ATOMIC COORDINATES FOR FERRICYTOCHROME c, OF RHODOSPIRILLUM RUBRUM

F. R. Salemme, S. T. Freer, R. A. Alden and J. Kraut
Department of Chemistry
University of California, San Diego
La Jolla, California 92037

Received July 12, 1973

Summary: Atomic coordinates and backbone torsion angles are tabulated for ferricytochrome c_0 of Rhodospirillum rubrum.

The three-dimensional structure of ferricytochrome \underline{c}_2 of the photosynthetic bacterium Rhodospirillum rubrum has been described in a previous publication (1). This protein, of MW = 12,480, functions as the electron donor to bacteriochlorophyll in the cyclic photophosphorylating electron transport chain of the bacterium, and is of interest because of its sequential and structural similarity with eucaryotic mitochondrial cytochrome \underline{c} (2-4).

Cytochrome \underline{c}_2 is composed of a single polypeptide chain of 112 amino acid residues and contains a single protoheme IX covalently bonded to the polypeptide chain through thioether linkages formed between the heme vinyl side chains and cysteine residues 14 and 17. The heme iron is coordinated to the Ne2 nitrogen atom of histidine 18 and the S δ sulfur atom of methionine 91 in the fifth and sixth positions, respectively. The heme group is planar, as expected for a low-spin ferriheme coordinate complex (5). The S δ sulfur atom of methionine 91 appears, however, to be slightly displaced (about 0.3 Å) from its expected axial position in a regular octahedral iron complex (ref. 1, Fig. 5).

Coordinates of cytochrome \underline{c}_2 were initially measured by means of an automated coordinate measuring device (6) on a model built in a Richards optical comparator (7) from a 2 \mathring{A} multiple-isomorphous-replacement phased map. These initial coordinates were subsequently refined by techniques which will be described in detail in a communication currently in preparation (8).

						Tai	ble I				
GLU		X Y Z 6.0 4.4 26.5 5.4 3.1 26.5	C ¥S	17 CB 17 SG	X	LEU	32 CD2	X Y Z 13.7 20.1 21.9 9.6 19.9 22.5	TTR		X y Z
	1 CR 1 CB 1 CG	4.0 3.0 25.9 3.7 4.2 24.9		17 C 17 O	19.1 22.0 25.2 18.7 23.2 25.0	PHE	32 O 33 N	9.7 18.7 22.6 8.5 20.6 23.0		46 CZ 46 OH 46 CE2	18.0 28.7 21.1 19.3 28.2 21.1 17.4 28.9 19.8
