ATOMIC COORDINATES FOR T4 PHAGE LYSOZYME

S. J. Remington, L. F. Ten Eyck and B. W. Matthews

Institute of Molecular Biology and Departments of Physics and Chemistry, University of Oregon, Eugene, Oregon 97403, U.S.A.

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Summary: Atomic coordinates are presented for the lysozyme from T4 bacteriophage. The coordinates were derived from a 2.4 Å resolution electron density map based on two isomorphous heavy-atom derivatives, interpreted in terms of the known amino acid sequence, and adjusted to have stereochemically acceptable bond lengths and angles.

T4 phage lysozyme is an endoacetylmuramidase produced in cells of Escherichia coli after infection by bacteriophage T4, and coded by the phage genome. The amino acid sequence of the enzyme is known (1) and a preliminary description of the lysozyme structure, determined by X-ray crystallography, has been presented (2).

Subsequently, the accuracy of the crystallographic analysis has been improved by the incorporation of additional diffraction data including anomalous scattering data for the mercury and platinum derivatives used in the original structure determination. The resultant electron density map, calculated to a nominal resolution of 2.4 Å, has revealed the approximate conformation of most of the molecule without ambiguity.

Preliminary atomic coordinates for the lysozyme molecule were obtained by building a skeletal model (Cambridge Repetition Engineers, Cambridge, U.K.) in a Richards optical comparator (3, 4) and then placing markers in the electron density map to agree, as well as possible, with both the model and the electron density. The advantages of this procedure have been described elsewhere (5).

The "raw" coordinates were then checked and idealized by using a least squares procedure in which bond length, bond angle and planarity constraints are enforced by constraining the interatomic distances between selected pairs

