ATOMIC COORDINATES FOR SUBTILISIN BPN' (OR NOVO)

Richard A. Alden, Jens J. Birktoft, Joseph Kraut,
Jon D. Robertus and Christine S. Wright*

Department of Chemistry, University of California, San Diego
La Jolla, California 92037

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Summary: Atomic coordinates and backbone torsion angles are tabulated for the active form of subtilisin BPN' (or Novo). Coordinates are also given for well defined solvent molecules inside the structure and in the neighborhood of the catalytic site.

The three dimensional structure of phenylmethanesulfonyl subtilisin BPN' (PMS•BPN') at 2.5 Å resolution has been described in previous publications (1,2). We have now reinterpreted the electron-density map, rebuilt the model, determined the structure of the active enzyme, and located 150 solvent molecules. In order to enable other investigators to construct their own models, we present here a list of Cartesian coordinates for all the atoms in active subtilisin BPN', or subtilisin Novo which is an identical enzyme from a different commercial source (3,4). Backbone torsion angles ϕ and ψ are also given, as well as coordinates for selected solvent molecules.

To facilitate a more careful and detailed interpretation the original 2.5 Å electron-density map of PMS•BPN' was recalculated on a grid of a/64, b/80 and c/60, contoured at 0.1, 0.2, 0.4, 0.6...e/Å^3 and sections of constant y were plotted on a scale of 2 cm = 1 Å. A new model of PMS•BPN' was then constructed with the aid of an optical comparitor (5). The new model is almost identical to the original one described earlier by Wright et al. (1). The backbone and most of the side chains were not significantly altered. A few side chains which did require adjustment were all far from the catalytic site and conclusions previously reached (1,2) remain valid.

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*present address: Medical Research Council Laboratory of Molecular Biology Hills Road, Cambridge, England.

The structure of the active enzyme (ACT•BPN') was arrived at by examination of a difference electron-density map calculated with coefficients [F(PMS•BPN')-F(ACT•BPN')] and the original isomorphous replacement phases for PMS•BPN'. The active enzyme structure was further confirmed with the aid of a second map calculated with the same phases but with coefficients [2F(ACT•BPN')-F(PMS•BPN')], which approximates the electron density of the active enzyme itself.

Coordinates for the active subtilisin molecule were measured directly on the model and checked for gross errors by calculating bond lengths and angles. Coordinates were also recorded for 150 clearly defined solvent molecules, of which three are unambiguously inside the protein molecule. All coordinates except those for 26 atoms whose locations remained relatively uncertain were then used to compute structure factors to 2 Å (intensities to 2 Å having meanwhile been measured on ACT•BPN'), resulting in a conventional R-factor of 44%. The new calculated phases were used in turn to compute F_o-F_c and $2F_o-F_c$ maps which now permitted placement of the uncertain atoms and confirmation or correction of solvent molecule locations. As examination of these maps progressed, it became evident, as expected, that many coordinates required slight revision. However these corrections are estimated as 2 Å or less, most of them less than 1 Å.

In Table 1 are listed the atomic coordinates for active subtilisin BPN' and 17 solvent molecules (assumed to be water) which are located either in the neighborhood of the catalytic site or in the interior of the protein molecule. These coordinates were obtained directly from the model, with the exception of residues 11-26, 232-253, and 268-275, where the coordinates listed are the output of a refinement by Diamond's model building program (6). For convenient model building the coordinates are given in Ångstrom units in a Cartesian system. Monoclinic crystallographic fractional coordinates can be obtained by the following transformation.

