.00	18.64	H
ATOM	3570	N	ASP	H	90	15.783	15.757	-40.968	1.00	16.04	H
ATOM	3571	CA	ASP	H	90	14.350	15.813	-40.832	1.00	13.47	H
ATOM	3572	CB	ASP	H	90	13.901	17.237	-40.509	1.00	13.36	H
ATOM	3573	CG	ASP	H	90	14.319	17.678	-39.111	1.00	13.47	H
ATOM	3574	OD1	ASP	H	90	14.207	16.875	-38.153	1.00	12.70	H
ATOM	3575	OD2	ASP	H	90	14.747	18.841	-38.960	1.00	13.27	H
ATOM	3576	C	ASP	H	90	13.639	15.296	-42.083	1.00	11.74	H
ATOM	3577	O	ASP	H	90	12.421	15.162	-42.082	1.00	11.55	H
ATOM	3578	N	THR	H	91	14.379	15.000	-43.150	1.00	10.83	H
ATOM	3579	CA	THR	H	91	13.739	14.477	-44.359	1.00	9.48	H
ATOM	3580	CB	THR	H	91	14.758	14.316	-45.534	1.00	7.81	H
ATOM	3581	OG1	THR	H	91	15.200	15.615	-45.947	1.00	7.57	H
ATOM	3582	CG2	THR	H	91	14.111	13.659	-46.748	1.00	6.29	H
ATOM	3583	C	THR	H	91	13.084	13.138	-44.019	1.00	8.73	H
ATOM	3584	O	THR	H	91	13.738	12.204	-43.531	1.00	8.19	H
ATOM	3585	N	ALA	H	92	11.776	13.068	-44.241	1.00	8.36	H
ATOM	3586	CA	ALA	H	92	11.017	11.852	-43.951	1.00	8.03	H
ATOM	3587	CB	ALA	H	92	11.149	11.491	-42.471	1.00	6.60	H
ATOM	3588	C	ALA	H	92	9.548	12.009	-44.290	1.00	6.21	H
ATOM	3589	O	ALA	H	92	9.092	13.092	-44.669	1.00	3.46	H
ATOM	3590	N	ILE	H	93	8.823	10.905	-44.157	1.00	6.09	H
ATOM	3591	CA	ILE	H	93	7.399	10.905	-44.390	1.00	6.84	H
ATOM	3592	CB	ILE	H	93	6.920	9.571	-44.932	1.00	6.37	H
ATOM	3593	CG2	ILE	H	93	5.416	9.615	-45.139	1.00	6.16	H
ATOM	3594	CG1	ILE	H	93	7.606	9.289	-46.259	1.00	7.33	H

ATOM	3595	CD1	ILE	H	93	7.328	7.897	-46.781	1.00	8.98	H
ATOM	3596	C	ILE	H	93	6.796	11.126	-43.023	1.00	6.45	H
ATOM	3597	O	ILE	H	93	6.982	10.309	-42.134	1.00	7.71	H
ATOM	3598	N	TYR	H	94	6.127	12.254	-42.828	1.00	7.32	H
ATOM	3599	CA	TYR	H	94	5.536	12.521	-41.527	1.00	8.20	H
ATOM	3600	CB	TYR	H	94	5.547	14.022	-41.207	1.00	7.72	H
ATOM	3601	CG	TYR	H	94	6.930	14.526	-40.868	1.00	6.95	H
ATOM	3602	CD1	TYR	H	94	7.942	14.513	-41.825	1.00	6.29	H
ATOM	3603	CE1	TYR	H	94	9.235	14.867	-41.513	1.00	6.51	H
ATOM	3604	CD2	TYR	H	94	7.252	14.927	-39.569	1.00	7.60	H
ATOM	3605	CE2	TYR	H	94	8.552	15.290	-39.241	1.00	8.06	H
ATOM	3606	CZ	TYR	H	94	9.544	15.250	-40.232	1.00	7.37	H
ATOM	3607	OH	TYR	H	94	10.844	15.565	-39.926	1.00	7.51	H
ATOM	3608	C	TYR	H	94	4.128	11.974	-41.467	1.00	8.37	H
ATOM	3609	O	TYR	H	94	3.231	12.385	-42.217	1.00	8.36	H
ATOM	3610	N	TYR	H	95	3.950	11.015	-40.572	1.00	7.89	H
ATOM	3611	CA	TYR	H	95	2.658	10.387	-40.373	1.00	7.44	H
ATOM	3612	CB	TYR	H	95	2.824	8.887	-40.112	1.00	7.20	H
ATOM	3613	CG	TYR	H	95	3.349	8.085	-41.279	1.00	6.80	H
ATOM	3614	CD1	TYR	H	95	2.508	7.660	-42.295	1.00	6.39	H
ATOM	3615	CE1	TYR	H	95	2.994	6.925	-43.365	1.00	8.93	H
ATOM	3616	CD2	TYR	H	95	4.689	7.757	-41.360	1.00	6.07	H
ATOM	3617	CE2	TYR	H	95	5.186	7.027	-42.419	1.00	8.64	H
ATOM	3618	CZ	TYR	H	95	4.336	6.608	-43.425	1.00	10.04	H
ATOM	3619	OH	TYR	H	95	4.834	5.866	-44.482	1.00	13.38	H
ATOM	3620	C	TYR	H	95	1.888	10.998	-39.209	1.00	6.27	H
ATOM	3621	O	TYR	H	95	2.431	11.316	-38.153	1.00	4.94	H
ATOM	3622	N	CYS	H	96	0.593	11.129	-39.431	1.00	8.19	H
ATOM	3623	CA	CYS	H	96	-0.370	11.655	-38.470	1.00	7.75	H
ATOM	3624	C	CYS	H	96	-1.075	10.462	-37.805	1.00	6.55	H
ATOM	3625	O	CYS	H	96	-1.678	9.647	-38.505	1.00	6.33	H
ATOM	3626	CB	CYS	H	96	-1.396	12.450	-39.250	1.00	8.73	H
ATOM	3627	SG	CYS	H	96	-2.753	13.021	-38.248	1.00	18.02	H
ATOM	3628	N	ALA	H	97	-1.024	10.343	-36.482	1.00	5.62	H
ATOM	3629	CA	ALA	H	97	-1.708	9.217	-35.842	1.00	6.65	H
ATOM	3630	CB	ALA	H	97	-0.705	8.135	-35.433	1.00	4.88	H
ATOM	3631	C	ALA	H	97	-2.591	9.600	-34.652	1.00	7.14	H
ATOM	3632	O	ALA	H	97	-2.270	10.525	-33.889	1.00	6.80	H
ATOM	3633	N	LYS	H	98	-3.706	8.876	-34.504	1.00	7.33	H
ATOM	3634	CA	LYS	H	98	-4.695	9.107	-33.435	1.00	6.92	H
ATOM	3635	CB	LYS	H	98	-6.118	9.141	-34.047	1.00	7.96	H
ATOM	3636	CG	LYS	H	98	-7.243	8.683	-33.099	1.00	8.65	H
ATOM	3637	CD	LYS	H	98	-8.577	8.713	-33.793	1.00	7.93	H
ATOM	3638	CE	LYS	H	98	-9.632	8.044	-32.957	1.00	8.38	H
ATOM	3639	NZ	LYS	H	98	-9.289	6.614	-32.781	1.00	11.17	H
ATOM	3640	C	LYS	H	98	-4.631	8.081	-32.291	1.00	5.55	H
ATOM	3641	O	LYS	H	98	-4.677	6.876	-32.522	1.00	4.02	H
ATOM	3642	N	ALA	H	99	-4.526	8.582	-31.063	1.00	5.94	H
ATOM	3643	CA	ALA	H	99	-4.466	7.744	-29.870	1.00	6.05	H
ATOM	3644	CB	ALA	H	99	-3.893	8.530	-28.713	1.00	5.32	H
ATOM	3645	C	ALA	H	99	-5.851	7.215	-29.498	1.00	6.38	H
ATOM	3646	O	ALA	H	99	-6.880	7.829	-29.806	1.00	6.74	H
ATOM	3647	N	LYS	H	100	-5.863	6.073	-28.823	1.00	6.25	H
ATOM	3648	CA	LYS	H	100	-7.109	5.446	-28.432	1.00	6.98	H
ATOM	3649	CB	LYS	H	100	-6.862	4.012	-27.966	1.00	7.85	H
ATOM	3650	CG	LYS	H	100	-8.137	3.260	-27.666	1.00	8.20	H
ATOM	3651	CD	LYS	H	100	-7.854	1.843	-27.230	1.00	10.16	H
ATOM	3652	CE	LYS	H	100	-7.573	0.930	-28.401	1.00	11.45	H
ATOM	3653	NZ	LYS	H	100	-8.683	0.917	-29.389	1.00	10.69	H
ATOM	3654	C	LYS	H	100	-7.833	6.209	-27.337	1.00	7.43	H
ATOM	3655	O	LYS	H	100	-9.067	6.222	-27.292	1.00	7.57	H

ATOM	3656	N	ARG	H	101	-7.068	6.848	-26.455	1.00	6.66	H
ATOM	3657	CA	ARG	H	101	-7.667	7.591	-25.355	1.00	5.82	H
ATOM	3658	CB	ARG	H	101	-7.125	7.080	-24.033	1.00	7.35	H
ATOM	3659	CG	ARG	H	101	-6.901	5.583	-24.024	1.00	8.88	H
ATOM	3660	CD	ARG	H	101	-6.708	5.089	-22.605	1.00	10.61	H
ATOM	3661	NE	ARG	H	101	-7.985	4.767	-21.985	1.00	11.45	H
ATOM	3662	CZ	ARG	H	101	-8.324	5.114	-20.755	1.00	13.93	H
ATOM	3663	NH1	ARG	H	101	-7.479	5.808	-19.996	1.00	17.72	H
ATOM	3664	NH2	ARG	H	101	-9.504	4.753	-20.281	1.00	12.33	H
ATOM	3665	C	ARG	H	101	-7.432	9.085	-25.459	1.00	4.76	H
ATOM	3666	O	ARG	H	101	-6.777	9.534	-26.393	1.00	6.34	H
ATOM	3667	N	VAL	H	102	-7.960	9.848	-24.501	1.00	3.31	H
ATOM	3668	CA	VAL	H	102	-7.815	11.302	-24.516	1.00	1.00	H
ATOM	3669	CB	VAL	H	102	-8.656	12.030	-23.457	1.00	2.44	H
ATOM	3670	CG1	VAL	H	102	-9.799	12.724	-24.127	1.00	1.07	H
ATOM	3671	CG2	VAL	H	102	-9.099	11.083	-22.353	1.00	1.00	H
ATOM	3672	C	VAL	H	102	-6.434	11.817	-24.301	1.00	1.00	H
ATOM	3673	O	VAL	H	102	-6.142	12.932	-24.688	1.00	1.36	H
ATOM	3674	N	GLY	H	103	-5.592	11.034	-23.650	1.00	1.00	H
ATOM	3675	CA	GLY	H	103	-4.246	11.501	-23.422	1.00	2.80	H
ATOM	3676	C	GLY	H	103	-3.334	10.895	-24.457	1.00	5.14	H
ATOM	3677	O	GLY	H	103	-3.778	10.171	-25.335	1.00	5.99	H
ATOM	3678	N	ALA	H	104	-2.057	11.224	-24.381	1.00	7.98	H
ATOM	3679	CA	ALA	H	104	-1.081	10.647	-25.281	1.00	11.22	H
ATOM	3680	CB	ALA	H	104	0.259	11.310	-25.052	1.00	12.12	H
ATOM	3681	C	ALA	H	104	-1.080	9.230	-24.730	1.00	13.71	H
ATOM	3682	O	ALA	H	104	-0.454	8.956	-23.703	1.00	16.89	H
ATOM	3683	N	THR	H	105	-1.808	8.339	-25.383	1.00	12.18	H
ATOM	3684	CA	THR	H	105	-1.913	6.979	-24.889	1.00	10.87	H
ATOM	3685	CB	THR	H	105	-3.137	6.300	-25.540	1.00	11.27	H
ATOM	3686	OG1	THR	H	105	-4.258	7.186	-25.458	1.00	11.02	H
ATOM	3687	CG2	THR	H	105	-3.497	5.020	-24.828	1.00	11.22	H
ATOM	3688	C	THR	H	105	-0.646	6.143	-25.097	1.00	10.95	H
ATOM	3689	O	THR	H	105	-0.193	5.472	-24.173	1.00	11.18	H
ATOM	3690	N	GLY	H	106	-0.080	6.193	-26.303	1.00	9.89	H
ATOM	3691	CA	GLY	H	106	1.108	5.422	-26.610	1.00	8.03	H
ATOM	3692	C	GLY	H	106	0.873	4.532	-27.821	1.00	9.08	H
ATOM	3693	O	GLY	H	106	1.806	4.189	-28.551	1.00	8.94	H
ATOM	3694	N	TYR	H	107	-0.381	4.152	-28.041	1.00	9.04	H
ATOM	3695	CA	TYR	H	107	-0.722	3.318	-29.178	1.00	7.70	H
ATOM	3696	CB	TYR	H	107	-1.167	1.918	-28.728	1.00	7.28	H
ATOM	3697	CG	TYR	H	107	-2.176	1.870	-27.621	1.00	6.75	H
ATOM	3698	CD1	TYR	H	107	-3.531	1.704	-27.889	1.00	7.50	H
ATOM	3699	CE1	TYR	H	107	-4.461	1.622	-26.868	1.00	9.33	H
ATOM	3700	CD2	TYR	H	107	-1.773	1.954	-26.308	1.00	7.00	H
ATOM	3701	CE2	TYR	H	107	-2.680	1.871	-25.281	1.00	8.83	H
ATOM	3702	CZ	TYR	H	107	-4.029	1.706	-25.552	1.00	11.18	H
ATOM	3703	OH	TYR	H	107	-4.940	1.646	-24.498	1.00	13.47	H
ATOM	3704	C	TYR	H	107	-1.793	4.036	-29.970	1.00	8.28	H
ATOM	3705	O	TYR	H	107	-2.670	4.694	-29.404	1.00	8.79	H
ATOM	3706	N	PHE	H	108	-1.707	3.904	-31.290	1.00	8.59	H
ATOM	3707	CA	PHE	H	108	-2.618	4.594	-32.194	1.00	7.43	H
ATOM	3708	CB	PHE	H	108	-1.803	5.633	-32.928	1.00	6.07	H
ATOM	3709	CG	PHE	H	108	-0.641	6.100	-32.138	1.00	3.15	H
ATOM	3710	CD1	PHE	H	108	-0.828	6.931	-31.033	1.00	3.84	H
ATOM	3711	CD2	PHE	H	108	0.631	5.640	-32.428	1.00	1.87	H
ATOM	3712	CE1	PHE	H	108	0.251	7.304	-30.206	1.00	1.62	H
ATOM	3713	CE2	PHE	H	108	1.720	5.998	-31.621	1.00	2.47	H
ATOM	3714	CZ	PHE	H	108	1.529	6.834	-30.503	1.00	1.15	H
ATOM	3715	C	PHE	H	108	-3.343	3.712	-33.189	1.00	7.78	H
ATOM	3716	O	PHE	H	108	-2.716	3.093	-34.041	1.00	7.98	H

ATOM	3717	N	ASP	H	109	-4.671	3.703	-33.092	1.00	7.48	H
ATOM	3718	CA	ASP	H	109	-5.522	2.904	-33.958	1.00	6.76	H
ATOM	3719	CB	ASP	H	109	-6.827	2.525	-33.251	1.00	8.37	H
ATOM	3720	CG	ASP	H	109	-7.497	3.708	-32.566	1.00	9.76	H
ATOM	3721	OD1	ASP	H	109	-7.446	4.836	-33.080	1.00	12.11	H
ATOM	3722	OD2	ASP	H	109	-8.092	3.513	-31.496	1.00	11.64	H
ATOM	3723	C	ASP	H	109	-5.867	3.540	-35.287	1.00	6.63	H
ATOM	3724	O	ASP	H	109	-6.497	2.904	-36.137	1.00	7.36	H
ATOM	3725	N	LEU	H	110	-5.466	4.782	-35.500	1.00	5.24	H
ATOM	3726	CA	LEU	H	110	-5.786	5.398	-36.781	1.00	5.19	H
ATOM	3727	CB	LEU	H	110	-7.013	6.295	-36.650	1.00	4.04	H
ATOM	3728	CG	LEU	H	110	-7.465	6.907	-37.979	1.00	4.58	H
ATOM	3729	CD1	LEU	H	110	-7.936	5.827	-38.912	1.00	1.00	H
ATOM	3730	CD2	LEU	H	110	-8.592	7.914	-37.717	1.00	6.43	H
ATOM	3731	C	LEU	H	110	-4.624	6.200	-37.298	1.00	5.51	H
ATOM	3732	O	LEU	H	110	-4.076	7.038	-36.592	1.00	6.65	H
ATOM	3733	N	TRP	H	111	-4.247	5.957	-38.538	1.00	4.26	H
ATOM	3734	CA	TRP	H	111	-3.132	6.702	-39.088	1.00	4.57	H