	1 CD 1 OE1 1 OE2	3.7 3.8 23.4 4.7 3.3 22.9 2.7 4.2 22.9	HIS	18 CA 18 CB	16.4 20.9 25.4 16.9 21.0 25.4 16.4 20.2 24.3		33 CA 33 CB 33 CG	7.4 15.9 23.6 7.2 20.4 25.0		46 CD2 46 C	16.1 29.4 19.8 14.6 32.5 20.1
	10	6.3 2.2 25.6 6.6 2.5 24.5		18 CG 18 ND1	16.4 20.2 24.3 11.0 20.5 22.9 16.6 21.5 22.1		33 CE1	5.8 2C.2 25.6 5.7 19.2 26.6 4.4 15.0 27.2	ALA	46 O 47 H 47 CA	14.0 33.0 19.2 15.9 32.5 20.2 16.7 13.2 19.2
GLY	2 N 2 CA	6.8 1.1 26.2 7.6 .1 25.5		18 CE1 18 NE2	17.4 21.4 21.0 18.2 20.4 21.1		33 CZ 33 CZ2	3.3 15.8 26.8 3.5 20.9 26.0		47 CB 47 C	18.0 33.6 19.8 17.3 32.2 18.1
ASP	2 C 2 O 3 N	8.2 .8 24.3 9.4 .8 24.0 7.3 1.3 23.5		18 CD2 18 C 18 O	18.0 19.8 22.3 16.2 20.6 26.7 16.8 20.1 27.6		33 CL2 33 C 33 O	4.8 21.0 25.3 6.5 20.5 22.5 6.6 21.6 22.1	TYR	47 0 48 N 48 CA	18.4 31.8 18.2 16.4 31.9 17.2 16.8 3C.9 16.2
	3 CA 3 CB	7.8 2.0 22.2 6.5 2.3 21.3	THE	19 N 19 CA	14.9 20.8 26.6 14.1 20.4 27.8	GLY	34 N 34 CA	5.6 19.6 22.0 4.7 20.0 20.9		48 CB 48 CG	15.5 30.5 15.4
	3 CG 3 OD1 3 OD2	6.6 1.4 20.1 6.1 .3 20.0 7.0 2.0 19.1		19 CB 19 OG1 19 CG2	13.9 21.6 28.7 12.7 22.3 28.2 15.1 22.5 28.6	VAL	34 C 34 D 35 N	5.5 20.5 19.7 5.1 21.5 19.0 6.6 15.8 19.4		48 CD1 48 CE1	14.6 28.1 15.5 13.8 27.1 16.2
	3 C 3 O	8.5 3.3 22.5 9.7 3.4 22.1		19 C 19 O	12.8 19.9 27.0 12.6 20.4 25.9	***	35 CA 35 CB	7.5 26.2 18.3 8.9 26.1 18.7		48 CZ 48 OH 48 CE2	13.1 27.4 17.3 12.4 26.4 17.9 13.2 28.7 17.9
ALA	4 N 4 CA 4 CB	7.8 4.3 22.9 8.4 5.6 23.2	984	20 N	12.1 19.0 27.5 10.9 18.4 26.9		35 CG1	9.4 18.8 19.3 9.9 25.6 17.6		48 CD2 48 C	14.0 29.7 17.3 17.8 31.5 15.2
	4 0	7.2 6.6 23.6 9.3 5.5 24.4 10.0 6.5 24.8		26 CB 20 CG 20 CD1	11.1 17.0 26.5 12.2 16.7 25.5 13.5 16.5 26.0	PHE	35 C 35 D 36 N	7.3 19.3 17.0 7.5 19.7 15.9 6.9 18.1 17.3	SER	49 N 49 CA	18.2 32.6 15.3 18.2 30.6 14.3 19.2 31.1 13.3
ALA	5 N 5 CA	9.2 4.3 25.0 10.1 4.1 26.2		20 CE1 20 CZ	14.6 16.2 25.1 14.3 16.1 23.8		36 CA 36 CB	6.7 17.1 16.2 5.4 16.3 16.5		49 CB 49 OG	20.3 3C.C 13.1 21.1 29.9 14.3
	5 CB 5 C 5 O	9.8 2.7 26.8 11.5 4.2 25.9 12.3 4.9 26.5		20 C#2 20 CD2 20 C	13.1 16.2 23.3 12.0 16.6 24.2 9.7 18.6 27.7		36 CG 36 CD1 36 CE1	5.3 15.1 15.6 6.3 14.2 15.4 6.3 13.1 14.6	GIU	49 C 49 O 50 N	18.5 31.3 12.0 17.7 30.5 11.5 18.8 32.5 11.4
ATA	6 N 6 CA	11.9 3.5 24.9 13.3 3.4 24.4	ASP	20 O 21 N	8.6 18.1 27.5 9.9 19.4 28.8		36 CZ 36 CE2	5.1 12.7 14.1 4.0 13.5 14.3	310	50 CA 50 CB	18.2 32.8 10.1 19.2 33.5 9.1