Table I

ALA	1	N	35.7	6.8	12.9
	1	CA	36.3	6.7	14.1
	1	CB	37.9	6.8	13.8
	1	C	36.0	8.1	14.9
	1	O	34.9	8.3	15.3
GLN	2	N	37.1	8.9	14.9
	2	CA	37.0	10.1	15.7
	2	CB	38.1	10.4	16.8
	2	CG	38.2	11.9	17.0
	2	CD	39.0	12.4	18.1
	2	OE1*	40.3	12.0	18.1
	2	NE2	38.5	13.1	19.0
	2	C	37.2	11.3	14.6
	2	O	38.0	11.2	13.7
SER	3	N	36.3	12.3	14.8
	3	CA	36.3	13.4	13.9
	3	CB	35.0	13.4	13.1
	3	OG	35.0	12.1	12.4
	3	C	36.3	14.9	14.4
	3	O	35.7	15.2	15.3
VAL	4	N	37.2	15.7	13.9
	4	CA	37.3	17.1	14.1
	4	CB	38.9	17.5	13.9
	4	CG1	39.1	19.0	14.1
	4	CG2	39.7	16.7	14.9
	4	C	36.3	17.9	13.3
	4	O	36.4	18.0	12.0
PRO	5	N	35.5	18.4	14.0
	5	CA	34.4	19.3	13.7
	5	CB	33.7	19.6	15.0
	5	CG	34.0	18.6	16.0
	5	CD	35.3	18.0	15.4
	5	C	35.0	20.6	13.1
	5	O	36.0	21.3	13.6
TYR	6	N	34.4	21.0	11.9
	6	CA	34.8	22.1	11.1
	6	CB	33.9	22.2	10.0
	6	CG	32.8	23.3	10.2
	6	CD1	33.0	24.7	10.2
	6	CE1	32.0	25.5	10.5
	6	CZ	30.6	25.0	10.7
	6	OH	29.7	26.0	10.9
	6	CE2	30.3	23.7	10.4
	6	CD2	31.3	22.9	10.3
	6	C	35.0	23.4	11.9
	6	O	36.1	24.0	11.9
GLY	7	N	34.1	23.7	12.9
	7	CA	34.2	25.0	13.6
	7	C	35.5	24.9	14.7
	7	O	35.9	26.0	14.9
VAL	8	N	35.8	23.7	15.1
	8	CA	36.8	23.7	16.1
	8	CB	36.9	22.2	16.6
	8	CG1	38.0	22.1	17.8
	8	CG2	35.6	21.9	17.4
	8	C	38.2	24.2	15.6
	8	O	38.7	25.1	16.1
SER	9	N	38.6	23.7	14.4
	9	CA	39.9	24.1	13.8
	9	CB	40.2	23.3	12.6
	9	OG *	41.5	23.7	12.0
	9	C	39.8	25.7	13.4
	9	O	40.7	26.4	13.6
GLN	10	N	38.5	26.0	12.9
	10	CA	38.3	27.3	12.4
	10	CB	36.8	27.2	11.9
	10	CG *	36.3	28.7	11.4
	10	CD *	34.8	28.5	10.9
	10	OE1*	34.3	27.4	10.6
	10	NE2*	34.2	29.8	10.9
	10	C	38.4	28.6	13.3
	10	O	38.8	29.6	12.7
ILE	11	N	38.5	28.2	14.5
	11	CD1	37.2	28.2	18.9
	11	CG1	37.9	28.1	17.6
	11	CB	37.8	29.3	16.6
	11	CG2	36.5	29.5	15.8
	11	CA *	38.8	29.3	15.4
	11	C *	40.3	29.0	15.9
	11	O *	41.2	29.9	16.2
LYS	12	N	40.5	27.7	16.1
	12	CA	41.9	27.3	16.6
	12	CB	43.0	28.3	16.2
	12	CG	43.3	28.3	14.7
	12	CD	44.1	29.6	14.3
	12	CE	43.1	30.8	14.1
	12	NZ *	42.8	31.4	15.4
	12	C	42.1	27.0	18.1
	12	O	43.1	27.6	18.8
ALA	13	N	41.2	26.3	18.7
	13	CA	41.5	25.6	20.0
	13	CB	40.3	24.9	20.5
	13	C	42.7	24.6	20.0
	13	O	43.4	24.3	21.0
PRO	14	N	42.8	24.0	18.8
	14	CA	43.8	22.9	18.6
	14	CB	43.3	22.1	17.5
	14	CG	42.2	22.9	16.8
	14	CD	41.7	23.9	17.8
	14	C	45.3	23.5	18.5
	14	O	46.3	22.8	18.6
ALA	15	N	45.3	24.9	18.3
	15	CA	46.6	25.6	18.5
	15	CB	46.3	27.1	18.1
	15	C	46.9	25.5	20.0
	15	O	48.1	25.3	20.4
LEU	16	N	45.9	25.8	20.8
	16	CA	46.1	25.7	22.3
	16	CB	45.0	26.6	23.0
	16	CG	45.2	28.1	23.0
	16	CD1*	45.1	28.6	21.6
	16	CD2*	44.1	28.7	23.9
	16	C *	46.2	24.3	22.8
	16	O *	46.8	23.9	23.9
HIS	17	N	45.5	23.4	22.0
	17	CA	45.4	22.0	22.4
	17	CB *	44.4	21.3	21.5
	17	CG	42.9	21.6	21.9
	17	ND1	41.9	21.2	21.1
	17	CE1	40.7	21.6	21.6
	17	NE2	40.9	22.2	22.8
	17	CD2	42.3	22.3	23.0
	17	C	46.8	21.3	22.3
	17	O	47.4	20.6	23.3
SER	18	N	47.5	21.5	21.1
	18	CA	48.8	20.9	20.9
	18	CB	49.0	20.9	19.4
	18	OG	49.4	22.2	18.8
	18	C	49.9	21.8	21.6
	18	O	51.2	21.5	21.5
GLN	19	N	49.5	22.7	22.4
	19	CA	50.4	23.6	23.1
	19	CB	49.9	25.0	23.0
	19	CG	50.7	26.0	23.8
	19	CD	50.9	27.4	23.1
	19	OE1	50.9	27.4	21.8
	19	NE2	51.1	28.5	23.8
	19	C	50.4	22.9	24.5
	19	O	51.3	23.1	25.5
GLY	20	N	49.3	22.0	24.7
	20	CA	49.2	21.3	26.0
	20	C	48.0	21.7	26.9
	20	O	47.5	20.9	27.8
TYR	21	N	47.5	22.9	26.6
	21	CA	46.3	23.4	27.4
	21	CB	46.4	24.9	27.5
	21	CG	48.0	25.3	27.6
	21	CD1	48.6	25.2	28.8
	21	CE1	50.0	25.6	28.9
	21	CZ	50.7	26.1	27.8
	21	OH	52.0	26.5	27.9
	21	CE2	50.0	26.2	26.6
	21	CD2	48.6	25.8	26.5
	21	C	44.9	23.0	26.8
	21	O	44.5	23.3	25.6
THR	22	N	44.1	22.3	27.7
	22	CA	42.8	21.9	27.3
	22	CB	42.9	20.3	27.1
	22	OG1	43.4	19.8	28.4
	22	CG2	43.8	20.0	25.9
	22	C	41.7	22.3	28.4
	22	O	40.4	22.1	28.3
GLY	23	N	42.2	23.0	29.4
	23	CA	41.3	23.5	30.5
	23	C	41.0	22.4	31.6
	23	O	39.9	22.1	32.1
SER	24	N	42.1	21.7	31.9
	24	CA	42.0	20.5	32.9
	24	CB	43.4	20.0	33.2
	24	OG	44.2	19.6	32.0
	24	C	41.3	21.0	34.2
	24	O	40.2	20.5	34.7
ASN	25	N	41.9	22.0	34.8
	25	CA	41.4	22.5	36.1
	25	CB *	42.6	23.1	37.0
	25	CG	43.3	21.9	37.7
	25	OD1	43.9	21.0	37.1
	25	ND2	43.4	22.0	39.1
	25	C	40.3	23.7	36.0
	25	O	40.0	24.5	36.9
VAL	26	N	39.7	23.7	34.8
	26	CA	38.6	24.7	34.5
	26	CB	38.9	25.3	33.1
	26	CG1	37.7	26.1	32.5
	26	CG2	40.3	25.9	33.0
	26	C	37.2	24.1	34.6
	26	O	36.9	22.8	34.3
LYS	27	N	36.3	25.2	35.3
	27	CA	35.0	24.6	35.1
	27	CB	34.4	24.3	36.4
	27	CG	35.7	23.5	37.2
	27	CD *	35.2	23.3	38.7
	27	CE *	36.3	22.6	39.5
	27	NZ *	35.8	22.3	40.8
	27	C	34.0	25.5	34.3
	27	O	33.9	26.8	34.5
VAL	28	N	33.3	24.9	33.3
	28	CA	32.3	25.5	32.5
	28	CB	32.8	25.3	31.0
	28	CG1	32.0	26.1	30.0
	28	CG2	34.3	25.4	31.0
	28	C	31.0	25.0	33.0
	28	O	30.9	23.7	33.0
ALA	29	N	30.0	25.6	33.3
	29	CA	28.7	25.1	33.7
	29	CB	28.0	25.9	34.8
	29	C	27.9	25.2	32.3
	29	O	27.7	26.3	31.9
VAL	30	N	27.3	24.1	32.0
	30	CA	26.5	24.1	30.9
	30	CB	26.6	22.9	30.0
	30	CG1	25.6	22.9	28.9
	30	CG2	28.0	22.8	29.4
	30	C	25.0	24.3	31.3
	30	O	24.4	23.3	31.8
ILE	31	N	24.5	25.6	31.1
	31	CA	23.2	26.0	31.6
	31	CB	23.1	27.3	32.2
	31	CG1	24.1	27.3	33.4
	31	CD1	24.0	28.8	34.0
	31	CG2	21.6	27.6	32.8
	31	C	22.1	25.8	30.4
	31	O	22.0	26.6	29.5
ASP	32	N	21.6	24.5	30.5
	32	CA	20.7	24.1	29.5
	32	CB	21.4	23.5	28.4
	32	CG	20.9	23.6	26.9
	32	OD1	21.0	24.7	26.4
	32	OD2	20.3	22.8	26.4
	32	C	19.7	23.1	30.1
	32	O	19.0	23.4	31.1
SER	33	N	19.5	22.0	29.5
	33	CA *	18.4	21.1	29.9
	33	CB	17.4	21.0	29.9
	33	OG	18.0	20.7	27.6
	33	C	18.9	19.7	30.3
	33	O	18.1	19.0	30.9
GLY	34	N	20.3	19.4	30.3
	34	CA	20.8	18.1	30.5
	34	C	22.0	17.9	29.9
	34	O	22.7	18.6	29.3
ILE	35	N	22.3	16.5	30.0
	35	CA	23.8	16.0	29.7
	35	CB	25.0	16.7	30.3
	35	CG1	24.8	18.3	30.2
	35	CD1	26.0	19.0	30.7
	35	CG2	26.2	16.2	29.7
	35	C	23.8	14.4	30.1
	35	O	23.8	14.1	31.2
ASP	36	N	23.8	13.7	29.0
	36	CA	23.7	12.1	29.3
	36	CB	23.2	11.6	28.0
	36	CG	23.1	10.0	28.3
	36	OD1	23.1	9.6	29.4
	36	OD2	23.0	9.3	27.3
	36	C	25.1	11.8	29.7
	36	O	26.1	12.0	29.0
SER	37	N	25.1	11.1	31.0
	37	CA	26.4	10.8	31.5
	37	CB	26.1	10.5	33.0
	37	OG	25.5	11.6	33.5
	37	C	27.0	9.4	31.0
	37	O	28.2	9.1	31.0
SER	38	N	26.1	8.6	30.3
	38	CA	26.5	7.3	29.8
	38	CB	25.3	6.3	29.8
	38	OG	24.3	6.7	29.0
	38	C	26.9	7.8	28.2
	38	O	27.1	6.8	27.4
HIS	39	N	27.0	9.0	27.9
	39	CA	27.5	9.3	26.5
	39	CB	27.3	10.8	26.0
	39	CG	27.5	10.8	24.5
	39	ND1	28.5	10.0	23.9
	39	CE1	28.1	10.0	22.5
	39	NE2	27.0	10.6	22.4
	39	CD2	26.5	11.1	23.6
	39	C	29.1	9.1	26.4
	39	O	30.0	9.9	27.0
PRO	40	N	29.4	8.1	25.6
	40	CA	30.9	7.7	25.4
	40	CB	30.8	6.4	24.5
	40	CG	29.2	6.0	24.5
	40	CD	28.4	7.3	24.9
	40	C	31.9	8.8	25.0
	40	O	33.0	8.6	25.5
ASP	41	N	31.4	9.9	24.5
	41	CA	32.2	11.0	24.4
	41	CB	32.3	11.7	23.0
	41	CG	32.9	10.8	22.0
	41	OD1*	33.8	9.9	22.4
	41	OD2*	32.5	10.8	20.9
	41	C	32.2	12.0	25.6
	41	O	33.0	13.0	25.5
LEU	42	N	31.3	11.9	26.6
	42	CA	31.3	12.9	27.6
	42	CB	29.8	13.4	27.8
	42	CG	29.4	14.1	26.4
	42	CD1	27.9	14.4	26.4
	42	CD2	30.1	15.4	26.1
	42	C	31.8	12.4	29.0
	42	O	31.5	11.2	29.3
LYS	43	N	32.5	13.2	29.7
	43	CA	32.9	13.1	31.1
	43	CB	34.5	12.9	31.3
	43	CG	34.8	12.9	32.8
	43	CD *	34.9	11.6	33.5
	43	CE	35.3	11.8	35.0
	43	NZ	35.3	10.4	35.8
	43	C	32.3	14.3	31.7
	43	O	32.8	15.4	31.4
VAL	44	N	31.3	14.1	32.5
	44	CA	30.7	15.1	33.3
	44	CB	29.1	14.9	33.3
	44	CG1	28.5	15.9	34.2
	44	CG2	28.5	15.0	31.9
	44	C	31.1	15.0	34.7
	44	O	31.6	13.9	35.2
ALA	45	N	31.3	16.1	35.2
	45	CA	32.0	16.2	36.5
	45	CB	33.0	17.4	36.5
	45	C	31.0	16.3	37.5
	45	O	31.1	15.7	38.6
GLY	46	N	29.9	17.0	37.3
	46	CA	28.8	17.0	38.2
	46	C	27.7	18.0	37.9
	46	O	27.6	18.4	36.7
GLY	47	N	27.0	18.6	38.8
	47	CA	26.0	19.7	38.5
	47	C	24.9	19.9	39.4
	47	O	25.0	20.0	40.7
ALA	48	N	23.7	19.9	38.9
	48	CA	22.4	19.9	39.7
	48	CB	22.4	20.8	41.0
	48	C	21.2	20.3	38.8
	48	O	21.4	21.0	37.8
SER	49	N	20.1	20.0	39.3
	49	CA	19.0	20.6	38.6
	49	CB	17.9	19.5	38.5
	49	OG	17.0	19.7	37.5
	49	C	18.3	21.8	39.3
	49	O	18.1	21.8	40.7
MET	50	N	18.0	22.8	38.7
	50	CA	17.0	23.8	39.1
	50	CB *	17.8	25.1	38.8
	50	CG *	19.1	25.1	39.2
	50	SD	19.1	24.9	41.0
	50	CE *	20.2	23.4	41.2
	50	C	15.6	23.8	38.6
	50	O	14.9	24.7	38.8
VAL	51	N	15.3	22.5	38.1
	51	CA	14.0	22.3	37.7
	51	CB	14.0	21.8	36.3
	51	CG1	12.6	21.4	35.8
	51	CG2	14.8	22.6	35.3
	51	C	13.3	21.4	38.7
	51	O	13.4	20.1	38.6
PRO	52	N	12.3	22.0	39.4
	52	CA	11.5	21.3	40.3
	52	CB	10.2	22.2	40.3
	52	CG	10.7	23.7	39.8
	52	CD	12.1	23.5	39.3
	52	C	11.1	19.9	40.0
	52	O	11.3	19.0	41.0
SER	53	N	10.7	19.6	38.9
	53	CA	9.9	18.2	38.7
	53	CB	8.9	18.5	37.7
	53	OG	9.4	18.9	36.3
	53	C	10.9	17.1	38.1
	53	O	10.6	16.0	38.0
GLU	54	N	12.1	17.5	37.8
	54	CA	13.1	16.7	37.0
	54	CB	13.4	17.2	35.7
	54	CG	12.3	17.1	34.7
	54	CD	12.6	15.9	33.9
	54	OE1*	12.2	14.8	34.3
	54	OE2	12.9	15.9	32.6
	54	C	14.2	16.4	38.0
	54	O	15.2	17.1	37.9
THR	55	N	14.2	15.3	38.8
	55	CA	15.2	14.9	39.7
	55	CB	15.1	13.7	40.3
	55	OG1	14.3	13.6	41.4
	55	CG2	16.6	13.3	40.9
	55	C	16.6	15.1	38.9
	55	O	17.3	15.9	39.0
PRO	56	N	16.9	13.9	38.2
	56	CA	18.2	13.9	37.5
	56	CB	18.1	12.6	36.6
	56	CG	16.8	11.9	36.9
	56	CD	16.1	12.6	38.0
	56	C	18.4	15.1	36.7
	56	O	17.9	15.3	35.7
ASN	57	N	19.8	15.6	37.0
	57	CA	20.3	16.6	36.3
	57	CB	21.4	17.0	37.2
	57	CG *	22.1	18.2	36.8
	57	OD1*	21.7	19.0	36.0
	57	ND2*	23.7	18.3	37.0
	57	C	21.0	15.9	35.0
	57	O	21.5	16.6	34.0
PHE	58	N	21.0	14.5	35.0
	58	CA	21.7	13.9	34.0
	58	CB	22.4	12.6	34.8
	58	CG	23.4	13.1	35.8
	58	CD1	24.3	14.1	35.7
	58	CE1	25.0	14.6	36.8
	58	CZ	24.9	14.0	38.0
	58	CE2	24.0	12.9	38.2
	58	CD2	23.2	12.6	37.1
	58	C	20.8	13.1	33.0
	58	O	20.9	11.9	32.7
GLN	59	N	19.7	13.9	32.8
	59	CA	18.5	13.4	32.0
	59	CB	17.4	12.9	33.0
	59	CG *	17.9	11.9	34.0
	59	CD *	18.0	10.6	33.3
	59	OE1*	17.8	10.4	32.0
	59	NE2*	18.2	9.6	34.0
	59	C	18.1	14.4	31.0
	59	O	17.4	15.4	31.3
ASP	60	N	18.5	14.3	29.8
	60	CA	18.2	15.2	28.9
	60	CB	19.7	15.6	28.1
	60	CG	19.4	16.5	26.9
	60	OD1	18.3	16.6	26.3
	60	OD2	20.4	17.1	26.4
	60	C	17.3	14.6	27.7
	60	O	17.5	13.6	27.0
ASP	61	N	16.0	15.2	27.7
	61	CA	14.9	14.8	26.9
	61	CB	13.8	14.9	27.8
	61	CG	13.8	13.9	28.9
	61	OD1	13.9	12.6	28.5
	61	OD2	13.8	14.1	30.0
	61	C	15.0	15.7	25.6
	61	O	14.9	15.2	24.5
ASN	62	N	15.2	17.0	25.9
	62	CA	15.4	18.0	24.9
	62	CB	15.4	19.4	25.5

Table I (continued)