ATOM	3735	CB	TRP	H	111	-1.912	5.790	-39.296	1.00	3.02	H
ATOM	3736	CG	TRP	H	111	-1.291	5.208	-38.059	1.00	1.95	H
ATOM	3737	CD2	TRP	H	111	0.081	5.316	-37.665	1.00	1.00	H
ATOM	3738	CE2	TRP	H	111	0.246	4.528	-36.503	1.00	1.00	H
ATOM	3739	CE3	TRP	H	111	1.189	6.001	-38.187	1.00	1.00	H
ATOM	3740	CD1	TRP	H	111	-1.890	4.389	-37.140	1.00	2.44	H
ATOM	3741	NE1	TRP	H	111	-0.971	3.975	-36.206	1.00	1.00	H
ATOM	3742	CZ2	TRP	H	111	1.482	4.401	-35.851	1.00	1.00	H
ATOM	3743	CZ3	TRP	H	111	2.412	5.882	-37.549	1.00	1.00	H
ATOM	3744	CH2	TRP	H	111	2.553	5.084	-36.387	1.00	2.97	H
ATOM	3745	C	TRP	H	111	-3.534	7.310	-40.423	1.00	5.19	H
ATOM	3746	O	TRP	H	111	-4.602	7.016	-40.963	1.00	4.62	H
ATOM	3747	N	GLY	H	112	-2.669	8.178	-40.933	1.00	6.36	H
ATOM	3748	CA	GLY	H	112	-2.917	8.808	-42.209	1.00	7.94	H
ATOM	3749	C	GLY	H	112	-1.848	8.270	-43.134	1.00	9.94	H
ATOM	3750	O	GLY	H	112	-0.962	7.545	-42.674	1.00	7.59	H
ATOM	3751	N	ARG	H	113	-1.911	8.609	-44.420	1.00	12.17	H
ATOM	3752	CA	ARG	H	113	-0.918	8.130	-45.387	1.00	14.63	H
ATOM	3753	CB	ARG	H	113	-1.415	8.357	-46.821	1.00	19.69	H
ATOM	3754	CG	ARG	H	113	-2.716	7.645	-47.220	1.00	26.76	H
ATOM	3755	CD	ARG	H	113	-3.136	7.992	-48.682	1.00	32.39	H
ATOM	3756	NE	ARG	H	113	-3.098	9.435	-48.981	1.00	36.17	H
ATOM	3757	CZ	ARG	H	113	-3.435	9.974	-50.154	1.00	39.14	H
ATOM	3758	NH1	ARG	H	113	-3.844	9.194	-51.153	1.00	40.77	H
ATOM	3759	NH2	ARG	H	113	-3.348	11.291	-50.334	1.00	39.73	H
ATOM	3760	C	ARG	H	113	0.459	8.801	-45.236	1.00	13.93	H
ATOM	3761	O	ARG	H	113	1.454	8.288	-45.747	1.00	14.13	H
ATOM	3762	N	GLY	H	114	0.508	9.949	-44.560	1.00	12.46	H
ATOM	3763	CA	GLY	H	114	1.763	10.660	-44.373	1.00	10.52	H
ATOM	3764	C	GLY	H	114	2.053	11.683	-45.468	1.00	9.35	H
ATOM	3765	O	GLY	H	114	1.436	11.642	-46.527	1.00	8.23	H
ATOM	3766	N	THR	H	115	2.963	12.618	-45.192	1.00	8.71	H
ATOM	3767	CA	THR	H	115	3.398	13.635	-46.151	1.00	6.50	H
ATOM	3768	CB	THR	H	115	3.021	15.043	-45.753	1.00	7.27	H
ATOM	3769	OG1	THR	H	115	1.952	14.999	-44.822	1.00	9.76	H
ATOM	3770	CG2	THR	H	115	2.636	15.855	-46.966	1.00	7.54	H
ATOM	3771	C	THR	H	115	4.925	13.624	-46.129	1.00	7.01	H
ATOM	3772	O	THR	H	115	5.554	13.574	-45.055	1.00	2.98	H
ATOM	3773	N	LEU	H	116	5.511	13.699	-47.318	1.00	6.85	H
ATOM	3774	CA	LEU	H	116	6.953	13.701	-47.463	1.00	6.07	H
ATOM	3775	CB	LEU	H	116	7.352	13.132	-48.812	1.00	5.44	H
ATOM	3776	CG	LEU	H	116	8.812	13.352	-49.199	1.00	5.58	H
ATOM	3777	CD1	LEU	H	116	9.727	12.426	-48.399	1.00	3.24	H

ATOM	3778	CD2	LEU	H	116	8.941	13.099	-50.685	1.00	5.27	H
ATOM	3779	C	LEU	H	116	7.531	15.082	-47.350	1.00	7.43	H
ATOM	3780	O	LEU	H	116	7.132	15.997	-48.059	1.00	9.44	H
ATOM	3781	N	VAL	H	117	8.481	15.228	-46.443	1.00	9.93	H
ATOM	3782	CA	VAL	H	117	9.151	16.500	-46.275	1.00	11.48	H
ATOM	3783	CB	VAL	H	117	9.107	16.966	-44.817	1.00	11.24	H
ATOM	3784	CG1	VAL	H	117	9.929	18.231	-44.648	1.00	11.87	H
ATOM	3785	CG2	VAL	H	117	7.675	17.217	-44.418	1.00	11.74	H
ATOM	3786	C	VAL	H	117	10.587	16.250	-46.706	1.00	11.33	H
ATOM	3787	O	VAL	H	117	11.247	15.342	-46.187	1.00	10.03	H
ATOM	3788	N	THR	H	118	11.049	17.032	-47.677	1.00	11.55	H
ATOM	3789	CA	THR	H	118	12.412	16.898	-48.182	1.00	13.80	H
ATOM	3790	CB	THR	H	118	12.469	16.720	-49.714	1.00	12.54	H
ATOM	3791	OG1	THR	H	118	11.597	15.658	-50.113	1.00	17.37	H
ATOM	3792	CG2	THR	H	118	13.880	16.398	-50.147	1.00	11.46	H
ATOM	3793	C	THR	H	118	13.156	18.177	-47.889	1.00	15.05	H
ATOM	3794	O	THR	H	118	12.809	19.235	-48.422	1.00	16.32	H
ATOM	3795	N	VAL	H	119	14.176	18.102	-47.048	1.00	14.62	H
ATOM	3796	CA	VAL	H	119	14.932	19.302	-46.763	1.00	15.25	H
ATOM	3797	CB	VAL	H	119	15.212	19.441	-45.249	1.00	15.70	H
ATOM	3798	CG1	VAL	H	119	15.740	18.137	-44.684	1.00	18.79	H
ATOM	3799	CG2	VAL	H	119	16.205	20.559	-45.013	1.00	14.10	H
ATOM	3800	C	VAL	H	119	16.242	19.309	-47.544	1.00	15.85	H
ATOM	3801	O	VAL	H	119	17.170	18.567	-47.232	1.00	15.88	H
ATOM	3802	N	SER	H	120	16.297	20.129	-48.589	1.00	17.32	H
ATOM	3803	CA	SER	H	120	17.511	20.245	-49.385	1.00	18.51	H
ATOM	3804	CB	SER	H	120	17.491	19.307	-50.597	1.00	18.68	H
ATOM	3805	OG	SER	H	120	17.034	19.984	-51.754	1.00	16.68	H
ATOM	3806	C	SER	H	120	17.669	21.665	-49.879	1.00	19.18	H
ATOM	3807	O	SER	H	120	16.789	22.509	-49.698	1.00	16.51	H
ATOM	3808	N	SER	H	121	18.808	21.908	-50.518	1.00	21.95	H
ATOM	3809	CA	SER	H	121	19.120	23.215	-51.069	1.00	23.17	H
ATOM	3810	CB	SER	H	121	20.568	23.602	-50.719	1.00	22.76	H
ATOM	3811	OG	SER	H	121	20.655	24.126	-49.404	1.00	23.27	H
ATOM	3812	C	SER	H	121	18.890	23.299	-52.584	1.00	23.84	H
ATOM	3813	O	SER	H	121	18.862	24.394	-53.122	1.00	24.66	H

Table IX. Amino acid sequences of the rBLG-His6, rBLG-His6 T18Y and rBLG-His6 T18Y/E45Y/L57Y are shown. The His6 tag is in italics, mutated amino acids are bolded and underlined.

rBLG-His6:

```

1      LIVTQTMKGL DIQKVAGTWY SLAMAASDIS LLDAQSAPLR
41     VYVEELKPTP EGDLEILLQK WENGECQKK  IIAEKTIPA
81     VFKIDALNEN KVLVLDTDYK KYLLFCMENS AEPEQSLVCQ
121    CLVRTPEVDD EALEKFDKAL KALPMHIRLS FNPTQLEEQC
161    HHHHHHHH (SEQ ID NO:9)

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rBLG-His6 T18Y:

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1      LIVTQTMKGL DIQKVAGYWY SLAMAASDIS LLDAQSAPLR
41     VYVEELKPTP EGDLEILLQK WENGECQKK  IIAEKTIPA
81     VFKIDALNEN KVLVLDTDYK KYLLFCMENS AEPEQSLVCQ
121    CLVRTPEVDD EALEKFDKAL KALPMHIRLS FNPTQLEEQC
161    HHHHHHHH (SEQ ID NO:10)

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rBLG-His6 T18Y/E45Y/L57Y:

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1      LIVTQTMKGL DIQKVAGYWY SLAMAASDIS LLDAQSAPLR
41     VYVEYLKPTP EGDLEIYLQK WENGECQKK  IIAEKTIPA
81     VFKIDALNEN KVLVLDTDYK KYLLFCMENS AEPEQSLVCQ
121    CLVRTPEVDD EALEKFDKAL KALPMHIRLS FNPTQLEEQC
161    HHHHHHHH (SEQ ID NO:11)

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Table X. The primers used for the PCR amplification of rBLG-His6, rBLG-His6 T18Y and rBLG-His6 T18Y/E45Y/L57Y mutant. Restriction enzyme sites are shown in italics. Overlapping areas and stop codons are underlined. Mutated codons are bolded, underlined and in italics.

SfiI *NcoI*
Primer 1. GAA TCC GCG ***GCC CAG CCG*** GCC ATG GCC CTG ATT GTG ACC

HindIII Stop
Primer 2. TTA CTC AAG CTT TTA ATG GTG ATG GTG ATG ATG AAT ATG GCA CTG TTC TTC CAG C

StuI
Primer 3. CC ATG AAA GGC CTG GAT ATT CAG AAA GTG GCG GGC ***TAC*** TGG TAT AGC C

Overlapping area with the primer 5
Primer 4. ***ATA*** AAT TTC CAG ATC GCC TTC CGG GGT CGG TTT CAG ***ATA*** TTC CAC ATA CAC ACG C

Overlapping area with the primer 4
Primer 5. GGC GAT CTG GAA ATT ***TAT*** CTG CAG AAA TGG G

Table XI. The association and dissociation constants of the D1 IgE Fab to nBLG, rBLG-His6 and its mutants (see Figure 24).

	nBLG	rBLGhis	T18Y	Triple mutant
Kd (1/s)	4.8e ⁻³	8.2e ⁻³	8.2e ⁻²	-
Ka (1/Ms)	1.8e ⁶	9.61e ⁵	1.3e ⁵	-
KD (M)	2.7e ⁻⁹	8.5e ⁻⁹	6.1e ⁻⁷	-
KA (1/M)	3.2e ⁸	1.2e ⁸	1.6e ⁶	-

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The embodiments of the invention in which an exclusive property or privilege is claimed are defined as follows:

1. A method for producing a modified allergenic polypeptide, the method comprising the steps of:
 - (a) modifying nucleic acid sequence encoding an allergenic polypeptide comprising a planar surface so that in the polypeptide expressed from the modified nucleic acid the structure of the planar surface of said polypeptide is altered;
 - (b) expressing or producing the modified allergenic polypeptide from the modified nucleic acid; and
 - (c) selecting those modified allergenic polypeptides towards which an IgE-antibody specific to said allergenic polypeptide shows at least tenfold lower affinity;

wherein said planar surface has an area of 600-900 Å² and is determined by computational analysis to be as the allergenic epitope of β-lactoglobulin defined by the structure or 3D-coordinates of β-lactoglobulin amino acids Trp19-Tyr20, Val43-Lys47, Leu57-Gln59, Cys66-Gln68, Pro126-Glu127, and Thr154-Glu157 of SEQ ID NO:8 in an antibody-β-lactoglobulin immunocomplex.
2. The method of claim 1, wherein said allergenic polypeptide is
 - a) Bos d 5, Beta-lactoglobulin;
 - b) Equ c 1, horse skin;
 - c) Bet v 1, birch pollen;
 - d) Bos d 2, bovine dander;
 - e) Cyp c 1, carp parvalbumin; or
 - f) Hev b 6, latex.
3. A method for identifying a molecule binding to the planar surface structure of an allergenic polypeptide, said molecule being capable to inhibit or hinder the binding of a specific IgE-antibody to said allergenic polypeptide; comprising the steps of: (a) contacting a particle comprising the allergenic epitope and a candidate binder molecule; and (b) isolating those candidate binder molecules which are able to bind to the planar surface of said allergen;

wherein said planar surface has an area of 600-900 Å² and is determined by computational analysis to be as the allergenic epitope of β-lactoglobulin defined by the structure or 3D-coordinates of β-lactoglobulin amino acids Trp19-Tyr20, Val43-Lys47, Leu57-Gln59, Cys66-Gln68, Pro126-Glu127, and Thr154-Glu157 of SEQ ID NO:8 in an antibody-β-lactoglobulin immunocomplex.

4. The method of claim 3, wherein said allergenic polypeptide is
 - a) Bos d 5, Beta-lactoglobulin;
 - b) Equ c 1, horse skin;
 - c) Bet v 1, birch pollen;
 - d) Bos d 2, bovine dander;
 - e) Cyp c 1, carp parvalbumin; or
 - f) Hev b 6, latex.
