ATOMIC COORDINATES FOR TOSYL-ELASTASE

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Summary: The full set of non-hydrogen, atomic coordinates of porcine tosyl elastase is given. This includes the tosyl group and the internal water molecules.

The structure of porcine pancreatic elastase has been determined at 3.5Å resolution (1, 2, 3). Recently, we have extended the resolution of the structure determination of tosyl-elastase to 2.5Å and have built an accurate atomic model of the enzyme, the coordinates of which are reported here.

High resolution X-ray data were collected from crystals, of the same derivatives as were used previously (2). The phases obtained from these new data were of high accuracy, the mean figure of merit being 0.86 for all reflexions between 3.64Å and 2.5Å, and this resulted in a clear and unambiguously interpretable electron density map.

The polypeptide main chain appears in the map as a continuous ribbon of high density with clearly defined protrusions indicating the positions of almost all of the peptide carbonyl oxygen atoms. Density representing the amino-acid side chains is also clear, with the exception of the extremities of some surface polar residues. Dimpling of six-membered rings and forking of branched side-chains is, for the most part, obvious. Sulphur atoms of disulphide bridges are just resolved and

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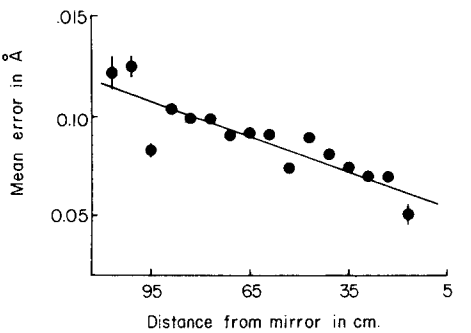

Figure I The mean error in the x-coordinate plotted as a function of the distance from the mirror. Error bars indicate the points averaged over less than 100 observations.

appear at twice the main-chain density. The majority of the residues can be identified from the electron density alone, confirming the chemically determined primary structure (5). It is known from the sequence work that Asn-186 is very susceptible to deamidation and, indeed, the electron density map at that point is more consistent with an aspartic acid. In addition to the density associated with protein, peaks representing the positions of the tosyl group attached to the active centre serine residue, a surface-bound sulphate ion (4), twenty five internal and many surface water molecules, are also well defined.

Using an optical comparator with a vertical mirror (6,7), a model has been constructed from Kendrew-Watson skeletal components (Cambridge Repetition Engineers, Greens Road, Cambridge, England) which fits accurately the electron density map of tosyl-elastase. From this model, the coordinates of all non-hydrogen atoms including those of the tosyl group, sulphate ion and

TABLE 1(see pp. 946-951)

The measured coordinates are recorded in Ångstrom units (0.1nm) measured from the origin of the unit cell ($P2_12_12_1$), along the crystallographic axes. Amino-acid residues are identified by their number in the chymotrypsinogen-A numbering scheme (5) to facilitate comparison. Atoms are identified according to the IUPAC-IUB conventions, 1970 (9) using Latin equivalents of Greek characters. η has been transliterated as EH rather than H. The positions of the amino group and oxygen atom of amide side-chains have been determined from stereochemical considerations. An asterisk preceding an atomic coordinate indicates that that atom is not clearly visible in the electron density map. Such atoms belong to freely rotating surface residues and were built fully staggered.