	62	CG *	13.9	19.9	25.8
	62	OD1	13.3	19.0	26.5
	62	ND2	13.6	20.7	25.0
	62	C	16.6	18.1	23.9
	62	O	16.5	18.4	22.8
SER	63	N	17.7	17.3	24.3
	63	CA	18.8	16.9	23.5
	63	CB	18.0	16.1	22.4
	63	OG	19.0	15.7	21.4
	63	C	19.8	18.0	23.3
	63	O	20.9	17.8	22.8
HIS	64	N	19.4	19.3	23.7
	64	CA	20.3	20.3	23.4
	64	CB	19.4	21.6	23.6
	64	CG	19.8	23.0	23.1
	64	ND1	20.1	24.0	23.8
	64	CE1	20.2	25.0	23.0
	64	NE2	20.0	24.6	21.8
	64	CD2	19.5	23.3	21.9
	64	C	21.4	20.4	24.3
	64	O	22.6	20.9	24.0
GLY	65	N	21.2	20.0	25.5
	65	CA	22.1	20.0	26.8
	65	C	23.4	19.4	26.0
	65	O	24.4	19.9	25.9
THR	66	N	23.2	18.1	25.9
	66	CA	24.3	17.1	25.4
	66	CB	23.6	15.8	25.2
	66	OG1	23.3	15.4	26.4
	66	CG2	24.8	14.9	24.8
	66	C	24.9	17.8	24.1
	66	O	26.1	17.9	24.0
HIS	67	N	24.0	18.1	23.1
	67	CA	24.5	18.8	21.9
	67	CB	23.3	19.4	21.1
	67	CG	23.7	19.7	19.8
	67	ND1	24.5	20.9	19.4
	67	CE1	24.8	20.8	18.0
	67	NE2	24.3	19.5	17.6
	67	CD2	23.8	18.9	18.6
	67	C	25.5	19.9	22.2
	67	O	26.6	19.8	21.7
VAL	68	N	25.1	20.8	23.0
	68	CA	26.0	21.9	23.4
	68	CB	25.1	22.8	24.3
	68	CG1*	26.1	24.0	24.6
	68	CG2	23.9	23.4	23.5
	68	C	27.2	21.3	24.1
	68	O	28.4	21.5	23.6
ALA	69	N	27.1	20.7	25.2
	69	CA	28.2	20.1	26.0
	69	CB	27.8	19.3	27.2
	69	C	29.2	19.3	25.1
	69	O	30.2	18.6	25.6
GLY	70	N	29.1	19.4	23.8
	70	CA	30.0	18.7	22.9
	70	C	30.9	19.6	22.0
	70	O	32.0	19.1	21.8
THR	71	N	30.4	20.9	21.8
	71	CA	31.5	21.7	21.1
	71	CB	30.7	22.9	20.4
	71	OG1	30.0	22.4	19.5
	71	CG2	31.9	23.8	19.8
	71	C	32.3	22.0	22.3
	71	O	33.7	22.1	22.1
VAL	72	N	31.9	22.3	23.5
	72	CA	32.6	22.5	24.6
	72	CB	31.8	22.9	25.9
	72	CG1	32.7	23.5	27.0
	72	CG2	30.8	24.0	25.4
	72	C	33.7	21.3	24.9
	72	O	34.8	21.6	24.9
ALA	73	N	33.2	20.1	25.0
	73	CA	34.1	19.0	25.3
	73	CB	34.5	19.1	26.8
	73	C	33.8	17.5	25.1
	73	O	34.0	16.8	26.0
ALA	74	N	33.5	17.1	23.9
	74	CA	33.5	15.6	23.5
	74	CB	33.3	15.9	22.0
	74	C	34.8	14.9	23.6
	74	O	35.8	15.4	23.0
LEU	75	N	34.8	13.6	24.0
	75	CA	36.0	12.7	24.0
	75	CB	36.3	12.1	22.7
	75	CG	35.0	11.7	21.9
	75	CD1	34.0	12.9	21.9
	75	CD2	35.5	11.3	20.5
	75	C	37.3	13.3	24.0
	75	O	37.6	14.6	24.1
ASN	76	N	38.2	12.4	23.9
	76	CA	39.8	12.4	23.7
	76	CB *	40.5	13.3	24.6
	76	CG *	41.7	15.2	23.4
	76	OD1*	42.1	28.7	21.9
	76	ND2*	43.4	15.3	23.2
	76	C	40.2	10.9	23.6
	76	O	40.7	10.4	24.4
ASN	77	N	39.9	10.4	22.3
	77	CA	40.2	8.9	22.1
	77	CB	39.0	8.1	23.0
	77	CG	37.9	8.9	23.5
	77	OD1	37.8	9.1	24.8
	77	ND2	37.0	9.1	22.8
	77	C	39.9	8.6	20.7
	77	O	40.4	9.3	19.9
SER	78	N	39.2	7.4	20.6
	78	CA	39.0	6.9	19.1
	78	CB	39.9	5.6	19.0
	78	OG	39.5	4.8	20.0
	78	C	37.4	6.8	18.9
	78	O	37.2	5.8	18.1
ILE	79	N	36.7	7.7	19.2
	79	CA	35.2	7.5	19.0
	79	CB	34.1	6.8	19.6
	79	CG1	33.8	7.2	21.1
	79	CD1	32.5	6.7	21.5
	79	CG2	34.5	5.2	19.8
	79	C	34.8	9.1	18.9
	79	O	35.6	10.0	19.0
GLY	80	N	33.3	9.2	18.3
	80	CA	32.8	10.4	18.0
	80	C	33.6	11.6	17.6
	80	O *	34.0	11.6	16.4
VAL	81	N	33.5	12.7	18.2
	81	CA	34.2	13.9	17.8
	81	CB	33.0	14.9	17.5
	81	CG1	32.3	14.6	16.2
	81	CG2	32.0	15.0	18.6
	81	C	35.3	14.6	18.5
	81	O *	36.3	13.9	18.7
LEU	82	N	35.3	15.9	18.8
	82	CA	36.3	16.5	19.4
	82	CB	37.7	16.9	18.5
	82	CG	38.8	17.5	19.4
	82	CD1	39.3	16.5	20.4
	82	CD2	39.9	18.0	18.4
	82	C	36.0	17.9	20.0
	82	O	36.0	18.8	19.3
GLY	83	N	35.9	17.8	21.4
	83	CA	35.5	19.0	22.0
	83	C	36.4	20.1	22.0
	83	O	37.7	19.9	21.8
VAL	84	N	36.0	21.3	22.3
	84	CA	36.9	22.4	22.3
	84	CB	36.0	23.9	22.1
	84	CG1	37.1	24.9	22.6
	84	CG2*	35.8	24.1	20.6
	84	C	37.4	22.8	23.7
	84	O	38.7	23.1	23.6
ALA	85	N	37.0	22.4	24.8
	85	CA	37.7	22.5	26.0
	85	CB	37.3	23.6	27.0
	85	C	37.7	21.0	26.4
	85	O	37.0	20.7	27.5
PRO	86	N	38.2	20.3	25.7
	86	CA	38.2	18.9	25.8
	86	CB	39.3	18.4	24.8
	86	CG	39.8	19.6	24.0
	86	CD *	39.1	20.9	24.5
	86	C	38.7	18.4	27.2
	86	O	38.5	17.1	27.4
SER	87	N	39.1	19.3	28.0
	87	CA	39.6	18.8	29.3
	87	CB	41.3	19.0	29.4
	87	OG *	41.8	20.0	28.5
	87	C	38.9	19.4	30.5
	87	O	39.3	19.0	31.8
SER	88	N	38.0	20.3	30.3
	88	CA	37.3	21.0	31.4
	88	CB	36.2	21.8	30.6
	88	OG *	35.3	20.9	29.9
	88	C	36.7	20.1	32.3
	88	O	36.5	18.9	32.3
ALA	89	N	36.3	20.7	33.5
	89	CA	35.6	20.0	34.5
	89	CB	36.3	20.0	35.9
	89	C	34.2	20.6	34.1
	89	O	34.0	21.9	34.1
LEU	90	N	33.2	19.9	33.8
	90	CA	32.0	20.3	33.2
	90	CB	32.2	19.6	31.9
	90	CG	31.1	20.0	30.8
	90	CD1	31.3	21.4	30.2
	90	CD2	31.2	19.0	29.6
	90	C	30.9	20.0	34.1
	90	O	30.7	18.9	34.7
TYR	91	N	30.2	21.0	34.4
	91	CA	29.1	21.0	35.4
	91	CB	29.1	22.0	36.5
	91	CG	30.3	21.5	37.4
	91	CD1	31.8	21.8	37.1
	91	CE1	32.7	21.2	37.9
	91	CZ	32.4	20.4	39.1
	91	OH	33.3	20.0	39.8
	91	CE2	31.0	20.2	39.4
	91	CD2	30.0	20.7	38.6
	91	C	27.7	21.0	34.8
	91	O	27.3	22.1	34.0
ALA	92	N	27.1	19.9	34.8
	92	CA	25.7	19.8	34.3
	92	CB	25.4	18.3	34.3
	92	C	24.7	20.4	35.2
	92	O	24.1	20.0	36.2
VAL	93	N	24.3	21.8	34.9
	93	CA	23.3	22.5	35.5
	93	CB	23.9	23.9	35.8
	93	CG1	22.8	24.8	36.5
	93	CG2	25.2	23.8	36.6
	93	C	22.0	22.6	34.7
	93	O	22.0	23.0	33.4
LYS	94	N	21.0	22.0	35.2
	94	CA	19.8	22.0	34.5
	94	CB	19.1	20.6	34.8
	94	CG	17.9	20.6	34.0
	94	CD	17.1	19.1	34.0
	94	CE	17.0	18.4	32.8
	94	NZ	16.4	17.1	33.0
	94	C	18.8	23.1	34.8
	94	O	18.4	23.2	36.0
VAL	95	N	18.2	24.0	34.0
	95	CA	17.2	24.9	34.3
	95	CB	18.0	26.3	34.3
	95	CG1	19.0	26.3	35.3
	95	CG2	18.5	26.5	32.8
	95	C	16.1	25.0	33.3