	6 CB	13.5 2.4 23.3		21 CB	9.4 19.7 31.2 10.4 18.7 31.4		36 CD2	4.1 14.7 15.1 6.5 17.9 14.9		50 CG 50 CD	18.8 33.6 7.7 19.4 34.9 6.9
GLY	6 0 7 N 7 CA	14.8 5.1 23.6 12.6 5.6 23.5 12.8 6.9 22.9		21 CG 21 OD1 21 OD2	10.4 18.7 31.4 11.5 18.7 31.1 10.0 17.8 32.1	GLU	36 D 37 N 37 CA	7.5 18.1 14.1 5.3 18.2 14.6 4.9 18.9 13.3		50 0E1 50 0E2 50 C	19.6 35.9 7.4 19.6 34.5 5.7 17.6 31.6 9.4
	7 C 7 O	13.4 7.8 23.9 14.3 8.7 23.6		21 C 21 O	8.1 21.0 29.3 8.6 22.0 29.5		37 CB 37 CG	3.7 18.4 12.6 3.7 16.9 12.3	SER	50 0 51 N	16.5 31.5 9.0 18.5 30.6 9.2
GLU	B N B CA B CB	12.9 7.7 25.1 13.4 8.6 26.2 12.4 8.6 27.4	GlN	22 N 22 CA 22 CB	6.9 20.8 28.7 6.2 22.0 28.3 4.8 21.5 28.0		37 CD 37 OE1 37 OE2	2.6 76.0 13.0 1.6 16.5 13.4 3.0 14.8 12.9		5 1 CA 5 1 CB	18.1 29.4 8.5 19.3 28.7 7.9 20.5 28.7 8.8
	8 CG 8 CD	11.7 9.6 27.4		22 CG	3.6 22.7 28.0 2.3 22.3 27.9		37 C 37 O	4.7 2C.4 13.6 3.5 2C.9 13.4		51 06 51 C 51 0	20.5 28.7 8.8 17.5 28.4 9.5 18.0 27.3 9.8
	8 021 8 022	9.7 8.2 26.1 9.9 10.3 25.7		22 OF1	1.9 21.4 28.7 1.6 22.8 27.0	ASH	38 N 38 CA 38 CB	5.7 21.1 13.9 5.6 22.6 14.2	TYR	52 N 52 CA	16.3 28.8 10.0 15.6 28.0 11.0
LYS	8 C 8 0 9 N	14.8 8.3 26.7 15.5 9.2 27.2 15.1 7.0 26.7	GLY	22 C 22 O 23 N	6.2 23.2 29.2 5.6 23.1 30.3 6.9 24.2 28.8		38 CG 38 OD1	6.0 22.9 15.6 5.4 24.2 16.1 5.7 24.8 17.1		52 CB 52 CG 52 CD1	16.3 28.0 12.3 17.1 26.8 12.6 16.4 25.6 13.0
	9 CA 9 CB	16.4 6.5 27.2 16.6 5.0 26.9		23 CA 23 C	7.0 25.4 29.6 8.4 25.5 30.1		38 C	4.3 24.7 15.3 6.6 23.2 13.2		52 CE1 52 CZ	17.2 24.4 13.3 18.5 24.5 13.3
	9 CG 9 CD 9 CE	16.6 4.2 28.2 15.3 4.5 29.0 15.7 4.7 30.5	GLY	23 G 24 N 24 CA	8.9 26.5 30.7 9.1 24.4 29.9 10.5 24.3 30.4	THR	38 O 39 N 39 CA	7.4 22.5 12.5 6.5 24.5 13.1 7.4 25.3 12.1		52 CE2 52 CE2	19.3 23.4 13.6 19.2 25.6 12.9 18.5 26.8 12.6
	9 N Z 9 C	14.7 4.0 31.4 17.4 7.4 26.3		24 C 24 O	11.4 25.5 29.8 10.9 26.2 28.9		39 CB 39 OG1	7.2 26.8 12.4 5.7 26.9 12.6		52 C 52 C	14.2 28.6 10.9 13.2 28.0 10.7
VAL	9 0 10 N 10 CA	18.2 8.1 26.9 17.1 7.4 25.0 18.0 8.1 24.1	ALA	25 N 25 CA	12.5 25.7 30.5 13.4 26.8 30.1		39 CG2 39 C	7.6 27.6 11.2 8.8 24.9 12.3	THR	53 N 53 CA	14.2 3C.C 10.9 12.9 3C.7 10.9
	10 CB 10 CG1	18.0 8.1 24.1 17.6 7.8 22.6 18.8 7.2 21.8		25 CB 25 C 25 O	14.6 26.8 31.0 13.9 26.4 28.7 13.6 25.4 28.1	ALA	39 0 40 K 40 CA	9.2 24.0 13.2 9.7 25.4 11.5 11.1 25.1 11.6		53 CB 53 OG1 53 CG2	13.1 32.0 11.8 12.7 33.0 10.9 14.5 32.1 12.3
