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- (54) Benævnelse: **Lipolytiske enzymvarianter og fremgangsmåde til fremstilling deraf.**
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LIPOLYTIC ENZYME VARIANTS AND METHOD FOR THEIR PRODUCTION**FIELD OF THE INVENTION**

The present invention relates to a lipolytic enzyme variant and a method of producing such a variant. More particularly, the variant has a relatively high activity for one ester
 5 bond in an amphiphilic substrate with two lipophilic groups and a relatively low activity for the ester bond in an amphiphilic substrate with one lipophilic group, e.g. a relatively high phospholipase activity and a relatively low lysophospholipase activity.

BACKGROUND OF THE INVENTION

EP 870840, JP-A 10-42884, JP-A 4-135456 or JP-A 2-49593 describe the use of a
 10 phospholipase to hydrolyze a phospholipid to produce lysophospholipid.

US 4567046, WO 94/04035, EP 109244, EP 585988, WO 98/26057, WO 98/45453, WO 99/53769, WO 00/32758, WO 0139602 and EP 575133 describe the addition of various lipolytic enzymes to dough in the preparation of baked products and the preparation of lipolytic enzyme variants.

15 WO 00/32758 discloses that the substrate specificity of a lipolytic enzyme can be modified by making alterations to the amino acid sequence.

SUMMARY OF THE INVENTION

The invention provides a lipolytic enzyme which: (a) has an amino acid sequence having at least 90% identity to that of SEQ ID NO: 7; and (b) has phospholipase activity; and
 20 (c) has a lyso-phospholipase to phospholipase ratio below 1000; and (d) comprises at least one amino acid alteration corresponding to position H257W, S142A, V157D+S271P, S80T+A127T, D263G, Y21W, S80T, R274A+275YRSAESVDKR, or R274A+275YRSAESVDKAATMTDAELEKKLNSYVQMDKEYVKNNQARS in SEQ ID NO: 7; and wherein the lyso-phospholipase to phospholipase ratio is defined as the lysophospho-
 25 lipase activity divided by the phospholipase where phospholipase activity is determined at 30°C using 4% (w/v) lecithin in 50mM sodium acetate, 5mM CaCl₂, pH 5.0 and lysophospholipase activity is determined at 30°C using 1% (w/v) lysolecithin in 50mM sodium acetate, 5mM CaCl₂, pH 5.0.

The invention also provides a method of preparing a dough or a baked product made
 30 from dough, comprising adding the lipolytic enzyme to the dough, and use of the lipolytic enzyme in the production of pasta, noodles and cheese.

DETAILED DESCRIPTION OF THE INVENTION**Test substrates**

The invention uses two different polar lipids as test substrates. Both are amphiphilic (amphipolaric), having a hydrophilic part and one or two lipophilic groups, respectively.

5 First substrate

The first substrate has the general formula A-B-C where:

- A is an acyl group, particularly straight-chain and unsubstituted. It may be saturated or may have one or more double bonds. It may have an even number of carbon atoms, e.g. from 12 to 24

- B is O (oxygen) or S (sulfur) forming an ester or thioester bond between A and C.

- C is a polyol having B attached to an OH group, optionally having other functional groups and/or a hydrophilic group attached to an OH group. The polyol may be a sugar alcohol such as glycerol, e.g. having B attached in the sn1 or sn2 position of glycerol. The other functional groups may be one or more aldehyde, keto or carboxyl groups; thus, the polyol may be a monosaccharide or a corresponding uronic acid. The hydrophilic group linked to an OH group, e.g. in the sn3 position of glycerol, may be:

- A phosphate group, optionally linked to an alcohol such as choline, ethanolamine, serine or inositol.

- Mono- or digalactosyl link to C through a glycosidic bond.

The first substrate may be a lysophospholipid such as lyso-lecithin or a lyso-galactolipid such as digalactosyl monoglyceride (DGMG) or monogalactosyl monoglyceride (MGMG). The lyso-phospholipid may be a 1-lyso-phospholipid with an acyl group at the sn1-position or a 2-lyso-phospholipid with an acyl group at the sn2-position.

The activity of interest is a hydrolytic activity towards the bond B-C.

Second substrate

The second substrate has the general formula A'-B'- (A''-B''-) C where:

- A' is an acyl group defined as for A above.

- B' is O (oxygen) or S (sulfur) forming an ester or thioester bond between A' and C.

- A'' is an acyl or alkyl group particularly straight-chain and unsubstituted. It may be saturated or may have one or more double bonds. It may have an even number of carbon atoms, e.g. from 12 to 24

- B'' is O (oxygen), S (sulfur) or NH forming an ester, thioester, amide, ether or thioether bond between A'' and C.

- C is the same as for the first substrate.

A" and B" of the second substrate may be chosen identical to A and B of the second substrate and attached in the same position of C, or they may be chosen independently.

The second substrate may be a phospholipid such as lecithin or a galactolipid such as digalactosyl diglyceride (DGDG) or monogalactosyl diglyceride (MGDG), or it may be prepared synthetically by attaching a fatty alcohol through an ether bond or thioether bond to a lysophospholipid or a lyso-galactolipid.

The activity of interest is a hydrolytic activity towards the B'-C bond.

Lipolytic enzyme activities

The lipolytic enzyme of the invention has a low ratio of activity for the first substrate compared to activity for the second substrate. Thus, it has a relatively low hydrolytic activity towards the B-C (thio)ester bond of the first substrate and a relatively high hydrolytic activity towards the B'-C (thio)ester bond of the second substrate. The activity towards the second substrate may be phospholipase A1 (EC 3.1.1.32) or A2 (EC 3.1.1.4), or it may be a galactolipase activity.

The activity ratio may be found by contacting the lipolytic enzyme with each substrate separately or by contacting it with a mixture including both substrates. The activity ratio may be measured by the PLARN assay, the RLPLA assay or a plate assay described below. The lipolytic enzyme may have a ratio of lysophospholipase activity to phospholipase activity corresponding to PLARN below 1000 (particularly 500, below 200 or below 50) or RLPLA (0.1/2.5) below 2 (particularly below 1 or below 0.5).

The lipolytic enzyme of the invention may have phospholipase (PL) activity with a relatively low lysophospholipase (LPL) activity. The lyso-phospholipid may be a 1-lysophospholipid with an acyl group at the sn1-position or a 2-lysophospholipid with an acyl group at the sn2-position. The lipolytic enzyme may in particular have phospholipase A1 activity with low 1-lysophospholipase activity.

The lipolytic enzyme of the invention may have hydrolytic activity towards a carboxylic ester bond in DGDG (digalactosyl diglyceride) with a relatively low hydrolytic activity towards the ester bond in DGMG (digalactosyl monoglyceride).

Optionally, the lipolytic enzyme may also have triacylglycerol lipase activity (EC 3.1.1.3), i.e. hydrolytic activity for carboxylic ester bonds in triglycerides, e.g. 1,3-specific activity, particularly on long-chain triglycerides such as olive oil. The enzyme may have a substrate specificity for hydrolyzing long-chain fatty acyl groups rather than short-chain groups, e.g. expressed as a high ratio of activities on olive oil and tributyrin, e.g. a ratio SLU/LU>3 as described in WO 0032758.

LPL/PL ratio (PLARN)

Phospholipase activity is determined at 30 °C using 4% (w/v) lecithin (phosphatidyl choline) in 50 mM sodium acetate, 5 mM CaCl₂, pH 5.0. One unit of phospholipase activity is defined as 1 mmol free fatty acids released per minute per mg enzyme using the above conditions.

Lysophospholipase activity is determined at 30 °C using 1% (w/v) lysolecithin in 50 mM sodium acetate, 5 mM CaCl₂, pH 5.0. One unit of lysophospholipase activity is defined as 1 mmol free fatty acids released per minute per mg enzyme using the above conditions. The lysolecithin may be an equilibrium mixture or pure 1- lysolecithin in the case of a phospholipase A1 and pure 2- lysolecithin in the case of a phospholipase A2.

The PLARN ratio is defined as the lysophospholipase activity divided by the phospholipase activity, both determined by the above methods.

Relative activity on lysopholipids and phospholipids (RLPLA)

This activity measurement expresses the relative activity on lysophosphatidyl choline and phosphatidyl choline in an equimolar mixture.

More specifically the assay is carried out as follows: The activity at different concentrations of phospholipase is determined at 30°C blending 1:1 solutions of phosphatidyl choline (25mM) and lysophosphatidyl choline (25mM) in 50mM NaOAc buffer (pH 5). 50µl enzyme solution (e.g. having 0.1 or 2.5 mg enzyme protein per ml) is added to the substrate solution and allowed to react for 30 minutes. 100µl of the sample is inactivated at 95°C for 5 minutes and dissolved in 900µl CHCl₃/MeOH 50%/50%. The sample is centrifuged at 14000rpm for 2 minutes. The supernatant is analyzed by HPLC after filtering through a 0.45µm filter. Column: Microsorb-MV 100Si 250mm column (analytical instruments). Mobile phases: A: 80% CHCl₃, 19.5% MeOH, 0.5% NH₄OH; B: 60% CHCl₃, 34% MeOH, 0.5% NH₄OH, 5.5% H₂O. Gradient: 0-3 minutes 100% A, 3-23 minutes 100% B, 23-45 minutes 100% A. Injection volume 20µl Detector: Sedere, Sedex 75 light scattering, Temp 40°C, pressure 3.5 Bar. The RLPLA is then measured as the depletion of phosphatidyl choline relative to lysophosphatidyl choline. A variant with a lower RLPLA value indicates a higher accumulation of lysophospholipid under the conditions of analysis.

The relative activity can be expressed as "RLPLA ratio" by measuring lysolecithin hydrolysis at an enzyme dosage of 0.1 mg/ml and lecithin hydrolysis at a dosage of 2.5 mg/ml, and taking the ratio of the two.

Plate assay

Plates including each of the substrates may be prepared in analogy with WO 0032758 using suitable pH and substrate concentration. Optionally, other ingredients such as

flour may be included. A suitably diluted enzyme solution is applied to holes in the plates, and clearing zones are read after incubation for a suitable time at a suitable temperature.

Preparation of lipolytic enzyme

The lipolytic enzyme may be obtained by preparing variants of a parent lipolytic enzyme by altering its amino acid sequence and screening for a variant with an improved activity ratio. The parent lipolytic enzyme may have phospholipase activity, DGDG hydrolytic activity and/or triacylglycerol lipase activity. Variants may be prepared from the parent lipolytic enzyme by known methods, e.g. by subjecting a DNA sequence encoding the parent lipolytic enzyme to site-directed mutagenesis, localized random mutagenesis or site-saturation mutagenesis, e.g. using methods described in WO 0032758. Resulting DNA sequences may be further modified by gene shuffling and directed evolution.

Parent lipolytic enzyme

The lipolytic enzyme to be used in the present invention is one that can hydrolyze ester bonds. Such enzymes include, for example, lipases, such as triacylglycerol lipase (EC 3.1.1.3), lipoprotein lipase (EC 3.1.1.34), monoglyceride lipase (EC 3.1.1.23), phospholipase A1 or A2 (EC 3.1.1.26, 3.1.1.4), lysophospholipase (EC 3.1.1.5), galactolipase (EC 3.1.1.26), ferulic acid esterase and esterase (EC 3.1.1.1, EC 3.1.1.2).

The parent lipolytic enzyme may be the *Thermomyces lanuginosus* lipase (*Humicola lanuginosa* lipase) (EP 305216) or it may have an amino acid sequence with at least 50 % identity (e.g. at least 90 % identity). The amino acid sequence of the *T. lanuginosus* lipase is shown in US 5869438 and as seq14 in Fig. 2 of this application.

Thus, the parent lipolytic enzyme may be a naturally occurring enzyme as described at pages 5-6 of WO 0032758. Examples are the lipolytic enzymes from the following organisms. They are known in the prior art; and their amino acid sequences are given in the attached sequence listing.

1. *Absidia reflexa*
2. *Absidia corymbifera*
3. *Rhizmucor miehei*
4. *Rhizopus delemar (oryzae)*
5. *Aspergillus niger*
6. *Aspergillus tubingensis*
7. *Fusarium oxysporum*
8. *Fusarium heterosporum*
9. *Aspergillus oryzae*
10. *Penicillium camembertii*

11. *Aspergillus foetidus*
12. *Aspergillus niger*
13. *Aspergillus oryzae*
14. *Thermomyces lanuginosus (Humicola lanuginosa)*

5 As indicated above, the amino acid to be altered may be determined on the basis of an alignment of the parent lipolytic enzyme with the *T. lanuginosus* lipase. Fig. 2 shows an alignment of the amino acid sequences of the above fungal lipolytic enzymes, based on a comparison of the available 3-dimensional structures:

Other amino acid sequences may be aligned with those shown in Fig. 2 by using the
 10 GAP alignment to the most homologous sequence found by the GAP program. GAP is provided in the GCG program package (Program Manual for the Wisconsin Package, Version 8, August 1994, Genetics Computer Group, 575 Science Drive, Madison, Wisconsin, USA 53711) (Needleman, S.B. and Wunsch, C.D., (1970), Journal of Molecular Biology, 48, 443-45). The following settings are used for polypeptide sequence comparison: GAP creation
 15 penalty of 3.0 and GAP extension penalty of 0.1.

Alternatively, the parent lipolytic used in the present invention may be a variant of the above, e.g. a variant of the *T. lanuginosus* lipase (SEQ ID NO: 14) or the *F. oxysporum* lipase/phospholipase (SEQ ID NO: 7). A variant with phospholipase activity or galactolipase activity may be used, e.g. as described in Example 5, 6 or 13 of WO 0032758. Particular ex-
 20 amples are variants of SEQ ID NO: 14 with the following amino acid alterations:

L259S
G266D
G91A+ D96W +E99K +G263Q +L264A +I265T +G266D +T267A +L269N +270A +271G +272G +273F +274S
G266E
G263A +G266A
E1SPCRPRP +E239C +Q249R +G266A
E1SPCRPRP +E239C +Q249R +G266S
D96S +G266A
D96S +G266S
D96S +G266W
E1SPPCGRRP +D96S +E239C +Q249R +G263D +L264I +I265N +G266E +T267GS

Three-dimensional model

Fig. 1 gives the coordinates of a three-dimensional model of the *T. lanuginosus* lipase docked with a phospholipid as substrate: 1-palmitoyl-2-oleylglycero-sn-3-phosphocholine (POPC). This may be used as a starting point for building a similar model for any given fungal lipolytic enzyme. Using this model, the following amino acid residues are found to be within 10 Å, 7 Å and 5 Å of an atom of the substrate (LIP1 in the pdb structure shown in Fig. 1):

10 Å: 17-18, 20-23, 26, 37, 39, 62, 64, 80-96, 110-113, 144-151, 171-177, 200-211, 213, 215, 227, 253-261, 263-269.

7 Å: 21, 81-95, 110, 113, 145-148, 150, 172-175, 201-208, 213, 254-256, 258-259, 264-269.

5 Å: 21, 82-86, 89-90, 92-93, 95, 110, 113, 145-147, 174, 202-203, 206-208, 255, 258-259, 265-268.

More particularly, amino acid alterations may be made at one or more positions corresponding to the following amino acids in the *T. lanuginosus* lipase (SEQ ID NO: 14): Y212, R84, S85, E87, D96, V203, L206, L227, P253, D254, P256, P257 and/or Y261, particularly one or more alterations corresponding to Y21V/K, R84W/A/G/Y/S, S85D, E87A, D96F/K/G, V203I, L206F, P253Q, D254*, P256N, P257S and/or Y261Q.

Further, amino acid alterations may be made at one or more positions corresponding to H257, S142, S80, D263 and/or Y21 of the *F. oxysporum* lipase/phospholipase (SEQ ID NO: 7), particularly one or more corresponding to H257W, S142A, S80T, D263G and/or Y21W.

Also, amino acid alterations may be made at the C-terminal or at any position downstream of L269 of SEQ ID NO: 14. Such alteration may be addition or deletion of a peptide extension or deletion of a peptide extension of one or more amino acids (e.g. 1-50 amino acids such as 2-15) at the C-terminal.

Amino acid alteration

The amino acid alteration may be substitution with a larger amino acid. The amino acid residues are ranked by size as follows from smallest to largest:

G, A, S, C, V, T, P, L, I, N, D, M, E, Q, K, H, R, F, Y, W

An amino acid residue within 10 Å (or 7 Å or 5 Å) of a C atom in the alkyl group R of R-COO attached to sn1 of the lyso-phospholipid may be substituted with an amino acid residue which is larger or more hydrophilic.

An amino acid residue within 10 Å (or 7 Å or 5 Å) of an atom (other than H) of the phosphate group attached to sn3 (i.e. the O atom at sn3 or any atom beyond that) may be substituted with an amino acid which is larger or more hydrophobic.

Amino acid residues are ranked as follows from most hydrophilic to most hydrophobic:

R, K, E, D, N, Q, H, S, T, Y, C, M, G, A, V, P, L, I, F, W

Lipolytic enzyme variant

5 Starting from a variant having phospholipase activity derived from the *T. lanuginosus* lipase, and improvement regarding increased ratio of lecithin/lysolecithin(sn1) activity and lowered activity against lysolecithin (sn1) of lysolecithin in general, or/and with improved sn1 lecithase activity may be achieved by use of the following concepts.

10 One concept is to lower the binding energy of sn1 acyl chain and in this way increase the ratio of activity lecithin/lysolecithin(sn1). Secondary to increase sn2 binding to favour lecithin rather than lysolecithin.

Thus, 206, 95, 203 and 93 may be made smaller and more hydrophilic. Also, positions 253, 255 and 256 may be made bigger. Some particular examples of such variants are:

L206V/S/T/A

15 V203T/S/A

F95I/L/Y

L93V/I/A/T

A doped library 206/203 and 95/93. appr. 90% wt and appr 10% variant may be used.

20 A second concept is to make libraries in the contacts to both acyl chains found docked structures, and in the regions close to the substrate found by comparison of good and bad lysolecithase active homologous enzymes. The regions will be doped according to the homologous enzymes sequence.

25 Thus, region 265-269 is of interest, e.g. P253. Some particular examples of such variants are:

A doped library 247-260 may be used, optionally together with doped I202P and L206V. The doping may be appr. 90%wt and appr. 10% variants.

P253TG/L

D254S/L

30 I255

P256L/A

A257D/A

L259

W260H

35 Proline removal(s):

P256X

P253X

together with I202P

L227D

Library 247-260 and 206, 95, 203 and 93 may be combined.

5 Amino acid identity

The lipolytic enzyme of the invention and the parent lipolytic enzyme may have an amino acid identity of at least 50 % (particularly at least 90 %, e.g. more than 95 % or more than 98 %) with the *T. lanuginosus* lipase (SEQ ID NO: 14).

The degree of identity may be suitably determined by means of computer programs known in the art, such as GAP provided in the GCG program package (Program Manual for the Wisconsin Package, Version 8, August 1994, Genetics Computer Group, 575 Science Drive, Madison, Wisconsin, USA 53711) (Needleman, S.B. and Wunsch, C.D., (1970), Journal of Molecular Biology, 48, 443-45), using GAP with the following settings for polypeptide sequence comparison: GAP creation penalty of 3.0 and GAP extension penalty of 0.1.

15 Use of lipolytic enzyme variant

Hydrolysis of phospholipid

A variant with phospholipase activity can be used to prepare lysophospholipid (e.g. lyso-lecithin) by treating the corresponding phospholipid with the variant, e.g. as described in EP 870840, JP-A 10-42884, JP-A 4-135456 or JP-A 2-49593. The variant can also be used to make mayonnaise, e.g. as described in EP 628256, EP 398666 or EP 319064.

Advantageously, a low ratio of lysophospholipase/phospholipase activity can lead to a high degree of phospholipid hydrolysis with a low degree of lysophospholipid hydrolysis. This may allow the use of long reaction time and the use of phospholipid with a high lysophospholipid content, e.g. from cereals such as oats.

25 Baking

Lipolytic enzymes according to the invention have improved baking performance, e.g. a lower dough stickiness, a better dough extensibility and elasticity, a better dough stability, a better crumb structure of the baked product, a larger loaf volume and/or improved resistance to over-proofing or other abuse.

The invention provides a baking additive in the form of a granulate, an agglomerated powder or a stabilized liquid, comprising a lipolytic enzyme which:

- a) has phospholipase activity, and
- b) has a lysophospholipase to phospholipase ratio corresponding to PLARN below 500 or RLPLA (0.1/2,5) .below 1.0.

The baking additive may have a narrow particle size distribution with more than 95 % (by weight) of the particles in the range from 25 to 500 μm .

Granulates and agglomerated powders may be prepared by conventional methods, e.g. by spraying the lipolytic enzyme onto a carrier in a fluid-bed granulator. The carrier may consist of particulate cores having a suitable particle size. The carrier may be soluble or insoluble, e.g. a salt (such as NaCl or sodium sulfate), a sugar (such as sucrose or lactose), a sugar alcohol (such as sorbitol), starch, rice, corn grits, or soy. Liquid enzyme preparations may, for instance, be stabilized by adding a polyol such as propylene glycol, a sugar or sugar alcohol, lactic acid or boric acid according to established methods.

10 The invention further relates to a pre-mix comprising flour and the lipolytic enzyme described above. The pre-mix may contain other dough-improving and/or bread-improving additives, e.g. any of the additives, including enzymes, mentioned above.

The invention also provides a method of preparing a dough or a baked product prepared from dough. The method may comprise preparing a variant by the above method and adding it to the dough. Alternatively, the method may comprise:

- a) testing at least one lipolytic enzyme for its hydrolytic activities towards intact phospholipid (PL) and lyso-phospholipid (LPL),
- b) selecting a lipolytic enzyme having a hydrolytic activity ratio for LPL/PL corresponding to PLARN below 500, and
- 20 c) adding the selected lipolytic enzyme to the dough.

Dough

The dough generally comprises wheat meal or wheat flour and/or other types of meal, flour or starch such as corn flour, corn starch, rye meal, rye flour, oat flour, oat meal, soy flour, sorghum meal, sorghum flour, rice starch, rice flour, potato meal, potato flour or potato starch. The dough may be fresh, frozen or par-baked. It may particularly be a leavened dough.

The dough may also comprise other conventional dough ingredients, e.g.: proteins, such as milk powder, gluten, and soy; eggs (either whole eggs, egg yolks or egg whites); an oxidant such as ascorbic acid, potassium bromate, potassium iodate, azodicarbonamide (ADA) or ammonium persulfate; an amino acid such as L-cysteine; a sugar; a salt such as sodium chloride, calcium acetate, sodium sulfate or calcium sulfate.

The dough may comprise fat (triglyceride) such as granulated fat or shortening, but the invention is particularly applicable to a dough where less than 1 % by weight of fat (triglyceride) is added, and particularly to a dough which is made without addition of fat.

35 The dough may further comprise an emulsifier such as mono- or diglycerides, diacetyl tartaric acid esters of mono- or diglycerides, sugar esters of fatty acids, polyglycerol esters

of fatty acids, lactic acid esters of monoglycerides, acetic acid esters of monoglycerides, polyoxyethylene stearates, or lysolecithin, but the invention is particularly applicable to a dough which is made without addition of emulsifiers (other than optionally phospholipid).

Baked product

5 The process of the invention may be used for any kind of baked product prepared from dough, either of a soft or a crisp character, either of a white, light or dark type. Examples are bread (in particular white, whole-meal or rye bread), typically in the form of loaves or rolls, French baguette-type bread, pita bread, tortillas, cakes, pancakes, biscuits, cookies, muffins, pie crusts, crisp bread, steamed bread, pizza and the like.

10 Additional enzyme

 Optionally, an additional enzyme may be used together with the lipolytic enzyme. The additional enzyme may be a second lipolytic enzyme (e.g. as described in PCT/DK01/00472), an amylase, particularly an anti-staling amylase, an amyloglucosidase, a cyclodextrin glucanotransferase, or the additional enzyme may be a peptidase, in particular an
15 exopeptidase, a transglutaminase, a cellulase, a hemicellulase, in particular a pentosanase such as xylanase, a protease, a protein disulfide isomerase, e.g., a protein disulfide isomerase as disclosed in WO 95/00636, a glycosyltransferase, a branching enzyme (1,4- α -glucan branching enzyme), a 4- α -glucanotransferase (dextrin glycosyltransferase), a lactase (galactosidase), or an oxidoreductase, e.g., a peroxidase, a laccase, a glucose oxidase, a pyranose
20 oxidase, a lipoxygenase, an L-amino acid oxidase or a carbohydrate oxidase.

 The amylase may be a fungal or bacterial α -amylase, e.g. from *Bacillus*, particularly *B. licheniformis* or *B. amyloliquefaciens*, or from *Aspergillus*, particularly *A. oryzae*, a β -amylase, e.g. from plant (e.g. soy bean) or from microbial sources (e.g. *Bacillus*). The amylase may be an anti-staling amylase, as described in WO 99/53769, i.e. an amylase that is
25 effective in retarding the staling (crumb firming) of baked products, particularly a maltogenic α -amylase, e.g. from *Bacillus stearothermophilus* strain NCIB 11837.

Other uses

 The lipolytic enzyme variant may also be used in the production of pasta and noodles in analogy with EP 1057415.

30 A lipolytic enzyme variant with phospholipase activity may be used in cheese production as described in WO 00/54601.

EMBODIMENTS

1. A method of producing a lipolytic enzyme variant comprising:

- a) selecting a parent fungal lipolytic enzyme,
- b) selecting at least one amino acid residue which comprises an atom (excluding H atoms) which in a three-dimensional model lies within 10 Å of an atom (excluding H atoms) of a phospholipid docked with the parent lipolytic enzyme, or which is the C-terminal amino acid,
- c) altering the selected amino acid,
- d) optionally, altering one or more amino acids other than those selected,
- e) preparing the variant resulting from the preceding steps,
- f) testing hydrolytic activities of the variant towards the bond B-C of a first substrate having the general formula A-B-C and towards the bond B'-C of a second substrate having the general formula A'-B'- (A''-B''-) C where:
 - i) A and A' are fatty acyl groups,
 - ii) B and B' are oxygen or sulfur
 - iii) C is a polyol with B, B' and B'' attached to OH groups, optionally having other functional groups, and optionally having a hydrophilic group attached to an OH group,
- g) selecting a variant having a ratio of activity on the first substrate to activity on the second substrate which is lower than the parent lipolytic enzyme, and
- h) producing the selected variant.

2. A method of producing a lipolytic enzyme variant comprising:

- a) selecting a parent fungal lipolytic enzyme,
- b) in the parent lipolytic enzyme selecting at least one amino acid residue corresponding to any of residues 17-18, 20-23, 26, 37, 39, 62, 64, 80-96, 110-113, 144-151, 171-177, 200-211, 213, 215, 227, 253-261 and 263-269 of the *T. lanuginosus* lipase (SEQ ID NO: 14),
- c) altering the selected amino acid,
- d) optionally, altering one or more amino acids other than those selected,
- e) preparing the variant resulting from the preceding steps,
- f) testing hydrolytic activities of the variant towards the bond B-C of a first substrate having the general formula A-B-C and towards the bond B'-C of a second substrate having the general formula A'-B'- (A''-B''-) C where:
 - i) A and A' are fatty acyl groups,
 - ii) B and B' are oxygen or sulfur
 - iii) C is a polyol with B, B' and B'' attached to OH groups, optionally having other functional groups, and optionally having a hydrophilic group attached to an OH group,
- g) selecting a variant having a ratio of activity on the first substrate to activity on the second substrate which is lower than the parent lipolytic enzyme, and

h) producing the selected variant.

3. The method of either preceding embodiment wherein the first substrate is a lyso-phospholipid and the second substrate is a phospholipid.

4. The method of the preceding embodiment wherein the parent lipolytic enzyme has phos-
5 pholipase activity, particularly phospholipase A1 activity.

5. The method of the preceding embodiment wherein the parent lipolytic enzyme also has digalactosyl diglyceride hydrolyzing activity and optionally triacylglycerol lipase activity.

6. The method of any preceding embodiment wherein the parent lipolytic enzyme has an amino acid sequence which is at least 50 % (particularly at least 90 %) identical to that of the
10 *Thermomyces lanuginosus* lipase (SEQ ID NO: 14).

7. The method of the preceding embodiment wherein the alterations comprise substitution of at least one of L93, F95, V203 and L206 with an amino acid residue which is smaller and/or more hydrophilic.

8. The method of the preceding embodiment wherein the alterations comprise at least one of
15 the substitutions L206V/S/T/A, V203T/S/A, F95I/L/Y and L93V/I/A/T.

9. The method of embodiment 5 wherein the alterations comprise substitution of at least one of P253, I255 and P256 with an amino acid which is larger.

10. The method of embodiment 5 wherein the alterations comprise an amino acid alteration in the region 247-260 or 265-269.

20 11. The method of the preceding embodiment wherein the alterations comprise substitution of at least one of P253 and P256 with a different amino acid residue.

12. The method of embodiment 5 wherein the alterations comprise a substitution L227D, P253T/G/L, D254S/L, I255, P256L/A, A257D/A, L259 or W260H.

13. The method of embodiment 5 wherein the alterations comprise an amino acid alteration in
25 the region 247-260 and an alteration of amino acid L93, F95, V203 and L206.

14. The method of any of embodiments 5-12 wherein the parent lipolytic enzyme compared to the *T. lanuginosus* lipase (SEQ ID NO: 14) comprises an amino acid alteration at a position

corresponding to R81, R84, S85, G263, L264, I265, G266, T267 or L269 and/or a peptide extension of 1-10 amino acids at the C-terminal.

15. A method of preparing a dough or a baked product made from dough, comprising preparing a lipolytic enzyme variant by the method of any preceding embodiment and adding the
5 lipolytic enzyme variant to the dough.

16. A variant of a parent fungal lipolytic enzyme which variant comprises an amino acid alteration corresponding to R84G/A/Y/S or L206F of SEQ ID NO: 14, has phospholipase activity and has a lysophospholipase to phospholipase ratio corresponding to PLARN below 500 or RLPLA below 1.0.

10 17. A lipolytic enzyme having an amino acid sequence derived from the *T. lanuginosus* lipase (SEQ ID NO: 14) comprising the following amino acid alterations:

a) R84W +G91A +D96F +E99K +G263Q +L264A +I265T +G266D +T267A +L269N,

15 b) G91A +D96W +E99K +L227G +G263Q +L264A +I265T +G266D +T267A +L269N,

c) R84W +G91A:D96F +E99K +G263Q +L264A +I265T +G266S +T267A +L269N +270A +271G +272G +273F +274S,

d) SPPCGRRP(-E) +Y21K +E99N +N101S +E239C +Q249R,

e) G91A +D96K +E99K +G263Q +L264A +I265T +G266D +T267A +L269N,

20 f) Y21V +R84G +G91A:D96F +E99K +G263Q +L264A +I265T +G266D +T267A +L269N +270A +271G +272G +273F +274S,

g) V60G +D62W +R84W +G91A +D96F +E99K +G263Q +L264A +I265T +G266D +T267A +L269N,

25 h) V60A +D62S +G91A +D96W +E99K +W221R +G263Q +L264A +I265T +G266D +T267A +L269N +270A +271G +272G +273F +274S,

i) R84A + S85D + E87A +G91A +D96G +K98E +E99D,

j) G91A +D96W +E99K +P250N +G263Q +L264A +I265T +G266D +T267A +L269N +270A +271G +272G +273F +274S,

30 k) G91A +D96W +E99K +P256N +G263Q +L264A +I265T +G266D +T267A +L269N +270A +271G +272G +273F +274S,

l) R84W +G91A +D96W +E99K +Y261Q +G263Q +L264A +I265T +G266D +T267A +L269N +270A +271G +272G +273F +274S,

m) G91A +D96W +E99K +P250L +P253Q +D254DEL +P257S +G263Q +L264A +I265T +G266D +T267A +L269N +270A +271G +272G +273F +274S,

35 n) R84Y +G91A +D96F +E99K +G263Q +L264A +I265T +G266D +T267A +L269N,
or

o) R84S +G91A +D96F +E99K +E129A +V203i +L206F +G263Q +L264A +I265T
+G266D +T267A +L269N.

18. A lipolytic enzyme having an amino acid sequence derived from a *Fusarium* lipase comprising at least one amino acid alteration corresponding to the following in the *Fusarium ox-*

5 *ysporum* lipase(phospholipase (SEQ ID NO: 7):

a) H257W,

b) S142A,

c) V157D,

d) S271P,

10 e) S80T,

f) A127T,

g) D263G,

h) Y21W,

i) S80T,

15 j) R274A,

k) 275YRSAESVDKR or

l) 275YRSAESVDKAATMTDAELEKKLNSYVQMDKEYVKNNQARS

19. A lipolytic enzyme which:

20 a) has an amino acid sequence having at least 90 % identity to that of the *Thermomyces lanuginosus* lipase (SEQ ID NO: 14) or the *Fusarium oxysporum* lipase/phospholipase (SEQ ID NO: 7),

b) has phospholipase activity, and

c) has a lysophospholipase to phospholipase ratio corresponding to PLARN below 500 or RLPLA below 1.0.

25

EXAMPLES**Example 1: Variants based on a *T. lanuginosus* lipase variant**

A prior-art variant of the *T. lanuginosus* lipase with phospholipase activity was chosen as the starting point (parent lipolytic enzyme), and variants were prepared by introducing
 5 further amino acid alterations into the prior-art variant.