	95	O	15.0	25.5	33.5
LEU	96	N	16.3	24.2	32.2
	96	CA	15.3	24.0	31.2
	96	CB	15.8	24.0	29.8
	96	CG	16.3	25.3	29.3
	96	CD1	17.0	24.8	28.0
	96	CD2	15.0	26.3	28.9
	96	C	14.4	22.5	31.5
	96	O	14.9	21.5	31.7
GLY	97	N	13.1	23.0	31.2
	97	CA	12.2	22.0	31.1
	97	C	12.1	21.3	29.9
	97	O	12.1	22.0	28.8
ASP	98	N *	11.9	20.0	29.9
	98	CA *	11.6	19.3	28.6
	98	CB *	11.0	17.9	29.0
	98	CG *	10.7	17.0	27.8
	98	OD1*	11.2	17.2	26.6
	98	OD2*	9.9	16.0	27.9
	98	C *	10.5	20.1	27.9
	98	O *	9.5	20.8	28.4
ALA	99	N *	10.6	20.0	26.4
	99	CA *	9.7	20.8	25.7
	99	CB *	8.1	20.7	26.1
	99	C *	10.1	22.3	25.5
	99	O *	9.7	23.0	24.6
GLY	100	N *	10.9	22.7	26.5
	100	CA *	11.3	24.0	26.4
	100	C *	10.9	24.8	27.6
	100	O *	10.7	26.0	27.4
SER	101	N *	10.9	24.3	28.8
	101	CA *	10.4	25.0	30.0
	101	CB *	10.4	24.0	31.1
	101	OG *	9.8	23.0	30.9
	101	C *	11.3	26.1	30.3
	101	O *	12.5	26.0	30.6
GLY	102	N *	10.7	27.4	30.3
	102	CA *	11.3	28.8	30.4
	102	C *	11.1	29.4	31.8
	102	O *	10.3	30.5	31.6
GLN	103	N	11.4	29.0	33.0
	103	CA	11.1	29.7	34.1
	103	CB	10.5	28.9	35.2
	103	CG	10.1	29.8	36.4
	103	CD	8.6	29.7	36.7
	103	OE1	7.8	29.5	35.7
	103	NE2	8.2	29.9	37.9
	103	C	12.4	30.5	34.5
	103	O	13.4	30.0	35.0
TYR	104	N	12.3	31.9	34.3
	104	CA	13.3	32.7	34.7
	104	CB	12.9	34.2	34.3
	104	CG *	13.4	34.5	33.0
	104	CD1*	13.4	33.5	32.0
	104	CE1*	13.9	33.8	30.8
	104	CZ *	14.4	35.1	30.3
	104	OH *	14.8	35.4	29.1
	104	CE2*	14.3	36.0	31.3
	104	CD2*	13.9	35.8	32.7
	104	C	13.8	32.5	36.1
	104	O	15.0	32.8	36.3
SER	105	N	12.9	32.0	37.0
	105	CA	13.3	31.9	38.3
	105	CB	12.3	31.5	39.3
	105	OG	11.6	30.3	38.9
	105	C	14.3	30.5	38.3
	105	O	15.1	30.5	39.3
TRP	106	N	14.3	29.7	37.4
	106	CA	15.0	28.5	37.3
	106	CB	14.4	27.4	36.7
	106	CG	13.0	27.0	37.0
	106	CD1	12.6	27.1	38.3
	106	NE1	11.1	26.5	38.3
	106	CE2	11.0	26.0	37.0
	106	CZ2	9.8	25.4	36.6
	106	CH2	9.9	25.0	35.2
	106	CZ3	10.9	25.2	34.5
	106	CE3	12.1	26.0	35.0
	106	CD2	12.1	26.3	36.3
	106	C	16.4	28.9	36.9
	106	O	17.5	28.4	37.4
ILE	107	N	16.5	29.9	35.9
	107	CA	17.6	30.4	35.3
	107	CB	17.3	31.4	34.3
	107	CG1	16.5	30.7	33.1
	107	CD1	16.2	31.8	32.0
	107	CG2	18.6	32.1	33.7
	107	C	18.5	31.0	36.3
	107	O	19.7	30.6	36.5
ILE	108	N	17.9	32.0	37.1
	108	CA	18.7	32.7	38.2
	108	CB	17.7	33.7	38.9
	108	CG1*	17.3	34.7	37.8
	108	CD1*	16.8	35.9	38.5
	108	CG2	18.3	34.3	40.1
	108	C	19.3	31.7	39.3
	108	O	20.5	31.6	39.5
ASN	109	N	18.5	30.9	40.0
	109	CA	19.0	30.0	41.0
	109	CB	18.0	29.1	41.8
	109	CG	17.0	30.0	42.3
	109	OD1	17.0	30.1	43.7
	109	ND2	16.0	30.5	41.7
	109	C	20.1	29.0	40.3
	109	O	21.2	28.9	41.0
GLY	110	N	20.0	28.8	39.0
	110	CA *	21.0	28.1	38.2
	110	C	22.3	29.0	38.3
	110	O	23.3	28.5	38.8
ILE	111	N	22.3	30.3	37.9
	111	CA	23.6	31.0	38.0
	111	CB	23.3	32.8	37.8
	111	CG1	22.9	33.0	36.4
	111	CD1*	23.0	34.5	36.2
	111	CG2*	24.9	33.2	37.9
	111	C	24.0	30.7	39.3
	111	O *	25.2	30.2	39.5
GLU	112	N	23.2	31.0	40.3
	112	CA	23.5	30.7	41.8
	112	CB	22.3	31.0	42.6
	112	CG	21.8	32.7	42.4
	112	CD	22.5	33.3	43.2
	112	OE1	23.9	33.3	43.2
	112	OE2	22.0	34.3	44.0
	112	C	24.3	29.6	42.2
	112	O	25.4	29.8	42.7
TRP	113	N	23.8	28.3	42.2
	113	CA	24.5	27.2	42.3
	113	CB	23.5	26.0	42.0
	113	CG	24.4	24.6	42.3
	113	CD1	24.5	23.9	43.3
	113	NE1	25.6	22.9	43.3
	113	CE2	26.1	23.1	42.0
	113	CZ2	27.1	22.4	41.5
	113	CH2	27.6	22.9	40.2
	113	CZ3	27.0	23.9	39.7
	113	CE3	26.0	24.6	40.1
	113	CD2	25.5	24.2	41.5
	113	C	25.8	27.1	41.7
	113	O	26.7	26.5	42.2
ALA	114	N	25.9	27.9	40.5
	114	CA	27.1	28.1	39.8
	114	CB *	27.0	28.5	38.3
	114	C	28.2	29.0	40.5
	114	O	29.4	28.9	40.3
ILE	115	N	27.7	30.0	41.1
	115	CA	28.4	31.0	42.0
	115	CB	27.5	32.3	42.3
	115	CG1	27.0	33.0	41.1
	115	CD1	26.2	34.3	41.6
	115	CG2	28.3	33.1	43.3
	115	C	28.9	30.1	43.2
	115	O	30.1	29.9	43.3
ALA	116	N	28.0	29.5	43.8
	116	CA	28.3	28.8	45.0
	116	CB	27.0	28.1	45.4
	116	C	29.4	27.6	44.7
	116	O	30.1	27.3	45.7
ASN	117	N	29.6	27.1	43.5
	117	CA	30.8	26.1	43.6
	117	CB	30.2	24.6	43.6
	117	CG	28.9	24.4	44.4
	117	OD1	28.9	24.0	45.5
	117	ND2	27.8	25.0	44.0
	117	C	32.0	26.5	42.8
	117	O	32.7	25.7	42.3
ASN	118	N	32.1	27.9	42.8
	118	CA	33.2	28.4	42.1
	118	CB	34.5	28.2	42.8
	118	CG	34.4	28.8	44.3
	118	OD1	34.9	30.0	44.4
	118	ND2	34.0	28.0	45.2
	118	C	33.3	27.9	40.6
	118	O	34.3	27.1	40.3
MET	119	N	32.5	28.3	39.9
	119	CA	32.5	28.1	38.3
	119	CB	31.1	28.1	37.8
	119	CG	30.4	27.0	38.0
	119	SD	30.8	25.3	37.4
	119	CE	31.0	24.4	39.0
	119	C	33.5	29.1	37.8
	119	O	33.5	30.3	38.4
ASP	120	N	34.2	29.0	36.8
	120	CA	35.2	29.9	36.2
	120	CB	36.5	29.1	35.9
	120	CG	37.0	28.6	37.3
	120	OD1	36.9	27.4	37.6
	120	OD2	37.9	29.3	38.0
	120	C	34.6	30.4	34.9
	120	O	34.7	31.7	34.7
VAL	121	N	33.9	29.6	34.3
	121	CA	33.3	29.9	33.0
	121	CB *	33.9	29.3	31.8
	121	CG1*	33.2	29.5	30.4
	121	CG2*	35.4	29.6	31.6
	121	C	31.7	29.6	33.0
	121	O	31.3	28.5	33.5
ILE	122	N	30.9	30.5	32.6
	122	CA	29.5	30.3	32.7
	122	CB	28.6	31.2	33.4
	122	CG1	28.7	30.9	35.0
	122	CD1	28.1	32.1	35.8
	122	CG2	27.1	31.0	33.0
	122	C	28.9	30.3	31.1
	122	O	29.0	31.3	30.4
ASN	123	N	28.1	29.3	30.9
	123	CA	27.5	29.2	29.5
	123	CB *	28.2	28.1	28.8
	123	CG	28.0	28.4	27.1
	123	OD1	28.6	29.0	26.4
	123	ND2	26.8	27.8	26.8
	123	C	26.0	28.9	29.6
	123	O	25.5	27.9	30.0
MET	124	N	25.3	29.9	29.0

