ATOMIC CO-ORDINATES FOR TOSYL-α-CHYMOTRYPSIN

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In previous reports the crystal structure of tosyl-α-chymotrypsin has been described (1, 2). Recalculation of the phase angles following further refinement of the heavy atom parameters has resulted in a greatly improved electron density map, which has enabled a more detailed and more certain interpretation to be made.

A model of tosyl-α-chymotrypsin was built with Kendrew-Watson skeletal models (Cambridge Repetition Engineers, Greens Road, Cambridge). The use of an optical device described by Richards (3) made it possible to fit the model very precisely to the electron-density map. The model was first built to fit the electron-density distribution obtained by averaging the electron-densities corresponding to each of the two crystallographically independent molecules in the asymmetric unit of the crystal. The model was then adjusted to eliminate short interatomic contact distances, and where difficulties of interpretation arose, reference was made to the electron-density maps for the individual molecules.

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The polypeptide backbone seems to assume different conformations in the two molecules in two places - at residues 9-13 and 73-77. These differences appear to be due to intermolecular contacts. Elsewhere, the only differences between the molecules are in the orientations of side-chains on the surface of the molecule. In these ambiguous regions the model has been made to conform to the more clearly indicated alternative. In the few cases where neither molecule indicated the conformation of a side chain, the fully extended chain conformation was chosen.

Although the process of perfecting the model can be continued further, it seems unlikely, except in the regions referred to, that atomic positions would be changed by as much as an Angstrom unit. The co-ordinates given in table I have been obtained directly from the model. Due to the considerable uncertainty about residues 9-13, they have been omitted. Model-building computer programs (4 ; M. Levitt, personal communication) have been used for checking the co-ordinates. The co-ordinates are measured in $\mathring{A}$, on a Cartesian reference system whose x, y, and z axes are parallel to the crystallographic directions a^{*}, b, and c for one of the molecules (Molecule 1). The origin of the co-ordinates is on a non-crystallographic two-fold axis at the level $x_{crystallographic} = 0$. Thus the line $y = 0$, $z = 0$ in the Cartesian system represents one of the non-crystallographic two-fold axes (Dyad A, see ref. 2). The amino acid sequence is due to Hartley (5 - 7).

A full description of the molecular structure corresponding to table I is in preparation.