	N	-10.1	33.0	35.1		CB	4.9	39.9	44.1		N	6.3	25.8	25.9		O	12.8	29.8	45.1
VAL	16					CA	3.8	39.0	43.5	TRP	38					N	12.8	28.6	47.0
	CG2	-9.2	34.2	37.8		C'	4.3	37.5	44.1		CD2	8.6	25.1	29.3	ASN	50			
	CG1	-11.1	35.6	37.5		O	5.4	37.3	44.2		CE3	7.9	24.1	30.3		ND2	14.9	25.9	49.2
	CB	-10.1	34.8	36.8		N	3.3	36.8	44.4		CZ3	8.8	23.2	31.0		OD1	13.1	27.2	49.2
	CA	-11.1	34.0	36.1	SER	29					CH2	10.2	23.2	30.8		CG	14.8	26.6	48.6
	C'	-12.8	34.4	35.3		OG	1.2	35.4	46.2		CZ2	10.6	24.0	29.8		CB	14.3	26.6	47.1
	O	-12.1	35.6	34.5		CB	2.8	35.3	46.4		CE2	10.0	24.8	29.1		CA	13.8	27.4	46.4
	N	-13.2	33.9	35.7		CA	3.5	35.5	44.9		NE1	10.1	25.8	28.1		C'	11.9	26.4	46.4
VAL	17					C'	2.9	34.5	44.8		CD1	8.9	26.4	27.7		O	12.1	25.3	46.2
	CG2	-15.3	32.2	34.2		O	2.8	33.1	44.1		CG	7.9	25.9	28.4		N	10.8	26.8	46.8
	CG1	-16.9	34.2	34.4		N	2.8	34.9	43.8		CB	6.4	26.2	28.3	TRP	51			
	CB	-15.6	33.4	35.4	GLN	30					CA	5.6	25.6	27.2		CD2	9.9	22.9	48.7
	CA	-14.6	34.4	35.1		NE2	-0.7	32.4	39.9		C'	4.3	26.2	27.1		CE3	8.9	22.1	48.2
	C'	-15.1	35.6	35.6		OE1	-1.9	33.9	41.0		O	4.0	27.3	26.6		CZ3	9.1	20.7	48.3
	O	-15.3	35.8	37.1		CD	-1.1	33.6	40.3		N	3.2	25.7	27.8		CH2	10.1	20.1	48.9
	N	-15.5	36.8	35.2		CG	0.1	34.6	39.9	ALA	39					CZ2	11.2	21.0	49.4
GLY	18					CB	0.8	35.3	41.2		CB	1.0	25.2	27.2		CE2	11.0	22.3	49.3
	CA	-15.7	37.9	35.6		CA	1.5	34.3	42.0		CA	1.8	26.2	27.9		NE1	11.9	23.3	49.8
	C'	-14.7	38.5	36.4		C'	2.6	33.8	41.0		C'	1.4	26.2	29.4		CD1	11.3	24.5	49.5
	O	-14.9	39.1	37.5		O	3.6	34.4	40.7		O	1.8	25.6	30.3		CG	10.1	24.4	48.8
	N	-13.3	38.4	36.0		N	2.3	32.4	40.7		N	0.4	27.0	29.6		CB	9.2	25.5	48.4
GLY	19				ILE	31				HIS	40					CA	9.6	26.0	46.9
	CA	-12.4	38.9	36.6		CD1	3.0	28.6	39.9		CD2	-2.6	28.6	32.9		C'	8.1	26.6	46.5
	C'	-12.8	40.2	35.9		CG1	3.4	29.5	41.8		NE2	-2.7	28.8	34.2		O	7.9	27.8	46.9
	O	-12.3	40.6	34.8		CB	4.1	30.8	40.5		CE1	-1.6	29.3	34.6		N	7.5	25.9	45.7
	N	-11.0	41.0	36.5		CG2	4.9	31.6	41.6		ND1	-0.7	29.3	33.5	VAL	52			
THR	20					CA	3.2	31.7	39.8		CG	-1.4	28.9	32.4		CG2	6.8	27.5	43.1
	CG2	-12.2	43.3	37.6		C'	2.3	31.0	38.8		CB	-0.8	28.6	31.1		CG1	4.6	26.4	43.4
	OG1	-9.7	43.5	37.9		O	1.1	30.7	39.0		CA	-0.2	27.2	31.0		CB	6.1	26.3	43.7
	CB	-10.7	43.4	37.0		N	2.8	30.8	37.6		C'	-1.3	26.1	31.3		CA	6.1	26.4	45.3
	CA	-10.3	42.1	36.0	SER	32					O	-2.2	25.9	30.5		C'	5.2	25.4	45.8
	C'	-8.9	41.9	36.0		OG	2.3	30.0	34.1		N	-1.1	25.6	32.5		O	5.2	24.2	45.9
	O	-8.3	40.9	36.6		CB	2.4	30.9	35.2	THR	41					N	3.9	26.1	45.9
	N	-8.1	42.6	35.1		CA	2.1	30.1	36.4		CG2	-0.6	23.4	34.4	MET	53			
GLU	21					C'	2.8	28.8	36.3		OG1	-2.2	22.3	33.3		CE	0.1	27.6	49.3
	OE2	-5.1	44.3	31.7		O	4.1	28.8	36.3		CB	-1.3	23.3	33.1		SD	0.2	25.9	49.5
	OE1	-3.1	44.3	32.5		N	2.1	27.7	36.3		CA	-2.1	24.6	32.9		CG	0.9	25.3	48.0
	CD	-4.4	44.0	32.6	LEU	33					C'	-2.6	25.2	34.3		CB	2.1	26.1	47.6
	CG	-4.7	43.4	33.9		CD2	2.0	23.8	37.9		O	-3.9	25.2	34.5		CA	2.7	25.4	46.3
	CB	-6.1	43.3	33.9		CD1	4.1	24.3	37.4		N	-1.8	25.5	35.1		C'	1.6	25.5	45.3
	CA	-6.9	42.6	35.1		CG	2.6	24.1	37.0	CYS	42					O	1.4	26.5	44.6
	C'	-6.1	43.8	36.4		CB	1.8	25.4	37.1		CA	-0.7	28.9	38.6		N	1.1	24.3	45.8
	O	-6.7	43.9	37.1		CA	2.6	26.4	36.2		CB	-2.4	21.4	38.6	THR	54			
	N	-5.2	42.5	36.6		C'	2.5	26.1	34.7		SG	-2.7	22.5	38.9		CG2	1.2	22.6	42.5
ALA	22					O	1.6	26.3	34.0		SG	-2.9	23.4	37.1		OG1	-0.5	23.9	41.7
	CB	-3.8	41.6	38.5		N	3.5	25.7	34.1		CB	-1.8	24.6	37.2		CB	0.4	24.8	42.6
	CA	-4.3	42.8	37.8	GLN	34					CA	-2.8	25.9	36.4		CA	-0.1	24.2	44.8
	C'	-3.8	43.8	37.5		NE2	3.9	30.2	31.1		C'	-1.4	27.1	37.1		C'	-0.8	22.8	44.4
	O	-2.5	43.8	36.5		OE1	5.8	28.9	31.4		O	-0.4	27.6	36.8		O	-0.6	22.1	45.3
	N	-2.7	44.3	38.5		CD	4.6	29.8	31.4		N	-2.1	27.6	38.1		N	-1.9	22.7	43.7
GLN	23					CG	3.7	27.9	31.9	GLY	43				ALA	55			
	NE2	-4.0	48.6	40.8		CB	4.5	26.6	32.0		CA	-1.6	28.6	39.8		CB	-4.1	21.8	43.3
	OE1	-1.9	48.8	41.6		CA	3.7	25.5	32.7		C'	-0.9	27.9	40.1		CA	-2.8	21.5	43.9
	CD	-2.7	47.9	40.8		C'	4.4	24.2	32.5		O	-0.9	26.8	40.3		C'	-2.2	20.3	43.2
	CG	-2.7	47.0	39.6		O	5.3	23.8	33.1		N	-0.2	26.7	40.8		O	-2.1	20.3	42.8
	CB	-1.4	46.1	39.6		N	3.7	23.6	31.4	GLY	44					N	-2.3	19.3	43.9
	CA	-1.4	45.1	38.5	TYR	35					CA	0.4	28.3	42.0	ALA	56			
	C'	-0.1	44.3	38.7		OEH	-1.1	21.2	27.9		C'	0.9	29.4	42.9		CB	-2.5	16.8	44.4
	O	-0.1	43.3	39.5		CD2	2.3	20.9	28.7		O	0.9	30.6	42.5		CA	-1.8	17.9	43.4
	N	0.8	44.6	37.9		CE2	1.4	21.8	28.1		N	1.4	29.1	44.8		C'	-2.2	17.7	41.9
ARG	24					CZ	0.1	21.2	28.7	THR	45					O	-1.5	17.3	41.1
	NEH2	2.8	45.4	31.2		CE1	0.1	21.5	30.0		CG2	1.4	31.3	47.1		N	-3.4	18.1	41.8
	NEH1	3.8	44.2	32.9		CD1	1.1	21.5	30.7		OG1	-0.3	30.7	45.6	HIS	57			
	CZ	3.3	45.3	32.5		CG	2.5	21.1	30.1		CB	0.9	30.3	46.1		CD2	-7.9	17.9	39.8
	NE	2.8	46.0	33.5		CB	3.8	21.0	31.0		CA	2.0	30.1	44.9		NE2	-8.1	17.8	38.9
	CD	3.4	45.8	34.8		CA	4.6	22.3	31.0		C'	3.6	29.8	45.4		CE1	-7.7	16.5	38.2
	CG	2.5	45.0	35.7		C'	5.3	22.6	29.5		O	3.8	28.6	45.8		ND1	-6.1	16.9	38.8
	CB	2.9	44.7	37.1		O	4.6	23.6	28.9		N	4.1	30.8	45.5		CG	-6.3	17.8	39.7
	CA	2.1	43.8	37.9		N	5.9	21.8	29.2	LEU	46					CB	-5.4	18.5	40.5
	C'	2.7	43.6	39.2	ARG	36					CD2	8.5	33.0	45.4		CA	-4.0	17.9	40.4
	O	3.4	42.6	39.4		• NEH2	12.3	19.7	23.8		CD1	8.3	30.5	45.1		C'	-3.3	18.3	39.2
	N	2.5	44.3	40.2		• NEH1	12.6	19.5	26.1		CG	7.6	31.7	45.9		O	-3.1	17.5	38.2
ASN	25					• CZ	11.9	19.8	25.1		CB	6.1	32.0	45.6		N	-2.8	19.4	39.3
	ND2	2.8	47.9	41.0		• NE	10.6	20.2	25.3		CA	5.4	30.8	46.1	CYS	58			
	OD1	1.1	46.5	42.2		• CD	10.3	20.4	26.6		C'	5.3	30.9	47.6		CA	-0.4	24.3	36.7
	CG	2.4	46.7	41.7		• CG	8.8	21.0	26.5		O	4.8	31.9	48.0		CB	-1.8	24.6	37.2
	CB	3.5	45.8	41.8		CB	8.1	21.8	27.9		N	6.0	30.1	48.3		SG	-2.9	23.4	37.1
	CA	2.9	44.3	41.6		CA	6.8	21.8	27.9	ILE	47					SG	-2.7	22.5	38.9
	C'	1.9	43.8	42.7		C'	5.8	21.1	26.9		CD1	4.5	26.7	50.2		CB	-1.5	21.4	38.6
	O	2.2	43.6	43.9		O	5.3	19.9	27.1		CG1	5.7	27.8	49.8		CA	-2.8	20.8	38.1
	N	0.7	43.7	42.4		N	5.3	21.9	26.8		CB	5.3	29.1	50.4		C'	-0.9	19.1	37.8
SER	26				SER	36A					CG2	3.8	29.3	50.1		O	-0.4	19.2	36.8
	OG	-2.6	44.5	42.8		OG	2.2	21.3	24.3		CA	6.1	30.2	49.8		N	-0.4	18.3	38.7
	CB	-1.6	43.4	42.4		CB	3.2	22.3	24.5		C'	7.5	30.3	50.2	VAL	59			
	CA	-0.5	43.4	43.3		CA	4.4	21.4	24.9		O	7.7	30.4	51.4		CG2	1.8	17.9	41.8
	C'	-0.2	41.9	43.9		C'	5.5	21.3	23.7		N	8.4	30.1	49.4		CG1	2.8	19.5	39.3
	O	-0.4	41.9	45.2		O	5.7	22.1	22.9	ARG	48					CB	1.7	18.8	39.6
	N	0.8	40.9	43.2		N	6.8	20.8	23.7		NEH2	8.4	27.8	55.5		CA	0.8	17.6	38.5
TRP	27				GLY	36B					NEH1	7.7	29.3	53.8		C'	0.5	16.1	38.4
	CD2	-3.1	39.6	44.5		CA	7.1	19.6	22.7		CZ	8.7	28.6	54.4		O	1.3	15.3	38.5
	CE3	-3.2	39.1	45.8		C'	8.0	20.9	22.5		NE	9.9	28.5	53.9		N	-0.9	15.7	38.2
	CZ3	-4.2	39.4	46.6		O	8.9	21.1	23.3		CD	10.2	29.2	52.6	ASP	60			
	CH2	-5.1	40.3	46.2		N	7.5	21.7	21.5		CG	9.7	28.4	51.5		OD2	-4.1	14.2	39.8
	CZ2	-5.1	40.8	45.0	SER	36C					CB	10.4	28.7	50.1		OD1	-2.4	13.3	40.1
	CE2	-4.1	40.5	44.1		OG	7.7	22.7	18.7		CA	9.9	30.1	49.6		CG	-3.8	13.9	39.4
	NE1	-4.0	40.8	42.8		CB	7.6	23.5	19.8		C'	10.6	30.3	48.3		CB	-2.6	14.2	38.8
	CD1	-2.7	40.2	42.4		CA	8.2	22.9	21.1		O	10.1	30.0	47.2		CA	-1.1	14.3	38.0
	CG	-2.2	39.5	43.5		C'	8.4	24.1	22.2		N	11.8	30.8	48.3		C'	-0.4	13.8	36.8
	CB	-1.0	38.7	43.5		O	9.5	24.6	22.0	GLN	49					O	-0.3	12.5	36.6
	CA	0.2	39.6	43.8		N	7.3	24.3	22.8		NE2	15.4	34.5	47.4		N	-0.1	14.5	35.8
	C'	1.5	39.8	43.2	SER	37					OE1	15.6	33.7	49.5	ARG	61			
	O	1.3	38.2	42.3		OG	5.3	25.8	22.6		CD	14.9	33.8	48.4		• NEH2	-5.8	14.8	38.9
	N	2.5	39.4	43.8		CB	6.3	26.5	23.2		CG	13.6	33.1	48.2		• NEH1	-4.1	16.8	38.8
PRO	28					CA	7.3	25.4	23.8		CB	13.9	31.8	47.5		• CZ	-4.6	15.2	31.8
	CG	4.1	40.8	45.2		C'	6.6	24.9	25.1		CA	12.5	31.1	47.1		• NE	-3.7	14.6	31.9
	CD	2.6	40.4	45.8		O	6.3	23.7	25.3		C'	12.8	29.8	46.3		• CD	-2.2	15.1	32.8