5. The method of claim 3, wherein said molecule is a peptide.
6. A method for identifying a molecule binding to the allergenic epitope of β-lactoglobulin defined by structure coordinates of β-lactoglobulin amino acids Trp19 and Tyr20 of SEQ ID NO:8 from beta-strand A and Glu44 of SEQ ID NO:8 from beta-strand B in an antibody-β-lactoglobulin immunocomplex; comprising the steps of:
 - (a) contacting a molecule comprising the allergenic epitope of β-lactoglobulin and a candidate binder molecule; and
 - (b) isolating those candidate binder molecules which were able to bind to said allergenic epitope of β-lactoglobulin.
7. The method according to claim 6, wherein the method is performed as an affinity chromatography.
8. A method for identifying a molecule binding to the allergenic epitope of β-lactoglobulin defined by structure coordinates of β-lactoglobulin amino acids Val43-Lys47 and Leu57-Gln59 of SEQ ID NO:8 in an antibody-β-lactoglobulin immunocomplex; comprising the steps of:

(a) contacting a molecule comprising the allergenic epitope of β -lactoglobulin and a candidate binder molecule; and

(b) isolating those candidate binder molecules which were able to bind to said allergenic epitope of β -lactoglobulin.

9. The method according to claim 8, wherein the method is performed as an affinity chromatography.

10. A method for identifying a modulator of binding between the allergenic epitope of β -lactoglobulin and its ligand, said allergenic epitope of β -lactoglobulin being defined by structure coordinates of β -lactoglobulin amino acids Trp19 and Tyr20 of SEQ ID NO:8 from beta-strand A and Glu44 of SEQ ID NO:8 from beta-strand B in an antibody- β -lactoglobulin immunocomplex; comprising the steps of:

(a) contacting a molecule comprising the allergenic epitope of β -lactoglobulin and its ligand in the presence and in the absence of a putative modulator compound;

(b) detecting binding between the allergenic epitope of β -lactoglobulin and its ligand in the presence and absence of the putative modulator; and

(c) identifying a modulator compound in view of decreased or increased binding between the allergenic epitope of β -lactoglobulin and its ligand in the presence of the putative modulator, as compared to binding in the absence of the putative modulator.

11. The method according to claim 10, further comprising a step of:

(d) making a modulator composition by formulating a modulator identified according to step (c) in a pharmaceutically acceptable carrier.

12. The method according to claim 10, wherein said ligand is a monoclonal antibody of IgE class having binding specificity to an allergenic epitope on β -lactoglobulin of SEQ ID NO:8, or a functional fragment having said specificity, wherein said antibody or the fragment thereof comprises Arg101 of CDR-H3 loop of SEQ ID NO:2 as a key residue in binding of the antibody to said allergenic epitope of β -lactoglobulin.

13. A method for identifying a modulator of binding between the allergenic epitope of β -lactoglobulin and its ligand, said allergenic epitope of β -lactoglobulin being defined by structure coordinates of β -lactoglobulin amino acids Val43-Lys47 and Leu57-Gln59 of SEQ ID NO:8 in an antibody- β -lactoglobulin immunocomplex; comprising the steps of:

(a) contacting a molecule comprising the allergenic epitope of β -lactoglobulin and its ligand in the presence and in the absence of a putative modulator compound;

(b) detecting binding between the allergenic epitope of β -lactoglobulin and its ligand in the presence and absence of the putative modulator; and

(c) identifying a modulator compound in view of decreased or increased binding between the allergenic epitope of β -lactoglobulin and its ligand in the presence of the putative modulator, as compared to binding in the absence of the putative modulator.

14. The method according to claim 13, further comprising a step of:

(d) making a modulator composition by formulating a modulator identified according to step (c) in a pharmaceutically acceptable carrier.

15. The method according to claim 13, wherein said ligand is a monoclonal antibody of IgE class having binding specificity to an allergenic epitope on β -lactoglobulin of SEQ ID NO:8, or a functional fragment having said specificity, wherein said antibody or the fragment thereof comprises Arg101 of CDR-H3 loop of SEQ ID NO:2 as a key residue in binding of the antibody to said allergenic epitope of β -lactoglobulin.

16. A method for producing a modified allergenic polypeptide, the method comprising the steps of:

(a) detecting by structural analysis or molecular modelling techniques a potential IgE binding site in an allergenic polypeptide;

(b) determining by computational analysis of a three-dimensional structure of said allergenic polypeptide whether said potential IgE binding site contains a planar or flat surface area of 600-900 Å² as the planar surface as defined by the 3D-coordinates of β -lactoglobulin amino acids Val43-Lys47 and Leu57-Gln59 of SEQ ID NO:8 in an

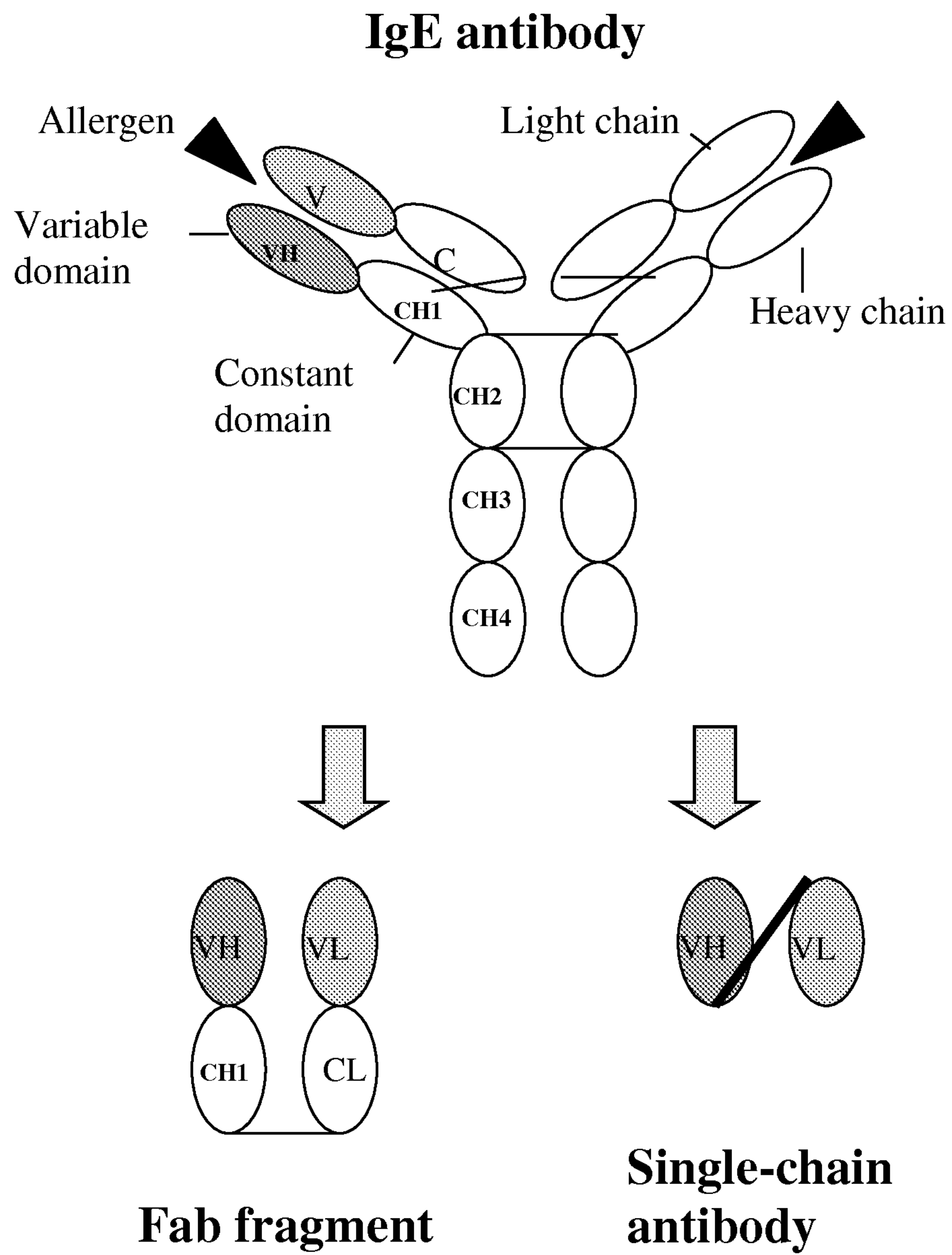
antibody- β -lactoglobulin immunocomplex, if a planar or flat surface as the one in β -lactoglobulin is found, the method is continued by

(c) modifying a nucleic acid sequence encoding said polypeptide so that in the polypeptide expressed from the modified nucleic acid the structure of the planar or flat surface of said polypeptide is altered; and

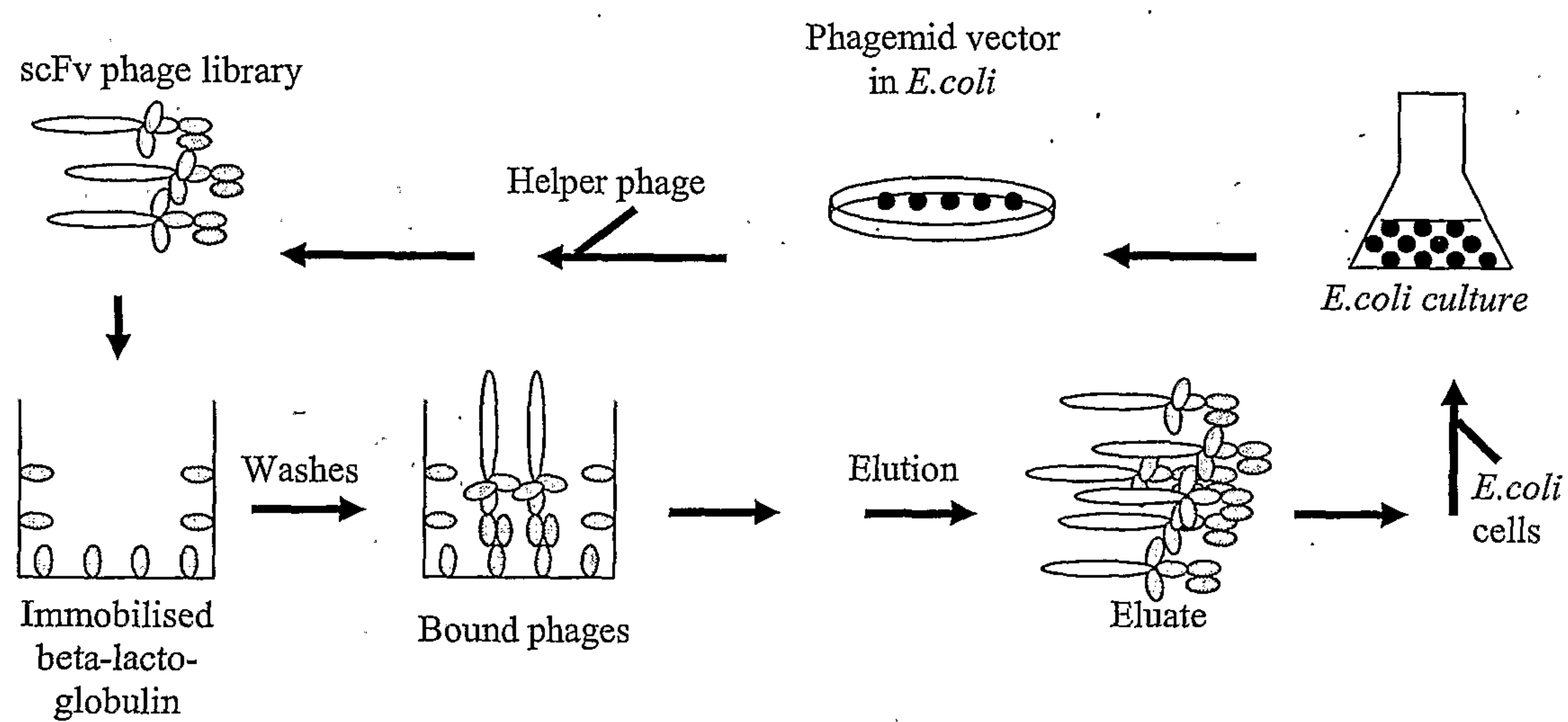
(d) expressing or producing a modified allergenic polypeptide from the modified nucleic acid obtained from step c).

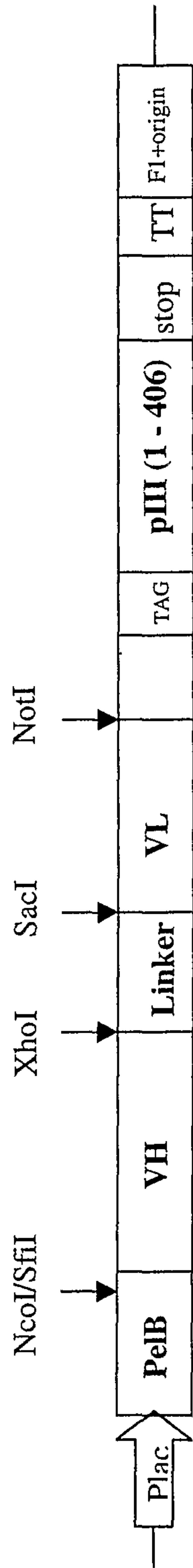
17. The method according to claim 16, wherein in step (b) the three-dimensional structure of said allergenic polypeptide is compared to the three-dimensional structure of β -lactoglobulin.