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TABLE I

	1	N	6.6	-5.4	31.4		24	N	2.4	-15.9	15.6		37	OG1	-0.8	5.6	0.0		51	CD1	4.6	7.5	25.1
CYS	1	SG	9.8	-4.5	30.3	PRO	24	CD	2.1	-17.2	15.0		37	CB	-2.2	6.1	-0.1		51	CG	5.2	7.4	24.9
	1	CB	7.9	-4.2	29.5		24	CG	3.6	-17.1	14.4		37	CA	-3.0	5.9	1.3		51	CB	5.5	6.2	24.1
	1	CA	7.1	-5.3	30.0		24	CB	0.0	-15.7	14.8		37	C	-3.3	4.5	1.4		51	CA	4.4	5.7	23.2
	1	C	7.9	-6.6	29.5		24	CA	1.3	-15.0	15.5		37	O	-4.0	3.7	0.8		51	C	5.1	4.8	22.4
	1	O	8.5	-7.3	30.3		24	C	0.9	-14.5	16.9		38	N	-2.6	4.1	2.6		51	O	5.2	3.5	22.7
	2	N	7.9	-6.7	28.3		24	O	0.4	-15.5	17.8	GLY	38	CA	-2.7	2.8	3.3		52	N	6.0	5.2	21.6
GLY	2	CA	8.5	-7.8	27.3		25	N	1.0	-13.2	17.2		38	C	-1.5	1.9	3.4	VAL	52	CG2	4.4	3.6	19.3
	2	C	8.5	-9.3	27.7	GLY	25	CA	0.6	-12.7	18.5		38	O	-1.8	0.8	3.8		52	CG1	6.7	3.2	18.2
	2	O	9.3	-10.1	27.6		25	C	2.0	-12.7	19.5		39	N	-0.3	2.3	3.0		52	CB	5.8	4.3	19.1
	3	N	7.2	-9.6	28.3		25	O	1.9	-12.3	20.7	PHE	39	CD2	4.0	0.9	1.5		52	CA	6.4	4.5	20.5
VAL	3	CG2	7.7	-10.7	30.9		26	N	2.9	-13.4	18.8		39	CE2	4.9	-0.1	1.3		52	C	7.8	4.8	19.9
	3	CG1	5.9	-12.4	30.5	SER	26	OG	5.9	-14.5	17.9		39	CZ	4.6	-1.4	1.2		52	O	7.8	5.8	19.9
	3	CB	6.4	-11.0	30.1		26	CB	5.0	-14.9	18.9		39	CE1	3.3	-1.8	1.4		53	N	8.8	4.3	19.7
	3	CA	6.6	-11.0	28.5		26	CA	4.2	-13.9	19.7		39	CD1	2.3	-0.9	1.5	VAL	53	CG2	12.5	4.7	18.9
	3	C	5.5	-11.3	27.7		26	C	5.1	-12.7	19.6		39	CG	2.6	0.5	1.6		53	CG1	11.6	2.7	20.1
	3	O	4.4	-11.2	28.3		26	O	6.2	-13.1	20.2		39	CB	1.4	1.5	1.7		53	CB	11.4	4.1	19.8
	4	N	5.7	-11.8	26.5		27	N	5.0	-11.5	19.1		39	CA	0.8	1.3	3.1		53	CA	10.0	4.3	19.1
PRO	4	CD	7.0	-11.9	25.8	TRY	27	CD2	8.8	-11.8	18.3		39	C	2.0	1.4	4.2		53	C	10.1	3.8	17.7
	4	CG	6.6	-12.4	24.3		27	CE3	9.6	-11.6	19.3		39	O	2.1	2.5	4.6		53	O	9.8	2.6	17.7
	4	CB	5.1	-12.6	24.2		27	CZ3	10.9	-12.4	19.5		40	N	2.6	0.3	4.6		54	N	10.7	4.3	16.6
	4	CA	4.5	-12.1	25.6		27	CEE2	11.2	-13.4	18.7	HIS	40	CD2	6.3	-2.3	6.1	THR	54	CG2	10.2	5.6	14.1
	4	C	3.6	-13.1	26.1		27	CZ2	10.4	-13.7	17.7		40	NE2	7.0	-2.2	7.3		54	OG1	10.7	3.5	13.1
	4	O	4.0	-14.1	26.7		27	CE2	9.1	-12.9	17.4		40	CE1	6.1	-1.9	8.2		54	CB	10.3	4.2	14.2
	5	N	2.3	-12.9	25.9		27	NE1	8.1	-13.0	16.4		40	ND1	4.9	-1.8	7.7		54	CA	11.2	3.7	15.4
ALA	5	CB	0.1	-13.6	26.9		27	CD1	7.2	-12.0	16.7		40	CG	5.0	-1.7	6.4		54	C	12.5	4.6	15.1
	5	CA	1.5	-14.0	26.5		27	CG	7.7	-11.2	17.8		40	CB	3.9	-1.4	5.3		54	O	13.3	5.1	16.0
	5	C	1.9	-15.2	25.6		27	CB	7.0	-10.1	18.2		40	CA	3.7	0.1	5.4		55	N	12.9	4.5	13.8
	5	O	1.4	-16.3	26.0		27	CA	5.9	-10.3	19.3		40	C	5.0	0.6	4.8	ALA	55	CB	15.1	4.2	12.5
	6	N	1.7	-15.0	24.3		27	C	5.0	-9.0	19.6		40	O	5.4	0.1	3.7		55	CA	14.3	5.1	13.3
ILE	6	CD1	-0.9	-14.6	24.7		27	O	4.8	-8.3	18.7		41	N	5.6	1.5	5.5		55	C	13.9	6.2	12.4
	6	CG1	-0.4	-15.2	22.2		28	N	4.4	-9.1	20.7	PHE	41	CD2	4.7	4.4	5.6		55	O	12.8	6.3	11.8
	6	CB	1.2	-15.2	21.8	PRO	28	CD	4.7	-10.1	21.8		41	CE2	4.3	5.4	6.8		56	N	14.8	7.1	12.5
	6	CG2	1.4	-16.2	20.8		28	CG	3.9	-9.8	22.9		41	CZ	5.3	6.2	7.6	ALA	56	CB	16.0	9.1	12.7
	6	CA	1.8	-15.8	23.2		28	CB	3.1	-8.5	22.6		41	CE1	6.6	5.7	7.5		56	CA	14.7	8.4	12.1
	6	C	3.4	-15.8	23.2		28	CA	3.2	-8.2	21.2		41	CD1	7.1	5.0	6.4		56	C	14.7	8.8	10.5
	6	O	4.0	-14.9	22.9		28	C	3.5	-6.9	20.7		41	CG	6.0	4.6	5.5		56	O	13.8	9.4	10.2
	7	N	4.0	-16.9	23.7		28	O	2.6	-6.1	20.7		41	CB	6.7	3.4	4.5		57	N	15.6	8.2	9.9
GLN	7	NOE2	5.5	-18.8	28.1		29	N	4.8	-6.4	20.7		41	CA	6.9	2.2	4.9	HIS	57	CD2	15.9	5.6	6.3
	7	NOE1	6.8	-19.8	26.3	THY	29	CD2	7.8	-6.9	22.2		41	C	8.1	2.0	6.0		57	NE2	15.6	4.3	6.4
	7	CD	6.0	-19.0	27.8		29	CE3	7.3	-7.3	23.5		41	O	9.3	2.2	5.6		57	CE1	16.1	3.6	7.4
	7	CG	5.2	-18.0	26.0		29	CZ3	7.8	-8.5	24.0		42	N	7.9	1.8	7.2		57	ND1	16.8	4.7	8.1
	7	CB	6.0	-18.0	24.7		29	CEE2	8.8	-9.2	23.4	CYS	42	SG	11.0	3.5	7.7		57	CG	16.6	5.8	7.4
	7	CA	5.5	-16.9	23.7		29	CZ2	9.4	-8.8	22.0		42	CB	9.9	2.6	8.7		57	CB	17.1	7.3	7.9
	7	C	6.0	-17.1	22.1		29	CE2	8.9	-7.7	21.6		42	CA	9.0	1.4	8.1		57	CA	15.7	8.1	8.4
	7	O	5.4	-17.9	21.8		29	NE1	9.1	-6.9	20.3		42	C	8.4	0.7	9.4		57	C	14.3	7.9	7.8
	8	N	7.0	-16.6	21.7		29	CD1	8.2	-5.8	20.1		42	O	7.2	0.4	9.5		57	O	14.2	8.5	6.8
PRO	8	CD	7.9	-15.6	22.4		29	CG	7.4	-5.7	21.3		43	N	9.4	0.0	10.1		58	N	13.3	7.3	8.4
	8	CG	9.0	-15.2	21.3		29	CB	6.3	-4.8	21.7	GLY	43	CA	9.1	-0.9	11.2	CYS	58	SG	12.2	4.5	8.9
	8	CB	8.8	-15.6	20.1		29	CA	5.1	-5.1	20.7		43	C	9.3	-2.1	12.5		58	CB	11.3	6.2	9.0
	8	CA	7.5	-16.8	20.3		29	C	5.3	-4.5	19.2		43	O	9.9	0.9	12.6		58	CA	12.0	7.2	8.1
	8	C	8.1	-18.3	20.3		29	O	5.3	-3.4	19.1		44	N	8.6	-0.5	13.7		58	C	13.8	8.2	7.8
	8	O	8.9	-18.7	21.0		30	N	5.4	-5.2	18.2	GLY	44	CA	8.7	-2.1	15.0		58	O	9.7	7.7	7.5
	16	N	13.1	-8.7	5.6	GLN	30	NOE2	7.3	-4.1	13.9		44	C	8.2	-0.8	16.1		59	N	11.0	9.4	8.1
ILE	16	CD1	13.6	-9.7	10.1		30	NOE1	8.0	-6.2	14.2		44	O	7.6	-1.8	15.6	GLY	59	CA	10.1	10.6	7.8