Table I (continued)

	124	CA	23.9	29.9	28.9
	124	CB	23.1	31.1	29.4
	124	CG *	22.8	30.9	31.0
	124	SD	22.0	32.3	31.8
	124	CE	23.6	33.3	31.9
	124	C	23.5	29.9	27.3
	124	O	23.6	31.0	26.9
SER	125	N	23.3	28.9	26.7
	125	CA	23.0	29.0	25.2
	125	CB	23.5	28.0	24.2
	125	OG	24.9	27.6	24.4
	125	C	21.5	29.1	25.1
	125	O	20.8	28.2	24.4
LEU	126	N	20.9	30.0	25.9
	126	CA	19.4	30.3	25.9
	126	CB	18.9	29.8	27.0
	126	CG	19.5	30.0	28.3
	126	CD1	18.9	31.2	29.0
	126	CD2	19.6	28.9	29.4
	126	C	19.2	31.9	25.9
	126	O	20.2	32.7	25.8
GLY	127	N	18.0	32.3	26.1
	127	CA	17.8	33.8	26.3
	127	C	16.3	34.0	25.9
	127	O	15.4	33.0	25.6
GLY	128	N	15.9	35.3	25.9
	128	CA	14.5	35.6	25.4
	128	C	14.4	37.1	25.0
	128	O	15.2	38.0	25.2
PRO	129	N	13.1	37.3	24.5
	129	CA	12.8	38.7	24.0
	129	CB *	11.4	38.4	23.1
	129	CG	11.1	37.0	23.3
	129	CD	12.1	36.4	24.4
	129	C	12.5	39.7	25.3
	129	O	12.9	40.8	25.1
SER	130	N	12.1	39.2	26.3
	130	CA	11.9	40.0	27.6
	130	CB	10.5	39.8	28.1
	130	OG	10.6	39.1	29.5
	130	C	13.0	39.5	28.6
	130	O	13.6	38.4	28.8
GLY	131	N	13.3	40.6	29.3
	131	CA	14.2	40.5	30.5
	131	C	13.6	40.4	31.9
	131	O	12.4	39.8	32.1
SER	132	N	14.2	41.0	32.8
	132	CA	13.9	41.0	34.2
	132	CB	13.7	39.5	34.5
	132	OG	13.4	39.4	36.0
	132	C	15.0	41.5	35.0
	132	O	16.3	41.3	34.9
ALA	133	N	14.5	42.3	36.0
	133	CA	15.4	43.0	36.9
	133	CB	14.7	44.0	37.8
	133	C	16.4	42.2	37.5
	133	O	17.5	42.4	37.7
ALA	134	N	16.0	41.0	38.0
	134	CA	16.9	39.9	38.8
	134	CB	16.0	38.9	39.3
	134	C	17.9	39.4	37.8
	134	O	19.1	39.4	38.0
LEU	135	N	17.5	38.9	36.7
	135	CA	18.3	38.2	35.7
	135	CB	17.7	38.3	34.2
	135	CG	18.3	37.3	33.3
	135	CD1	18.3	35.9	34.0
	135	CD2	17.6	37.3	31.9
	135	C	19.7	38.9	35.6
	135	O	20.7	38.3	36.0
LYS	136	N	19.5	40.2	35.2
	136	CA	20.5	41.1	35.1
	136	CB	20.1	42.3	34.4
	136	CG	21.3	43.3	34.3
	136	CD	20.7	44.8	34.0
	136	CE	22.2	45.7	33.5
	136	NZ	22.7	46.4	34.7
	136	C	21.2	41.5	36.5
	136	O	22.5	41.5	36.5
ALA	137	N	20.5	41.3	37.5
	137	CA	21.1	41.3	38.9
	137	CB	20.1	41.3	40.0
	137	C	22.2	40.1	39.0
	137	O	23.3	40.5	39.2
ALA	138	N	21.7	39.0	38.9
	138	CA	22.7	37.9	39.0
	138	CB	21.8	36.6	39.0
	138	C	23.8	37.9	38.0
	138	O	25.0	37.7	38.3
VAL	139	N	23.4	38.2	36.8
	139	CA	24.2	38.2	35.7
	139	CB	23.6	39.1	34.7
	139	CG1	24.6	39.5	33.5
	139	CG2*	22.4	38.3	34.0
	139	C	25.4	39.0	36.1
	139	O	26.6	38.8	36.0
ASP	140	N	25.2	40.3	36.9
	140	CA	26.2	41.0	37.3
	140	CB	25.5	42.3	37.9
	140	CG	25.1	43.2	36.8
	140	OD1	25.5	42.9	35.5
	140	OD2	24.4	44.3	36.9
	140	C	27.0	40.2	38.3
	140	O	28.2	40.1	38.2
LYS	141	N	26.4	39.7	39.4
	141	CA	27.0	38.9	40.4
	141	CB	26.0	38.0	41.1
	141	CG	25.0	39.0	42.0
	141	CD *	24.4	37.8	42.8
	141	CE *	23.4	38.5	43.9
	141	NZ *	22.8	37.6	44.8
	141	C	28.0	38.0	39.8
	141	O	29.3	38.0	40.0
ALA	142	N	27.7	37.0	38.9
	142	CA *	28.8	36.0	38.5
	142	CB	28.2	35.0	37.5
	142	C	30.0	36.6	38.0
	142	O	31.1	36.0	38.2
VAL	143	N	30.0	37.7	37.3
	143	CA	31.2	38.3	36.8
	143	CB	30.7	39.3	35.7
	143	CG1	31.9	39.7	34.8
	143	CG2	29.6	38.7	34.8
	143	C	31.9	39.1	37.9
	143	O	33.1	39.3	38.0
ALA	144	N	31.1	39.5	38.9
	144	CA	31.5	40.3	40.0
	144	CB	30.4	40.9	40.8
	144	C	32.5	39.5	40.8
	144	O	33.7	39.8	41.1
SER	145	N	32.0	38.3	41.1
	145	CA	32.8	37.3	41.9
	145	CB	31.9	36.0	42.1
	145	OG	31.0	36.3	43.0
	145	C	34.0	37.0	41.0
	145	O	35.2	37.1	41.5
GLY	146	N	33.8	36.8	39.8
	146	CA	34.9	36.4	38.8
	146	C	34.5	35.3	37.8
	146	O	35.5	34.5	37.3
VAL	147	N	33.3	35.3	37.4
	147	CA	32.9	34.3	36.4
	147	CB	31.6	33.7	37.0
	147	CG1*	31.0	33.0	35.6
	147	CG2*	31.9	32.5	38.0
	147	C	32.7	35.0	35.0
	147	O	32.0	36.2	35.0
VAL	148	N	33.0	34.4	34.0
	148	CA	32.9	34.9	32.7
	148	CB	34.0	34.2	32.0
	148	CG1	33.8	34.5	30.4
	148	CG2	35.4	34.5	32.3
	148	C	31.5	34.3	32.1
	148	O	31.4	33.1	31.8
VAL	149	N	30.6	35.2	32.0
	149	CA	29.3	34.8	31.6
	149	CB	28.3	35.4	32.5
	149	CG1	26.9	34.9	32.1
	149	CG2	28.6	35.0	34.0
	149	C	29.1	35.0	30.0
	149	O	29.4	36.0	29.4
VAL	150	N	28.9	33.8	29.5
	150	CA	28.9	33.6	28.0
	150	CB	30.0	32.6	27.7
	150	CG1	30.1	32.5	26.0
	150	CG2	31.3	33.0	28.3
	150	C	27.4	33.0	27.6
	150	O	27.0	31.9	28.0
ALA	151	N	26.8	33.7	26.7
	151	CA	25.5	33.3	26.1
	151	CB	24.4	34.3	26.9
	151	C	25.4	33.5	24.5
	151	O	26.0	34.1	23.9
ALA	152	N	24.3	32.8	24.3
	152	CA	23.8	32.9	22.9
	152	CB	22.5	31.9	22.9
	152	C	23.1	34.3	22.8
	152	O	22.5	34.8	23.8
ALA	153	N	23.3	35.0	21.7
	153	CA	22.8	36.4	21.6
	153	CB *	23.6	37.3	20.8
	153	C	21.3	36.2	21.1
	153	O	20.4	37.0	21.6
GLY	154	N	21.1	35.2	20.3
	154	CA	19.9	34.9	20.0
	154	C	19.8	34.7	18.4
	154	O	20.5	35.0	17.6
ASN	155	N	18.6	33.9	18.0
	155	CA	18.3	33.5	16.8
	155	CB	17.8	32.0	17.1
	155	CG	18.8	31.0	17.5
	155	OD1	20.0	31.1	17.2
	155	ND2	18.5	30.0	18.1
	155	C	17.0	34.3	16.1
	155	O	16.1	33.8	15.6
GLU	156	N	17.1	35.8	16.1
	156	CA	16.2	36.5	15.4
	156	CB	15.4	37.5	16.2
	156	CG	15.1	37.1	17.6
	156	CD *	14.6	35.8	18.0
	156	OE1*	13.4	35.2	17.5
	156	OE2*	15.3	35.0	18.7
	156	C	17.0	37.0	14.1
	156	O	18.0	36.3	13.9
GLY	157	N	16.6	38.0	13.5
	157	CA	17.5	38.4	12.4
	157	C	17.7	40.0	12.3
	157	O	17.9	40.7	13.3
SER	158	N	17.1	40.4	11.2
	158	CA *	16.7	41.9	11.4
	158	CB	16.7	42.1	9.8
	158	OG	17.0	41.0	9.1
	158	C	15.1	42.0	11.9
	158	O	14.3	41.0	11.9
THR	159	N	14.8	43.1	12.1
	159	CA	13.4	43.7	12.3
	159	CB	12.6	43.3	13.7
	159	OG1*	11.3	43.7	13.6
	159	CG2*	13.2	43.8	15.0
	159	C *	13.9	45.1	12.4
	159	O	14.3	45.6	13.4
GLY	160	N	13.8	45.8	11.3
	160	CA	14.4	47.0	10.9
	160	C	15.9	47.0	11.4
	160	O	16.8	46.3	10.9
SER	161	N	16.1	47.8	12.3
	161	CA	17.5	48.2	12.9
	161	CB	17.5	49.7	12.4
	161	OG *	17.6	49.7	11.0
	161	C	17.4	48.1	14.4
	161	O	18.5	48.4	15.1
SER	162	N	16.3	47.9	15.0
	162	CA *	16.4	48.0	16.5
	162	CB	14.9	48.2	17.1
	162	OG	15.0	48.1	18.5
	162	C	17.1	46.6	16.7
	162	O	17.8	46.0	15.9
SER	163	N	17.0	46.2	18.0
	163	CA	17.8	45.0	18.3
	163	CB	18.9	45.8	19.2
	163	OG	19.9	44.8	19.5
	163	C	17.0	43.7	18.9
	163	O	16.3	43.7	19.6
THR	164	N	17.6	42.7	18.1
	164	CA	17.0	41.3	18.5
	164	CB	16.6	40.9	17.0
	164	OG1	17.6	40.8	16.1
	164	CG2	15.6	42.0	16.7
	164	C	18.0	40.5	19.3
	164	O	17.6	39.3	19.4
VAL	165	N	19.0	41.0	19.9
	165	CA	19.7	40.1	20.9
	165	CB	21.1	40.8	21.0
	165	CG1	21.6	40.4	22.5
	165	CG2	22.0	40.3	20.0
	165	C	18.8	40.1	22.1
	165	O	18.3	41.1	22.5
GLY	166	N	18.7	39.0	22.6
	166	CA	17.9	38.7	23.7
	166	C	18.6	38.8	25.0
	166	O	19.8	39.0	25.0
TYR	167	N	17.9	38.4	26.1
	167	CA	18.3	38.5	27.4
	167	CB	17.3	39.0	28.4
	167	CG	17.0	40.3	28.1
	167	CD1	16.0	40.7	27.0
	167	CE1	15.7	42.0	26.8
	167	CZ	16.1	43.0	27.5
	167	OH	15.9	44.3	27.2
	167	CE2	17.0	42.8	28.6
	167	CD2	17.5	41.4	28.9
	167	C	18.9	37.0	27.8
	167	O	18.1	36.1	27.3
PRO	168	N	19.9	36.9	28.6
	168	CA	20.7	37.8	29.3
	168	CB	21.4	37.0	30.4
	168	CG	21.3	35.4	30.0
	168	CD	20.4	35.3	28.9
	168	C	21.8	38.3	28.4
	168	O	22.7	39.1	29.0
GLY	169	N	21.8	38.0	27.1
	169	CA	22.9	38.3	26.2
	169	C	23.1	39.9	26.1
	169	O	24.3	40.3	26.1
LYS	170	N	22.0	40.7	26.0
	170	CA	21.9	42.2	25.9
	170	CB	20.3	42.3	25.9
	170	CG	20.0	43.9	25.6
	170	CD	18.4	44.0	25.4
	170	CE	18.3	45.3	24.6
	170	NZ	18.6	45.3	23.1
	170	C	22.4	42.9	27.0
	170	O	22.8	44.0	26.9
TYR	171	N	22.5	42.3	28.1
	171	CA	23.0	42.9	29.3
	171	CB	22.6	42.3	30.6
	171	CG	21.1	42.0	31.0
	171	CD1	20.1	43.0	31.0
	171	CE1	18.9	42.8	31.4
	171	CZ	18.3	41.5	31.7
	171	OH	17.0	41.3	32.0
	171	CE2	19.3	40.4	31.8
	171	CD2	20.6	40.7	31.3
	171	C	24.5	42.6	29.3
	171	O	25.1	41.7	29.1
PRO	172	N	25.2	44.0	29.3
	172	CA	26.6	44.2	29.0
	172	CB	27.0	45.8	29.4
	172	CG	25.5	46.4	29.5
	172	CD	24.4	45.3	29.6
	172	C	27.8	43.4	29.8
	172	O	28.9	43.6	29.4
SER	173	N	27.4	42.6	30.8
	173	CA	28.5	42.0	31.5
	173	CB	28.2	42.0	33.0
	173	OG	27.1	41.1	33.3
	173	C	28.7	40.5	30.9
	173	O	29.4	39.8	31.3
VAL	174	N	27.9	40.3	29.8
	174	CA	28.0	39.2	29.1
	174	CB	26.4	38.7	28.9
	174	CG1	26.5	37.4	28.0
	174	CG2	25.7	38.4	30.2
	174	C	28.6	39.1	27.8
	174	O	28.8	40.1	27.0
ILE	175	N	29.0	38.0	27.4
	175	CA *	29.7	37.9	26.0
	175	CB	31.1	37.2	26.0
	175	CG1	32.0	37.9	27.1
	175	CD1	33.0	36.8	27.7
	175	CG2	31.6	37.3	24.6
	175	C	28.7	37.2	25.1
	175	O	28.5	36.0	25.4
ALA	176	N	28.0	37.9	24.2
	176	CA	27.0	37.4	23.4
	176	CB	26.1	38.8	23.1
	176	C	27.5	36.9	22.0
	176	O	28.4	37.6	21.4
VAL	177	N	27.1	35.7	21.6
	177	CA	27.7	35.1	20.4
	177	CB	28.5	33.8	21.0
	177	CG1*	29.4	33.3	19.9
	177	CG2	29.4	34.3	22.3
	177	C	26.8	35.0	19.3
	177	O	25.8	34.1	19.3
GLY	178	N	27.0	35.6	18.3
	178	CA	26.5	35.6	17.0
	178	C	27.1	34.3	16.1
	178	O	28.3	34.0	16.3
ALA	179	N	26.3	33.8	15.3
	179	CA	26.9	32.6	14.4
	179	CB	25.8	31.6	14.3
	179	C	27.3	33.0	13.0
	179	O	26.6	33.8	12.3
VAL	180	N	28.4	32.5	12.8
	180	CA	29.0	32.6	11.4
	180	CB	30.5	33.0	11.6
	180	CG1	30.5	34.6	12.1
	180	CG2	31.2	32.2	12.6
	180	C	29.1	31.1	10.9
	180	O	29.0	30.1	11.5
ASP	181	N	29.4	31.0	9.4
	181	CA	29.7	29.7	8.9
	181	CB	28.9	29.4	7.8
	181	CG	29.1	30.3	6.4
	181	OD1	30.2	30.9	6.3
	181	OD2	28.2	30.4	5.7
	181	C	31.3	29.4	8.6
	181	O	32.0	30.3	9.1
SER	182	N	31.5	28.4	7.9
	182	CA	33.0	28.3	7.8
	182	CB	33.2	27.0	6.8
	182	OG	32.4	27.1	5.8
	182	C	33.3	29.5	6.8
	182	O	34.7	29.4	6.8
SER	183	N	32.7	30.3	6.2
	183	CA	33.2	31.2	5.2
	183	CB	32.8	31.3	3.8
	183	OG	33.0	30.0	3.2
	183	C	33.0	32.7	5.9
	183	O	33.3	33.7	5.3
ASN	184	N	32.8	32.6	7.2
	184	CA	32.7	33.7	8.1
	184	CB	34.0	34.4	8.3
	184	CG	35.2	33.4	8.7
	184	OD1	35.4	33.1	9.9
	184	ND2	35.9	33.1	7.7
	184	C	31.6	34.8	7.7
	184	O	31.7	35.9	7.9
GLN	185	N	30.7	34.2	6.9
	185	CA	29.4	35.0	6.5
	185	CB	28.9	34.5	5.3
	185	CG	29.9	34.4	4.2
	185	CD	30.3	35.9	3.6
	185	OE1	29.4	36.8	3.4
	185	NE2	31.5	36.1	3.5
	185	C	28.6	34.9	7.8
	185	O	28.5	33.8	8.4
ARG	186	N	27.9	36.0	8.1
	186	CA	27.0	35.8	9.3
	186	CB	26.6	37.2	9.9
	186	CG	25.4	37.3	10.6
	186	CD	25.0	38.9	10.6
	186	NE	23.7	39.0	11.0
	186	CZ	22.6	39.0	10.4
	186	NH1	22.6	38.8	8.9
	186	NH2	21.3	39.2	10.9
	186	C	25.7	35.1	8.8
	186	O	25.0	35.4	7.7
ALA	187	N	25.4	34.1	9.6
	187	CA	24.2	33.3	9.4
	187	CB	24.2	32.1	10.3
	187	C	22.9	34.1	9.4
	187	O	22.7	35.0	10.3
SER	188	N	22.0	33.9	8.4
	188	CA	20.8	34.7	8.3
	188	CB	19.7	33.8	7.8
	188	OG	20.1	32.9	6.8
	188	C	20.0	34.8	9.6
	188	O	19.3	35.8	9.8
PHE	189	N	20.0	33.8	10.4
	189	CA	19.3	33.8	11.7
	189	CB	18.9	32.2	12.0
	189	CG	20.1	31.4	12.1
	189	CD1	21.0	31.7	13.4
	189	CE1	22.2	30.9	13.4
	189	CZ	22.4	29.9	12.7
	189	CE2	21.6	29.6	11.4
	189	CD2	20.4	30.3	11.4
	189	C	20.0	34.3	12.9
	189	O	19.5	34.3	14.1
SER	190	N	21.2	35.0	12.8
	190	CA	21.9	35.4	13.9
	190	CB	23.4	35.3	13.6
	190	OG	24.1	35.9	14.8
	190	C	21.3	37.0	14.1
	190	O	21.5	38.0	13.4
SER	191	N	21.0	37.0	15.4
	191	CA	20.5	38.3	16.0
	191	CB	20.2	38.1	17.5