Experiment A

Activities of the new variants were determined with lecithin and lysolecithin (pure 1-phosphatidyl choline, 1-lysolecithin) as substrates by the methods described above. More specifically, 1.7 mL of the reaction mixture was shaken for between 15 and 90 min in an Eppendorf tube shaken at 1300 rpm by an “Eppendorf Thermomixer comfort”. The enzyme was
 10 inactivated at 95 C for 5 min, and centrifuged at 14000 rpm by Eppendorf centrifuge 5417R. The liberated fatty acids were determined (relative to a control sample where the enzyme was inactivated before it was added to the substrate) by NEFA C test from Wako following the ACS-ACOD method described for the NEFA-C test.

15 Three variants were found to have phospholipase activity and a to have a lower ratio of lysophospholipase to phospholipase than the prior-art variant.

R84W +G91A +D96F +E99K +G263Q +L264A +I265T +G266D +T267A +L269N

G91A +D96W +E99K +L227G +G263Q +L264A +I265T +G266D +T267A +L269N

R84W +G91A +D96F +E99K +G263Q +L264A +I265T +G266S +T267A +L269N
 20 +270A +271G +272G +273F +274S

Experiment B

Activities of further variants were determined with lecithin and lysolecithin (mixture of 1- and 2-lysolecithin) as substrates at 0.1 and 2.5 mg/ml by the RLPLA method described above. All variants were found to have a high activity on lysolecithin compared to lecithin.

25 Variants having the following amino acid alterations compared to SEQ ID NO: 14 were found to have phospholipase activity and a to have a lower ratio of lysophospholipase to phospholipase than the prior-art variant.

SPPCGRRP(-E) +Y21K +E99N +N101S +E239C +Q249R
G91A +D96K +E99K +G263Q +L264A +I265T +G266D +T267A +L269N
Y21V +R84G +G91A +D96F +E99K +G263Q +L264A +I265T +G266D +T267A +L269N +270A +271G +272G +273F +274S

V60G +D62W +R84W +G91A +D96F +E99K +G263Q +L264A +I265T +G266D +T267A +L269N
V60A +D62S +G91A +D96W +E99K +W221R +G263Q +L264A +I265T +G266D +T267A +L269N +270A +271G +272G +273F +274S
R84A + S85D + E87A +G91A +D96G +K98E +E99D
G91A +D96W +E99K +P250N +G263Q +L264A +I265T +G266D +T267A +L269N +270A +271G +272G +273F +274S
G91A +D96W +E99K +P256N +G263Q +L264A +I265T +G266D +T267A +L269N +270A +271G +272G +273F +274S
R84W +G91A +D96W +E99K +Y261Q +G263Q +L264A +I265T +G266D +T267A +L269N +270A +271G +272G +273F +274S
G91A +D96W +E99K +P250L +P253Q +D254DEL +P257S +G263Q +L264A +I265T +G266D +T267A +L269N +270A +271G +272G +273F +274S
R84Y +G91A +D96F +E99K +G263Q +L264A +I265T +G266D +T267A +L269N
R84S +G91A +D96F +E99K +E129A +V203i +L206F +G263Q +L264A +I265T +G266D +T267A +L269N

Example 2: Variants of *F. oxysporum* lipase/phospholipase

Variants of the *F. oxysporum* lipase/phospholipase were prepared, having the following amino acid alterations compared to SEQ ID NO: 7:

- 5 H257W
 S142A
 V157D +S271P
 S80T +A127T
 D263G
 10 Y21W
 S80T

The following variants with modified C-terminal sequences were prepared by making the substitutions R274A and/or R284A to remove one or two cleavage points for the Kex-2 protease:

- 15 R274A +275YRSAESVDKR
 R274A +275YRSAESVDKAATMTDAELEKKLNSYVQMDKEYVKNNQARS

Activities of the variants and the parent enzyme were determined as in Example 2. Compared to the parent enzyme, the variants were found to have lower activity on lysolecithin and a lower ratio of lysolecithin activity to lecithin activity.

Example 3: Preparation of dough

5 Doughs were prepared from Meneba flour according to the European straight dough method (ABF-SP 1201.1) with 40 ppm Fungamyl Super MA (Novozymes), 40 ppm ascorbic acid, and different dosages of lipolytic enzyme.

The stickiness of the dough was evaluated on a 1-10 scale by the baker as the degree to which a dough adheres to one's hands or other surfaces, where 5 is identical to a control without addition of lipolytic enzyme, 1 is the lowest degree of stickiness and 10 is the highest degree of stickiness.

The extensibility of the dough was evaluated on a 1-10 scale by the baker as the degree to which a dough can be stretched without tearing, where 5 is identical to a control without addition of lipolytic enzyme, 1 indicates the lowest (shortest) extensibility and 10 indicates the highest (longest) extensibility.

The elasticity of the dough was evaluated on a 1-10 scale by the baker as the degree to which a dough tends to recover its original shape after release from a deforming force, where 5 is identical to a control without addition of lipolytic enzyme, 1 indicates the lowest (weakest) elasticity and 10 indicates the highest (strongest) elasticity.

20 A lipolytic enzyme prepared in Example 1 was tested, and the prior-art variant was tested for comparison. The results were as follows

Experiment A

Lipolytic enzyme	Dosage	PLARN ratio	Stickiness	Extensibility	Elasticity
Invention	0.2 mg/kg dough	690	5	6	4
Prior art	250 LU/kg dough	5800	5	7	3

Experiment B

Lipolytic enzyme	Dosage	RLPLA ratio	Stickiness	Extensibility	Elasticity
Invention	0.2 mg/kg flour	1.06	4	4	6
Prior art	250 LU/kg dough	1.58	5	5	5

25

The results show that lipolytic enzymes with a lower ratio of lysolecithin activity to lecithin activity make doughs with a desirable combination of lower extensibility and higher elasticity than the prior-art lipolytic enzymes, and they furthermore tend to make a less sticky dough.

5

GB SQ listing ST25
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<120> Lipolytic Enzymes

<130> 10248-EP-ETD

<160> 14

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35 40 45

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50 55 60

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65 70 75 80

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85 90 95

Val Pro Val Asn Tyr Pro Pro Val Asn Gly Ala Lys Val His Lys Gly
100 105 110

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115 120 125

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145 150 155 160

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 50 55 60

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 65 70 75 80

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 100 105 110

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180 185 190

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195 200 205

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 195 200 205

Arg His Thr Ser Pro Glu Tyr Trp Leu Asn Gly Gly Pro Leu Asp Lys
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 225 230 235 240

Met Cys Asn Gly Gly Thr Ile Gly Leu Asp Ile Leu Ala His Ile Thr
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250

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Lys Leu Asn Cys Ser Val Gly Asn Cys Pro Asp Val Glu Ala Ala Gly
 35 40 45

Ser Thr Val Lys Leu Ser Phe Ser Asp Asp Thr Ile Thr Asp Thr Ala
 50 55 60

Gly Phe Val Ala Val Asp Asn Thr Asn Lys Ala Ile Val Val Ala Phe
 65 70 75 80

Arg Gly Ser Tyr Ser Ile Arg Asn Trp Val Thr Asp Ala Thr Phe Pro
 85 90 95

Gln Thr Asp Pro Gly Leu Cys Asp Gly Cys Lys Ala Glu Leu Gly Phe
 100 105 110

Trp Thr Ala Trp Lys Val Val Arg Asp Arg Ile Ile Lys Thr Leu Asp
 115 120 125

Glu Leu Lys Pro Glu His Ser Asp Tyr Lys Ile Val Val Val Gly His
 130 135 140

Ser Leu Gly Ala Ala Ile Ala Ser Leu Ala Ala Asp Leu Arg Thr
 145 150 155 160

Lys Asn Tyr Asp Ala Ile Leu Tyr Ala Tyr Ala Ala Pro Arg Val Ala
 165 170 175

Asn Lys Pro Leu Ala Glu Phe Ile Thr Asn Gln Gly Asn Asn Tyr Arg
 180 185 190

Phe Thr His Asn Asp Asp Pro Val Pro Lys Leu Pro Leu Leu Thr Met
 195 200 205

GB SQ listing ST25

Gly Tyr Val His Ile Ser Pro Glu Tyr Tyr Ile Thr Ala Pro Asp Asn
 210 215 220

Thr Thr Val Thr Asp Asn Gln Val Thr Val Leu Asp Gly Tyr Val Asn
 225 230 235 240

Phe Lys Gly Asn Thr Gly Thr Ser Gly Gly Leu Pro Asp Leu Leu Ala
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Phe His Ser His Val Trp Tyr Phe Ile His Ala Asp Ala Cys Lys Gly
 260 265 270

Pro Gly Leu Pro Leu Arg
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 20 25 30

Lys Leu Ser Cys Ser Lys Gly Asn Cys Pro Glu Val Glu Ala Thr Gly
 35 40 45

Ala Thr Val Ser Tyr Asp Phe Ser Asp Ser Thr Ile Thr Asp Thr Ala
 50 55 60

Gly Tyr Ile Ala Val Asp His Thr Asn Ser Ala Val Val Leu Ala Phe
 65 70 75 80

Arg Gly Ser Tyr Ser Val Arg Asn Trp Val Ala Asp Ala Thr Phe Val
 85 90 95

His Thr Asn Pro Gly Leu Cys Asp Gly Cys Leu Ala Glu Leu Gly Phe
 100 105 110

Trp Ser Ser Trp Lys Leu Val Arg Asp Asp Ile Ile Lys Glu Leu Lys
 115 120 125

Glu Val Val Ala Gln Asn Pro Asn Tyr Glu Leu Val Val Val Gly His
 130 135 140

Ser Leu Gly Ala Ala Val Ala Thr Leu Ala Ala Thr Asp Leu Arg Gly
 145 150 155 160

Lys Gly Tyr Pro Ser Ala Lys Leu Tyr Ala Tyr Ala Ser Pro Arg Val

GB SQ listing ST25																	
165								170								175	
Gly	Asn	Ala	Ala 180	Leu	Ala	Lys	Tyr	Ile 185	Thr	Ala	Gln	Gly	Asn 190	Asn	Phe		
Arg	Phe	Thr 195	His	Thr	Asn	Asp	Pro 200	Val	Pro	Lys	Leu	Pro 205	Leu	Leu	Ser		
Met	Gly 210	Tyr	Val	His	Val	Ser 215	Pro	Glu	Tyr	Trp	Ile 220	Thr	Ser	Pro	Asn		
Asn 225	Ala	Thr	Val	Ser	Thr 230	Ser	Asp	Ile	Lys	Val 235	Ile	Asp	Gly	Asp	Val 240		
Ser	Phe	Asp	Gly	Asn 245	Thr	Gly	Thr	Gly	Leu 250	Pro	Leu	Leu	Thr	Asp 255	Phe		
Glu	Ala	His	Ile 260	Trp	Tyr	Phe	Val	Gln 265	Val	Asp	Ala	Gly	Lys 270	Gly	Pro		
Gly	Leu	Pro 275	Phe	Lys	Arg												
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Ser	Ala	Ala	Ala 20	Tyr	Cys	Ser	Asn	Asn 25	Ile	Asp	Ser	Lys	Asp 30	Ser	Asn		
Leu	Thr	Cys 35	Thr	Ala	Asn	Ala	Cys 40	Pro	Ser	Val	Glu	Glu 45	Ala	Ser	Thr		
Thr	Met 50	Leu	Leu	Glu	Phe	Asp 55	Leu	Thr	Asn	Asp	Phe 60	Gly	Gly	Thr	Ala		
Gly 65	Phe	Leu	Ala	Ala	Asp 70	Asn	Thr	Asn	Lys	Arg 75	Leu	Val	Val	Ala	Phe 80		
Arg	Gly	Ser	Ser	Thr 85	Ile	Glu	Asn	Trp	Ile 90	Ala	Asn	Leu	Asp	Phe 95	Ile		
Leu	Glu	Asp	Asn 100	Asp	Asp	Leu	Cys	Thr 105	Gly	Cys	Lys	Val	His 110	Thr	Gly		
Phe	Trp	Lys 115	Ala	Trp	Glu	Ser	Ala 120	Ala	Asp	Glu	Leu	Thr 125	Ser	Lys	Ile		

GB SQ listing ST25

Lys Ser Ala Met Ser Thr Tyr Ser Gly Tyr Thr Leu Tyr Phe Thr Gly
130 135 140

His Ser Leu Gly Gly Ala Leu Ala Thr Leu Gly Ala Thr Val Leu Arg
145 150 155 160

Asn Asp Gly Tyr Ser Val Glu Leu Tyr Thr Tyr Gly Cys Pro Arg Ile
165 170 175

Gly Asn Tyr Ala Leu Ala Glu His Ile Thr Ser Gln Gly Ser Gly Ala
180 185 190

Asn Phe Arg Val Thr His Leu Asn Asp Ile Val Pro Arg Val Pro Pro
195 200 205

Met Asp Phe Gly Phe Ser Gln Pro Ser Pro Glu Tyr Trp Ile Thr Ser
210 215 220

Gly Asn Gly Ala Ser Val Thr Ala Ser Asp Ile Glu Val Ile Glu Gly
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Ala His Leu Trp Tyr Phe Phe Ala Ile Ser Glu Cys Leu Leu
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20 25 30

Val Thr Cys Thr Ala Asp Ala Cys Pro Ser Val Glu Glu Ala Ser Thr
35 40 45

Lys Met Leu Leu Glu Phe Asp Leu Thr Asn Asn Phe Gly Gly Thr Ala
50 55 60

Gly Phe Leu Ala Ala Asp Asn Thr Asn Lys Arg Leu Val Val Ala Phe
65 70 75 80

Arg Gly Ser Ser Thr Ile Lys Asn Trp Ile Ala Asp Leu Asp Phe Ile
85 90 95

Leu Gln Asp Asn Asp Asp Leu Cys Thr Gly Cys Lys Val His Thr Gly
Page 13

GB SQ listing ST25															
100				105				110							
Phe	Trp	Lys 115	Ala	Trp	Glu	Ala	Ala 120	Ala	Asp	Asn	Leu	Thr 125	Ser	Lys	Ile
Lys	Ser 130	Ala	Met	Ser	Thr	Tyr 135	Ser	Gly	Tyr	Thr	Leu 140	Tyr	Phe	Thr	Gly
His 145	Ser	Leu	Gly	Gly	Ala 150	Leu	Ala	Thr	Leu	Gly 155	Ala	Thr	Val	Leu	Arg 160
Asn	Asp	Gly	Tyr	Ser 165	Val	Glu	Leu	Tyr	Thr 170	Tyr	Gly	Cys	Pro	Arg 175	Val
Gly	Asn	Tyr	Ala 180	Leu	Ala	Glu	His	Ile 185	Thr	Ser	Gln	Gly	Ser 190	Gly	Ala
Asn	Phe	Pro 195	Val	Thr	His	Leu	Asn 200	Asp	Ile	Val	Pro	Arg 205	Val	Pro	Pro
Met	Asp 210	Phe	Gly	Phe	Ser	Gln 215	Pro	Ser	Pro	Glu	Tyr 220	Trp	Ile	Thr	Ser
Gly 225	Thr	Gly	Ala	Ser	Val 230	Thr	Ala	Ser	Asp	Ile 235	Glu	Leu	Ile	Glu	Gly 240
Ile	Asn	Ser	Thr	Ala 245	Gly	Asn	Ala	Gly	Glu 250	Ala	Thr	Val	Asp	Val 255	Leu
Ala	His	Leu	Trp 260	Tyr	Phe	Phe	Ala	Ile 265	Ser	Glu	Cys	Leu	Leu 270		
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Ser	Ala	Ala	Ala 20	Tyr	Cys	Asp	Glu	Asn 25	Leu	Asn	Ser	Thr	Gly 30	Thr	Lys
Leu	Thr	Cys 35	Ser	Val	Gly	Asn	Cys 40	Pro	Leu	Val	Glu	Ala 45	Ala	Ser	Thr
Gln	Ser 50	Leu	Asp	Glu	Phe	Asn 55	Glu	Ser	Ser	Ser	Tyr 60	Gly	Asn	Pro	Ala
Gly 65	Tyr	Leu	Ala	Ala	Asp 70	Glu	Thr	Asn	Lys	Leu 75	Leu	Val	Leu	Ser	Phe 80

GB SQ listing ST25

Arg Gly Ser Ala Asp Leu Ala Asn Trp Val Ala Asn Leu Asn Phe Gly
85 90 95

Leu Glu Asp Ala Ser Asp Leu Cys Ser Gly Cys Glu Val His Ser Gly
100 105 110

Phe Trp Lys Ala Trp Ser Glu Ile Ala Asp Thr Ile Thr Ser Lys Val
115 120 125

Glu Ser Ala Leu Ser Asp His Ser Asp Tyr Ser Leu Val Leu Thr Gly
130 135 140

His Ser Tyr Gly Ala Ala Leu Ala Ala Leu Ala Ala Thr Ala Leu Arg
145 150 155 160

Asn Ser Gly His Ser Val Glu Leu Tyr Asn Tyr Gly Gln Pro Arg Leu
165 170 175

Gly Asn Glu Ala Leu Ala Thr Tyr Ile Thr Asp Gln Asn Lys Gly Gly
180 185 190

Asn Tyr Arg Val Thr His Thr Asn Asp Ile Val Pro Lys Leu Pro Pro
195 200 205

Thr Leu Leu Gly Tyr His His Phe Ser Pro Glu Tyr Tyr Ile Ser Ser
210 215 220

Ala Asp Glu Ala Thr Val Thr Thr Thr Asp Val Thr Glu Val Thr Gly
225 230 235 240

Ile Asp Ala Thr Gly Gly Asn Asp Gly Thr Asp Gly Thr Ser Ile Asp
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Ala His Arg Trp Tyr Phe Ile Tyr Ile Ser Glu Cys Ser
260 265

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<400> 14

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20 25 30

Asn Ile Thr Cys Thr Gly Asn Ala Cys Pro Glu Val Glu Lys Ala Asp
35 40 45

Ala Thr Phe Leu Tyr Ser Phe Glu Asp Ser Gly Val Gly Asp Val Thr
Page 15

GB SQ listing ST25															
50				55				60							
Gly 65	Phe	Leu	Ala	Leu	Asp 70	Asn	Thr	Asn	Lys	Leu 75	Ile	Val	Leu	Ser	Phe 80
Arg	Gly	Ser	Arg	Ser 85	Ile	Glu	Asn	Trp	Ile 90	Gly	Asn	Leu	Asn	Phe 95	Asp
Leu	Lys	Glu	Ile 100	Asn	Asp	Ile	Cys	Ser 105	Gly	Cys	Arg	Gly	His 110	Asp	Gly
Phe	Thr	Ser 115	Ser	Trp	Arg	Ser	Val 120	Ala	Asp	Thr	Leu	Arg 125	Gln	Lys	Val
Glu	Asp 130	Ala	Val	Arg	Glu	His 135	Pro	Asp	Tyr	Arg	Val 140	Val	Phe	Thr	Gly
His 145	Ser	Leu	Gly	Gly	Ala 150	Leu	Ala	Thr	Val	Ala 155	Gly	Ala	Asp	Leu	Arg 160
Gly	Asn	Gly	Tyr	Asp 165	Ile	Asp	Val	Phe	Ser 170	Tyr	Gly	Ala	Pro	Arg 175	Val
Gly	Asn	Arg	Ala 180	Phe	Ala	Glu	Phe	Leu 185	Thr	Val	Gln	Thr	Gly 190	Gly	Thr
Leu	Tyr	Arg 195	Ile	Thr	His	Thr	Asn 200	Asp	Ile	Val	Pro	Arg 205	Leu	Pro	Pro
Arg	Glu 210	Phe	Gly	Tyr	Ser	His 215	Ser	Ser	Pro	Glu	Tyr 220	Trp	Ile	Lys	Ser
Gly 225	Thr	Leu	Val	Pro	Val 230	Thr	Arg	Asn	Asp	Ile 235	Val	Lys	Ile	Glu	Gly 240
Ile	Asp	Ala	Thr	Gly 245	Gly	Asn	Asn	Gln	Pro 250	Asn	Ile	Pro	Asp	Ile 255	Pro
Ala	His	Leu	Trp 260	Tyr	Phe	Gly	Leu	Ile 265	Gly	Thr	Cys	Leu			

LIPOLYTISKE ENZYMVARIANTER OG FREMGANGSMÅDE TIL FREMSTILLING DERAFT

PATENTKRAV

1. Lipolytisk enzym, som:
 - 5 a) har en aminosyresekvens, der udviser mindst 90% identitet til den i SEQ ID NO: 7; og
 - b) har phospholipaseaktivitet og
 - c) har et forhold mellem lysophospholipase og phospholipase på mindre end 1000 og
 - 10 d) omfatter mindst én aminosyreændring svarende til position H257W, S142A, V157D+S271P, S80T+A127T, D263G, Y21W, S80T, R274A+275YRSAESVDKR eller R274A+275YRSAESVDKAATMTDAELEKKLNSYVQMDKEYVKNNQARS i SEQ ID NO: 7; og hvor forholdet mellem lysophospholipase og phospholipase er defineret som lysophospholipaseaktiviteten divideret med phospholipaseaktiviteten, hvor
 - 15 phospholipaseaktivitet er bestemt ved 30°C ved anvendelse af 4% (vægt/volumen) lecithin i 50mM natriumacetat, 5mM CaCl₂, pH 5,0, og lysophospholipaseaktivitet er bestemt ved 30°C ved anvendelse af 1% (vægt/volumen) lysolecithin i 50mM natriumacetat, 5mM CaCl₂, pH 5,0.
2. Lipolytisk enzym ifølge krav 1, som har et forhold mellem lysophospholipase og
 - 20 phospholipase på mindre end 1000, og som omfatter en aminosyresekvens, der er afledt fra en *Fusarium*-lipase der omfatter mindst én aminosyreændring svarende til SEQ ID NO: 7:
 - a. H257W;
 - b. S142A;
 - 25 c. V157D+S271P;
 - d. S80T+A127T;
 - e. D263G;
 - f. Y21W;
 - g. S80T;
 - 30 h. R274A+275YRSAESVDKR;
 - i. R274A+275YRSAESVDKAATMTDAELEKKLNSYVQMDKEYVKNNQARS; og

5 hvor forholdet mellem lysophospholipase og phospholipase er defineret som lysophospholipaseaktiviteten divideret med phospholipaseaktiviteten, hvor phospholipaseaktivitet er bestemt ved 30°C ved anvendelse af 4% (vægt/volumen) lecithin i 50mM natriumacetat, 5mM CaCl₂, pH 5,0, og lysophospholipaseaktivitet er bestemt ved 30°C ved anvendelse af 1% (vægt/volumen) lysolecithin i 50mM natriumacetat, 5mM CaCl₂, pH 5,0.

- 10 3. Fremgangsmåde til fremstilling af en dej eller et bagt produkt fremstillet af dej, hvilken fremgangsmåde omfatter tilsætning af det lipolytiske enzym ifølge et hvilket som helst af kravene 1-2 til dejen.
4. Anvendelse af det lipolytiske enzym ifølge et hvilket som helst af kravene 1-2 ved fremstilling af pasta.
- 15 5. Anvendelse af det lipolytiske enzym ifølge et hvilket som helst af kravene 1-2 ved fremstilling af nudler.
6. Anvendelse af det lipolytiske enzym ifølge et hvilket som helst af kravene 1-2 ved ostefremstilling.
- 20

Fig. 1
3D structure of *Thermomyces lanuginosus* lipase docked with lecithin

ATOM	1	N	GLU	B	1	-20.466	-0.687	-7.615	0.00	0.00	N
ATOM	2	CA	GLU	B	1	-20.359	-1.989	-6.986	0.00	0.00	C
ATOM	3	C	GLU	B	1	-19.088	-2.775	-7.345	0.00	0.00	C
ATOM	4	O	GLU	B	1	-18.379	-2.717	-8.352	0.00	0.00	O
ATOM	5	CB	GLU	B	1	-21.505	-2.986	-7.267	0.00	0.00	C
ATOM	6	CG	GLU	B	1	-22.640	-3.127	-6.294	0.00	0.00	C
ATOM	7	CD	GLU	B	1	-22.816	-3.646	-4.918	0.00	0.00	C
ATOM	8	OE1	GLU	B	1	-23.898	-4.183	-4.595	0.00	0.00	O
ATOM	9	OE2	GLU	B	1	-21.911	-3.529	-4.045	0.00	0.00	O
ATOM	10	N	VAL	B	2	-18.891	-3.622	-6.331	0.00	0.00	N
ATOM	11	CA	VAL	B	2	-17.758	-4.540	-6.297	0.00	0.00	C
ATOM	12	C	VAL	B	2	-17.940	-5.789	-5.453	0.00	0.00	C
ATOM	13	O	VAL	B	2	-18.520	-5.817	-4.344	0.00	0.00	O
ATOM	14	CB	VAL	B	2	-16.625	-3.596	-5.795	0.00	0.00	C
ATOM	15	CG1	VAL	B	2	-16.528	-3.620	-4.292	0.00	0.00	C
ATOM	16	CG2	VAL	B	2	-15.360	-3.922	-6.542	0.00	0.00	C
ATOM	17	N	SER	B	3	-17.361	-6.824	-6.068	0.00	0.00	N
ATOM	18	CA	SER	B	3	-17.298	-8.144	-5.411	0.00	0.00	C
ATOM	19	C	SER	B	3	-16.576	-7.883	-4.089	0.00	0.00	C
ATOM	20	O	SER	B	3	-15.806	-6.889	-4.045	0.00	0.00	O
ATOM	21	CB	SER	B	3	-16.515	-9.110	-6.270	0.00	0.00	C
ATOM	22	OG	SER	B	3	-15.546	-9.683	-5.389	0.00	0.00	O
ATOM	23	N	GLN	B	4	-16.743	-8.657	-3.040	0.00	0.00	N
ATOM	24	CA	GLN	B	4	-15.969	-8.293	-1.796	0.00	0.00	C
ATOM	25	C	GLN	B	4	-14.564	-8.801	-2.124	0.00	0.00	C
ATOM	26	O	GLN	B	4	-13.647	-8.204	-1.547	0.00	0.00	O
ATOM	27	CB	GLN	B	4	-16.623	-8.685	-0.541	0.00	0.00	C
ATOM	28	CG	GLN	B	4	-16.654	-8.513	0.906	0.00	0.00	C
ATOM	29	CD	GLN	B	4	-16.396	-7.253	1.657	0.00	0.00	C
ATOM	30	OE1	GLN	B	4	-15.532	-6.465	1.274	0.00	0.00	O
ATOM	31	NE2	GLN	B	4	-17.094	-6.999	2.770	0.00	0.00	N
ATOM	32	N	ASP	B	5	-14.435	-9.846	-2.923	0.00	0.00	N
ATOM	33	CA	ASP	B	5	-13.122	-10.372	-3.317	0.00	0.00	C
ATOM	34	C	ASP	B	5	-12.524	-9.498	-4.444	0.00	0.00	C
ATOM	35	O	ASP	B	5	-11.328	-9.717	-4.741	0.00	0.00	O
ATOM	36	CB	ASP	B	5	-12.934	-11.835	-3.756	0.00	0.00	C
ATOM	37	CG	ASP	B	5	-11.448	-12.248	-3.619	0.00	0.00	C
ATOM	38	OD1	ASP	B	5	-10.664	-12.482	-4.568	0.00	0.00	O
ATOM	39	OD2	ASP	B	5	-11.016	-12.294	-2.432	0.00	0.00	O
ATOM	40	N	LEU	B	6	-13.332	-8.722	-5.157	0.00	0.00	N
ATOM	41	CA	LEU	B	6	-12.674	-7.931	-6.220	0.00	0.00	C
ATOM	42	C	LEU	B	6	-12.054	-6.747	-5.478	0.00	0.00	C
ATOM	43	O	LEU	B	6	-10.898	-6.366	-5.536	0.00	0.00	O
ATOM	44	CB	LEU	B	6	-13.562	-7.459	-7.347	0.00	0.00	C
ATOM	45	CG	LEU	B	6	-12.813	-6.791	-8.502	0.00	0.00	C
ATOM	46	CD1	LEU	B	6	-11.383	-7.312	-8.617	0.00	0.00	C
ATOM	47	CD2	LEU	B	6	-13.611	-7.084	-9.774	0.00	0.00	C
ATOM	48	N	PHE	B	7	-12.981	-6.261	-4.658	0.00	0.00	N
ATOM	49	CA	PHE	B	7	-12.747	-5.102	-3.803	0.00	0.00	C
ATOM	50	C	PHE	B	7	-11.401	-5.345	-3.134	0.00	0.00	C
ATOM	51	O	PHE	B	7	-10.436	-4.593	-3.256	0.00	0.00	O
ATOM	52	CB	PHE	B	7	-13.882	-4.975	-2.775	0.00	0.00	C
ATOM	53	CG	PHE	B	7	-13.684	-3.819	-1.846	0.00	0.00	C
ATOM	54	CD1	PHE	B	7	-14.259	-2.582	-2.150	0.00	0.00	C
ATOM	55	CD2	PHE	B	7	-12.885	-3.954	-0.722	0.00	0.00	C
ATOM	56	CE1	PHE	B	7	-14.033	-1.506	-1.320	0.00	0.00	C

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Fig. 1 cont.

ATOM	57	CE2	PHE	B	7	-12.660	-2.875	0.130	0.00	0.00	C
ATOM	58	CZ	PHE	B	7	-13.246	-1.642	-0.176	0.00	0.00	C
ATOM	59	N	ASN	B	8	-11.355	-6.490	-2.507	0.00	0.00	N
ATOM	60	CA	ASN	B	8	-10.198	-6.952	-1.722	0.00	0.00	C
ATOM	61	C	ASN	B	8	-8.904	-6.951	-2.523	0.00	0.00	C
ATOM	62	O	ASN	B	8	-7.919	-6.377	-1.964	0.00	0.00	O
ATOM	63	CB	ASN	B	8	-10.664	-8.270	-1.072	0.00	0.00	C
ATOM	64	CG	ASN	B	8	-11.217	-8.078	0.333	0.00	0.00	C
ATOM	65	OD1	ASN	B	8	-10.712	-7.260	1.111	0.00	0.00	O
ATOM	66	ND2	ASN	B	8	-12.247	-8.837	0.679	0.00	0.00	N
ATOM	67	N	GLN	B	9	-8.842	-7.446	-3.740	0.00	0.00	N
ATOM	68	CA	GLN	B	9	-7.563	-7.399	-4.483	0.00	0.00	C
ATOM	69	C	GLN	B	9	-7.145	-5.943	-4.695	0.00	0.00	C
ATOM	70	O	GLN	B	9	-6.014	-5.512	-4.363	0.00	0.00	O
ATOM	71	CB	GLN	B	9	-7.669	-8.111	-5.815	0.00	0.00	C
ATOM	72	CG	GLN	B	9	-8.771	-9.152	-5.839	0.00	0.00	C
ATOM	73	CD	GLN	B	9	-8.305	-10.386	-6.564	0.00	0.00	C
ATOM	74	OE1	GLN	B	9	-7.162	-10.790	-6.347	0.00	0.00	O
ATOM	75	NE2	GLN	B	9	-9.150	-10.943	-7.410	0.00	0.00	N
ATOM	76	N	PHE	B	10	-8.083	-5.111	-5.120	0.00	0.00	N
ATOM	77	CA	PHE	B	10	-7.988	-3.698	-5.423	0.00	0.00	C
ATOM	78	C	PHE	B	10	-7.230	-2.939	-4.340	0.00	0.00	C
ATOM	79	O	PHE	B	10	-6.509	-2.009	-4.674	0.00	0.00	O
ATOM	80	CB	PHE	B	10	-9.328	-2.959	-5.466	0.00	0.00	C
ATOM	81	CG	PHE	B	10	-10.128	-3.134	-6.707	0.00	0.00	C
ATOM	82	CD1	PHE	B	10	-9.601	-3.828	-7.793	0.00	0.00	C
ATOM	83	CD2	PHE	B	10	-11.389	-2.561	-6.779	0.00	0.00	C
ATOM	84	CE1	PHE	B	10	-10.319	-3.980	-8.958	0.00	0.00	C
ATOM	85	CE2	PHE	B	10	-12.129	-2.708	-7.959	0.00	0.00	C
ATOM	86	CZ	PHE	B	10	-11.580	-3.414	-9.035	0.00	0.00	C
ATOM	87	N	ASN	B	11	-7.499	-3.364	-3.154	0.00	0.00	N
ATOM	88	CA	ASN	B	11	-6.851	-2.799	-1.990	0.00	0.00	C
ATOM	89	C	ASN	B	11	-5.360	-3.072	-1.799	0.00	0.00	C
ATOM	90	O	ASN	B	11	-4.469	-2.220	-1.689	0.00	0.00	O
ATOM	91	CB	ASN	B	11	-7.731	-3.465	-0.897	0.00	0.00	C
ATOM	92	CG	ASN	B	11	-7.901	-2.270	0.044	0.00	0.00	C
ATOM	93	OD1	ASN	B	11	-8.910	-1.601	-0.177	0.00	0.00	O
ATOM	94	ND2	ASN	B	11	-6.872	-2.145	0.870	0.00	0.00	N
ATOM	95	N	LEU	B	12	-5.077	-4.365	-1.812	0.00	0.00	N
ATOM	96	CA	LEU	B	12	-3.764	-4.979	-1.623	0.00	0.00	C
ATOM	97	C	LEU	B	12	-2.773	-4.582	-2.720	0.00	0.00	C
ATOM	98	O	LEU	B	12	-1.603	-4.282	-2.407	0.00	0.00	O
ATOM	99	CB	LEU	B	12	-3.962	-6.511	-1.509	0.00	0.00	C
ATOM	100	CG	LEU	B	12	-2.706	-7.270	-1.944	0.00	0.00	C
ATOM	101	CD1	LEU	B	12	-1.876	-7.434	-0.686	0.00	0.00	C
ATOM	102	CD2	LEU	B	12	-3.105	-8.566	-2.607	0.00	0.00	C
ATOM	103	N	PHE	B	13	-3.263	-4.607	-3.947	0.00	0.00	N
ATOM	104	CA	PHE	B	13	-2.482	-4.200	-5.114	0.00	0.00	C
ATOM	105	C	PHE	B	13	-2.294	-2.684	-5.081	0.00	0.00	C
ATOM	106	O	PHE	B	13	-1.384	-2.192	-5.747	0.00	0.00	O
ATOM	107	CB	PHE	B	13	-3.070	-4.668	-6.433	0.00	0.00	C
ATOM	108	CG	PHE	B	13	-3.208	-6.165	-6.446	0.00	0.00	C
ATOM	109	CD1	PHE	B	13	-4.428	-6.756	-6.744	0.00	0.00	C
ATOM	110	CD2	PHE	B	13	-2.109	-6.969	-6.154	0.00	0.00	C
ATOM	111	CE1	PHE	B	13	-4.575	-8.127	-6.734	0.00	0.00	C
ATOM	112	CE2	PHE	B	13	-2.216	-8.354	-6.129	0.00	0.00	C
ATOM	113	CZ	PHE	B	13	-3.471	-8.917	-6.421	0.00	0.00	C
ATOM	114	N	ALA	B	14	-3.180	-1.986	-4.391	0.00	0.00	N
ATOM	115	CA	ALA	B	14	-3.124	-0.540	-4.236	0.00	0.00	C

Fig. 1 cont.