	16	CG1	13.9	-9.0	8.7		30	CD	7.2	-5.4	14.1		45	N	8.3	-0.5	17.2		59	C	8.7	10.4	8.5
	16	CB	13.8	-10.1	7.7		30	CG	5.7	-5.8	14.5	SER	45	OG	10.1	-2.5	18.4		59	O	7.7	11.7	7.8
	16	CG2	14.8	-11.3	8.0		30	CB	5.5	-6.1	16.0		45	CB	9.3	-1.7	19.2		60	N	8.7	9.7	9.7
	16	CA	14.2	-9.4	6.2		30	CA	5.5	-4.9	16.8		45	CA	7.9	-1.2	18.5	VAL	60	CG2	8.0	7.4	10.8
	16	C	14.4	-10.7	5.3		30	C	4.2	-4.2	16.3		45	C	7.6	-0.4	19.7		60	CG1	5.9	8.3	11.9
	16	O	13.7	-11.8	4.9		30	O	3.0	-4.5	16.2		45	O	8.5	0.5	20.2		60	CB	7.3	8.7	11.4
	17	N	15.7	-10.8	4.8		31	N	4.4	-3.1	15.8		46	N	6.6	-0.7	20.5		60	CA	7.2	9.8	10.2
VAL	17	CG2	16.4	-9.8	2.4	VAL	31	CG2	5.0	-0.2	15.7	LEU	46	CD2	3.0	1.2	21.2		60	C	6.7	11.1	10.4
	17	CG1	17.4	-12.0	1.7		31	CG1	3.1	-0.7	17.3		46	CD1	2.5	-1.5	21.4		60	O	7.4	12.0	10.9
	17	CB	17.1	-11.2	2.8		31	CB	3.6	-0.7	15.8		46	CG	3.6	-0.2	21.1		61	N	5.4	11.4	9.9
	17	CA	16.1	-11.8	3.9		31	CA	3.5	-2.1	15.0		46	CB	4.7	-0.9	22.1	THR	61	CG2	5.6	13.2	7.7
	17	C	16.7	-13.1	4.5		31	C	4.2	-2.0	13.8		46	CA	6.0	-0.3	21.7		61	OG1	3.5	12.4	8.0
	17	O	17.7	-13.2	5.2		31	O	5.3	-2.4	13.5		46	C	6.8	-0.7	22.9		61	CB	4.4	13.1	8.7
	18	N	16.0	-14.1	4.2		32	N	3.4	-1.4	12.7		46	O	6.9	-2.0	23.0		61	CA	4.7	12.6	10.0
ASN	18	NOD2	18.4	-18.3	4.0	SER	32	OG	2.4	-1.7	9.3		47	N	7.0	0.2	23.7		61	C	3.6	12.2	11.1
	18	NOD1	16.7	-16.3	5.5		32	CB	2.3	-1.8	10.8	ILE	47	CD1	9.6	3.9	24.4		61	O	2.9	11.1	11.0
	18	CG	17.5	-17.7	4.5		32	CA	3.6	-1.2	11.3		47	CG1	8.4	2.7	24.4		62	N	2.9	13.3	11.7
	18	CB	17.4	-16.2	4.1		32	C	3.3	0.2	11.1		47	CB	8.9	1.4	24.9	THR	62	CG2	3.1	14.3	14.1
	18	CA	16.1	-15.6	4.7		32	O	2.3	0.7	11.4		47	CG2	10.1	1.0	24.1		62	OG1	2.5	15.0	13.8
	18	C	15.9	-15.7	6.2		33	N	4.2	1.0	10.3		47	CA	7.8	0.4	24.9		62	CB	1.5	14.4	13.2
	18	O	16.8	-16.0	7.1	LEU	33	CD2	3.9	3.5	11.7		47	C	6.9	1.0	26.2		62	CA	1.7	13.1	12.5
	19	N	14.7	-15.6	6.5		33	CD1	6.7	4.0	12.2		47	O	7.0	0.9	27.5		62	C	0.7	12.4	11.6
GLY	19	CA	14.1	-15.7	7.8		33	CG	5.3	3.7	11.7		48	N	5.8	1.7	25.9		62	O	-0.5	12.0	12.1
	19	C	12.8	-16.4	7.7		33	CB	5.3	3.1	10.1	ASN	48	NOD2	5.4	3.7	29.2		63	N	0.7	12.6	10.3
	19	O	12.5	-17.3	7.0		33	CA	4.0	2.4	9.8		48	NOD1	6.0	4.9	27.7	SER	63	OG	-1.5	12.5	7.2
	20	N	11.8	-16.3	8.7		33	C	3.4	2.3	8.4		48	CG	5.4	3.9	27.9		63	CB	-0.3	12.8	7.9
GLU	20	OE2	12.9	-20.6	12.0		33	O	4.0	1.8	7.5		48	CB	4.5	3.2	27.0		63	CA	-0.4	12.2	9.2
	20	OE1	10.9	-20.1	12.3		34	N	2.2	2.8	8.3		48	CA	4.6	1.8	26.6		63	C	-0.4	10.6	9.0
	20	CD	11.9	-19.8	11.6	GLN	34	NOE2	-2.2	-0.3	7.3		48	C	3.3	1.6	25.8		63	O	-1.5	10.2	8.6
	20	CG	12.0	-18.9	10.2		34	NOE1	-2.6	1.6	7.0		48	O	3.4	1.3	24.5		64	N	0.6	9.7	9.1
	20	CB	10.7	-18.2	10.1		34	CD	-1.9	0.9	7.1		49	N	2.3	1.7	26.3	ASP	64	OD2	3.9	9.0	7.7
	20	CA	10.6	-17.1	9.0		34	CG	-0.4	1.1	7.1	GLU	49	OE2	-2.6	1.2	29.2		64	OD1	2.0	9.1	7.0
	20	C	9.2	-16.3	9.4		34	CB	-0.1	2.6	7.5		49	OE1	-2.1	-0.7	28.4		64	CG	2.8	8.8	7.7
	20	O	9.3	-15.2	9.9		34	CA	1.4	3.2	7.2		49	CD	-2.1	0.6	28.3		64	CB	2.1	7.9	9.0
	21	N	8.2	-16.9	9.3		34	C	1.2	4.8	6.9		49	CG	-1.5	1.2	27.1		64	CA	0.6	6.4	8.9
GLU	21	OF2	1.9	-17.4	9.5		34	O	1.0	5.4	7.9		49	CB	0.1	1.8	27.3		64	C	-0.1	7.9	10.3
	21	OE1	3.3	-18.3	8.0		35	N	1.5	4.9	5.7		49	CA	0.8	1.9	26.0		64	O	-0.7	8.6	11.2
	21	CD	3.1	-17.6	9.1	ASP	35	OD2	1.6	5.3	1.2		49	C	0.5	3.3	25.2		65	N	-0.2	6.6	10.2
	21	CG	4.3	-16.8	9.8		35	OD1	3.1	5.4	2.8		49	O	-0.3	3.1	24.3	VAL	65	CG2	-3.3	6.1	10.6
	21	CB	5.6	-17.3	9.3		35	CG	1.9	5.5	2.4		50	N	1.1	4.3	25.5		65	CG1	-2.6	4.4	12.2
	21	CA	6.8	-16.6	9.8		35	CB	0.6	5.6	3.4	ASN	50	NOD2	-0.3	5.5	28.3		65	CB	-2.1	5.1	11.4
	21	C	6.9	-16.9	11.4		35	CA	1.1	6.1	4.7		50	NOD1	-1.2	6.9	26.8		65	CA	-1.8	5.7	11.4
	21	O	7.0	-18.1	11.9		35	C	-0.5	6.5	5.2		50	CG	-0.3	6.2	27.2		65	C	0.1	4.7	11.7
	22	N	7.0	-15.8	12.0		35	O	-1.0	6.1	6.2		50	CB	1.0	6.5	26.3		65	O	0.8	4.2	11.1
ALA	22	CB	6.6	-14.3	14.0		36	N	-1.1	7.3	4.3		50	CA	1.1	5.5	25.2		66	N	-0.1	4.6	13.0
	22	CA	6.9	-15.6	13.5	LYS	36	NZ	2.2	10.6	4.8		50	C	2.1	6.0	24.1	VAL	66	CG2	1.7	4.8	15.3
	22	C	5.6	-16.1	13.9		36	CE	0.8	11.1	5.2		50	O	1.9	7.1	23.6		66	CG1	1.5	2.4	15.8
	22	O	4.5	-16.1	13.5		36	CD	-0.1	10.6	4.6		51	N	3.1	5.4	23.9		66	CB	0.7	3.5	15.2
	23	N	5.6	-16.4	15.3		36	CG	-1.5	10.1	5.1	TRY	51	CD2	5.7	8.8	24.7		66	CA	0.4	3.2	13.8
VAL	23	CG2	5.4	-18.8	16.4		36	CB	-2.6	9.3	4.1		51	CE3	6.3	9.4	23.6		66	C	-0.6	1.9	13.8
	23	CG1	3.2	-18.5	17.6		36	CA	-2.4	7.7	4.4		51	CZ3	6.6	10.8	23.7		66	O	-1.7	2.3	14.4
	23	CB	4.4	-17.7	17.1		36	C	-3.1	7.0	3.2		51	CEE2	6.3	11.6	24.7		67	N	-0.2	1.8	13.5
	23	CA	4.2	-16.7	15.9		36	O	-4.3	6.8	3.4		51	CZ2	5.7	11.0	25.8	VAL	67	CG2	-1.5	0.6	11.2
	23	C	3.5	-15.6	16.3		37	N	-2.4	6.5	2.4		51	CE2	5.3	9.6	25.9		67	CG1	-2.3	-1.9	11.7
	23	O	3.8	-14.6	16.8	THR	37	CG2	-2.2	7.5	-0.7		51	NE1	4.6	8.9	26.7		67	CB	-1.2	-0.7	11.9