* CG	-1.6	14.4	33.1
CB	-0.1	14.7	33.3
CA	0.4	14.0	34.5
C'	2.0	14.1	34.6
O	2.6	15.3	34.7
N	2.5	13.1	34.6
GLU 62			
OE2	4.3	8.8	36.3
OE1	6.5	9.4	36.1
CD	5.3	9.6	36.2
CG	4.7	11.1	36.1
CB	4.5	11.6	34.6
CA	4.8	13.0	34.6
C'	4.5	13.8	33.4
O	5.0	13.3	32.5
N	4.4	15.1	33.6
LEU 63			
CD2	2.9	16.1	30.1
CD1	1.5	17.6	31.6
CG	2.7	16.5	31.6
CB	4.0	17.1	32.2
CA	5.0	16.8	32.5
C'	6.3	16.7	33.1
O	6.6	16.6	34.3
N	6.8	17.4	32.2
THR 64			
CG2	10.4	19.3	31.8
OG1	9.7	17.8	31.4
CB	9.0	18.3	31.5
CA	8.0	18.3	32.6
C'	7.4	19.7	32.8
O	7.3	20.4	31.9
N	7.3	20.1	34.8
PHE 65			
CD2	5.3	19.8	36.8
CE2	4.4	18.8	36.8
CZ	3.1	18.2	35.6
CE1	2.9	19.5	35.2
CD1	3.6	20.6	35.2
CG	4.9	20.4	35.6
CB	5.9	21.5	35.6
CA	6.7	21.5	34.3
C'	7.9	22.5	34.5
O	9.1	22.1	34.7
N	7.6	23.7	34.3
ARG 65A			
NEH2	8.1	38.1	29.5
NEH1	10.8	28.7	29.6
CZ	8.8	29.1	30.8
NE	8.3	28.4	31.8
CD	9.8	27.3	31.6
CG	8.2	26.5	32.7
CB	9.2	25.5	33.4
CA	8.5	24.8	34.6
C'	7.6	25.8	35.4
O	6.5	25.9	35.2
N	8.3	26.6	36.3
VAL 66			
CG2	7.1	26.3	39.2
CG1	8.8	28.6	39.3
CB	8.8	27.3	38.6
CA	7.6	27.5	37.1
C'	8.1	29.8	36.7
O	9.4	29.1	36.5
N	7.3	29.8	36.5
VAL 67			
CG2	7.4	30.6	33.7
CG1	7.8	33.1	34.4
CB	7.1	31.6	34.8
CA	7.5	31.2	36.2
C'	6.9	32.1	37.2
O	5.8	32.2	37.5
N'	7.9	32.9	37.8
VAL 68			
CG2	10.8	34.1	39.6
CG1	8.3	32.8	40.8
CB	8.6	34.1	40.8
CA	7.6	34.8	38.7
C'	7.7	35.4	38.8
O	8.9	35.6	37.3
N	7.1	36.4	38.2
GLY 69			
CA	7.8	37.8	37.7
C'	6.5	37.8	36.3
O	6.6	38.5	35.4
N	5.4	36.9	36.2
GLU 70			
OE2	5.3	34.3	31.9
OE1	5.8	36.4	31.6
CD	4.6	35.2	32.2
CG	3.6	35.2	33.2
CB	4.3	35.3	34.7
CA	4.5	36.8	35.8
C'	3.1	37.6	35.1
O	2.5	37.5	36.1
N	3.1	38.5	34.1
HIS 71			
CD2	8.2	42.2	33.1
NE2	-0.8	42.8	33.6
CE1	-0.8	42.6	34.9
NO1	8.3	41.8	35.2
CG	8.9	41.6	34.1
CB	2.1	40.8	34.8
CA	1.7	39.3	34.1
C'	1.1	38.9	32.8
O	-0.2	38.7	32.7
N	1.9	39.8	31.8
ASN 72			
* ND2	8.2	48.8	27.6
* OD1	8.8	38.6	27.6
* CG	8.9	39.7	28.1
CB	1.5	39.9	29.4
CA	1.4	38.7	30.3
C'	2.8	37.5	29.8
O	3.3	37.5	29.6
N	1.5	36.4	29.7
LEU 73			
CD2	1.4	33.1	31.3
CD1	-0.9	32.6	30.1
CG	0.2	33.7	30.4
CB	0.9	34.0	29.8
CA	2.1	35.1	29.2
C'	2.8	35.3	27.9
O	3.9	35.1	27.7
N	2.0	35.9	26.9
ASN 74			
ND2	1.0	33.8	25.8
OD1	-1.0	35.8	24.7
CG	0.4	35.0	24.7
CB	1.3	36.2	24.6
CA	2.6	36.1	25.5
C'	3.4	37.3	25.2
O	3.7	37.5	24.2
N	3.6	38.1	26.3
GLN 75			
* NE2	4.8	44.2	26.1
* OE1	2.1	43.8	25.8
* CD	3.5	43.1	25.9
* CG	4.4	41.8	25.9
CB	3.6	40.5	26.2
CA	4.5	39.3	26.2
C'	5.5	39.2	27.2
O	5.5	38.8	27.8
N	6.7	40.0	26.9
ASN 76			
ND2	11.1	41.6	27.7
OD1	10.6	39.6	28.7
CG	10.3	40.5	27.8
CB	9.1	40.4	26.9
CA	7.8	40.6	27.8
C'	7.5	41.4	28.6
O	7.5	42.5	28.1
N	7.1	41.1	29.8
ASN 77			
ND2	3.8	41.9	31.2
OD1	4.4	39.9	32.2
CG	4.8	41.1	31.8
CB	6.1	41.6	32.1
CA	6.8	42.2	30.9
C'	8.1	42.8	31.4
O	8.1	43.9	32.8
N	9.1	41.9	31.2
GLY 78			
CA	10.6	42.3	31.6
C'	11.8	41.9	33.8
O	12.1	42.2	33.5
N	10.2	41.1	33.7
THR 79			
CG2	9.4	42.9	35.8
OG1	7.8	41.8	35.2
CB	9.1	41.3	35.8
CA	10.4	40.8	35.1
C'	10.4	39.3	35.4
O	10.4	38.8	36.5
N	10.2	38.5	34.3
GLU 80			
OE2	8.4	38.8	38.5
OE1	8.5	39.1	32.3
CD	8.4	38.8	31.7
CG	8.5	36.6	32.4
CB	10.8	36.5	33.8
CA	10.1	37.8	34.5
C'	11.4	36.3	35.1
O	12.6	36.8	34.9
N	11.2	35.2	35.8
GLN 81			
NE2	13.3	36.5	40.1
OE1	14.6	34.6	40.3
CD	13.9	35.4	39.7
CG	13.8	35.1	38.1
CB	12.4	34.4	37.8
CA	12.2	34.4	36.3
C'	11.6	33.8	35.8
O	10.6	32.6	36.1
N	12.5	32.2	35.1
TYR 82			
OEH	9.9	35.1	30.2
CD2	10.4	31.8	31.9
CE2	9.7	32.9	31.2
CZ	10.4	34.1	31.8
CE1	11.8	34.2	31.4
CD1	12.4	33.2	32.1
CG	11.7	32.8	32.3
CB	12.5	30.9	33.1
CA	12.2	30.9	34.6
C'	13.8	29.8	35.4
O	14.2	29.8	35.3
N	12.3	29.8	36.1
VAL 83			
CG2	14.1	27.8	39.1
CG1	11.7	28.6	39.1
CB	13.1	28.6	38.3
CA	12.8	27.9	36.9
C'	12.0	26.6	36.8
O	10.8	26.4	36.8
N	12.8	25.5	36.8
GLY 84			
CA	12.3	24.2	36.8
C'	12.2	23.6	38.0
O	12.7	24.1	39.0
N	11.6	22.5	38.0
VAL 85			
CG2	8.9	22.4	38.8
CG1	9.4	20.3	40.1
CB	9.8	21.2	39.0
CA	11.3	21.7	39.2
C'	12.3	20.5	39.3
O	12.5	19.9	38.2
N	12.7	20.1	40.4
GLN 86			
NE2	16.7	19.5	44.5
OE1	17.4	19.8	42.4
CD	16.5	19.6	43.2
CG	15.0	19.7	42.8
CB	14.9	19.4	41.2
CA	13.6	19.8	40.6
C'	13.1	18.8	41.5
O	13.5	16.8	41.6
N	11.8	18.2	42.3
LYS 87			
NZ	14.2	16.8	47.7
CE	13.3	15.9	46.4
CD	11.8	16.3	46.8
CG	11.2	16.3	45.5
CB	11.9	17.3	44.6
CA	11.2	17.3	43.2
C'	9.8	17.7	43.4
O	9.4	18.9	43.7
N	8.9	16.6	43.3
ILE 88			
CD1	6.6	17.2	39.7
CG1	7.3	17.6	41.0
CB	6.8	16.4	42.1
CG2	5.2	16.4	42.2
CA	7.4	16.8	43.4
C'	6.9	15.9	44.6
O	6.9	14.8	44.6
N	6.3	16.5	45.4
VAL 89			
CG2	7.7	16.8	47.9
CG1	5.5	15.7	49.1
CB	6.1	16.3	47.9
CA	5.5	16.8	46.6
C'	4.1	16.3	46.6
O	3.7	17.5	46.9
N	3.3	15.4	46.3
VAL 90			
CG2	-0.3	14.9	45.3
CG1	1.5	13.5	45.4
CB	1.2	14.7	45.3
CA	1.8	15.5	46.4
C'	1.3	14.9	47.7
O	1.9	13.9	48.1
N	0.3	15.3	48.3
HIS 91			
CD2	-1.4	15.9	52.2
NE2	-1.9	15.4	53.5
CE1	-2.4	14.1	53.1
ND1	-2.2	14.8	51.8
CG	-1.8	15.1	51.3
CB	-1.4	15.3	49.8
CA	-0.1	14.7	49.5
C'	-0.4	13.1	49.3
O	-0.7	12.5	48.2
N	-0.1	12.4	50.3
PRO 92			
CG	0.7	11.9	52.6
CD	0.2	13.1	51.6
CB	0.4	10.7	51.8
CA	-0.1	11.0	50.5
C'	-1.5	10.4	50.3
O	-1.6	9.3	50.8
N	-2.3	11.3	50.5
TYR 93			
OEH	-4.5	8.8	56.4
CD2	-4.8	11.6	54.8
CE2	-4.7	10.9	55.2
CZ	-4.5	9.5	55.3
CE1	-4.4	8.8	54.1
CD1	-4.2	9.4	53.0
CG	-4.5	10.8	53.0
CB	-4.8	11.7	51.6
CA	-3.9	10.9	50.5
C'	-4.4	11.3	49.2
O	-5.9	11.1	49.1
N	-3.8	11.9	48.2
TRP 94			
CD2	-5.3	14.3	44.8
CE3	-6.1	14.8	45.6
CZ3	-7.3	15.5	45.2
CEH2	-7.4	15.7	43.8
CZ2	-6.5	15.2	42.9
CE2	-5.3	14.5	43.4
NE1	-4.4	14.8	42.8
CD1	-3.6	13.4	43.7
CG	-4.8	13.6	45.8
CB	-3.3	13.1	46.3
CA	-4.4	12.2	47.8
C'	-4.6	11.8	46.2
O	-4.1	10.1	45.9
N	-5.9	11.1	45.7
ASN 95			
ND2	-8.1	8.3	43.5
OD1	-9.4	7.7	45.2
CG	-8.2	8.3	44.8
CB	-7.2	9.1	45.6
CA	-6.5	10.1	44.8
C'	-7.2	10.9	43.8
O	-8.6	11.3	44.0
N	-6.5	11.1	42.6
THR 96			
CG2	-6.6	12.4	39.2
OG1	-4.7	11.7	40.6
CB	-6.2	11.6	40.3
CA	-7.1	11.9	41.5
C'	-8.3	11.6	41.1
O	-9.2	12.5	40.7
N	-8.0	10.4	41.3
ASP 97			
OD2	-9.8	6.5	40.1
OD1	-9.4	8.3	38.8
CG	-9.5	7.7	39.9
CB	-10.3	8.4	41.1
CA	-10.1	9.9	41.2
C'	-11.2	10.3	42.3
O	-12.0	10.2	42.2
N	-10.7	11.0	43.3
ASP 98			
OD2	-12.8	9.7	47.2
OD1	-13.7	11.1	45.8
CG	-12.7	10.4	46.2
CB	-11.4	10.5	45.6
CA	-11.6	11.5	44.4
C'	-10.9	12.7	44.9
O	-10.2	12.9	45.8
N	-11.4	13.8	44.1
VAL 99			
CG2	-12.2	16.3	42.7
CG1	-9.8	15.3	42.2
CB	-11.1	16.1	43.2
CA	-11.1	15.2	44.5
C'	-11.9	15.8	45.4
O	-11.5	16.6	46.3
N	-13.2	15.4	45.3
ALA 99A			
CB	-15.8	15.3	45.8
CA	-14.8	15.9	46.2
C'	-13.8	15.3	47.6
O	-14.5	15.5	48.6
N	-12.6	14.5	47.6
ALA 99B			
CB	-11.8	12.5	48.5
CA	-12.4	13.9	48.8
C'	-11.3	14.8	49.4
O	-11.1	14.6	50.6
N	-10.6	15.6	48.7
GLY 100			
CA	-9.6	16.5	49.1
C'	-8.1	15.9	48.9
O	-8.1	15.8	48.2
N	-7.3	16.5	49.6
TYR 101			
OEH	-8.6	13.3	54.3
CD2	-7.7	13.0	50.8
CE2	-8.2	13.4	51.9
CZ	-8.0	13.5	53.2
CE1	-6.7	14.0	53.4
CD1	-6.1	14.5	52.3
CG	-6.4	14.4	51.0
CB	-5.7	14.8	49.7
CA	-5.9	16.3	49.6
C'	-5.3	16.8	48.2
O	-4.4	16.5	47.8
N	-6.8	17.8	47.5
ASP 102			
OD2	-7.4	19.7	43.6
OD1	-5.3	19.3	44.8
CG	-6.6	19.5	44.4
CB	-7.8	19.8	45.8
CA	-5.8	18.5	46.5
C'	-4.6	19.5	46.8
O	-4.8	20.7	46.8
N	-3.6	19.2	46.9
ILE 103			
CD1	-1.1	21.8	50.3
CG1	-1.2	21.3	48.8
CB	-2.4	20.5	48.6
CG2	-2.5	19.3	49.5
CA	-2.4	20.1	47.1
C'	-1.8	19.3	46.9
O	-1.8	18.1	47.1
N	0.8	20.1	46.6
ALA 104			
CB	1.2	18.9	45.8
CA	1.2	19.6	46.4
C'	2.3	20.7	46.4
O	2.8	21.9	46.2
N	3.4	20.3	46.7
LEU 105			
CD2	4.3	23.1	49.6
CD1	4.8	20.8	50.3
CG	4.1	21.7	49.1
CB	5.3	21.3	48.1
CA	4.5	21.2	46.7
C'	5.7	20.9	45.7
O	6.8	19.8	45.5
N	6.1	21.9	45.1
LEU 106			