ATOM	116	C	ALA	B	14	-1.882	-0.274	-3.383	0.00	0.00	C
ATOM	117	O	ALA	B	14	-1.146	0.666	-3.628	0.00	0.00	O
ATOM	118	CB	ALA	B	14	-4.318	0.060	-3.550	0.00	0.00	C
ATOM	119	N	GLN	B	15	-1.756	-1.128	-2.394	0.00	0.00	N
ATOM	120	CA	GLN	B	15	-0.704	-1.247	-1.375	0.00	0.00	C
ATOM	121	C	GLN	B	15	0.559	-1.754	-2.048	0.00	0.00	C
ATOM	122	O	GLN	B	15	1.654	-1.190	-1.939	0.00	0.00	O
ATOM	123	CB	GLN	B	15	-1.188	-2.116	-0.206	0.00	0.00	C
ATOM	124	CG	GLN	B	15	-2.449	-1.571	0.394	0.00	0.00	C
ATOM	125	CD	GLN	B	15	-2.970	-1.835	1.764	0.00	0.00	C
ATOM	126	OE1	GLN	B	15	-4.107	-1.456	2.111	0.00	0.00	O
ATOM	127	NE2	GLN	B	15	-2.164	-2.466	2.610	0.00	0.00	N
ATOM	128	N	TYR	B	16	0.452	-2.767	-2.869	0.00	0.00	N
ATOM	129	CA	TYR	B	16	1.567	-3.317	-3.641	0.00	0.00	C
ATOM	130	C	TYR	B	16	2.258	-2.273	-4.500	0.00	0.00	C
ATOM	131	O	TYR	B	16	3.491	-2.305	-4.656	0.00	0.00	O
ATOM	132	CB	TYR	B	16	1.012	-4.476	-4.512	0.00	0.00	C
ATOM	133	CG	TYR	B	16	1.501	-5.737	-3.838	0.00	0.00	C
ATOM	134	CD1	TYR	B	16	2.833	-6.087	-4.067	0.00	0.00	C
ATOM	135	CD2	TYR	B	16	0.746	-6.508	-2.982	0.00	0.00	C
ATOM	136	CE1	TYR	B	16	3.392	-7.213	-3.464	0.00	0.00	C
ATOM	137	CE2	TYR	B	16	1.292	-7.641	-2.384	0.00	0.00	C
ATOM	138	CZ	TYR	B	16	2.610	-8.000	-2.625	0.00	0.00	C
ATOM	139	OH	TYR	B	16	3.154	-9.119	-2.057	0.00	0.00	O
ATOM	140	N	SER	B	17	1.497	-1.384	-5.124	0.00	0.00	N
ATOM	141	CA	SER	B	17	1.893	-0.269	-5.978	0.00	0.00	C
ATOM	142	C	SER	B	17	2.422	0.945	-5.181	0.00	0.00	C
ATOM	143	O	SER	B	17	3.353	1.669	-5.548	0.00	0.00	O
ATOM	144	CB	SER	B	17	0.790	0.316	-6.843	0.00	0.00	C
ATOM	145	OG	SER	B	17	-0.135	-0.480	-7.501	0.00	0.00	O
ATOM	146	N	ALA	B	18	1.764	1.193	-4.077	0.00	0.00	N
ATOM	147	CA	ALA	B	18	2.010	2.304	-3.159	0.00	0.00	C
ATOM	148	C	ALA	B	18	3.390	2.255	-2.537	0.00	0.00	C
ATOM	149	O	ALA	B	18	4.116	3.200	-2.225	0.00	0.00	O
ATOM	150	CB	ALA	B	18	0.907	2.295	-2.102	0.00	0.00	C
ATOM	151	N	ALA	B	19	3.768	1.031	-2.322	0.00	0.00	N
ATOM	152	CA	ALA	B	19	4.938	0.445	-1.745	0.00	0.00	C
ATOM	153	C	ALA	B	19	6.150	0.686	-2.612	0.00	0.00	C
ATOM	154	O	ALA	B	19	7.223	0.600	-2.018	0.00	0.00	O
ATOM	155	CB	ALA	B	19	4.773	-1.064	-1.589	0.00	0.00	C
ATOM	156	N	ALA	B	20	5.930	0.899	-3.888	0.00	0.00	N
ATOM	157	CA	ALA	B	20	7.065	1.078	-4.819	0.00	0.00	C
ATOM	158	C	ALA	B	20	7.666	2.467	-4.756	0.00	0.00	C
ATOM	159	O	ALA	B	20	8.719	2.812	-5.320	0.00	0.00	O
ATOM	160	CB	ALA	B	20	6.578	0.651	-6.193	0.00	0.00	C
ATOM	161	N	TYR	B	21	6.978	3.337	-4.029	0.00	0.00	N
ATOM	162	CA	TYR	B	21	7.486	4.702	-3.859	0.00	0.00	C
ATOM	163	C	TYR	B	21	8.584	4.536	-2.816	0.00	0.00	C
ATOM	164	O	TYR	B	21	9.631	5.109	-3.127	0.00	0.00	O
ATOM	165	CB	TYR	B	21	6.405	5.726	-3.539	0.00	0.00	C
ATOM	166	CG	TYR	B	21	5.690	6.063	-4.829	0.00	0.00	C
ATOM	167	CD1	TYR	B	21	6.026	7.147	-5.628	0.00	0.00	C
ATOM	168	CD2	TYR	B	21	4.660	5.228	-5.249	0.00	0.00	C
ATOM	169	CE1	TYR	B	21	5.345	7.426	-6.811	0.00	0.00	C
ATOM	170	CE2	TYR	B	21	3.966	5.497	-6.433	0.00	0.00	C
ATOM	171	CZ	TYR	B	21	4.308	6.597	-7.213	0.00	0.00	C
ATOM	172	OH	TYR	B	21	3.587	6.756	-8.355	0.00	0.00	O
ATOM	173	N	CYS	B	22	8.357	3.790	-1.762	0.00	0.00	N
ATOM	174	CA	CYS	B	22	9.346	3.537	-0.698	0.00	0.00	C

Fig. 1 cont.

ATOM	175	C	CYS	B	22	10.706	3.061	-1.219	0.00	0.00	C
ATOM	176	O	CYS	B	22	10.976	1.911	-1.618	0.00	0.00	O
ATOM	177	CB	CYS	B	22	8.865	2.514	0.328	0.00	0.00	C
ATOM	178	SG	CYS	B	22	7.222	2.816	0.947	0.00	0.00	S
ATOM	179	N	GLY	B	23	11.631	4.004	-1.120	0.00	0.00	N
ATOM	180	CA	GLY	B	23	13.031	3.972	-1.513	0.00	0.00	C
ATOM	181	C	GLY	B	23	13.829	2.809	-0.956	0.00	0.00	C
ATOM	182	O	GLY	B	23	14.857	2.395	-1.536	0.00	0.00	O
ATOM	183	N	LYS	B	24	13.386	2.274	0.167	0.00	0.00	N
ATOM	184	CA	LYS	B	24	13.938	1.097	0.834	0.00	0.00	C
ATOM	185	C	LYS	B	24	13.631	-0.095	-0.085	0.00	0.00	C
ATOM	186	O	LYS	B	24	14.483	-0.954	-0.379	0.00	0.00	O
ATOM	187	CB	LYS	B	24	13.362	0.979	2.236	0.00	0.00	C
ATOM	188	CG	LYS	B	24	13.741	-0.174	3.157	0.00	0.00	C
ATOM	189	CD	LYS	B	24	13.192	-0.065	4.589	0.00	0.00	C
ATOM	190	CE	LYS	B	24	13.833	-0.999	5.606	0.00	0.00	C
ATOM	191	NZ	LYS	B	24	13.491	-0.704	7.025	0.00	0.00	N
ATOM	192	N	ASN	B	25	12.429	-0.171	-0.645	0.00	0.00	N
ATOM	193	CA	ASN	B	25	12.002	-1.280	-1.502	0.00	0.00	C
ATOM	194	C	ASN	B	25	12.473	-1.194	-2.950	0.00	0.00	C
ATOM	195	O	ASN	B	25	12.139	-2.050	-3.808	0.00	0.00	O
ATOM	196	CB	ASN	B	25	10.482	-1.415	-1.382	0.00	0.00	C
ATOM	197	CG	ASN	B	25	9.960	-1.596	0.017	0.00	0.00	C
ATOM	198	OD1	ASN	B	25	8.764	-1.844	0.251	0.00	0.00	O
ATOM	199	ND2	ASN	B	25	10.826	-1.493	1.023	0.00	0.00	N
ATOM	200	N	ASN	B	26	13.276	-0.201	-3.245	0.00	0.00	N
ATOM	201	CA	ASN	B	26	13.757	-0.040	-4.632	0.00	0.00	C
ATOM	202	C	ASN	B	26	15.110	-0.651	-4.905	0.00	0.00	C
ATOM	203	O	ASN	B	26	15.326	-0.959	-6.072	0.00	0.00	O
ATOM	204	CB	ASN	B	26	13.756	1.453	-4.934	0.00	0.00	C
ATOM	205	CG	ASN	B	26	12.399	1.831	-5.475	0.00	0.00	C
ATOM	206	OD1	ASN	B	26	12.348	3.012	-5.821	0.00	0.00	O
ATOM	207	ND2	ASN	B	26	11.469	0.898	-5.548	0.00	0.00	N
ATOM	208	N	ASP	B	27	15.897	-0.716	-3.862	0.00	0.00	N
ATOM	209	CA	ASP	B	27	17.231	-1.325	-3.966	0.00	0.00	C
ATOM	210	C	ASP	B	27	17.608	-1.565	-2.484	0.00	0.00	C
ATOM	211	O	ASP	B	27	18.175	-0.768	-1.761	0.00	0.00	O
ATOM	212	CB	ASP	B	27	18.242	-0.649	-4.840	0.00	0.00	C
ATOM	213	CG	ASP	B	27	18.413	-1.386	-6.171	0.00	0.00	C
ATOM	214	OD1	ASP	B	27	18.457	-0.761	-7.248	0.00	0.00	O
ATOM	215	OD2	ASP	B	27	18.517	-2.636	-6.209	0.00	0.00	O
ATOM	216	N	ALA	B	28	17.156	-2.743	-2.174	0.00	0.00	N
ATOM	217	CA	ALA	B	28	16.934	-3.807	-1.278	0.00	0.00	C
ATOM	218	C	ALA	B	28	17.392	-5.178	-1.831	0.00	0.00	C
ATOM	219	O	ALA	B	28	17.369	-5.454	-3.039	0.00	0.00	O
ATOM	220	CB	ALA	B	28	15.434	-4.089	-1.007	0.00	0.00	C
ATOM	221	N	PRO	B	29	17.775	-6.044	-0.888	0.00	0.00	N
ATOM	222	CA	PRO	B	29	18.296	-7.387	-1.168	0.00	0.00	C
ATOM	223	C	PRO	B	29	17.273	-8.465	-1.437	0.00	0.00	C
ATOM	224	O	PRO	B	29	16.174	-8.628	-0.881	0.00	0.00	O
ATOM	225	CB	PRO	B	29	19.170	-7.711	0.041	0.00	0.00	C
ATOM	226	CG	PRO	B	29	18.957	-6.649	1.078	0.00	0.00	C
ATOM	227	CD	PRO	B	29	17.831	-5.767	0.567	0.00	0.00	C
ATOM	228	N	ALA	B	30	17.672	-9.351	-2.318	0.00	0.00	N
ATOM	229	CA	ALA	B	30	16.910	-10.491	-2.816	0.00	0.00	C
ATOM	230	C	ALA	B	30	16.166	-11.355	-1.816	0.00	0.00	C
ATOM	231	O	ALA	B	30	15.312	-12.173	-2.282	0.00	0.00	O
ATOM	232	CB	ALA	B	30	17.910	-11.310	-3.670	0.00	0.00	C
ATOM	233	N	GLY	B	31	16.362	-11.293	-0.517	0.00	0.00	N

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Fig. 1 cont.

ATOM	234	CA	GLY	B	31	15.579	-12.209	0.331	0.00	0.00	C
ATOM	235	C	GLY	B	31	14.662	-11.499	1.304	0.00	0.00	C
ATOM	236	O	GLY	B	31	13.683	-12.078	1.800	0.00	0.00	O
ATOM	237	N	THR	B	32	15.037	-10.278	1.541	0.00	0.00	N
ATOM	238	CA	THR	B	32	14.358	-9.366	2.473	0.00	0.00	C
ATOM	239	C	THR	B	32	12.854	-9.431	2.419	0.00	0.00	C
ATOM	240	O	THR	B	32	12.248	-9.999	1.492	0.00	0.00	O
ATOM	241	CB	THR	B	32	15.049	-7.976	2.137	0.00	0.00	C
ATOM	242	OG1	THR	B	32	16.408	-8.228	2.685	0.00	0.00	O
ATOM	243	CG2	THR	B	32	14.470	-6.666	2.657	0.00	0.00	C
ATOM	244	N	ASN	B	33	12.226	-8.845	3.424	0.00	0.00	N
ATOM	245	CA	ASN	B	33	10.767	-8.746	3.607	0.00	0.00	C
ATOM	246	C	ASN	B	33	10.216	-7.432	3.061	0.00	0.00	C
ATOM	247	O	ASN	B	33	10.762	-6.417	3.533	0.00	0.00	O
ATOM	248	CB	ASN	B	33	10.545	-8.934	5.114	0.00	0.00	C
ATOM	249	CG	ASN	B	33	9.530	-10.011	5.460	0.00	0.00	C
ATOM	250	OD1	ASN	B	33	9.752	-10.846	6.362	0.00	0.00	O
ATOM	251	ND2	ASN	B	33	8.396	-10.006	4.735	0.00	0.00	N
ATOM	252	N	ILE	B	34	9.239	-7.310	2.175	0.00	0.00	N
ATOM	253	CA	ILE	B	34	8.760	-6.007	1.672	0.00	0.00	C
ATOM	254	C	ILE	B	34	7.968	-5.254	2.747	0.00	0.00	C
ATOM	255	O	ILE	B	34	6.778	-5.406	3.005	0.00	0.00	O
ATOM	256	CB	ILE	B	34	8.020	-6.090	0.296	0.00	0.00	C
ATOM	257	CG1	ILE	B	34	6.869	-7.113	0.145	0.00	0.00	C
ATOM	258	CG2	ILE	B	34	9.022	-6.426	-0.843	0.00	0.00	C
ATOM	259	CD1	ILE	B	34	6.721	-7.771	-1.281	0.00	0.00	C
ATOM	260	N	THR	B	35	8.660	-4.348	3.411	0.00	0.00	N
ATOM	261	CA	THR	B	35	8.248	-3.465	4.496	0.00	0.00	C
ATOM	262	C	THR	B	35	7.982	-2.054	3.991	0.00	0.00	C
ATOM	263	O	THR	B	35	8.667	-1.714	3.009	0.00	0.00	O
ATOM	264	CB	THR	B	35	9.349	-3.508	5.633	0.00	0.00	C
ATOM	265	OG1	THR	B	35	9.551	-2.079	5.916	0.00	0.00	O
ATOM	266	CG2	THR	B	35	10.646	-4.240	5.278	0.00	0.00	C
ATOM	267	N	CYS	B	36	7.071	-1.297	4.588	0.00	0.00	N
ATOM	268	CA	CYS	B	36	6.762	0.067	4.124	0.00	0.00	C
ATOM	269	C	CYS	B	36	6.857	1.120	5.230	0.00	0.00	C
ATOM	270	O	CYS	B	36	6.224	1.052	6.288	0.00	0.00	O
ATOM	271	CB	CYS	B	36	5.390	0.154	3.447	0.00	0.00	C
ATOM	272	SG	CYS	B	36	5.298	-0.969	2.017	0.00	0.00	S
ATOM	273	N	THR	B	37	7.692	2.103	4.937	0.00	0.00	N
ATOM	274	CA	THR	B	37	8.015	3.264	5.759	0.00	0.00	C
ATOM	275	C	THR	B	37	6.712	3.847	6.316	0.00	0.00	C
ATOM	276	O	THR	B	37	5.967	4.504	5.572	0.00	0.00	O
ATOM	277	CB	THR	B	37	8.882	4.339	4.992	0.00	0.00	C
ATOM	278	OG1	THR	B	37	10.252	3.815	4.873	0.00	0.00	O
ATOM	279	CG2	THR	B	37	8.919	5.708	5.678	0.00	0.00	C
ATOM	280	N	GLY	B	38	6.477	3.569	7.597	0.00	0.00	N
ATOM	281	CA	GLY	B	38	5.263	4.009	8.301	0.00	0.00	C
ATOM	282	C	GLY	B	38	3.989	3.569	7.558	0.00	0.00	C
ATOM	283	O	GLY	B	38	3.807	2.435	7.076	0.00	0.00	O
ATOM	284	N	ASN	B	39	3.086	4.519	7.454	0.00	0.00	N
ATOM	285	CA	ASN	B	39	1.755	4.458	6.849	0.00	0.00	C
ATOM	286	C	ASN	B	39	1.617	3.286	5.880	0.00	0.00	C
ATOM	287	O	ASN	B	39	1.386	2.125	6.249	0.00	0.00	O
ATOM	288	CB	ASN	B	39	1.388	5.822	6.247	0.00	0.00	C
ATOM	289	CG	ASN	B	39	1.971	7.015	6.989	0.00	0.00	C
ATOM	290	OD1	ASN	B	39	1.992	7.062	8.233	0.00	0.00	O
ATOM	291	ND2	ASN	B	39	2.487	8.035	6.283	0.00	0.00	N
ATOM	292	N	ALA	B	40	1.719	3.610	4.635	0.00	0.00	N

Fig. 1 cont.

ATOM	293	CA	ALA	B	40	1.687	2.879	3.407	0.00	0.00	C
ATOM	294	C	ALA	B	40	1.391	1.424	3.149	0.00	0.00	C
ATOM	295	O	ALA	B	40	0.983	1.266	1.949	0.00	0.00	O
ATOM	296	CB	ALA	B	40	3.193	2.962	2.934	0.00	0.00	C
ATOM	297	N	CYS	B	41	1.605	0.398	3.958	0.00	0.00	N
ATOM	298	CA	CYS	B	41	1.279	-0.974	3.424	0.00	0.00	C
ATOM	299	C	CYS	B	41	1.041	-2.130	4.377	0.00	0.00	C
ATOM	300	O	CYS	B	41	1.651	-3.189	4.239	0.00	0.00	O
ATOM	301	CB	CYS	B	41	2.385	-1.253	2.433	0.00	0.00	C
ATOM	302	SG	CYS	B	41	3.830	-2.286	2.566	0.00	0.00	S
ATOM	303	N	PRO	B	42	0.073	-2.014	5.271	0.00	0.00	N
ATOM	304	CA	PRO	B	42	-0.260	-3.024	6.261	0.00	0.00	C
ATOM	305	C	PRO	B	42	-0.574	-4.416	5.776	0.00	0.00	C
ATOM	306	O	PRO	B	42	-0.172	-5.381	6.432	0.00	0.00	O
ATOM	307	CB	PRO	B	42	-1.507	-2.441	6.965	0.00	0.00	C
ATOM	308	CG	PRO	B	42	-1.393	-0.935	6.811	0.00	0.00	C
ATOM	309	CD	PRO	B	42	-0.719	-0.768	5.460	0.00	0.00	C
ATOM	310	N	GLU	B	43	-1.287	-4.560	4.694	0.00	0.00	N
ATOM	311	CA	GLU	B	43	-1.748	-5.771	4.026	0.00	0.00	C
ATOM	312	C	GLU	B	43	-0.641	-6.615	3.409	0.00	0.00	C
ATOM	313	O	GLU	B	43	-0.770	-7.850	3.306	0.00	0.00	O
ATOM	314	CB	GLU	B	43	-2.769	-5.490	2.898	0.00	0.00	C
ATOM	315	CG	GLU	B	43	-4.224	-5.876	3.155	0.00	0.00	C
ATOM	316	CD	GLU	B	43	-5.010	-5.022	4.098	0.00	0.00	C
ATOM	317	OE1	GLU	B	43	-6.232	-4.990	4.063	0.00	0.00	O
ATOM	318	OE2	GLU	B	43	-4.405	-4.338	4.961	0.00	0.00	O
ATOM	319	N	VAL	B	44	0.369	-5.933	2.908	0.00	0.00	N
ATOM	320	CA	VAL	B	44	1.548	-6.572	2.292	0.00	0.00	C
ATOM	321	C	VAL	B	44	2.482	-7.084	3.388	0.00	0.00	C
ATOM	322	O	VAL	B	44	2.929	-8.250	3.426	0.00	0.00	O
ATOM	323	CB	VAL	B	44	2.117	-5.536	1.309	0.00	0.00	C
ATOM	324	CG1	VAL	B	44	3.582	-5.676	0.930	0.00	0.00	C
ATOM	325	CG2	VAL	B	44	1.216	-5.561	0.081	0.00	0.00	C
ATOM	326	N	GLU	B	45	2.723	-6.181	4.347	0.00	0.00	N
ATOM	327	CA	GLU	B	45	3.613	-6.451	5.478	0.00	0.00	C
ATOM	328	C	GLU	B	45	3.099	-7.736	6.123	0.00	0.00	C
ATOM	329	O	GLU	B	45	3.741	-8.813	5.991	0.00	0.00	O
ATOM	330	CB	GLU	B	45	3.616	-5.486	6.651	0.00	0.00	C
ATOM	331	CG	GLU	B	45	3.559	-3.980	6.455	0.00	0.00	C
ATOM	332	CD	GLU	B	45	4.935	-3.425	6.197	0.00	0.00	C
ATOM	333	OE1	GLU	B	45	5.893	-4.156	6.389	0.00	0.00	O
ATOM	334	OE2	GLU	B	45	5.015	-2.243	5.813	0.00	0.00	O
ATOM	335	N	LYS	B	46	1.857	-7.657	6.607	0.00	0.00	N
ATOM	336	CA	LYS	B	46	1.268	-8.849	7.261	0.00	0.00	C
ATOM	337	C	LYS	B	46	1.258	-10.043	6.309	0.00	0.00	C
ATOM	338	O	LYS	B	46	0.673	-11.017	6.838	0.00	0.00	O
ATOM	339	CB	LYS	B	46	0.056	-8.580	8.090	0.00	0.00	C
ATOM	340	CG	LYS	B	46	-1.246	-7.968	7.687	0.00	0.00	C
ATOM	341	CD	LYS	B	46	-2.391	-8.744	8.364	0.00	0.00	C
ATOM	342	CE	LYS	B	46	-2.643	-8.208	9.768	0.00	0.00	C
ATOM	343	NZ	LYS	B	46	-3.220	-6.827	9.617	0.00	0.00	N
ATOM	344	N	ALA	B	47	1.646	-10.075	5.040	0.00	0.00	N
ATOM	345	CA	ALA	B	47	1.636	-11.403	4.383	0.00	0.00	C
ATOM	346	C	ALA	B	47	3.024	-12.034	4.547	0.00	0.00	C
ATOM	347	O	ALA	B	47	3.766	-11.717	5.524	0.00	0.00	O
ATOM	348	CB	ALA	B	47	1.139	-11.216	2.949	0.00	0.00	C
ATOM	349	N	ASP	B	48	3.696	-12.555	3.571	0.00	0.00	N
ATOM	350	CA	ASP	B	48	4.980	-13.223	3.428	0.00	0.00	C
ATOM	351	C	ASP	B	48	5.474	-12.868	2.012	0.00	0.00	C

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Fig. 1 cont.

ATOM	352	O	ASP	B	48	5.419	-13.703	1.081	0.00	0.00	O
ATOM	353	CB	ASP	B	48	4.846	-14.731	3.623	0.00	0.00	C
ATOM	354	CG	ASP	B	48	6.062	-15.586	3.305	0.00	0.00	C
ATOM	355	OD1	ASP	B	48	6.945	-15.783	4.180	0.00	0.00	O
ATOM	356	OD2	ASP	B	48	6.141	-16.074	2.150	0.00	0.00	O
ATOM	357	N	ALA	B	49	5.927	-11.618	1.950	0.00	0.00	N
ATOM	358	CA	ALA	B	49	6.366	-11.113	0.611	0.00	0.00	C
ATOM	359	C	ALA	B	49	7.812	-10.721	0.802	0.00	0.00	C
ATOM	360	O	ALA	B	49	8.289	-9.998	1.672	0.00	0.00	O
ATOM	361	CB	ALA	B	49	5.346	-10.093	0.194	0.00	0.00	C
ATOM	362	N	THR	B	50	8.519	-11.344	-0.105	0.00	0.00	N
ATOM	363	CA	THR	B	50	9.972	-11.363	-0.218	0.00	0.00	C
ATOM	364	C	THR	B	50	10.201	-10.907	-1.645	0.00	0.00	C
ATOM	365	O	THR	B	50	9.476	-11.443	-2.495	0.00	0.00	O
ATOM	366	CB	THR	B	50	10.631	-12.772	0.110	0.00	0.00	C
ATOM	367	OG1	THR	B	50	10.516	-13.752	-1.012	0.00	0.00	O
ATOM	368	CG2	THR	B	50	10.085	-13.458	1.388	0.00	0.00	C
ATOM	369	N	PHE	B	51	11.228	-10.107	-1.759	0.00	0.00	N
ATOM	370	CA	PHE	B	51	11.555	-9.543	-3.066	0.00	0.00	C
ATOM	371	C	PHE	B	51	12.320	-10.624	-3.824	0.00	0.00	C
ATOM	372	O	PHE	B	51	12.993	-11.336	-3.049	0.00	0.00	O
ATOM	373	CB	PHE	B	51	12.552	-8.410	-2.920	0.00	0.00	C
ATOM	374	CG	PHE	B	51	12.227	-7.206	-2.120	0.00	0.00	C
ATOM	375	CD1	PHE	B	51	11.833	-6.049	-2.806	0.00	0.00	C
ATOM	376	CD2	PHE	B	51	12.323	-7.176	-0.730	0.00	0.00	C
ATOM	377	CE1	PHE	B	51	11.521	-4.883	-2.118	0.00	0.00	C
ATOM	378	CE2	PHE	B	51	12.024	-6.005	-0.011	0.00	0.00	C
ATOM	379	CZ	PHE	B	51	11.626	-4.849	-0.716	0.00	0.00	C
ATOM	380	N	LEU	B	52	12.129	-10.782	-5.151	0.00	0.00	N
ATOM	381	CA	LEU	B	52	13.014	-11.819	-5.701	0.00	0.00	C
ATOM	382	C	LEU	B	52	13.758	-11.090	-6.817	0.00	0.00	C
ATOM	383	O	LEU	B	52	14.749	-11.684	-7.302	0.00	0.00	O
ATOM	384	CB	LEU	B	52	12.224	-12.943	-6.339	0.00	0.00	C
ATOM	385	CG	LEU	B	52	10.712	-12.901	-6.297	0.00	0.00	C
ATOM	386	CD1	LEU	B	52	10.012	-13.831	-7.279	0.00	0.00	C
ATOM	387	CD2	LEU	B	52	10.385	-13.317	-4.864	0.00	0.00	C
ATOM	388	N	TYR	B	53	13.540	-9.800	-6.884	0.00	0.00	N
ATOM	389	CA	TYR	B	53	14.198	-8.857	-7.786	0.00	0.00	C
ATOM	390	C	TYR	B	53	13.697	-7.461	-7.373	0.00	0.00	C
ATOM	391	O	TYR	B	53	12.464	-7.336	-7.445	0.00	0.00	O
ATOM	392	CB	TYR	B	53	14.005	-9.070	-9.286	0.00	0.00	C
ATOM	393	CG	TYR	B	53	14.978	-8.244	-10.117	0.00	0.00	C
ATOM	394	CD1	TYR	B	53	16.329	-8.116	-9.768	0.00	0.00	C
ATOM	395	CD2	TYR	B	53	14.548	-7.599	-11.281	0.00	0.00	C
ATOM	396	CE1	TYR	B	53	17.194	-7.355	-10.551	0.00	0.00	C
ATOM	397	CE2	TYR	B	53	15.400	-6.835	-12.077	0.00	0.00	C
ATOM	398	CZ	TYR	B	53	16.729	-6.723	-11.705	0.00	0.00	C
ATOM	399	OH	TYR	B	53	17.568	-5.982	-12.491	0.00	0.00	O
ATOM	400	N	SER	B	54	14.590	-6.569	-7.056	0.00	0.00	N
ATOM	401	CA	SER	B	54	14.169	-5.201	-6.641	0.00	0.00	C
ATOM	402	C	SER	B	54	15.130	-4.272	-7.364	0.00	0.00	C
ATOM	403	O	SER	B	54	16.353	-4.401	-7.203	0.00	0.00	O
ATOM	404	CB	SER	B	54	14.128	-5.128	-5.136	0.00	0.00	C
ATOM	405	OG	SER	B	54	14.909	-4.052	-4.674	0.00	0.00	O
ATOM	406	N	PHE	B	55	14.573	-3.362	-8.147	0.00	0.00	N
ATOM	407	CA	PHE	B	55	15.322	-2.476	-9.034	0.00	0.00	C
ATOM	408	C	PHE	B	55	14.992	-1.006	-9.120	0.00	0.00	C
ATOM	409	O	PHE	B	55	13.827	-0.604	-9.083	0.00	0.00	O
ATOM	410	CB	PHE	B	55	15.104	-3.068	-10.445	0.00	0.00	C

Fig. 1 cont.