Table I (continued)

	67	CA	-1.0	-0.3	13.3		82	CG	-6.2	0.2	11.8		95	CB	24.3	12.4	11.1		109	O	-4.3	9.7	22.8
	67	C	-0.3	-1.3	14.4		82	CB	-6.1	1.2	13.0		95	CA	23.0	12.9	10.6		110	N	-4.7	8.1	21.2
	67	O	1.0	-1.5	14.3		82	CA	-4.8	1.1	13.8		95	C	22.8	12.5	9.2	THR	110	CG2	-7.6	6.2	22.9
	68	N	-1.1	-2.0	15.4		82	C	-4.8	2.4	14.7		95	O	23.4	11.4	8.7		110	OG1	-7.0	8.4	21.5
ALA	68	CB	-0.5	-2.3	17.7		82	O	-5.9	2.9	14.9		96	N	21.9	13.1	8.4		110	CB	-6.5	6.9	21.8
	68	CA	-0.6	-3.0	16.3		83	N	-3.8	3.1	15.2	SER	96	OG	20.6	15.6	7.3		110	CA	-5.1	7.2	22.3
	68	C	-1.5	-4.3	16.5	LEU	83	CD2	-4.9	2.6	18.3		96	CB	21.7	14.8	6.8		110	C	-4.2	6.0	22.5
	68	O	-2.8	-4.0	16.2		83	CD1	-2.8	1.6	19.1		96	CA	21.7	13.2	7.0		110	O	-3.7	5.3	21.4
	69	N	-1.1	-5.3	17.1		83	CG	-3.5	2.3	17.9		96	C	22.8	12.7	6.1		111	N	-3.7	5.8	23.7
GLY	69	CA	-1.9	-6.6	17.2		83	CB	-2.9	3.8	17.4		96	O	22.4	12.6	5.0	ALA	111	CB	-4.3	4.4	25.1
	69	C	-2.0	-6.9	15.7		83	CA	-3.7	4.2	16.0		97	N	24.0	12.6	6.5		111	CA	-3.1	4.7	24.1
	69	O	-2.9	-7.5	15.3		83	C	-2.9	5.3	15.6	LEU	97	CD2	24.0	13.8	3.5		111	C	-3.2	3.5	23.2
	70	N	-1.0	-6.8	14.9		83	O	-1.9	5.3	14.9		97	CD1	25.6	15.8	3.9		111	O	-4.4	3.3	22.7
GLU	70	OE2	-2.4	-4.8	9.4		84	N	-3.7	6.4	15.8		97	CG	25.0	14.4	4.4		112	N	-2.4	2.5	23.2
	70	OE1	-0.3	-4.3	9.8	LYS	84	NZ	-9.5	9.1	13.6		97	CB	25.9	13.2	5.1	ALA	112	CB	-1.6	3.2	22.2
	70	CD	-1.3	-5.0	10.2		84	CE	-8.1	8.3	13.7		97	CA	25.0	12.1	5.5		112	CA	-2.7	1.1	22.9
	70	CG	-1.3	-6.1	11.2		84	CD	-7.0	9.1	14.7		97	C	25.8	10.9	6.0		112	C	-3.2	1.2	24.1
	70	CB	-1.0	-5.8	12.6		84	CG	-5.7	8.2	14.4		97	O	26.6	10.4	5.3		112	O	-2.7	0.2	25.3
	70	CA	-1.1	-7.1	13.3		84	CB	-4.6	8.7	15.4		98	N	25.7	10.5	7.2		113	N	-4.2	-0.4	23.7
	70	C	-0.3	-8.2	12.9		84	CA	-3.4	7.9	15.3	THR	98	CG2	28.0	9.6	10.1	SER	113	OG	-6.6	-2.0	23.3
	70	O	1.0	-8.3	13.1		84	C	-2.4	8.4	16.4		98	OG1	27.9	11.2	8.4		113	CB	-6.1	-1.8	24.7
	71	N	-0.9	-8.8	12.1		84	O	-2.5	8.3	17.6		98	CB	27.1	10.3	9.1		113	CA	-4.6	-1.5	24.6
PHE	71	CD2	-1.1	-13.5	10.8		85	N	-1.3	8.9	15.8		98	CA	26.4	9.5	8.1		113	C	-3.9	-2.8	24.0
	71	CE2	-0.4	-14.7	10.3	ILE	85	CD1	2.6	7.9	14.1		98	C	25.3	8.4	8.3		113	O	-3.9	-3.6	23.0
	71	CZ	1.1	-14.6	10.5		85	CG1	1.2	8.0	15.0		98	O	25.5	7.3	8.4		114	N	-3.4	-3.4	25.2
	71	CE1	1.7	-13.6	11.2		85	CB	1.1	9.5	15.5		99	N	24.2	8.9	8.8	PHE	114	CD2	-2.8	-3.3	27.4
	71	CD1	1.0	-12.6	11.7		85	CG2	2.7	10.5	15.7	ILE	99	CD1	22.3	8.2	6.4		114	CE2	2.0	-2.2	26.6
	71	CG	-0.5	-12.5	11.5		85	CA	-0.2	9.6	16.4		99	CG1	22.9	7.1	7.2		114	CZ	2.3	-1.8	25.1
	71	CB	-1.2	-11.4	12.1		85	C	-0.6	11.1	16.4		99	CB	22.8	6.9	8.7		114	CE1	0.9	-2.0	24.4
	71	CA	-0.4	-10.1	11.4		85	O	-1.5	11.7	15.7		99	CG2	21.3	6.6	9.2		114	CD1	-0.1	-2.8	24.7
	71	C	-0.4	-10.0	9.9		86	N	-0.1	11.7	17.5		99	CA	23.0	8.2	9.4		114	CG	-0.2	-3.2	26.1
	71	O	0.8	-9.7	9.4	ALA	86	CB	-0.3	13.2	19.6		99	C	23.4	7.8	10.9		114	CB	-1.3	-4.2	26.6
	72	N	-1.4	-10.0	9.1		86	CA	-0.2	13.2	18.1		99	O	22.9	6.6	11.3		114	CA	-2.3	-4.6	25.6
ASP	72	OD2	-1.9	-12.4	5.1		86	C	1.1	13.9	17.7		100	N	24.1	8.5	11.6		114	C	-3.5	-5.4	25.9
	72	OD1	-2.6	-10.6	4.7		86	O	1.1	14.8	17.0	ASN	100	ND2	26.7	9.2	15.4		114	O	-4.6	-5.5	26.6
	72	CG	-2.1	-11.2	5.6		87	N	2.2	13.5	18.5		100	OD1	26.2	7.0	14.7		115	N	-3.2	-6.7	25.3
	72	CB	-1.6	-11.2	7.0	LYS	87	NZ	5.5	19.1	21.6		100	CG	26.3	8.4	14.5	SER	115	OG	-4.9	-7.6	23.1
	72	CA	-1.4	-9.9	7.7		87	CE	5.3	18.4	20.5		100	CB	25.8	8.9	13.1		115	CB	-4.9	-7.9	24.3
	72	C	-2.1	-8.8	7.1		87	CD	4.5	17.0	20.7		100	CA	24.3	8.3	13.0		115	CA	-3.9	-8.0	25.4
	72	O	-3.4	-8.6	7.2		87	CG	4.5	16.1	19.4		100	C	23.2	9.1	13.6		115	C	-2.9	-6.2	25.5
	73	N	-1.3	-8.1	6.4		87	CA	3.6	14.2	18.3		100	O	22.8	10.0	12.9		115	O	-1.8	-6.7	24.7
GLN	73	NDE2	2.5	-4.9	7.0		87	CB	3.7	15.0	19.4		101	N	22.8	8.8	14.8		116	N	-3.3	-5.4	25.1
	73	NDE1	2.6	-5.4	4.8		87	C	4.6	13.3	17.9	ASN	101	ND2	23.8	11.3	16.8	GLN	116	NOE2	-5.4	-14.9	26.8
	73	CD	1.9	-5.4	5.8		87	O	4.8	12.2	18.6		101	ND1	23.3	9.8	18.4		116	NDE1	-5.4	-14.1	24.6
	73	CG	0.5	-6.0	6.1		88	N	5.4	13.6	17.0		101	CG	22.9	10.4	17.3		116	CD	-5.0	-13.9	25.8
	73	CB	-0.4	-6.4	4.9	VAL	88	CG2	5.8	12.4	14.2		101	CB	21.6	10.2	16.4		116	CG	-3.9	-13.3	26.0
	73	CA	-1.7	-7.0	5.5		88	CG1	8.3	12.3	14.7		101	CA	21.6	8.9	15.7		116	CB	-3.2	-12.8	24.6
	73	C	-2.7	-7.3	4.5		88	CB	7.0	13.0	15.0		101	C	20.3	8.7	14.8		116	CA	-2.3	-11.5	24.8
	73	O	-3.3	-6.2	4.2		88	CA	6.6	13.0	16.4		101	O	19.5	9.5	14.8		116	C	-1.7	-11.2	23.5
	74	N	-2.9	-8.2	3.7		88	C	7.8	13.6	17.4		102	N	20.2	7.5	14.2		116	O	-0.5	-11.1	23.6
GLY	74	CA	-3.8	-8.4	2.6		88	O	7.9	14.9	17.1	ASP	102	OD2	18.1	5.0	10.7		117	N	-2.1	-10.2	22.5
	74	C	-5.3	-8.9	3.3		89	N	8.4	12.8	18.0		102	OD1	17.5	6.8	11.6	THR	117	CG2	-2.5	-11.2	19.6
	74	O	-6.3	-9.3	2.5	PHE	89	CD2	8.8	14.6	21.8		102	CG	18.4	5.8	11.5		117	OG1	-3.2	-8.8	20.1
	75	N	-5.3	-9.1	4.6		89	CE2	7.8	15.3	22.6		102	CB	19.3	6.2	12.3		117	CB	-2.1	-9.7	20..
SER	75	OG	-6.9	-11.4	6.7		89	CZ	6.8	14.8	22.6		102	CA	18.9	7.3	13.3		117	CA	-1.2	-11.0	21.3