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Table 1

	1 N	36.5	-24.8	9.1		14 NE	51.9	-8.2	14.2		27 CD1	47.5	-5.2	21.0	SER	44 CA	43.6	5.1	28.2
MET	1 CA	36.9	-23.4	8.7		14 CZ	52.2	-7.6	13.0		27 CG2	43.9	-3.8	21.3		44 C	42.6	4.0	27.8
	1 C	35.4	-22.8	9.3		14 NEE1	52.0	-6.3	12.8		28 N	45.5	-6.6	19.3		44 O	42.0	3.4	28.7
	1 O	34.6	-23.4	9.5		14 NEE2	52.6	-8.4	12.0	GLY	28 CA	45.0	-8.0	19.7		44 CB	42.9	6.3	27.7
	1 CB	36.5	-23.2	7.2		15 N	50.2	-8.9	20.2		28 C	44.9	-8.6	18.3		44 OG	41.5	6.5	27.9
	1 CG	37.4	-22.1	6.6	LEU	15 CA	50.1	-9.0	21.6		28 O	45.9	-8.9	17.6		45 N	42.4	3.7	26.5
	1 SD	39.0	-22.1	7.3		15 C	50.7	-7.7	22.1		29 N	43.7	-8.7	17.8	GLU	45 CA	41.3	2.9	26.1
	1 CE	39.2	-20.4	7.9		15 O	50.9	-7.5	23.3	ILE	29 CA	43.3	-9.4	16.6		45 C	41.7	1.5	26.5
	2 N	35.8	-21.5	9.7		15 CB	51.0	-10.1	22.3		29 C	42.3	-8.5	15.9		45 O	40.8	0.7	26.6
ASN	2 CA	34.8	-20.7	10.4		15 CG	50.2	-11.3	22.7		29 O	41.1	-8.7	16.0		45 CB	41.0	2.8	24.6
	2 C	33.5	-19.6	10.5		15 CD1	50.5	-12.6	21.8		29 CB	42.4	-10.6	16.8		45 CG	40.8	4.2	23.9
	2 O	36.7	-19.2	10.5		15 CD2	50.3	-11.7	24.2		29 CG1	43.2	-11.9	17.1		45 CD	39.3	4.3	23.7
	2 CB	34.3	-21.0	11.7		16 N	50.9	-6.8	21.2		29 CD1	42.4	-12.9	18.0		45 OE1	38.7	3.8	22.7
	2 CG	35.3	-21.3	12.7	LYS	16 CA	51.4	-5.4	21.5		29 CG2	41.6	-10.9	15.5		45 OE2	38.7	5.0	24.6
	2 ND21	36.1	-20.3	13.0		16 C	50.9	-4.5	20.5		30 N	42.8	-7.4	15.3		46 N	42.9	1.3	26.6
	2 ND22	35.5	-22.4	13.2		16 O	50.7	-4.9	19.3	GLY	30 CA	42.5	-6.4	14.4	LEU	46 CA	43.5	-0.0	26.8
	3 N	34.7	-18.3	10.8		16 CB	52.9	-5.3	21.2		30 C	41.4	-5.6	15.2		46 C	42.9	-0.5	28.1
ILE	3 CA	34.8	-16.8	10.6		16 CG	53.6	-4.1	21.8		30 O	40.3	-5.3	14.6		46 O	42.0	-1.3	28.2
	3 C	35.8	-16.5	11.7		16 CD	55.1	-4.0	21.6		31 N	41.7	-5.3	16.4		46 CB	45.0	-0.1	27.1
	3 O	36.7	-15.6	11.6		16 CE	55.7	-2.7	22.0	HIS	31 CA	40.7	-4.8	17.4		46 CG	45.7	-1.3	26.6
	3 CB	33.7	-16.0	11.0		16 NZ	57.2	-2.7	21.8		31 C	41.1	-3.3	17.5		46 CD1	45.6	-2.5	27.6
	3 CG1	32.5	-16.8	11.7		17 N	50.6	-3.2	20.9		31 O	42.2	-3.0	17.9		46 CD2	45.3	-1.8	25.2
	3 CD1	32.6	-16.9	13.2	ILE	17 CA	49.7	-2.2	20.3		31 CB	40.9	-5.1	18.9		47 N	43.4	0.1	29.3
	3 CG2	33.3	-15.0	10.0		17 C	50.6	-1.7	19.2		31 CG	40.0	-4.5	19.8	ASP	47 CA	43.2	-0.4	30.6
	4 N	35.8	-17.3	12.8		17 O	51.8	-1.5	19.4		31 ND1	38.7	-4.6	19.8		47 C	41.7	-0.6	30.9
PHE	4 CA	36.5	-17.0	13.9		17 CB	49.6	-1.0	21.2		31 CE1	38.2	-3.9	20.8		47 O	41.3	-0.9	31.8
	4 C	37.9	-17.3	13.5		17 CG1	48.7	-1.4	22.4		31 CD2	40.4	-3.8	20.9		47 CB	43.7	0.6	31.6
	4 O	38.8	-16.5	13.4		17 CD1	48.7	-0.4	23.6		31 NE2	39.2	-3.4	21.6		47 CG	44.9	1.2	30.8
	4 CB	36.3	-17.8	15.1		17 CG2	49.2	0.3	20.5		32 N	40.2	-2.4	17.1		47 OD1	46.0	0.5	30.7
	4 CG	35.4	-17.3	16.2		18 N	50.1	-1.5	17.9	LEU	32 CA	40.4	-1.0	16.8		47 OD2	44.7	2.3	30.1
	4 CD1	34.1	-17.6	16.3	TYR	18 CA	50.5	-1.3	16.5		32 C	40.2	-0.4	18.2		48 N	40.9	0.3	30.0
	4 CE1	33.3	-17.1	17.3		18 C	49.5	-0.5	15.8		32 O	39.1	-0.5	18.8	LYS	48 CA	39.5	0.6	30.2
	4 CZ	33.9	-16.1	18.2		18 O	48.6	0.0	16.3		32 CB	39.1	-0.5	16.1		48 C	38.9	-0.6	29.5
	4 CE2	35.2	-15.8	18.0		18 CB	50.6	-2.6	15.8		32 CG	39.4	0.8	15.2		48 O	37.8	-1.1	29.9
	4 CD2	36.0	-16.4	17.0		18 CG	49.6	-3.5	15.4		32 CD1	38.7	2.1	15.8		48 CB	39.0	1.7	29.3
	5 N	38.1	-18.6	13.0		18 CD1	49.2	-3.6	14.1		32 CD2	40.9	1.0	14.8		48 CG	37.6	2.2	29.6
GLU	5 CA	39.4	-19.0	12.8		18 CE1	48.2	-4.5	13.7		33 N	41.2	0.2	18.8		48 CD	37.2	3.4	28.7
	5 C	39.7	-18.5	11.4		18 CZ	47.5	-5.2	14.7	LEU	33 CA	41.7	0.8	20.0		48 CE	36.9	3.1	27.2
	5 O	40.6	-19.0	10.7		18 CE2	47.9	-5.1	16.0		33 C	41.2	2.2	20.0		48 NZ	36.1	4.1	26.5
	5 CB	39.6	-20.5	12.7		18 CD2	48.9	-4.2	16.4		33 O	40.4	2.6	20.8		49 N	39.6	-1.0	28.4
	5 CG	39.2	-21.3	11.5		18 OEE	46.5	-6.0	14.3		33 CB	43.1	0.7	20.5	ALA	49 CA	38.9	-2.0	27.6
	5 CD	39.1	-22.8	11.9		19 N	49.6	-0.6	14.4		33 CG	43.4	0.2	21.9		49 C	38.9	-3.2	28.5
	5 OE1	38.7	-23.5	11.0	LYS	19 CA	49.0	0.4	13.6		33 CD1	42.3	-0.4	22.7		49 O	37.9	-3.8	28.9
	5 OE2	39.5	-23.1	13.0		19 C	48.1	-0.4	12.6		33 CD2	44.7	-0.7	22.0		49 CB	39.8	-2.5	26.3
	6 N	38.9	-17.5	10.9		19 O	48.3	-1.6	12.5		34 N	41.7	3.0	19.1		50 N	40.1	-3.6	28.9
MET	6 CA	38.8	-17.1	9.5		19 CB	50.0	1.0	12.5	THR	34 CA	41.2	4.4	19.1	ILE	50 CA	40.2	-5.0	29.5
	6 C	39.4	-15.7	9.6		19 CG	49.9	2.5	12.3		34 C	41.9	5.1	17.9		50 C	40.3	-4.8	31.0
	6 O	40.0	-15.2	8.6		19 CD	50.6	3.3	13.5		34 O	43.1	4.8	17.7		50 O	40.1	-5.8	31.7
	6 CB	37.5	-16.8	9.0		19 CE	50.4	4.9	13.2		34 CB	41.9	5.2	20.2		50 CB	41.6	-5.6	29.4
	6 CG	37.4	-16.3	7.5		19 NZ	51.7	5.5	14.0		34 OG1	41.3	6.5	20.5		50 CG1	41.9	-6.0	27.9
	6 SD	35.8	-15.6	7.0		20 N	47.2	0.3	12.0		34 CG2	43.4	5.1	20.2		50 CD1	42.1	-6.8	27.0
	6 CE	36.0	-15.5	5.2	ASP	20 CA	46.0	-0.1	11.2		35 N	41.1	5.9	17.2		50 CG2	41.8	-6.8	30.4
	7 N	39.2	-15.0	10.7		20 C	46.6	0.1	9.8	LYS	35 CA	41.4	6.5	15.9		51 N	40.4	-3.5	31.4
LEU	7 CA	39.4	-13.6	11.1		20 O	47.5	0.9	9.7		35 C	42.3	7.6	16.2	GLY	51 CA	40.1	-2.9	32.6
	7 C	40.7	-13.5	11.7		20 CB	44.9	0.9	11.1		35 O	42.8	8.3	15.3		51 C	41.2	-3.3	33.6
	7 O	41.3	-12.4	11.7		20 CG	43.6	0.2	11.3		35 CB	40.2	7.2	15.3		51 O	41.0	-4.0	34.5
	7 CB	38.5	-13.1	12.2		20 OD1	43.0	-0.1	10.2		35 CG	39.7	6.7	13.9		52 N	42.4	-2.7	33.3