ATOM	411	CG	PHE	B	55	13.663	-3.167	-10.849	0.00	0.00	C
ATOM	412	CD1	PHE	B	55	12.826	-4.171	-10.376	0.00	0.00	C
ATOM	413	CD2	PHE	B	55	13.151	-2.216	-11.749	0.00	0.00	C
ATOM	414	CE1	PHE	B	55	11.505	-4.247	-10.801	0.00	0.00	C
ATOM	415	CE2	PHE	B	55	11.826	-2.287	-12.169	0.00	0.00	C
ATOM	416	CZ	PHE	B	55	10.988	-3.304	-11.694	0.00	0.00	C
ATOM	417	N	GLU	B	56	16.068	-0.259	-9.248	0.00	0.00	N
ATOM	418	CA	GLU	B	56	16.130	1.201	-9.324	0.00	0.00	C
ATOM	419	C	GLU	B	56	17.111	1.656	-10.403	0.00	0.00	C
ATOM	420	O	GLU	B	56	17.960	0.981	-10.993	0.00	0.00	O
ATOM	421	CB	GLU	B	56	16.489	1.911	-8.007	0.00	0.00	C
ATOM	422	CG	GLU	B	56	17.867	2.498	-7.799	0.00	0.00	C
ATOM	423	CD	GLU	B	56	18.354	2.943	-6.475	0.00	0.00	C
ATOM	424	OE1	GLU	B	56	18.632	4.070	-6.102	0.00	0.00	O
ATOM	425	OE2	GLU	B	56	18.548	2.045	-5.639	0.00	0.00	O
ATOM	426	N	ASP	B	57	16.884	2.890	-10.774	0.00	0.00	N
ATOM	427	CA	ASP	B	57	17.512	3.810	-11.717	0.00	0.00	C
ATOM	428	C	ASP	B	57	17.927	3.104	-12.996	0.00	0.00	C
ATOM	429	O	ASP	B	57	18.886	3.461	-13.672	0.00	0.00	O
ATOM	430	CB	ASP	B	57	18.610	4.591	-10.959	0.00	0.00	C
ATOM	431	CG	ASP	B	57	18.098	5.867	-10.288	0.00	0.00	C
ATOM	432	OD1	ASP	B	57	18.050	6.034	-9.044	0.00	0.00	O
ATOM	433	OD2	ASP	B	57	17.720	6.798	-11.056	0.00	0.00	O
ATOM	434	N	SER	B	58	17.171	2.139	-13.442	0.00	0.00	N
ATOM	435	CA	SER	B	58	17.216	1.216	-14.538	0.00	0.00	C
ATOM	436	C	SER	B	58	16.722	1.489	-15.945	0.00	0.00	C
ATOM	437	O	SER	B	58	15.525	1.769	-16.133	0.00	0.00	O
ATOM	438	CB	SER	B	58	16.253	0.061	-14.119	0.00	0.00	C
ATOM	439	OG	SER	B	58	16.883	-1.095	-13.656	0.00	0.00	O
ATOM	440	N	GLY	B	59	17.567	1.292	-16.925	0.00	0.00	N
ATOM	441	CA	GLY	B	59	17.249	1.426	-18.333	0.00	0.00	C
ATOM	442	C	GLY	B	59	17.032	2.850	-18.835	0.00	0.00	C
ATOM	443	O	GLY	B	59	17.780	3.778	-18.449	0.00	0.00	O
ATOM	444	N	VAL	B	60	15.989	2.970	-19.684	0.00	0.00	N
ATOM	445	CA	VAL	B	60	15.770	4.333	-20.215	0.00	0.00	C
ATOM	446	C	VAL	B	60	14.984	5.232	-19.293	0.00	0.00	C
ATOM	447	O	VAL	B	60	15.801	6.116	-18.825	0.00	0.00	O
ATOM	448	CB	VAL	B	60	15.351	4.234	-21.683	0.00	0.00	C
ATOM	449	CG1	VAL	B	60	15.503	5.572	-22.394	0.00	0.00	C
ATOM	450	CG2	VAL	B	60	16.178	3.227	-22.458	0.00	0.00	C
ATOM	451	N	GLY	B	61	13.744	5.269	-18.902	0.00	0.00	N
ATOM	452	CA	GLY	B	61	13.363	6.397	-17.995	0.00	0.00	C
ATOM	453	C	GLY	B	61	13.541	6.263	-16.525	0.00	0.00	C
ATOM	454	O	GLY	B	61	12.576	6.613	-15.816	0.00	0.00	O
ATOM	455	N	ASP	B	62	14.631	5.808	-15.949	0.00	0.00	N
ATOM	456	CA	ASP	B	62	14.696	5.636	-14.492	0.00	0.00	C
ATOM	457	C	ASP	B	62	13.712	4.510	-14.166	0.00	0.00	C
ATOM	458	O	ASP	B	62	12.931	4.738	-13.216	0.00	0.00	O
ATOM	459	CB	ASP	B	62	14.283	6.844	-13.657	0.00	0.00	C
ATOM	460	CG	ASP	B	62	14.705	6.733	-12.205	0.00	0.00	C
ATOM	461	OD1	ASP	B	62	15.057	7.681	-11.480	0.00	0.00	O
ATOM	462	OD2	ASP	B	62	14.713	5.589	-11.710	0.00	0.00	O
ATOM	463	N	VAL	B	63	13.692	3.386	-14.842	0.00	0.00	N
ATOM	464	CA	VAL	B	63	12.698	2.348	-14.437	0.00	0.00	C
ATOM	465	C	VAL	B	63	12.989	1.767	-13.050	0.00	0.00	C
ATOM	466	O	VAL	B	63	13.992	1.159	-12.630	0.00	0.00	O
ATOM	467	CB	VAL	B	63	12.626	1.422	-15.657	0.00	0.00	C
ATOM	468	CG1	VAL	B	63	11.434	0.476	-15.550	0.00	0.00	C
ATOM	469	CG2	VAL	B	63	12.629	2.188	-16.980	0.00	0.00	C

Fig. 1 cont.

ATOM	470	N	THR	B	64	12.043	1.890	-12.133	0.00	0.00	N
ATOM	471	CA	THR	B	64	11.956	1.508	-10.753	0.00	0.00	C
ATOM	472	C	THR	B	64	10.747	0.751	-10.245	0.00	0.00	C
ATOM	473	O	THR	B	64	9.594	1.073	-10.546	0.00	0.00	O
ATOM	474	CB	THR	B	64	11.924	2.883	-9.926	0.00	0.00	C
ATOM	475	OG1	THR	B	64	13.206	3.478	-10.219	0.00	0.00	O
ATOM	476	CG2	THR	B	64	11.615	2.647	-8.463	0.00	0.00	C
ATOM	477	N	GLY	B	65	10.978	-0.269	-9.450	0.00	0.00	N
ATOM	478	CA	GLY	B	65	9.835	-1.091	-8.935	0.00	0.00	C
ATOM	479	C	GLY	B	65	10.585	-2.168	-8.137	0.00	0.00	C
ATOM	480	O	GLY	B	65	11.589	-1.805	-7.538	0.00	0.00	O
ATOM	481	N	PHE	B	66	9.969	-3.309	-8.033	0.00	0.00	N
ATOM	482	CA	PHE	B	66	10.400	-4.572	-7.485	0.00	0.00	C
ATOM	483	C	PHE	B	66	9.533	-5.712	-8.081	0.00	0.00	C
ATOM	484	O	PHE	B	66	8.381	-5.542	-8.492	0.00	0.00	O
ATOM	485	CB	PHE	B	66	10.388	-4.726	-5.961	0.00	0.00	C
ATOM	486	CG	PHE	B	66	9.012	-4.583	-5.400	0.00	0.00	C
ATOM	487	CD1	PHE	B	66	8.044	-5.570	-5.581	0.00	0.00	C
ATOM	488	CD2	PHE	B	66	8.672	-3.428	-4.716	0.00	0.00	C
ATOM	489	CE1	PHE	B	66	6.761	-5.420	-5.090	0.00	0.00	C
ATOM	490	CE2	PHE	B	66	7.379	-3.262	-4.207	0.00	0.00	C
ATOM	491	CZ	PHE	B	66	6.421	-4.263	-4.392	0.00	0.00	C
ATOM	492	N	LEU	B	67	10.074	-6.904	-8.027	0.00	0.00	N
ATOM	493	CA	LEU	B	67	9.318	-8.101	-8.436	0.00	0.00	C
ATOM	494	C	LEU	B	67	9.289	-8.841	-7.090	0.00	0.00	C
ATOM	495	O	LEU	B	67	10.380	-8.759	-6.464	0.00	0.00	O
ATOM	496	CB	LEU	B	67	9.891	-8.877	-9.591	0.00	0.00	C
ATOM	497	CG	LEU	B	67	9.088	-10.160	-9.863	0.00	0.00	C
ATOM	498	CD1	LEU	B	67	7.772	-9.828	-10.557	0.00	0.00	C
ATOM	499	CD2	LEU	B	67	9.903	-11.123	-10.729	0.00	0.00	C
ATOM	500	N	ALA	B	68	8.176	-9.402	-6.673	0.00	0.00	N
ATOM	501	CA	ALA	B	68	8.103	-10.060	-5.363	0.00	0.00	C
ATOM	502	C	ALA	B	68	7.333	-11.383	-5.406	0.00	0.00	C
ATOM	503	O	ALA	B	68	6.699	-11.701	-6.419	0.00	0.00	O
ATOM	504	CB	ALA	B	68	7.469	-9.259	-4.249	0.00	0.00	C
ATOM	505	N	LEU	B	69	7.503	-12.100	-4.298	0.00	0.00	N
ATOM	506	CA	LEU	B	69	6.878	-13.383	-4.034	0.00	0.00	C
ATOM	507	C	LEU	B	69	6.011	-13.207	-2.774	0.00	0.00	C
ATOM	508	O	LEU	B	69	6.529	-12.840	-1.719	0.00	0.00	O
ATOM	509	CB	LEU	B	69	7.836	-14.507	-3.706	0.00	0.00	C
ATOM	510	CG	LEU	B	69	7.222	-15.902	-3.782	0.00	0.00	C
ATOM	511	CD1	LEU	B	69	6.656	-16.103	-5.186	0.00	0.00	C
ATOM	512	CD2	LEU	B	69	8.302	-16.921	-3.461	0.00	0.00	C
ATOM	513	N	ASP	B	70	4.770	-13.549	-2.977	0.00	0.00	N
ATOM	514	CA	ASP	B	70	3.742	-13.424	-1.906	0.00	0.00	C
ATOM	515	C	ASP	B	70	3.368	-14.897	-1.836	0.00	0.00	C
ATOM	516	O	ASP	B	70	2.692	-15.467	-2.678	0.00	0.00	O
ATOM	517	CB	ASP	B	70	2.688	-12.444	-2.343	0.00	0.00	C
ATOM	518	CG	ASP	B	70	1.652	-12.023	-1.343	0.00	0.00	C
ATOM	519	OD1	ASP	B	70	0.867	-12.854	-0.885	0.00	0.00	O
ATOM	520	OD2	ASP	B	70	1.630	-10.824	-1.000	0.00	0.00	O
ATOM	521	N	ASN	B	71	3.849	-15.417	-0.730	0.00	0.00	N
ATOM	522	CA	ASN	B	71	3.712	-16.890	-0.475	0.00	0.00	C
ATOM	523	C	ASN	B	71	2.521	-17.085	0.444	0.00	0.00	C
ATOM	524	O	ASN	B	71	2.230	-18.212	0.853	0.00	0.00	O
ATOM	525	CB	ASN	B	71	5.086	-17.283	-0.129	0.00	0.00	C
ATOM	526	CG	ASN	B	71	5.807	-18.547	0.016	0.00	0.00	C
ATOM	527	OD1	ASN	B	71	6.316	-18.746	1.141	0.00	0.00	O
ATOM	528	ND2	ASN	B	71	5.937	-19.359	-1.017	0.00	0.00	N

Fig. 1 cont.

ATOM	529	N	THR	B	72	1.821	-15.999	0.663	0.00	0.00	N
ATOM	530	CA	THR	B	72	0.581	-16.054	1.467	0.00	0.00	C
ATOM	531	C	THR	B	72	-0.585	-15.908	0.505	0.00	0.00	C
ATOM	532	O	THR	B	72	-1.480	-16.784	0.507	0.00	0.00	O
ATOM	533	CB	THR	B	72	0.748	-15.071	2.678	0.00	0.00	C
ATOM	534	OG1	THR	B	72	1.691	-15.884	3.479	0.00	0.00	O
ATOM	535	CG2	THR	B	72	-0.588	-14.659	3.279	0.00	0.00	C
ATOM	536	N	ASN	B	73	-0.599	-14.943	-0.392	0.00	0.00	N
ATOM	537	CA	ASN	B	73	-1.719	-14.802	-1.353	0.00	0.00	C
ATOM	538	C	ASN	B	73	-1.523	-15.727	-2.541	0.00	0.00	C
ATOM	539	O	ASN	B	73	-2.431	-15.988	-3.351	0.00	0.00	O
ATOM	540	CB	ASN	B	73	-1.877	-13.313	-1.703	0.00	0.00	C
ATOM	541	CG	ASN	B	73	-2.178	-12.693	-0.338	0.00	0.00	C
ATOM	542	OD1	ASN	B	73	-1.303	-12.095	0.292	0.00	0.00	O
ATOM	543	ND2	ASN	B	73	-3.416	-13.016	0.017	0.00	0.00	N
ATOM	544	N	LYS	B	74	-0.296	-16.211	-2.611	0.00	0.00	N
ATOM	545	CA	LYS	B	74	0.062	-17.125	-3.711	0.00	0.00	C
ATOM	546	C	LYS	B	74	-0.099	-16.289	-4.976	0.00	0.00	C
ATOM	547	O	LYS	B	74	-0.876	-16.578	-5.894	0.00	0.00	O
ATOM	548	CB	LYS	B	74	-0.753	-18.414	-3.644	0.00	0.00	C
ATOM	549	CG	LYS	B	74	-0.292	-19.287	-2.447	0.00	0.00	C
ATOM	550	CD	LYS	B	74	-0.407	-20.776	-2.775	0.00	0.00	C
ATOM	551	CE	LYS	B	74	0.572	-21.645	-2.006	0.00	0.00	C
ATOM	552	NZ	LYS	B	74	0.790	-23.002	-2.588	0.00	0.00	N
ATOM	553	N	LEU	B	75	0.708	-15.228	-4.942	0.00	0.00	N
ATOM	554	CA	LEU	B	75	0.860	-14.208	-5.960	0.00	0.00	C
ATOM	555	C	LEU	B	75	2.359	-13.889	-6.141	0.00	0.00	C
ATOM	556	O	LEU	B	75	3.160	-13.963	-5.240	0.00	0.00	O
ATOM	557	CB	LEU	B	75	0.259	-12.820	-5.746	0.00	0.00	C
ATOM	558	CG	LEU	B	75	-0.766	-12.474	-4.718	0.00	0.00	C
ATOM	559	CD1	LEU	B	75	-0.419	-11.126	-4.090	0.00	0.00	C
ATOM	560	CD2	LEU	B	75	-2.148	-12.406	-5.357	0.00	0.00	C
ATOM	561	N	ILE	B	76	2.663	-13.480	-7.328	0.00	0.00	N
ATOM	562	CA	ILE	B	76	3.956	-13.002	-7.802	0.00	0.00	C
ATOM	563	C	ILE	B	76	3.613	-11.603	-8.315	0.00	0.00	C
ATOM	564	O	ILE	B	76	3.202	-11.445	-9.473	0.00	0.00	O
ATOM	565	CB	ILE	B	76	4.463	-13.967	-8.913	0.00	0.00	C
ATOM	566	CG1	ILE	B	76	4.578	-15.400	-8.357	0.00	0.00	C
ATOM	567	CG2	ILE	B	76	5.780	-13.438	-9.533	0.00	0.00	C
ATOM	568	CD1	ILE	B	76	5.168	-16.401	-9.392	0.00	0.00	C
ATOM	569	N	VAL	B	77	3.921	-10.590	-7.545	0.00	0.00	N
ATOM	570	CA	VAL	B	77	3.570	-9.211	-7.850	0.00	0.00	C
ATOM	571	C	VAL	B	77	4.803	-8.463	-8.327	0.00	0.00	C
ATOM	572	O	VAL	B	77	5.856	-8.608	-7.727	0.00	0.00	O
ATOM	573	CB	VAL	B	77	2.964	-8.539	-6.606	0.00	0.00	C
ATOM	574	CG1	VAL	B	77	1.931	-7.515	-7.052	0.00	0.00	C
ATOM	575	CG2	VAL	B	77	2.434	-9.530	-5.581	0.00	0.00	C
ATOM	576	N	LEU	B	78	4.558	-7.729	-9.403	0.00	0.00	N
ATOM	577	CA	LEU	B	78	5.581	-6.905	-10.068	0.00	0.00	C
ATOM	578	C	LEU	B	78	4.973	-5.497	-9.982	0.00	0.00	C
ATOM	579	O	LEU	B	78	3.942	-5.266	-10.630	0.00	0.00	O
ATOM	580	CB	LEU	B	78	5.845	-7.316	-11.509	0.00	0.00	C
ATOM	581	CG	LEU	B	78	7.170	-6.967	-12.173	0.00	0.00	C
ATOM	582	CD1	LEU	B	78	6.985	-6.589	-13.636	0.00	0.00	C
ATOM	583	CD2	LEU	B	78	7.865	-5.790	-11.500	0.00	0.00	C
ATOM	584	N	SER	B	79	5.660	-4.626	-9.297	0.00	0.00	N
ATOM	585	CA	SER	B	79	5.181	-3.267	-9.083	0.00	0.00	C
ATOM	586	C	SER	B	79	6.164	-2.263	-9.643	0.00	0.00	C
ATOM	587	O	SER	B	79	7.336	-2.419	-9.260	0.00	0.00	O

Fig. 1 cont.

ATOM	588	CB	SER	B	79	5.083	-3.125	-7.583	0.00	0.00	C
ATOM	589	OG	SER	B	79	4.329	-2.132	-6.979	0.00	0.00	O
ATOM	590	N	PHE	B	80	5.640	-1.299	-10.403	0.00	0.00	N
ATOM	591	CA	PHE	B	80	6.521	-0.241	-10.934	0.00	0.00	C
ATOM	592	C	PHE	B	80	6.094	1.136	-10.343	0.00	0.00	C
ATOM	593	O	PHE	B	80	4.963	1.561	-10.070	0.00	0.00	O
ATOM	594	CB	PHE	B	80	6.640	-0.053	-12.410	0.00	0.00	C
ATOM	595	CG	PHE	B	80	6.784	-1.157	-13.375	0.00	0.00	C
ATOM	596	CD1	PHE	B	80	5.724	-2.038	-13.610	0.00	0.00	C
ATOM	597	CD2	PHE	B	80	7.982	-1.297	-14.088	0.00	0.00	C
ATOM	598	CE1	PHE	B	80	5.833	-3.070	-14.532	0.00	0.00	C
ATOM	599	CE2	PHE	B	80	8.104	-2.336	-15.030	0.00	0.00	C
ATOM	600	CZ	PHE	B	80	7.033	-3.229	-15.223	0.00	0.00	C
ATOM	601	N	ARG	B	81	7.178	1.869	-10.131	0.00	0.00	N
ATOM	602	CA	ARG	B	81	7.094	3.217	-9.560	0.00	0.00	C
ATOM	603	C	ARG	B	81	6.624	4.230	-10.614	0.00	0.00	C
ATOM	604	O	ARG	B	81	7.106	4.260	-11.739	0.00	0.00	O
ATOM	605	CB	ARG	B	81	8.405	3.711	-8.927	0.00	0.00	C
ATOM	606	CG	ARG	B	81	8.268	4.834	-7.898	0.00	0.00	C
ATOM	607	CD	ARG	B	81	9.605	5.342	-7.478	0.00	0.00	C
ATOM	608	NE	ARG	B	81	10.427	5.827	-8.567	0.00	0.00	N
ATOM	609	CZ	ARG	B	81	11.546	6.527	-8.411	0.00	0.00	C
ATOM	610	NH1	ARG	B	81	11.994	6.814	-7.193	0.00	0.00	N
ATOM	611	NH2	ARG	B	81	12.233	6.957	-9.471	0.00	0.00	N
ATOM	612	N	GLY	B	82	5.715	5.046	-10.134	0.00	0.00	N
ATOM	613	CA	GLY	B	82	5.117	6.157	-10.859	0.00	0.00	C
ATOM	614	C	GLY	B	82	6.262	7.186	-10.878	0.00	0.00	C
ATOM	615	O	GLY	B	82	7.430	6.899	-10.576	0.00	0.00	O
ATOM	616	N	SER	B	83	5.913	8.399	-11.243	0.00	0.00	N
ATOM	617	CA	SER	B	83	6.981	9.408	-11.325	0.00	0.00	C
ATOM	618	C	SER	B	83	7.433	9.979	-10.003	0.00	0.00	C
ATOM	619	O	SER	B	83	6.682	10.264	-9.078	0.00	0.00	O
ATOM	620	CB	SER	B	83	6.447	10.478	-12.293	0.00	0.00	C
ATOM	621	OG	SER	B	83	5.756	9.722	-13.291	0.00	0.00	O
ATOM	622	N	ARG	B	84	8.726	10.222	-9.968	0.00	0.00	N
ATOM	623	CA	ARG	B	84	9.414	10.841	-8.861	0.00	0.00	C
ATOM	624	C	ARG	B	84	10.555	11.736	-9.338	0.00	0.00	C
ATOM	625	O	ARG	B	84	10.577	12.931	-9.031	0.00	0.00	O
ATOM	626	CB	ARG	B	84	10.008	9.823	-7.876	0.00	0.00	C
ATOM	627	CG	ARG	B	84	10.727	10.457	-6.693	0.00	0.00	C
ATOM	628	CD	ARG	B	84	10.369	9.855	-5.388	0.00	0.00	C
ATOM	629	NE	ARG	B	84	8.997	10.157	-5.025	0.00	0.00	N
ATOM	630	CZ	ARG	B	84	8.344	9.490	-4.065	0.00	0.00	C
ATOM	631	NH1	ARG	B	84	8.879	8.490	-3.373	0.00	0.00	N
ATOM	632	NH2	ARG	B	84	7.078	9.829	-3.789	0.00	0.00	N
ATOM	633	N	SER	B	85	11.505	11.152	-10.021	0.00	0.00	N
ATOM	634	CA	SER	B	85	12.707	11.842	-10.469	0.00	0.00	C
ATOM	635	C	SER	B	85	12.457	12.646	-11.713	0.00	0.00	C
ATOM	636	O	SER	B	85	11.570	12.163	-12.421	0.00	0.00	O
ATOM	637	CB	SER	B	85	13.825	10.844	-10.787	0.00	0.00	C
ATOM	638	OG	SER	B	85	13.575	10.207	-12.019	0.00	0.00	O
ATOM	639	N	ILE	B	86	13.251	13.675	-11.958	0.00	0.00	N
ATOM	640	CA	ILE	B	86	13.029	14.436	-13.194	0.00	0.00	C
ATOM	641	C	ILE	B	86	13.188	13.514	-14.403	0.00	0.00	C
ATOM	642	O	ILE	B	86	12.459	13.832	-15.364	0.00	0.00	O
ATOM	643	CB	ILE	B	86	13.835	15.766	-13.399	0.00	0.00	C
ATOM	644	CG1	ILE	B	86	14.953	15.542	-14.455	0.00	0.00	C
ATOM	645	CG2	ILE	B	86	14.412	16.391	-12.115	0.00	0.00	C
ATOM	646	CD1	ILE	B	86	15.271	16.841	-15.228	0.00	0.00	C
ATOM	647	N	GLU	B	87	14.034	12.507	-14.423	0.00	0.00	N

Fig. 1 cont.

ATOM	648	CA	GLU	B	87	14.188	11.631	-15.597	0.00	0.00	C
ATOM	649	C	GLU	B	87	12.893	10.874	-15.890	0.00	0.00	C
ATOM	650	O	GLU	B	87	12.668	10.406	-17.028	0.00	0.00	O
ATOM	651	CB	GLU	B	87	15.344	10.673	-15.565	0.00	0.00	C
ATOM	652	CG	GLU	B	87	16.078	10.249	-14.329	0.00	0.00	C
ATOM	653	CD	GLU	B	87	17.169	11.108	-13.768	0.00	0.00	C
ATOM	654	OE1	GLU	B	87	16.979	11.942	-12.897	0.00	0.00	O
ATOM	655	OE2	GLU	B	87	18.282	10.848	-14.292	0.00	0.00	O
ATOM	656	N	ASN	B	88	12.064	10.682	-14.896	0.00	0.00	N
ATOM	657	CA	ASN	B	88	10.758	10.035	-14.966	0.00	0.00	C
ATOM	658	C	ASN	B	88	9.781	10.982	-15.686	0.00	0.00	C
ATOM	659	O	ASN	B	88	9.155	10.662	-16.689	0.00	0.00	O
ATOM	660	CB	ASN	B	88	10.187	9.704	-13.600	0.00	0.00	C
ATOM	661	CG	ASN	B	88	10.444	8.508	-12.754	0.00	0.00	C
ATOM	662	OD1	ASN	B	88	10.749	8.620	-11.557	0.00	0.00	O
ATOM	663	ND2	ASN	B	88	10.309	7.270	-13.216	0.00	0.00	N
ATOM	664	N	TRP	B	89	9.699	12.166	-15.108	0.00	0.00	N
ATOM	665	CA	TRP	B	89	8.822	13.281	-15.509	0.00	0.00	C
ATOM	666	C	TRP	B	89	9.197	13.845	-16.871	0.00	0.00	C
ATOM	667	O	TRP	B	89	8.246	13.894	-17.690	0.00	0.00	O
ATOM	668	CB	TRP	B	89	8.812	14.263	-14.352	0.00	0.00	C
ATOM	669	CG	TRP	B	89	8.019	14.122	-13.114	0.00	0.00	C
ATOM	670	CD1	TRP	B	89	8.509	14.091	-11.835	0.00	0.00	C
ATOM	671	CD2	TRP	B	89	6.586	14.087	-12.976	0.00	0.00	C
ATOM	672	NE1	TRP	B	89	7.477	14.033	-10.928	0.00	0.00	N
ATOM	673	CE2	TRP	B	89	6.292	13.994	-11.599	0.00	0.00	C
ATOM	674	CE3	TRP	B	89	5.533	14.074	-13.894	0.00	0.00	C
ATOM	675	CZ2	TRP	B	89	4.994	13.875	-11.115	0.00	0.00	C
ATOM	676	CZ3	TRP	B	89	4.231	13.965	-13.425	0.00	0.00	C
ATOM	677	CH2	TRP	B	89	3.963	13.867	-12.043	0.00	0.00	C
ATOM	678	N	ILE	B	90	10.417	14.147	-17.266	0.00	0.00	N
ATOM	679	CA	ILE	B	90	10.741	14.656	-18.605	0.00	0.00	C
ATOM	680	C	ILE	B	90	10.349	13.599	-19.652	0.00	0.00	C
ATOM	681	O	ILE	B	90	10.243	13.799	-20.879	0.00	0.00	O
ATOM	682	CB	ILE	B	90	12.197	15.204	-18.809	0.00	0.00	C
ATOM	683	CG1	ILE	B	90	12.612	16.387	-17.898	0.00	0.00	C
ATOM	684	CG2	ILE	B	90	12.463	15.635	-20.295	0.00	0.00	C
ATOM	685	CD1	ILE	B	90	13.902	17.121	-18.382	0.00	0.00	C
ATOM	686	N	GLY	B	91	10.223	12.365	-19.261	0.00	0.00	N
ATOM	687	CA	GLY	B	91	9.834	11.151	-19.953	0.00	0.00	C
ATOM	688	C	GLY	B	91	8.342	11.121	-20.268	0.00	0.00	C
ATOM	689	O	GLY	B	91	7.936	10.507	-21.267	0.00	0.00	O
ATOM	690	N	ASN	B	92	7.555	11.732	-19.395	0.00	0.00	N
ATOM	691	CA	ASN	B	92	6.083	11.757	-19.545	0.00	0.00	C
ATOM	692	C	ASN	B	92	5.732	12.655	-20.717	0.00	0.00	C
ATOM	693	O	ASN	B	92	4.739	12.406	-21.407	0.00	0.00	O
ATOM	694	CB	ASN	B	92	5.380	12.054	-18.225	0.00	0.00	C
ATOM	695	CG	ASN	B	92	5.670	10.911	-17.238	0.00	0.00	C
ATOM	696	OD1	ASN	B	92	6.208	11.222	-16.159	0.00	0.00	O
ATOM	697	ND2	ASN	B	92	5.364	9.662	-17.590	0.00	0.00	N
ATOM	698	N	LEU	B	93	6.566	13.653	-20.927	0.00	0.00	N
ATOM	699	CA	LEU	B	93	6.402	14.610	-22.005	0.00	0.00	C
ATOM	700	C	LEU	B	93	7.057	14.063	-23.255	0.00	0.00	C
ATOM	701	O	LEU	B	93	7.692	14.870	-23.937	0.00	0.00	O
ATOM	702	CB	LEU	B	93	7.011	15.964	-21.653	0.00	0.00	C
ATOM	703	CG	LEU	B	93	7.296	16.324	-20.209	0.00	0.00	C
ATOM	704	CD1	LEU	B	93	8.493	17.270	-20.139	0.00	0.00	C
ATOM	705	CD2	LEU	B	93	6.065	16.988	-19.605	0.00	0.00	C
ATOM	706	N	ASN	B	94	6.962	12.806	-23.559	0.00	0.00	N
ATOM	707	CA	ASN	B	94	7.532	12.165	-24.743	0.00	0.00	C

Fig. 1 cont.

ATOM	708	C	ASN	B	94	6.353	11.529	-25.460	0.00	0.00	C
ATOM	709	O	ASN	B	94	6.494	10.359	-25.788	0.00	0.00	O
ATOM	710	CB	ASN	B	94	8.600	11.095	-24.454	0.00	0.00	C
ATOM	711	CG	ASN	B	94	9.822	11.680	-25.162	0.00	0.00	C
ATOM	712	OD1	ASN	B	94	9.550	12.170	-26.266	0.00	0.00	O
ATOM	713	ND2	ASN	B	94	10.974	11.644	-24.546	0.00	0.00	N
ATOM	714	N	PHE	B	95	5.298	12.302	-25.551	0.00	0.00	N
ATOM	715	CA	PHE	B	95	4.020	11.861	-26.101	0.00	0.00	C
ATOM	716	C	PHE	B	95	4.072	11.598	-27.600	0.00	0.00	C
ATOM	717	O	PHE	B	95	2.899	11.286	-27.989	0.00	0.00	O
ATOM	718	CB	PHE	B	95	2.851	12.786	-25.931	0.00	0.00	C
ATOM	719	CG	PHE	B	95	2.172	13.645	-24.981	0.00	0.00	C
ATOM	720	CD1	PHE	B	95	0.813	13.975	-25.158	0.00	0.00	C
ATOM	721	CD2	PHE	B	95	2.840	14.230	-23.890	0.00	0.00	C
ATOM	722	CE1	PHE	B	95	0.156	14.839	-24.268	0.00	0.00	C
ATOM	723	CE2	PHE	B	95	2.202	15.103	-22.991	0.00	0.00	C
ATOM	724	CZ	PHE	B	95	0.835	15.387	-23.176	0.00	0.00	C
ATOM	725	N	ASP	B	96	5.100	11.656	-28.424	0.00	0.00	N
ATOM	726	CA	ASP	B	96	4.637	11.319	-29.812	0.00	0.00	C
ATOM	727	C	ASP	B	96	4.261	9.832	-29.643	0.00	0.00	C
ATOM	728	O	ASP	B	96	4.550	9.218	-28.609	0.00	0.00	O
ATOM	729	CB	ASP	B	96	5.486	11.670	-30.975	0.00	0.00	C
ATOM	730	CG	ASP	B	96	6.977	11.485	-30.809	0.00	0.00	C
ATOM	731	OD1	ASP	B	96	7.379	10.780	-29.865	0.00	0.00	O
ATOM	732	OD2	ASP	B	96	7.620	12.106	-31.693	0.00	0.00	O
ATOM	733	N	LEU	B	97	3.670	9.374	-30.729	0.00	0.00	N
ATOM	734	CA	LEU	B	97	3.243	7.956	-30.695	0.00	0.00	C
ATOM	735	C	LEU	B	97	4.299	7.299	-31.604	0.00	0.00	C
ATOM	736	O	LEU	B	97	4.476	7.650	-32.763	0.00	0.00	O
ATOM	737	CB	LEU	B	97	1.799	7.835	-31.089	0.00	0.00	C
ATOM	738	CG	LEU	B	97	0.605	8.375	-30.358	0.00	0.00	C
ATOM	739	CD1	LEU	B	97	0.473	9.880	-30.517	0.00	0.00	C
ATOM	740	CD2	LEU	B	97	-0.611	7.687	-30.986	0.00	0.00	C
ATOM	741	N	LYS	B	98	4.909	6.307	-30.988	0.00	0.00	N
ATOM	742	CA	LYS	B	98	6.014	5.501	-31.539	0.00	0.00	C
ATOM	743	C	LYS	B	98	5.284	4.210	-31.845	0.00	0.00	C
ATOM	744	O	LYS	B	98	4.296	3.999	-31.127	0.00	0.00	O
ATOM	745	CB	LYS	B	98	7.093	5.381	-30.537	0.00	0.00	C
ATOM	746	CG	LYS	B	98	8.518	5.045	-30.928	0.00	0.00	C
ATOM	747	CD	LYS	B	98	9.165	4.397	-29.701	0.00	0.00	C
ATOM	748	CE	LYS	B	98	10.477	3.719	-30.000	0.00	0.00	C
ATOM	749	NZ	LYS	B	98	11.491	4.692	-30.515	0.00	0.00	N
ATOM	750	N	GLU	B	99	5.728	3.445	-32.805	0.00	0.00	N
ATOM	751	CA	GLU	B	99	5.027	2.246	-33.282	0.00	0.00	C
ATOM	752	C	GLU	B	99	5.326	0.959	-32.540	0.00	0.00	C
ATOM	753	O	GLU	B	99	6.476	0.711	-32.147	0.00	0.00	O
ATOM	754	CB	GLU	B	99	5.470	1.992	-34.745	0.00	0.00	C
ATOM	755	CG	GLU	B	99	5.389	3.020	-35.872	0.00	0.00	C
ATOM	756	CD	GLU	B	99	4.816	2.677	-37.224	0.00	0.00	C
ATOM	757	OE1	GLU	B	99	3.707	2.216	-37.467	0.00	0.00	O
ATOM	758	OE2	GLU	B	99	5.541	2.892	-38.230	0.00	0.00	O
ATOM	759	N	ILE	B	100	4.309	0.155	-32.207	0.00	0.00	N
ATOM	760	CA	ILE	B	100	4.517	-1.112	-31.496	0.00	0.00	C
ATOM	761	C	ILE	B	100	3.560	-2.182	-32.010	0.00	0.00	C
ATOM	762	O	ILE	B	100	2.751	-2.823	-31.308	0.00	0.00	O
ATOM	763	CB	ILE	B	100	4.247	-0.891	-29.972	0.00	0.00	C
ATOM	764	CG1	ILE	B	100	2.963	-0.025	-29.783	0.00	0.00	C
ATOM	765	CG2	ILE	B	100	5.395	-0.263	-29.176	0.00	0.00	C
ATOM	766	CD1	ILE	B	100	2.252	-0.419	-28.457	0.00	0.00	C
ATOM	767	N	ASN	B	101	3.879	-2.569	-33.253	0.00	0.00	N

Fig. 1 cont.