	75	CB	-6.8	-10.0	6.6		89	CE1	6.1	13.7	21.9		102	C	17.9	6.7	14.2		117	C	-0.7	-8.6	21.4
	75	CA	-6.7	-9.4	5.1		89	CD1	7.1	12.9	21.1		102	O	17.5	5.5	14.2		117	O	0.1	-8.3	22.3
	75	C	-7.5	-8.1	4.8		89	CG	8.5	13.4	21.1		103	N	17.4	7.6	15.0		118	N	-0.8	-7.6	22.2
	75	O	-7.2	-7.0	4.7		89	CB	9.6	12.8	20.3	ILE	103	CD1	16.2	5.6	19.4	VAL	118	CG2	-2.2	-5.9	20.6
	76	N	-8.8	-8.5	4.8		89	CA	9.5	13.1	18.8		103	CG1	15.8	6.1	18.0		118	CG1	-0.7	-3.9	21.4
SER	76	OG	-11.2	-9.6	3.6		89	C	10.7	12.7	17.9		103	CB	16.9	6.9	17.3		118	CB	-1.2	-5.3	21.7
	76	CB	-11.4	-8.5	4.6		89	O	11.2	11.6	17.8		103	CG2	17.4	8.1	18.0		118	CA	-0.2	-6.2	22.1
	76	CA	-10.0	-7.6	4.7		90	N	11.2	13.6	17.0		103	CA	16.2	7.4	15.9		118	C	0.3	-5.9	23.5
	76	C	-10.0	-6.9	5.9	LYS	90	NZ	10.8	18.4	12.3		103	C	15.1	8.2	16.2		118	O	-0.2	-6.0	24.6
	76	O	-10.3	-5.6	5.9		90	CE	10.5	16.9	12.6		103	O	15.4	9.4	16.5		119	N	1.6	-5.4	23.5
	77	N	-9.6	-7.5	6.8		90	CD	11.4	16.6	13.9		104	N	13.9	7.8	16.3	SER	119	OG	1.3	-7.4	25.2
SER	77	OG	-10.8	-5.9	10.1		90	CG	11.1	15.2	14.3	THR	104	CG2	12.6	9.8	15.6		119	CB	2.7	-6.7	25.5
	77	CB	-11.1	-6.7	8.8		90	CB	12.2	15.1	15.3		104	OG1	12.7	10.2	14.6		119	CA	2.5	-5.3	24.9
	77	CA	-9.7	-7.1	8.3		90	CA	12.4	13.6	16.1		104	CB	12.1	9.2	15.3		119	C	3.8	-4.8	24.4
	77	C	-9.1	-8.1	9.2		90	C	13.5	13.6	17.2		104	CA	12.8	8.8	16.7		119	O	4.1	-4.7	23.2
	77	O	-9.7	-9.2	9.1		90	O	13.5	14.4	18.1		104	C	11.6	8.0	17.5		120	N	4.6	-4.4	25.4
	78	N	-8.2	-8.1	10.3		91	N	14.5	12.8	17.0		104	O	11.5	6.6	17.4	ALA	120	CB	5.8	-2.4	26.2
GLU	78	OE2	-4.3	-10.2	12.3	ASN	91	ND2	18.3	11.4	19.4		105	N	10.7	8.6	18.3		120	CA	5.9	-3.6	25.2
	78	OE1	-3.9	-11.2	10.7		91	ND1	19.2	12.7	17.8	LEU	105	CD2	12.0	8.7	21.8		120	C	7.1	-4.5	25.5
	78	CD	-4.7	-10.8	11.4		91	CG	18.3	12.1	18.1		105	CD1	10.0	7.1	22.3		120	O	7.0	-5.3	26.2
	78	CG	-6.2	-10.6	10.9		91	CB	17.0	11.9	17.6		105	CG	10.4	8.0	21.8		121	N	8.1	-4.2	24.8
	78	CB	-6.5	-9.3	11.7		91	CA	15.9	13.2	17.7		105	CB	9.5	9.1	20.5	VAL	121	CG2	11.7	-5.5	24..
	78	CA	-8.0	-8.8	11.4		91	C	16.8	14.2	16.9		105	CA	9.6	8.2	19.1		121	CG1	11.7	-3.4	23..
	78	C	-8.3	-7.8	12.5		91	O	17.2	14.0	15.8		105	C	8.3	8.7	18.7		121	CB	10.4	-4.9	23.6
	78	O	-8.8	-6.6	12.3		92	N	17.0	15.2	17.7		105	O	8.3	9.9	18.5		121	CA	9.5	-4.8	24.9
	79	N	-8.2	-8.2	13.8	SER	92	OG	17.8	17.3	20.0		106	N	7.3	7.9	18.8		121	C	10.2	-3.8	26..
LYS	79	NZ	-12.5	-10.3	19.5		92	CB	18.5	16.8	18.8	LEU	106	CD2	6.3	8.8	15.6		121	O	9.5	-2.8	26..
	79	CE	-11.2	-9.2	19.1		92	CA	17.8	16.2	17.6		106	CD1	5.6	6.4	15.2		122	N	11.4	-4.2	26.5
	79	CD	-10.3	-9.5	18.0		92	C	19.3	15.9	16.8		106	CG	6.2	7.4	16.3	CYS	122	SG	10.9	-5.5	29.2
	79	CG	-9.5	-8.4	17.3		92	O	19.8	16.8	16.2		106	CB	5.2	7.4	17.6		122	CB	12.2	-4.6	28.6
	79	CB	-8.8	-8.8	16.1		93	N	19.8	14.9	16.9		106	CA	5.7	8.4	18.7		122	CA	12.0	-3.5	27.6
	79	CA	-8.5	-7.6	15.0	LYS	93	NZ	23.7	18.0	20.3		106	C	5.1	8.5	20.0		122	C	13.2	-2.5	27.9
	79	C	-7.3	-6.7	15.5		93	CE	23.4	16.5	20.0		106	O	5.4	8.2	21.0		122	O	13.5	-2.8	25.8
	79	O	-6.5	-6.9	16.5		93	CD	23.1	16.0	18.6		107	N	4.1	9.5	20.1		123	N	13.8	-1.6	27.6
	80	N	-7.3	-5.6	14.9		93	CG	22.5	14.7	18.7	LYS	107	NZ	2.3	12.3	26.3	LEU	123	CD2	14.3	1.5	25.2
ILE	80	CD1	-6.0	-3.4	11.1		93	CB	22.2	14.2	17.2		107	CE	2.1	12.9	25.2		123	CD1	12.5	1.9	27..
	80	CG1	-6.7	-3.8	12.4		93	CA	21.2	14.9	16.3		107	CD	3.1	12.6	24.0		123	CG	14.0	1.6	26.8
	80	CB	-5.8	-4.5	13.4		93	C	21.4	13.8	15.1		107	CG	2.8	11.3	23.3		123	CB	15.0	0.7	27.5
	80	CG2	-5.4	-5.7	12.9		93	O	22.4	13.2	14.7		107	CA	3.5	9.6	21.4		123	CA	15.0	-0.9	27.4
	80	CA	-6.2	-4.6	14.9		94	N	20.2	13.5	14.4		107	CB	3.6	11.1	21.9		123	C	16.5	-1.2	28.2
	80	C	-6.5	-3.4	15.4	TYR	94	OEE	18.3	9.6	7.8		107	C	1.9	9.7	20.8		123	O	16.6	-1.8	29.3
	80	O	-7.7	-3.1	15.5		94	CD2	18.0	12.4	10.2		107	O	1.8	10.5	19.8		124	N	17.4	-0.9	27.4
	81	N	-5.5	-2.8	16.2		94	CE2	17.9	11.6	9.1		108	N	1.0	8.8	21.1	PRO	124	CD	17.0	-0.2	26.0
GLN	81	NOE2	-5.3	-3.4	20.7		94	CZ	18.4	10.4	8.8	LEU	108	CD2	0.6	6.7	18.3		124	CG	18.4	0.2	25.5
	81	NDE1	-5.3	-1.1	21.2		94	CE1	18.9	9.9	10.1		108	CD1	0.0	4.9	20.0		124	CB	19.5	-0.3	26.3
	81	CD	-5.5	-2.1	20.4		94	CD1	19.0	10.6	11.3		108	CG	0.4	6.2	19.8		124	CA	18.8	-0.9	27.5
	81	CG	-6.0	-2.2	18.9		94	CG	18.6	12.0	11.4		108	CB	-0.7	7.0	20.5		124	C	19.2	0.0	28.6
	81	CB	-4.8	-1.5	18.1		94	CB	18.6	12.7	12.7		108	CA	-0.3	8.5	20.4		124	O	18.4	-0.8	28.9
	81	CA	-5.3	-1.4	16.7		94	CA	20.1	12.8	13.2		108	C	-1.6	9.3	21.0		125	N	20.5	0.0	29.0
	81	C	-4.7	-0.7	15.4		94	C	21.2	13.3	12.1		108	O	-1.6	9.5	22.2	SER	125	OG	19.8	0.0	31.8
	81	O	-3.4	-1.2	15.2		94	O	21.5	14.6	12.1		109	N	-2.4	9.5	20.1		125	CB	21.1	-0.5	31.5
	82	N	-5.1	0.3	15.0		95	N	21.9	12.4	11.5	SER	109	OG	-5.9	10.8	19.2		125	CA	21.1	1.1	30.3
LYS	82	NZ	-9.2	0.2	9.2	ASN	95	ND2	26.3	13.7	10.1		109	CB	-4.6	10.3	19.0		125	C	22.5	1.4	29.4
	82	CE	-7.8	-0.2	9.5		95	ND1	24.5	13.6	8.9		109	CA	-3.7	10.2	20.4		125	O	23.4	0.7	29..
	82	CD	-7.6	0.6	10.9		95	CG	25.1	13.3	10.0		109	C	-4.3	9.3	21.6		126	N	22.6	2.8	29.5