	7 CG	37.4	-12.0	11.7		20 OD2	43.3	-0.1	12.4		35 CD	39.4	5.1	13.9	ARG	52 CA	43.6	-2.9	34.1
	7 CD1	37.2	-12.2	10.1		21 N	46.0	-0.6	8.8		35 CE	38.9	4.7	12.5		52 C	44.7	-2.2	33.2
	7 CD2	36.1	-12.0	12.5	THR	21 CA	46.4	-0.6	7.5		35 NZ	37.4	4.5	12.5		52 O	44.4	-2.1	32.0
	8 N	41.3	-14.6	12.2		21 C	46.1	0.9	7.1		36 N	42.6	7.9	17.5		52 CB	44.1	-4.3	34.0
ARG	8 CA	42.4	-14.8	13.0		21 O	46.7	1.4	6.1	SER	36 CA	43.2	9.1	18.0		52 CG	44.8	-4.7	32.8
	8 C	43.5	-14.6	12.0		21 CB	45.5	-1.3	6.5		36 C	44.7	8.8	17.8		52 CD	45.3	-6.1	32.7
	8 O	44.6	-14.3	12.3		21 OG1	44.4	-2.0	7.3		36 O	45.2	7.8	18.3		52 NE	46.7	-6.3	33.0
	8 CB	42.6	-16.2	13.7		21 CG2	46.3	-2.4	5.7		36 CB	43.3	9.0	19.6		52 CZ	47.4	-6.9	32.0
	8 CG	43.7	-17.1	13.3		22 N	45.3	1.5	7.9		36 OG	43.0	10.3	20.1		52 NEE1	48.7	-6.9	32.0
	8 CD	44.9	-17.2	14.2	GLU	22 CA	44.8	2.8	7.4		37 N	45.4	9.7	17.1		52 NEE2	46.7	-7.5	31.3
	8 NE	46.1	-16.8	13.6		22 C	45.3	3.8	8.5	PRO	37 CA	46.8	9.6	16.6		53 N	45.8	-1.8	33.8
	8 CZ	47.0	-16.4	14.4		22 O	44.9	5.0	8.4		37 C	47.7	9.7	17.8	ASN	53 CA	46.8	-0.8	33.4
	8 NEE1	47.6	-16.8	15.7		22 CB	43.3	3.0	7.5		37 O	48.9	10.0	17.6		53 C	47.7	-1.6	32.6
	8 NEE2	48.1	-15.8	14.0		22 CG	42.7	2.9	6.1		37 CB	47.0	10.9	15.9		53 O	48.7	-2.1	33.1
	9 N	43.3	-15.2	10.8		22 CD	41.2	2.8	6.2		37 CG	45.7	11.6	15.6		53 CB	47.7	-0.4	34.6
ILE	9 CA	44.2	-15.6	9.8		22 OE1	40.7	3.1	7.3		37 CD	44.7	10.7	16.2		53 CG	47.7	1.1	34.4
	9 C	44.2	-14.6	8.7		22 OE2	40.3	2.4	5.2		38 N	47.2	9.5	19.0		53 ND01	47.3	1.8	35.5
	9 O	45.0	-14.5	7.8		23 N	46.1	3.3	9.4	SER	38 CA	47.8	9.7	20.3		53 ND02	47.9	1.6	33.3
	9 CB	43.5	-16.9	9.0	GLY	23 CA	47.1	4.1	10.1		38 C	48.0	8.4	20.9		54 N	47.5	-1.7	31.3
	9 CG1	42.9	-16.8	7.8		23 C	46.9	4.3	11.5		38 O	47.1	7.5	20.7	CYH	54 CA	48.0	-2.5	30.2
	9 CD1	43.5	-17.5	6.5		23 O	47.0	5.1	12.3		38 CB	46.8	10.3	21.3		54 C	49.3	-2.0	29.6
	9 CG2	43.5	-18.1	9.9		24 N	45.5	3.5	11.8		38 OG	46.5	11.6	21.1		54 O	50.2	-2.8	29.4
	10 N	43.3	-13.6	8.8	TYR	24 CA	44.7	3.8	13.0		39 N	49.1	8.1	21.5		54 CB	47.1	-2.9	29.0
ASP	10 CA	43.1	-12.7	7.7		24 C	45.1	2.6	13.9	LEU	39 CA	49.7	6.8	21.9		54 SG	45.6	-4.1	29.4
	10 C	43.7	-11.4	8.2		24 O	45.5	1.5	13.4		39 C	49.3	6.7	23.4		55 N	49.3	-0.7	29.4
	10 O	44.0	-10.5	7.4		24 CB	43.2	3.5	12.6		39 O	49.3	5.6	23.9	ASN	55 CA	50.5	0.0	29.0
	10 CB	41.6	-12.2	7.5		24 CG	42.6	4.6	11.8		39 CB	51.2	6.7	22.0		55 C	50.9	-0.6	27.6
	10 CG	41.3	-12.5	6.0		24 CD1	41.8	4.5	10.8		39 CG	51.7	5.3	22.4		55 O	51.9	-0.2	27.1
	10 CD1	42.3	-12.9	5.3		24 CE1	41.3	5.6	10.1		39 CD1	51.1	4.8	23.8		55 CB	51.8	-0.3	29.7
	10 CD2	40.1	-12.4	5.7		24 CZ	41.7	6.9	10.5		39 CD2	51.5	4.2	21.3		55 CG	52.8	-0.6	29.1
	11 N	44.0	-11.4	9.5		24 CE2	42.6	7.0	11.6		40 N	49.0	7.8	24.0		55 ND01	52.6	1.8	28.7
GLU	11 CA	44.5	-10.1	9.9		24 CD2	43.1	5.9	12.2	ASN	40 CA	48.9	8.1	25.4		55 ND02	54.0	0.2	29.1
	11 C	45.4	-10.2	11.1		24 OEE	41.3	8.0	9.8		40 C	47.4	7.9	25.6		56 N	50.1	-1.5	27.1
	11 O	45.5	-9.2	11.6		25 N	45.0	2.8	15.2		40 O	46.9	7.6	26.7	GLY	56 CA	50.2	-1.7	25.7
	11 CB	43.5	-9.2	10.5	TYR	25 CA	45.9	2.2	16.2		40 CB	49.1	9.5	25.8		56 C	50.6	-3.1	25.5
	11 CG	42.1	-9.8	10.7		25 C	45.0	1.1	16.7		40 CG	49.8	9.5	27.0		56 O	51.1	-3.4	24.4
	11 CD	41.3	-8.6	11.2		25 O	43.8	1.3	17.0		40 ND01	51.0	8.8	27.0		57 N	50.3	-4.0	26.4
	11 OE1	40.5	-7.8	10.3		25 CB	46.0	3.0	17.4		40 ND02	49.4	10.1	28.1	VAL	57 CA	50.6	-5.3	26.0
	11 OE2	41.0	-8.6	12.4		25 CG	47.1	3.9	17.8		41 N	46.6	8.1	24.5		57 C	49.8	-6.2	27.0
	12 N	45.5	-11.4	11.7		25 CD1	46.9	5.3	17.9	ALA	41 CA	45.2	8.3	24.6		57 O	49.5	-5.8	28.1
GLY	12 CA	46.4	-12.0	12.4		25 CE1	48.0	6.2	17.9		41 C	44.7	6.9	24.3		57 CB	52.0	-5.7	26.5
	12 C	46.3	-11.8	13.9		25 CZ	49.3	5.6	17.7		41 O	43.6	6.4	24.7		57 CG1	52.7	-4.6	25.5
	12 O	45.1	-11.6	14.2		25 CE2	49.4	4.3	17.6		41 CB	44.6	9.0	23.3		57 CG2	52.1	-6.2	27.9
	13 N	47.3	-11.7	14.7		25 CD2	48.3	3.4	17.6		42 N	45.6	6.1	23.5		58 N	49.4	-7.4	26.5
LEU	13 CA	47.1	-11.4	16.1		25 OEE	50.3	6.9	17.7	ALA	42 CA	45.2	4.9	22.8	ILE	58 CA	48.5	-8.3	27.1
	13 C	48.5	-11.0	16.7		26 N	45.3	-0.2	16.7		42 C	45.6	4.0	24.0		58 C	48.9	-9.6	26.5
	13 O	49.5	-11.7	16.5	THR	26 CA	44.8	-1.5	16.7		42 O	45.0	2.8	23.9		58 O	50.0	-9.9	26.2
	13 CB	46.8	-12.6	17.0		26 C	45.6	-2.3	17.6		42 CB	46.4	4.4	22.0		58 CB	47.1	-8.3	26.5
	13 CG	47.6	-12.8	18.3		26 O	46.8	-2.1	17.8		43 N	46.0	4.4	25.1		58 CG1	47.1	-8.2	25.0
	13 CD1	46.7	-12.7	19.6		26 CB	45.0	-2.2	15.4	LYS	43 CA	46.5	3.7	26.2		58 CD1	46.3	-9.3	24.3
	13 CD2	48.3	-14.1	18.3		26 OG1	44.7	-1.4	14.2		43 C	45.4	3.6	27.2		58 CG2	46.2	-7.2	27.2
	14 N	48.5	-9.9	17.4		26 CG2	44.1	-3.5	15.3		43 O	45.2	2.6	27.8		59 N	47.9	-10.5	26.4
ARG	14 CA	49.7	-9.1	17.8		27 N	45.0	-3.3	18.3		43 CB	47.6	4.3	27.0	THR	59 CA	48.1	-11.9	26.4
	14 C	49.3	-8.7	19.2	ILE	27 CA	45.5	-4.2	19.3		43 CG	49.0	3.8	26.5		59 C	47.1	-12.4	25.5
	14 O	48.1	-8.3	19.5		27 C	44.0	-5.5	19.1		43 CD	48.8	2.9	25.2		59 O	46.2	-11.8	25.1
	14 CB	49.8	-7.8	17.2		27 O	43.6	-5.6	18.0		43 CE	50.1	2.7	24.3		59 CB	47.5	-13.4	27.8
	14 CG	49.9	-7.9	15.6		27 CB	45.3	-3.9	20.7		43 NZ	50.9	1.6	24.9		59 OG1	46.2	-12.0	27.9
	14 CD	51.1	-7.3	14.9		27 CG1	46.2	-4.7	21.7		44 N	44.7	4.7	27.3		59 CG2	48.4	-12.0	28.9