ATOM	768	CA	ASN	B	101	3.072	-3.590	-33.977	0.00	0.00	C
ATOM	769	C	ASN	B	101	3.747	-4.947	-33.799	0.00	0.00	C
ATOM	770	O	ASN	B	101	3.528	-5.936	-34.465	0.00	0.00	O
ATOM	771	CB	ASN	B	101	2.688	-3.165	-35.380	0.00	0.00	C
ATOM	772	CG	ASN	B	101	3.747	-2.952	-36.413	0.00	0.00	C
ATOM	773	OD1	ASN	B	101	4.257	-1.827	-36.555	0.00	0.00	O
ATOM	774	ND2	ASN	B	101	4.073	-3.998	-37.177	0.00	0.00	N
ATOM	775	N	ASP	B	102	4.525	-4.980	-32.776	0.00	0.00	N
ATOM	776	CA	ASP	B	102	5.383	-5.871	-32.023	0.00	0.00	C
ATOM	777	C	ASP	B	102	4.491	-6.281	-30.831	0.00	0.00	C
ATOM	778	O	ASP	B	102	4.657	-7.367	-30.254	0.00	0.00	O
ATOM	779	CB	ASP	B	102	6.679	-5.173	-31.738	0.00	0.00	C
ATOM	780	CG	ASP	B	102	7.447	-5.164	-30.462	0.00	0.00	C
ATOM	781	OD1	ASP	B	102	7.303	-5.987	-29.543	0.00	0.00	O
ATOM	782	OD2	ASP	B	102	8.303	-4.236	-30.370	0.00	0.00	O
ATOM	783	N	ILE	B	103	3.541	-5.403	-30.520	0.00	0.00	N
ATOM	784	CA	ILE	B	103	2.589	-5.705	-29.458	0.00	0.00	C
ATOM	785	C	ILE	B	103	1.301	-6.163	-30.160	0.00	0.00	C
ATOM	786	O	ILE	B	103	0.755	-7.217	-29.816	0.00	0.00	O
ATOM	787	CB	ILE	B	103	2.228	-4.583	-28.437	0.00	0.00	C
ATOM	788	CG1	ILE	B	103	3.465	-4.393	-27.540	0.00	0.00	C
ATOM	789	CG2	ILE	B	103	0.929	-4.904	-27.649	0.00	0.00	C
ATOM	790	CD1	ILE	B	103	3.261	-3.840	-26.106	0.00	0.00	C
ATOM	791	N	CYS	B	104	0.875	-5.286	-31.064	0.00	0.00	N
ATOM	792	CA	CYS	B	104	-0.369	-5.638	-31.779	0.00	0.00	C
ATOM	793	C	CYS	B	104	-0.377	-4.812	-33.054	0.00	0.00	C
ATOM	794	O	CYS	B	104	0.272	-3.794	-33.196	0.00	0.00	O
ATOM	795	CB	CYS	B	104	-1.617	-5.473	-30.952	0.00	0.00	C
ATOM	796	SG	CYS	B	104	-1.567	-4.045	-29.846	0.00	0.00	S
ATOM	797	N	SER	B	105	-1.171	-5.430	-33.907	0.00	0.00	N
ATOM	798	CA	SER	B	105	-1.363	-4.900	-35.274	0.00	0.00	C
ATOM	799	C	SER	B	105	-2.227	-3.658	-35.165	0.00	0.00	C
ATOM	800	O	SER	B	105	-3.328	-3.733	-34.596	0.00	0.00	O
ATOM	801	CB	SER	B	105	-1.929	-5.960	-36.205	0.00	0.00	C
ATOM	802	OG	SER	B	105	-0.898	-6.803	-36.743	0.00	0.00	O
ATOM	803	N	GLY	B	106	-1.657	-2.576	-35.677	0.00	0.00	N
ATOM	804	CA	GLY	B	106	-2.441	-1.321	-35.639	0.00	0.00	C
ATOM	805	C	GLY	B	106	-2.009	-0.448	-34.482	0.00	0.00	C
ATOM	806	O	GLY	B	106	-1.971	0.774	-34.727	0.00	0.00	O
ATOM	807	N	CYS	B	107	-1.701	-1.026	-33.345	0.00	0.00	N
ATOM	808	CA	CYS	B	107	-1.275	-0.282	-32.155	0.00	0.00	C
ATOM	809	C	CYS	B	107	-0.146	0.714	-32.375	0.00	0.00	C
ATOM	810	O	CYS	B	107	0.567	0.706	-33.391	0.00	0.00	O
ATOM	811	CB	CYS	B	107	-0.911	-1.358	-31.133	0.00	0.00	C
ATOM	812	SG	CYS	B	107	-2.286	-2.530	-31.050	0.00	0.00	S
ATOM	813	N	ARG	B	108	-0.086	1.634	-31.426	0.00	0.00	N
ATOM	814	CA	ARG	B	108	0.866	2.755	-31.316	0.00	0.00	C
ATOM	815	C	ARG	B	108	0.879	3.159	-29.834	0.00	0.00	C
ATOM	816	O	ARG	B	108	-0.153	3.115	-29.141	0.00	0.00	O
ATOM	817	CB	ARG	B	108	0.501	3.882	-32.239	0.00	0.00	C
ATOM	818	CG	ARG	B	108	1.282	4.818	-33.106	0.00	0.00	C
ATOM	819	CD	ARG	B	108	0.751	5.009	-34.499	0.00	0.00	C
ATOM	820	NE	ARG	B	108	1.324	6.106	-35.244	0.00	0.00	N
ATOM	821	CZ	ARG	B	108	1.249	7.392	-34.863	0.00	0.00	C
ATOM	822	NH1	ARG	B	108	0.620	7.723	-33.735	0.00	0.00	N
ATOM	823	NH2	ARG	B	108	1.773	8.443	-35.523	0.00	0.00	N
ATOM	824	N	GLY	B	109	2.022	3.565	-29.343	0.00	0.00	N
ATOM	825	CA	GLY	B	109	2.249	3.987	-27.978	0.00	0.00	C
ATOM	826	C	GLY	B	109	3.064	5.244	-27.722	0.00	0.00	C
ATOM	827	O	GLY	B	109	3.887	5.780	-28.480	0.00	0.00	O

Fig. 1 cont.

ATOM	828	N	HIS	B	110	2.930	5.644	-26.475	0.00	0.00	N
ATOM	829	CA	HIS	B	110	3.560	6.869	-25.959	0.00	0.00	C
ATOM	830	C	HIS	B	110	5.020	6.506	-25.846	0.00	0.00	C
ATOM	831	O	HIS	B	110	5.480	5.645	-25.107	0.00	0.00	O
ATOM	832	CB	HIS	B	110	2.875	7.196	-24.634	0.00	0.00	C
ATOM	833	CG	HIS	B	110	3.506	8.313	-23.873	0.00	0.00	C
ATOM	834	ND1	HIS	B	110	4.854	8.458	-23.657	0.00	0.00	N
ATOM	835	CD2	HIS	B	110	2.884	9.348	-23.247	0.00	0.00	C
ATOM	836	CE1	HIS	B	110	5.014	9.555	-22.930	0.00	0.00	C
ATOM	837	NE2	HIS	B	110	3.849	10.117	-22.678	0.00	0.00	N
ATOM	838	N	ASP	B	111	5.775	7.280	-26.629	0.00	0.00	N
ATOM	839	CA	ASP	B	111	7.219	7.145	-26.855	0.00	0.00	C
ATOM	840	C	ASP	B	111	7.992	6.875	-25.561	0.00	0.00	C
ATOM	841	O	ASP	B	111	8.772	5.909	-25.543	0.00	0.00	O
ATOM	842	CB	ASP	B	111	7.811	8.387	-27.534	0.00	0.00	C
ATOM	843	CG	ASP	B	111	9.260	8.248	-27.962	0.00	0.00	C
ATOM	844	OD1	ASP	B	111	9.736	9.084	-28.762	0.00	0.00	O
ATOM	845	OD2	ASP	B	111	9.942	7.289	-27.517	0.00	0.00	O
ATOM	846	N	GLY	B	112	7.732	7.709	-24.575	0.00	0.00	N
ATOM	847	CA	GLY	B	112	8.387	7.574	-23.291	0.00	0.00	C
ATOM	848	C	GLY	B	112	8.040	6.304	-22.545	0.00	0.00	C
ATOM	849	O	GLY	B	112	8.863	5.922	-21.707	0.00	0.00	O
ATOM	850	N	PHE	B	113	6.869	5.733	-22.661	0.00	0.00	N
ATOM	851	CA	PHE	B	113	6.466	4.519	-21.913	0.00	0.00	C
ATOM	852	C	PHE	B	113	6.999	3.283	-22.640	0.00	0.00	C
ATOM	853	O	PHE	B	113	7.577	2.327	-22.128	0.00	0.00	O
ATOM	854	CB	PHE	B	113	4.965	4.537	-21.664	0.00	0.00	C
ATOM	855	CG	PHE	B	113	4.219	5.638	-21.010	0.00	0.00	C
ATOM	856	CD1	PHE	B	113	4.787	6.641	-20.240	0.00	0.00	C
ATOM	857	CD2	PHE	B	113	2.827	5.679	-21.136	0.00	0.00	C
ATOM	858	CE1	PHE	B	113	4.017	7.631	-19.634	0.00	0.00	C
ATOM	859	CE2	PHE	B	113	2.016	6.672	-20.558	0.00	0.00	C
ATOM	860	CZ	PHE	B	113	2.635	7.667	-19.791	0.00	0.00	C
ATOM	861	N	THR	B	114	6.790	3.328	-23.943	0.00	0.00	N
ATOM	862	CA	THR	B	114	7.181	2.309	-24.897	0.00	0.00	C
ATOM	863	C	THR	B	114	8.673	2.042	-24.831	0.00	0.00	C
ATOM	864	O	THR	B	114	9.156	0.920	-24.665	0.00	0.00	O
ATOM	865	CB	THR	B	114	6.832	2.804	-26.367	0.00	0.00	C
ATOM	866	OG1	THR	B	114	5.397	2.588	-26.396	0.00	0.00	O
ATOM	867	CG2	THR	B	114	7.645	2.110	-27.461	0.00	0.00	C
ATOM	868	N	SER	B	115	9.372	3.153	-24.939	0.00	0.00	N
ATOM	869	CA	SER	B	115	10.835	3.193	-24.941	0.00	0.00	C
ATOM	870	C	SER	B	115	11.361	2.609	-23.630	0.00	0.00	C
ATOM	871	O	SER	B	115	12.077	1.590	-23.619	0.00	0.00	O
ATOM	872	CB	SER	B	115	11.240	4.639	-25.185	0.00	0.00	C
ATOM	873	OG	SER	B	115	12.613	4.844	-24.973	0.00	0.00	O
ATOM	874	N	SER	B	116	10.863	3.217	-22.550	0.00	0.00	N
ATOM	875	CA	SER	B	116	11.223	2.818	-21.194	0.00	0.00	C
ATOM	876	C	SER	B	116	10.824	1.360	-21.018	0.00	0.00	C
ATOM	877	O	SER	B	116	11.520	0.608	-20.298	0.00	0.00	O
ATOM	878	CB	SER	B	116	10.582	3.604	-20.075	0.00	0.00	C
ATOM	879	OG	SER	B	116	11.426	4.672	-19.665	0.00	0.00	O
ATOM	880	N	TRP	B	117	9.716	0.957	-21.619	0.00	0.00	N
ATOM	881	CA	TRP	B	117	9.473	-0.468	-21.342	0.00	0.00	C
ATOM	882	C	TRP	B	117	10.499	-1.349	-22.036	0.00	0.00	C
ATOM	883	O	TRP	B	117	11.326	-2.034	-21.390	0.00	0.00	O
ATOM	884	CB	TRP	B	117	8.011	-0.885	-21.576	0.00	0.00	C
ATOM	885	CG	TRP	B	117	8.097	-2.055	-20.628	0.00	0.00	C
ATOM	886	CD1	TRP	B	117	8.517	-2.032	-19.323	0.00	0.00	C
ATOM	887	CD2	TRP	B	117	7.902	-3.411	-20.993	0.00	0.00	C

Fig. 1 cont.

ATOM	888	NE1	TRP	B	117	8.545	-3.312	-18.818	0.00	0.00	N
ATOM	889	CE2	TRP	B	117	8.169	-4.169	-19.825	0.00	0.00	C
ATOM	890	CE3	TRP	B	117	7.502	-4.025	-22.171	0.00	0.00	C
ATOM	891	CZ2	TRP	B	117	8.050	-5.550	-19.791	0.00	0.00	C
ATOM	892	CZ3	TRP	B	117	7.388	-5.394	-22.141	0.00	0.00	C
ATOM	893	CH2	TRP	B	117	7.660	-6.133	-20.987	0.00	0.00	C
ATOM	894	N	ARG	B	118	10.583	-1.191	-23.348	0.00	0.00	N
ATOM	895	CA	ARG	B	118	11.500	-1.897	-24.227	0.00	0.00	C
ATOM	896	C	ARG	B	118	12.913	-1.863	-23.659	0.00	0.00	C
ATOM	897	O	ARG	B	118	13.740	-2.688	-24.052	0.00	0.00	O
ATOM	898	CB	ARG	B	118	11.508	-1.257	-25.611	0.00	0.00	C
ATOM	899	CG	ARG	B	118	10.871	-1.909	-26.828	0.00	0.00	C
ATOM	900	CD	ARG	B	118	11.405	-1.415	-28.139	0.00	0.00	C
ATOM	901	NE	ARG	B	118	12.713	-1.911	-28.518	0.00	0.00	N
ATOM	902	CZ	ARG	B	118	13.751	-1.533	-29.255	0.00	0.00	C
ATOM	903	NH1	ARG	B	118	13.884	-0.395	-29.948	0.00	0.00	N
ATOM	904	NH2	ARG	B	118	14.794	-2.388	-29.313	0.00	0.00	N
ATOM	905	N	SER	B	119	13.289	-0.895	-22.850	0.00	0.00	N
ATOM	906	CA	SER	B	119	14.588	-0.645	-22.252	0.00	0.00	C
ATOM	907	C	SER	B	119	15.001	-1.703	-21.259	0.00	0.00	C
ATOM	908	O	SER	B	119	15.987	-2.414	-21.353	0.00	0.00	O
ATOM	909	CB	SER	B	119	14.496	0.711	-21.546	0.00	0.00	C
ATOM	910	OG	SER	B	119	13.872	0.426	-20.331	0.00	0.00	O
ATOM	911	N	VAL	B	120	14.200	-1.869	-20.269	0.00	0.00	N
ATOM	912	CA	VAL	B	120	14.195	-2.765	-19.122	0.00	0.00	C
ATOM	913	C	VAL	B	120	13.612	-4.094	-19.551	0.00	0.00	C
ATOM	914	O	VAL	B	120	12.865	-4.758	-18.812	0.00	0.00	O
ATOM	915	CB	VAL	B	120	13.651	-1.975	-17.917	0.00	0.00	C
ATOM	916	CG1	VAL	B	120	12.149	-1.786	-17.918	0.00	0.00	C
ATOM	917	CG2	VAL	B	120	14.125	-2.577	-16.599	0.00	0.00	C
ATOM	918	N	ALA	B	121	13.588	-4.465	-20.772	0.00	0.00	N
ATOM	919	CA	ALA	B	121	13.237	-5.563	-21.616	0.00	0.00	C
ATOM	920	C	ALA	B	121	13.253	-7.047	-21.241	0.00	0.00	C
ATOM	921	O	ALA	B	121	12.419	-7.744	-20.647	0.00	0.00	O
ATOM	922	CB	ALA	B	121	14.385	-5.395	-22.706	0.00	0.00	C
ATOM	923	N	ASP	B	122	14.344	-7.644	-21.674	0.00	0.00	N
ATOM	924	CA	ASP	B	122	14.972	-8.925	-21.667	0.00	0.00	C
ATOM	925	C	ASP	B	122	15.158	-9.329	-20.207	0.00	0.00	C
ATOM	926	O	ASP	B	122	14.757	-10.449	-19.848	0.00	0.00	O
ATOM	927	CB	ASP	B	122	16.289	-8.808	-22.460	0.00	0.00	C
ATOM	928	CG	ASP	B	122	16.108	-9.110	-23.944	0.00	0.00	C
ATOM	929	OD1	ASP	B	122	16.559	-10.192	-24.377	0.00	0.00	O
ATOM	930	OD2	ASP	B	122	15.517	-8.270	-24.663	0.00	0.00	O
ATOM	931	N	THR	B	123	15.662	-8.447	-19.366	0.00	0.00	N
ATOM	932	CA	THR	B	123	15.855	-8.681	-17.951	0.00	0.00	C
ATOM	933	C	THR	B	123	14.565	-8.935	-17.190	0.00	0.00	C
ATOM	934	O	THR	B	123	14.579	-9.948	-16.483	0.00	0.00	O
ATOM	935	CB	THR	B	123	16.516	-7.423	-17.246	0.00	0.00	C
ATOM	936	OG1	THR	B	123	17.713	-7.195	-18.046	0.00	0.00	O
ATOM	937	CG2	THR	B	123	16.729	-7.619	-15.748	0.00	0.00	C
ATOM	938	N	LEU	B	124	13.553	-8.087	-17.329	0.00	0.00	N
ATOM	939	CA	LEU	B	124	12.277	-8.251	-16.593	0.00	0.00	C
ATOM	940	C	LEU	B	124	11.521	-9.489	-17.049	0.00	0.00	C
ATOM	941	O	LEU	B	124	10.805	-10.076	-16.230	0.00	0.00	O
ATOM	942	CB	LEU	B	124	11.442	-6.984	-16.646	0.00	0.00	C
ATOM	943	CG	LEU	B	124	11.733	-5.761	-15.799	0.00	0.00	C
ATOM	944	CD1	LEU	B	124	10.775	-5.681	-14.611	0.00	0.00	C
ATOM	945	CD2	LEU	B	124	13.192	-5.834	-15.350	0.00	0.00	C
ATOM	946	N	ARG	B	125	11.647	-9.862	-18.292	0.00	0.00	N
ATOM	947	CA	ARG	B	125	11.015	-11.069	-18.840	0.00	0.00	C

Fig. 1 cont.

ATOM	948	C	ARG B 125	11.523	-12.336	-18.160	0.00	0.00	C
ATOM	949	O	ARG B 125	10.766	-13.279	-17.890	0.00	0.00	O
ATOM	950	CB	ARG B 125	11.335	-11.135	-20.331	0.00	0.00	C
ATOM	951	CG	ARG B 125	10.964	-12.381	-21.104	0.00	0.00	C
ATOM	952	CD	ARG B 125	10.609	-12.026	-22.492	0.00	0.00	C
ATOM	953	NE	ARG B 125	9.892	-13.001	-23.292	0.00	0.00	N
ATOM	954	CZ	ARG B 125	9.057	-12.619	-24.280	0.00	0.00	C
ATOM	955	NH1	ARG B 125	8.821	-11.321	-24.562	0.00	0.00	N
ATOM	956	NH2	ARG B 125	8.422	-13.540	-25.006	0.00	0.00	N
ATOM	957	N	GLN B 126	12.820	-12.400	-17.913	0.00	0.00	N
ATOM	958	CA	GLN B 126	13.607	-13.492	-17.331	0.00	0.00	C
ATOM	959	C	GLN B 126	13.487	-13.792	-15.856	0.00	0.00	C
ATOM	960	O	GLN B 126	13.277	-14.990	-15.581	0.00	0.00	O
ATOM	961	CB	GLN B 126	15.122	-13.281	-17.601	0.00	0.00	C
ATOM	962	CG	GLN B 126	16.075	-14.430	-17.413	0.00	0.00	C
ATOM	963	CD	GLN B 126	17.534	-14.074	-17.202	0.00	0.00	C
ATOM	964	OE1	GLN B 126	17.893	-13.504	-16.160	0.00	0.00	O
ATOM	965	NE2	GLN B 126	18.456	-14.378	-18.133	0.00	0.00	N
ATOM	966	N	LYS B 127	13.573	-12.872	-14.913	0.00	0.00	N
ATOM	967	CA	LYS B 127	13.458	-13.218	-13.473	0.00	0.00	C
ATOM	968	C	LYS B 127	12.091	-13.842	-13.200	0.00	0.00	C
ATOM	969	O	LYS B 127	11.831	-14.702	-12.358	0.00	0.00	O
ATOM	970	CB	LYS B 127	13.755	-12.023	-12.565	0.00	0.00	C
ATOM	971	CG	LYS B 127	15.124	-11.445	-12.889	0.00	0.00	C
ATOM	972	CD	LYS B 127	16.186	-11.196	-11.833	0.00	0.00	C
ATOM	973	CE	LYS B 127	17.551	-11.433	-12.458	0.00	0.00	C
ATOM	974	NZ	LYS B 127	18.672	-10.555	-12.111	0.00	0.00	N
ATOM	975	N	VAL B 128	11.124	-13.374	-13.952	0.00	0.00	N
ATOM	976	CA	VAL B 128	9.698	-13.648	-14.062	0.00	0.00	C
ATOM	977	C	VAL B 128	9.410	-15.043	-14.605	0.00	0.00	C
ATOM	978	O	VAL B 128	8.292	-15.554	-14.353	0.00	0.00	O
ATOM	979	CB	VAL B 128	9.030	-12.460	-14.821	0.00	0.00	C
ATOM	980	CG1	VAL B 128	7.523	-12.597	-15.019	0.00	0.00	C
ATOM	981	CG2	VAL B 128	9.358	-11.132	-14.120	0.00	0.00	C
ATOM	982	N	GLU B 129	10.306	-15.598	-15.401	0.00	0.00	N
ATOM	983	CA	GLU B 129	10.081	-16.997	-15.945	0.00	0.00	C
ATOM	984	C	GLU B 129	10.646	-17.903	-14.851	0.00	0.00	C
ATOM	985	O	GLU B 129	10.050	-18.866	-14.361	0.00	0.00	O
ATOM	986	CB	GLU B 129	10.539	-17.106	-17.350	0.00	0.00	C
ATOM	987	CG	GLU B 129	10.932	-17.938	-18.517	0.00	0.00	C
ATOM	988	CD	GLU B 129	10.822	-17.401	-19.931	0.00	0.00	C
ATOM	989	OE1	GLU B 129	10.350	-16.307	-20.268	0.00	0.00	O
ATOM	990	OE2	GLU B 129	11.268	-18.222	-20.787	0.00	0.00	O
ATOM	991	N	ASP B 130	11.796	-17.485	-14.325	0.00	0.00	N
ATOM	992	CA	ASP B 130	12.493	-18.139	-13.232	0.00	0.00	C
ATOM	993	C	ASP B 130	11.440	-18.107	-12.096	0.00	0.00	C
ATOM	994	O	ASP B 130	11.339	-19.144	-11.423	0.00	0.00	O
ATOM	995	CB	ASP B 130	13.755	-17.507	-12.697	0.00	0.00	C
ATOM	996	CG	ASP B 130	14.895	-17.325	-13.666	0.00	0.00	C
ATOM	997	OD1	ASP B 130	14.808	-17.666	-14.864	0.00	0.00	O
ATOM	998	OD2	ASP B 130	15.903	-16.814	-13.110	0.00	0.00	O
ATOM	999	N	ALA B 131	10.772	-16.967	-11.966	0.00	0.00	N
ATOM	1000	CA	ALA B 131	9.784	-16.831	-10.900	0.00	0.00	C
ATOM	1001	C	ALA B 131	8.613	-17.792	-11.056	0.00	0.00	C
ATOM	1002	O	ALA B 131	8.260	-18.365	-10.007	0.00	0.00	O
ATOM	1003	CB	ALA B 131	9.246	-15.409	-10.778	0.00	0.00	C
ATOM	1004	N	VAL B 132	8.045	-17.918	-12.239	0.00	0.00	N
ATOM	1005	CA	VAL B 132	6.865	-18.823	-12.347	0.00	0.00	C
ATOM	1006	C	VAL B 132	7.198	-20.290	-12.493	0.00	0.00	C
ATOM	1007	O	VAL B 132	6.382	-21.101	-11.975	0.00	0.00	O

Fig. 1 cont.

ATOM	1008	CB	VAL	B	132	5.850	-18.268	-13.360	0.00	0.00	C
ATOM	1009	CG1	VAL	B	132	4.713	-19.235	-13.650	0.00	0.00	C
ATOM	1010	CG2	VAL	B	132	5.334	-16.941	-12.806	0.00	0.00	C
ATOM	1011	N	ARG	B	133	8.309	-20.650	-13.118	0.00	0.00	N
ATOM	1012	CA	ARG	B	133	8.637	-22.095	-13.181	0.00	0.00	C
ATOM	1013	C	ARG	B	133	8.658	-22.621	-11.732	0.00	0.00	C
ATOM	1014	O	ARG	B	133	7.875	-23.542	-11.473	0.00	0.00	O
ATOM	1015	CB	ARG	B	133	9.987	-22.431	-13.710	0.00	0.00	C
ATOM	1016	CG	ARG	B	133	10.463	-22.071	-15.114	0.00	0.00	C
ATOM	1017	CD	ARG	B	133	11.731	-22.884	-15.295	0.00	0.00	C
ATOM	1018	NE	ARG	B	133	12.327	-22.936	-13.951	0.00	0.00	N
ATOM	1019	CZ	ARG	B	133	13.467	-22.403	-13.574	0.00	0.00	C
ATOM	1020	NH1	ARG	B	133	14.289	-21.765	-14.402	0.00	0.00	N
ATOM	1021	NH2	ARG	B	133	13.791	-22.527	-12.295	0.00	0.00	N
ATOM	1022	N	GLU	B	134	9.422	-21.968	-10.855	0.00	0.00	N
ATOM	1023	CA	GLU	B	134	9.426	-22.454	-9.478	0.00	0.00	C
ATOM	1024	C	GLU	B	134	8.030	-22.548	-8.865	0.00	0.00	C
ATOM	1025	O	GLU	B	134	7.778	-23.606	-8.217	0.00	0.00	O
ATOM	1026	CB	GLU	B	134	10.136	-21.589	-8.448	0.00	0.00	C
ATOM	1027	CG	GLU	B	134	11.043	-20.501	-9.014	0.00	0.00	C
ATOM	1028	CD	GLU	B	134	12.486	-20.839	-8.720	0.00	0.00	C
ATOM	1029	OE1	GLU	B	134	12.683	-21.541	-7.737	0.00	0.00	O
ATOM	1030	OE2	GLU	B	134	13.247	-20.332	-9.557	0.00	0.00	O
ATOM	1031	N	HIS	B	135	7.210	-21.499	-9.013	0.00	0.00	N
ATOM	1032	CA	HIS	B	135	5.872	-21.568	-8.390	0.00	0.00	C
ATOM	1033	C	HIS	B	135	4.674	-21.407	-9.297	0.00	0.00	C
ATOM	1034	O	HIS	B	135	3.951	-20.386	-9.236	0.00	0.00	O
ATOM	1035	CB	HIS	B	135	5.724	-20.493	-7.284	0.00	0.00	C
ATOM	1036	CG	HIS	B	135	6.922	-20.273	-6.439	0.00	0.00	C
ATOM	1037	ND1	HIS	B	135	6.958	-20.400	-5.070	0.00	0.00	N
ATOM	1038	CD2	HIS	B	135	8.171	-19.898	-6.793	0.00	0.00	C
ATOM	1039	CE1	HIS	B	135	8.194	-20.140	-4.645	0.00	0.00	C
ATOM	1040	NE2	HIS	B	135	8.957	-19.848	-5.690	0.00	0.00	N
ATOM	1041	N	PRO	B	136	4.356	-22.395	-10.131	0.00	0.00	N
ATOM	1042	CA	PRO	B	136	3.201	-22.337	-11.035	0.00	0.00	C
ATOM	1043	C	PRO	B	136	1.851	-22.566	-10.366	0.00	0.00	C
ATOM	1044	O	PRO	B	136	0.894	-22.895	-11.128	0.00	0.00	O
ATOM	1045	CB	PRO	B	136	3.463	-23.373	-12.136	0.00	0.00	C
ATOM	1046	CG	PRO	B	136	4.777	-24.005	-11.802	0.00	0.00	C
ATOM	1047	CD	PRO	B	136	5.069	-23.668	-10.334	0.00	0.00	C
ATOM	1048	N	ASP	B	137	1.709	-22.402	-9.053	0.00	0.00	N
ATOM	1049	CA	ASP	B	137	0.342	-22.613	-8.500	0.00	0.00	C
ATOM	1050	C	ASP	B	137	-0.195	-21.194	-8.235	0.00	0.00	C
ATOM	1051	O	ASP	B	137	-1.367	-20.976	-7.915	0.00	0.00	O
ATOM	1052	CB	ASP	B	137	0.248	-23.615	-7.385	0.00	0.00	C
ATOM	1053	CG	ASP	B	137	1.268	-23.781	-6.288	0.00	0.00	C
ATOM	1054	OD1	ASP	B	137	2.495	-23.713	-6.526	0.00	0.00	O
ATOM	1055	OD2	ASP	B	137	0.746	-23.998	-5.152	0.00	0.00	O
ATOM	1056	N	TYR	B	138	0.717	-20.279	-8.425	0.00	0.00	N
ATOM	1057	CA	TYR	B	138	0.667	-18.838	-8.272	0.00	0.00	C
ATOM	1058	C	TYR	B	138	0.152	-18.017	-9.449	0.00	0.00	C
ATOM	1059	O	TYR	B	138	0.467	-18.231	-10.641	0.00	0.00	O
ATOM	1060	CB	TYR	B	138	2.139	-18.442	-7.969	0.00	0.00	C
ATOM	1061	CG	TYR	B	138	2.621	-18.623	-6.554	0.00	0.00	C
ATOM	1062	CD1	TYR	B	138	1.892	-19.283	-5.565	0.00	0.00	C
ATOM	1063	CD2	TYR	B	138	3.871	-18.116	-6.187	0.00	0.00	C
ATOM	1064	CE1	TYR	B	138	2.375	-19.400	-4.264	0.00	0.00	C
ATOM	1065	CE2	TYR	B	138	4.363	-18.247	-4.887	0.00	0.00	C
ATOM	1066	CZ	TYR	B	138	3.609	-18.871	-3.908	0.00	0.00	C
ATOM	1067	OH	TYR	B	138	4.111	-18.945	-2.638	0.00	0.00	O

Fig. 1 cont.