	10 CG2 10 C	16.4 7.0 22.6 17.9 9.7 24.3	AS N	26 N 26 CA	14.6 27.3 28.1 15.3 27.1 26.8		40 CB 40 C	11.8 25.6 10.3 11.7 25.9 12.7		53 C 53 O	12.6 31.1 9.4
SER	10 0 11 H 11 CR	18.9 10.4 24.2 16.6 10.1 24.6 16.4 11.5 24.8		26 CB 26 CG 26 OE1	15.3 28.4 26.0 14.0 28.6 25.3 13.1 27.8 25.2	ALA	40 O 43 N 41 CA	12.7 25.5 13.3 11.1 27.1 13.0	G LU	54 N 54 CA 54 CB	12.5 30.2 8.6 12.2 30.4 7.2 13.1 30.1 6.2
	11 CB 11 OG	14.9 11.8 25.2 14.8 12.7 26.3		26 ND2 26 C	13.7 29.9 24.9 16.8 26.6 26.9		41 CB 41 C	11.6 27.9 14.1 11.5 29.4 13.7 10.5 27.8 15.2		54 CG 54 CD	14.8 3C.3 6.8 15.7 31.1 5.8
• • •	11 C	17.3 12.1 25.9 17.5 13.3 25.9	LYS	26 O 27 K	17.0 25.4 26.6 17.6 27.4 27.4	HIS	41 O	9.9 28.7 15.7 10.3 26.5 15.6		54 OB1	15.4 32.0 5.1 16.8 30.5 5.8
LYS	12 N 12 CA 12 CB	17.8 11.2 26.7 18.7 11.6 27.8 19.2 10.4 28.6		27 CA 27 CB 27 CG	19.0 27.1 27.6 19.2 26.0 28.7 18.0 25.9 29.6		42 CA 42 CB 42 CG	9.4 26.2 16.7 10.0 25.3 17.7 9.1 24.5 18.6	net	54 C 54 O 55 N	10.9 29.5 6.9 10.0 29.9 6.2 11.0 28.4 7.5
	12 CG 12 CD	18.6 10.2 29.9 18.4 8.8 30.2		27 CB 27 CE 27 N2	17.5 24.4 30.1 18.6 23.5 29.3		42 ND1	9.5 13.9 19.8 8.5 23.3 20.3		55 CA 55 CB	9.9 27.4 7.3 9.5 26.8 8.7
	12 CE 12 NZ 12 C	16.9 8.5 30.6 16.8 7.7 31.8 19.8 12.4 27.1		27 C 27 C	19.1 27.3 30.1 19.7 26.4 26.4 19.4 25.3 26.0		42 HE2 42 CD2 42 C	7.4 23.6 19.6 7.8 24.3 18.5 8.8 27.5 17.4		55 CG 55 SD 55 CE	8.8 27.8 9.6 9.9 29.2 9.9 9.0 29.9 11.J
LYS	12 O 13 N	20.3 13.5 27.6 20.2 12.0 26.0	VAL	28 N 28 CA	20.6 27.2 25.7 21.3 26.7 24.5	175	42 O 43 N	8.3 28.4 16.7 8.9 27.5 18.7		55 C 55 O	8.6 28.0 6.7 7.7 27.3 6.2
	13 CA 13 CB 13 CG	21.3 12.6 25.2 21.8 11.8 24.1 22.6 10.6 24.5		28 CB 28 CG1 28 CG2	22.0 25.4 24.8 23.0 25.0 23.8 22.5 25.4 26.2		43 CA 43 CB 43 CG	8.4 28.6 19.5 8.4 28.3 20.9 8.9 26.9 21.3	LYS	56 N 56 CA 56 CB	8.6 29.3 6.7 7.4 30.0 6.1 7.4 31.5 6.5
	13 CD 13 CE	23.1 9.8 23.3 22.2 8.6 23.0		28 C 28 D	20.2 26.6 23.4 19.9 27.5 22.7		43 CE	8.4 26.5 22.7 7,7 25.1 22.6		56 CG 56 CD	8.7 32.1 6.8 8.7 33.1 7.9
	13 H Z 13 C 13 D	22.3 7.6 24.2 21.0 14.0 24.6 21.9 14.5 23.9	GLY	29 N 29 CA 29 C	19.6 25.4 23.4		43 NZ 43 C	6.2 25.4 22.3 9.1 29.9 19.4		56 CB 56 NZ	10.0 33.9 8.1