Table 1 (Continued 1)

	60 N	47.3	-13.7	25.0		74 C	28.0	-8.0	14.1		88 CD2	24.0	-12.5	8.3		L03 CG2	29.1	-5.9	8.8
LYS	60 CA	46.5	-14.9	24.0		74 O	26.9	-7.4	13.9		88 OEE	25.3	-13.2	10.5		104 N	33.8	-6.7	9.4
	60 C	45.2	-14.8	24.7		74 CB	30.1	-8.1	13.5		89 N	20.1	-13.3	5.3	PHE	104 CA	34.5	-6.6	10.6
	60 O	44.2	-14.6	24.1		75 N	28.0	-9.3	14.2	ASP	89 CA	19.1	-14.3	5.4		104 C	35.4	-5.4	10.4
	60 CB	46.9	-15.8	23.7	VAL	75 CA	27.0	-10.3	13.8		89 C	19.2	-14.8	4.0		104 O	35.4	-4.5	11.2
	60 CG	47.1	-16.2	22.2		75 C	25.8	-9.7	14.3		89 O	18.7	-15.9	3.7		104 CB	35.5	-7.8	10.8
	60 CD	47.0	-17.7	21.9		75 O	24.7	-9.7	13.5		89 CB	17.7	-13.8	5.5		104 CG	36.0	-9.1	12.1
	60 CE	47.4	-18.0	20.4		75 CB	27.1	-11.6	14.3		89 CG	17.6	-13.5	7.0		104 CD1	37.4	-7.7	12.4
	60 NZ	48.2	-19.2	20.3		75 CG1	26.7	-11.9	15.8		89 OD1	16.4	-13.4	7.5		104 CE1	37.9	-7.9	13.6
	61 N	45.3	-14.3	26.0		75 CG2	28.9	-12.8	13.4		89 OD2	18.6	-13.3	7.7		104 CZ	37.2	-8.5	14.6
ASP	61 CA	44.2	-14.5	26.9		76 N	25.7	-9.1	15.4		90 N	19.8	-14.0	3.1		104 CE2	35.9	-8.9	14.4
	61 C	43.3	-13.3	26.5	ARG	76 CA	24.5	-8.8	16.2	SER	90 CA	19.8	-14.3	1.7		104 CD2	35.3	-8.7	13.1
	61 O	42.0	-13.5	26.5		76 C	24.1	-7.5	15.6		90 C	20.8	-15.3	1.5		105 N	30.2	-5.5	9.3
	61 CB	44.4	-14.1	28.4		76 O	22.8	-7.2	15.5		90 O	20.8	-16.1	0.6	GLN	105 CA	27.4	-4.5	9.3
	61 CG	43.7	-15.3	29.0		76 CB	24.0	-8.4	17.6		90 CB	20.1	-13.2	0.8		105 C	26.7	-3.2	8.9
	61 OD1	42.5	-15.1	29.3		76 CG	24.2	-9.6	18.6		90 OG	21.4	-12.7	0.8		105 O	27.4	-2.2	8.9
	61 OD2	44.3	-16.4	29.3		76 CD	24.8	-9.2	20.1		91 N	21.9	-15.3	2.3		105 CB	28.3	-4.7	8.1
	62 A	43.9	-12.2	26.3		76 NE	25.8	-8.3	20.3	LEU	91 CA	23.1	-15.9	2.0		105 CG	27.7	-5.7	7.1
GLU	62 CA	43.1	-10.9	26.4		76 CZ	26.2	-7.5	21.5		91 C	23.1	-17.3	2.8		105 CD	28.6	-5.5	5.9
	62 C	42.6	-10.8	25.0		76 NEE1	25.9	-8.6	22.7		91 O	22.2	-17.5	3.6		105 NOE1	28.4	-6.4	4.9
	62 O	41.4	-10.4	24.8		76 NEE2	27.1	-7.0	21.6		91 CB	24.3	-15.3	2.5		105 NOE2	29.5	-4.7	5.9
	62 CB	43.9	-9.8	26.8		77 N	25.0	-6.7	15.1		91 CG	24.3	-14.1	1.7		106 N	35.5	-3.2	8.4
	62 CG	43.4	-8.8	27.8	GLY	77 CA	25.1	-5.4	14.5		91 CD1	24.5	-14.3	0.2	MET	106 CA	35.1	-2.1	7.5
	62 CD	44.1	-9.0	29.1		77 C	24.1	-5.7	13.3		91 CD2	24.2	-12.8	2.2		106 C	34.1	-1.3	8.3
	62 CE1	45.4	-8.7	29.1		77 O	23.0	-5.1	13.3		92 N	24.0	-18.1	2.5		106 O	34.0	-0.1	8.2
	62 CE2	43.5	-9.5	30.0		78 N	24.3	-6.5	12.4	ASP	92 CA	24.3	-19.5	2.9		106 CB	34.2	-2.4	6.3
	63 N	43.4	-11.1	24.0	ILE	78 CA	23.9	-6.7	11.1		92 C	25.5	-19.3	3.9		106 CG	35.1	-3.8	5.2
ALA	63 CA	43.3	-10.9	22.6		78 C	22.5	-6.8	11.3		92 O	25.9	-18.2	4.3		106 SD	34.5	-3.8	3.9
	63 C	42.0	-11.6	22.3		78 O	21.6	-6.1	10.8		92 CB	24.7	-20.5	1.9		106 CE	35.9	-1.9	2.8
	63 O	41.3	-11.2	21.4		78 CB	24.2	-7.8	10.3		92 CG	25.9	-19.9	1.1		107 N	33.2	-2.0	9.1
	63 CB	44.3	-11.7	21.7		78 CG1	26.0	-7.6	10.0		92 OD1	27.1	-20.0	1.7	GLY	107 CA	32.4	-1.2	9.9
	64 N	41.8	-12.8	22.9		78 CD1	26.8	-8.9	9.5		92 OD2	25.7	-19.3	0.0		107 C	31.0	-1.6	9.5
GLU	64 CA	40.8	-13.7	22.6		78 CG2	23.8	-8.4	9.0		93 N	25.9	-20.4	4.4		107 O	30.8	-2.1	8.4
	64 C	39.5	-13.2	23.2		79 N	22.1	-7.7	12.2	ALA	93 CA	26.6	-20.4	5.7		108 N	30.0	-1.4	10.4
	64 O	38.4	-13.6	22.8	LEU	79 CA	20.8	-8.3	12.6		93 C	28.0	-19.8	5.5	GLU	108 CA	28.7	-1.9	10.3
	64 CB	41.1	-15.2	23.0		79 C	19.7	-7.1	13.0		93 O	28.3	-18.7	5.9		108 C	28.2	-1.1	9.2
	64 CG	41.2	-16.2	21.9		79 O	18.7	-7.2	12.8		93 CB	26.7	-21.7	6.4		108 O	27.5	-1.6	8.2
	64 CD	42.5	-17.0	22.0		79 CB	20.9	-9.1	13.9		94 N	28.8	-20.6	4.8		108 CB	27.7	-1.5	11.4
	64 OE1	43.0	-17.2	23.2		79 CG	20.6	-10.6	13.7	VAL	94 CA	30.1	-20.1	4.5		108 CG	26.4	-2.5	11.5
	64 OE2	43.1	-17.3	21.0		79 CD1	21.5	-11.2	12.6		94 C	30.1	-18.8	3.9		108 CD	25.4	-1.7	12.3
	65 N	39.6	-12.3	24.2		79 CD2	20.7	-11.4	15.0		94 O	31.1	-18.1	3.9		108 OE1	24.5	-1.1	11.7
LYS	65 CA	38.5	-11.8	25.1		80 N	20.5	-6.1	13.5		94 CB	30.8	-20.9	3.4		108 OE2	25.6	-1.7	13.5
	65 C	37.7	-10.9	24.1	ARG	80 CA	19.7	-5.1	14.0		94 CG1	29.8	-21.4	2.3		109 N	28.4	0.2	9.2
	65 O	36.5	-11.0	24.0		80 C	19.6	-3.9	13.1		94 CG2	32.1	-20.3	2.9	THR	109 CA	27.6	1.2	8.9
	65 CB	38.7	-11.0	26.3		80 O	19.1	-2.8	13.5		95 N	29.0	-18.4	3.3		109 C	28.5	1.5	7.2
	65 CG	37.6	-10.8	27.3		80 CB	20.2	-4.4	15.3	ARG	95 CA	29.0	-17.2	2.5		109 O	28.0	2.4	6.4
	65 CD	37.7	-11.4	28.7		80 CG	21.1	-3.2	15.3		95 C	28.8	-16.1	3.5		109 CB	27.4	2.6	8.9
	65 CE	36.3	-11.6	29.4		80 CD	21.7	-2.6	16.5		95 O	29.1	-14.9	3.2		109 OG1	26.3	3.1	8.3
	65 NZ	36.3	-12.5	30.5		80 NE	22.3	-3.4	17.5		95 CB	28.0	-16.9	1.4		109 CG2	28.6	3.6	9.0
	66 N	38.5	-13.0	23.5		80 CZ	23.6	-3.2	17.6		95 CG	28.4	-17.2	-0.0		110 N	29.5	0.7	6.8
LEU	66 CA	38.1	-8.6	22.8		80 NEE1	24.2	-2.2	16.9		95 CD	27.4	-17.4	-1.1	GLY	110 CA	30.4	1.1	5.7
	66 C	37.6	-9.4	21.5		80 NEE2	24.3	-3.9	18.4		95 NE	27.8	-17.4	-2.5		110 C	30.1	0.1	4.6
	66 O	36.7	-8.9	20.8		81 N	19.9	-4.1	11.8		95 CZ	27.5	-18.6	-3.1		110 O	30.4	0.3	3.5
	66 CB	39.2	-7.9	22.4	ASN	81 CA	20.0	-3.0	10.8		95 NEE1	26.7	-19.4	-2.5		111 N	29.4	-1.0	5.3
	66 CG	39.7	-7.1	23.6		81 C	19.4	-3.6	9.6		95 NEE2	27.9	-18.9	-4.3	VAL	111 CA	29.4	-2.1	4.0
	66 CD1	40.6	-8.0	24.6		81 O	19.9	-4.6	9.0		96 N	28.3	-16.5	4.7		111 C	28.0	-1.8	3.4
	66 CD2	40.3	-5.6	23.3		81 CB	21.5	-3.0	10.3	ARG	96 CA	27.8	-15.5	5.6		111 O	27.8	-2.1	2.2