Table I (continued)

ALA126	CB	23.7	4.9	29.6	142	N	9.7	-6.4	5.8	157	CG	11.3	-14.5	14.1	171	C	33.5	-2.7	5.2
126	CA	23.9	3.5	29.0	GLY142	CA	10.4	-6.3	4.5	157	CB	12.6	-13.9	12.9	171	O	33.6	-2.4	4.1
126	C	25.1	2.7	29.6	142	C	10.8	-7.4	3.7	157	CA	11.6	-12.8	12.1	172	N	33.2	-2.0	6.3
126	O	26.3	2.6	29.5	142	O	10.8	-8.7	3.8	157	C	12.8	-13.5	11.4	TRY172	CD2	29.7	-1.2	5.6
127	N	24.8	2.4	30.8	143	N	11.1	-6.9	2.5	157	O	12.8	-14.3	10.6	172	CE3	29.9	-0.3	4.5
SER127	OG	24.1	0.7	32.8	LEU143	CD2	10.9	-6.3	-1.1	158	N	13.9	-13.0	12.0	172	CZ3	29.1	-0.1	3.5
127	CB	25.3	1.3	32.9	143	CD1	12.9	-5.0	-1.3	ALA158	CB	16.2	-13.1	10.7	172	CEE2	27.8	-0.7	3.5
127	CA	25.9	1.6	31.4	143	CG	11.9	-5.6	-0.2	158	CA	15.2	-13.6	11.8	172	CZ2	27.5	-1.6	4.5
127	C	26.1	0.1	31.1	143	CB	12.7	-6.8	0.7	158	C	16.2	-13.2	13.1	172	CE2	28.4	-1.9	5.4
127	O	26.0	-0.3	32.3	143	CA	11.6	-7.7	1.3	158	O	16.1	-12.3	13.8	172	NE1	28.5	-2.8	6.7
128	N	25.4	-0.5	30.2	143	C	12.4	-9.0	1.8	159	N	17.1	-14.1	13.5	172	CD1	29.5	-2.6	7.3
ASP128	OD2	22.1	-2.6	31.3	143	O	13.4	-8.8	2.5	SER159	OG	16.6	-15.0	15.8	172	CG	30.3	-1.5	6.6
128	OD1	22.8	-1.1	30.0	144	N	12.1	-10.2	1.4	159	CB	17.9	-15.1	15.3	172	CB	31.5	-0.7	7.1
128	CG	22.9	-2.1	30.8	THR144	CG2	10.6	-12.0	3.1	159	CA	18.0	-13.9	14.4	172	CA	32.8	-0.6	6.1
128	CB	24.4	-2.3	31.3	144	OG1	11.0	-12.6	0.8	159	C	19.5	-14.0	13.9	172	C	33.6	0.6	6.4
128	CA	25.6	-2.0	30.2	144	CB	11.6	-12.5	2.0	159	O	19.9	-14.6	12.8	172	O	33.2	1.6	5.9
128	C	26.0	-2.7	28.9	144	CA	12.7	-11.4	1.7	160	N	20.4	-13.2	14.6	173	N	34.9	0.5	7.1
128	O	26.8	-2.2	28.3	144	C	13.9	-11.7	0.7	LEU160	CD2	20.1	-10.5	14.7	GLY173	CA	35.8	1.5	7.4
129	N	25.8	-4.0	28.7	144	O	14.7	-12.6	1.3	160	CD1	21.2	-9.6	12.7	173	C	35.5	2.7	8.3
ASP129	OD2	29.3	-5.2	26.4	145	N	14.1	-11.3	-0.5	160	CG	21.4	-10.6	13.9	173	O	34.8	2.8	9.4
129	OD1	28.3	-6.9	27.0	ARG145	NEE2	17.1	-15.1	-5.9	160	CB	21.8	-11.9	13.2	174	N	36.0	3.8	7.9
129	CG	28.5	-5.6	27.2	145	NEE1	15.0	-15.6	-5.8	160	CA	21.7	-13.1	14.2	THR174	CG2	36.3	7.4	7.9
129	CB	27.6	-5.0	28.1	145	CZ	16.0	-15.2	-5.1	160	C	22.7	-12.8	15.5	174	OG1	37.8	5.9	6.9
129	CA	26.3	-4.6	27.5	145	NE	16.1	-15.0	-3.9	160	O	22.3	-12.3	16.5	174	CB	36.5	6.1	7.2
129	C	25.5	-5.7	27.1	145	CD	15.0	-15.0	-3.0	161	N	24.0	-12.9	15.1	174	CA	35.8	5.2	8.2
129	O	24.8	-6.5	27.7	145	CG	14.9	-14.0	-1.9	PRO161	CD	24.5	-13.5	13.8	174	C	34.3	5.4	8.4
130	N	25.6	-5.7	25.8	145	CB	15.2	-12.7	-2.3	161	CG	25.9	-13.5	13.8	174	O	33.9	6.3	9.0
PHE130	CD2	22.0	-6.2	25.2	145	CA	15.3	-11.5	-1.3	161	CB	26.4	-13.0	15.2	175	N	33.6	4.7	7.9
130	CE2	21.0	-5.8	26.0	145	C	15.5	-10.1	-2.1	161	CA	25.1	-12.6	16.0	LYS175	NZ	32.9	4.5	3.4
130	CZ	21.1	-4.7	26.7	145	O	14.6	-9.4	-2.3	161	C	25.3	-11.0	16.1	175	CE	31.8	3.4	3.7
130	CE1	22.3	-3.9	26.6	146	N	16.7	-9.9	-2.5	161	O	25.4	-10.4	15.0	175	CD	30.6	4.3	4.4
130	CD1	23.3	-4.3	25.7	TYR146	OEE	19.0	-3.6	-6.6	162	N	25.8	-10.5	17.2	175	CG	31.1	4.9	5.7
130	CG	23.1	-5.4	25.0	146	CD2	18.6	-7.0	-5.8	LEU162	CD2	24.4	-7.3	18.0	175	CB	31.3	4.0	7.0
130	CB	24.2	-5.8	24.0	146	CE2	18.8	-5.7	-6.6	162	CD1	24.4	-8.2	20.3	175	CA	32.1	4.8	8.1
130	CA	25.2	-6.6	24.7	146	CZ	19.0	-4.7	-5.7	162	CG	24.7	-8.5	18.8	175	C	31.7	4.3	9.5
130	C	26.6	-6.7	23.9	146	CE1	18.9	-4.8	-4.4	162	CB	26.2	-8.6	18.7	175	O	31.5	4.6	9.7
130	O	27.0	-5.7	23.5	146	CD1	18.7	-5.8	-3.8	162	CA	26.4	-9.1	17.2	176	N	32.5	3.8	10.4
131	N	27.2	-7.7	24.3	146	CG	18.5	-7.0	-4.4	162	C	27.9	-9.1	17.0	ILE176	CD1	32.1	-0.5	11.7
ALA131	CB	28.8	-9.2	24.9	146	CB	18.5	-8.4	-3.8	162	O	28.8	-9.9	17.5	176	CG1	31.9	0.9	11.0
131	CA	28.6	-8.1	23.8	146	CA	17.0	-8.7	-3.2	163	N	28.4	-8.1	16.2	176	CB	32.2	2.0	12.1
131	C	28.7	-8.9	22.5	146	C	16.0	-8.7	-4.5	LEU163	CD2	30.1	-7.6	12.1	176	CG2	31.4	1.8	13.5
131	O	27.7	-9.5	22.1	146	O	15.7	-7.7	-5.2	163	CD1	28.4	-9.1	13.5	176	CA	32.0	3.5	11.8
132	N	29.8	-8.8	21.8	146	O	15.7	-9.8	-4.8	163	CG	29.8	-8.6	13.4	176	C	32.3	4.4	12.9
ALA132	CB	31.7	-9.2	20.1	149	N	6.1	-10.9	-6.3	163	CB	30.0	-7.5	14.6	176	O	33.3	4.5	13.2
132	CA	30.2	-9.3	20.5	ALA149	CB	6.4	-8.8	-5.2	163	CA	29.7	-7.9	16.1	177	N	31.1	4.9	13.4
132	C	29.8	-10.8	20.4	149	CA	7.2	-9.9	-5.7	163	C	30.3	-6.7	16.9	LYS177	NZ	31.8	8.7	9.7
132	O	30.2	-11.5	21.3	149	C	7.8	-10.7	-4.6	163	O	29.7	-5.7	17.5	177	CE	31.4	8.9	11.1
133	N	29.0	-11.2	19.5	149	O	7.8	-12.0	-4.2	164	N	31.7	-6.7	16.9	177	CD	31.0	7.5	11.8
GLY133	CA	28.7	-12.7	19.2	150	N	8.5	-9.9	-3.8	SER164	OG	33.5	-7.1	19.0	177	CG	33.5	7.8	13.1
133	C	27.3	-13.1	20.0	ASN150	NOD2	12.2	-10.6	-5.0	164	CB	33.9	-6.4	17.9	177	CB	29.9	6.8	14.1
133	O	27.0	-14.3	19.5	150	NOD1	11.2	-11.9	-4.4	164	CA	32.7	-5.7	17.4	177	CA	31.0	5.7	14.6
134	N	27.0	-12.4	21.0	150	CG	11.5	-10.7	-4.2	164	C	32.8	-4.8	16.3	177	C	30.5	5.2	15.9
THR134	CG2	24.1	-11.1	23.3	150	CB	10.8	-10.0	-3.0	164	O	32.9	-5.1	15.1	177	O	29.5	4.5	16.1
134	OG1	26.6	-11.2	23.3	150	CA	9.3	-10.1	-2.6	165	N	32.8	-3.5	16.5	178	N	31.2	5.8	16.8
134	CB	25.4	-11.2	22.5	150	C	8.9	-9.4	-1.4	ASN165	NOD2	31.1	0.3	17.1	ASP178	OD2	32.8	8.3	17.7