CYS	14 B 14 CA	19.8 14.5 24.8 19.5 15.8 24.2	PRC	29 O 30 N	17.1 25.3 22.9 16.9 25.2 24.1 16.2 25.5 22.0	ASP	43 0 44 K 44 Ck	10.4 3C.0 19.4 8.4 31.0 19.3 8.9 32.3 19.3	ALA	56 C 56 O 57 P	7.6 29.9 4.6 6.7 29.6 3.8 8.8 30.2 4.1
	14 CB 14 SG 14 C	18.0 15.5 24.2 17.4 14.5 22.7 19.3 16.9 25.3		30 CA	14.6 25.6 22.3 14.1 25.8 21.0		44 CB	7.9 33.3 18.8 6.5 32.7 18.6		57 CB	9.1 30.1 2.7
LEG	14 0 15 N	19.5 18.1 25.0 18.9 16.5 26.5		30 CG 30 CD 30 C	15.2 25.8 19.9 16.3 25.0 20.6 14.3 24.3 22.9		44 0D2 44 CD2	6.3 32.0 17.6 5.8 32.8 19.5 9.6 33.1 20.4	LYS	57 C 57 O 58 N	9.5 28.6 2.7 10.5 28.2 3.2 8.6 27.9 2.1
	15 CA 15 CB	18.7 17.5 27.6 17.9 16.8 28.7	ASN	30 O 31 N	14.8 23.2 72.6 13.1 24.4 23.6	ASN	44 O 45 N	9.7 34.4 20.4	•	58 CA 58 CB	8.8 26.4 2.1 10.2 26.0 2.4
	15 CG 15 CD1 15 CD2	18.2 15.3 29.0 19.6 15.2 29.6 17.2 14.8 30.0		31 CB 31 CB 31 CG	12.5 23.2 24.2 11.9 23.6 25.6 10.7 24.5 25.4		45 CA 45 CB 45 CG	10.6 33.0 22.6 9.9 32.5 23.9 10.2 31.1 24.2		58 CG 58 CD 58 CE	11.2 27.0 1.8 12.6 26.2 1.7 13.1 26.4 .3
	15 C 15 O	20.1 17.9 28.0 20.9 17.0 28.5		31 OD1	10.8 25.7 25.3 9.5 23.9 25.2		45 0D1 45 MD2	10.8 3C.6 25.1 9.6 3C.2 23.3		58 NZ 58 C	14.4 25.6 .1 7.8 25.7 3.0
ALA	16 H 16 CA 16 CB	20.4 19.1 27.7 21.8 19.6 28.0 23.0 18.9 27.5	LEO	31 C 31 D 32 N	11.5 22.7 23.2 10.6 23.4 22.8	T IR	45 C 45 Q 46 N	12.1 32.6 22.6 12.8 32.7 23.6	GLT	58 0 59 N 59 CA	7.2 24.7 2.7 7.8 26.2 4.3 6.9 25.6 5.3
	16 C 16 D	21.6 20.9 27.2 22.1 22.0 27.5	-40	32 CA 32 CB	11.6 21.4 22.9 10.7 20.8 21.9 11.4 19.9 20.9	1 18	46 CB	13.9 31.7 21.3 14.0 30.2 21.0		59 C 59 O	7.6 24.5 6.1 7.0 23.9 6.9
CYS	17 H 17 CA	20.9 20.7 26.1 20.6 21.8 25.1		32 CG 32 CD1	12.6 19.1 21.4 13.2 18.3 20.3		46 CG 46 CD1	15.4 29.6 21.0 16.0 29.4 22.3	LEU	60 W	8.9 24.4 5.B 9.7 23.3 6.4

Table I (continued)

					, ,	DIC	T (COLICII	iueu				
		х у	z		x y	z			, X , ,)	/ Z			x y z
LEO	60 CB 60 CG	11.1 23.9 12.2 22.9	6.8 AS	N 73 OD1 73 ND2	26.8 15.3 26.4 17.3	8.2 9.0	ALA	87 C 87 O	24.7 27. 25.6 27.	9 7.4	G LU	100 OE1	15.9 10.2 13.2 17.1 10.2 11.4
	60 CD1	12.0 22.2	8.4	73 C	23.0 17.1	10.1	LYS	98 N	24.5 28.	4 8.7		100 C	16.0 7.9 15.2
	60 CD2	12.2 21.8 8.8 23.0	5.9 7.6 PR	730 0 74 N	22.2 17.5 23.0 17.8	9.1 11.2		88 CA 88 CB	25.5 28. 26.4 29.		ILE	100 O	15.2 8.6 15.7 15.7 6.7 14.6
	60 0	8.4 23.6	8.4	74 CA	22.2 19.0	11.5		88 CG	25.9 30.	3 10.9		101 CA	14.3 6.2 14.6