	67 N	38.2	-10.5	21.0		81 CG	21.5	-2.0	9.2		96 C	28.9	-14.8	6.3		111 CB	29.2	-3.4	4.7
PHE	67 CA	38.0	-11.1	19.7		81 ND1	20.6	-2.1	8.2		96 O	28.8	-13.7	6.8		111 CG1	29.6	-3.4	6.1
	67 C	36.6	-11.6	19.8		81 ND2	22.3	-1.0	9.2		96 CB	27.0	-16.0	6.8		111 CG2	28.6	-4.6	4.1
	67 O	35.8	-11.1	19.0		82 N	18.5	-2.9	9.0		96 CG	25.4	-16.0	6.7		112 N	27.1	-1.2	4.1
	67 CB	38.7	-12.4	19.4	ALA	82 CA	17.5	-3.0	8.0		96 CD	24.9	-16.4	7.9	ALA	112 CA	25.8	-1.0	3.9
	67 CG	38.9	-12.9	18.0		82 C	18.1	-3.1	6.7		96 NE	23.3	-16.6	8.0		112 C	26.0	0.1	2.7
	67 CD1	39.3	-14.2	17.8		82 O	17.4	-3.8	5.8		96 CZ	22.9	-17.8	7.7		112 O	25.0	0.8	2.2
	67 CE1	39.4	-14.7	16.5		82 CB	16.7	-1.7	7.6		96 NEE1	23.7	-18.8	7.4		112 CB	24.8	-0.4	4.6
	67 CZ	39.0	-13.9	15.4		83 N	19.4	-3.0	6.5		96 NEE2	21.6	-18.1	7.7		113 N	27.2	0.4	2.3
	67 CE2	38.5	-12.6	15.7	LYS	83 CA	20.0	-3.0	5.2		97 N	30.1	-15.5	6.3	GLY	113 CA	27.5	1.4	1.3
	67 CD2	38.5	-12.1	17.0		83 C	20.7	-4.4	5.2	CYH	97 CA	31.2	-15.2	7.1		113 C	27.9	0.6	0.1
	68 N	36.3	-12.5	20.7		83 O	20.8	-5.0	4.1		97 C	31.9	-14.2	6.2		113 O	28.0	1.0	-0.8
ASN	68 CA	35.2	-13.3	20.8		83 CB	21.2	-2.1	5.0		97 O	32.6	-13.3	6.7		114 N	27.4	-0.7	0.0
	68 C	34.1	-12.3	21.0		83 CG	21.0	-1.1	3.8		97 CB	32.2	-16.3	7.1	PHE	114 CA	27.7	-1.4	-1.2
	68 O	32.9	-12.6	20.8		83 CD	21.2	0.4	4.1		97 SG	31.7	-17.6	8.3		114 C	26.4	-2.0	-1.5
	68 CB	35.0	-14.2	21.9		83 CE	21.1	1.4	3.0		98 N	31.8	-14.3	4.9		114 O	26.2	-3.3	-1.6
	68 CG	35.4	-15.6	21.5		83 NZ	21.2	2.8	3.3	ALA	98 CA	32.4	-13.6	3.9		114 CB	28.6	-2.6	-1.0
	68 ND01	36.7	-15.8	21.3		84 N	21.1	-4.8	6.3		98 C	31.8	-12.2	4.1		114 CG	29.9	-2.3	-0.5
	68 ND02	34.6	-16.5	21.4	LEU	84 CA	22.1	-5.8	6.4		98 O	32.6	-11.3	4.3		114 CD1	31.0	-2.4	-1.4
	69 N	34.4	-11.1	21.4		84 C	21.3	-7.1	6.6		98 CB	31.8	-13.8	2.5		114 CE1	32.3	-2.0	-0.9
GLN	69 CA	33.7	-10.0	22.0		84 O	21.5	-8.0	5.8		99 N	30.5	-12.1	4.2		114 CZ	32.5	-1.5	0.4
	69 C	33.1	-9.2	20.9		84 CB	23.1	-5.8	7.6	LEU	99 CA	29.9	-10.8	4.3		114 CE2	31.4	-1.4	1.2
	69 O	31.9	-9.4	21.0		84 CG	24.2	-5.7	7.3		99 C	30.3	-10.4	5.6		114 CD2	30.1	-1.8	0.8
	69 CB	34.8	-9.0	23.0		84 CD1	24.8	-5.5	5.7		99 O	30.5	-9.2	5.9		115 N	25.3	-2.2	-1.8
	69 CG	33.6	-8.1	23.9		84 CD2	25.4	-4.8	8.1		99 CB	28.4	-10.8	4.4	THR	115 CA	23.9	-1.1	-2.0
	69 CD	34.4	-7.9	25.2		85 N	20.5	-7.2	7.7		99 CG	27.7	-9.5	4.4		115 C	23.8	-2.0	-3.3
	69 OE1	34.1	-8.7	26.2	LYS	85 CA	19.7	-8.3	8.1		99 CD1	27.6	-8.7	3.1		115 O	22.7	-2.6	-3.5
	69 NOE2	35.2	-7.0	25.3		85 C	19.2	-9.0	6.9		99 CD2	26.2	-9.6	5.0		115 CB	23.4	0.3	-2.4
	70 N	33.6	-8.9	19.8		85 O	19.3	-10.3	6.9		100 N	30.3	-11.4	6.6		115 OG1	23.6	1.1	-1.3
ASP	70 CA	33.7	-7.9	18.8		85 CB	18.5	-7.9	8.9	ILE	100 CA	30.4	-11.2	8.0		115 CG2	22.0	0.3	-2.9
	70 C	32.9	-8.5	17.7		85 CG	18.2	-8.9	10.0		100 C	31.8	-10.5	8.1		116 N	24.8	-2.0	-4.1
	70 O	32.1	-7.8	17.0		85 CD	17.0	-9.9	9.6		100 O	31.9	-9.5	8.9	ASN	116 CA	24.6	-2.6	-5.4
	70 CB	34.9	-7.5	18.1		85 CE	16.3	-10.5	10.8		100 CB	30.5	-12.4	8.8		116 C	25.2	-4.0	-5.2
	70 CG	35.7	-6.5	19.0		85 NZ	14.8	-10.5	10.6		100 CG1	29.1	-13.0	9.2		116 O	24.8	-4.9	-5.9
	70 OD1	35.0	-5.6	19.5		86 N	18.7	-8.4	5.9		100 CD1	28.7	-12.7	10.6		116 CB	25.5	-2.0	-6.5
	70 OD2	36.9	-6.7	19.2	PRO	86 CA	17.9	-9.1	4.9		100 CG2	31.3	-12.3	10.2		116 CG	24.0	-0.8	-6.9
	71 N	33.1	-9.6	17.4		86 C	18.9	-9.8	4.0		101 N	32.8	-11.1	7.5		116 NOD1	23.4	-1.1	-7.1
VAL	71 CA	32.7	-10.5	16.2		86 O	18.7	-10.9	3.5	ASN	101 CA	34.2	-10.9	7.6		116 ND02	25.1	-0.1	-7.1
	71 C	31.3	-10.7	16.4		86 CB	17.5	-8.0	3.8		101 C	34.3	-9.4	7.0		117 N	26.2	-4.1	-4.3
	71 O	30.5	-10.9	15.5		86 CG	17.3	-6.8	4.7		101 O	35.3	-8.6	7.3	SER	117 CA	26.8	-5.4	-4.4
	71 CB	33.2	-11.9	16.1		86 CD	18.1	-7.0	6.0		101 CB	35.0	-11.6	6.8		117 C	25.8	-6.3	-3.7
	71 CG1	32.2	-13.0	15.7		87 N	20.1	-9.2	4.0		101 CG	36.5	-11.3	6.9		117 O	25.6	-7.4	-4.0
	71 CG2	34.6	-12.1	15.4	VAL	87 CA	21.2	-9.6	3.1		101 ND01	37.3	-12.3	7.4		117 CB	28.0	-5.5	-3.5
	72 N	30.8	-10.7	17.7		87 C	21.7	-10.9	3.7		101 ND02	36.9	-10.2	6.6		117 OG	29.2	-5.3	-4.3
ASP	72 CA	29.6	-11.1	18.2		87 O	22.3	-11.7	2.9		102 N	33.3	-9.0	6.3		118 N	25.2	-5.7	-2.7
	72 C	28.9	-9.8	18.2		87 CB	22.4	-8.7	2.9	MET	102 CA	33.2	-7.8	5.5	LEU	118 CA	24.2	-6.3	-1.8
	72 O	27.6	-9.7	18.2		87 CG1	23.8	-9.3	3.0		102 C	33.0	-6.7	6.5		118 C	23.1	-6.7	-2.8
	72 CB	29.6	-11.4	19.7		87 CG2	22.3	-7.9	1.5		102 O	33.7	-5.6	6.5		118 O	22.9	-7.9	-2.9
	72 CG	28.3	-11.6	20.1		88 N	21.6	-11.1	5.0		102 CB	32.0	-7.5	4.6		118 CB	23.5	-5.1	-1.0
	72 OD1	27.4	-11.0	20.5	TYR	88 CA	22.2	-12.1	5.8		102 CG	32.2	-6.4	3.6		118 CG	24.2	-4.9	0.4
	72 OD2	28.0	-13.1	20.1		88 C	21.4	-13.4	5.4		102 SD	32.3	-6.9	1.8		118 CD1	24.5	-6.3	0.8
	73 N	29.6	-8.7	18.0		88 O	22.0	-14.5	5.2		102 CE	32.5	-5.3	1.0		118 CD2	23.5	-4.1	0.1
ALA	73 CA	29.3	-7.4	18.2		88 CB	21.8	-12.1	7.3		103 N	32.2	-6.9	7.5		119 N	22.4	-5.8	-3.4
	73 C	28.7	-7.0	16.8		88 CG	22.7	-12.8	8.3	VAL	103 CA	31.7	-5.9	8.4	ARG	119 CA	21.4	-5.9	-4.4
	73 O	27.7	-6.4	16.7		88 CD1	22.2	-13.8	9.1		103 C	32.8	-5.8	9.4		119 C	21.4	-7.3	-5.0
	73 CB	30.5	-6.4	18.1		88 CE1	23.1	-14.7	9.8		103 O	32.8	-4.8	10.2		119 O	21.1	-8.2	-4.9
	74 N	29.4	-7.5	15.8		88 CZ	24.4	-14.4	9.8		103 CB	30.5	-6.4	9.3		119 CB	21.6	-5.0	-5.6
ALA	74 CA	29.3	-7.3	14.3		88 CE2	24.9	-13.3	9.1		103 CG1	30.6	-6.0	10.8		119 CG	20.3	-4.4	-6.0