ATOM	1068	N	ARG B 139	-0.583	-16.986	-9.050	0.00	0.00	N
ATOM	1069	CA	ARG B 139	-1.220	-15.962	-9.876	0.00	0.00	C
ATOM	1070	C	ARG B 139	-0.200	-14.800	-9.917	0.00	0.00	C
ATOM	1071	O	ARG B 139	0.105	-14.247	-8.854	0.00	0.00	O
ATOM	1072	CB	ARG B 139	-2.481	-15.284	-9.341	0.00	0.00	C
ATOM	1073	CG	ARG B 139	-3.575	-14.969	-10.332	0.00	0.00	C
ATOM	1074	CD	ARG B 139	-4.168	-13.620	-10.392	0.00	0.00	C
ATOM	1075	NE	ARG B 139	-5.116	-13.253	-9.346	0.00	0.00	N
ATOM	1076	CZ	ARG B 139	-5.758	-12.068	-9.358	0.00	0.00	C
ATOM	1077	NH1	ARG B 139	-5.597	-11.141	-10.303	0.00	0.00	N
ATOM	1078	NH2	ARG B 139	-6.582	-11.883	-8.334	0.00	0.00	N
ATOM	1079	N	VAL B 140	0.233	-14.487	-11.106	0.00	0.00	N
ATOM	1080	CA	VAL B 140	1.227	-13.408	-11.285	0.00	0.00	C
ATOM	1081	C	VAL B 140	0.397	-12.152	-11.562	0.00	0.00	C
ATOM	1082	O	VAL B 140	-0.437	-12.267	-12.479	0.00	0.00	O
ATOM	1083	CB	VAL B 140	2.284	-13.797	-12.340	0.00	0.00	C
ATOM	1084	CG1	VAL B 140	2.238	-15.265	-12.792	0.00	0.00	C
ATOM	1085	CG2	VAL B 140	2.344	-12.904	-13.577	0.00	0.00	C
ATOM	1086	N	VAL B 141	0.546	-11.108	-10.758	0.00	0.00	N
ATOM	1087	CA	VAL B 141	-0.201	-9.849	-10.896	0.00	0.00	C
ATOM	1088	C	VAL B 141	0.702	-8.635	-11.174	0.00	0.00	C
ATOM	1089	O	VAL B 141	1.613	-8.414	-10.363	0.00	0.00	O
ATOM	1090	CB	VAL B 141	-1.092	-9.478	-9.694	0.00	0.00	C
ATOM	1091	CG1	VAL B 141	-2.078	-8.369	-10.092	0.00	0.00	C
ATOM	1092	CG2	VAL B 141	-1.796	-10.674	-9.116	0.00	0.00	C
ATOM	1093	N	PHE B 142	0.413	-7.870	-12.209	0.00	0.00	N
ATOM	1094	CA	PHE B 142	1.262	-6.683	-12.540	0.00	0.00	C
ATOM	1095	C	PHE B 142	0.644	-5.392	-12.037	0.00	0.00	C
ATOM	1096	O	PHE B 142	-0.462	-5.034	-12.434	0.00	0.00	O
ATOM	1097	CB	PHE B 142	1.530	-6.719	-14.040	0.00	0.00	C
ATOM	1098	CG	PHE B 142	2.630	-7.626	-14.500	0.00	0.00	C
ATOM	1099	CD1	PHE B 142	3.368	-8.396	-13.582	0.00	0.00	C
ATOM	1100	CD2	PHE B 142	2.922	-7.735	-15.866	0.00	0.00	C
ATOM	1101	CE1	PHE B 142	4.376	-9.254	-14.005	0.00	0.00	C
ATOM	1102	CE2	PHE B 142	3.927	-8.599	-16.318	0.00	0.00	C
ATOM	1103	CZ	PHE B 142	4.653	-9.353	-15.376	0.00	0.00	C
ATOM	1104	N	THR B 143	1.328	-4.706	-11.139	0.00	0.00	N
ATOM	1105	CA	THR B 143	0.833	-3.478	-10.487	0.00	0.00	C
ATOM	1106	C	THR B 143	1.675	-2.211	-10.657	0.00	0.00	C
ATOM	1107	O	THR B 143	2.841	-2.236	-11.118	0.00	0.00	O
ATOM	1108	CB	THR B 143	0.441	-3.731	-8.968	0.00	0.00	C
ATOM	1109	OG1	THR B 143	-0.698	-2.821	-8.720	0.00	0.00	O
ATOM	1110	CG2	THR B 143	1.531	-3.499	-7.936	0.00	0.00	C
ATOM	1111	N	GLY B 144	0.944	-1.090	-10.555	0.00	0.00	N
ATOM	1112	CA	GLY B 144	1.539	0.222	-10.715	0.00	0.00	C
ATOM	1113	C	GLY B 144	0.709	1.447	-10.523	0.00	0.00	C
ATOM	1114	O	GLY B 144	-0.346	1.497	-11.189	0.00	0.00	O
ATOM	1115	N	HIS B 145	1.147	2.465	-9.848	0.00	0.00	N
ATOM	1116	CA	HIS B 145	0.368	3.711	-9.752	0.00	0.00	C
ATOM	1117	C	HIS B 145	0.820	4.669	-10.860	0.00	0.00	C
ATOM	1118	O	HIS B 145	2.040	4.800	-11.106	0.00	0.00	O
ATOM	1119	CB	HIS B 145	0.567	4.508	-8.477	0.00	0.00	C
ATOM	1120	CG	HIS B 145	0.332	5.958	-8.315	0.00	0.00	C
ATOM	1121	ND1	HIS B 145	1.317	6.837	-7.940	0.00	0.00	N
ATOM	1122	CD2	HIS B 145	-0.793	6.720	-8.391	0.00	0.00	C
ATOM	1123	CE1	HIS B 145	0.819	8.059	-7.818	0.00	0.00	C
ATOM	1124	NE2	HIS B 145	-0.462	8.022	-8.102	0.00	0.00	N
ATOM	1125	N	SER B 146	-0.150	5.260	-11.534	0.00	0.00	N
ATOM	1126	CA	SER B 146	0.140	6.293	-12.546	0.00	0.00	C
ATOM	1127	C	SER B 146	1.170	5.951	-13.595	0.00	0.00	C

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ATOM	1128	O	SER B 146	0.839	5.205	-14.530	0.00	0.00	O
ATOM	1129	CB	SER B 146	0.554	7.570	-11.761	0.00	0.00	C
ATOM	1130	OG	SER B 146	1.403	8.471	-12.379	0.00	0.00	O
ATOM	1131	N	LEU B 147	2.398	6.477	-13.458	0.00	0.00	N
ATOM	1132	CA	LEU B 147	3.441	6.191	-14.456	0.00	0.00	C
ATOM	1133	C	LEU B 147	3.561	4.664	-14.471	0.00	0.00	C
ATOM	1134	O	LEU B 147	3.487	4.139	-15.603	0.00	0.00	O
ATOM	1135	CB	LEU B 147	4.727	6.925	-14.174	0.00	0.00	C
ATOM	1136	CG	LEU B 147	5.810	7.093	-15.227	0.00	0.00	C
ATOM	1137	CD1	LEU B 147	7.185	6.801	-14.613	0.00	0.00	C
ATOM	1138	CD2	LEU B 147	5.621	6.186	-16.435	0.00	0.00	C
ATOM	1139	N	GLY B 148	3.640	4.035	-13.304	0.00	0.00	N
ATOM	1140	CA	GLY B 148	3.716	2.574	-13.248	0.00	0.00	C
ATOM	1141	C	GLY B 148	2.589	1.739	-13.832	0.00	0.00	C
ATOM	1142	O	GLY B 148	2.850	0.615	-14.311	0.00	0.00	O
ATOM	1143	N	GLY B 149	1.351	2.160	-13.752	0.00	0.00	N
ATOM	1144	CA	GLY B 149	0.136	1.531	-14.252	0.00	0.00	C
ATOM	1145	C	GLY B 149	0.182	1.569	-15.781	0.00	0.00	C
ATOM	1146	O	GLY B 149	-0.259	0.696	-16.532	0.00	0.00	O
ATOM	1147	N	ALA B 150	0.740	2.677	-16.219	0.00	0.00	N
ATOM	1148	CA	ALA B 150	1.004	3.001	-17.625	0.00	0.00	C
ATOM	1149	C	ALA B 150	2.106	2.032	-18.025	0.00	0.00	C
ATOM	1150	O	ALA B 150	1.975	1.362	-19.062	0.00	0.00	O
ATOM	1151	CB	ALA B 150	1.286	4.467	-17.630	0.00	0.00	C
ATOM	1152	N	LEU B 151	3.142	1.840	-17.229	0.00	0.00	N
ATOM	1153	CA	LEU B 151	4.250	0.904	-17.451	0.00	0.00	C
ATOM	1154	C	LEU B 151	3.858	-0.575	-17.366	0.00	0.00	C
ATOM	1155	O	LEU B 151	4.145	-1.456	-18.210	0.00	0.00	O
ATOM	1156	CB	LEU B 151	5.376	1.243	-16.441	0.00	0.00	C
ATOM	1157	CG	LEU B 151	6.601	1.872	-17.096	0.00	0.00	C
ATOM	1158	CD1	LEU B 151	7.655	2.384	-16.126	0.00	0.00	C
ATOM	1159	CD2	LEU B 151	7.174	0.766	-17.989	0.00	0.00	C
ATOM	1160	N	ALA B 152	3.115	-0.826	-16.292	0.00	0.00	N
ATOM	1161	CA	ALA B 152	2.573	-2.146	-15.939	0.00	0.00	C
ATOM	1162	C	ALA B 152	1.680	-2.689	-17.053	0.00	0.00	C
ATOM	1163	O	ALA B 152	1.819	-3.834	-17.510	0.00	0.00	O
ATOM	1164	CB	ALA B 152	1.802	-2.036	-14.632	0.00	0.00	C
ATOM	1165	N	THR B 153	0.790	-1.859	-17.556	0.00	0.00	N
ATOM	1166	CA	THR B 153	-0.082	-2.224	-18.665	0.00	0.00	C
ATOM	1167	C	THR B 153	0.749	-2.631	-19.885	0.00	0.00	C
ATOM	1168	O	THR B 153	0.548	-3.753	-20.398	0.00	0.00	O
ATOM	1169	CB	THR B 153	-1.072	-1.069	-19.140	0.00	0.00	C
ATOM	1170	OG1	THR B 153	-0.218	0.123	-19.244	0.00	0.00	O
ATOM	1171	CG2	THR B 153	-2.292	-0.670	-18.295	0.00	0.00	C
ATOM	1172	N	VAL B 154	1.685	-1.794	-20.328	0.00	0.00	N
ATOM	1173	CA	VAL B 154	2.459	-2.092	-21.560	0.00	0.00	C
ATOM	1174	C	VAL B 154	3.340	-3.350	-21.465	0.00	0.00	C
ATOM	1175	O	VAL B 154	3.642	-4.091	-22.405	0.00	0.00	O
ATOM	1176	CB	VAL B 154	3.299	-0.905	-22.098	0.00	0.00	C
ATOM	1177	CG1	VAL B 154	2.798	0.471	-21.706	0.00	0.00	C
ATOM	1178	CG2	VAL B 154	4.785	-1.077	-21.767	0.00	0.00	C
ATOM	1179	N	ALA B 155	3.796	-3.516	-20.237	0.00	0.00	N
ATOM	1180	CA	ALA B 155	4.629	-4.644	-19.838	0.00	0.00	C
ATOM	1181	C	ALA B 155	3.738	-5.841	-20.072	0.00	0.00	C
ATOM	1182	O	ALA B 155	4.080	-6.898	-20.607	0.00	0.00	O
ATOM	1183	CB	ALA B 155	4.958	-4.280	-18.410	0.00	0.00	C
ATOM	1184	N	GLY B 156	2.482	-5.680	-19.680	0.00	0.00	N
ATOM	1185	CA	GLY B 156	1.372	-6.623	-19.759	0.00	0.00	C
ATOM	1186	C	GLY B 156	1.042	-6.981	-21.201	0.00	0.00	C
ATOM	1187	O	GLY B 156	0.679	-8.144	-21.409	0.00	0.00	O

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ATOM	1188	N	ALA	B	157	1.155	-6.017	-22.103	0.00	0.00	N
ATOM	1189	CA	ALA	B	157	0.843	-6.308	-23.518	0.00	0.00	C
ATOM	1190	C	ALA	B	157	1.821	-7.282	-24.171	0.00	0.00	C
ATOM	1191	O	ALA	B	157	1.372	-8.239	-24.839	0.00	0.00	O
ATOM	1192	CB	ALA	B	157	0.713	-4.980	-24.264	0.00	0.00	C
ATOM	1193	N	ASP	B	158	3.109	-7.086	-23.999	0.00	0.00	N
ATOM	1194	CA	ASP	B	158	4.164	-7.917	-24.549	0.00	0.00	C
ATOM	1195	C	ASP	B	158	4.295	-9.299	-23.920	0.00	0.00	C
ATOM	1196	O	ASP	B	158	4.951	-10.157	-24.546	0.00	0.00	O
ATOM	1197	CB	ASP	B	158	5.575	-7.274	-24.444	0.00	0.00	C
ATOM	1198	CG	ASP	B	158	6.439	-7.713	-25.621	0.00	0.00	C
ATOM	1199	OD1	ASP	B	158	6.725	-8.885	-25.938	0.00	0.00	O
ATOM	1200	OD2	ASP	B	158	6.859	-6.753	-26.324	0.00	0.00	O
ATOM	1201	N	LEU	B	159	3.987	-9.527	-22.676	0.00	0.00	N
ATOM	1202	CA	LEU	B	159	4.191	-10.798	-21.977	0.00	0.00	C
ATOM	1203	C	LEU	B	159	3.049	-11.776	-21.905	0.00	0.00	C
ATOM	1204	O	LEU	B	159	3.210	-12.952	-21.545	0.00	0.00	O
ATOM	1205	CB	LEU	B	159	4.700	-10.323	-20.596	0.00	0.00	C
ATOM	1206	CG	LEU	B	159	6.026	-9.593	-20.771	0.00	0.00	C
ATOM	1207	CD1	LEU	B	159	6.660	-9.461	-19.387	0.00	0.00	C
ATOM	1208	CD2	LEU	B	159	6.969	-10.284	-21.750	0.00	0.00	C
ATOM	1209	N	ARG	B	160	1.913	-11.139	-22.107	0.00	0.00	N
ATOM	1210	CA	ARG	B	160	0.607	-11.796	-22.022	0.00	0.00	C
ATOM	1211	C	ARG	B	160	0.693	-13.089	-22.799	0.00	0.00	C
ATOM	1212	O	ARG	B	160	1.453	-13.191	-23.768	0.00	0.00	O
ATOM	1213	CB	ARG	B	160	-0.526	-10.882	-22.494	0.00	0.00	C
ATOM	1214	CG	ARG	B	160	-1.621	-10.827	-21.431	0.00	0.00	C
ATOM	1215	CD	ARG	B	160	-1.872	-9.421	-21.038	0.00	0.00	C
ATOM	1216	NE	ARG	B	160	-2.767	-9.301	-19.900	0.00	0.00	N
ATOM	1217	CZ	ARG	B	160	-4.048	-8.947	-20.013	0.00	0.00	C
ATOM	1218	NH1	ARG	B	160	-4.584	-8.687	-21.201	0.00	0.00	N
ATOM	1219	NH2	ARG	B	160	-4.773	-8.864	-18.913	0.00	0.00	N
ATOM	1220	N	GLY	B	161	-0.050	-14.047	-22.299	0.00	0.00	N
ATOM	1221	CA	GLY	B	161	-0.179	-15.397	-22.848	0.00	0.00	C
ATOM	1222	C	GLY	B	161	1.001	-16.043	-23.539	0.00	0.00	C
ATOM	1223	O	GLY	B	161	0.973	-16.732	-24.577	0.00	0.00	O
ATOM	1224	N	ASN	B	162	2.125	-15.874	-22.868	0.00	0.00	N
ATOM	1225	CA	ASN	B	162	3.443	-16.406	-23.255	0.00	0.00	C
ATOM	1226	C	ASN	B	162	3.527	-17.743	-22.491	0.00	0.00	C
ATOM	1227	O	ASN	B	162	4.613	-18.324	-22.380	0.00	0.00	O
ATOM	1228	CB	ASN	B	162	4.521	-15.396	-22.980	0.00	0.00	C
ATOM	1229	CG	ASN	B	162	5.410	-14.752	-24.012	0.00	0.00	C
ATOM	1230	OD1	ASN	B	162	6.478	-15.330	-24.311	0.00	0.00	O
ATOM	1231	ND2	ASN	B	162	5.090	-13.567	-24.554	0.00	0.00	N
ATOM	1232	N	GLY	B	163	2.421	-18.222	-21.955	0.00	0.00	N
ATOM	1233	CA	GLY	B	163	2.200	-19.450	-21.229	0.00	0.00	C
ATOM	1234	C	GLY	B	163	1.469	-19.136	-19.929	0.00	0.00	C
ATOM	1235	O	GLY	B	163	0.716	-19.905	-19.331	0.00	0.00	O
ATOM	1236	N	TYR	B	164	1.734	-17.913	-19.518	0.00	0.00	N
ATOM	1237	CA	TYR	B	164	1.315	-17.205	-18.311	0.00	0.00	C
ATOM	1238	C	TYR	B	164	0.233	-16.136	-18.532	0.00	0.00	C
ATOM	1239	O	TYR	B	164	0.244	-15.266	-19.421	0.00	0.00	O
ATOM	1240	CB	TYR	B	164	2.560	-16.605	-17.578	0.00	0.00	C
ATOM	1241	CG	TYR	B	164	3.881	-16.376	-18.263	0.00	0.00	C
ATOM	1242	CD1	TYR	B	164	4.528	-17.410	-18.966	0.00	0.00	C
ATOM	1243	CD2	TYR	B	164	4.574	-15.160	-18.227	0.00	0.00	C
ATOM	1244	CE1	TYR	B	164	5.749	-17.272	-19.623	0.00	0.00	C
ATOM	1245	CE2	TYR	B	164	5.805	-14.978	-18.867	0.00	0.00	C
ATOM	1246	CZ	TYR	B	164	6.400	-16.030	-19.574	0.00	0.00	C
ATOM	1247	OH	TYR	B	164	7.615	-15.858	-20.209	0.00	0.00	O
ATOM	1248	N	ASP	B	165	-0.734	-16.264	-17.635	0.00	0.00	N
ATOM	1249	CA	ASP	B	165	-1.924	-15.444	-17.458	0.00	0.00	C

Fig. 1 cont.

ATOM	1250	C	ASP B 165	-1.593	-14.237	-16.549	0.00	0.00	C
ATOM	1251	O	ASP B 165	-1.359	-14.398	-15.331	0.00	0.00	O
ATOM	1252	CB	ASP B 165	-3.044	-16.196	-16.795	0.00	0.00	C
ATOM	1253	CG	ASP B 165	-4.301	-16.609	-17.490	0.00	0.00	C
ATOM	1254	OD1	ASP B 165	-5.360	-16.119	-17.034	0.00	0.00	O
ATOM	1255	OD2	ASP B 165	-4.193	-17.425	-18.441	0.00	0.00	O
ATOM	1256	N	ILE B 166	-1.634	-13.057	-17.172	0.00	0.00	N
ATOM	1257	CA	ILE B 166	-1.340	-11.824	-16.439	0.00	0.00	C
ATOM	1258	C	ILE B 166	-2.519	-10.863	-16.301	0.00	0.00	C
ATOM	1259	O	ILE B 166	-3.024	-10.105	-17.117	0.00	0.00	O
ATOM	1260	CB	ILE B 166	-0.082	-11.066	-17.018	0.00	0.00	C
ATOM	1261	CG1	ILE B 166	1.094	-12.035	-17.262	0.00	0.00	C
ATOM	1262	CG2	ILE B 166	0.314	-9.885	-16.094	0.00	0.00	C
ATOM	1263	CD1	ILE B 166	2.226	-11.529	-18.195	0.00	0.00	C
ATOM	1264	N	ASP B 167	-2.885	-10.791	-15.055	0.00	0.00	N
ATOM	1265	CA	ASP B 167	-3.895	-10.013	-14.373	0.00	0.00	C
ATOM	1266	C	ASP B 167	-3.036	-8.783	-13.990	0.00	0.00	C
ATOM	1267	O	ASP B 167	-1.915	-8.936	-13.451	0.00	0.00	O
ATOM	1268	CB	ASP B 167	-4.457	-10.782	-13.187	0.00	0.00	C
ATOM	1269	CG	ASP B 167	-5.771	-11.480	-13.467	0.00	0.00	C
ATOM	1270	OD1	ASP B 167	-6.571	-11.624	-12.533	0.00	0.00	O
ATOM	1271	OD2	ASP B 167	-5.952	-11.827	-14.655	0.00	0.00	O
ATOM	1272	N	VAL B 168	-3.520	-7.623	-14.392	0.00	0.00	N
ATOM	1273	CA	VAL B 168	-2.856	-6.333	-14.146	0.00	0.00	C
ATOM	1274	C	VAL B 168	-3.765	-5.360	-13.417	0.00	0.00	C
ATOM	1275	O	VAL B 168	-4.945	-5.329	-13.818	0.00	0.00	O
ATOM	1276	CB	VAL B 168	-2.366	-5.716	-15.470	0.00	0.00	C
ATOM	1277	CG1	VAL B 168	-1.296	-6.466	-16.243	0.00	0.00	C
ATOM	1278	CG2	VAL B 168	-3.539	-5.494	-16.424	0.00	0.00	C
ATOM	1279	N	PHE B 169	-3.391	-4.638	-12.392	0.00	0.00	N
ATOM	1280	CA	PHE B 169	-4.217	-3.659	-11.669	0.00	0.00	C
ATOM	1281	C	PHE B 169	-3.606	-2.253	-11.762	0.00	0.00	C
ATOM	1282	O	PHE B 169	-2.526	-2.094	-11.146	0.00	0.00	O
ATOM	1283	CB	PHE B 169	-4.361	-3.942	-10.187	0.00	0.00	C
ATOM	1284	CG	PHE B 169	-5.213	-5.117	-9.853	0.00	0.00	C
ATOM	1285	CD1	PHE B 169	-6.391	-4.896	-9.126	0.00	0.00	C
ATOM	1286	CD2	PHE B 169	-4.823	-6.404	-10.246	0.00	0.00	C
ATOM	1287	CE1	PHE B 169	-7.209	-5.963	-8.795	0.00	0.00	C
ATOM	1288	CE2	PHE B 169	-5.630	-7.497	-9.930	0.00	0.00	C
ATOM	1289	CZ	PHE B 169	-6.817	-7.242	-9.203	0.00	0.00	C
ATOM	1290	N	SER B 170	-4.276	-1.328	-12.433	0.00	0.00	N
ATOM	1291	CA	SER B 170	-3.649	0.004	-12.533	0.00	0.00	C
ATOM	1292	C	SER B 170	-4.511	1.075	-11.891	0.00	0.00	C
ATOM	1293	O	SER B 170	-5.733	1.049	-11.974	0.00	0.00	O
ATOM	1294	CB	SER B 170	-3.246	0.400	-13.929	0.00	0.00	C
ATOM	1295	OG	SER B 170	-4.315	0.458	-14.813	0.00	0.00	O
ATOM	1296	N	TYR B 171	-3.747	1.919	-11.205	0.00	0.00	N
ATOM	1297	CA	TYR B 171	-4.224	3.063	-10.443	0.00	0.00	C
ATOM	1298	C	TYR B 171	-3.779	4.433	-10.954	0.00	0.00	C
ATOM	1299	O	TYR B 171	-2.567	4.714	-11.032	0.00	0.00	O
ATOM	1300	CB	TYR B 171	-3.716	2.928	-8.980	0.00	0.00	C
ATOM	1301	CG	TYR B 171	-4.193	1.650	-8.341	0.00	0.00	C
ATOM	1302	CD1	TYR B 171	-3.508	0.459	-8.603	0.00	0.00	C
ATOM	1303	CD2	TYR B 171	-5.315	1.646	-7.516	0.00	0.00	C
ATOM	1304	CE1	TYR B 171	-3.954	-0.732	-8.038	0.00	0.00	C
ATOM	1305	CE2	TYR B 171	-5.772	0.471	-6.935	0.00	0.00	C
ATOM	1306	CZ	TYR B 171	-5.080	-0.708	-7.194	0.00	0.00	C
ATOM	1307	OH	TYR B 171	-5.495	-1.887	-6.637	0.00	0.00	O
ATOM	1308	N	GLY B 172	-4.765	5.246	-11.290	0.00	0.00	N
ATOM	1309	CA	GLY B 172	-4.675	6.596	-11.795	0.00	0.00	C

Fig. 1 cont.

ATOM	1310	C	GLY B 172	-3.733	6.774	-12.965	0.00	0.00	C
ATOM	1311	O	GLY B 172	-3.042	7.810	-12.974	0.00	0.00	O
ATOM	1312	N	ALA B 173	-3.713	5.848	-13.901	0.00	0.00	N
ATOM	1313	CA	ALA B 173	-2.796	5.945	-15.047	0.00	0.00	C
ATOM	1314	C	ALA B 173	-3.311	6.647	-16.300	0.00	0.00	C
ATOM	1315	O	ALA B 173	-4.497	6.633	-16.622	0.00	0.00	O
ATOM	1316	CB	ALA B 173	-2.368	4.526	-15.474	0.00	0.00	C
ATOM	1317	N	PRO B 174	-2.362	7.224	-17.028	0.00	0.00	N
ATOM	1318	CA	PRO B 174	-2.672	7.938	-18.261	0.00	0.00	C
ATOM	1319	C	PRO B 174	-3.003	6.976	-19.396	0.00	0.00	C
ATOM	1320	O	PRO B 174	-3.107	5.731	-19.275	0.00	0.00	O
ATOM	1321	CB	PRO B 174	-1.422	8.757	-18.554	0.00	0.00	C
ATOM	1322	CG	PRO B 174	-0.299	7.966	-17.959	0.00	0.00	C
ATOM	1323	CD	PRO B 174	-0.917	7.291	-16.733	0.00	0.00	C
ATOM	1324	N	ARG B 175	-3.188	7.639	-20.530	0.00	0.00	N
ATOM	1325	CA	ARG B 175	-3.443	6.917	-21.786	0.00	0.00	C
ATOM	1326	C	ARG B 175	-1.976	6.646	-22.164	0.00	0.00	C
ATOM	1327	O	ARG B 175	-1.125	7.513	-21.843	0.00	0.00	O
ATOM	1328	CB	ARG B 175	-4.230	7.680	-22.826	0.00	0.00	C
ATOM	1329	CG	ARG B 175	-5.443	8.451	-22.337	0.00	0.00	C
ATOM	1330	CD	ARG B 175	-5.995	9.425	-23.330	0.00	0.00	C
ATOM	1331	NE	ARG B 175	-7.383	9.704	-23.024	0.00	0.00	N
ATOM	1332	CZ	ARG B 175	-7.983	10.770	-22.542	0.00	0.00	C
ATOM	1333	NH1	ARG B 175	-7.377	11.878	-22.235	0.00	0.00	N
ATOM	1334	NH2	ARG B 175	-9.281	10.602	-22.377	0.00	0.00	N
ATOM	1335	N	VAL B 176	-1.739	5.480	-22.737	0.00	0.00	N
ATOM	1336	CA	VAL B 176	-0.329	5.196	-23.091	0.00	0.00	C
ATOM	1337	C	VAL B 176	-0.307	5.055	-24.613	0.00	0.00	C
ATOM	1338	O	VAL B 176	0.798	4.955	-25.198	0.00	0.00	O
ATOM	1339	CB	VAL B 176	0.291	4.021	-22.321	0.00	0.00	C
ATOM	1340	CG1	VAL B 176	-0.232	3.742	-20.909	0.00	0.00	C
ATOM	1341	CG2	VAL B 176	0.204	2.700	-23.071	0.00	0.00	C
ATOM	1342	N	GLY B 177	-1.503	5.065	-25.214	0.00	0.00	N
ATOM	1343	CA	GLY B 177	-1.533	4.904	-26.684	0.00	0.00	C
ATOM	1344	C	GLY B 177	-2.873	5.178	-27.329	0.00	0.00	C
ATOM	1345	O	GLY B 177	-3.773	5.768	-26.726	0.00	0.00	O
ATOM	1346	N	ASN B 178	-2.937	4.707	-28.565	0.00	0.00	N
ATOM	1347	CA	ASN B 178	-4.117	4.903	-29.423	0.00	0.00	C
ATOM	1348	C	ASN B 178	-5.233	3.884	-29.177	0.00	0.00	C
ATOM	1349	O	ASN B 178	-5.167	2.987	-28.338	0.00	0.00	O
ATOM	1350	CB	ASN B 178	-3.676	5.000	-30.871	0.00	0.00	C
ATOM	1351	CG	ASN B 178	-3.257	3.726	-31.552	0.00	0.00	C
ATOM	1352	OD1	ASN B 178	-2.442	3.865	-32.485	0.00	0.00	O
ATOM	1353	ND2	ASN B 178	-3.752	2.546	-31.193	0.00	0.00	N
ATOM	1354	N	ARG B 179	-6.276	4.113	-29.958	0.00	0.00	N
ATOM	1355	CA	ARG B 179	-7.562	3.420	-30.004	0.00	0.00	C
ATOM	1356	C	ARG B 179	-7.478	1.942	-30.370	0.00	0.00	C
ATOM	1357	O	ARG B 179	-8.273	1.172	-29.770	0.00	0.00	O
ATOM	1358	CB	ARG B 179	-8.553	4.180	-30.913	0.00	0.00	C
ATOM	1359	CG	ARG B 179	-9.507	3.339	-31.746	0.00	0.00	C
ATOM	1360	CD	ARG B 179	-10.696	4.124	-32.164	0.00	0.00	C
ATOM	1361	NE	ARG B 179	-11.788	4.080	-31.194	0.00	0.00	N
ATOM	1362	CZ	ARG B 179	-12.716	3.110	-31.120	0.00	0.00	C
ATOM	1363	NH1	ARG B 179	-12.683	2.068	-31.974	0.00	0.00	N
ATOM	1364	NH2	ARG B 179	-13.676	3.194	-30.181	0.00	0.00	N
ATOM	1365	N	ALA B 180	-6.602	1.552	-31.279	0.00	0.00	N
ATOM	1366	CA	ALA B 180	-6.466	0.118	-31.651	0.00	0.00	C
ATOM	1367	C	ALA B 180	-5.840	-0.591	-30.443	0.00	0.00	C
ATOM	1368	O	ALA B 180	-6.238	-1.671	-29.950	0.00	0.00	O
ATOM	1369	CB	ALA B 180	-5.674	-0.111	-32.919	0.00	0.00	C

Fig. 1 cont.

ATOM	1370	N	PHE B 181	-4.834	0.155	-29.954	0.00	0.00	N
ATOM	1371	CA	PHE B 181	-4.155	-0.334	-28.731	0.00	0.00	C
ATOM	1372	C	PHE B 181	-5.250	-0.329	-27.653	0.00	0.00	C
ATOM	1373	O	PHE B 181	-5.439	-1.350	-26.968	0.00	0.00	O
ATOM	1374	CB	PHE B 181	-2.907	0.442	-28.397	0.00	0.00	C
ATOM	1375	CG	PHE B 181	-1.981	-0.265	-27.451	0.00	0.00	C
ATOM	1376	CD1	PHE B 181	-1.895	-1.663	-27.467	0.00	0.00	C
ATOM	1377	CD2	PHE B 181	-1.196	0.454	-26.560	0.00	0.00	C
ATOM	1378	CE1	PHE B 181	-1.045	-2.345	-26.622	0.00	0.00	C
ATOM	1379	CE2	PHE B 181	-0.326	-0.241	-25.700	0.00	0.00	C
ATOM	1380	CZ	PHE B 181	-0.258	-1.633	-25.728	0.00	0.00	C
ATOM	1381	N	ALA B 182	-6.038	0.728	-27.555	0.00	0.00	N
ATOM	1382	CA	ALA B 182	-7.138	0.778	-26.579	0.00	0.00	C
ATOM	1383	C	ALA B 182	-8.081	-0.399	-26.821	0.00	0.00	C
ATOM	1384	O	ALA B 182	-8.532	-1.121	-25.918	0.00	0.00	O
ATOM	1385	CB	ALA B 182	-7.826	2.147	-26.617	0.00	0.00	C
ATOM	1386	N	GLU B 183	-8.405	-0.728	-28.053	0.00	0.00	N
ATOM	1387	CA	GLU B 183	-9.337	-1.824	-28.335	0.00	0.00	C
ATOM	1388	C	GLU B 183	-8.795	-3.167	-27.913	0.00	0.00	C
ATOM	1389	O	GLU B 183	-9.595	-4.053	-27.565	0.00	0.00	O
ATOM	1390	CB	GLU B 183	-9.762	-1.901	-29.812	0.00	0.00	C
ATOM	1391	CG	GLU B 183	-10.636	-0.682	-30.141	0.00	0.00	C
ATOM	1392	CD	GLU B 183	-11.136	-0.652	-31.561	0.00	0.00	C
ATOM	1393	OE1	GLU B 183	-10.402	-0.352	-32.501	0.00	0.00	O
ATOM	1394	OE2	GLU B 183	-12.357	-0.964	-31.590	0.00	0.00	O
ATOM	1395	N	PHE B 184	-7.483	-3.282	-28.013	0.00	0.00	N
ATOM	1396	CA	PHE B 184	-6.881	-4.594	-27.668	0.00	0.00	C
ATOM	1397	C	PHE B 184	-7.022	-4.923	-26.201	0.00	0.00	C
ATOM	1398	O	PHE B 184	-7.859	-5.819	-25.999	0.00	0.00	O
ATOM	1399	CB	PHE B 184	-5.431	-4.649	-28.057	0.00	0.00	C
ATOM	1400	CG	PHE B 184	-4.446	-5.717	-27.804	0.00	0.00	C
ATOM	1401	CD1	PHE B 184	-3.207	-5.367	-27.232	0.00	0.00	C
ATOM	1402	CD2	PHE B 184	-4.647	-7.047	-28.157	0.00	0.00	C
ATOM	1403	CE1	PHE B 184	-2.193	-6.283	-26.996	0.00	0.00	C
ATOM	1404	CE2	PHE B 184	-3.647	-8.011	-27.937	0.00	0.00	C
ATOM	1405	CZ	PHE B 184	-2.419	-7.613	-27.361	0.00	0.00	C
ATOM	1406	N	LEU B 185	-6.433	-4.149	-25.321	0.00	0.00	N
ATOM	1407	CA	LEU B 185	-6.389	-4.318	-23.870	0.00	0.00	C
ATOM	1408	C	LEU B 185	-7.739	-4.574	-23.204	0.00	0.00	C
ATOM	1409	O	LEU B 185	-7.885	-4.779	-21.991	0.00	0.00	O
ATOM	1410	CB	LEU B 185	-5.624	-3.133	-23.246	0.00	0.00	C
ATOM	1411	CG	LEU B 185	-4.156	-2.955	-23.589	0.00	0.00	C
ATOM	1412	CD1	LEU B 185	-3.714	-1.490	-23.510	0.00	0.00	C
ATOM	1413	CD2	LEU B 185	-3.267	-3.760	-22.635	0.00	0.00	C
ATOM	1414	N	THR B 186	-8.795	-4.379	-23.904	0.00	0.00	N
ATOM	1415	CA	THR B 186	-10.198	-4.541	-23.796	0.00	0.00	C
ATOM	1416	C	THR B 186	-10.495	-6.026	-23.991	0.00	0.00	C
ATOM	1417	O	THR B 186	-11.118	-6.751	-23.224	0.00	0.00	O
ATOM	1418	CB	THR B 186	-10.922	-3.708	-24.941	0.00	0.00	C
ATOM	1419	OG1	THR B 186	-10.217	-2.434	-25.056	0.00	0.00	O
ATOM	1420	CG2	THR B 186	-12.416	-3.496	-24.739	0.00	0.00	C
ATOM	1421	N	VAL B 187	-10.009	-6.450	-25.145	0.00	0.00	N
ATOM	1422	CA	VAL B 187	-10.152	-7.806	-25.680	0.00	0.00	C
ATOM	1423	C	VAL B 187	-9.128	-8.855	-25.291	0.00	0.00	C
ATOM	1424	O	VAL B 187	-9.416	-10.067	-25.496	0.00	0.00	O
ATOM	1425	CB	VAL B 187	-10.325	-7.644	-27.216	0.00	0.00	C
ATOM	1426	CG1	VAL B 187	-10.166	-8.964	-27.967	0.00	0.00	C
ATOM	1427	CG2	VAL B 187	-11.666	-6.954	-27.467	0.00	0.00	C
ATOM	1428	N	GLN B 188	-7.943	-8.434	-24.883	0.00	0.00	N
ATOM	1429	CA	GLN B 188	-6.874	-9.404	-24.571	0.00	0.00	C

Fig. 1 cont.