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Figure 1

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Figure 2



lac promoter
pelB: pectate lyase signal sequence
Heavy chain: VH = SfiI/NcoI - XhoI fragment
Linker: (Gly₄Ser)₃ = 15 aa
Light chain: VL = SacI - NotI fragment
Myc peptide: EQKLISEEDLN = 11 aa; Mab 9E10
TAG = Amber stop codon; supE+, E.coli strain TAG = Glu → scFv-pIII fusion
supE-, E.coli strain = stop codon → scFv
TT: transcription terminator
f1+: phage origin of replication

Figure 3

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Figure 4

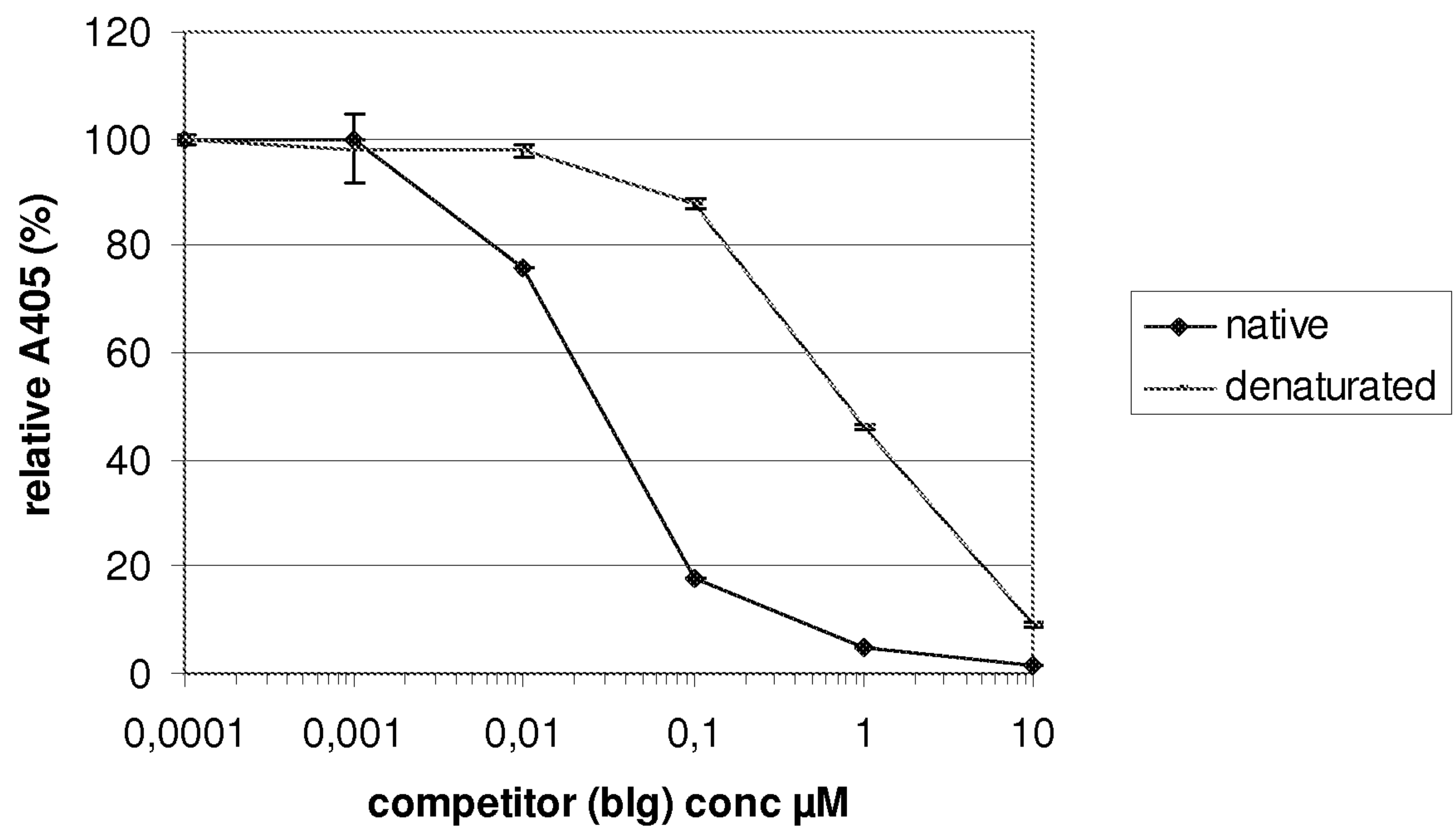
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D1VH	QVSLRESGGGLVQPGRSLRLSCTASGFTFR		