Table 1 (Continued 2)

	119 CD	20.0	-4.6	-7.5		133 N	32.6	-5.2	-6.3		146 N	41.1	-8.9	-0.2		159 OD2	38.6	-25.3	-1.5
	119 NE	18.9	-3.9	-8.0	LEU	133 CA	33.0	-4.8	-5.0	ALA	146 CA	40.0	-8.3	-0.9		160 N	39.9	-20.4	-0.0
	119 CZ	19.2	-3.3	-9.1		133 C	34.4	-4.5	-5.2		146 C	39.4	-9.6	-1.6	ALA	160 CA	40.5	-19.1	-0.0
	119 NEE1	20.4	-3.4	-9.7		133 O	35.0	-3.7	-4.4		146 O	38.2	-9.9	-1.3		160 C	41.4	-19.1	1.1
	119 NEE2	18.4	-2.3	-9.7		133 CB	33.1	-6.0	-4.0		146 CB	40.5	-7.6	-2.2		160 O	42.6	-18.3	1.0
	120 N	23.0	-7.3	-5.6		133 CG	31.8	-6.5	-3.4		147 N	40.2	-10.3	-2.4		160 CB	39.6	-17.9	0.3
MET	120 CA	23.2	-8.5	-6.6		133 CD1	31.5	-7.9	-3.9	LYS	147 CA	39.4	-11.2	-3.2		161 N	40.9	-19.4	2.3
	120 C	23.6	-9.5	-5.9		133 CD2	31.7	-6.4	-1.9		147 C	39.5	-12.4	-2.3	TYR	161 CA	41.7	-19.3	3.5
	120 O	23.9	-10.5	-6.6		134 N	35.1	-5.0	-6.2		147 O	39.0	-13.5	-2.7		161 C	42.1	-20.7	3.6
	120 CB	24.4	-8.0	-7.5	ALA	134 CA	36.5	-5.0	-6.5		147 CB	40.4	-11.7	-4.3		161 O	42.4	-21.3	4.7
	120 CG	24.2	-6.9	-8.6		134 C	36.7	-3.5	-6.9		147 CG	41.7	-10.8	-4.4		161 CB	43.8	-19.0	4.7
	120 SD	25.5	-6.7	-9.8		134 O	37.9	-3.1	-6.9		147 CD	42.7	-11.2	-5.4		161 CG	44.0	-17.8	4.5
	120 CE	26.2	-5.1	-9.3		134 CB	36.9	-5.7	-7.7		147 CE	42.7	-10.2	-6.6		161 CD1	40.2	-16.8	5.3
	121 N	23.7	-9.5	-4.6		135 N	35.7	-2.8	-7.2		147 NZ	44.1	-10.0	-7.0		161 CE1	39.4	-15.6	5.1
LEU	121 CA	24.2	-10.6	-3.9	LYS	135 CA	35.8	-1.5	-7.9		148 N	40.0	-12.2	-1.1		161 CZ	38.6	-15.5	3.9
	121 C	23.0	-11.4	-3.3		135 C	35.5	-0.6	-6.8	ARG	148 CA	40.3	-13.2	-0.1		161 CE2	38.4	-16.6	3.1
	121 O	23.0	-12.5	-3.0		135 O	34.7	0.4	-7.0		148 C	38.9	-13.4	0.5		161 CD2	39.2	-17.8	3.4
	121 CB	25.0	-10.3	-2.6		135 CB	34.7	-1.2	-8.8		148 O	38.5	-14.5	0.8		161 OEE	37.9	-14.4	3.6
	121 CG	26.5	-10.2	-2.9		135 CG	34.4	0.3	-9.2		148 CB	41.1	-12.9	1.1		162 N	42.1	-21.5	2.5
	121 CD1	27.0	-11.5	-3.8		135 CD	33.8	0.5	-10.6		148 CG	41.8	-14.0	1.7	LYS	162 CA	42.4	-22.8	2.1
	121 CD2	27.4	-9.9	-1.7		135 CE	34.5	1.6	-11.3		148 CD	43.0	-14.5	0.9		162 C	43.5	-23.3	2.9
	122 N	21.9	-10.5	-3.1		135 NZ	34.3	2.9	-10.6		148 NE	44.3	-14.6	1.6		162 O	43.3	-24.3	3.7
GLN	122 CA	20.8	-10.9	-2.4		136 N	36.0	-0.8	-5.6		148 CZ	44.3	-13.8	2.6		162 CB	42.7	-23.1	0.7
	122 C	20.1	-11.9	-3.3	SER	136 CA	35.6	0.0	-4.4		148 NEE1	43.3	-13.8	3.5		162 CG	44.1	-22.6	0.1
	122 O	19.5	-12.9	-2.9		136 C	37.2	0.2	-3.8		148 NEE2	45.4	-13.1	2.9		162 CD	44.2	-22.9	-1.4
	122 CB	19.7	-9.8	-2.4		136 O	38.1	-0.3	-4.4		149 N	38.1	-12.3	0.5		162 CE	45.6	-23.1	-1.8
	122 CG	19.5	-9.4	-0.9		136 CB	35.1	-0.7	-3.3	VAL	149 CA	36.9	-12.2	1.2		162 NZ	45.9	-24.4	-2.4
	122 CD	18.5	-8.2	-1.0		136 OG	35.0	-1.9	-2.9		149 C	35.9	-12.3	0.1		163 N	44.7	-22.8	2.7
	122 NOE1	17.3	-8.5	-0.5		137 N	37.3	0.8	-2.7		149 O	34.7	-12.5	0.3	ASN	163 CA	46.0	-23.4	3.1
	122 NCE2	18.9	-7.1	-1.5	ARG	137 CA	38.4	1.4	-2.1		149 CB	36.5	-10.9	1.9		163 C	46.8	-22.4	3.9
	123 N	20.3	-11.7	-4.6		137 C	39.4	0.2	-1.5		149 CG1	35.1	-10.4	1.7		163 O	47.1	-22.6	5.0
GLN	123 CA	19.5	-12.5	-5.5		137 O	40.3	0.1	-1.5		149 CG2	37.0	-10.9	3.4		163 CB	46.9	-24.1	2.3
	123 C	20.5	-13.5	-6.0		137 CB	38.2	2.2	-0.8		150 N	36.4	-12.3	-1.2		163 CG	48.2	-23.5	2.1
	123 O	20.2	-14.3	-7.0		137 CG	39.0	3.5	-0.6	ILE	150 CA	35.5	-12.0	-2.3		163 NOD1	49.1	-23.6	3.1
	123 CB	19.3	-11.6	-6.8		137 CD	39.2	4.1	0.7		150 C	35.3	-13.4	-2.9		163 ND02	48.5	-22.8	1.1
	123 CG	18.3	-10.5	-6.5		137 NE	40.4	5.0	0.8		150 O	34.2	-13.6	-3.4		164 N	47.2	-21.3	3.2
	123 CD	18.8	-9.4	-7.4		137 CZ	40.9	5.1	2.0		150 CB	36.0	-11.1	-3.4	LEU	164 CA	47.8	-20.0	3.4
	123 NOE1	17.8	-8.8	-8.1		137 NEE1	40.4	4.6	3.0		150 CG1	36.2	-9.7	-2.8		164 C	48.7	-20.2	4.6
	123 NCE2	20.0	-9.0	-7.4		137 NEE2	42.1	5.8	2.1		150 CD1	36.2	-8.6	-3.9		164 O	48.9	-21.3	5.0
	124 N	21.6	-13.0	-5.3		138 N	38.3	-0.8	-1.1		150 CG2	35.3	-11.1	-4.7		164 CB	46.8	-19.0	4.0
LYS	124 CA	22.5	-14.7	-5.2	TRP	138 CA	38.5	-2.0	-0.3		151 N	36.3	-14.2	-2.9		164 CG	46.6	-17.7	3.3
	124 C	23.3	-14.7	-6.5		138 C	39.4	-2.8	-1.1	THR	151 CA	36.4	-15.4	-3.7		164 CD1	45.6	-17.8	2.1
	124 O	23.2	-15.7	-7.3		138 O	40.4	-3.2	-0.7		151 C	35.4	-16.4	-3.0		164 CD2	46.3	-16.5	4.2
	124 CB	21.8	-16.1	-5.3		138 CB	37.3	-2.9	-0.4		151 O	34.8	-17.2	-3.7		164 O-	49.2	-19.1	5.1
	124 CG	21.2	-16.4	-3.9		138 CG	37.1	-4.0	0.5		151 CB	37.7	-16.1	-3.6					
	124 CD	20.3	-17.7	-3.9		138 CD2	36.6	-5.2	-0.0		151 OG1	38.7	-15.5	-4.5					
	124 CE	20.3	-18.3	-2.5		138 CE3	35.9	-5.6	-1.1		151 CG2	37.8	-17.6	-3.6					
	124 NZ	20.5	-17.5	-1.5		138 CZ3	35.3	-6.8	-1.2		152 N	35.3	-16.2	-1.7					
	125 N	23.9	-13.6	-6.8		138 CD1	37.9	-4.3	1.6	THR	152 CA	34.4	-17.1	-1.0					
ARG	125 CA	24.5	-13.3	-8.1		138 CE2	36.9	-6.2	0.9		152 C	33.1	-16.8	-1.7					
	125 C	26.0	-13.1	-7.8		138 CZ2	36.4	-7.6	0.8		152 O	32.4	-17.6	-2.2					
	125 O	26.5	-12.0	-7.6		138 NE1	37.7	-5.7	1.9		152 CB	34.4	-16.5	0.4					