ATOM	1430	C	GLN	B	188	-7.293	-10.399	-23.473	0.00	0.00	C
ATOM	1431	O	GLN	B	188	-8.019	-10.292	-22.501	0.00	0.00	O
ATOM	1432	CB	GLN	B	188	-5.495	-8.825	-24.246	0.00	0.00	C
ATOM	1433	CG	GLN	B	188	-4.300	-9.751	-24.334	0.00	0.00	C
ATOM	1434	CD	GLN	B	188	-2.951	-9.086	-24.431	0.00	0.00	C
ATOM	1435	OE1	GLN	B	188	-1.937	-9.595	-24.927	0.00	0.00	O
ATOM	1436	NE2	GLN	B	188	-2.859	-7.841	-23.961	0.00	0.00	N
ATOM	1437	N	THR	B	189	-6.660	-11.497	-23.800	0.00	0.00	N
ATOM	1438	CA	THR	B	189	-6.598	-12.812	-23.238	0.00	0.00	C
ATOM	1439	C	THR	B	189	-5.226	-13.161	-22.654	0.00	0.00	C
ATOM	1440	O	THR	B	189	-4.134	-12.884	-23.171	0.00	0.00	O
ATOM	1441	CB	THR	B	189	-7.024	-13.863	-24.373	0.00	0.00	C
ATOM	1442	OG1	THR	B	189	-8.413	-14.212	-24.058	0.00	0.00	O
ATOM	1443	CG2	THR	B	189	-6.143	-15.108	-24.530	0.00	0.00	C
ATOM	1444	N	GLY	B	190	-5.432	-13.859	-21.549	0.00	0.00	N
ATOM	1445	CA	GLY	B	190	-4.365	-14.428	-20.719	0.00	0.00	C
ATOM	1446	C	GLY	B	190	-4.337	-13.581	-19.448	0.00	0.00	C
ATOM	1447	O	GLY	B	190	-3.231	-13.171	-19.080	0.00	0.00	O
ATOM	1448	N	GLY	B	191	-5.513	-13.394	-18.892	0.00	0.00	N
ATOM	1449	CA	GLY	B	191	-5.672	-12.581	-17.666	0.00	0.00	C
ATOM	1450	C	GLY	B	191	-6.550	-11.363	-18.023	0.00	0.00	C
ATOM	1451	O	GLY	B	191	-7.056	-11.138	-19.154	0.00	0.00	O
ATOM	1452	N	THR	B	192	-6.698	-10.509	-17.003	0.00	0.00	N
ATOM	1453	CA	THR	B	192	-7.512	-9.294	-17.110	0.00	0.00	C
ATOM	1454	C	THR	B	192	-6.820	-8.034	-16.621	0.00	0.00	C
ATOM	1455	O	THR	B	192	-5.795	-8.041	-15.916	0.00	0.00	O
ATOM	1456	CB	THR	B	192	-8.864	-9.536	-16.326	0.00	0.00	C
ATOM	1457	OG1	THR	B	192	-9.236	-8.239	-15.765	0.00	0.00	O
ATOM	1458	CG2	THR	B	192	-8.785	-10.592	-15.222	0.00	0.00	C
ATOM	1459	N	LEU	B	193	-7.418	-6.931	-17.020	0.00	0.00	N
ATOM	1460	CA	LEU	B	193	-7.025	-5.554	-16.734	0.00	0.00	C
ATOM	1461	C	LEU	B	193	-8.128	-4.854	-15.935	0.00	0.00	C
ATOM	1462	O	LEU	B	193	-9.299	-4.769	-16.333	0.00	0.00	O
ATOM	1463	CB	LEU	B	193	-6.719	-4.938	-18.092	0.00	0.00	C
ATOM	1464	CG	LEU	B	193	-5.822	-3.765	-18.392	0.00	0.00	C
ATOM	1465	CD1	LEU	B	193	-6.191	-3.116	-19.746	0.00	0.00	C
ATOM	1466	CD2	LEU	B	193	-5.911	-2.681	-17.327	0.00	0.00	C
ATOM	1467	N	TYR	B	194	-7.720	-4.359	-14.793	0.00	0.00	N
ATOM	1468	CA	TYR	B	194	-8.439	-3.591	-13.792	0.00	0.00	C
ATOM	1469	C	TYR	B	194	-7.917	-2.150	-13.755	0.00	0.00	C
ATOM	1470	O	TYR	B	194	-6.967	-1.849	-13.002	0.00	0.00	O
ATOM	1471	CB	TYR	B	194	-8.212	-4.191	-12.376	0.00	0.00	C
ATOM	1472	CG	TYR	B	194	-8.843	-5.565	-12.442	0.00	0.00	C
ATOM	1473	CD1	TYR	B	194	-10.235	-5.628	-12.434	0.00	0.00	C
ATOM	1474	CD2	TYR	B	194	-8.099	-6.715	-12.599	0.00	0.00	C
ATOM	1475	CE1	TYR	B	194	-10.870	-6.855	-12.508	0.00	0.00	C
ATOM	1476	CE2	TYR	B	194	-8.736	-7.944	-12.699	0.00	0.00	C
ATOM	1477	CZ	TYR	B	194	-10.110	-8.001	-12.644	0.00	0.00	C
ATOM	1478	OH	TYR	B	194	-10.749	-9.198	-12.749	0.00	0.00	O
ATOM	1479	N	ARG	B	195	-8.623	-1.282	-14.456	0.00	0.00	N
ATOM	1480	CA	ARG	B	195	-8.232	0.133	-14.592	0.00	0.00	C
ATOM	1481	C	ARG	B	195	-9.063	0.975	-13.643	0.00	0.00	C
ATOM	1482	O	ARG	B	195	-10.257	1.212	-13.848	0.00	0.00	O
ATOM	1483	CB	ARG	B	195	-8.389	0.529	-16.043	0.00	0.00	C
ATOM	1484	CG	ARG	B	195	-7.731	1.696	-16.716	0.00	0.00	C
ATOM	1485	CD	ARG	B	195	-8.141	1.924	-18.132	0.00	0.00	C
ATOM	1486	NE	ARG	B	195	-9.312	2.701	-18.414	0.00	0.00	N
ATOM	1487	CZ	ARG	B	195	-9.894	3.862	-18.218	0.00	0.00	C
ATOM	1488	NH1	ARG	B	195	-9.376	4.849	-17.492	0.00	0.00	N
ATOM	1489	NH2	ARG	B	195	-11.098	4.120	-18.767	0.00	0.00	N

Fig. 1 cont.

ATOM	1490	N	ILE B 196	-8.330	1.409	-12.613	0.00	0.00	N
ATOM	1491	CA	ILE B 196	-8.897	2.240	-11.560	0.00	0.00	C
ATOM	1492	C	ILE B 196	-8.289	3.651	-11.660	0.00	0.00	C
ATOM	1493	O	ILE B 196	-7.107	3.910	-11.704	0.00	0.00	O
ATOM	1494	CB	ILE B 196	-8.741	1.832	-10.081	0.00	0.00	C
ATOM	1495	CG1	ILE B 196	-9.371	0.440	-9.904	0.00	0.00	C
ATOM	1496	CG2	ILE B 196	-9.326	2.866	-9.098	0.00	0.00	C
ATOM	1497	CD1	ILE B 196	-8.367	-0.708	-10.220	0.00	0.00	C
ATOM	1498	N	THR B 197	-9.291	4.471	-11.742	0.00	0.00	N
ATOM	1499	CA	THR B 197	-9.428	5.904	-11.842	0.00	0.00	C
ATOM	1500	C	THR B 197	-10.252	6.367	-10.633	0.00	0.00	C
ATOM	1501	O	THR B 197	-11.151	5.620	-10.182	0.00	0.00	O
ATOM	1502	CB	THR B 197	-10.086	6.372	-13.178	0.00	0.00	C
ATOM	1503	OG1	THR B 197	-11.525	6.170	-13.038	0.00	0.00	O
ATOM	1504	CG2	THR B 197	-9.523	5.611	-14.386	0.00	0.00	C
ATOM	1505	N	HIS B 198	-9.853	7.492	-10.099	0.00	0.00	N
ATOM	1506	CA	HIS B 198	-10.461	8.119	-8.930	0.00	0.00	C
ATOM	1507	C	HIS B 198	-11.025	9.489	-9.312	0.00	0.00	C
ATOM	1508	O	HIS B 198	-10.417	10.260	-10.063	0.00	0.00	O
ATOM	1509	CB	HIS B 198	-9.540	8.373	-7.737	0.00	0.00	C
ATOM	1510	CG	HIS B 198	-10.043	9.025	-6.496	0.00	0.00	C
ATOM	1511	ND1	HIS B 198	-11.264	8.955	-5.893	0.00	0.00	N
ATOM	1512	CD2	HIS B 198	-9.284	9.784	-5.653	0.00	0.00	C
ATOM	1513	CE1	HIS B 198	-11.204	9.661	-4.785	0.00	0.00	C
ATOM	1514	NE2	HIS B 198	-10.026	10.194	-4.589	0.00	0.00	N
ATOM	1515	N	THR B 199	-12.213	9.661	-8.780	0.00	0.00	N
ATOM	1516	CA	THR B 199	-13.051	10.869	-8.915	0.00	0.00	C
ATOM	1517	C	THR B 199	-12.635	11.718	-10.097	0.00	0.00	C
ATOM	1518	O	THR B 199	-12.923	11.418	-11.272	0.00	0.00	O
ATOM	1519	CB	THR B 199	-13.046	11.511	-7.465	0.00	0.00	C
ATOM	1520	OG1	THR B 199	-14.180	12.434	-7.419	0.00	0.00	O
ATOM	1521	CG2	THR B 199	-11.732	12.177	-7.064	0.00	0.00	C
ATOM	1522	N	ASN B 200	-11.937	12.777	-9.915	0.00	0.00	N
ATOM	1523	CA	ASN B 200	-11.319	13.843	-10.639	0.00	0.00	C
ATOM	1524	C	ASN B 200	-9.847	13.778	-11.028	0.00	0.00	C
ATOM	1525	O	ASN B 200	-9.305	14.790	-11.513	0.00	0.00	O
ATOM	1526	CB	ASN B 200	-11.240	14.928	-9.519	0.00	0.00	C
ATOM	1527	CG	ASN B 200	-11.958	16.225	-9.660	0.00	0.00	C
ATOM	1528	OD1	ASN B 200	-11.869	17.044	-8.723	0.00	0.00	O
ATOM	1529	ND2	ASN B 200	-12.644	16.364	-10.788	0.00	0.00	N
ATOM	1530	N	ASP B 201	-9.098	12.760	-10.720	0.00	0.00	N
ATOM	1531	CA	ASP B 201	-7.639	12.678	-10.969	0.00	0.00	C
ATOM	1532	C	ASP B 201	-7.309	13.261	-12.318	0.00	0.00	C
ATOM	1533	O	ASP B 201	-7.962	12.820	-13.286	0.00	0.00	O
ATOM	1534	CB	ASP B 201	-7.373	11.213	-10.681	0.00	0.00	C
ATOM	1535	CG	ASP B 201	-5.917	10.867	-10.728	0.00	0.00	C
ATOM	1536	OD1	ASP B 201	-5.582	9.687	-10.611	0.00	0.00	O
ATOM	1537	OD2	ASP B 201	-5.137	11.816	-10.919	0.00	0.00	O
ATOM	1538	N	ILE B 202	-6.385	14.199	-12.460	0.00	0.00	N
ATOM	1539	CA	ILE B 202	-6.142	14.764	-13.802	0.00	0.00	C
ATOM	1540	C	ILE B 202	-5.419	13.802	-14.729	0.00	0.00	C
ATOM	1541	O	ILE B 202	-5.599	13.795	-15.957	0.00	0.00	O
ATOM	1542	CB	ILE B 202	-5.396	16.152	-13.765	0.00	0.00	C
ATOM	1543	CG1	ILE B 202	-5.216	16.807	-15.161	0.00	0.00	C
ATOM	1544	CG2	ILE B 202	-4.002	16.050	-13.079	0.00	0.00	C
ATOM	1545	CD1	ILE B 202	-6.393	17.010	-16.154	0.00	0.00	C
ATOM	1546	N	VAL B 203	-4.601	12.986	-14.118	0.00	0.00	N
ATOM	1547	CA	VAL B 203	-3.733	12.027	-14.853	0.00	0.00	C
ATOM	1548	C	VAL B 203	-4.451	11.107	-15.812	0.00	0.00	C
ATOM	1549	O	VAL B 203	-3.993	11.118	-17.001	0.00	0.00	O

Fig. 1 cont.

ATOM	1550	CB	VAL	B	203	-2.762	11.461	-13.799	0.00	0.00	C
ATOM	1551	CG1	VAL	B	203	-1.631	10.768	-14.542	0.00	0.00	C
ATOM	1552	CG2	VAL	B	203	-2.318	12.560	-12.830	0.00	0.00	C
ATOM	1553	N	PRO	B	204	-5.531	10.406	-15.498	0.00	0.00	N
ATOM	1554	CA	PRO	B	204	-6.254	9.543	-16.451	0.00	0.00	C
ATOM	1555	C	PRO	B	204	-6.877	10.173	-17.696	0.00	0.00	C
ATOM	1556	O	PRO	B	204	-7.437	9.598	-18.659	0.00	0.00	O
ATOM	1557	CB	PRO	B	204	-7.330	8.902	-15.562	0.00	0.00	C
ATOM	1558	CG	PRO	B	204	-6.889	9.077	-14.126	0.00	0.00	C
ATOM	1559	CD	PRO	B	204	-6.064	10.352	-14.127	0.00	0.00	C
ATOM	1560	N	ARG	B	205	-6.832	11.486	-17.767	0.00	0.00	N
ATOM	1561	CA	ARG	B	205	-7.295	12.478	-18.703	0.00	0.00	C
ATOM	1562	C	ARG	B	205	-6.170	12.966	-19.604	0.00	0.00	C
ATOM	1563	O	ARG	B	205	-6.429	13.672	-20.601	0.00	0.00	O
ATOM	1564	CB	ARG	B	205	-7.938	13.673	-17.984	0.00	0.00	C
ATOM	1565	CG	ARG	B	205	-9.319	13.491	-17.375	0.00	0.00	C
ATOM	1566	CD	ARG	B	205	-9.754	14.662	-16.568	0.00	0.00	C
ATOM	1567	NE	ARG	B	205	-11.060	14.485	-15.964	0.00	0.00	N
ATOM	1568	CZ	ARG	B	205	-11.798	15.406	-15.346	0.00	0.00	C
ATOM	1569	NH1	ARG	B	205	-11.439	16.679	-15.187	0.00	0.00	N
ATOM	1570	NH2	ARG	B	205	-12.967	14.966	-14.857	0.00	0.00	N
ATOM	1571	N	LEU	B	206	-4.966	12.564	-19.296	0.00	0.00	N
ATOM	1572	CA	LEU	B	206	-3.730	12.871	-20.047	0.00	0.00	C
ATOM	1573	C	LEU	B	206	-3.183	11.597	-20.651	0.00	0.00	C
ATOM	1574	O	LEU	B	206	-3.350	10.551	-19.988	0.00	0.00	O
ATOM	1575	CB	LEU	B	206	-2.812	13.591	-19.029	0.00	0.00	C
ATOM	1576	CG	LEU	B	206	-3.219	15.078	-18.999	0.00	0.00	C
ATOM	1577	CD1	LEU	B	206	-2.927	15.703	-17.657	0.00	0.00	C
ATOM	1578	CD2	LEU	B	206	-2.470	15.769	-20.132	0.00	0.00	C
ATOM	1579	N	PRO	B	207	-2.558	11.575	-21.809	0.00	0.00	N
ATOM	1580	CA	PRO	B	207	-2.290	12.694	-22.713	0.00	0.00	C
ATOM	1581	C	PRO	B	207	-3.569	12.941	-23.511	0.00	0.00	C
ATOM	1582	O	PRO	B	207	-4.276	11.979	-23.835	0.00	0.00	O
ATOM	1583	CB	PRO	B	207	-1.095	12.172	-23.478	0.00	0.00	C
ATOM	1584	CG	PRO	B	207	-0.748	10.774	-23.114	0.00	0.00	C
ATOM	1585	CD	PRO	B	207	-2.014	10.323	-22.389	0.00	0.00	C
ATOM	1586	N	PRO	B	208	-3.850	14.208	-23.778	0.00	0.00	N
ATOM	1587	CA	PRO	B	208	-5.044	14.660	-24.489	0.00	0.00	C
ATOM	1588	C	PRO	B	208	-5.531	13.679	-25.533	0.00	0.00	C
ATOM	1589	O	PRO	B	208	-4.670	13.023	-26.153	0.00	0.00	O
ATOM	1590	CB	PRO	B	208	-4.573	15.995	-25.058	0.00	0.00	C
ATOM	1591	CG	PRO	B	208	-3.670	16.588	-24.012	0.00	0.00	C
ATOM	1592	CD	PRO	B	208	-3.014	15.375	-23.382	0.00	0.00	C
ATOM	1593	N	ARG	B	209	-6.856	13.597	-25.712	0.00	0.00	N
ATOM	1594	CA	ARG	B	209	-7.490	12.712	-26.715	0.00	0.00	C
ATOM	1595	C	ARG	B	209	-7.250	13.324	-28.112	0.00	0.00	C
ATOM	1596	O	ARG	B	209	-6.894	12.633	-29.091	0.00	0.00	O
ATOM	1597	CB	ARG	B	209	-8.978	12.402	-26.651	0.00	0.00	C
ATOM	1598	CG	ARG	B	209	-9.739	12.422	-25.365	0.00	0.00	C
ATOM	1599	CD	ARG	B	209	-9.917	13.753	-24.757	0.00	0.00	C
ATOM	1600	NE	ARG	B	209	-8.983	14.421	-23.866	0.00	0.00	N
ATOM	1601	CZ	ARG	B	209	-9.319	14.984	-22.696	0.00	0.00	C
ATOM	1602	NH1	ARG	B	209	-8.411	15.600	-21.929	0.00	0.00	N
ATOM	1603	NH2	ARG	B	209	-10.556	14.956	-22.196	0.00	0.00	N
ATOM	1604	N	GLU	B	210	-7.425	14.630	-28.219	0.00	0.00	N
ATOM	1605	CA	GLU	B	210	-7.157	15.397	-29.430	0.00	0.00	C
ATOM	1606	C	GLU	B	210	-5.925	14.914	-30.197	0.00	0.00	C
ATOM	1607	O	GLU	B	210	-5.957	14.776	-31.426	0.00	0.00	O
ATOM	1608	CB	GLU	B	210	-6.883	16.864	-29.062	0.00	0.00	C
ATOM	1609	CG	GLU	B	210	-6.420	17.266	-27.667	0.00	0.00	C

Fig. 1 cont.

ATOM	1610	CD	GLU	B	210	-7.466	17.629	-26.653	0.00	0.00	C
ATOM	1611	OE1	GLU	B	210	-7.523	17.373	-25.460	0.00	0.00	O
ATOM	1612	OE2	GLU	B	210	-8.386	18.321	-27.156	0.00	0.00	O
ATOM	1613	N	PHE	B	211	-4.805	14.670	-29.548	0.00	0.00	N
ATOM	1614	CA	PHE	B	211	-3.530	14.207	-30.044	0.00	0.00	C
ATOM	1615	C	PHE	B	211	-3.371	12.731	-30.422	0.00	0.00	C
ATOM	1616	O	PHE	B	211	-2.280	12.359	-30.938	0.00	0.00	O
ATOM	1617	CB	PHE	B	211	-2.470	14.463	-28.949	0.00	0.00	C
ATOM	1618	CG	PHE	B	211	-2.144	15.920	-28.878	0.00	0.00	C
ATOM	1619	CD1	PHE	B	211	-1.472	16.526	-29.949	0.00	0.00	C
ATOM	1620	CD2	PHE	B	211	-2.518	16.664	-27.763	0.00	0.00	C
ATOM	1621	CE1	PHE	B	211	-1.147	17.878	-29.925	0.00	0.00	C
ATOM	1622	CE2	PHE	B	211	-2.202	18.020	-27.720	0.00	0.00	C
ATOM	1623	CZ	PHE	B	211	-1.516	18.613	-28.801	0.00	0.00	C
ATOM	1624	N	GLY	B	212	-4.358	11.896	-30.155	0.00	0.00	N
ATOM	1625	CA	GLY	B	212	-4.275	10.491	-30.515	0.00	0.00	C
ATOM	1626	C	GLY	B	212	-4.578	9.455	-29.470	0.00	0.00	C
ATOM	1627	O	GLY	B	212	-4.924	8.315	-29.855	0.00	0.00	O
ATOM	1628	N	TYR	B	213	-4.469	9.803	-28.206	0.00	0.00	N
ATOM	1629	CA	TYR	B	213	-4.706	8.794	-27.151	0.00	0.00	C
ATOM	1630	C	TYR	B	213	-6.179	8.460	-26.955	0.00	0.00	C
ATOM	1631	O	TYR	B	213	-7.089	9.159	-27.413	0.00	0.00	O
ATOM	1632	CB	TYR	B	213	-3.935	9.296	-25.920	0.00	0.00	C
ATOM	1633	CG	TYR	B	213	-2.446	9.368	-26.174	0.00	0.00	C
ATOM	1634	CD1	TYR	B	213	-1.598	8.415	-25.589	0.00	0.00	C
ATOM	1635	CD2	TYR	B	213	-1.858	10.353	-26.967	0.00	0.00	C
ATOM	1636	CE1	TYR	B	213	-0.214	8.443	-25.771	0.00	0.00	C
ATOM	1637	CE2	TYR	B	213	-0.479	10.386	-27.180	0.00	0.00	C
ATOM	1638	CZ	TYR	B	213	0.341	9.432	-26.579	0.00	0.00	C
ATOM	1639	OH	TYR	B	213	1.689	9.483	-26.778	0.00	0.00	O
ATOM	1640	N	SER	B	214	-6.388	7.336	-26.294	0.00	0.00	N
ATOM	1641	CA	SER	B	214	-7.666	6.721	-25.951	0.00	0.00	C
ATOM	1642	C	SER	B	214	-7.464	5.780	-24.763	0.00	0.00	C
ATOM	1643	O	SER	B	214	-6.297	5.447	-24.523	0.00	0.00	O
ATOM	1644	CB	SER	B	214	-8.295	5.989	-27.139	0.00	0.00	C
ATOM	1645	OG	SER	B	214	-9.264	6.883	-27.700	0.00	0.00	O
ATOM	1646	N	HIS	B	215	-8.509	5.385	-24.076	0.00	0.00	N
ATOM	1647	CA	HIS	B	215	-8.560	4.499	-22.909	0.00	0.00	C
ATOM	1648	C	HIS	B	215	-9.364	3.232	-23.193	0.00	0.00	C
ATOM	1649	O	HIS	B	215	-10.255	3.324	-24.046	0.00	0.00	O
ATOM	1650	CB	HIS	B	215	-9.186	5.227	-21.719	0.00	0.00	C
ATOM	1651	CG	HIS	B	215	-8.319	5.873	-20.697	0.00	0.00	C
ATOM	1652	ND1	HIS	B	215	-7.129	5.411	-20.228	0.00	0.00	N
ATOM	1653	CD2	HIS	B	215	-8.554	7.008	-19.974	0.00	0.00	C
ATOM	1654	CE1	HIS	B	215	-6.655	6.226	-19.299	0.00	0.00	C
ATOM	1655	NE2	HIS	B	215	-7.501	7.203	-19.117	0.00	0.00	N
ATOM	1656	N	SER	B	216	-9.194	2.106	-22.588	0.00	0.00	N
ATOM	1657	CA	SER	B	216	-9.777	0.773	-22.694	0.00	0.00	C
ATOM	1658	C	SER	B	216	-11.167	0.466	-22.142	0.00	0.00	C
ATOM	1659	O	SER	B	216	-11.753	1.481	-21.645	0.00	0.00	O
ATOM	1660	CB	SER	B	216	-8.706	-0.116	-22.020	0.00	0.00	C
ATOM	1661	OG	SER	B	216	-7.800	0.692	-21.276	0.00	0.00	O
ATOM	1662	N	SER	B	217	-11.746	-0.770	-22.155	0.00	0.00	N
ATOM	1663	CA	SER	B	217	-13.143	-0.896	-21.623	0.00	0.00	C
ATOM	1664	C	SER	B	217	-13.437	-1.283	-20.244	0.00	0.00	C
ATOM	1665	O	SER	B	217	-12.531	-0.371	-19.968	0.00	0.00	O
ATOM	1666	CB	SER	B	217	-14.085	-1.773	-22.492	0.00	0.00	C
ATOM	1667	OG	SER	B	217	-15.201	-2.464	-21.915	0.00	0.00	O
ATOM	1668	N	PRO	B	218	-13.801	-1.534	-19.061	0.00	0.00	N
ATOM	1669	CA	PRO	B	218	-13.858	-1.249	-17.719	0.00	0.00	C

Fig. 1 cont.

ATOM	1670	C	PRO	B	218	-12.879	-0.171	-17.310	0.00	0.00	C
ATOM	1671	O	PRO	B	218	-11.702	-0.129	-17.638	0.00	0.00	O
ATOM	1672	CB	PRO	B	218	-13.595	-2.547	-16.931	0.00	0.00	C
ATOM	1673	CG	PRO	B	218	-14.294	-3.501	-17.835	0.00	0.00	C
ATOM	1674	CD	PRO	B	218	-14.881	-2.553	-18.921	0.00	0.00	C
ATOM	1675	N	GLU	B	219	-13.516	0.618	-16.503	0.00	0.00	N
ATOM	1676	CA	GLU	B	219	-12.777	1.661	-15.776	0.00	0.00	C
ATOM	1677	C	GLU	B	219	-13.537	1.424	-14.459	0.00	0.00	C
ATOM	1678	O	GLU	B	219	-14.785	1.347	-14.491	0.00	0.00	O
ATOM	1679	CB	GLU	B	219	-12.822	3.004	-16.400	0.00	0.00	C
ATOM	1680	CG	GLU	B	219	-13.884	4.020	-16.028	0.00	0.00	C
ATOM	1681	CD	GLU	B	219	-13.375	5.430	-16.124	0.00	0.00	C
ATOM	1682	OE1	GLU	B	219	-13.063	5.953	-17.176	0.00	0.00	O
ATOM	1683	OE2	GLU	B	219	-13.309	5.924	-14.989	0.00	0.00	O
ATOM	1684	N	TYR	B	220	-12.758	1.271	-13.413	0.00	0.00	N
ATOM	1685	CA	TYR	B	220	-13.460	1.064	-12.116	0.00	0.00	C
ATOM	1686	C	TYR	B	220	-13.080	2.470	-11.593	0.00	0.00	C
ATOM	1687	O	TYR	B	220	-11.903	2.847	-11.544	0.00	0.00	O
ATOM	1688	CB	TYR	B	220	-13.115	-0.143	-11.269	0.00	0.00	C
ATOM	1689	CG	TYR	B	220	-13.155	-1.473	-12.006	0.00	0.00	C
ATOM	1690	CD1	TYR	B	220	-12.275	-1.680	-13.079	0.00	0.00	C
ATOM	1691	CD2	TYR	B	220	-14.015	-2.486	-11.656	0.00	0.00	C
ATOM	1692	CE1	TYR	B	220	-12.238	-2.856	-13.789	0.00	0.00	C
ATOM	1693	CE2	TYR	B	220	-14.012	-3.685	-12.348	0.00	0.00	C
ATOM	1694	CZ	TYR	B	220	-13.130	-3.858	-13.406	0.00	0.00	C
ATOM	1695	OH	TYR	B	220	-13.159	-5.043	-14.124	0.00	0.00	O
ATOM	1696	N	TRP	B	221	-14.186	3.126	-11.283	0.00	0.00	N
ATOM	1697	CA	TRP	B	221	-14.173	4.503	-10.815	0.00	0.00	C
ATOM	1698	C	TRP	B	221	-14.573	4.535	-9.343	0.00	0.00	C
ATOM	1699	O	TRP	B	221	-15.668	4.174	-8.892	0.00	0.00	O
ATOM	1700	CB	TRP	B	221	-15.168	5.339	-11.625	0.00	0.00	C
ATOM	1701	CG	TRP	B	221	-15.076	6.815	-11.430	0.00	0.00	C
ATOM	1702	CD1	TRP	B	221	-13.921	7.541	-11.419	0.00	0.00	C
ATOM	1703	CD2	TRP	B	221	-16.138	7.769	-11.300	0.00	0.00	C
ATOM	1704	NE1	TRP	B	221	-14.198	8.872	-11.262	0.00	0.00	N
ATOM	1705	CE2	TRP	B	221	-15.546	9.036	-11.163	0.00	0.00	C
ATOM	1706	CE3	TRP	B	221	-17.518	7.673	-11.272	0.00	0.00	C
ATOM	1707	CZ2	TRP	B	221	-16.275	10.206	-11.006	0.00	0.00	C
ATOM	1708	CZ3	TRP	B	221	-18.248	8.831	-11.104	0.00	0.00	C
ATOM	1709	CH2	TRP	B	221	-17.658	10.085	-10.971	0.00	0.00	C
ATOM	1710	N	ILE	B	222	-13.615	5.119	-8.640	0.00	0.00	N
ATOM	1711	CA	ILE	B	222	-13.813	5.256	-7.172	0.00	0.00	C
ATOM	1712	C	ILE	B	222	-14.501	6.622	-7.290	0.00	0.00	C
ATOM	1713	O	ILE	B	222	-14.019	7.411	-8.133	0.00	0.00	O
ATOM	1714	CB	ILE	B	222	-12.500	5.158	-6.372	0.00	0.00	C
ATOM	1715	CG1	ILE	B	222	-11.619	3.947	-6.791	0.00	0.00	C
ATOM	1716	CG2	ILE	B	222	-12.762	5.120	-4.834	0.00	0.00	C
ATOM	1717	CD1	ILE	B	222	-10.234	3.921	-6.055	0.00	0.00	C
ATOM	1718	N	LYS	B	223	-15.620	6.780	-6.613	0.00	0.00	N
ATOM	1719	CA	LYS	B	223	-16.437	7.993	-6.634	0.00	0.00	C
ATOM	1720	C	LYS	B	223	-16.324	8.779	-5.321	0.00	0.00	C
ATOM	1721	O	LYS	B	223	-16.679	9.975	-5.316	0.00	0.00	O
ATOM	1722	CB	LYS	B	223	-17.924	7.692	-6.780	0.00	0.00	C
ATOM	1723	CG	LYS	B	223	-18.288	6.919	-8.030	0.00	0.00	C
ATOM	1724	CD	LYS	B	223	-19.795	6.761	-8.180	0.00	0.00	C
ATOM	1725	CE	LYS	B	223	-20.478	8.119	-8.108	0.00	0.00	C
ATOM	1726	NZ	LYS	B	223	-21.949	8.003	-8.173	0.00	0.00	N
ATOM	1727	N	SER	B	224	-15.890	8.053	-4.299	0.00	0.00	N
ATOM	1728	CA	SER	B	224	-15.700	8.525	-2.925	0.00	0.00	C
ATOM	1729	C	SER	B	224	-14.593	9.569	-2.942	0.00	0.00	C

Fig. 1 cont.

ATOM	1730	O	SER B 224	-13.688	9.389	-3.753	0.00	0.00	O
ATOM	1731	CB	SER B 224	-15.391	7.373	-1.998	0.00	0.00	C
ATOM	1732	OG	SER B 224	-14.005	7.068	-1.863	0.00	0.00	O
ATOM	1733	N	GLY B 225	-14.656	10.577	-2.122	0.00	0.00	N
ATOM	1734	CA	GLY B 225	-13.711	11.681	-2.085	0.00	0.00	C
ATOM	1735	C	GLY B 225	-12.286	11.415	-1.681	0.00	0.00	C
ATOM	1736	O	GLY B 225	-11.888	10.239	-1.641	0.00	0.00	O
ATOM	1737	N	THR B 226	-11.576	12.497	-1.392	0.00	0.00	N
ATOM	1738	CA	THR B 226	-10.187	12.416	-0.919	0.00	0.00	C
ATOM	1739	C	THR B 226	-10.278	12.270	0.598	0.00	0.00	C
ATOM	1740	O	THR B 226	-11.231	12.614	1.328	0.00	0.00	O
ATOM	1741	CB	THR B 226	-9.277	13.568	-1.442	0.00	0.00	C
ATOM	1742	OG1	THR B 226	-9.062	13.167	-2.833	0.00	0.00	O
ATOM	1743	CG2	THR B 226	-7.922	13.760	-0.766	0.00	0.00	C
ATOM	1744	N	LEU B 227	-9.291	11.582	1.152	0.00	0.00	N
ATOM	1745	CA	LEU B 227	-9.030	11.213	2.534	0.00	0.00	C
ATOM	1746	C	LEU B 227	-10.237	10.510	3.167	0.00	0.00	C
ATOM	1747	O	LEU B 227	-10.335	10.351	4.402	0.00	0.00	O
ATOM	1748	CB	LEU B 227	-8.491	12.411	3.304	0.00	0.00	C
ATOM	1749	CG	LEU B 227	-7.190	13.117	2.978	0.00	0.00	C
ATOM	1750	CD1	LEU B 227	-6.844	14.102	4.109	0.00	0.00	C
ATOM	1751	CD2	LEU B 227	-6.003	12.184	2.815	0.00	0.00	C
ATOM	1752	N	VAL B 228	-11.090	9.971	2.320	0.00	0.00	N
ATOM	1753	CA	VAL B 228	-12.243	9.224	2.759	0.00	0.00	C
ATOM	1754	C	VAL B 228	-12.164	7.824	2.125	0.00	0.00	C
ATOM	1755	O	VAL B 228	-12.038	7.663	0.921	0.00	0.00	O
ATOM	1756	CB	VAL B 228	-13.605	9.867	2.518	0.00	0.00	C
ATOM	1757	CG1	VAL B 228	-13.639	11.098	1.614	0.00	0.00	C
ATOM	1758	CG2	VAL B 228	-14.636	8.857	1.976	0.00	0.00	C
ATOM	1759	N	PRO B 229	-12.347	6.885	3.045	0.00	0.00	N
ATOM	1760	CA	PRO B 229	-12.395	5.442	2.806	0.00	0.00	C
ATOM	1761	C	PRO B 229	-13.186	4.879	1.642	0.00	0.00	C
ATOM	1762	O	PRO B 229	-14.435	5.041	1.653	0.00	0.00	O
ATOM	1763	CB	PRO B 229	-13.122	4.937	4.084	0.00	0.00	C
ATOM	1764	CG	PRO B 229	-13.714	6.165	4.734	0.00	0.00	C
ATOM	1765	CD	PRO B 229	-12.535	7.130	4.513	0.00	0.00	C
ATOM	1766	N	VAL B 230	-12.567	4.185	0.689	0.00	0.00	N
ATOM	1767	CA	VAL B 230	-13.497	3.695	-0.376	0.00	0.00	C
ATOM	1768	C	VAL B 230	-14.297	2.615	0.366	0.00	0.00	C
ATOM	1769	O	VAL B 230	-14.069	2.312	1.542	0.00	0.00	O
ATOM	1770	CB	VAL B 230	-12.944	3.279	-1.746	0.00	0.00	C
ATOM	1771	CG1	VAL B 230	-11.510	3.769	-2.009	0.00	0.00	C
ATOM	1772	CG2	VAL B 230	-13.076	1.799	-2.053	0.00	0.00	C
ATOM	1773	N	THR B 231	-15.280	2.131	-0.353	0.00	0.00	N
ATOM	1774	CA	THR B 231	-16.134	1.051	0.105	0.00	0.00	C
ATOM	1775	C	THR B 231	-16.753	0.613	-1.248	0.00	0.00	C
ATOM	1776	O	THR B 231	-16.835	1.256	-2.288	0.00	0.00	O
ATOM	1777	CB	THR B 231	-17.228	1.182	1.199	0.00	0.00	C
ATOM	1778	OG1	THR B 231	-18.465	1.266	0.377	0.00	0.00	O
ATOM	1779	CG2	THR B 231	-17.219	2.315	2.225	0.00	0.00	C
ATOM	1780	N	ARG B 232	-17.172	-0.604	-1.116	0.00	0.00	N
ATOM	1781	CA	ARG B 232	-17.738	-1.457	-2.148	0.00	0.00	C
ATOM	1782	C	ARG B 232	-18.680	-0.762	-3.090	0.00	0.00	C
ATOM	1783	O	ARG B 232	-18.561	-0.974	-4.314	0.00	0.00	O
ATOM	1784	CB	ARG B 232	-18.365	-2.669	-1.447	0.00	0.00	C
ATOM	1785	CG	ARG B 232	-17.296	-3.459	-0.676	0.00	0.00	C
ATOM	1786	CD	ARG B 232	-17.233	-4.870	-1.122	0.00	0.00	C
ATOM	1787	NE	ARG B 232	-18.450	-5.373	-1.745	0.00	0.00	N
ATOM	1788	CZ	ARG B 232	-19.637	-5.540	-1.139	0.00	0.00	C
ATOM	1789	NH1	ARG B 232	-19.880	-5.235	0.140	0.00	0.00	N

Fig. 1 cont.