	40	50	60
	<u>HHGMTWVRQAPGKGLEWVASLSGSGTKTHF</u>		
	70	80	90
	<u>ADSVKGRFTISRDN</u> SNNTLYLQMDNVRDED		
	100	110	120
	TAIYYCAKAKRVGATGYFDLWGRGTLVTVSS		

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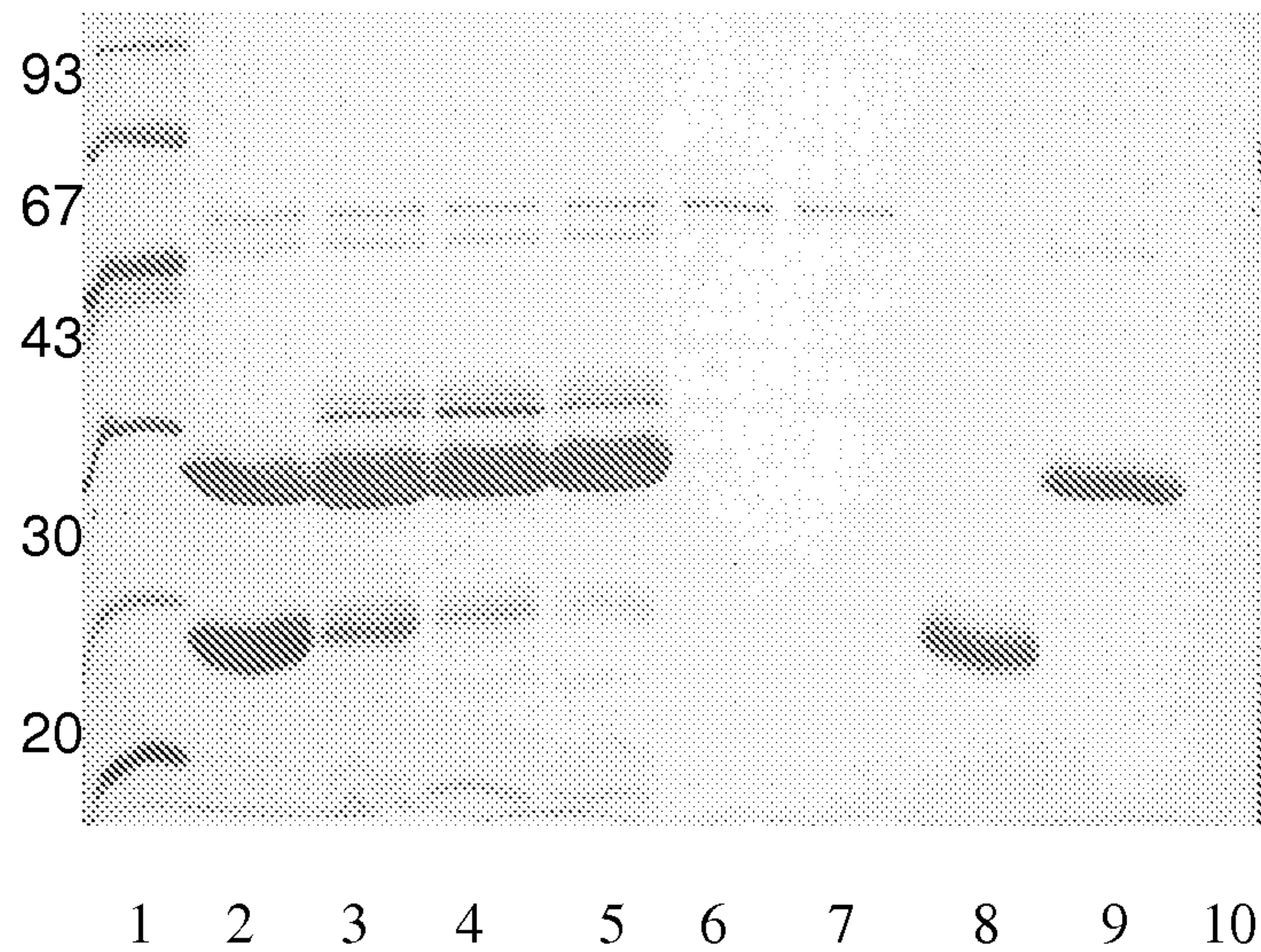
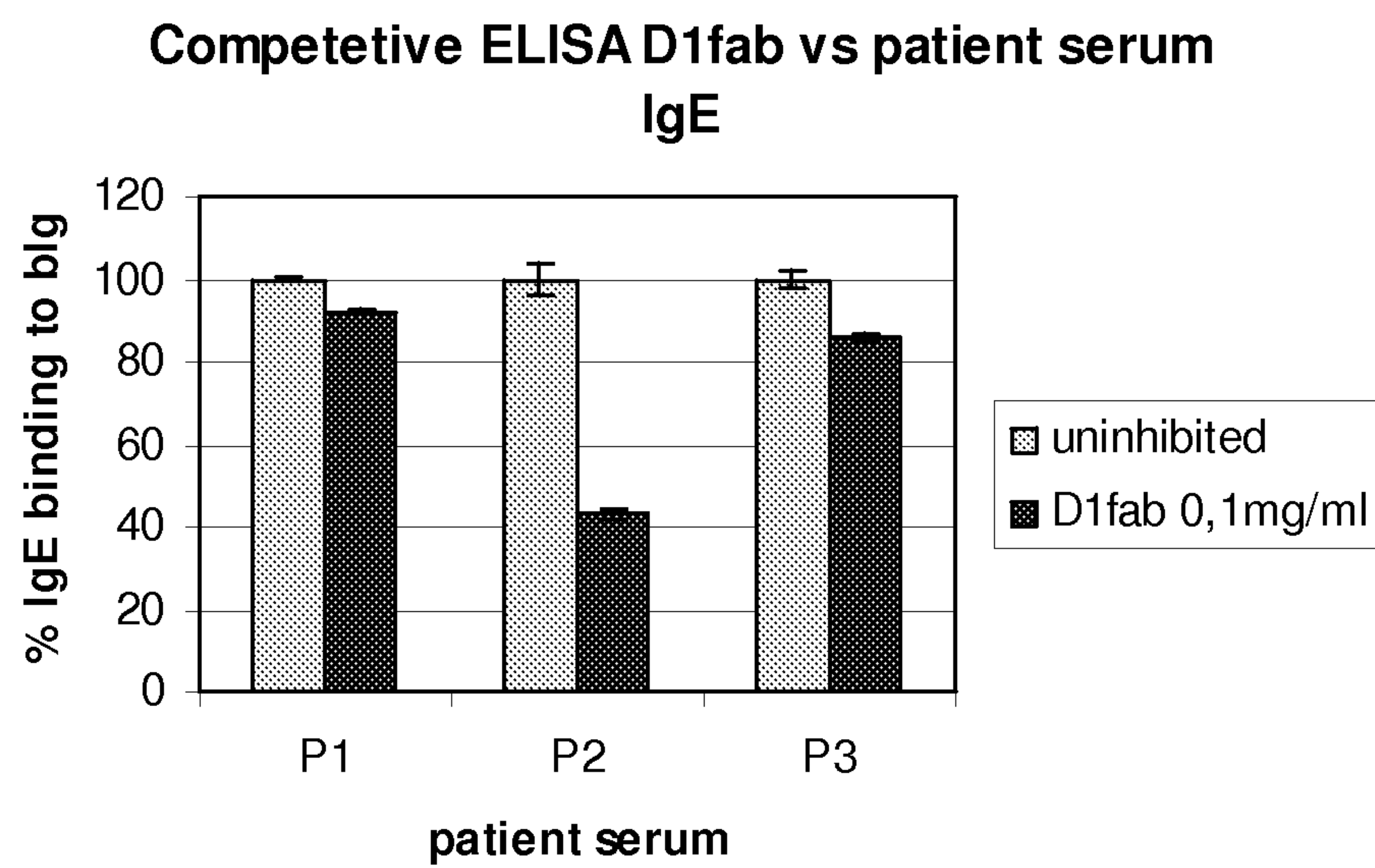
Figure 5

	10	20	30
D1VL	DIVMTQSPSSLSASVGDRVTITCRAS <u>QGIS</u>		
	40	50	60
	<u>SRLAWYQQKPGKAPKLLIYAASSLQSGVPS</u>		
	70	80	90
	RFSGSGSGTEFTLTISSLQPEDFATYYC <u>QQ</u>		
	100		
	<u>YHSYPWTFGQGTKVEIKR</u>		

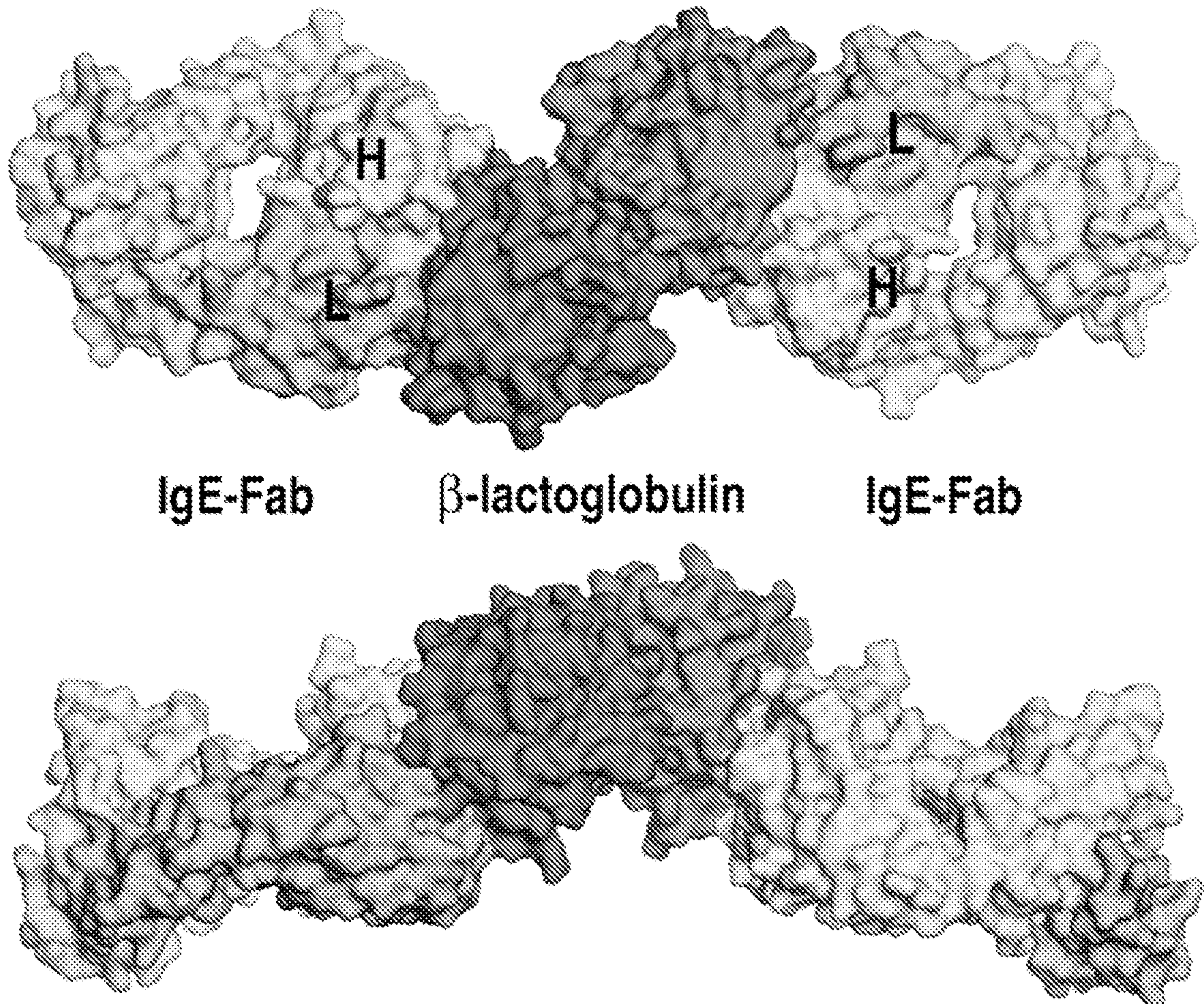
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Figure 6

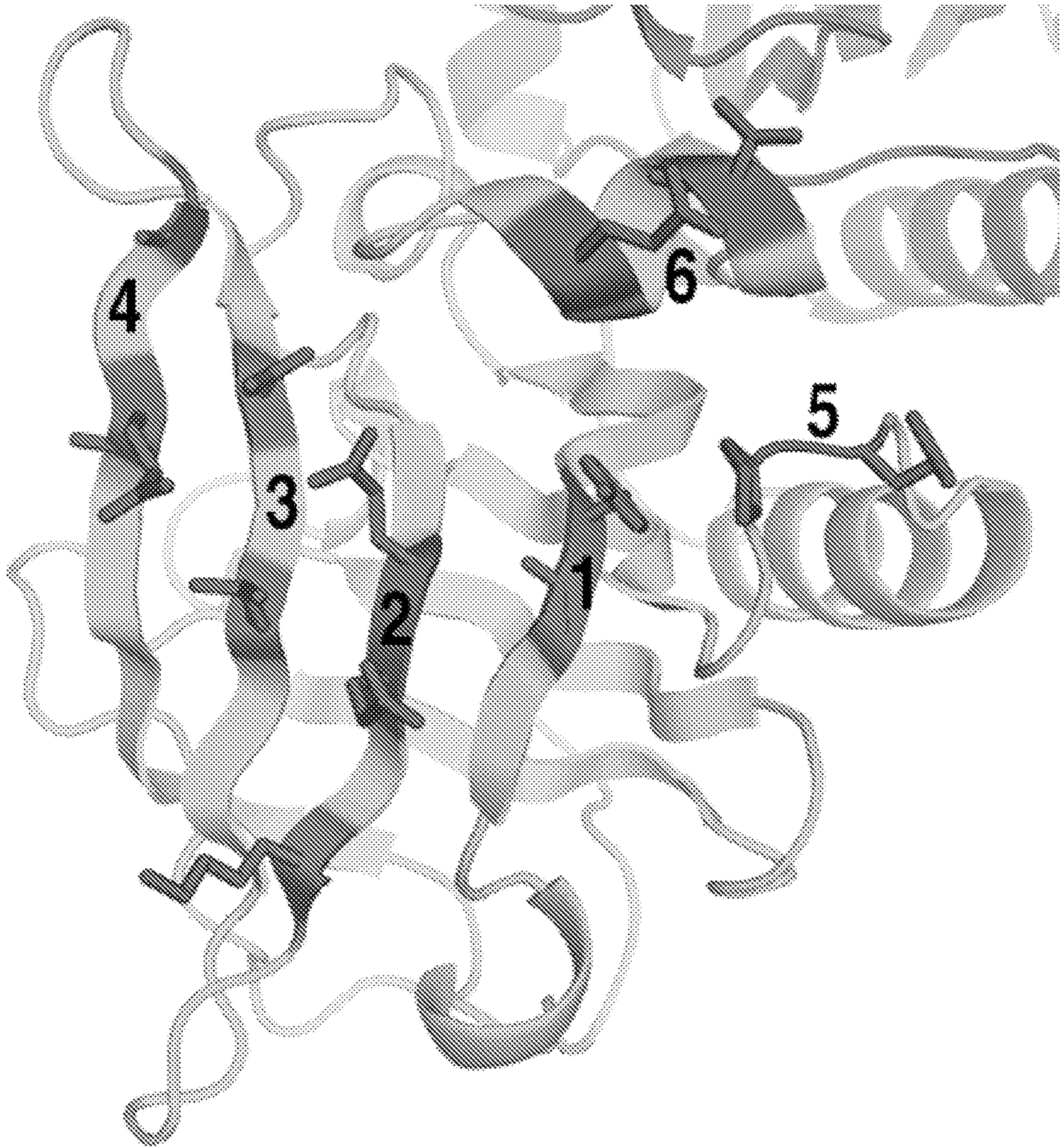
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Figure 7**Figure 8**