	125 CB	24.2	-11.9	-8.6		138 CEE2	35.6	-7.8	-0.3		152 OG1	35.8	-16.5	0.8					
	125 CG	23.6	-12.0	-9.5		139 N	39.0	-3.0	-2.4		152 CG2	33.6	-17.2	1.5					
	125 CD	22.9	-11.0	-10.7	TYR	139 CA	39.7	-4.0	-3.1		153 N	32.7	-15.5	-1.6					
	125 NE	21.5	-11.0	-11.2		139 C	41.0	-3.3	-3.5	PHE	153 CA	31.3	-15.1	-1.8					
	125 CZ	21.3	-10.3	-12.3		139 O	42.0	-4.0	-3.8		153 C	31.0	-15.7	-3.1					
	125 NEE1	22.3	-9.6	-12.8		139 CB	39.1	-4.3	-4.5		153 O	29.8	-16.0	-3.4					
	125 NEE2	20.1	-10.2	-12.8		139 CG	39.7	-5.3	-5.4		153 CB	31.2	-13.6	-1.9					
	126 N	26.7	-14.3	-7.9		139 CD1	39.6	-6.6	-5.3		153 CG	30.9	-12.8	-0.8					
TRP	126 CA	28.0	-14.6	-7.4		139 CE1	40.2	-7.5	-6.1		153 CD1	31.8	-11.8	-0.4					
	126 C	28.9	-13.9	-8.3		139 CZ	41.1	-7.0	-7.1		153 CE1	31.4	-10.9	0.7					
	126 O	29.4	-12.8	-8.1		139 CE2	41.2	-5.6	-7.3		153 CZ	30.2	-11.1	1.3					
	126 CB	28.3	-16.0	-7.2		139 CD2	40.5	-4.8	-6.4		153 CE2	29.4	-12.1	1.0					
	126 CG	27.3	-16.7	-6.4		139 OEE	41.8	-7.8	-8.0		153 CD2	29.7	-12.9	-0.1					
	126 CD2	26.5	-16.1	-5.4		140 N	41.0	-2.0	-3.4		154 N	32.0	-15.9	-3.9					
	126 CE3	26.6	-14.9	-4.8	ASN	140 CA	42.1	-1.2	-3.9	ARG	154 CA	32.1	-16.3	-5.3					
	126 CZ3	25.7	-14.6	-3.7		140 C	43.1	-1.2	-2.8		154 C	31.7	-17.7	-5.4					
	126 CD1	26.7	-18.0	-6.6		140 O	44.3	-1.2	-3.1		154 O	30.9	-18.0	-6.4					
	126 CE2	25.6	-17.1	-4.9		140 CB	41.8	0.3	-4.2		154 CB	33.4	-16.2	-6.3					
	126 CZ2	24.7	-16.8	-3.8		140 CG	41.8	0.2	-5.7		154 CG	33.4	-15.7	-7.4					
	126 NE1	25.7	-18.2	-5.7		140 NOD1	40.8	0.9	-6.3		154 CD	34.8	-15.8	-8.2					
	126 CEE2	24.6	-15.6	-3.3		140 ND02	42.6	-0.5	-6.3		154 NE	35.3	-14.6	-8.8					
	127 N	29.3	-14.5	-9.5		141 N	42.7	-1.3	-1.6		154 CZ	36.2	-14.9	-9.7					
ASP	127 CA	30.2	-14.4	-10.6	GLN	141 CA	43.7	-0.9	-0.5		154 NEE1	36.6	-16.1	-9.8					
	127 C	30.4	-13.0	-10.8		141 C	44.2	-2.2	0.0		154 NEE2	36.7	-13.9	-10.4					
	127 O	31.5	-12.5	-11.1		141 O	45.4	-2.2	0.5		155 N	32.2	-16.6	-4.6					
	127 CB	29.8	-15.0	-11.9		141 CB	43.2	-0.1	0.6	THR	155 CA	32.1	-20.0	-4.9					
	127 CG	30.8	-16.1	-12.3		141 CG	44.2	0.8	1.4		155 C	31.5	-20.7	-3.7					
	127 OD1	30.6	-17.0	-11.5		141 CD	44.0	1.9	0.5		155 O	30.8	-21.8	-3.9					
	127 OD2	31.4	-15.9	-13.4		141 NOE1	45.6	2.7	0.8		155 CB	33.5	-20.6	-4.8					
	128 N	29.4	-12.1	-10.7		141 NOE2	43.4	2.1	-0.6		155 OG1	34.0	-20.8	-3.5					
GLU	128 CA	29.4	-10.8	-11.3		142 N	43.4	-3.3	0.0		155 CG2	34.5	-19.9	-5.8					
	128 C	29.4	-9.8	-10.2	THR	142 CA	43.9	-4.5	0.6		156 N	31.6	-20.2	-2.5					
	128 O	29.5	-8.6	-10.4		142 C	43.7	-5.6	-0.5	GLY	156 CA	30.6	-20.7	-1.6					
	128 CB	28.1	-10.5	-12.0		142 O	42.8	-6.4	-0.4		156 C	31.3	-21.8	-0.9					
	128 CG	26.6	-10.8	-11.2		142 CB	42.9	-5.0	1.7		156 O	30.7	-22.8	-0.5					
	128 CD	26.5	-12.2	-11.8		142 OG1	42.1	-3.9	2.2		157 N	32.6	-21.7	-0.7					
	128 CE1	27.3	-13.1	-11.7		142 CG2	43.7	-5.5	2.9	THR	157 CA	33.5	-22.8	-0.1					
	128 CE2	25.3	-12.3	-12.2		143 N	44.6	-5.5	-1.5		157 C	34.8	-22.0	0.2					
	129 N	29.2	-10.3	-8.9	PRO	143 CA	44.6	-6.1	-2.8		157 O	35.0	-20.9	-0.4					
ALA	129 CA	29.6	-9.3	-7.9		143 C	44.2	-7.5	-2.6		157 CB	34.0	-23.6	-1.3					
	129 C	30.3	-9.3	-7.2		143 O	43.2	-7.9	-3.3		157 OG1	35.3	-23.8	-1.5					
	129 O	30.6	-8.4	-6.4		143 CB	46.1	-6.3	-3.0		157 CG2	33.1	-23.4	-2.6					
	129 CB	28.1	-9.9	-6.8		143 CG	46.7	-5.0	-2.4		158 N	35.8	-22.5	1.1					
	130 N	31.2	-10.3	-7.6		143 CD	45.6	-4.5	-1.5	TRP	158 CA	36.6	-21.7	1.8					
ALA	130 CA	32.5	-10.5	-7.1		144 N	44.8	-8.3	-1.7		158 C	37.9	-22.3	1.3					
	130 C	33.3	-9.4	-7.8	ASN	144 CA	44.8	-9.7	-1.5		158 O	38.6	-22.9	2.1					
	130 O	34.5	-9.3	-7.5		144 C	43.5	-10.0	-0.8		158 CB	36.8	-22.0	3.3					
	130 CB	33.1	-11.7	-7.7		144 O	42.6	-10.4	-1.5		158 CG	35.7	-22.1	4.3					
	131 N	32.6	-8.6	-8.5		144 CB	45.8	-10.1	-0.4		158 CD2	35.3	-21.0	5.1					
VAL	131 CA	33.4	-7.8	-9.4		144 CG	47.1	-10.1	-1.3		158 CE3	35.7	-19.7	5.3					
	131 C	33.1	-6.3	-9.1		144 NOD1	48.2	-10.4	-0.7		158 CZ3	35.1	-18.9	6.2					
	131 O	34.0	-5.5	-9.4		144 ND02	47.3	-9.9	-2.5		158 CD1	34.9	-23.1	4.5					
	131 CB	33.0	-7.9	-10.9		145 N	43.4	-9.7	0.5		158 CE2	34.3	-21.5	5.9					
	131 CG1	31.7	-8.2	-11.1	ARG	145 CA	42.4	-10.1	1.4		158 CZ2	33.9	-20.7	6.9					
	131 CG2	33.2	-6.0	-11.8		145 C	41.1	-9.8	0.7		158 NE1	34.1	-22.8	5.6					
	132 N	32.0	-6.0	-8.5		145 O	40.1	-10.5	1.0		158 CEE2	34.0	-19.4	7.0					
ASN	132 CA	31.4	-4.7	-8.4		145 CB	42.3	-9.1	2.6		159 N	38.2	-22.0	0.0					
	132 C	32.0	-4.3	-7.0		145 CG	41.4	-9.4	3.8	ASP	159 CA	39.3	-22.7	-0.6					
	132 O	31.9	-3.1	-6.6		145 CD	41.4	-8.4	4.9		159 C	40.3	-21.5	-0.6					
	132 CB	30.0	-4.6	-8.2		145 NE	40.6	-8.7	6.0		159 O	41.4	-21.6	-1.1					
	132 CG	29.5	-3.3	-7.7		145 CZ	40.8	-8.0	7.1		159 CB	39.1	-22.8	-2.1					
	132 NOD1	29.4	-3.2	-6.4		145 NEE1	41.7	-7.0	7.1		159 CG	38.6	-24.3	-2.3					
	132 ND02	29.2	-2.4	-8.5		145 NEE2	40.1	-8.3	8.2		159 OD1	38.3	-24.6	-3.4					