134	CA	25.5	-12.5	21.6	150	O	9.5	-9.4	-0.3	165	NOD1	30.4	-1.7	16.3	178	OD1	32.9	6.5	18.9
134	C	24.4	-12.4	20.4	151	N	7.8	-8.8	-1.5	165	CG	31.3	-0.8	16.4	178	CG	32.3	7.4	18.4
134	O	24.1	-11.6	19.7	THR151	CG2	4.9	-6.5	-0.2	165	CB	32.8	-1.0	15.9	178	CB	31.0	6.9	19.0
135	N	23.6	-13.6	20.5	151	OG1	6.5	-6.3	-1.8	165	CA	32.9	-2.4	15.4	178	CA	31.8	5.5	18.3
THR135	CG2	21.2	-15.7	19.0	151	CB	5.7	-7.3	-1.0	165	C	34.2	-2.6	14.8	178	C	29.2	5.1	18.3
135	OG1	23.4	-15.9	18.8	151	CA	7.0	-8.1	-0.4	165	O	34.3	-2.9	13.6	178	O	29.1	4.2	19.2
135	CB	22.5	-15.4	19.5	151	C	6.0	-9.1	0.3	166	N	35.3	-2.7	15.5	179	N	28.3	5.7	17.7
135	CA	22.6	-13.8	19.6	151	O	5.1	-9.6	-0.4	THR166	CG2	38.5	-4.5	16.3	ALA179	CB	26.1	6.5	17.6
135	C	21.2	-13.3	19.9	152	N	6.3	-9.5	1.5	166	OG1	37.4	-2.8	17.3	179	CA	26.9	5.3	18.0
135	O	20.8	-13.7	21.1	PRO152	CD	7.5	-9.0	2.2	166	CB	37.1	-3.8	16.4	179	C	26.2	4.3	17.1
136	N	20.5	-12.4	19.2	152	CG	7.6	-9.7	3.6	166	CA	36.6	-3.1	15.1	179	O	25.0	4.4	17.4
CYS136	SG	21.2	-10.0	21.0	152	CB	6.5	-10.7	3.7	166	C	36.4	-4.0	14.0	180	N	26.8	3.4	16.3
136	CB	19.9	-10.3	19.7	152	CA	5.4	-10.5	2.6	166	O	36.7	-3.9	12.8	MET180	CE	27.3	5.4	11.8
136	CA	19.2	-11.8	19.5	152	C	4.1	-9.8	2.9	167	N	35.5	-5.1	14.2	180	SD	27.3	3.7	11.7
136	C	18.4	-11.9	18.3	152	O	4.4	-8.6	3.5	ASN167	NOD2	35.4	-8.7	15.0	180	CG	27.7	3.2	13.3
136	O	18.7	-12.4	17.3	153	N	3.0	-10.2	3.1	167	NOD1	33.3	-8.0	15.8	180	CB	26.3	2.7	14.1
137	N	17.1	-11.3	18.4	ASP153	OD2	-0.1	-9.8	0.5	167	CG	34.2	-7.9	14.9	180	CA	26.3	2.4	15.5
VAL137	CG2	15.0	-13.5	18.4	153	OD1	1.7	-9.1	1.1	167	CB	34.1	-7.2	13.6	180	C	27.0	1.0	16.0
137	CG1	13.7	-12.3	17.0	153	CG	0.7	-9.7	1.5	167	CA	35.1	-6.0	13.3	180	O	28.0	1.0	16.8
137	CB	14.7	-12.0	17.9	153	CB	0.5	-10.3	2.8	167	C	34.7	-5.4	12.0	181	N	26.3	-0.1	15.7
137	CA	16.1	-11.4	17.4	153	CA	1.8	-9.9	3.6	167	O	35.2	-6.1	10.9	ILE181	CD1	24.4	-3.0	19.4
137	C	15.6	-10.0	16.8	153	C	2.0	-10.3	5.1	168	N	33.6	-4.9	12.1	181	CG1	25.4	-3.0	18.2
137	O	15.5	-9.1	17.5	153	O	1.4	-9.7	6.0	CYS168	SG	29.9	-3.2	10.9	181	CB	25.4	-1.6	17.5
138	N	15.3	-9.9	15.5	154	N	2.9	-11.2	5.6	168	CB	31.6	-3.7	11.8	181	CG2	24.0	-1.4	16.8
THR138	CG2	16.0	-8.8	12.6	ARG154	NEE2	3.0	-17.4	4.2	168	CA	32.8	-4.3	11.2	181	CA	26.4	-1.5	16.4
138	OG1	15.0	-6.8	13.5	154	NEE1	1.7	-17.9	5.6	168	C	33.7	-3.3	10.3	181	C	26.3	-2.5	15.1
138	CB	15.7	-7.8	13.8	154	CZ	0.8	-17.0	5.1	168	O	33.7	-3.3	9.1	181	O	25.4	-2.2	14.3
138	CA	14.8	-8.8	14.8	154	NE	0.9	-15.7	5.5	169	N	34.6	-2.6	10.9	182	N	27.2	-3.4	14.9
138	C	13.6	-9.3	14.0	154	CD	1.8	-15.1	6.3	LYS169	NZ	36.6	3.2	14.0	CYS182	SG	28.9	-2.7	12.7
138	O	13.7	-10.4	13.4	154	CG	1.9	-13.5	6.7	169	CE	36.1	2.3	12.9	182	CB	28.8	-4.4	13.5
139	N	12.6	-8.4	13.9	154	CB	2.9	-13.1	7.1	169	CD	37.0	1.2	12.3	182	CA	27.2	-4.4	13.9
THR139	CG2	10.4	-10.4	15.3	154	CA	3.0	-11.5	7.2	169	CG	36.1	0.1	11.6	182	C	26.4	-5.7	14.0
139	OG1	9.9	-7.9	15.1	154	C	4.5	-11.3	7.6	169	CB	36.6	-0.9	10.8	182	O	26.6	-6.3	15.0
139	CB	10.2	-9.1	14.4	154	O	5.3	-11.8	7.2	169	CA	35.5	-1.8	10.3	183	N	25.5	-6.1	13.2
139	CA	11.3	-8.9	13.2	155	N	4.6	-10.6	8.7	169	C	36.3	-2.4	9.1	ALA183	CB	23.6	-7.4	13.9
139	C	10.9	-7.9	12.2	LEU155	CD2	5.8	-9.7	13.4	169	O	36.8	-1.9	8.2	183	CA	25.1	-7.4	13.3
139	O	11.3	-6.7	12.3	155	CD1	6.4	-8.1	11.6	170	N	36.1	-3.8	8.8	183	C	24.7	-8.2	11.9
140	N	10.3	-8.1	11.2	155	CG	6.3	-9.4	11.9	LYS170	NZ	39.3	-9.2	11.2	183	O	24.4	-7.4	10.9
GLY140	CA	9.9	-7.1	10.1	155	CB	5.3	-10.1	10.9	170	CE	39.3	-7.9	10.7	184	N	24.8	-9.4	12.0
140	C	9.0	-7.6	9.0	155	CA	5.8	-10.2	9.4	170	CD	38.0	-7.5	9.8	GLY184	CA	24.5	-10.4	11.8
140	O	9.0	-8.7	8.4	155	C	6.9	-11.3	9.6	170	CG	37.9	-6.1	9.4	184	C	25.6	-11.0	12.0
141	N	8.5	-6.7	8.3	155	O	6.8	-12.1	10.4	170	CB	36.8	-5.9	8.2	184	O	26.8	-10.8	12.5
TRY141	CD2	4.8	-6.1	9.3	156	N	8.1	-11.2	8.8	170	CA	36.7	-4.5	7.8	185	N	25.4	-11.8	8.7
141	CE3	5.3	-5.2	10.2	GLN156	NOE2	7.3	-13.9	6.7	170	C	36.0	-4.4	6.5	ALA185	CB	28.1	-10.4	8.1
141	CZ3	4.6	-4.9	11.4	156	NOE1	9.4	-14.7	6.6	170	O	36.4	-4.5	5.4	185	CA	26.7	-11.1	7.9
141	CEE2	3.5	-5.6	11.7	156	CD	8.7	-13.7	6.6	171	N	34.6	-4.1	6.7	185	C	26.8	-12.7	8.1
141	CZ2	3.0	-6.4	10.9	156	CG	9.0	-12.3	6.6	TYR171	OEE	32.4	-9.9	8.2	185	O	27.9	-13.3	8.1
141	CE2	3.6	-6.8	9.6	156	CB	10.0	-12.1	7.7	171	CD2	32.5	-6.1	8.1	186	N	25.7	-13.3	8.5
141	NE1	3.4	-7.7	8.6	156	CA	9.2	-12.1	9.1	171	CE2	32.5	-7.4	8.6	SER186	OG	24.2	-13.8	10.7
141	CD1	4.4	-7.5	7.6	156	C	9.8	-11.7	10.5	171	CZ	32.5	-8.5	7.7	186	CB	25.4	-14.3	10.5
141	CG	5.3	-6.4	8.2	156	O	9.6	-10.5	10.9	171	CE1	32.6	-8.4	6.3	186	CA	25.7	-14.7	8.9
141	CB	6.3	-6.0	7.3	157	N	10.6	-12.6	11.1	171	CD1	32.6	-7.0	5.8	186	C	24.6	-15.6	8.6
141	CA	7.6	-6.9	7.1	GLN157	NOE2	10.6	-16.8	14.2	171	CG	32.6	-5.9	6.6	186	O	24.4	-16.6	9.2
141	C	8.3	-6.5	5.9	157	NOE1	9.1	-15.3	14.9	171	CB	32.5	-4.6	6.3	187	N	24.0	-15.2	7.6
141	O	7.7	-6.3	4.9	157	CO	10.2	-15.6	14.6	171	CA	33.7	-4.3	5.6	GLY187	CA	22.9	-15.6	6.5