CD2	5.2	20.6	42.4
CD1	5.2	22.7	40.8
CG	5.3	22.1	42.3
CB	6.8	22.6	42.9
CA	7.1	21.8	44.1
C'	8.5	22.4	44.6
O	8.4	23.6	44.9
N	9.6	21.6	44.6
ARG107			
* NEH2	16.7	21.8	48.4
* NEH1	14.6	21.3	49.1
* CZ	15.4	21.2	48.1
* NE	15.2	20.8	46.9
CD	13.9	20.3	46.6
CG	13.8	21.5	46.1
CB	11.7	20.9	45.6
CA	10.8	22.1	45.8
C'	11.6	22.5	43.6
O	11.6	21.8	42.7
N	12.8	23.8	43.7
LEU108			
CD2	10.4	25.8	41.6
CD1	11.1	27.9	42.5
CG	11.1	26.4	42.7
CB	12.6	25.9	42.6
CA	12.6	24.3	42.5
C'	14.1	23.8	42.5
O	14.8	23.5	43.4
N	14.6	24.0	41.1
ALA109			
CB	15.9	23.3	39.2
CA	15.9	23.5	40.7
C'	16.9	24.6	41.1
O	18.1	24.4	41.3
N	16.3	25.8	41.2
GLN110			
* NE2	21.3	29.8	39.9
* OE1	19.5	28.9	38.5
* CD	20.1	28.7	39.5
CG	19.4	28.1	40.8
CB	17.8	27.8	40.4
CA	17.2	27.8	41.7
C'	16.8	27.9	42.4
O	14.8	27.8	42.3
N	16.6	28.8	43.2
SER111			
OG	16.8	29.8	46.1
CB	16.8	30.1	45.3
CA	15.9	29.8	44.0
C'	15.7	31.1	43.3
O	16.6	31.7	42.8
N	14.5	31.6	43.3
VAL112			
CG2	12.8	33.3	43.9
CG1	12.4	31.9	41.8
CB	12.7	33.1	42.5
CA	14.3	32.9	42.8
C'	14.7	34.1	43.6
O	14.9	34.8	44.9
N	14.9	35.2	43.8
THR113			
CG2	16.1	38.8	43.3
OG1	17.5	36.7	42.7
CB	16.8	37.4	42.8
CA	15.1	36.4	43.7
C'	13.8	37.2	43.9
O	13.8	37.4	43.8
N	13.6	37.7	45.1
LEU114			
CD2	11.3	36.8	46.7
CD1	12.2	36.8	49.8
CG	12.3	36.9	47.4
CB	12.2	38.3	47.8
CA	12.4	38.4	45.4
C'	12.6	39.9	45.8
O	13.6	40.4	44.8
N	11.3	40.4	44.7
ASN115			
ND2	12.4	48.5	41.8
OD1	10.3	41.3	41.5
CG	11.4	41.3	41.8
CB	12.8	42.1	42.9
CA	11.4	41.8	44.4
C'	9.9	42.2	44.3
O	8.9	41.3	44.6
N	9.6	43.5	44.1
SER116			
OG	8.6	45.5	42.3
CB	8.3	45.5	43.6
CA	8.2	44.8	44.1
C'	7.3	43.2	43.2
O	6.1	43.2	43.3
N	7.9	42.5	42.2
TYR117			
OEH	8.1	47.1	37.7
CD2	9.4	43.8	38.9
CE2	9.3	45.1	38.4
CZ	8.1	45.8	38.2
CE1	7.8	45.2	38.5
CD1	6.8	43.8	39.0
CG	8.1	43.2	39.3
CB	7.8	41.8	39.8
CA	7.4	41.7	41.2
C'	7.4	40.2	41.6
O	6.4	39.4	41.8
N	7.9	39.9	42.6
VAL118			
CG2	9.1	37.6	40.8
CG1	9.5	36.5	43.1
CB	9.3	37.0	42.4
CA	8.0	38.5	43.1
C'	8.3	38.4	44.6
O	9.4	38.6	45.0
N	7.3	38.2	45.4
GLN119			
NE2	8.9	39.8	49.0
OE1	9.6	41.3	47.5
CD	8.6	40.6	48.0
CG	7.2	40.5	47.5
CB	6.7	39.0	47.6
CA	7.5	38.0	46.8
C'	7.0	36.6	47.3
O	6.6	35.8	46.5
N	7.2	36.5	48.6
LEU120			
CD2	8.9	33.3	48.7
CD1	10.0	33.9	50.9
CG	9.1	34.4	49.8
CB	7.7	34.9	50.3
CA	6.8	35.2	49.2
C'	5.3	35.3	49.8
O	4.8	36.4	50.2
N	4.6	34.3	49.6
GLY121			
CA	3.3	34.2	49.8
C'	3.1	34.8	51.4
O	3.7	33.1	51.9
N	2.0	34.9	51.9
VAL122			
CG2	2.7	37.1	53.7
CG1	1.1	35.8	55.4
CB	1.6	36.3	53.8
CA	1.8	34.8	53.3
C'	0.9	33.8	53.5
O	-0.4	33.9	53.3
N	1.4	32.6	54.2
LEU123			
CD2	0.5	28.9	52.9
CD1	2.8	28.5	53.8
CG	1.7	29.6	53.6
CB	1.1	30.1	55.0
CA	0.4	31.5	54.7
C'	-0.3	31.9	56.0
O	0.1	32.6	56.8
N	-1.4	31.3	56.2
PRO124			
CG	-3.5	30.1	55.5
CD	-2.1	30.4	55.1
CB	-3.7	30.9	56.9
CA	-2.3	31.5	57.3
C'	-1.8	30.6	58.5
O	-0.9	29.9	58.3
N	-2.3	30.8	59.6
ARG125			
* NEH2	8.8	35.7	64.1
* NEH1	-8.7	34.5	65.4
* CZ	8.0	34.8	64.2
* NE	-8.3	33.8	63.3
* CD	-1.1	32.8	63.3
CG	-1.3	32.0	62.0
CB	-2.3	30.9	62.0
CA	-2.1	30.8	60.8
C'	-3.2	28.8	60.8
O	-4.2	28.9	60.5
N	-2.5	27.6	61.0
ALA126			
CB	-2.6	25.3	61.5
CA	-3.4	26.4	61.0
C'	-4.8	26.6	61.8
O	-4.9	27.1	62.9
N	-5.8	25.9	61.1
GLY127			
CA	-6.8	25.8	61.7
C'	-7.8	27.0	61.5
O	-9.2	26.9	61.6
N	-7.3	28.1	61.3
THR128			
CG2	-8.8	31.6	59.9
OG1	-6.2	30.8	61.3
CB	-7.2	30.4	60.4
CA	-8.1	29.3	61.0
C'	-9.2	29.0	59.9
O	-8.9	28.7	58.9
N	-10.4	29.4	60.5
ILE129			
CD1	-11.5	26.5	59.8
CG1	-11.9	27.1	60.4
CB	-12.6	28.5	60.3
CG2	-13.6	28.4	59.3
CA	-11.6	29.4	59.6
C'	-12.1	30.8	59.5
O	-12.6	31.5	60.5
N	-12.3	31.2	58.3
LEU130			
CD2	-10.6	34.3	57.3
CD1	-10.8	33.5	55.0
CG	-10.9	33.3	56.4
CB	-12.6	32.9	56.6
CA	-12.9	32.5	58.0
C'	-14.5	32.4	58.0
O	-15.1	31.6	57.6
N	-14.8	33.5	58.7
ALA131			
CB	-16.5	35.3	59.5
CA	-16.0	33.9	58.7
C'	-16.5	33.9	57.3
O	-15.9	34.1	56.5
N	-17.9	33.8	57.2
ASN132			
ND2	-21.5	33.8	54.7
OD1	-20.1	32.3	54.1
CG	-20.7	33.0	54.9
CB	-20.0	33.2	56.2
CA	-18.5	33.8	55.9
C'	-18.6	35.2	55.4
O	-18.7	36.2	56.0
N	-18.2	35.2	54.0
ASN133			
ND2	-19.9	37.6	51.4
OD1	-21.6	37.3	52.8
CG	-20.4	37.4	52.7
CB	-19.6	37.2	53.8
CA	-18.4	36.4	53.3
C'	-16.8	37.1	53.5
O	-17.0	38.4	53.3
N	-16.0	36.5	53.9
SER134			
OG	-14.3	35.9	56.0
CB	-13.9	36.1	54.7
CA	-15.1	37.2	54.0
C'	-14.3	37.5	52.6
O	-14.4	36.8	51.7
N	-13.9	38.6	52.6
PRO135			
CG	-13.2	40.9	53.3
CD	-13.9	39.5	53.7
CB	-12.8	40.6	51.9
CA	-13.3	39.3	51.5
C'	-12.0	38.5	50.9
O	-11.1	38.4	51.5
N	-12.3	37.9	49.8
CYS136			
CA	-9.2	35.5	54.0
CB	-9.0	35.7	52.5
SG	-9.7	34.5	51.3
SG	-11.5	35.2	51.1
CB	-11.5	35.0	49.4
CA	-11.2	37.1	49.2
C'	-11.1	37.3	47.6
O	-12.0	37.5	47.0
N	-10.0	37.2	47.2
TYR137			
OEH	-11.6	43.5	45.2
CD2	-9.5	40.8	46.6
CE2	-10.4	41.9	46.5
CZ	-10.7	42.2	45.3
CE1	-10.6	41.4	44.2
CD1	-9.9	40.3	44.3
CG	-9.3	39.9	45.5
CB	-8.6	38.6	45.6
CA	-9.6	37.4	45.8
C'	-8.8	36.2	45.1
O	-7.9	35.6	45.7
N	-9.3	36.0	43.9
ILE138			
CD1	-9.9	31.7	41.6
CG1	-8.8	32.8	41.9
CB	-9.7	33.9	42.7
CG2	-10.4	34.6	41.7
CA	-8.6	35.8	43.2
C'	-8.1	35.7	41.9
O	-8.4	36.5	41.2
N	-6.6	35.2	41.6
THR139			
CG2	-5.1	37.8	41.6
OG1	-4.1	35.4	42.2
CB	-4.7	36.3	41.1
CA	-6.1	35.6	40.5
C'	-5.5	34.5	39.7
O	-5.3	33.4	40.2
N	-5.4	34.7	38.4
GLY140			
CA	-5.3	33.7	37.5
C'	-5.2	34.2	36.8
O	-5.8	35.1	35.7
N	-4.8	33.2	35.2
TRP141			
CD2	-1.5	34.2	34.3
CE3	-1.1	33.4	35.3
CZ3	-0.1	33.6	36.1
CEH2	0.6	34.7	35.9
CZ2	0.2	35.6	34.8
CE2	-0.9	35.4	34.1
NE1	-1.4	35.9	32.9
CD1	-2.6	35.3	32.6
CG	-2.4	34.1	33.5
CB	-3.5	32.9	33.3
CA	-4.8	33.3	33.8
C'	-5.8	32.5	33.8
O	-6.1	32.6	31.6
N	-6.4	31.6	33.7
GLY142			
CA	-7.4	30.7	33.2
C'	-8.7	31.3	32.3
O	-8.5	32.7	32.1
N	-9.4	30.7	31.8
LEU143			
CD2	-9.6	28.9	29.4
CD1	-11.7	27.8	29.5
CG	-10.8	28.6	30.4
CB	-11.4	29.9	30.9
CA	-10.4	31.0	31.0
C'	-11.1	32.5	31.6
O	-11.1	32.6	32.8
N	-11.8	33.1	30.7
THR144			
CG2	-10.7	35.8	30.0
OG1	-12.5	34.9	28.8
CB	-12.1	35.3	30.0
CA	-12.6	34.3	30.9
C'	-13.9	33.9	30.9
O	-15.1	34.5	31.5
N	-14.1	32.9	30.2
ARG145			
NEH2	-20.3	34.9	26.4
NEH1	-20.4	33.8	28.4
CZ	-19.6	34.4	27.4
NE	-18.2	34.6	27.6
CD	-17.7	34.0	28.9
CG	-16.5	34.8	28.5
CB	-16.2	32.3	28.7
CA	-15.4	32.1	30.0
C'	-15.3	30.7	30.2
O	-14.5	30.0	30.1
N	-16.1	29.9	30.4
THR147			
CG2	-17.5	26.4	30.9
OG1	-17.7	28.4	32.3
CB	-17.8	28.0	30.9
CA	-16.3	28.5	30.4
C'	-16.2	28.1	28.8
O	-16.9	28.5	28.1
N	-15.3	27.4	28.6
ASN148			
ND2	-17.6	24.7	27.7
OD1	-15.7	24.1	27.8
CG	-16.5	25.8	27.4
CB	-16.1	26.1	26.7
CA	-14.9	26.8	27.3
C'	-14.4	28.0	26.4
O	-14.8	28.1	25.1
N	-13.6	28.8	26.9
GLY149			
CA	-13.1	30.0	26.2
C'	-11.4	29.8	26.2
O	-10.9	28.8	26.2
N	-11.1	31.0	26.2
GLN150			
* NE2	-9.1	33.4	22.7
* OE1	-9.8	35.3	23.6
* CD	-9.5	34.8	23.6
CG	-9.9	33.5	24.9
CB	-9.2	31.8	24.9
CA	-9.7	30.9	26.1
C'	-8.9	31.4	27.4
O	-9.6	32.0	28.2
N	-7.8	31.3	27.6
LEU151			
CD2	-6.2	29.3	30.7
CD1	-4.4	29.8	28.8
CG	-5.9	29.5	29.1
CB	-5.7	31.1	29.0
CA	-7.1	31.7	28.8
C'	-6.8	33.2	28.6
O	-6.6	33.9	27.5
N	-6.6	33.8	29.7
ALA152			
CB	-6.8	35.8	31.0
CA	-6.4	35.3	29.7
C'	-4.9	35.4	29.5
O	-4.8	34.7	29.9
N	-4.5	36.4	28.7
GLN153			
* NE2	-2.9	39.1	24.6
* OE1	-5.2	38.7	24.2
* CD	-4.1	38.4	24.8
CG	-4.1	37.4	26.8
CB	-3.3	37.9	27.2
CA	-3.4	36.9	28.3
C'	-2.6	37.3	29.5
O	-1.4	37.2	29.8
N	-3.3	38.0	30.4
THR154			
CG2	-2.8	40.7	30.4
OG1	-4.3	40.6	31.8
CB	-3.8	40.2	31.4
CA	-2.8	38.6	31.6
C'	-3.5	38.2	32.8
O	-4.8	37.9	32.8
N	-2.9	38.1	34.0
LEU155			
CD2	-1.7	38.3	38.7
CD1	-2.3	36.2	37.6
CG	-2.6	37.7	37.6
CB	-2.4	38.4	36.3
CA	-3.4	37.9	35.3
C'	-4.7	38.5	35.4
O	-4.8	39.8	35.5
N	-5.8	37.8	35.8
GLN156			
NE2	-6.8	39.9	33.1
OE1	-9.2	39.6	33.4
CD	-7.8	39.1	33.4
CG	-7.7	37.7	33.7
CB	-7.9	37.3	35.1
CA	-6.8	38.1	36.8
C'	-7.3	38.8	37.5
O	-6.8	37.8	38.1