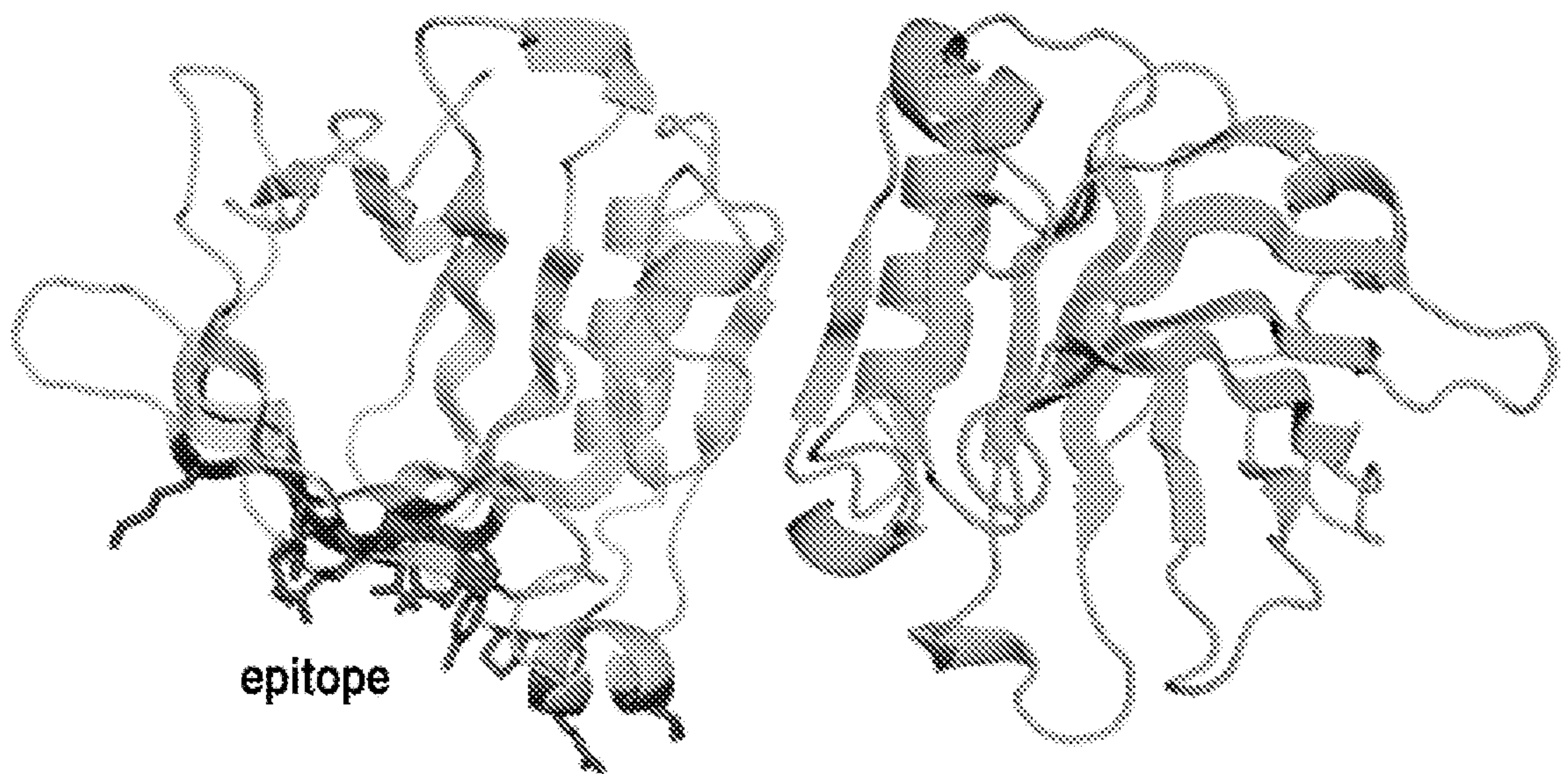
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Figure 9

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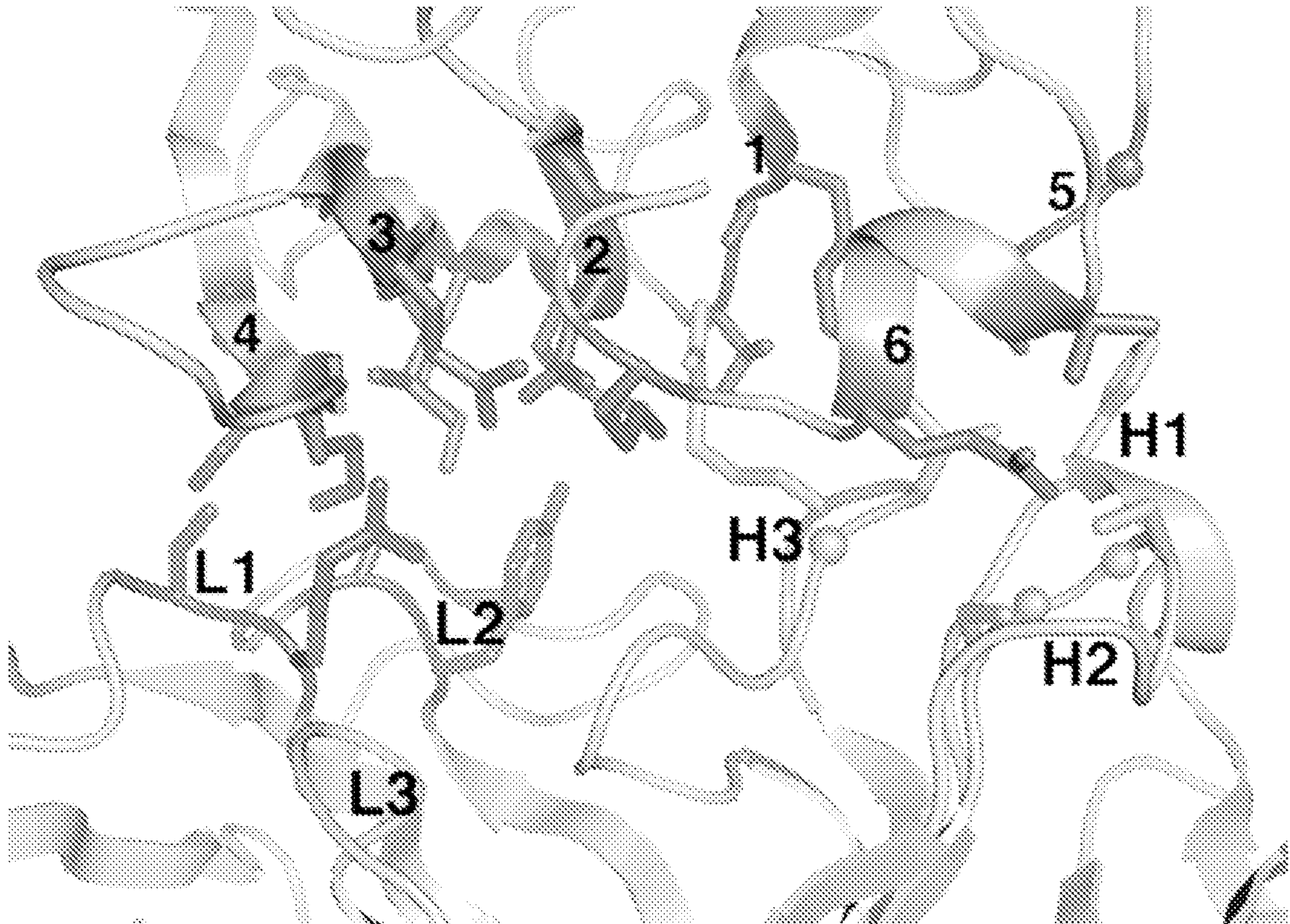
Figure 10

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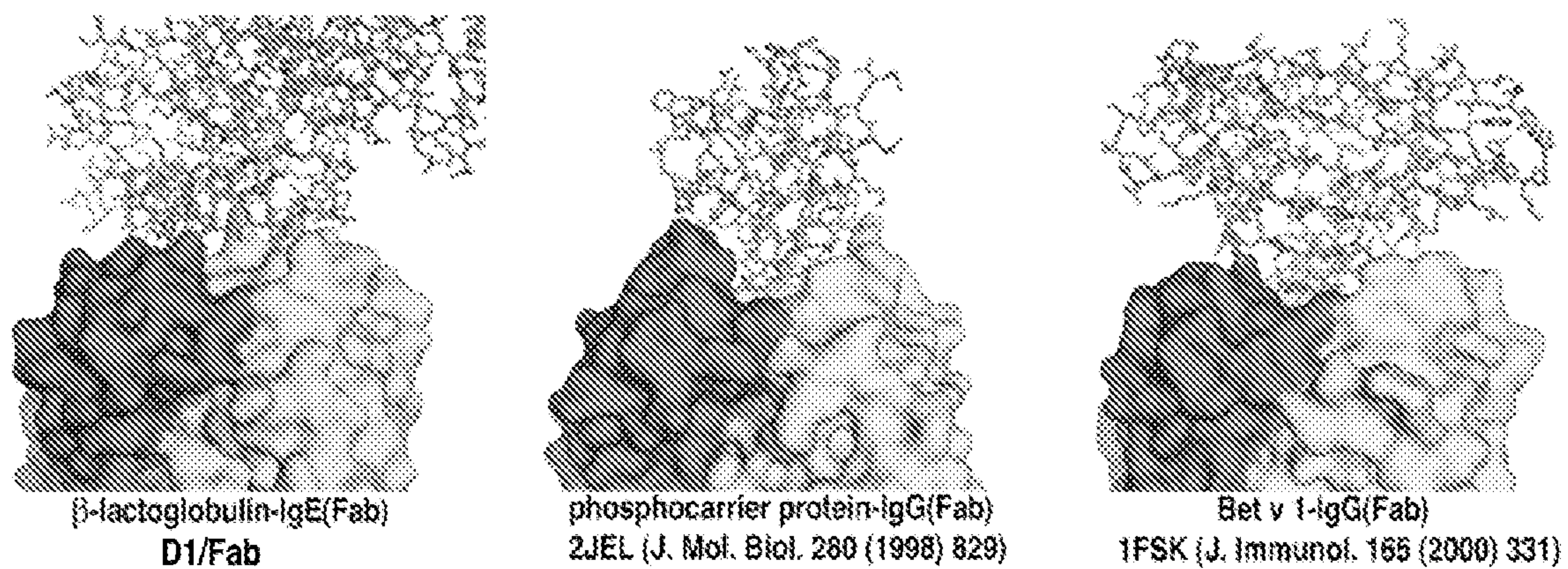
Figure 11

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Figure 12

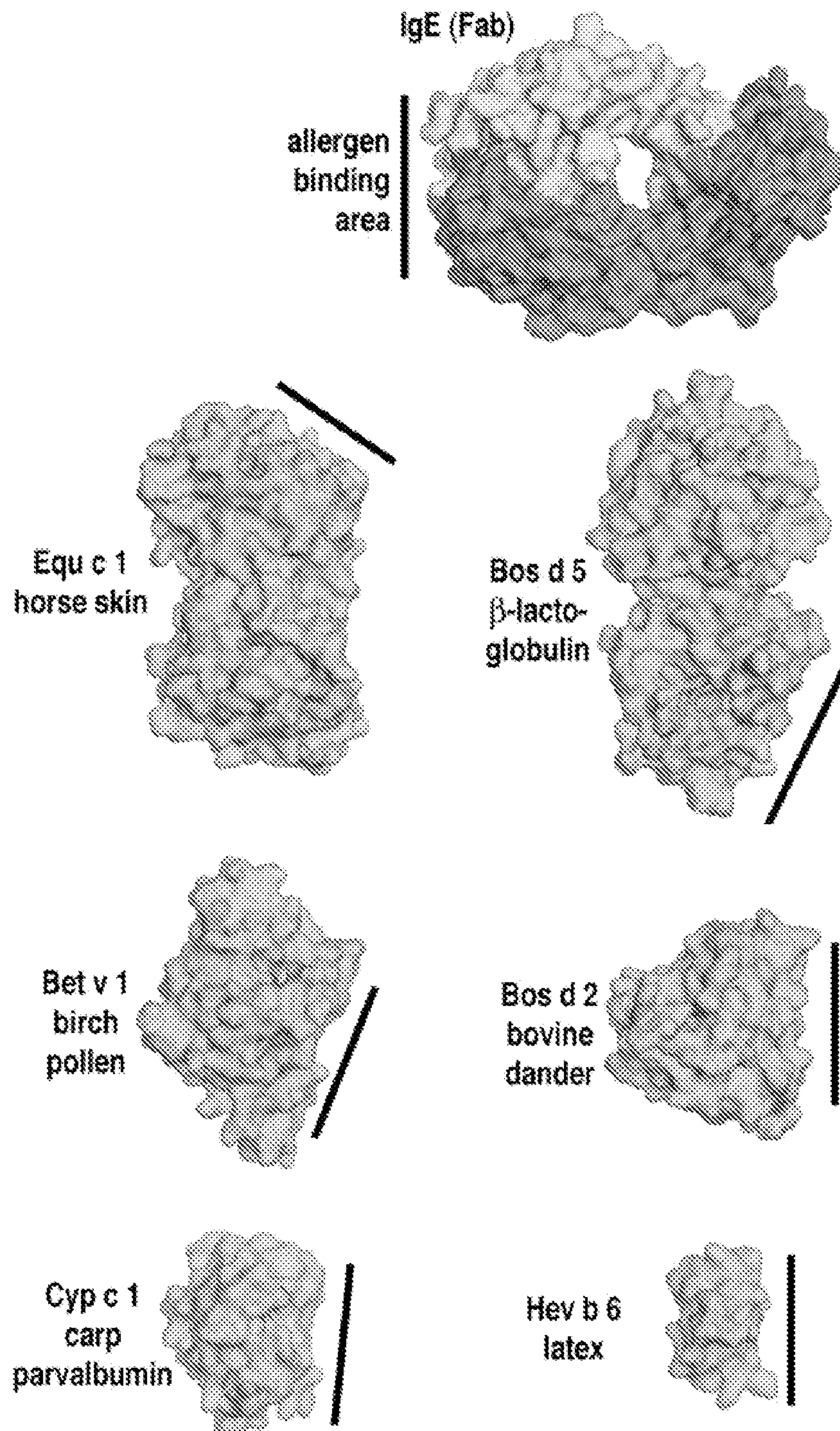


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Figure 13

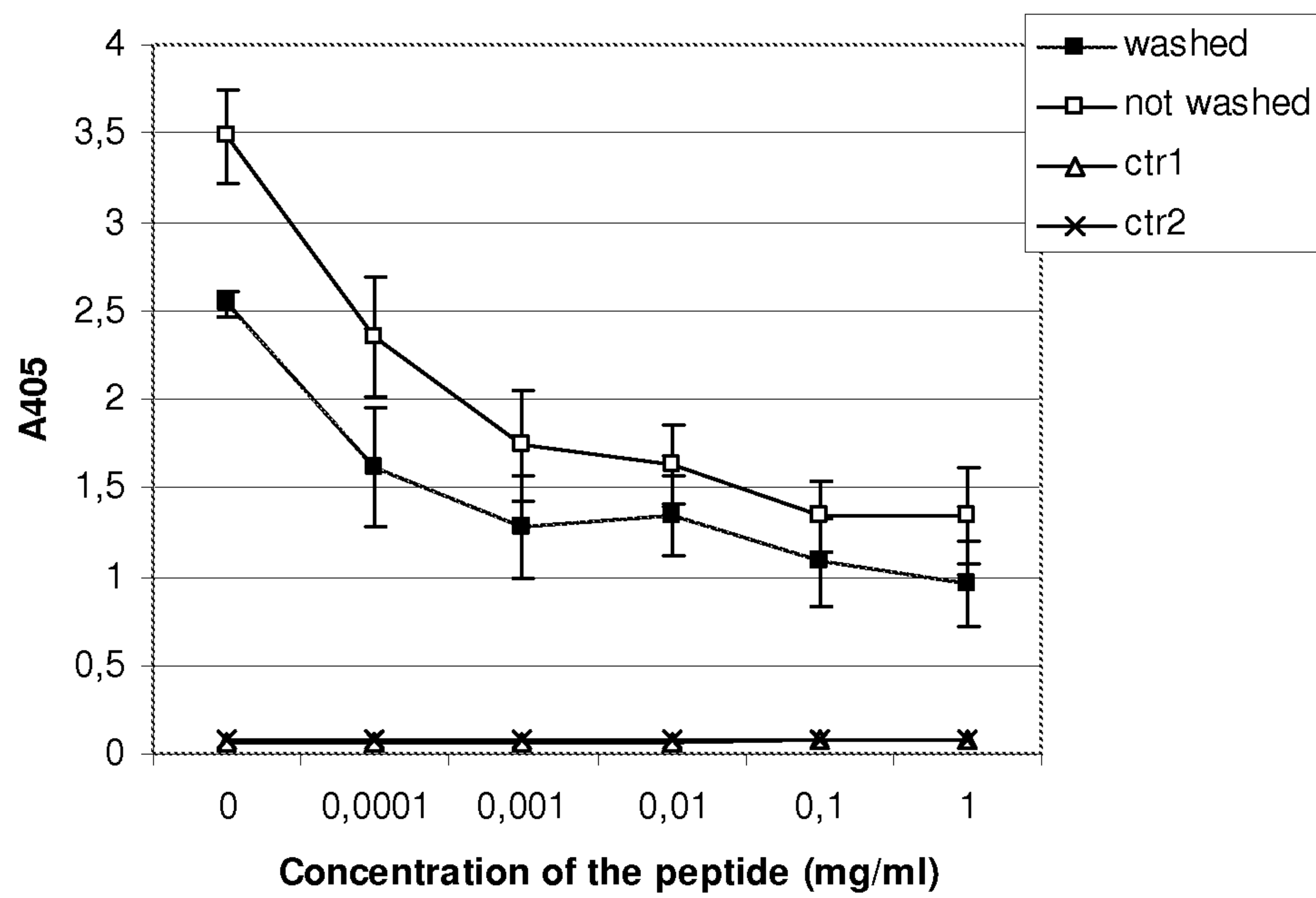
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Figure 14.



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Figure 15.



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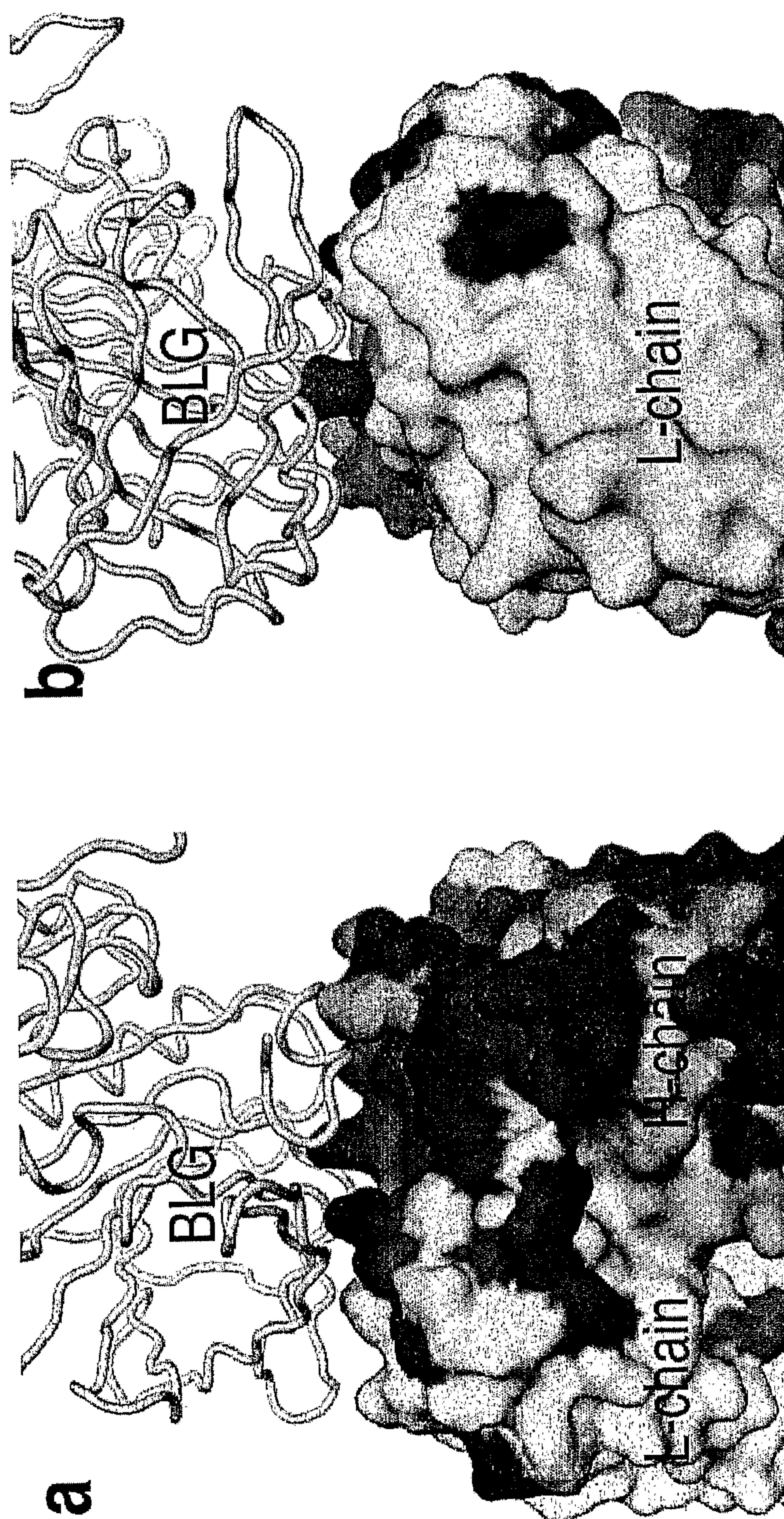