Table I (continued)

	191	OG	19.2	37.1	17.6
	191	C	21.6	39.4	15.7
	191	O	22.8	39.0	15.3
VAL	192	N	21.1	40.8	15.8
	192	CA	21.9	41.9	15.4
	192	CB	21.5	42.3	14.0
	192	CG1	21.5	41.1	13.1
	192	CG2	20.0	42.9	13.9
	192	C	21.6	42.9	16.6
	192	O	20.5	43.0	17.1
GLY	193	N	22.7	43.5	16.9
	193	CA	22.5	44.4	18.0
	193	C	24.0	45.0	18.3
	193	O	25.0	44.8	17.9
PRO	194	N	23.9	46.1	19.1
	194	CA	25.0	46.8	19.7
	194	CB	24.5	48.1	20.3
	194	CG	23.0	48.2	20.0
	194	CD	22.5	46.8	19.5
	194	C	25.9	46.0	20.7
	194	O	27.1	46.3	20.9
GLU	195	N	25.1	45.2	21.2
	195	CA	25.1	44.3	22.4
	195	CB	23.5	44.5	23.0
	195	CG	23.3	46.0	23.2
	195	CD	21.8	46.1	23.1
	195	OE1	21.0	45.5	22.5
	195	OE2	21.3	47.2	23.6
	195	C	25.6	42.8	22.0
	195	O	25.7	41.9	22.8
LEU	196	N	25.9	42.8	20.6
	196	CA	26.5	41.7	20.0
	196	CB	26.1	41.8	18.6
	196	CG	26.8	40.8	17.6
	196	CD1	26.5	39.3	18.3
	196	CD2	26.0	40.9	16.3
	196	C	28.1	41.8	20.2
	196	O	28.5	42.8	19.9
ASP	197	N	28.5	41.0	20.9
	197	CA	30.1	41.0	21.3
	197	CB	30.0	40.8	22.9
	197	CG	29.5	41.8	23.5
	197	OD1	29.8	43.0	23.1
	197	OD2	28.6	41.7	24.5
	197	C	31.0	40.3	20.3
	197	O	31.9	41.0	19.8
VAL	198	N	30.9	39.0	20.0
	198	CA	31.7	38.3	19.0
	198	CB	32.8	37.5	19.6
	198	CG1	33.8	38.4	20.6
	198	CG2	32.1	36.4	20.6
	198	C	30.9	37.3	18.1
	198	O	29.6	37.1	18.4
MET	199	N	31.5	36.9	17.1
	199	CA	30.9	36.0	16.2
	199	CB	30.9	36.5	14.8
	199	CG	30.3	38.0	14.9
	199	SD	28.5	37.7	15.1
	199	CE	28.0	37.0	13.4
	199	C	31.4	34.7	16.3
	199	O	32.7	34.5	16.4
ALA	200	N	30.8	33.5	16.1
	200	CA	31.3	32.1	16.2
	200	CB	31.3	31.8	17.8
	200	C	30.5	31.0	15.5
	200	O	29.2	31.1	15.1
PRO	201	N	31.1	29.9	15.3
	201	CA	30.8	28.9	14.6
	201	CB	31.9	27.7	14.8
	201	CG	33.0	28.3	15.4
	201	CD	32.7	29.9	15.6
	201	C	29.2	28.4	15.1
	201	O	29.0	27.8	16.0
GLY	202	N	28.3	28.9	14.3
	202	CA	26.9	28.5	14.6
	202	C	26.1	27.6	13.5
	202	O	25.0	27.1	13.8
VAL	203	N	26.7	27.4	12.3
	203	CA	26.0	26.7	11.3
	203	CB	26.1	27.5	10.0
	203	CG1	25.6	26.6	8.9
	203	CG2	25.4	28.8	10.1
	203	C	26.7	25.3	11.2
	203	O	27.9	24.9	11.1
SER	204	N	25.8	24.4	11.1
	204	CA	25.9	23.0	10.9
	204	CB	26.1	22.6	9.4
	204	OG *	25.0	23.1	8.7
	204	C	27.1	22.5	11.8
	204	O	28.1	21.9	11.3
ILE	205	N	27.0	22.7	13.1
	205	CA	28.0	22.5	14.1
	205	CB	27.9	23.6	15.1
	205	CG1	28.5	24.9	14.5
	205	CD1	29.8	24.6	13.6
	205	CG2	28.6	23.1	16.4
	205	C	27.5	21.1	14.6
	205	O	26.5	21.0	15.3
GLN	206	N	28.2	20.1	14.4
	206	CA	27.9	18.8	14.8
	206	CB	28.3	17.8	13.8
	206	CG	28.6	16.4	14.3
	206	CD	27.3	15.5	13.9
	206	OE1	26.3	16.0	13.5
	206	NE2	27.5	14.1	14.0
	206	C	28.4	18.4	16.1
	206	O	29.5	18.5	16.4
SER	207	N	27.5	17.9	17.0
	207	CA	27.9	17.5	18.3
	207	CB	27.6	18.7	19.1
	207	OG	28.0	18.4	20.5
	207	C	27.0	16.1	18.8
	207	O	26.4	15.4	18.0
THR	208	N	27.3	15.9	20.0
	208	CA	26.9	14.8	20.8
	208	CB	27.5	14.4	22.0
	208	OG1	27.6	15.6	22.9
	208	CG2	29.0	13.9	21.8
	208	C	25.4	14.9	21.0
	208	O	24.8	15.9	21.0
LEU	209	N	24.9	13.6	21.0
	209	CA	23.4	13.4	21.0
	209	CB	22.9	13.1	19.7
	209	CG	22.8	14.3	18.9
	209	CD1	22.4	14.1	17.4
	209	CD2	21.8	15.3	19.4
	209	C	23.3	12.0	21.9
	209	O	24.0	11.1	21.6
PRO	210	N	22.3	12.0	22.8
	210	CA	22.0	10.8	23.4
	210	CB	20.9	10.9	24.3
	210	CG	20.3	12.4	24.1
	210	CD	21.1	13.0	23.0
	210	C	21.7	9.6	22.5
	210	O	21.0	9.7	21.4
GLY	211	N	22.0	8.4	23.0
	211	CA	21.9	7.0	22.8
	211	C	23.0	6.7	21.8
	211	O	22.9	6.3	20.6
ASN	212	N	24.1	6.7	22.3
	212	CA	25.3	6.4	21.6
	212	CB	25.3	4.9	21.2
	212	CG	26.5	4.4	20.3
	212	OD1	27.6	5.1	20.3
	212	ND2*	26.3	3.5	19.4
	212	C	25.3	7.2	20.1
	212	O	25.4	6.6	19.0
LYS	213	N	25.1	8.4	20.2
	213	CA	24.9	9.1	19.0
	213	CB	23.5	9.9	19.0
	213	CG	22.4	8.6	18.9
	213	CD	21.0	9.2	18.7
	213	CE	20.1	8.1	18.9
	213	NZ	18.7	8.8	18.9
	213	C	25.5	10.7	19.0
	213	O	26.0	11.1	20.0
TYR	214	N	25.4	11.3	17.9
	214	CA	26.0	12.6	17.6
	214	CB	27.3	12.2	17.0
	214	CG	28.2	11.3	17.9
	214	CD1	28.1	9.9	17.6
	214	CE1	29.0	9.1	18.3
	214	CZ	30.0	9.5	19.3
	214	OH	30.9	8.9	20.0
	214	CE2	30.0	10.9	19.4
	214	CD2	29.1	11.8	18.7
	214	C	25.0	13.1	16.4
	214	O	24.5	12.4	15.7
GLY	215	N	25.0	14.5	16.4
	215	CA	24.3	15.1	15.3
	215	C	24.5	16.7	15.1
	215	O	25.3	17.1	15.9
ALA	216	N	24.0	17.1	14.1
	216	CA	24.3	18.6	13.9
	216	CB	24.9	18.5	12.3
	216	C	23.2	19.7	13.9
	216	O	22.1	19.6	13.4
TYR	217	N	23.5	20.9	14.4
	217	CA	22.5	21.9	14.7
	217	CB	22.2	22.1	16.2
	217	CG *	21.3	21.0	16.5
	217	CD1*	20.1	20.9	15.9
	217	CE1*	19.1	19.9	16.1
	217	CZ *	19.4	19.1	17.3
	217	OH *	18.5	18.1	17.6
	217	CE2*	20.6	19.2	18.0
	217	CD2*	21.4	20.2	17.8
	217	C	23.1	23.2	14.2
	217	O	24.3	23.5	14.1
ASN	218	N	22.0	24.0	13.9
	218	CA	22.3	25.5	13.4
	218	CB	21.9	25.7	12.1
	218	CG	22.4	24.7	11.1
	218	OD1	23.8	24.5	11.1
	218	ND2	21.7	24.0	10.3
	218	C	21.8	26.4	14.6
	218	O	20.5	26.3	14.9
GLY	219	N	22.6	27.1	15.1
	219	CA	22.1	27.9	16.4
	219	C	23.0	29.0	16.9
	219	O	24.3	28.7	17.0
THR	220	N	22.6	30.0	17.2
	220	CA	23.4	31.0	17.9
	220	CB	22.8	32.3	18.4
	220	OG1	23.7	33.3	18.9
	220	CG2	21.7	32.2	19.4
	220	C	23.8	30.4	19.2
	220	O	24.7	30.8	19.9
SER	221	N	23.1	29.1	19.4
	221	CA	23.4	28.5	20.7
	221	CB	22.1	27.9	21.3
	221	OG	21.4	27.0	20.6
	221	C	24.4	27.2	20.5
	221	O	24.6	26.7	21.5
MET	222	N	24.9	27.0	19.4
	222	CA	26.0	26.0	19.0
	222	CB	25.6	25.4	17.8
	222	CG	24.6	24.2	17.8
	222	SD	22.9	25.0	17.9
	222	CE	22.5	24.6	19.5
	222	C	27.3	26.9	18.9
	222	O	28.4	26.2	19.1
ALA	223	N	27.1	28.2	18.6
	223	CA	28.3	29.0	18.6
	223	CB	27.9	30.2	17.7
	223	C	28.8	29.4	20.0
	223	O	29.9	29.1	20.3
SER	224	N	27.9	29.8	20.8
	224	CA	28.0	30.1	22.1
	224	CB	26.6	30.0	22.9
	224	OG	26.8	30.5	24.3
	224	C	29.0	29.0	23.0
	224	O	29.7	29.	23.8
PRO	225	N	28.9	27.7	22.5
	225	CA	29.7	26.8	23.1
	225	CB	29.0	25.4	22.8
	225	CG	27.9	25.6	21.8
	225	CD *	27.9	27.2	21.6
	225	C	31.1	26.9	22.6
	225	O	32.0	26.7	23.4
HIS	226	N	31.3	27.2	21.3
	226	CA	32.8	27.4	20.9
	226	CB	32.7	28.0	19.4
	226	CG	32.4	26.9	18.4
	226	ND1	31.1	26.4	18.2
	226	CE1	31.2	25.4	17.3
	226	NE2	32.7	25.3	17.0
	226	CD2	33.3	26.1	17.8
	226	C	33.3	28.4	21.8
	226	O	34.5	28.1	22.3
VAL	227	N	32.8	29.5	21.9
	227	CA	33.2	30.7	22.6
	227	CB	32.0	31.9	22.7
	227	CG1	32.2	33.0	23.6
	227	CG2	32.0	32.4	21.3
	227	C	33.6	30.4	24.1
	227	O	34.6	31.0	24.5
ALA	228	N	32.8	29.8	24.9
	228	CA	33.0	29.4	26.3
	228	CB	31.8	28.7	26.9
	228	C	34.3	28.6	26.6
	228	O	34.8	28.7	27.8
GLY	229	N	34.7	27.8	25.6
	229	CA	35.8	26.9	25.8
	229	C	37.1	27.6	25.4
	229	O	38.0	27.4	26.1
ALA	230	N	37.0	28.4	24.3
	230	CA	38.3	29.1	24.0
	230	CB	38.0	30.3	23.1
	230	C	38.8	29.6	25.4
	230	O	40.0	29.5	25.8
ALA	231	N	37.9	30.3	26.1
	231	CA	38.0	30.8	27.4
	231	CB	36.6	31.4	28.0
	231	C	38.5	29.9	28.5
	231	O	39.6	30.1	29.1
ALA	232	N	37.9	28.6	28.6
	232	CA	38.6	27.7	29.5
	232	CB	37.8	26.3	29.1
	232	C	40.0	27.6	29.6
	232	O	40.4	27.9	30.7
LEU	233	N	40.2	27.3	28.3
	233	CA	41.6	27.0	28.0
	233	CB	41.7	26.3	26.7
	233	CG	41.0	24.9	26.5
	233	CD1	39.6	25.1	26.9
	233	CD2	41.2	24.4	25.1
	233	C	42.5	28.3	28.0
	233	O	43.7	28.2	28.1
ILE	234	N	41.8	29.4	27.9
	234	CA	42.5	30.7	27.9
	234	CB	41.6	31.9	27.5
	234	CG1	41.5	32.2	26.0
	234	CD1	40.7	33.4	25.6
	234	CG2	42.1	33.0	28.4
	234	C	43.0	30.6	29.3
	234	O	44.1	30.7	29.7
LEU	235	N	42.0	30.4	30.2
	235	CA	42.2	30.3	31.6
	235	CB	40.9	30.1	32.4
	235	CG	40.4	31.2	33.3
	235	CD1	41.3	32.4	33.1
	235	CD2	39.0	31.5	33.1
	235	C	43.2	29.2	32.1
	235	O	43.8	29.3	33.1
SER	236	N	43.2	28.1	31.3
	236	CA	44.1	27.0	31.6
	236	CB	43.8	25.8	30.7
	236	OG	42.9	26.2	29.6
	236	C	45.6	27.4	31.5
	236	O	46.5	26.9	32.2
LYS	237	N	45.8	28.3	30.5
	237	CA	47.2	28.8	30.3
	237	CB	47.4	29.3	28.9
	237	CG	48.8	29.6	28.4
	237	CD	48.9	29.9	27.0
	237	CE	50.3	30.4	26.5
	237	NZ	50.5	30.2	25.1
	237	C	47.5	29.9	31.3
	237	O	48.5	29.8	32.1
HIS	238	N	46.6	30.8	31.4
	238	CA	46.7	32.0	32.3
	238	CB	46.6	33.3	31.5
	238	CG	47.6	33.5	30.5
	238	ND1	47.3	33.5	29.1
	238	CE1	48.3	33.7	28.4
	238	NE2	49.3	33.9	29.3
	238	CD2	48.9	33.8	30.5
	238	C	45.7	31.8	33.4
	238	O	44.9	32.7	33.7
PRO	239	N	45.7	30.6	34.0
	239	CA	44.8	30.4	35.1
	239	CB	45.2	29.0	35.7
	239	CG	46.7	29.0	35.4
	239	CD	46.9	29.7	34.0
	239	C	44.7	31.3	36.3
	239	O	44.0	31.1	37.3
ASN	240	N	45.6	32.3	36.3
	240	CA	45.7	33.3	37.3
	240	CB *	47.2	33.6	37.7
	240	CG *	48.0	33.7	36.4
	240	OD1*	47.8	34.3	35.4
	240	ND2*	49.2	32.9	36.5
	240	C	44.9	34.6	36.8
	240	O	44.5	35.4	37.7
TRP	241	N	44.8	34.7	35.5
	241	CA	44.1	35.8	34.9
	241	CB	43.9	35.5	33.5
	241	CG	45.1	35.8	32.5
	241	CD1	46.4	36.0	32.9
	241	NE1	47.2	36.3	31.7
	241	CE2	46.4	36.1	30.7
	241	CZ2	46.8	36.3	29.3
	241	CH2	45.8	36.1	28.4
	241	CZ3	44.5	35.9	28.9
	241	CE3	44.1	35.8	30.2
	241	CD2	45.1	35.9	31.1
	241	C	42.7	36.2	35.5
	241	O	42.0	35.3	36.1
THR	242	N	42.4	37.5	35.5
	242	CA	41.1	37.9	36.0
	242	CB	41.2	39.5	36.2
	242	OG1	42.6	39.8	35.7
	242	CG2	41.0	39.9	37.6
	242	C	39.9	37.5	35.1
	242	O	40.1	37.2	33.9
ASN	243	N	38.7	37.6	35.7
	243	CA	37.5	37.2	34.9
	243	CB	36.3	37.3	35.9
	243	CG	35.2	38.2	35.3
	243	OD1	34.2	37.8	34.9
	243	ND2	35.5	39.5	35.5
	243	C	37.5	38.3	33.8
	243	O	37.0	38.0	32.7
THR	244	N	38.0	39.5	34.2
	244	CA	38.0	40.6	33.2
	244	CB	37.9	41.9	34.0
	244	OG1	36.6	42.0	34.5
	244	CG2*	38.3	43.1	33.2
	244	C	39.3	40.5	32.3
	244	O	39.2	40.8	31.1
GLN	245	N	40.3	40.1	32.9
	245	CA	41.6	40.0	32.1
	245	CB	42.6	39.3	33.0
	245	CG	44.0	39.7	32.7
	245	CD	45.0	39.4	33.8
	245	OE1	44.7	39.3	35.0
	245	NE2	46.3	39.2	33.5
	245	C	41.2	39.3	30.9
	245	O	41.5	39.6	29.8
VAL	246	N	40.4	38.2	31.2
	246	CA	39.8	37.4	30.1
	246	CB	39.2	36.2	30.6
	246	CG1	38.8	35.1	29.6
	246	CG2	39.9	35.6	31.8
	246	C	38.8	37.8	29.0
	246	O	38.9	37.3	27.8
ARG	247	N	38.0	38.7	29.3
	247	CA	36.9	39.2	28.4
	247	CB	35.9	40.0	29.1
	247	CG *	35.2	41.1	28.2
	247	CD	33.8	41.4	28.7
	247	NE	32.7	41.0	27.8
	247	CZ	31.4	41.3	27.9
	247	NH1	30.6	41.3	26.9
	247	NH2	31.0	41.7	29.1
	247	C	37.9	40.0	27.5
	247	O	38.0	39.7	26.3
SER	248	N	38.6	40.9	28.1
	248	CA	39.5	41.7	27.3
	248	CB	40.5	42.4	28.2
	248	OG	39.9	43.2	29.3
	248	C	40.4	41.0	26.2
	248	O	40.5	41.5	25.1
SER	249	N	41.1	40.0	26.6
	249	CA	41.9	39.2	25.7
	249	CB	42.7	38.2	26.5
	249	OG	43.6	37.4	25.6
	249	C	41.1	38.5	24.6
	249	O	41.6	38.0	23.7
LEU	250	N	39.8	38.6	24.8
	250	CA	38.8	38.0	23.9
	250	CB	37.7	37.3	24.6
	250	CG	37.7	35.8	24.5
	250	CD1*	38.6	35.3	23.5
	250	CD2*	38.1	35.2	25.9
	250	C	38.2	39.0	22.9
	250	O	38.0	38.7	21.7
GLN	251	N	37.9	40.2	23.4
	251	CA	37.3	41.2	22.6
	251	CB	36.7	42.3	23.5
	251	CG	36.1	41.8	24.7
	251	CD	34.5	41.6	24.6
	251	OE1	33.9	41.5	25.6
	251	NE2	34.0	41.5	23.4
	251	C	38.3	41.7	21.6
	251	O	38.1	41.9	20.4
ASN	252	N	39.5	42.0	22.1
	252	CA	40.6	42.5	21.3
	252	CB	41.5	43.4	22.1