of atoms while requiring the idealized model to fit as closely as possible to the raw coordinates (6, 7). The "standard" dimensions of the peptide linkage and the amino acid side chains were taken from the CRC Handbook of Biochemistry and Molecular Biology (8).

Further refinement of the lysozyme coordinates, currently under way, will take some time. In the meantime, we present here the coordinates available at this time (Table I). These coordinates were obtained using the idealization procedure described above in which adherence to satisfactory stereochemistry was weighted ten times as heavily as adherence to the raw coordinates. The conventional crystallographic residual, calculated for 7700 reflections to a resolution of 2.4 Å, was 45.0% for the raw coordinates and 44.1% for the constrained ones. The decrease in the residual indicates that the idealized coordinates are not only superior to the raw coordinates so far as acceptable stereochemistry is concerned, but also they agree better with the crystallographic data.

The phage lysozyme coordinates quoted in Table I are in Angstroms relative to orthogonal axes parallel to the crystallographic axes $\underline{a}^*$, $\underline{b}$ and $\underline{c}$, with origin at the origin of the unit cell. Crystals of phage lysozyme have space group $P3_221$ with cell dimensions $\underline{a} = \underline{b} = 61.2$ Å, $\underline{c} = 96.8$ Å. The transformation giving the fractional crystallographic coordinates (x, y, z) in terms of the orthogonal coordinates (X, Y, Z) given in Table I, is

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Legend to Table I:

The atom names correspond to the standard nomenclature (9) with transliteration of the Greek subscripts, and using EE for eta (η). The distinction between the nitrogen and oxygen atoms of amide side chains is not indicated by the electron density map and these atoms are labeled NOD1, NOD2 for asparagine, and NOE1, NOE2 for glutamine. The atom labeled 1 is believed to be oxygen on stereochemical grounds.

$$x = 0.01887\ X$$

$$y = 0.00943\ X + 0.01634\ Y$$

$$z = 0.01033\ Z$$

We estimate that for most of the lysozyme molecule, the coordinates given in Table I have an average error of about 0.4 Å, except for the amino terminal residues 162-164, which are poorly defined in the electron density map and may be somewhat disordered in the crystal.

A full description of the structure determination and the molecular structure is in preparation.

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