N	-7.9	38.9	38.0
GLN157			
NE2	-7.8	43.3	41.1
OE1	-5.7	42.4	40.8
CD	-7.0	42.4	40.4
CG	-7.6	41.4	39.6
CB	-7.4	39.9	42.1
CA	-8.3	38.9	39.4
C'	-9.8	39.4	39.6
O	-10.1	40.3	38.9
N	-10.4	38.8	42.5
ALA158			
CB	-12.6	38.1	40.8
CA	-11.8	39.0	40.9
C'	-12.3	38.7	42.3
O	-11.4	37.8	43.2
N	-13.4	39.4	42.8
TYR159			
OEH	-14.8	41.2	49.9
CD2	-15.6	40.8	46.5
CE2	-15.8	41.8	47.9
CZ	-14.8	41.1	48.6
CE1	-13.7	41.8	48.8
CD1	-13.5	40.8	46.7
CG	-14.7	40.8	45.9
CB	-14.6	40.7	44.4
CA	-13.8	39.4	44.2
C'	-14.6	38.2	44.4
O	-15.5	38.1	44.8
N	-13.9	37.3	45.2
LEU160			
CD2	-13.7	32.8	43.7
CD1	-14.8	34.8	42.7
CG	-14.6	34.1	43.9
CB	-13.6	35.0	44.8
CA	-14.4	36.1	45.5
C'	-14.7	35.8	47.0
O	-13.4	35.8	47.5
N	-15.6	36.2	47.5
PR0161			
CG	-17.7	37.3	48.0
CD	-16.8	36.8	46.9
CB	-17.1	36.8	49.4
CA	-15.9	35.9	48.9
C'	-16.3	34.5	49.1
O	-16.6	33.8	48.4
N	-15.7	34.1	50.3
THR162			
CG2	-13.6	33.2	52.1
OG1	-15.0	33.7	53.1
CB	-15.2	32.8	52.3
CA	-15.6	32.9	50.9
C'	-17.4	32.7	51.4
O	-18.0	33.6	51.6
N	-17.5	31.4	51.5
VAL163			
CG2	-19.0	31.6	49.8
CG1	-21.0	29.9	51.1
CB	-19.5	30.4	50.7
CA	-19.0	30.8	51.9
C'	-18.5	29.7	52.9
O	-17.6	28.8	52.9
N	-19.0	29.7	54.0
ASP164			
OD2	-21.3	30.3	57.5
OD1	-21.7	28.9	55.9
CG	-20.9	29.5	56.6
CB	-19.2	29.2	56.6
CA	-18.9	28.8	55.0
C'	-19.5	27.4	54.7
O	-20.5	27.3	54.1
N	-18.0	26.4	55.2
TYR165			
OEH	-18.9	18.7	55.2
CD2	-19.4	22.8	56.9
CE2	-19.6	20.6	56.8
CZ	-19.1	20.8	55.5
CE1	-18.4	20.8	54.5
CD1	-18.3	22.2	54.7
CG	-18.8	22.7	55.8
CB	-18.5	24.3	56.1
CA	-19.3	25.1	55.0
C'	-21.0	24.8	55.4
O	-21.4	24.2	54.6
N	-21.6	25.4	56.3
ALA166			
CB	-23.2	26.6	57.5
CA	-22.9	25.4	56.8
C'	-23.6	25.3	55.5
O	-23.9	24.2	55.0
N	-23.3	26.4	54.7
ILE167			
CD1	-24.3	30.5	54.8
CG1	-24.2	28.8	54.3
CB	-23.8	28.8	53.2
CG2	-24.4	28.4	51.9
CA	-23.8	26.5	53.6
C'	-23.9	25.9	52.4
O	-24.5	25.1	51.8
N	-22.4	26.8	52.2
CYS168			
CA	-17.8	28.3	58.4
CB	-17.5	27.3	49.2
SG	-17.6	25.7	49.5
SG	-19.8	25.3	49.4
CB	-20.3	25.4	50.9
CA	-21.8	25.4	51.8
C'	-22.2	23.9	52.9
O	-22.8	23.3	49.8
N	-22.4	23.4	52.2
SER169			
OG	-21.2	21.6	54.1
CB	-22.4	21.5	53.7
CA	-22.8	21.8	52.2
C'	-24.2	21.7	51.8
O	-24.6	20.5	51.7
N	-25.2	22.8	51.5
SER170			
OG	-26.9	24.7	52.2
CB	-26.9	24.2	51.2
CA	-26.3	22.6	51.2
C'	-26.6	21.8	49.9
O	-25.8	21.6	49.1
N	-27.8	21.2	49.8
SER170A			
OG	-30.4	20.8	49.4
CB	-29.5	19.8	49.2
CA	-28.2	20.5	48.7
C'	-28.3	21.5	47.6
O	-28.3	21.2	46.5
N	-28.2	22.9	48.0
SER170B			
OG	-29.6	25.9	47.0
CB	-29.5	24.9	47.9
CA	-28.6	23.8	47.2
C'	-27.4	24.3	46.7
O	-27.0	24.8	45.6
N	-26.3	23.7	47.2
TYR171			
OEH	-25.3	30.5	48.5
CD2	-23.5	27.4	48.0
CE2	-24.0	28.7	48.1
CZ	-25.1	29.1	48.4
CE1	-25.9	28.2	48.6
CD1	-25.0	26.8	48.6
CG	-24.4	26.4	48.3
CB	-24.5	25.0	48.2
CA	-25.2	24.4	47.0
C'	-24.2	23.1	46.4
O	-24.4	22.8	45.3
N	-23.4	22.6	47.3
TRP172			
CD2	-19.9	22.2	44.9
CE3	-20.8	20.9	44.4
CZ3	-19.6	20.5	43.2
CEH2	-19.2	21.4	42.5
CZ2	-19.0	22.7	43.0
CE2	-19.5	23.0	44.2
NE1	-19.4	24.2	44.9
CD1	-19.9	24.0	46.1
CG	-20.4	22.8	46.1
CB	-21.1	22.1	47.3
CA	-22.5	21.6	46.8
C'	-22.7	20.3	47.4
O	-22.2	19.3	46.7
N	-23.4	20.1	48.4
GLY173			
CA	-23.6	18.8	48.8
C'	-22.4	18.3	49.6
O	-21.5	19.0	50.2
N	-22.2	16.9	49.7
SER174			
OG	-22.2	14.4	49.5
CB	-21.7	14.8	50.6
CA	-21.1	16.3	50.4
C'	-20.1	16.3	49.7
O	-19.8	15.8	50.1
N	-20.1	16.8	48.5
THR175			
CG2	-18.1	17.4	45.4
OG1	-20.2	16.8	45.8
CB	-19.4	17.5	46.4
CA	-18.9	16.9	47.7
C'	-17.8	17.8	48.4
O	-16.6	17.4	48.1
N	-18.1	18.7	49.4
VAL176			
CG2	-16.9	22.8	50.1
CG1	-19.2	21.8	50.4
CB	-17.9	21.8	49.6
CA	-17.2	19.5	49.7
C'	-17.8	19.2	51.1
O	-17.8	19.1	52.8
N	-15.9	18.9	51.4
LYS177			
NZ	-16.8	15.5	50.2
CE	-16.1	14.7	51.2
CD	-15.6	15.5	52.3
CG	-14.7	16.6	51.7
CB	-14.4	17.6	52.7
CA	-15.6	18.6	52.7
C'	-15.0	19.8	53.5
O	-14.6	20.9	53.8
N	-15.5	19.6	54.9
ASN178			
ND2	-15.8	21.9	58.6
OD1	-13.3	21.5	58.6
CG	-14.6	21.3	58.2
CB	-14.8	20.1	57.2
CA	-14.9	20.6	55.8
C'	-13.5	21.1	55.4