ATOM	1790	NH2	ARG	B	232	-20.563	-6.030	-1.958	0.00	0.00	N
ATOM	1791	N	ASN	B	233	-19.552	0.027	-2.540	0.00	0.00	N
ATOM	1792	CA	ASN	B	233	-20.533	0.761	-3.366	0.00	0.00	C
ATOM	1793	C	ASN	B	233	-19.970	2.087	-3.848	0.00	0.00	C
ATOM	1794	O	ASN	B	233	-20.832	2.879	-4.267	0.00	0.00	O
ATOM	1795	CB	ASN	B	233	-21.820	0.872	-2.552	0.00	0.00	C
ATOM	1796	CG	ASN	B	233	-22.245	-0.402	-1.839	0.00	0.00	C
ATOM	1797	OD1	ASN	B	233	-21.974	-0.688	-0.652	0.00	0.00	O
ATOM	1798	ND2	ASN	B	233	-22.987	-1.182	-2.620	0.00	0.00	N
ATOM	1799	N	ASP	B	234	-18.690	2.377	-3.843	0.00	0.00	N
ATOM	1800	CA	ASP	B	234	-18.168	3.652	-4.352	0.00	0.00	C
ATOM	1801	C	ASP	B	234	-17.366	3.445	-5.643	0.00	0.00	C
ATOM	1802	O	ASP	B	234	-16.771	4.372	-6.199	0.00	0.00	O
ATOM	1803	CB	ASP	B	234	-17.305	4.298	-3.305	0.00	0.00	C
ATOM	1804	CG	ASP	B	234	-17.981	4.513	-1.977	0.00	0.00	C
ATOM	1805	OD1	ASP	B	234	-18.174	3.585	-1.193	0.00	0.00	O
ATOM	1806	OD2	ASP	B	234	-18.325	5.672	-1.654	0.00	0.00	O
ATOM	1807	N	ILE	B	235	-17.369	2.232	-6.144	0.00	0.00	N
ATOM	1808	CA	ILE	B	235	-16.638	1.842	-7.338	0.00	0.00	C
ATOM	1809	C	ILE	B	235	-17.693	1.394	-8.338	0.00	0.00	C
ATOM	1810	O	ILE	B	235	-18.360	0.382	-8.053	0.00	0.00	O
ATOM	1811	CB	ILE	B	235	-15.629	0.683	-7.017	0.00	0.00	C
ATOM	1812	CG1	ILE	B	235	-14.430	1.118	-6.140	0.00	0.00	C
ATOM	1813	CG2	ILE	B	235	-15.100	-0.022	-8.307	0.00	0.00	C
ATOM	1814	CD1	ILE	B	235	-14.603	0.801	-4.649	0.00	0.00	C
ATOM	1815	N	VAL	B	236	-17.743	2.031	-9.492	0.00	0.00	N
ATOM	1816	CA	VAL	B	236	-18.702	1.761	-10.574	0.00	0.00	C
ATOM	1817	C	VAL	B	236	-17.859	1.308	-11.783	0.00	0.00	C
ATOM	1818	O	VAL	B	236	-16.698	1.706	-11.889	0.00	0.00	O
ATOM	1819	CB	VAL	B	236	-19.681	2.881	-11.007	0.00	0.00	C
ATOM	1820	CG1	VAL	B	236	-20.546	3.446	-9.887	0.00	0.00	C
ATOM	1821	CG2	VAL	B	236	-19.031	4.055	-11.717	0.00	0.00	C
ATOM	1822	N	LYS	B	237	-18.511	0.501	-12.600	0.00	0.00	N
ATOM	1823	CA	LYS	B	237	-17.805	0.001	-13.792	0.00	0.00	C
ATOM	1824	C	LYS	B	237	-18.517	0.677	-14.971	0.00	0.00	C
ATOM	1825	O	LYS	B	237	-19.730	0.677	-15.220	0.00	0.00	O
ATOM	1826	CB	LYS	B	237	-17.792	-1.492	-13.931	0.00	0.00	C
ATOM	1827	CG	LYS	B	237	-17.134	-2.025	-15.214	0.00	0.00	C
ATOM	1828	CD	LYS	B	237	-16.938	-3.532	-15.070	0.00	0.00	C
ATOM	1829	CE	LYS	B	237	-18.082	-4.341	-15.640	0.00	0.00	C
ATOM	1830	NZ	LYS	B	237	-19.396	-3.641	-15.491	0.00	0.00	N
ATOM	1831	N	ILE	B	238	-17.597	1.302	-15.722	0.00	0.00	N
ATOM	1832	CA	ILE	B	238	-17.959	2.076	-16.896	0.00	0.00	C
ATOM	1833	C	ILE	B	238	-17.331	1.515	-18.162	0.00	0.00	C
ATOM	1834	O	ILE	B	238	-16.158	1.770	-18.470	0.00	0.00	O
ATOM	1835	CB	ILE	B	238	-17.446	3.569	-16.709	0.00	0.00	C
ATOM	1836	CG1	ILE	B	238	-17.808	4.067	-15.290	0.00	0.00	C
ATOM	1837	CG2	ILE	B	238	-17.922	4.496	-17.868	0.00	0.00	C
ATOM	1838	CD1	ILE	B	238	-18.041	5.589	-15.169	0.00	0.00	C
ATOM	1839	N	GLU	B	239	-18.245	0.869	-18.877	0.00	0.00	N
ATOM	1840	CA	GLU	B	239	-17.868	0.264	-20.167	0.00	0.00	C
ATOM	1841	C	GLU	B	239	-17.818	1.283	-21.308	0.00	0.00	C
ATOM	1842	O	GLU	B	239	-18.341	2.404	-21.269	0.00	0.00	O
ATOM	1843	CB	GLU	B	239	-18.776	-0.891	-20.569	0.00	0.00	C
ATOM	1844	CG	GLU	B	239	-18.526	-2.189	-19.805	0.00	0.00	C
ATOM	1845	CD	GLU	B	239	-19.672	-2.829	-19.087	0.00	0.00	C
ATOM	1846	OE1	GLU	B	239	-20.866	-2.638	-19.268	0.00	0.00	O
ATOM	1847	OE2	GLU	B	239	-19.282	-3.648	-18.222	0.00	0.00	O
ATOM	1848	N	GLY	B	240	-17.102	0.785	-22.315	0.00	0.00	N
ATOM	1849	CA	GLY	B	240	-16.884	1.534	-23.553	0.00	0.00	C

Fig. 1 cont.

ATOM	1850	C	GLY B 240	-15.559	2.273	-23.662	0.00	0.00	C
ATOM	1851	O	GLY B 240	-15.087	2.914	-22.691	0.00	0.00	O
ATOM	1852	N	ILE B 241	-15.019	2.145	-24.892	0.00	0.00	N
ATOM	1853	CA	ILE B 241	-13.728	2.859	-25.123	0.00	0.00	C
ATOM	1854	C	ILE B 241	-14.168	4.308	-24.879	0.00	0.00	C
ATOM	1855	O	ILE B 241	-15.332	4.746	-24.949	0.00	0.00	O
ATOM	1856	CB	ILE B 241	-12.959	2.525	-26.432	0.00	0.00	C
ATOM	1857	CG1	ILE B 241	-12.125	1.221	-26.228	0.00	0.00	C
ATOM	1858	CG2	ILE B 241	-12.002	3.632	-26.961	0.00	0.00	C
ATOM	1859	CD1	ILE B 241	-12.538	0.007	-27.090	0.00	0.00	C
ATOM	1860	N	ASP B 242	-13.205	5.051	-24.404	0.00	0.00	N
ATOM	1861	CA	ASP B 242	-13.375	6.456	-24.062	0.00	0.00	C
ATOM	1862	C	ASP B 242	-14.727	6.799	-23.462	0.00	0.00	C
ATOM	1863	O	ASP B 242	-15.131	7.948	-23.760	0.00	0.00	O
ATOM	1864	CB	ASP B 242	-13.072	7.261	-25.347	0.00	0.00	C
ATOM	1865	CG	ASP B 242	-11.589	7.027	-25.659	0.00	0.00	C
ATOM	1866	OD1	ASP B 242	-11.233	6.448	-26.685	0.00	0.00	O
ATOM	1867	OD2	ASP B 242	-10.883	7.472	-24.731	0.00	0.00	O
ATOM	1868	N	ALA B 243	-15.372	5.978	-22.661	0.00	0.00	N
ATOM	1869	CA	ALA B 243	-16.643	6.398	-22.070	0.00	0.00	C
ATOM	1870	C	ALA B 243	-16.324	7.639	-21.221	0.00	0.00	C
ATOM	1871	O	ALA B 243	-15.232	7.952	-20.740	0.00	0.00	O
ATOM	1872	CB	ALA B 243	-17.309	5.317	-21.262	0.00	0.00	C
ATOM	1873	N	THR B 244	-17.394	8.374	-21.111	0.00	0.00	N
ATOM	1874	CA	THR B 244	-17.538	9.624	-20.355	0.00	0.00	C
ATOM	1875	C	THR B 244	-18.206	9.150	-19.063	0.00	0.00	C
ATOM	1876	O	THR B 244	-18.411	7.919	-19.048	0.00	0.00	O
ATOM	1877	CB	THR B 244	-18.359	10.747	-21.110	0.00	0.00	C
ATOM	1878	OG1	THR B 244	-19.725	10.259	-21.374	0.00	0.00	O
ATOM	1879	CG2	THR B 244	-17.702	11.247	-22.415	0.00	0.00	C
ATOM	1880	N	GLY B 245	-18.523	9.971	-18.089	0.00	0.00	N
ATOM	1881	CA	GLY B 245	-19.242	9.454	-16.937	0.00	0.00	C
ATOM	1882	C	GLY B 245	-18.637	9.048	-15.629	0.00	0.00	C
ATOM	1883	O	GLY B 245	-19.348	9.051	-14.590	0.00	0.00	O
ATOM	1884	N	GLY B 246	-17.379	8.668	-15.713	0.00	0.00	N
ATOM	1885	CA	GLY B 246	-16.573	8.286	-14.533	0.00	0.00	C
ATOM	1886	C	GLY B 246	-15.567	9.452	-14.511	0.00	0.00	C
ATOM	1887	O	GLY B 246	-16.005	10.593	-14.440	0.00	0.00	O
ATOM	1888	N	ASN B 247	-14.323	9.081	-14.545	0.00	0.00	N
ATOM	1889	CA	ASN B 247	-13.194	10.018	-14.544	0.00	0.00	C
ATOM	1890	C	ASN B 247	-13.422	11.012	-15.687	0.00	0.00	C
ATOM	1891	O	ASN B 247	-13.588	12.222	-15.428	0.00	0.00	O
ATOM	1892	CB	ASN B 247	-11.865	9.255	-14.606	0.00	0.00	C
ATOM	1893	CG	ASN B 247	-10.672	10.189	-14.436	0.00	0.00	C
ATOM	1894	OD1	ASN B 247	-10.469	10.604	-13.276	0.00	0.00	O
ATOM	1895	ND2	ASN B 247	-10.008	10.462	-15.558	0.00	0.00	N
ATOM	1896	N	ASN B 248	-13.437	10.499	-16.898	0.00	0.00	N
ATOM	1897	CA	ASN B 248	-13.649	11.246	-18.139	0.00	0.00	C
ATOM	1898	C	ASN B 248	-14.999	11.981	-18.169	0.00	0.00	C
ATOM	1899	O	ASN B 248	-16.145	11.612	-18.462	0.00	0.00	O
ATOM	1900	CB	ASN B 248	-13.480	10.318	-19.338	0.00	0.00	C
ATOM	1901	CG	ASN B 248	-13.055	11.031	-20.591	0.00	0.00	C
ATOM	1902	OD1	ASN B 248	-13.460	10.690	-21.701	0.00	0.00	O
ATOM	1903	ND2	ASN B 248	-12.188	12.030	-20.468	0.00	0.00	N
ATOM	1904	N	GLN B 249	-14.835	13.242	-17.790	0.00	0.00	N
ATOM	1905	CA	GLN B 249	-15.862	14.278	-17.703	0.00	0.00	C
ATOM	1906	C	GLN B 249	-15.148	15.627	-17.902	0.00	0.00	C
ATOM	1907	O	GLN B 249	-13.994	15.922	-17.505	0.00	0.00	O
ATOM	1908	CB	GLN B 249	-16.626	14.166	-16.406	0.00	0.00	C
ATOM	1909	CG	GLN B 249	-17.626	13.071	-16.091	0.00	0.00	C

Fig. 1 cont.

ATOM	1910	CD	GLN	B	249	-18.358	13.411	-14.792	0.00	0.00	C
ATOM	1911	OE1	GLN	B	249	-18.267	14.560	-14.329	0.00	0.00	O
ATOM	1912	NE2	GLN	B	249	-19.084	12.494	-14.155	0.00	0.00	N
ATOM	1913	N	PRO	B	250	-15.883	16.541	-18.529	0.00	0.00	N
ATOM	1914	CA	PRO	B	250	-15.469	17.938	-18.774	0.00	0.00	C
ATOM	1915	C	PRO	B	250	-15.913	18.653	-17.501	0.00	0.00	C
ATOM	1916	O	PRO	B	250	-16.894	19.398	-17.396	0.00	0.00	O
ATOM	1917	CB	PRO	B	250	-16.229	18.295	-20.025	0.00	0.00	C
ATOM	1918	CG	PRO	B	250	-17.582	17.680	-19.722	0.00	0.00	C
ATOM	1919	CD	PRO	B	250	-17.270	16.361	-19.023	0.00	0.00	C
ATOM	1920	N	ASN	B	251	-15.175	18.305	-16.484	0.00	0.00	N
ATOM	1921	CA	ASN	B	251	-15.266	18.634	-15.066	0.00	0.00	C
ATOM	1922	C	ASN	B	251	-14.023	19.428	-14.706	0.00	0.00	C
ATOM	1923	O	ASN	B	251	-13.163	19.660	-15.607	0.00	0.00	O
ATOM	1924	CB	ASN	B	251	-15.437	17.225	-14.465	0.00	0.00	C
ATOM	1925	CG	ASN	B	251	-15.390	17.037	-12.978	0.00	0.00	C
ATOM	1926	OD1	ASN	B	251	-16.319	16.482	-12.351	0.00	0.00	O
ATOM	1927	ND2	ASN	B	251	-14.317	17.486	-12.317	0.00	0.00	N
ATOM	1928	N	ILE	B	252	-13.903	19.852	-13.457	0.00	0.00	N
ATOM	1929	CA	ILE	B	252	-12.646	20.574	-13.117	0.00	0.00	C
ATOM	1930	C	ILE	B	252	-11.784	19.535	-12.417	0.00	0.00	C
ATOM	1931	O	ILE	B	252	-12.276	18.984	-11.427	0.00	0.00	O
ATOM	1932	CB	ILE	B	252	-12.929	21.912	-12.403	0.00	0.00	C
ATOM	1933	CG1	ILE	B	252	-12.667	23.017	-13.459	0.00	0.00	C
ATOM	1934	CG2	ILE	B	252	-12.114	22.025	-11.084	0.00	0.00	C
ATOM	1935	CD1	ILE	B	252	-12.703	22.656	-14.974	0.00	0.00	C
ATOM	1936	N	PRO	B	253	-10.631	19.306	-13.026	0.00	0.00	N
ATOM	1937	CA	PRO	B	253	-9.672	18.304	-12.547	0.00	0.00	C
ATOM	1938	C	PRO	B	253	-8.955	18.677	-11.255	0.00	0.00	C
ATOM	1939	O	PRO	B	253	-8.794	19.854	-10.885	0.00	0.00	O
ATOM	1940	CB	PRO	B	253	-8.709	18.107	-13.715	0.00	0.00	C
ATOM	1941	CG	PRO	B	253	-9.205	18.959	-14.848	0.00	0.00	C
ATOM	1942	CD	PRO	B	253	-10.136	19.992	-14.233	0.00	0.00	C
ATOM	1943	N	ASP	B	254	-8.513	17.615	-10.600	0.00	0.00	N
ATOM	1944	CA	ASP	B	254	-7.816	17.590	-9.322	0.00	0.00	C
ATOM	1945	C	ASP	B	254	-6.533	16.741	-9.319	0.00	0.00	C
ATOM	1946	O	ASP	B	254	-6.392	15.628	-9.854	0.00	0.00	O
ATOM	1947	CB	ASP	B	254	-8.786	17.071	-8.250	0.00	0.00	C
ATOM	1948	CG	ASP	B	254	-8.742	17.668	-6.866	0.00	0.00	C
ATOM	1949	OD1	ASP	B	254	-9.267	17.071	-5.896	0.00	0.00	O
ATOM	1950	OD2	ASP	B	254	-8.209	18.793	-6.688	0.00	0.00	O
ATOM	1951	N	ILE	B	255	-5.616	17.370	-8.579	0.00	0.00	N
ATOM	1952	CA	ILE	B	255	-4.288	16.732	-8.377	0.00	0.00	C
ATOM	1953	C	ILE	B	255	-4.169	15.903	-7.109	0.00	0.00	C
ATOM	1954	O	ILE	B	255	-3.779	14.719	-7.245	0.00	0.00	O
ATOM	1955	CB	ILE	B	255	-3.231	17.860	-8.653	0.00	0.00	C
ATOM	1956	CG1	ILE	B	255	-3.116	17.984	-10.194	0.00	0.00	C
ATOM	1957	CG2	ILE	B	255	-1.905	17.573	-7.923	0.00	0.00	C
ATOM	1958	CD1	ILE	B	255	-2.386	19.268	-10.675	0.00	0.00	C
ATOM	1959	N	PRO	B	256	-4.543	16.297	-5.908	0.00	0.00	N
ATOM	1960	CA	PRO	B	256	-4.481	15.474	-4.703	0.00	0.00	C
ATOM	1961	C	PRO	B	256	-5.470	14.320	-4.692	0.00	0.00	C
ATOM	1962	O	PRO	B	256	-5.573	13.510	-3.758	0.00	0.00	O
ATOM	1963	CB	PRO	B	256	-4.760	16.435	-3.545	0.00	0.00	C
ATOM	1964	CG	PRO	B	256	-5.650	17.460	-4.202	0.00	0.00	C
ATOM	1965	CD	PRO	B	256	-5.067	17.639	-5.606	0.00	0.00	C
ATOM	1966	N	ALA	B	257	-6.265	14.178	-5.720	0.00	0.00	N
ATOM	1967	CA	ALA	B	257	-7.225	13.109	-5.899	0.00	0.00	C
ATOM	1968	C	ALA	B	257	-6.401	11.992	-6.539	0.00	0.00	C
ATOM	1969	O	ALA	B	257	-6.770	10.820	-6.586	0.00	0.00	O

Fig. 1 cont.

ATOM	1970	CB	ALA	B	257	-8.351	13.362	-6.880	0.00	0.00	C
ATOM	1971	N	HIS	B	258	-5.287	12.420	-7.099	0.00	0.00	N
ATOM	1972	CA	HIS	B	258	-4.394	11.499	-7.806	0.00	0.00	C
ATOM	1973	C	HIS	B	258	-3.783	10.570	-6.764	0.00	0.00	C
ATOM	1974	O	HIS	B	258	-3.692	9.370	-7.081	0.00	0.00	O
ATOM	1975	CB	HIS	B	258	-3.314	12.205	-8.635	0.00	0.00	C
ATOM	1976	CG	HIS	B	258	-2.504	11.294	-9.495	0.00	0.00	C
ATOM	1977	ND1	HIS	B	258	-3.017	10.502	-10.487	0.00	0.00	N
ATOM	1978	CD2	HIS	B	258	-1.165	11.099	-9.507	0.00	0.00	C
ATOM	1979	CE1	HIS	B	258	-2.050	9.834	-11.072	0.00	0.00	C
ATOM	1980	NE2	HIS	B	258	-0.922	10.191	-10.505	0.00	0.00	N
ATOM	1981	N	LEU	B	259	-3.424	11.129	-5.621	0.00	0.00	N
ATOM	1982	CA	LEU	B	259	-2.774	10.396	-4.542	0.00	0.00	C
ATOM	1983	C	LEU	B	259	-3.693	9.688	-3.538	0.00	0.00	C
ATOM	1984	O	LEU	B	259	-3.175	9.257	-2.476	0.00	0.00	O
ATOM	1985	CB	LEU	B	259	-1.852	11.365	-3.789	0.00	0.00	C
ATOM	1986	CG	LEU	B	259	-0.731	12.171	-4.375	0.00	0.00	C
ATOM	1987	CD1	LEU	B	259	-0.678	12.273	-5.885	0.00	0.00	C
ATOM	1988	CD2	LEU	B	259	-0.985	13.545	-3.754	0.00	0.00	C
ATOM	1989	N	TRP	B	260	-4.967	9.587	-3.868	0.00	0.00	N
ATOM	1990	CA	TRP	B	260	-5.837	8.922	-2.890	0.00	0.00	C
ATOM	1991	C	TRP	B	260	-6.526	7.732	-3.538	0.00	0.00	C
ATOM	1992	O	TRP	B	260	-7.688	7.874	-3.914	0.00	0.00	O
ATOM	1993	CB	TRP	B	260	-6.856	9.840	-2.221	0.00	0.00	C
ATOM	1994	CG	TRP	B	260	-7.600	9.165	-1.110	0.00	0.00	C
ATOM	1995	CD1	TRP	B	260	-8.842	8.602	-1.170	0.00	0.00	C
ATOM	1996	CD2	TRP	B	260	-7.124	8.946	0.233	0.00	0.00	C
ATOM	1997	NE1	TRP	B	260	-9.184	8.088	0.052	0.00	0.00	N
ATOM	1998	CE2	TRP	B	260	-8.150	8.270	0.931	0.00	0.00	C
ATOM	1999	CE3	TRP	B	260	-5.954	9.251	0.904	0.00	0.00	C
ATOM	2000	CZ2	TRP	B	260	-8.034	7.897	2.262	0.00	0.00	C
ATOM	2001	CZ3	TRP	B	260	-5.852	8.904	2.228	0.00	0.00	C
ATOM	2002	CH2	TRP	B	260	-6.860	8.235	2.914	0.00	0.00	C
ATOM	2003	N	TYR	B	261	-5.784	6.642	-3.650	0.00	0.00	N
ATOM	2004	CA	TYR	B	261	-6.387	5.423	-4.240	0.00	0.00	C
ATOM	2005	C	TYR	B	261	-6.520	4.430	-3.115	0.00	0.00	C
ATOM	2006	O	TYR	B	261	-5.650	3.570	-2.974	0.00	0.00	O
ATOM	2007	CB	TYR	B	261	-5.570	4.925	-5.423	0.00	0.00	C
ATOM	2008	CG	TYR	B	261	-5.944	5.723	-6.660	0.00	0.00	C
ATOM	2009	CD1	TYR	B	261	-5.738	7.088	-6.803	0.00	0.00	C
ATOM	2010	CD2	TYR	B	261	-6.508	5.039	-7.727	0.00	0.00	C
ATOM	2011	CE1	TYR	B	261	-6.096	7.760	-7.952	0.00	0.00	C
ATOM	2012	CE2	TYR	B	261	-6.848	5.678	-8.916	0.00	0.00	C
ATOM	2013	CZ	TYR	B	261	-6.641	7.042	-9.018	0.00	0.00	C
ATOM	2014	OH	TYR	B	261	-7.012	7.624	-10.197	0.00	0.00	O
ATOM	2015	N	PHE	B	262	-7.584	4.513	-2.329	0.00	0.00	N
ATOM	2016	CA	PHE	B	262	-7.902	3.661	-1.186	0.00	0.00	C
ATOM	2017	C	PHE	B	262	-7.035	3.954	0.044	0.00	0.00	C
ATOM	2018	O	PHE	B	262	-7.107	3.226	1.039	0.00	0.00	O
ATOM	2019	CB	PHE	B	262	-7.683	2.169	-1.425	0.00	0.00	C
ATOM	2020	CG	PHE	B	262	-8.443	1.546	-2.528	0.00	0.00	C
ATOM	2021	CD1	PHE	B	262	-9.691	1.004	-2.278	0.00	0.00	C
ATOM	2022	CD2	PHE	B	262	-7.909	1.539	-3.816	0.00	0.00	C
ATOM	2023	CE1	PHE	B	262	-10.392	0.417	-3.319	0.00	0.00	C
ATOM	2024	CE2	PHE	B	262	-8.602	0.973	-4.887	0.00	0.00	C
ATOM	2025	CZ	PHE	B	262	-9.866	0.402	-4.620	0.00	0.00	C
ATOM	2026	N	GLY	B	263	-6.185	4.928	-0.053	0.00	0.00	N
ATOM	2027	CA	GLY	B	263	-5.229	5.338	0.958	0.00	0.00	C
ATOM	2028	C	GLY	B	263	-4.110	6.058	0.187	0.00	0.00	C
ATOM	2029	O	GLY	B	263	-4.221	6.225	-1.039	0.00	0.00	O

Fig. 1 cont.

ATOM	2030	N	LEU B 264	-3.092	6.451	0.939	0.00	0.00	N
ATOM	2031	CA	LEU B 264	-1.985	7.204	0.352	0.00	0.00	C
ATOM	2032	C	LEU B 264	-1.342	6.460	-0.792	0.00	0.00	C
ATOM	2033	O	LEU B 264	-1.273	5.247	-0.630	0.00	0.00	O
ATOM	2034	CB	LEU B 264	-0.934	7.477	1.411	0.00	0.00	C
ATOM	2035	CG	LEU B 264	-0.966	8.775	2.206	0.00	0.00	C
ATOM	2036	CD1	LEU B 264	-1.261	9.979	1.319	0.00	0.00	C
ATOM	2037	CD2	LEU B 264	-2.023	8.602	3.281	0.00	0.00	C
ATOM	2038	N	ILE B 265	-0.936	7.170	-1.803	0.00	0.00	N
ATOM	2039	CA	ILE B 265	-0.202	6.480	-2.895	0.00	0.00	C
ATOM	2040	C	ILE B 265	0.579	7.595	-3.587	0.00	0.00	C
ATOM	2041	O	ILE B 265	0.105	8.722	-3.736	0.00	0.00	O
ATOM	2042	CB	ILE B 265	-1.062	5.487	-3.700	0.00	0.00	C
ATOM	2043	CG1	ILE B 265	-0.088	4.986	-4.811	0.00	0.00	C
ATOM	2044	CG2	ILE B 265	-2.420	5.985	-4.260	0.00	0.00	C
ATOM	2045	CD1	ILE B 265	-0.434	3.570	-5.345	0.00	0.00	C
ATOM	2046	N	GLY B 266	1.836	7.293	-3.832	0.00	0.00	N
ATOM	2047	CA	GLY B 266	2.826	8.160	-4.451	0.00	0.00	C
ATOM	2048	C	GLY B 266	3.602	9.005	-3.468	0.00	0.00	C
ATOM	2049	O	GLY B 266	4.648	9.622	-3.715	0.00	0.00	O
ATOM	2050	N	THR B 267	3.113	9.067	-2.266	0.00	0.00	N
ATOM	2051	CA	THR B 267	3.565	9.781	-1.059	0.00	0.00	C
ATOM	2052	C	THR B 267	3.996	8.770	-0.004	0.00	0.00	C
ATOM	2053	O	THR B 267	3.253	8.529	0.963	0.00	0.00	O
ATOM	2054	CB	THR B 267	2.382	10.764	-0.687	0.00	0.00	C
ATOM	2055	OG1	THR B 267	2.224	10.884	0.747	0.00	0.00	O
ATOM	2056	CG2	THR B 267	0.998	10.348	-1.229	0.00	0.00	C
ATOM	2057	N	CYS B 268	5.109	8.084	-0.185	0.00	0.00	N
ATOM	2058	CA	CYS B 268	5.790	7.089	0.637	0.00	0.00	C
ATOM	2059	C	CYS B 268	7.300	7.370	0.255	0.00	0.00	C
ATOM	2060	O	CYS B 268	7.950	6.987	-0.703	0.00	0.00	O
ATOM	2061	CB	CYS B 268	5.730	5.554	0.663	0.00	0.00	C
ATOM	2062	SG	CYS B 268	7.097	4.714	1.604	0.00	0.00	S
ATOM	2063	N	LEU B 269	7.772	8.096	1.199	0.00	0.00	N
ATOM	2064	CA	LEU B 269	8.856	8.817	1.767	0.00	0.00	C
ATOM	2065	CB	LEU B 269	8.717	8.576	3.317	0.00	0.00	C
ATOM	2066	CG	LEU B 269	7.378	8.954	3.971	0.00	0.00	C
ATOM	2067	CD1	LEU B 269	6.584	7.774	4.558	0.00	0.00	C
ATOM	2068	CD2	LEU B 269	7.608	9.965	5.108	0.00	0.00	C
ATOM	2069	C	LEU B 269	10.275	8.611	1.206	0.00	0.00	C
ATOM	2070	OT	LEU B 269	10.582	7.650	0.464	0.00	0.00	O
ATOM	2071	OE	LEU B 269	11.013	9.581	1.572	0.00	0.00	O
ATOM	2072	N	LIP1 1	4.155	13.598	-1.915	0.00	0.00	N
ATOM	2073	C	LIP1 1	2.861	13.926	-1.250	0.00	0.00	C
ATOM	2074	C1	LIP1 1	4.774	14.860	-2.425	0.00	0.00	C
ATOM	2075	C2	LIP1 1	5.074	13.010	-0.886	0.00	0.00	C
ATOM	2076	C3	LIP1 1	3.966	12.591	-3.013	0.00	0.00	C
ATOM	2077	C4	LIP1 1	5.223	12.036	-3.755	0.00	0.00	C
ATOM	2078	P7	LIP1 1	6.100	11.437	-6.259	0.00	0.00	P
ATOM	2079	O	LIP1 1	7.395	12.033	-5.825	0.00	0.00	O
ATOM	2080	O1	LIP1 1	6.313	9.888	-6.596	0.00	0.00	O
ATOM	2081	O2	LIP1 1	5.692	12.177	-7.616	0.00	0.00	O
ATOM	2082	O3	LIP1 1	4.994	11.629	-5.114	0.00	0.00	O
ATOM	2083	C5	LIP1 1	4.465	12.841	-7.934	0.00	0.00	C
ATOM	2084	C6	LIP1 1	3.338	11.836	-8.307	0.00	0.00	C
ATOM	2085	O4	LIP1 1	3.696	11.455	-9.654	0.00	0.00	O
ATOM	2086	C7	LIP1 1	2.798	10.866	-10.467	0.00	0.00	C
ATOM	2087	O5	LIP1 1	1.642	10.851	-10.076	0.00	0.00	O
ATOM	2088	C8	LIP1 1	3.101	10.251	-11.822	0.00	0.00	C
ATOM	2089	C9	LIP1 1	1.969	12.593	-8.232	0.00	0.00	C

Fig. 1 cont.

[illegible]