Table I (continued)

187	C	21.6	-14.8	6.6	203	CE	21.2	-7.7	31.9	SER218	OG	24.9	-0.8	-2.5	LEU234	CD2	21.2	6.0	19.6
187	O	20.6	-15.3	6.0	203	CD	20.2	-7.6	30.8	218	CB	23.9	-1.7	-2.8	234	CD1	21.6	8.3	20.1
188	N	21.7	-13.7	7.3	203	CG	19.4	-9.0	30.6	218	CA	23.2	-2.2	-1.5	234	CG	20.5	7.3	20.0
VAL188	CG2	20.1	-12.7	9.9	203	CB	18.3	-9.0	29.6	218	C	22.2	-3.5	-1.7	234	CB	19.8	7.4	21.4
188	CG1	19.1	-14.3	8.1	203	CA	17.6	-10.3	29.6	218	O	21.1	-3.4	-2.1	234	CA	20.5	7.3	22.8
188	CB	19.6	-12.9	8.4	203	C	16.7	-10.5	31.0	219	N	22.9	-4.6	-1.7	234	C	19.4	7.4	23.8
188	CA	20.7	-12.7	7.3	203	O	15.4	-10.2	31.0	THR219	CG2	22.3	-8.0	-3.3	234	O	18.6	8.3	23.8
188	C	21.3	-11.2	7.1	204	N	17.1	-11.1	32.1	219	OG1	23.3	-5.9	-4.2	235	N	19.2	6.4	24.8
188	O	22.4	-10.9	7.2	ASN204	ND2	17.6	-8.7	35.6	219	CB	23.1	-6.6	-3.0	VAL235	CG2	17.2	4.3	26.8
189	N	20.2	-10.4	6.7	204	ND1	18.5	-10.4	34.6	219	CA	22.1	-5.7	-2.2	235	CG1	19.6	4.6	26.8
SER189	OG	20.0	-8.7	4.4	204	CG	17.6	-9.6	34.9	219	C	21.6	-6.5	-0.9	235	CB	18.3	4.8	26.0
189	CB	20.7	-8.2	5.3	204	CB	16.3	-10.0	34.1	219	O	21.3	-7.6	-1.1	235	CA	18.1	6.2	25.6
189	CA	20.3	-8.9	6.6	204	CA	16.2	-11.4	33.4	220	N	21.5	-5.9	0.2	235	C	17.8	7.3	26.8
189	C	18.8	-8.6	6.7	204	C	14.7	-11.7	32.9	CYS220	SG	18.1	-5.2	1.1	235	O	16.7	7.2	27.2
189	O	18.0	-9.2	6.2	204	O	13.9	-11.5	33.6	220	CB	19.3	-6.8	1.1	236	N	18.6	8.1	27.2
190	N	18.7	-7.4	7.2	205	N	14.7	-12.6	31.8	220	CA	20.9	-6.4	1.4	ASN236	ND2	21.6	8.3	29.7
SER190	OG	17.5	-5.7	9.6	GLY205	CA	13.6	-13.4	31.4	220	C	21.5	-7.8	1.5	236	ND1	19.8	7.5	30.6
190	CB	17.5	-5.3	8.1	205	C	12.6	-12.4	30.6	220	O	20.8	-8.8	1.7	236	CG	20.4	8.4	29.9
190	CA	17.6	-6.5	7.2	205	O	11.6	-13.0	30.1	221	N	22.8	-7.8	1.3	236	CB	19.6	9.4	29.3
190	C	17.7	-6.1	5.7	206	N	13.0	-11.1	30.2	SER221	OG	25.5	-10.2	0.2	236	CA	18.3	9.0	28.4
190	O	18.6	-6.0	5.2	ALA206	CB	11.5	-9.2	30.0	221	CB	25.0	-8.8	0.3	236	C	17.7	10.5	28.5
191	N	16.4	-5.9	5.2	206	CA	12.2	-10.4	29.2	221	CA	23.6	-9.0	1.2	236	O	17.1	11.0	29.5
CYS191	SG	16.3	-6.1	0.9	206	C	13.2	-9.8	28.1	221	C	23.8	-9.7	2.6	237	N	17.7	10.6	26.8
191	CB	16.1	-6.5	2.7	206	O	14.3	-9.4	28.3	221	O	23.7	-9.1	3.7	TRY237	CD2	16.0	11.5	22.7
191	CA	16.4	-5.3	3.7	207	N	12.5	-9.5	27.1	222	N	24.0	-10.9	2.4	237	CE3	16.0	10.1	22.3
191	C	15.2	-4.5	3.7	TRY207	CD2	12.6	-11.6	23.5	THR222	CG2	21.7	-12.6	2.3	237	CZ3	15.0	9.6	21.5
191	O	14.4	-4.2	4.6	207	CE3	13.7	-11.1	22.7	222	OG1	23.9	-13.5	1.7	237	CEE2	14.1	10.4	21.0
192	N	14.9	-4.1	2.5	207	CZ3	14.4	-11.8	22.0	222	CB	23.1	-13.0	2.8	237	CZ2	14.0	11.7	21.2
MET192	CE	16.9	-1.4	-1.2	207	CEE2	14.1	-13.3	22.1	222	CA	24.0	-11.9	3.6	237	CE2	14.8	12.3	22.1
192	SD	15.1	-1.4	-1.1	207	CZ2	13.2	-13.8	22.9	222	C	25.3	-12.3	3.9	237	NE1	15.1	13.6	22.6
192	CG	14.9	-2.0	0.7	207	CE2	12.4	-13.0	23.7	222	O	25.4	-13.0	5.0	237	CD1	16.1	13.7	23.4
192	CB	13.5	-2.6	1.0	207	NE1	11.3	-13.1	24.5	223	N	26.3	-11.8	3.4	237	CG	16.7	12.6	23.4
192	CA	13.8	-3.2	2.5	207	CD1	10.9	-11.9	25.0	SER223	OG	28.1	-11.5	1.3	237	CB	17.7	11.6	24.4
192	C	12.4	-3.8	3.0	207	CG	11.7	-10.9	24.4	223	CB	28.4	-12.3	2.4	237	CA	17.0	11.5	25.8
192	O	12.0	-4.8	2.7	207	CB	11.8	-9.4	24.7	223	CA	27.7	-11.8	3.7	237	C	15.6	11.0	25.8
193	N	11.8	-2.7	3.6	207	CA	13.0	-9.0	25.7	223	C	28.4	-10.5	4.3	237	O	14.6	11.3	26.3
GLY193	CA	10.6	-2.9	4.5	207	C	13.4	-7.5	25.8	223	O	29.6	-10.4	4.0	238	N	15.3	9.8	25.4
193	C	10.9	-2.9	5.9	207	O	12.4	-6.8	26.0	224	N	27.5	-9.5	4.4	VAL238	CG2	15.3	7.2	24.1
193	O	10.1	-2.8	6.7	208	N	14.6	-7.2	25.6	THR224	CG2	28.1	-5.7	3.8	238	CG1	13.3	6.6	25.4
194	N	12.2	-3.2	6.5	THR208	CG2	17.0	-4.3	26.9	224	OG1	28.5	-7.6	2.5	238	CB	14.6	7.4	25.4
ASP194	OD2	13.7	-6.7	6.8	208	OG1	15.9	-6.2	27.9	224	CB	27.8	-7.2	3.5	238	CA	14.1	8.9	25.6
194	OD1	12.0	-6.2	8.0	208	CB	16.4	-5.7	26.7	224	CA	27.9	-8.1	5.0	238	C	13.4	9.0	26.9
194	CG	13.1	-6.0	7.6	208	CA	15.1	-5.8	25.9	224	C	26.9	-7.7	5.9	238	O	12.2	9.2	27.1
194	CB	13.7	-4.5	7.7	208	C	15.5	-5.3	24.3	224	O	25.7	-7.9	5.8	239	N	14.1	8.7	28.0
194	CA	12.6	-3.4	7.8	208	O	16.0	-6.3	23.6	225	N	27.4	-7.2	7.0	GLN239	NOE2	14.0	4.1	29.8
194	C	13.2	-2.2	8.5	209	N	15.2	-4.2	23.8	PRO225	CD	28.9	-6.9	7.1	239	NDE1	12.6	5.7	30.3
194	O	13.0	-2.2	9.8	LEU209	CD2	13.9	-0.1	21.1	225	CG	29.0	-6.5	8.7	239	CD	13.8	5.3	30.0
195	N	13.7	-1.2	7.9	209	CD1	14.1	-2.5	20.1	225	CB	27.7	-6.5	9.4	239	CG	14.9	6.2	29.9
TOS195	CEE2	17.8	-1.9	4.3	209	CG	14.6	-1.5	21.1	225	CA	26.7	-6.9	8.2	239	CB	14.6	7.7	30.3
195	CTH2	18.9	-2.8	4.3	209	CB	14.4	-2.2	22.5	225	C	25.6	-5.7	7.9	239	CA	13.8	8.4	29.3
195	CKA	20.1	-3.9	5.4	209	CA	15.3	-3.5	22.7	225	O	25.9	-4.8	7.2	239	C	13.4	10.0	29.8
195	CIO	19.6	-2.9	5.5	209	C	16.8	-3.0	22.8	226	N	24.6	-5.7	8.7	239	O	12.3	10.3	30.1
195	CTH1	19.4	-2.1	6.6	209	O	17.2	-2.3	23.7	GLY226	CA	23.6	-4.8	8.8	240	N	14.2	10.8	29.9
195	CEE1	18.3	-1.3	6.6	210	N	17.8	-3.7	21.9	226	C	23.9	-3.8	9.9	GLN240	NOE2	18.6	13.8	31.5
195	CZ	17.6	-1.1	5.5	VAL210	CG2	19.8	-5.7	23.0	226	O	24.4	-4.3	11.0	240	NOE1	17.8	14.8	29.6
195	OE2	14.9	-0.6	5.0	210	CG1	21.5	-4.7	21.4	227	N	23.7	-2.6	9.7	240	CD	17.7	14.0	30.5
195	OE1	16.5	1.2	4.5	210	CB	20.0	-4.9	21.7	VAL227	CG2	26.4	-1.0	10.0	240	CG	16.5	13.0	30.7
195	SD	16.2	0.0	5.4	210	CA	19.1	-3.5	22.0	227	CG1	25.0	0.8	11.4	240	CB	15.2	13.3	29.8
SER195	OG	16.1	0.7	6.8	210	C	19.4	-2.6	20.7	227	CB	25.0	-0.3	10.2	240	CA	14.1	12.4	30.0
195	CB	14.7	1.0	7.4	210	O	20.3	-1.8	20.7	227	CA	24.0	-1.4	10.4	240	C	12.8	12.9	29.3
195	CA	14.1	0.1	8.6	211	N	18.5	-2.8	19.7	227	C	22.6	-0.8	11.0	240	O	11.9	13.5	29.8
195	C	13.2	0.5	9.7	GLY211	CA	18.7	-1.8	18.6	227	O	21.7	-0.2	10.3	241	N	12.9	12.7	27.9
195	O	11.9	0.6	9.5	211	C	17.5	-1.4	17.7	228	N	22.6	-0.7	12.3	THR241	CG2	13.7	12.6	24.9
196	N	13.7	0.9	10.8	211	O	16.4	-2.0	17.6	TYR228	OEE	19.8	-6.1	11.5	241	OG1	13.2	13.1	24.9
GLY196	CA	13.0	1.4	12.0	212	N	17.8	-0.4	16.8	228	CD2	19.7	-3.0	13.3	241	CB	12.2	12.4	25.6
196	C	12.7	0.4	13.1	ILE212	CD1	16.1	2.9	18.2	228	CE2	19.3	-4.2	12.7	241	CA	11.8	12.9	27.0
196	O	12.6	0.7	14.3	212	CG1	16.2	1.4	17.5	228	CZ	20.2	-5.1	12.1	241	C	10.4	12.3	27.3
197	N	12.6	-0.9	12.7	212	CB	16.7	1.5	16.1	228	CE1	21.6	-4.8	12.2	241	O	9.6	13.1	27.0
GLY197	CA	12.0	-1.9	13.7	212	CG2	15.7	2.4	15.2	228	CD1	22.0	-3.7	12.9	242	N	10.5	11.2	28.0
197	C	13.1	-2.5	14.7	212	CA	17.0	0.0	15.7	228	CG	21.1	-2.8	13.4	LEU242	CD2	8.4	8.7	26.3
197	O	14.1	-2.0	14.9	212	C	17.8	-0.1	14.4	228	CB	21.6	-1.5	14.2	242	CD1	9.3	6.7	27.6
198	N	12.4	-3.4	15.6	212	O	19.0	0.3	14.3	228	CA	21.6	-0.2	13.3	242	CG	9.5	8.2	27.3
PRO198	CD	11.1	-4.1	15.1	213	N	17.3	-0.7	13.4	228	C	22.4	0.9	14.0	242	CB	9.4	9.0	28.6
198	CG	10.8	-5.1	16.2	VAL213	CG2	16.3	-3.1	12.2	228	O	23.7	1.1	14.0	242	CA	9.3	10.6	28.5
198	CB	11.9	-5.0	17.4	213	CG1	17.2	-2.3	10.0	229	N	21.6	1.7	14.5	242	C	8.9	11.1	30.0
198	CA	13.0	-3.9	16.8	213	CB	16.6	-1.8	11.4	ALA229	CB	21.0	4.1	15.3	242	O	7.8	11.0	30.3
198	C	14.2	-4.7	16.6	213	CA	17.8	-0.9	12.0	229	CA	21.8	2.7	15.5	243	N	9.9	11.6	30.6
198	O	14.1	-5.5	15.7	213	C	17.9	0.4	11.2	229	C	21.6	2.1	16.9	ALA243	CB	11.2	12.6	32.2
199	N	15.5	-4.6	17.1	213	O	17.0	1.1	11.0	229	O	20.7	1.4	17.2	243	CA	9.8	12.3	31.9
LEU199	CD2	20.5	-5.3	16.6	214	N	19.1	0.6	10.7	230	N	22.5	2.4	17.7	243	C	8.9	13.6	31.9
199	CD1	18.0	-6.9	16.0	SER214	OG	20.6	3.7	11.4	ARG230	NEE2	29.0	-1.4	19.4	243	O	7.9	13.7	32.7
199	CG	19.1	-5.8	17.0	214	CB	20.7	3.0	10.2	230	NEE1	28.0	-1.3	21.4	244	N	9.2	14.2	30.9
199	CB	17.9	-4.8	16.8	214	CA	19.6	1.9	10.1	230	CZ	28.1	-0.9	20.2	ALA244	CB	9.1	16.6	29.7
199	CA	16.7	-5.5	17.3	214	C	19.9	1.7	8.5	230	NE	27.2	0.1	19.7	244	CA	8.5	15.6	30.8
199	C	16.7	-5.9	18.9	214	O	19.1	2.3	7.7	230	CD	26.3	0.7	20.5	244	C	7.3	15.5	29.8
199	O	16.8	-5.1	19.8	215	N	21.0	1.0	8.2	230	CG	24.7	0.7	20.4	244	O	6.6	16.6	29.7
200	N	16.4	-7.2	19.4	TRY215	CD2	24.9	2.2	6.8	230	CB	24.4	1.6	19.2	245	N	6.7	14.5	29.2
VAL200	CG2	14.1	-9.3	20.1	215	CE3	25.3	1.6	5.7	230	CA	22.7	1.8	19.1	ASN245	NOD2	8.3	15.0	26.5
200	CG1	13.7	-7.0	20.6	215	CZ3	26.6	1.4	5.4	230	C	22.0	2.4	20.2	245	NOD1	6.7	16.7	26.4
200	CB	14.6	-8.1	20.9	215	CEE2	27.5	1.8	6.3	230	O	22.4	3.5	20.6	245	CG	7.1	15.6	26.6
200	CA	16.2	-7.6	20.7	215	CZ2	27.1	2.4	7.5	231	N	21.1	1.7	20.7	245	CB	5.9	14.6	26.9
200	C	17.0	-8.9	21.2	215	CE2	25.8	2.7	7.8	VAL231	CG2	18.1	1.1	20.7	245	CA	5.5	14.6	28.4
200	O	17.3	-9.9	20.4	215	NE1	25.2	3.2	8.9	231	CG1	17.9	2.3	22.9	245	C	4.3	13.7	28.6
201	N	17.4	-8.8	22.5	215	CD1	23.7	3.1	8.6	231	CB	18.8	1.4	22.0	245	O	4.5	12.5	28.8
CYS201	SG	20.3	-8.4	21.9	215	CG	23.5	2.5	7.3	231	CA	20.2	2.3	21.8	245	O	3.1	14.2	28.5
201	CB	19.6	-9.1	23.5	215	CB	22.2	2.3	6.5	231	C	21.1	2.6	23.0					
201	CA	18.0	-9.7	23.3	215	CA	21.6	0.9	6.9	231	O	20.8	3.7	23.5					
201	C	17.3	-9.9	24.6	215	C	22.3	-0.4	6.6	232	N	21.9	1.7	23.5					
201	O	16.8	-8.9	25.1	215	O	22.6	-1.1	7.6	THR232	CG2	25.3	2.0	25.0					
202	N	17.1	-11.1	25.1	216	N	22.7	-0.6	5.3	232	OG1	24.2	0.1	24.3					
LYS202	NZ	13.3	-16.7	28.0	GLY216	CA	23.2	-1.9	4.7	232	CB	24.3	1.4	24.1					
202	CE	13.7	-15.2	28.1	216	C	24.2	-1.7	3.6	232	CA	22.9	2.1	24.5					
202	CD	14.5	-15.0	27.0	216	O	24.5	-0.7	3.2	232	C	23.2	3.7	24.7					
202	CG	14.8	-13.3	27.1	217	N	24.2	-3.0	3.1	232	O	23.4	4.2	25.8					
202	CB	15.8	-13.0	26.0	SER217	OG	24.7	-5.5	0.6	233	N	23.4	4.2	23.5					
202	CA	16.2	-11.5	26.3	217	CB	24.4	-5.1	1.8	ALA233	CB	25.1	5.6	22.4					
202	C	17.2	-11.2	27.4	217	CA	24.5	-3.5	1.9	233	CA	23.9	5.6	23.4					
202	O	18.2	-11.4	27.4	217	C	23.6	-2.9	0.8	233	C	22.9	6.5	23.1					
203	N	16.7	-10.5	28.5	217	O	22.4	-2.8	1.2	233	O	23.2	7.6	22.8					
LYS203	NZ	21.9	-6.3	32.2	218	N	24.0	-2.6	-0.3	234	N	21.6	6.3	23.0					

Legend to Table I

The names allocated to the atoms correspond to those in the proposed nomenclature for polypeptides (8) with transliteration of the Greek superscripts, and with the following exceptions:

In tryptophan, $C^{\varepsilon 1}$, $C^{\zeta 1}$, C^{η}, $C^{\zeta 2}$, $C^{\varepsilon 2}$ are called CE2, CZ2, CEE2, CZ3, CE3 respectively.

In valine and leucine, the subscripts 1 and 2 are interchanged, so that $C^{\gamma 1}$ is called CG2 and $C^{\gamma 2}$ is called CG1, for example.

The distinction between the amino group and the oxygen atom of amide side chains is not indicated by the diffraction results: hence these atoms are called NOD1, NOD2 (asparagine) or NOE1, NOE2 (glutamine). The atom labelled 1 is the one believed to be oxygen on stereochemical grounds.

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