O	-13.1	22.1	56.1
N	-12.8	20.5	54.6
SER179			
CG	-11.2	19.2	52.9
CB	-12.8	19.6	54.1
CA	-11.2	22.8	54.2
C'	-11.1	21.8	53.2
O	-12.2	22.1	52.4
N	-12.4	22.4	52.6
MET180			
CE	-13.4	18.8	49.2
SD	-14.1	22.4	49.2
CG	-13.2	21.1	52.2
CB	-13.4	22.6	52.6
CA	-12.6	23.2	51.5
C'	-12.9	24.5	51.9
O	-13.5	24.8	53.2
N	-13.1	25.3	52.9
VAL181			
CG2	-11.6	27.4	52.3
CG1	-13.1	29.1	51.2
CB	-12.5	27.8	51.2
CA	-13.6	26.8	51.1
C'	-14.1	27.0	49.8
O	-13.9	26.8	48.8
N	-15.5	27.5	52.0
CYS182			
CA	-20.7	26.9	51.4
CB	-20.3	25.4	50.9
SG	-19.8	25.3	49.4
SG	-17.6	25.7	49.5
CB	-17.5	27.3	49.2
CA	-16.3	27.8	48.9
C'	-16.1	29.3	48.8
O	-16.5	30.0	49.7
N	-16.2	29.7	47.6
ALA183			
CB	-14.4	31.6	46.9
CA	-16.0	31.1	47.3
C'	-16.9	31.5	46.1
O	-16.9	30.9	45.1
N	-17.6	32.6	46.1
GLY184			
CA	-18.2	33.0	45.0
C'	-19.5	32.7	45.0
O	-20.3	32.7	46.0
N	-20.3	32.3	44.0
GLY185			
CA	-21.5	31.9	43.7
C'	-22.4	32.9	43.2
O	-23.8	32.6	43.3
N	-22.0	33.9	42.9
ASP186			
CD2	-20.3	35.3	41.1
OD1	-20.1	37.4	41.6
CG	-20.8	36.4	41.6
CB	-22.0	36.5	42.3
CA	-22.8	35.0	42.3
C'	-22.9	34.7	40.8
O	-23.5	35.2	40.1
N	-22.0	33.8	42.3
GLY187			
CA	-22.2	33.4	39.0
C'	-21.6	34.3	38.0
O	-21.5	34.2	36.9
N	-21.8	35.4	38.6
VAL188			
CG2	-22.2	38.1	37.9
CG1	-19.9	38.8	37.5
CB	-20.9	37.9	38.2
CA	-20.3	36.4	37.7
C'	-18.9	36.2	37.9
O	-18.5	36.0	36.9
N	-18.3	36.3	39.0
ARG188A			
NEH2	-19.4	48.3	42.9
NEH1	-17.3	41.2	42.9
CZ	-18.3	40.3	42.5
NE	-18.0	39.4	41.6
CD	-16.8	39.5	40.9
CG	-16.9	38.4	39.8
CB	-16.4	37.0	40.3
CA	-16.8	36.1	39.3
C'	-16.7	34.5	39.7
O	-17.6	34.0	40.6
N	-15.9	34.0	39.5
SER189			
OG	-16.8	31.5	38.0
CB	-16.7	31.7	39.3
CA	-15.5	32.5	39.9
C'	-14.2	32.0	39.3
O	-13.8	32.7	38.5
N	-14.2	30.8	39.5
GLY190			
CA	-12.9	30.1	39.1
C'	-13.3	29.4	37.8
O	-14.4	29.4	37.5
N	-12.1	28.9	37.3
CYS191			
CA	-17.7	28.4	34.4
CB	-16.6	28.3	35.4
SG	-15.1	27.1	35.0
SG	-13.9	28.8	33.7
CB	-12.9	29.8	34.8
CA	-12.6	28.1	36.8
C'	-11.8	27.4	35.6
O	-10.8	27.6	36.2
N	-11.8	26.6	34.6
GLN192			
NE2	-13.7	23.8	33.9
OE1	-12.8	25.3	32.4
CD	-12.5	24.4	33.0
CG	-11.1	23.9	33.1
CB	-10.3	25.2	32.8
CA	-9.9	25.9	34.1
C'	-8.9	27.2	33.9
O	-9.2	28.0	33.2
N	-7.6	26.6	34.2
GLY193			
CA	-6.8	27.5	34.1
C'	-6.3	28.1	35.4
O	-5.1	28.4	35.5
N	-7.3	28.2	36.4
ASP194			
OD2	-9.1	31.3	36.6
OD1	-7.0	31.3	36.5
CG	-7.9	30.9	37.0
CB	-7.9	29.8	38.0
CA	-6.7	28.8	37.7
C'	-6.6	27.9	38.8
O	-6.0	28.3	39.9
N	-6.8	26.6	38.5
TOS195			
CEH2	-7.2	22.0	35.6
CTH2	-6.3	20.8	35.2
CKA	-5.8	18.3	35.5
C10	-6.5	19.6	36.0
CTH1	-7.3	19.7	37.2
CEH1	-7.8	20.9	37.6
CZ	-7.8	22.0	36.9
SD	-8.5	23.6	37.3
OE2	-9.9	23.6	37.1
OE1	-8.0	24.8	36.6
OG	-8.0	23.8	38.9
CB	-6.8	24.2	38.9
CA	-6.7	25.6	39.6
C'	-5.3	25.7	40.2
O	-4.4	26.1	39.6
N	-5.2	25.4	41.5
GLY196			
CA	-4.2	25.4	42.2
C'	-3.6	26.8	42.6
O	-2.7	27.0	43.3
N	-4.4	27.7	42.2
GLY197			
CA	-4.2	29.2	42.4
C'	-4.7	29.6	43.8
O	-5.3	29.1	44.5
N	-3.9	30.7	44.1
PR0198			
CG	-2.3	32.5	44.1
CD	-2.8	31.4	43.3
CB	-3.0	32.5	45.5
CA	-4.0	31.3	45.4
C'	-5.6	31.9	45.6
O	-6.1	32.4	44.6
N	-5.9	31.9	46.7
LEU199			
CD2	-10.4	31.7	48.6
CD1	-9.9	33.4	47.2
CG	-9.3	32.6	48.1
CB	-8.1	31.8	47.6
CA	-7.1	32.8	47.2
C'	-6.5	33.6	48.3
O	-6.2	33.2	49.4
N	-6.4	34.9	47.9
HIS200			
CD2	-4.9	36.3	45.8
NE2	-3.8	35.8	45.1
CE1	-2.7	35.8	46.0
ND1	-3.3	36.3	47.2
CG	-4.5	36.5	47.1
CB	-5.3	37.0	48.1
CA	-6.0	35.9	48.8
C'	-7.1	36.4	49.7
O	-8.2	37.1	49.1
N	-7.3	36.2	51.0
CYS201			
CA	-11.8	34.6	48.3
CB	-11.5	35.6	49.4
SG	-11.5	35.2	51.1
SG	-9.7	34.5	51.3
CB	-9.8	35.7	52.5
CA	-8.4	36.7	51.8
C'	-7.5	37.7	52.8
O	-6.3	37.7	53.2
N	-8.5	38.7	53.0
LEU202			
CD2	-6.4	42.3	53.4
CD1	-8.3	42.6	55.1
CG	-7.9	42.3	53.5
CB	-8.7	41.0	53.2
CA	-7.9	39.8	53.8
C'	-8.1	39.6	55.3
O	-9.2	39.5	55.7
N	-7.1	39.6	56.0
VAL203			
CG2	-8.1	37.1	57.8
CG1	-7.2	37.7	59.3
CB	-7.8	37.9	57.8
CA	-7.2	39.4	57.5
C'	-6.3	40.1	58.2
O	-5.8	39.9	58.8
N	-6.5	41.1	59.0
ASN204			
ND2	-6.3	41.8	62.4
OD1	-5.6	39.8	61.9