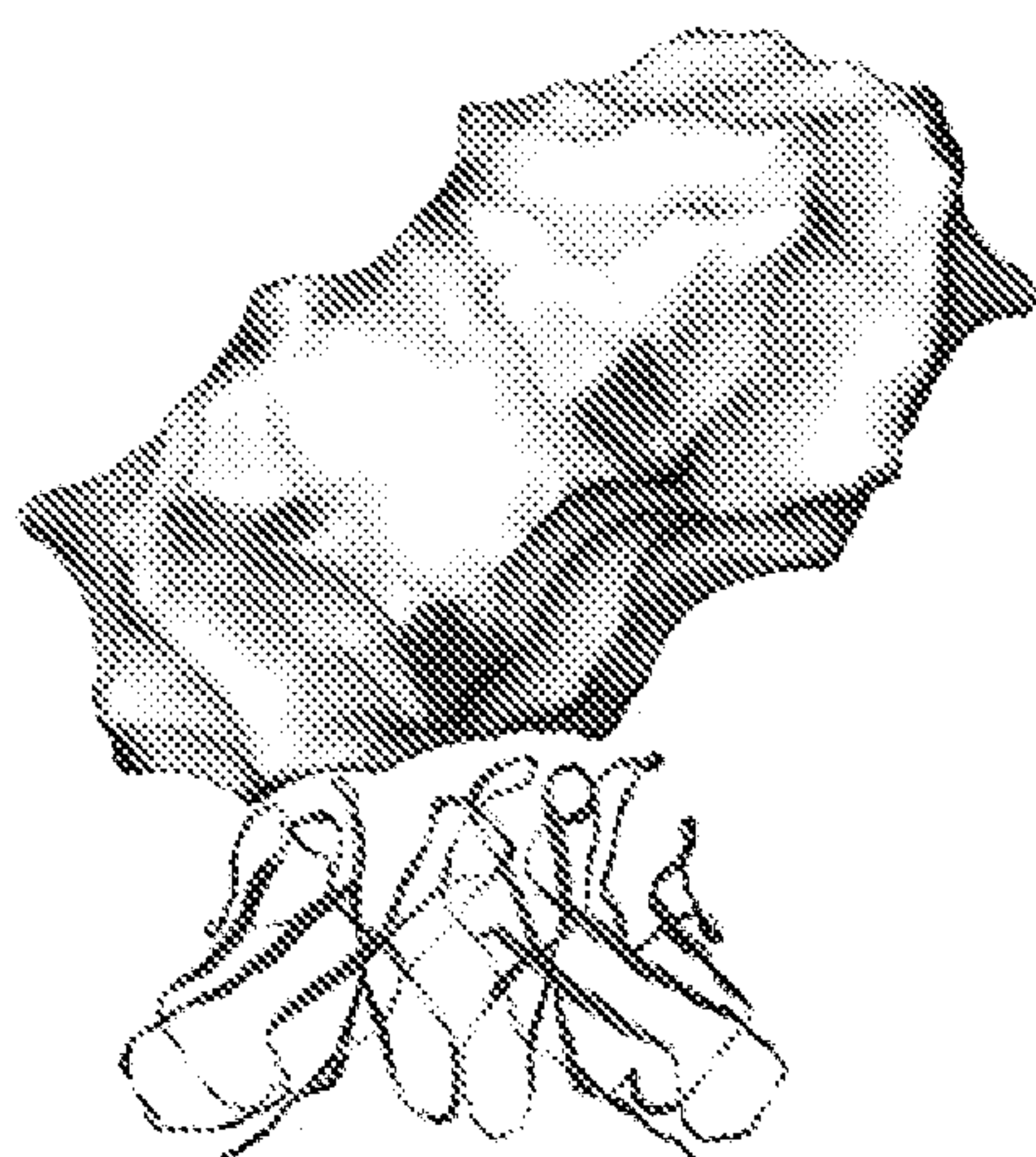


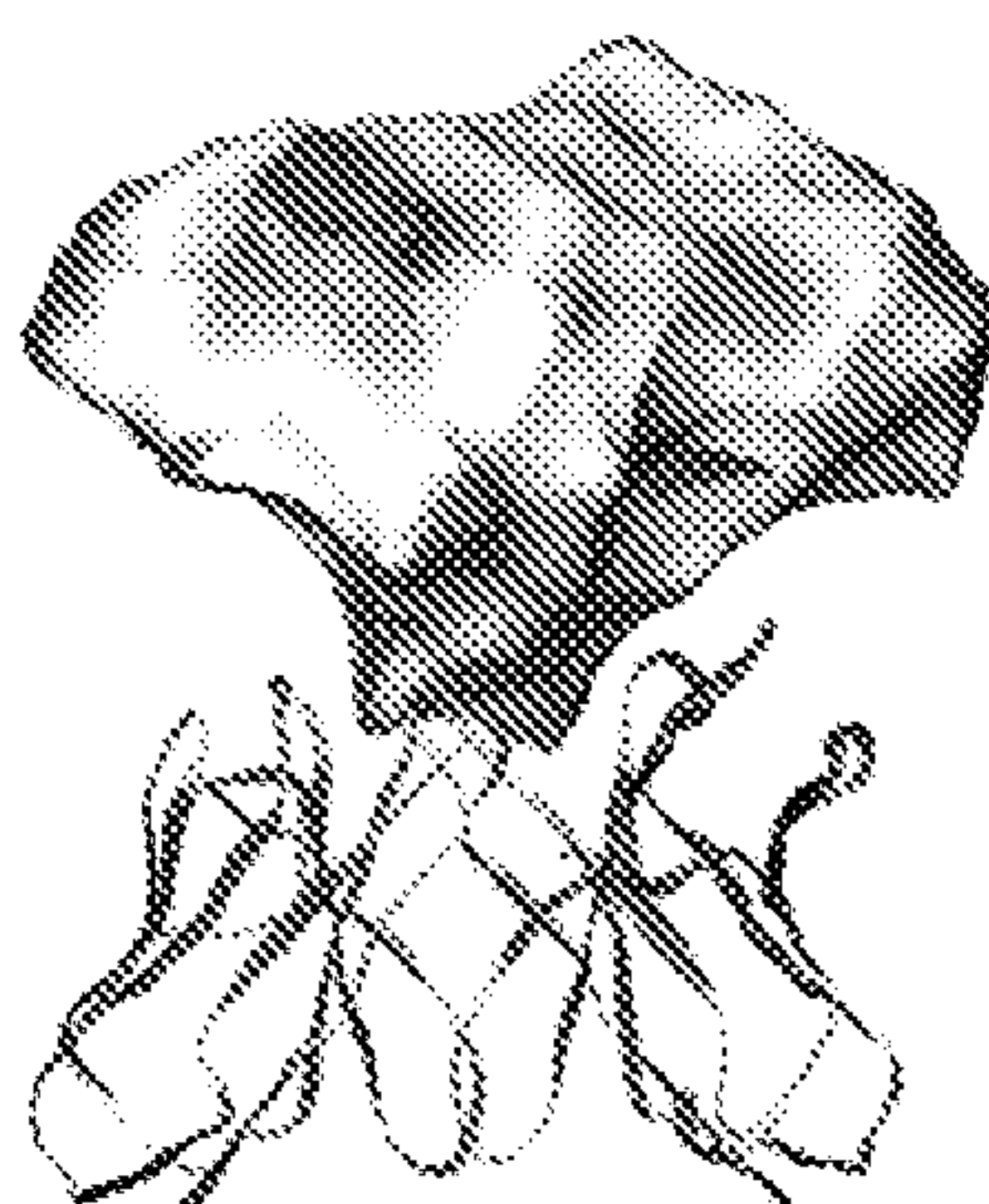
Figure 16

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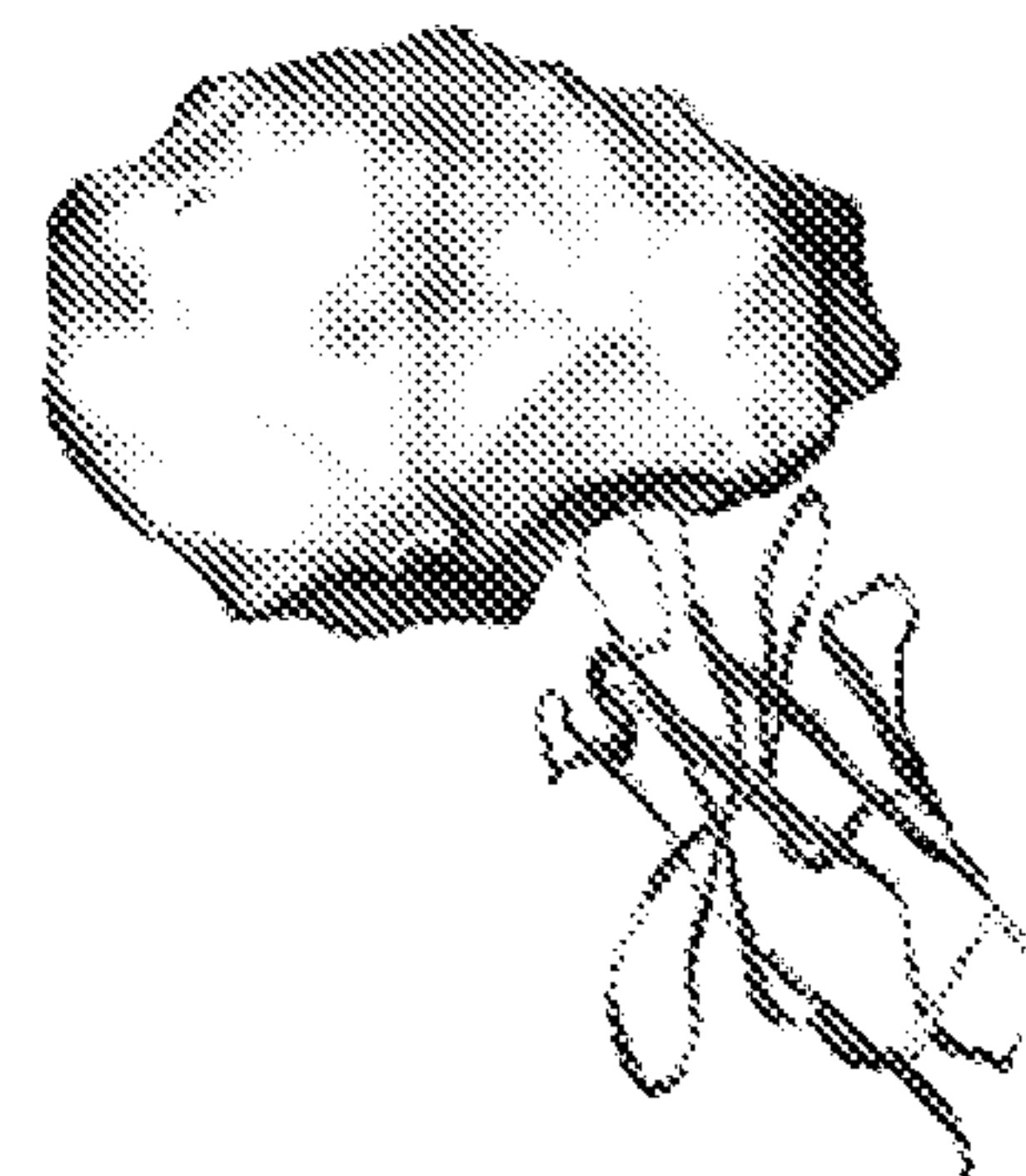
Figure 17.



BLG-IgE complex
flat epitope



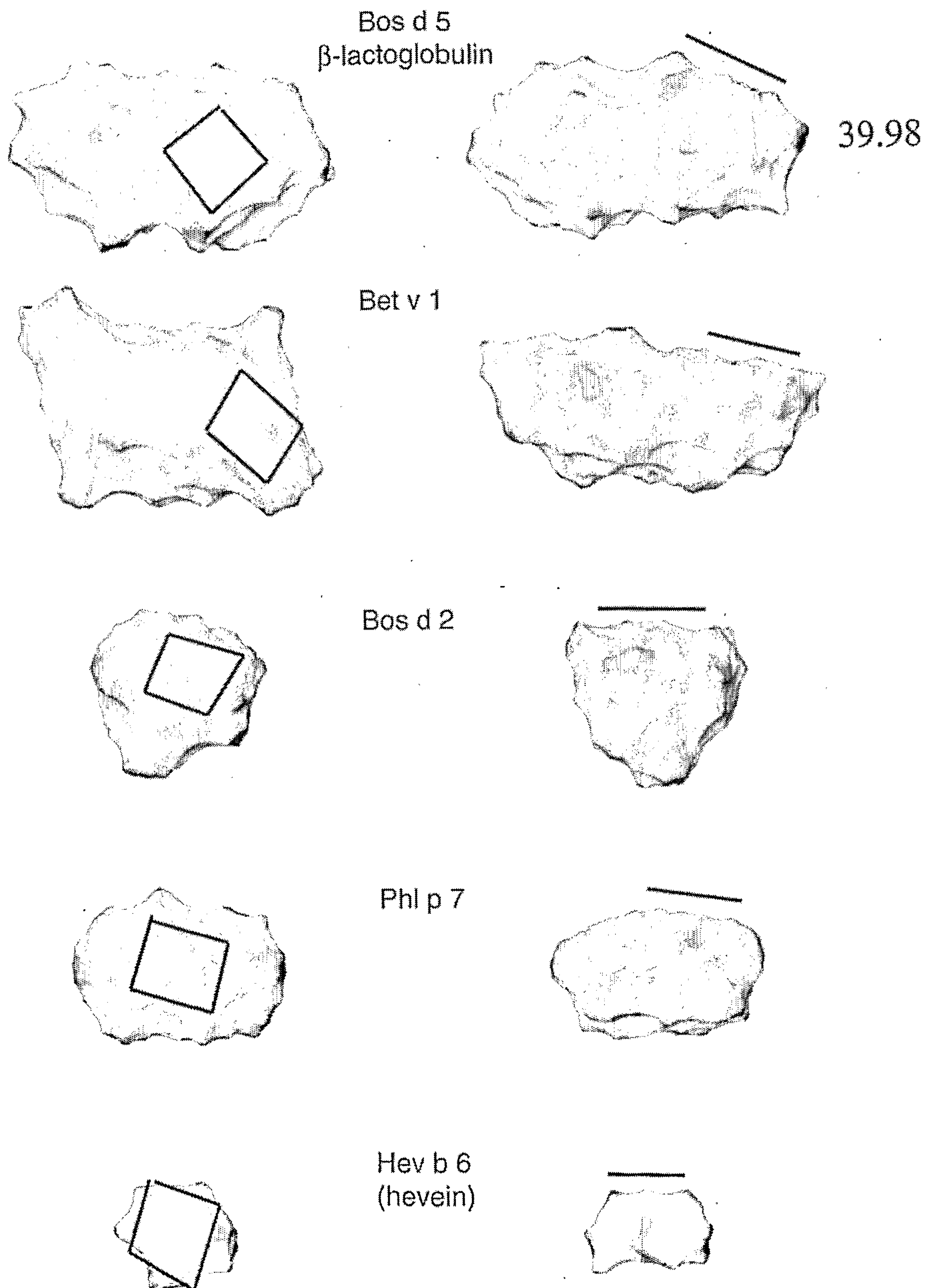
Bet v 1 -IgG complex
convex epitope



lysozyme-single chain
antibody complex
concave epitope

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Figure 18.



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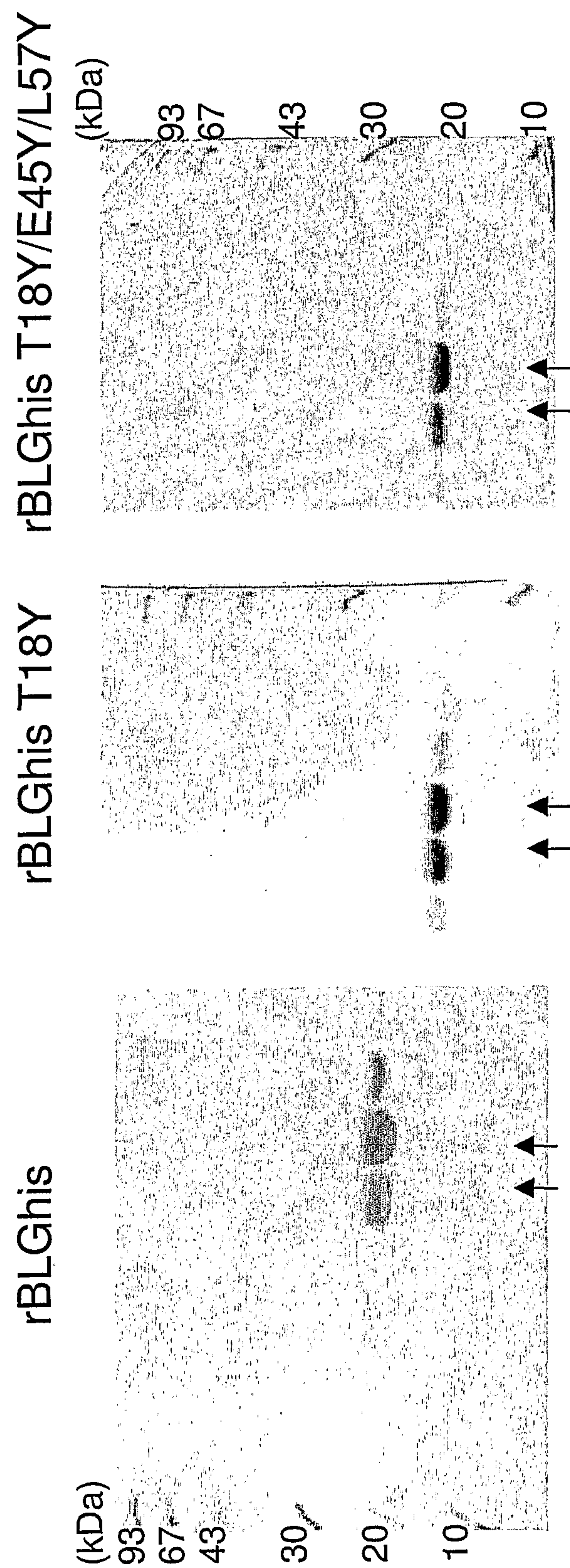
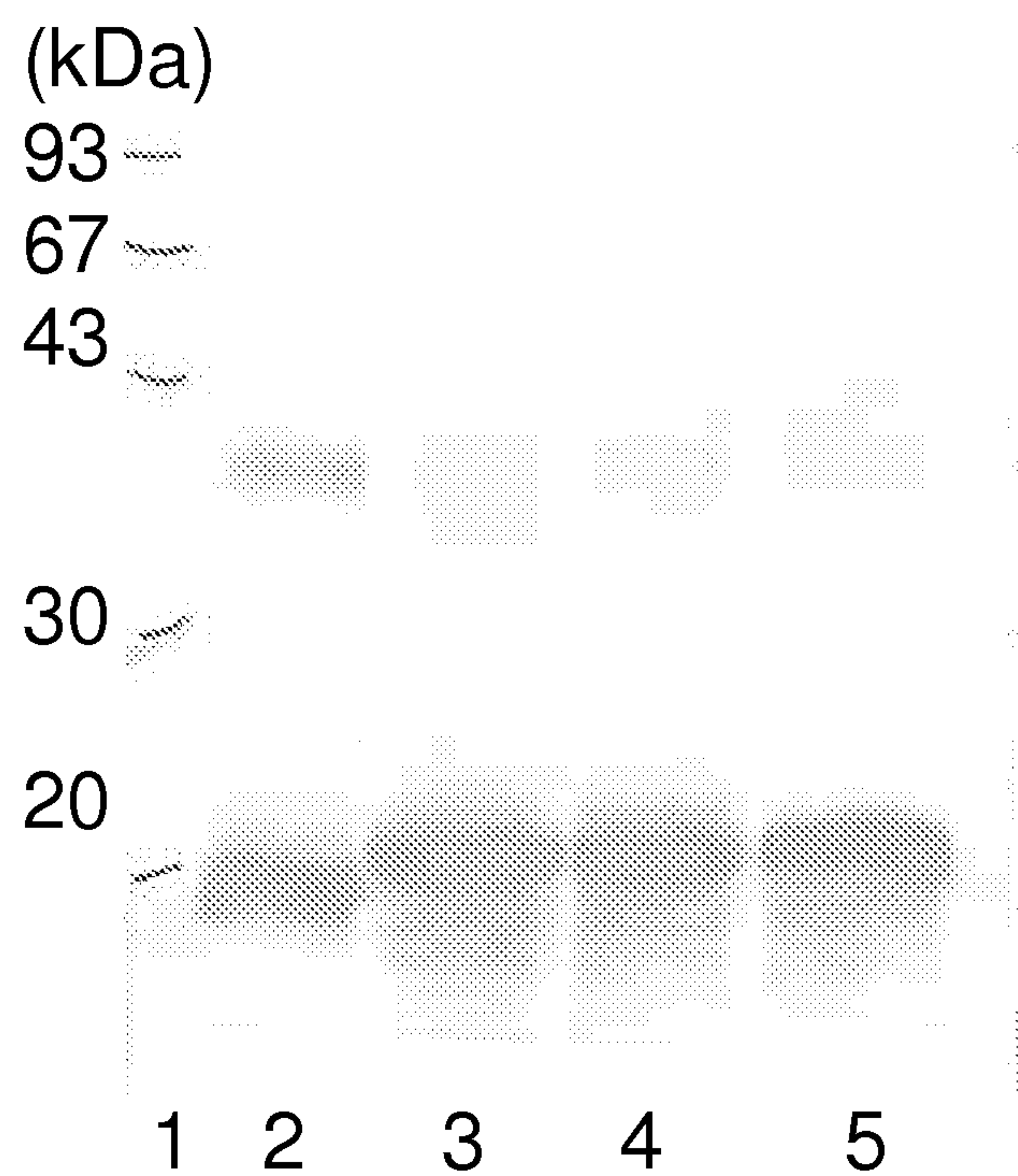


Figure 19

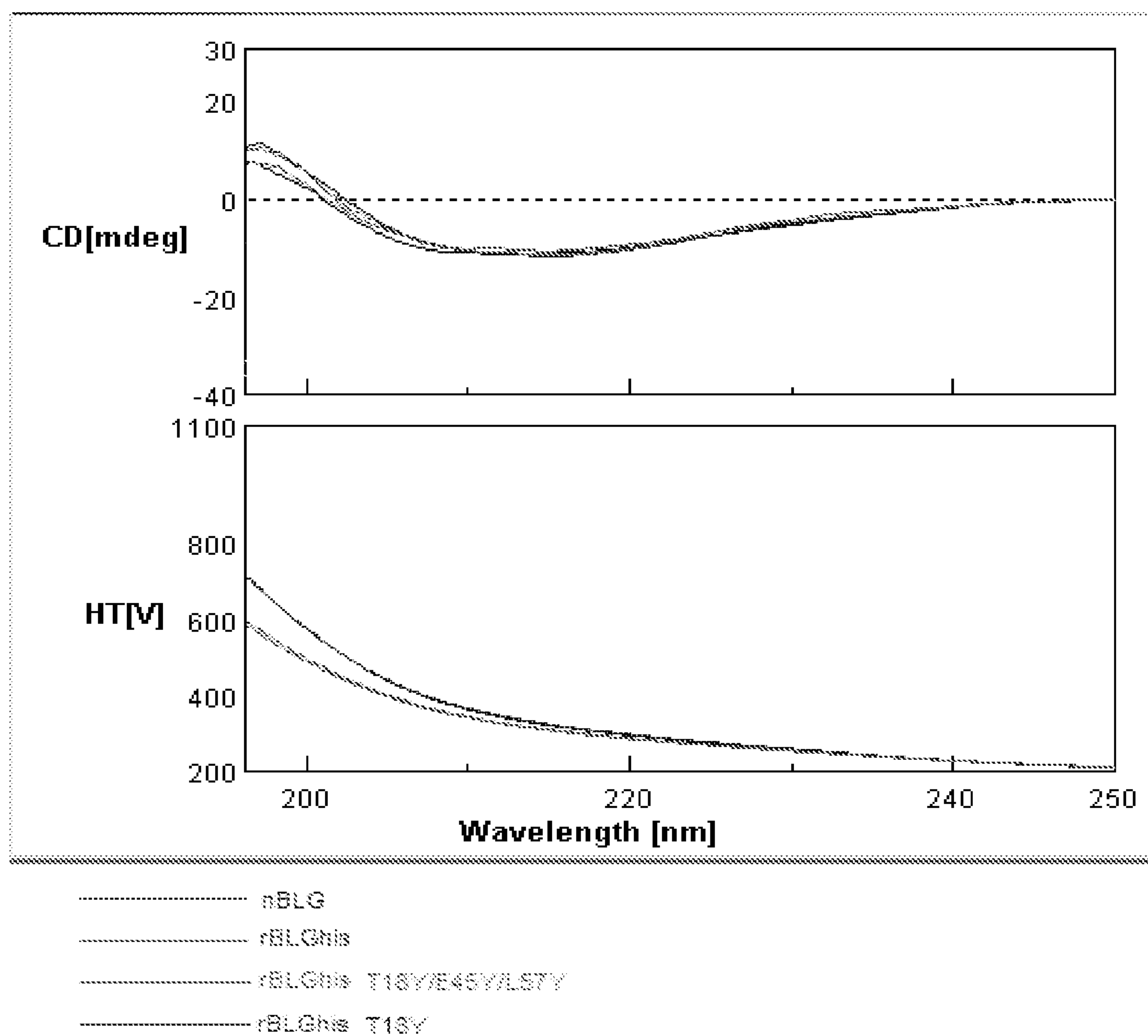
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Figure 20.