Table I (continued)

	252	CG	40.8	44.0	23.3
	252	OD1	39.6	43.8	23.6
	252	ND2	41.5	44.8	24.2
	252	C	41.6	41.7	20.5
	252	O	42.8	42.1	20.3
THR	253	N	41.2	40.5	20.1
	253	CA	42.1	39.6	19.3
	253	CB	42.8	38.7	20.4
	253	OG1	44.1	39.2	20.4
	253	CG2	42.7	37.3	19.9
	253	C	41.4	38.8	18.2
	253	O	42.1	38.0	17.6
THR	254	N	40.1	39.0	18.1
	254	CA	39.4	38.2	17.1
	254	CB	38.0	38.6	17.1
	254	OG1	37.9	40.0	17.2
	254	CG2	37.2	38.0	18.3
	254	C	39.9	38.5	15.8
	254	O	40.9	39.3	15.6
THR	255	N	39.3	38.0	14.9
	255	CA	39.3	38.2	13.4
	255	CB	39.4	37.0	12.6
	255	OG1	40.5	36.2	13.0
	255	CG2	39.5	37.3	11.1
	255	C	38.2	39.2	13.1
	255	O	37.0	38.9	13.3
LYS	256	N	38.4	40.3	12.5
	256	CA	37.3	41.3	12.1
	256	CB	38.0	42.6	11.7
	256	CG *	38.9	43.4	12.7
	256	CD *	39.4	44.8	12.2
	256	CE *	40.4	45.4	13.2
	256	NZ *	40.9	46.7	12.7
	256	C	36.5	40.7	10.9
	256	O	37.0	40.3	9.9
LEU	257	N	35.2	40.7	11.1
	257	CA	34.3	40.1	10.1
	257	CB	33.4	38.9	10.5
	257	CG	34.5	37.7	10.9
	257	CD1	33.5	36.4	11.0
	257	CD2	35.3	37.5	9.6
	257	C	33.5	41.0	9.4
	257	O	33.5	40.8	8.1
GLY	258	N	33.0	42.0	9.9
	258	CA	32.1	43.0	9.1
	258	C	31.4	43.8	10.1
	258	O	31.4	43.5	11.4
ASP	259	N	30.9	45.0	9.8
	259	CA	30.3	45.8	10.6
	259	CB	29.1	46.5	9.9
	259	CG	28.3	47.4	10.9
	259	OD1	27.7	47.0	11.9
	259	OD2	28.3	48.7	10.8
	259	C	29.8	45.3	11.9
	259	O	29.0	44.3	12.0
SER	260	N	30.2	45.8	13.0
	260	CA	30.0	45.6	14.4
	260	CB	30.0	46.9	15.2
	260	OG	31.3	47.5	14.9
	260	C	28.5	45.0	14.9
	260	O	28.4	44.2	15.8
PHE	261	N	27.4	45.5	14.2
	261	CA	26.1	45.2	14.5
	261	CB	25.3	46.2	13.7
	261	CG	23.9	46.3	14.1
	261	CD1	23.8	47.3	15.2
	261	CE1	22.4	47.7	15.6
	261	CZ	21.3	47.2	14.9
	261	CE2	21.5	46.4	13.7
	261	CD2	22.9	46.1	13.4
	261	C	25.4	43.8	14.0
	261	O	24.5	43.3	14.6
TYR	262	N	26.1	43.3	12.9
	262	CA	25.9	41.9	12.4
	262	CB	25.9	42.0	10.9
	262	CG	24.5	42.7	10.4
	262	CD1	24.5	44.2	10.4
	262	CE1	23.3	44.8	9.9
	262	CZ	22.3	44.0	9.2
	262	OH	21.1	44.5	8.6
	262	CE2	22.4	42.5	9.1
	262	CD2	23.5	42.0	9.8
	262	C	27.0	41.1	12.9
	262	O	26.8	39.9	13.1
TYR	263	N	28.2	41.6	13.2
	263	CA	29.4	40.8	13.5
	263	CB	30.4	41.0	12.3
	263	CG	30.0	40.4	11.0
	263	CD1	30.2	39.1	10.8
	263	CE1	29.9	38.7	9.4
	263	CZ	29.3	39.4	8.4
	263	OH	29.0	39.0	7.2
	263	CE2	29.1	40.8	8.8
	263	CD2	29.3	41.3	10.1
	263	C	30.1	41.0	14.9
	263	O	31.0	40.2	15.1
GLY	264	N	29.9	42.0	15.4
	264	CA	30.5	42.4	16.8
	264	C	32.0	42.6	16.5
	264	O	32.4	43.2	15.4
LYS	265	N	32.8	42.1	17.3
	265	CA	34.3	42.2	17.2
	265	CB	35.0	41.7	18.5
	265	CG	35.0	42.8	19.5
	265	CD	35.2	44.3	19.0
	265	CE *	35.1	45.3	20.2
	265	NZ *	35.4	46.7	19.6
	265	C	34.8	41.3	16.0
	265	O	36.0	41.4	15.7
GLY	266	N	34.0	40.5	15.6
	266	CA	34.3	39.5	14.6
	266	C	34.9	38.1	15.1
	266	O	33.9	37.8	16.1
LEU	267	N	35.6	37.3	14.7
	267	CA	35.8	36.0	15.1
	267	CB	36.2	35.3	13.8
	267	CG	36.3	33.8	13.9
	267	CD1	34.8	33.3	14.0
	267	CD2	37.0	33.1	12.8
	267	C	36.9	35.9	16.0
	267	O	38.0	36.6	15.9
ILE	268	N	36.4	35.1	17.1
	268	CA	37.3	34.8	18.3
	268	CB	36.4	34.3	19.5
	268	CG1	36.3	32.7	19.4
	268	CD1	37.3	32.0	20.4
	268	CG2	35.1	35.0	19.4
	268	C	38.4	33.9	18.0
	268	O	38.2	32.8	17.4
ASN	269	N	39.6	34.3	18.3
	269	CA	40.8	33.5	18.0
	269	CB	41.8	34.3	17.1
	269	CG	43.1	33.5	16.9
	269	OD1	43.4	32.5	17.4
	269	ND2	43.9	34.0	15.9
	269	C	41.4	33.0	19.3
	269	O	42.0	33.9	20.0
VAL	270	N	41.3	31.8	19.6
	270	CA	41.9	31.2	20.8
	270	CB	41.5	29.7	20.9
	270	CG1	41.3	29.2	22.3
	270	CG2	40.4	29.3	19.9
	270	C	43.4	31.4	20.9
	270	O	44.0	31.5	22.0
GLN	271	N	44.0	31.4	19.7
	271	CA	45.5	31.5	19.7
	271	CB	46.0	31.1	18.3
	271	CG	47.4	31.2	18.1
	271	CD	48.0	30.2	17.1
	271	OE1	49.2	29.7	17.3
	271	NE2	47.4	30.0	16.0
	271	C	46.0	33.0	19.9
	271	O	46.9	33.2	20.8
ALA	272	N	45.3	33.9	19.3
	272	CA	45.6	35.3	19.5
	272	CB	44.7	36.2	18.7
	272	C	45.3	35.6	21.1
	272	O	46.1	36.0	21.9
ALA	273	N	44.0	35.4	21.5
	273	CA	43.6	35.6	23.0
	273	CB	42.1	35.2	23.1
	273	C	44.3	34.8	24.1
	273	O	44.4	35.3	25.2
ALA	274	N	44.7	33.6	23.7
	274	CA	45.5	32.8	24.6
	274	CB	45.8	31.5	24.0
	274	C	46.9	33.4	24.9
	274	O	47.2	34.0	26.0
GLN	275	N	47.8	33.4	23.9
	275	CA	49.1	33.9	24.0
	275	CB	49.3	34.4	25.4
	275	CG	49.2	35.8	25.6
	275	CD	50.2	36.5	26.4
	275	OE1	50.4	36.2	27.6
	275	NE2	50.9	37.4	25.9
	275	C	49.9	32.6	23.6
	275	O	51.1	32.6	23.6
	275	O2	49.1	31.6	23.1
	38	WAT	30.6	20.7	12.6
	39	WAT	31.6	21.2	17.7
	76	WAT	23.6	26.3	27.8
	82	WAT	12.0	29.9	24.8
	83	WAT	11.7	33.0	26.6
	84	WAT	13.6	31.9	29.9
	88	WAT	15.9	30.1	24.3
	201	WAT	16.5	27.8	24.4
	202	WAT	19.3	26.9	19.6
	203	WAT	16.9	28.0	16.3
	205	WAT	15.2	29.7	19.6
	302	WAT	12.0	32.0	15.6
	304	WAT	13.0	26.8	23.1
	308	WAT	17.8	32.6	22.4
	309	WAT	32.5	22.7	16.4
	310	WAT	20.7	35.6	25.3
	315	WAT	22.8	21.4	31.6