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      CG    -5.6 40.3 61.7
      CB    -5.0 40.9 60.6
      CA    -5.7 41.9 59.8
      C'    -4.7 42.8 59.0
      O     -3.6 43.0 59.4
      N     -5.3 43.4 57.9
GLY205
      CA    -4.6 44.4 57.2
      C'    -3.4 43.6 56.4
      O     -2.4 44.2 55.9
      N     -3.5 42.3 56.2
GLN206
      NE2   -0.0 38.5 57.1
      OE1    1.7 39.9 56.5
      CD     0.4 39.6 56.4
      CG    -0.5 40.4 55.6
      CB    -1.8 40.6 56.3
      CA    -2.8 41.5 55.4
      C'    -3.4 40.6 54.5
      O     -4.8 40.0 54.8
      N     -2.9 40.3 53.3
TYR207
      OEH   -0.8 42.9 49.4
      CD2   -4.8 42.1 50.3
      CE2   -5.6 42.8 49.9
      CZ    -7.0 42.1 49.8
      CE1   -6.9 40.8 50.0
      CD1   -5.0 40.0 50.5
      CG    -4.7 40.7 50.5
      CB    -3.3 40.0 50.9
      CA    -3.4 39.4 52.4
      C'    -2.6 38.1 52.4
      O     -1.4 38.1 52.3
      N     -3.5 36.9 52.6
ALA208
      CB    -2.4 35.3 54.2
      CA    -2.6 35.7 52.7
      C'    -3.6 34.7 51.8
      O     -4.8 34.8 51.7
      N     -2.6 33.7 51.5
VAL209
      CG2   -1.5 33.0 49.1
      CG1   -2.8 30.9 48.9
      CB    -2.1 31.9 49.9
      CA    -3.3 32.6 50.7
      C'    -4.1 31.5 51.6
      O     -3.3 30.8 52.4
      N     -5.1 31.5 51.6
HIS210
      CD2   -5.9 33.2 54.3
      NE2   -5.8 33.6 55.7
      CE1   -6.6 32.6 56.3
      ND1   -6.9 31.7 55.5
      CG    -6.4 32.1 54.2
      CB    -7.3 31.4 52.8
      CA    -5.9 30.6 52.3
      C'    -6.6 29.4 51.5
      O     -6.8 28.3 52.1
      N     -6.7 29.6 50.3
GLY211
      CA    -7.3 28.6 49.4
      C'    -6.3 28.4 48.1
      O     -5.8 29.2 47.4
      N     -6.7 27.1 47.7
VAL212
      CG2   -4.1 25.9 47.8
      CG1   -4.6 24.9 45.5
      CB    -5.1 25.3 46.8
      CA    -6.8 26.5 46.4
      C'    -7.2 26.8 45.7
      O     -7.7 24.9 46.8
      N     -7.4 26.5 44.5
THR213
      CG2   -9.6 26.9 41.7
      OG1   -8.2 28.4 42.9
      CB    -8.6 27.0 42.5
      CA    -8.5 26.1 43.7
      C'    -8.4 24.7 43.3
      O     -7.3 24.1 43.1
      N     -9.5 24.8 43.3
SER214
      OG    -9.6 28.5 43.9
      CB   -10.8 21.8 44.2
      CA    -9.5 22.6 43.8
      C'   -10.3 22.5 41.8
      O     -9.9 22.1 40.7
      N    -11.9 22.7 42.1
PHE215
      CD2  -14.8 20.9 42.8
      CE2  -15.4 20.6 44.8
      CZ   -14.7 20.1 45.8
      CE1  -13.3 19.9 44.7
      CD1  -12.8 20.3 43.5
      CG   -13.7 20.7 42.6
      CB   -13.1 21.1 41.2
      CA   -12.6 22.6 41.0
      C'   -13.6 23.5 41.8
      O    -13.6 24.3 42.8
      N    -14.5 23.4 40.2
VAL216
      CG2  -15.4 24.7 37.7
      CG1  -14.8 26.3 39.6
      CB   -15.7 25.1 39.1
      CA   -15.9 24.8 40.1
      C'   -16.7 23.8 39.7
      O    -16.7 21.8 39.7
      N    -17.9 23.4 39.2
SER217
      OG   -21.5 22.8 38.5
      CB   -20.4 23.5 38.8
      CA   -19.0 22.6 38.8
      C'   -18.9 22.8 37.5
      O    -18.3 22.6 36.6
      N    -19.3 20.8 37.3
ARG217A
      NEH2 -22.5 16.1 35.4
      NEH1 -21.7 16.3 37.5
      CZ   -21.7 16.3 36.2
      NE   -20.3 16.3 35.7
      CD   -19.4 16.3 36.6
      CG   -18.7 17.8 36.6
      CB   -19.9 18.7 36.2
      CA   -19.2 20.1 36.1
      C'   -19.9 20.8 35.8
      O    -19.8 20.9 33.8
      N    -21.2 21.3 35.4
LEU218
      CD2  -24.1 20.8 34.8
      CD1  -25.3 21.1 36.8
      CG   -23.9 20.8 35.4
      CB   -23.3 22.2 35.1
      CA   -22.8 22.1 34.5
      C'   -21.6 23.6 34.1
      O    -22.2 24.3 33.4
      N    -20.4 24.0 34.8
GLY219
      CA   -19.9 25.3 34.5
      C'   -19.3 26.8 35.7
      O    -19.4 25.7 36.9
      N    -18.5 26.8 35.3
CYS220
      CA   -11.6 28.4 35.3
      CB   -12.9 29.0 34.8
      SG   -13.9 28.8 33.7
      SG   -15.1 27.1 35.8
      CB   -16.6 28.3 35.4
      CA   -17.7 27.5 36.2
      C'   -18.3 28.5 37.8
      O    -18.3 28.3 38.3
      N    -18.8 29.4 36.4
ASN221
      ND2  -20.9 32.5 34.5
      OD1  -19.2 31.1 34.8
      CG   -19.9 31.8 34.8
      CB   -19.3 31.9 36.3
      CA   -19.5 30.6 37.0
      C'   -21.1 30.5 37.1
      O    -21.8 31.2 36.7
      N    -21.4 29.2 37.8
VAL221A
      CG2  -23.8 27.3 36.3
      CG1  -24.6 27.3 38.5
      CB   -23.8 27.6 37.9
      CA   -22.8 28.9 38.8
      C'   -23.2 29.6 39.4
      O    -22.4 29.6 40.4
      N    -24.7 29.8 39.5
THR222
      CG2  -26.9 31.6 41.6
      OG1  -26.3 31.8 39.3
      CB   -26.3 30.9 40.4
      CA   -25.2 30.4 40.7
      C'   -24.9 29.3 41.8
      O    -25.5 28.1 41.5
      N    -24.6 29.7 43.0
ARG223
      NEH2 -30.8 31.1 44.3
    * NEH1 -29.9 29.1 43.5
    * CZ   -29.9 30.1 44.4
    * NE   -29.8 30.0 45.4
    * CD   -28.2 29.8 45.4
      CG   -26.9 29.5 44.9
      CB   -26.1 28.3 44.3
      CA   -24.9 28.8 44.8
      C'   -24.8 27.7 43.9
      O    -23.7 26.8 44.7
      N    -23.8 27.8 42.9
LYS224
      NZ   -24.7 23.2 42.9
      CE   -23.8 22.7 42.6
      CD   -22.8 23.8 42.5
      CG   -23.3 24.9 41.6
      CB   -22.3 26.0 41.3
      CA   -22.8 26.7 42.6
      C'   -20.9 27.3 42.7
      O    -20.2 27.3 41.8
      N    -20.4 27.0 43.8
PRO225
      CG   -20.3 28.3 46.1
      CD   -21.2 27.8 45.0
      CB   -19.8 28.8 45.5
      CA   -18.9 28.4 44.0
      C'   -17.8 27.5 43.7
      O    -18.8 26.3 43.6
      N    -16.7 28.2 43.5
THR226
      CG2  -13.3 28.3 42.5
      OG1  -15.3 29.3 41.6
      CB   -14.7 28.7 42.8
      CA   -15.5 27.6 43.3
      C'   -15.1 27.1 44.6
      O    -15.3 27.5 45.7
      N    -14.4 26.8 44.5
VAL227
      CG2  -15.6 23.5 46.2
      CG1  -13.1 23.0 46.3
      CB   -14.2 23.8 45.6
      CA   -14.0 25.3 45.7
      C'   -12.5 25.4 45.8
      O    -11.8 25.2 44.8
      N    -11.9 25.7 46.9
PHE228
      CD2  -11.8 28.0 46.3
      CE2  -11.6 29.8 45.2