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Figure 21.



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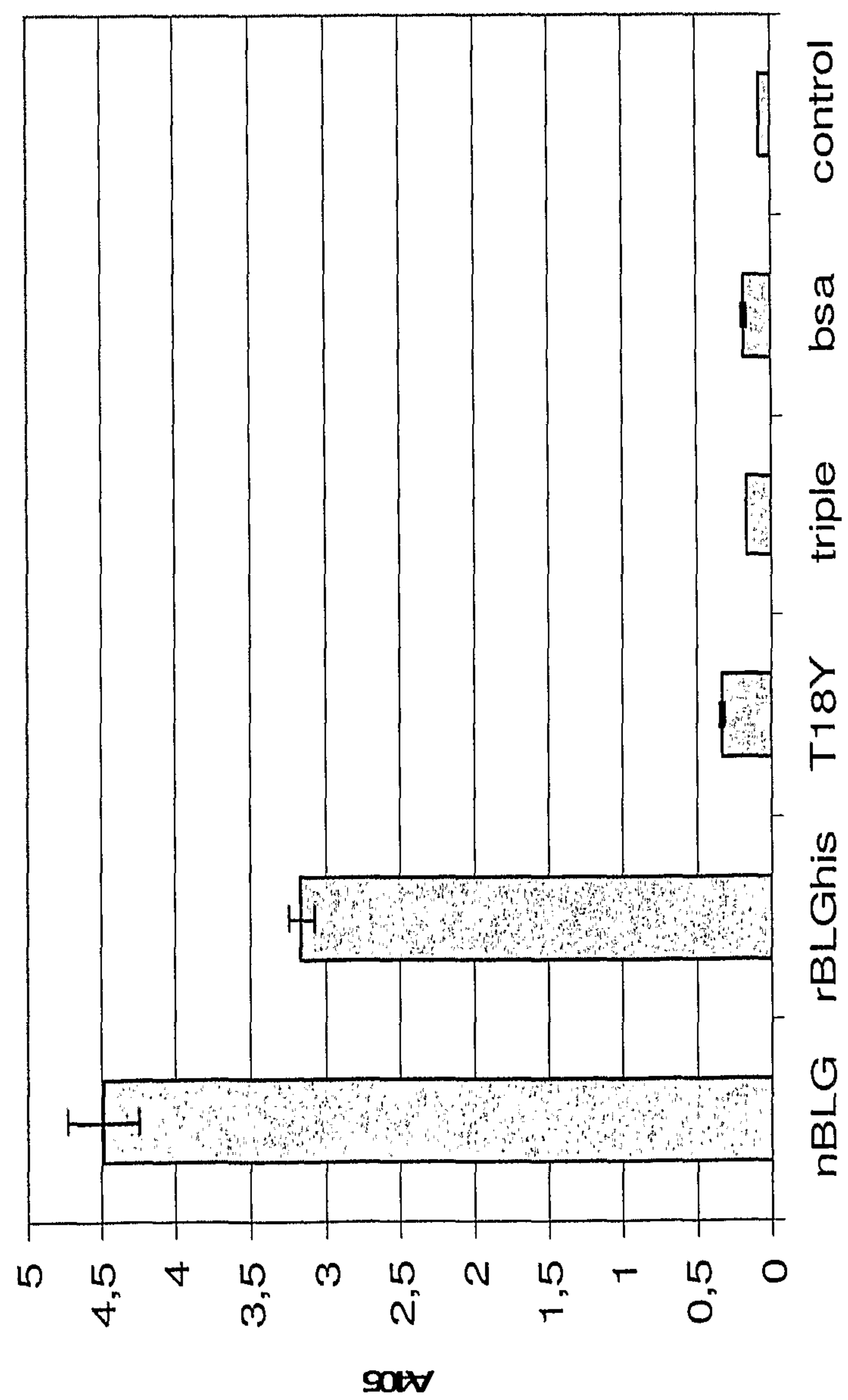
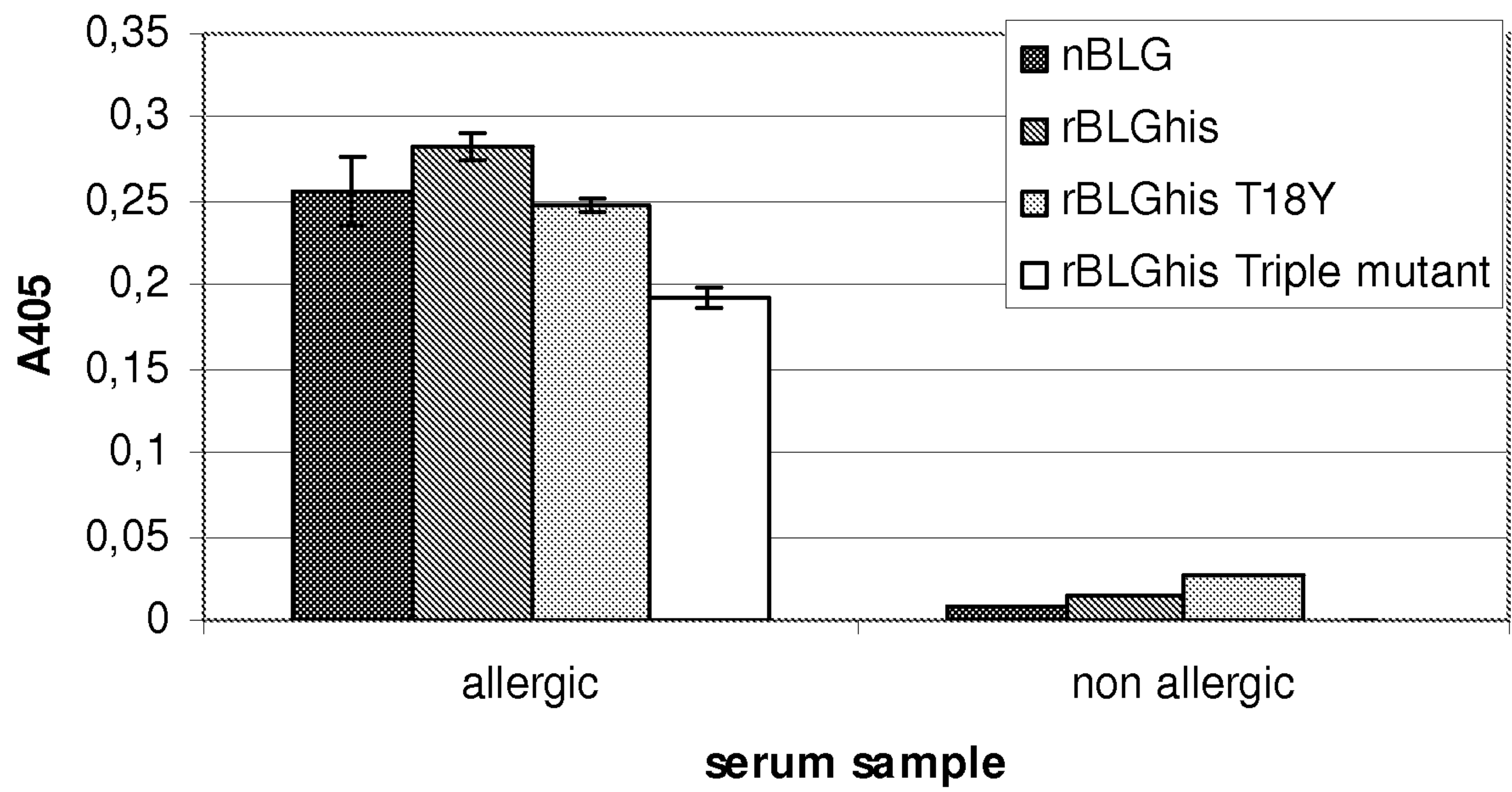


Figure 22

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Figure 23.



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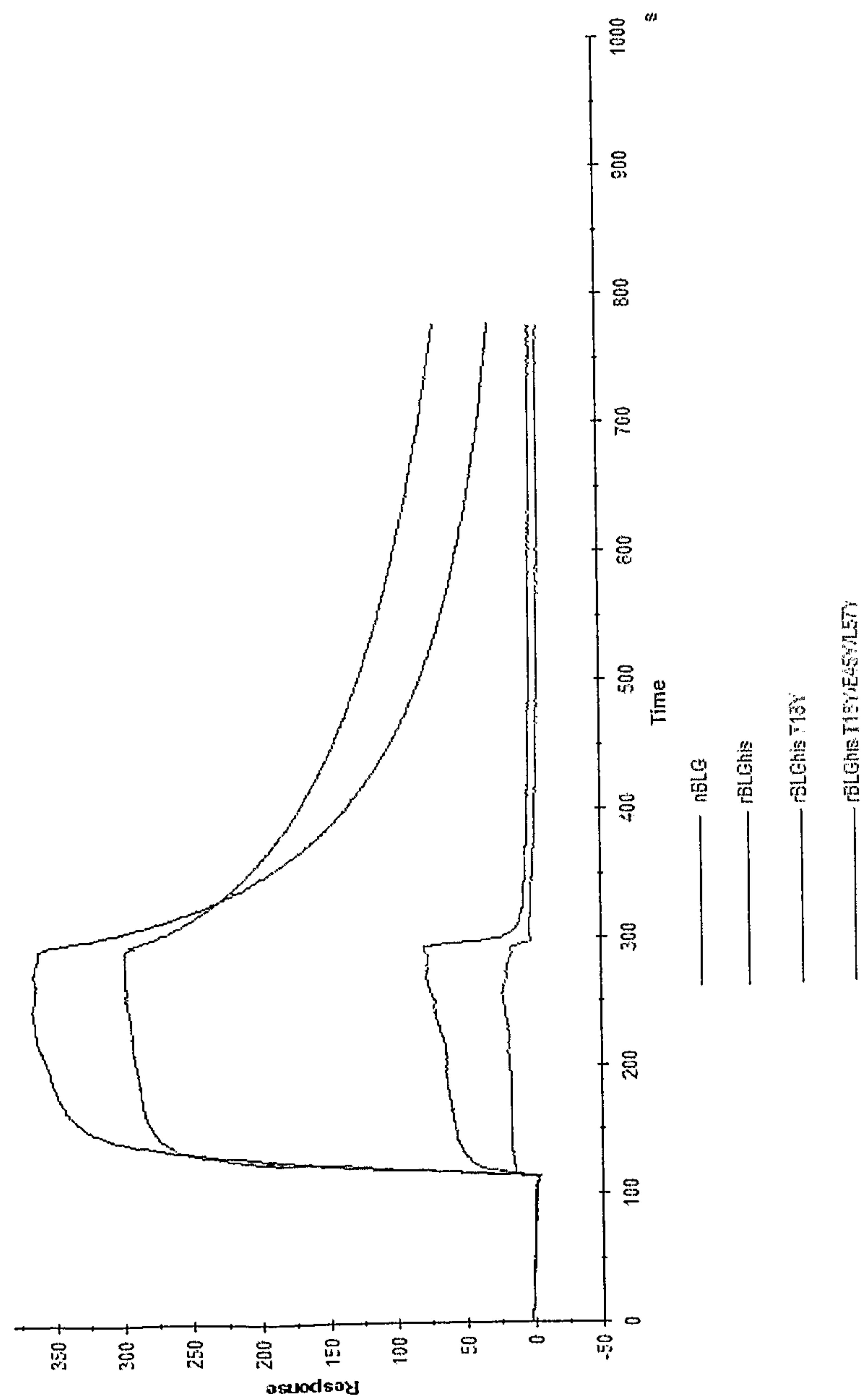


Figure 24