$$X_{cryst} = (150\ X - 1322)\ 10^{-4}$$

$$Y_{cryst} = (184\ Y - 3999)\ 10^{-4}$$

$$Z_{cryst} = (5\ X + 159\ Z - 1654)\ 10^{-4}$$

where X, Y, and Z are the Cartesian coordinates given in Table 1. The space group is C2, with a = 66.7 Å, b = 54.4 Å, c = 62.9 Å and $\beta = 91.9^\circ$. Atoms for which the F_o-F_c map indicates coordinate errors of more than about 1 Å are labeled with an asterisk (*). Most of these occur in surface side chains that are ill defined in the 2.5 Å PMS•BPN' map. In particular it should be emphasized that residues 98-102 are still very uncertain. Backbone chain torsion angles in degrees are listed in Table 2 with ϕ first, followed by ψ. Nomenclature and torsion angle conventions follow IUPAC-IUB (7) recommendations.

Table II

ALA	1	0	-101	PRO	56	-56	137	ILE	111	-47	-55	GLY	166	-96	-174	SER	221	-101	4
GLN	2	-119	137	ASN	57	-85	-10	GLU	112	-32	-74	TYR	167	-96	145	MET	222	-106	-19
SER	3	-132	130	PHE	58	-109	41	TRP	113	-45	-28	PRO	168	-86	13	ALA	223	-77	-53
VAL	4	-77	107	GLN	59	-133	99	ALA	114	-74	-32	GLY	169	-64	-44	SER	224	-35	-40
PRO	5	-56	127	ASP	60	-116	115	ILE	115	-63	-62	LYS	170	-66	-18	PRO	225	-71	-38
TYR	6	-49	-41	ASP	61	-96	-46	ALA	116	-54	-24	TYR	171	-84	120	HIS	226	-54	-57
GLY	7	-71	-26	ASN	62	-65	-15	ASN	117	-117	34	PRO	172	-53	-10	VAL	227	-42	-55
VAL	8	-68	-45	SER	63	69	-3	ASN	118	54	65	SER	173	-95	9	ALA	228	-59	-31
SER	9	-66	-40	HIS	64	-84	-29	MET	119	-79	149	VAL	174	-105	158	GLY	229	-88	-45
GLN	10	-61	-11	GLY	65	-50	-75	ASP	120	-110	-33	ILE	175	-108	108	ALA	230	-43	-47
ILE	11	-112	-37	THR	66	-45	-53	VAL	121	-127	132	ALA	176	-95	132	ALA	231	-54	-55
LYS	12	96	51	HIS	67	-44	-59	ILE	122	-120	132	VAL	177	-113	116	ALA	232	-32	-59
ALA	13	-69	-26	VAL	68	-60	-64	ASN	123	-131	120	GLY	178	-81	149	LEU	233	-77	-15
PRO	14	-76	-14	ALA	69	-44	10	MET	124	-119	103	ALA	179	-106	138	ILE	234	-70	-56
ALA	15	-66	-46	GLY	70	-115	-26	SER	125	-101	54	VAL	180	-117	165	LEU	235	-56	-29
LEU	16	-79	-24	THR	71	-79	-34	LEU	126	-139	-167	ASP	181	-100	-165	SER	236	-67	-34
HIS	17	-70	-49	VAL	72	-50	-61	GLY	127	153	-177	SER	182	-69	-9	LYS	237	-81	-55
SER	18	-79	7	ALA	73	-165	56	GLY	128	-162	-179	SER	183	-107	9	HIS	238	-106	56
GLN	19	-99	-15	ALA	74	-61	145	PRO	129	-81	-29	ASN	184	59	26	PRO	239	-57	-1
GLY	20	111	-19	LEU	75	24	-173	SER	130	-103	147	GLN	185	-75	142	ASN	240	-101	-21
TYR	21	-89	122	ASN	76	180	80	GLY	131	-101	-140	ARG	186	-81	130	TRP	241	-49	151
THR	22	-128	1	ASN	77	-177	-138	SER	132	163	134	ALA	187	-58	132	THR	242	-75	161
GLY	23	84	41	SER	78	-122	46	ALA	133	-52	-46	SER	188	-46	-38	ASN	243	-63	-32
SER	24	-51	-59	ILE	79	-151	169	ALA	134	-70	-56	PHE	189	-91	11	THR	244	-85	-37
ASN	25	-87	22	GLY	80	27	-125	LEU	135	-33	-67	SER	190	-88	129	GLN	245	-49	-44
VAL	26	-102	142	VAL	81	-112	-128	LYS	136	-64	-24	SER	191	-54	160	VAL	246	-67	-32
LYS	27	-122	132	LEU	82	-167	104	ALA	137	-54	-68	VAL	192	-138	139	ARG	247	-70	-58
VAL	28	-110	131	GLY	83	-69	166	ALA	138	-63	-41	GLY	193	-179	169	SER	248	-41	-51
ALA	29	-100	129	VAL	84	-102	-11	VAL	139	-47	-39	PRO	194	-69	-26	SER	249	-67	-8
VAL	30	-99	100	ALA	85	-126	64	ASP	140	-67	-59	GLU	195	-100	3	LEU	250	-101	-39
ILE	31	-93	92	PRO	86	-55	-8	LYS	141	-38	-62	LEU	196	-88	111	GLN	251	-70	-47
ASP	32	-145	-127	SER	87	-121	-5	ALA	142	-58	-34	ASP	197	-82	-64	ASN	252	-86	28
SER	33	-123	-1	SER	88	-52	168	VAL	143	-73	-25	VAL	198	-138	173	THR	253	-144	2
GLY	34	155	-165	ALA	89	-105	122	ALA	144	-73	-51	MET	199	-111	147	THR	254	-66	-172
ILE	35	173	106	LEU	90	-116	118	SER	145	-65	-44	ALA	200	-161	162	THR	255	-95	118
ASP	36	-77	128	TYR	91	-105	108	GLY	146	137	36	PRO	201	-42	94	LYS	256	-67	128
SER	37	-90	-10	ALA	92	-76	96	VAL	147	-109	144	GLY	202	-119	-6	LEU	257	-113	-38
SER	38	-99	18	VAL	93	-103	116	VAL	148	-98	109	VAL	203	-106	138	GLY	258	167	162
HIS	39	-78	109	LYS	94	-100	127	VAL	149	-90	113	SER	204	33	62	ASP	259	-21	126
PRO	40	-44	-23	VAL	95	-138	-2	VAL	150	-120	125	ILE	205	-102	110	SER	260	-30	-43
ASP	41	-92	-6	LEU	96	-95	134	ALA	151	-137	168	GLN	206	-85	128	PHE	261	-78	-19
LEU	42	-113	146	GLY	97	-86	138	ALA	152	-77	143	SER	207	-147	-172	TYR	262	-98	-35
LYS	43	-125	109	ASP	98	-38	145	ALA	153	-88	-33	THR	208	-73	149	TYR	263	-121	-20
VAL	44	-101	143	ALA	99	83	-26	GLY	154	132	156	LEU	209	-146	139	GLY	264	70	-138
ALA	45	-98	-34	GLY	100	123	31	ASN	155	-101	49	PRO	210	-55	154	LYS	265	-67	-21
GLY	46	167	-149	SER	101	-64	124	GLU	156	-104	-148	GLY	211	81	67	GLY	266	112	-134
GLY	47	156	-124	GLY	102	-109	62	GLY	157	-148	-114	ASN	212	48	56	LEU	267	-109	133
ALA	48	159	161	GLN	103	-102	103	SER	158	-96	177	LYS	213	-148	174	ILE	268	-74	127
SER	49	-106	137	TYR	104	-45	-28	THR	159	177	97	TYR	214	-156	158	ASN	269	-112	110
MET	50	-99	21	SER	105	-71	-24	GLY	160	46	-110	GLY	215	-169	172	VAL	270	-61	-30
VAL	51	-108	111	TRP	106	-79	-41	SER	161	-136	-6	ALA	216	-115	145	GLN	271	-75	-48
PRO	52	-38	-43	ILE	107	-61	-56	SER	162	-72	-162	TYR	217	-136	157	ALA	272	-60	-60
SER	53	-98	-6	ILE	108	-56	-58	SER	163	-124	136	ASN	218	-113	123	ALA	273	-58	-33
GLU	54	-111	83	ASN	109	-55	-28	THR	164	-111	15	GLY	219	-176	134	ALA	274	-64	-73
THR	55	-41	-84	GLY	110	-53	-68	VAL	165	-73	138	THR	220	-59	-10	GLN	275	127	0

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