      CZ   -10.5 30.1 44.7
      CE1   -9.3 29.6 45.0
      CD1   -9.2 28.5 46.0
      CG   -10.4 28.3 46.6
      CB   -10.4 27.3 47.7
      CA   -10.7 25.9 47.3
      C'   -10.2 24.8 48.2
      O    -11.0 24.6 49.2
      N    -8.9 24.5 48.2
THR229
      CG2   -6.7 21.8 49.6
      OG1   -7.7 22.2 47.4
      CB    -7.3 22.8 48.6
      CA    -8.4 23.7 49.2
      C'    -7.9 24.5 50.3
      O     -7.3 25.5 50.1
      N     -8.1 24.0 51.5
ARG230
      NEH2  -9.2 22.8 58.6
      NEH1 -10.6 23.8 57.8
      CZ    -9.7 23.7 57.6
      NE    -9.2 24.4 56.9
      CD    -9.8 25.3 56.8
      CG    -9.8 25.8 54.9
      CB    -8.6 24.4 53.9
      CA    -7.9 24.8 52.7
      C'    -6.4 24.6 53.2
      O     -5.8 23.6 53.9
      N     -5.4 25.6 52.8
VAL231
      CG2   -3.8 26.9 51.1
      CG1   -2.8 27.1 53.8
      CB    -3.6 26.9 52.6
      CA    -4.1 25.6 53.1
      C'    -3.9 25.5 54.6
      O     -3.8 24.7 55.1
      N     -4.7 26.1 55.4
SER232
      OG    -6.8 26.3 57.7
      CB    -5.4 27.8 57.4
      CA    -4.5 26.1 56.9
      C'    -4.6 24.7 57.5
      O     -4.3 24.6 58.8
      N     -5.1 23.7 56.8
ALA233
      CB    -6.4 21.8 56.8
      CA    -5.2 22.4 57.3
      C'    -3.8 21.4 56.8
      O     -3.7 20.2 57.2
      N     -2.9 22.0 56.8
TYR234
      OEH   -7.3 18.5 53.1
      CD2   -3.3 19.8 53.7
      CE2   -4.5 18.4 53.4
      CZ    -5.7 19.1 53.3
      CE1   -5.7 20.5 53.5
      CD1   -4.5 21.1 53.7
      CG    -3.3 20.4 53.8
      CB    -2.0 21.0 54.0
      CA    -1.9 21.3 55.5
      C'    -0.7 22.0 56.0
      O      0.5 21.8 55.5
      N     -0.9 23.0 56.8
ILE235
      CD1   -0.9 26.5 57.8
      CG1   -1.4 25.5 58.1
      CB    -0.3 24.6 58.6
      CG2    0.9 25.5 59.0
      CA     0.2 23.6 57.4
      C'     1.2 23.0 57.9
      O      2.6 23.0 57.6
      N      0.9 22.8 58.7
SER236
      OG     1.6 19.0 60.9
      CB     0.8 20.1 60.4
      CA     1.6 21.0 59.4
      C'     2.4 20.1 58.3
      O      3.6 20.0 58.4
      N      1.5 19.6 57.5
TRP237
      CD2    1.1 18.1 53.1
      CE3    1.0 19.3 52.4
      CZ3    1.1 19.4 51.0
      CEH2   1.6 18.3 50.3
      CZ2    1.8 17.1 50.9
      CE2    1.6 17.0 52.3
      NE1    1.6 15.9 53.3
      CD1    1.4 16.4 54.5
      CG     1.3 17.7 54.4
      CB     0.9 18.7 55.4
      CA     2.1 18.8 56.4
      C'     3.3 19.6 55.5
      O      4.2 19.2 55.4
      N      2.9 20.7 55.2
ILE238
      CD1    1.3 24.3 53.6
      CG1    1.8 23.0 53.6
      CB     3.1 23.1 54.4
      CG2    4.1 24.0 53.7
      CA     3.8 21.7 54.5
      C'     5.0 21.8 55.2
      O      6.1 21.5 54.7
      N      4.9 22.2 56.5
ASN239
      ND2    5.8 25.0 57.7
      OD1    4.6 24.8 59.6
      CG     5.4 24.3 58.8
      CB     5.9 22.9 58.8
      CA     6.1 22.4 57.3
      C'     6.9 21.1 57.4
      O      8.1 21.0 57.8
      N      6.3 20.1 57.8
ASN240
      ND2    6.2 17.8 60.5
      OD1    4.8 17.9 59.7
      CG     5.2 17.9 59.5
      CB     5.6 17.7 58.0
      CA     6.9 18.7 57.8
      C'     7.7 18.5 56.5
      O      9.1 18.3 56.6
      N      7.1 18.5 55.4
VAL241
      CG2    5.6 17.3 52.8
      CG1    7.5 18.7 51.6
      CB     6.6 18.5 53.8
      CA     7.6 18.3 54.1
      C'     9.0 19.3 53.9
      O     10.0 18.8 53.6
      N      8.8 20.7 54.0
ILE242
      CD1    7.5 24.7 52.9
      CG1    8.6 23.6 52.6
      CB     9.3 23.0 53.9
      CG2   10.3 24.0 54.3
      CA     9.0 21.6 53.6
      C'    10.9 21.4 54.5
      O     12.1 21.5 54.1
      N     10.8 21.0 55.8
ALA243
      CB    11.3 20.6 58.2
      CA    11.9 20.8 56.8
      C'    12.8 19.5 56.5
      O     14.1 19.5 56.5
      N     12.0 18.5 56.1
SER244
      OG    10.6 16.2 55.8
      CB    11.6 16.1 55.9
      CA    12.6 17.2 55.8
      C'    13.1 17.2 54.2
      O     13.4 16.1 53.7
      N     13.1 18.3 53.6
ASN245
      ND2   10.9 16.7 58.6
      OD1   12.8 17.3 49.6
      CG    12.8 17.5 50.5
      CB    12.1 18.7 51.4
      CA    13.4 18.5 52.2
      C'    14.3 19.8 52.0
      O     14.8 20.7 51.3
WAT  1
      OH2  -18.7 26.1 48.1
WAT  2
      OH2  -19.4 30.2 48.4
WAT  3
      OH2  -21.0 32.2 48.1
WAT  4
      OH2  -17.8 31.5 42.8
WAT  5
      OH2  -16.1 27.4 53.3
WAT  6
      OH2  -16.5 24.8 53.4
WAT  7
      OH2  -16.1 31.3 55.3
WAT  8
      OH2  -13.9 29.1 55.6
WAT  9
      OH2    8.9 48.6 37.5
WAT 10
      OH2    4.4 48.7 37.3
WAT 11
      OH2    5.7 42.3 35.7
WAT 12
      OH2    3.8 39.6 39.9
WAT 13
      OH2   -6.4 38.9 41.8
WAT 14
      OH2   -4.4 38.9 39.6
WAT 15
      OH2   -3.8 38.4 36.4
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WAT 16				WAT 19				WAT 22				WAT 25			
	OH2	-1.9	28.2 45.6		OH2	-9.6	18.6 46.4		OH2	5.1	36.1 41.2		OH2	5.2	37.8 38.1
WAT 17				WAT 20				WAT 23				SUL 1			
	OH2	-9.6	29.5 56.1		OH2	-9.2	19.6 48.3		OH2	4.4	35.1 38.2		SO4	-8.3	21.8 68.9
WAT 18				WAT 21				WAT 24							
	OH2	-7.1	28.5 54.7		OH2	-8.9	18.8 51.1		OH2	2.2	36.8 38.6				

internal waters have been measured using a simplified version of the device described by Salemmi and Fehr (8). Table 1 lists the coordinates as measured. Gross clerical errors in coordinate measurement have been eliminated using the output from a model-building programme (10). The r.m.s. deviation between the measured coordinates and those obtained by the model-building programme was 0.188Å. The problem of depth perception in the direction perpendicular to the mirror produces a systematic variation in the accuracy of the x-coordinate measurement as is shown in Figure I.

A full description of the structure and its determination is in preparation

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