THR	61 N 61 CA	0.6 21.7 7.8 21.2	7.8 8.9	74 CB 74 CG	21.9 18.9	12.9		88 CE	26.9 30. 26.3 31.			101 CB 101 CG1	14.3 4.8 14.1 15.5 4.3 13.3
	61 CB	6.3 21.1	8.4	74 CD	24.0 18.1	12.2		88 NZ	25.1 31.	3 13.5		101 CG2	12.9 4.8 13.3
	61 0G1 61 CG2		9.4	74 C 74 O	22.4 20.1 21.4 20.6	9.9		88 C	24.6 27. 23.7 28.	7 11.0		101 CD1	15.2 3.5 12.0
	61 C	8.4 19.8	8.3 9.3 LY		23.6 20.4	10.1	SER	89 N	24.7 26.	5 11.5		101 C 101 O	13.6 6.3 15.9 12.4 6.7 16.0
	610		8.5	75 CA	23.9 21.4	9.1		89 CA	24.0 26.	1 12.7	G LU		14.3 5.9 16.9
TRP	62 N 62 CA	8.4 19.5 1 8.9 18.3 1	1.1	75 CB 75 CG	25.4 21.7 26.3 20.8	9.1		89 CB 89 OG	23.0 25. 22.9 24.			102 CA 102 CB	13.8 5.9 18.3 14.7 5.2 19.3
	62 CB	9_4 18_5 1	2.6	75 CD	27.7 21.3			89 C	24.8 25.	7 13.9		162 CG	14.1 4.3 20.4
	62 CG 62 CD1	10.4 19.7 1		75 CE 75 NZ	27. E 22.1 26.5 21.9	11.4	1.75	89 O 90 N	25.9 25. 24.3 25.			102 CD 102 OB1	14.4 2.8 20.2 15.5 2.3 20.3
	62 NE1	11.3 21.7 1	13.4	75 C	23.5 21.0	7.7		90 CA	25.0 25.	5 16.3		102 OE 2	13.3 2.2 20.0
	62 CE2		2.8 2.6 AI	75 O a 76 N	23.3 21.8 23.3 19.7	6.8 7.6		90 CB	25.0 26. 25.7 27.	7 17.3 9 16.8		102 C 102 O	13.4 7.2 18.9 12.3 7.4 19.5
	62 CH2	14.3 20.6 1	2.0	76 C&	22.8 19.1	6.3		90 CD	24.9 29.	2 17.2	ASM	103 W	14.3 8.2 18.7
	62 CZ3		1.5	76 CB 76 C	23.4 17.7 21.3 19.0	6.0 6.4		90 CE 90 NZ	23.4 29.			103 CA	14.0 9.5 19.3
	62 CD2	11.7 19.8 1	2.4	76 C	20.8 18.2	7.2		90 C	22.7 30.	4 17.1		103 CB 103 CG	15.3 10.4 19.0 16.4 10.1 19.9
	62 C		11.1 PH		20.6 19.7	5. 5	HET	90 0	24.0 24.	5 18.3		103 OD1	16.4 9.2 20.7
THR	62 O 63 N		0.0	77 CB	19.1 19.7 18.7 18.8	5.5 6.7	HET	91 H 91 CA	24.7 23. 24.3 21.	9 17.3		103 ND2 103 C	17.6 10.9 19.6 12.8 10.1 18.6
	63 CA		9.8	77 CG	17.3 19.2	7.3		91 CB	22.8 21.	7 17.0		103 0	11.8 10.5 19.4
	63 CB 63 OG1		8.3 7.7	77 CD1 77 CE1	17.2 20.4 16.0 20.8	7.9 8.5		91 CG 91 SD	22.4 20. 20.6 2C.			104 N 104 CA	12.7 10.1 17.3 11.6 10.6 16.6
	63 CG2	5.9 16.4	7.7	77 CZ	14.9 20.0	8.3		91 CE	20.6 18.	2 17.2		164 CB	11.7 10.4 15.1
	63 C 63 O		0.4	77 CE2	15.0 18.9 16.2 18.4	7.6		91 C 91 O	25.1 20. 26.3 20.			104 CG1 104 CG2	10.4 10.7 14.3
GLU	64 N	8.6 14.1 1	0.9	77 C	16.9 21.2	5.7	THR	92 N	24.4 19.	8 16.1		104 C	10.3 10.0 17.1
	64 CA 64 CB	9.2 12.9 1	11.4 11.7 VA	77 O L 78 N	17.9 21.7 19.9 21.9	5.2 6.2		92 CA 92 CB	25.1 18. 26.4 19.	6 15.6	***	104 0	9.2 10.7 17.2
	64 CG	8.6 10.4 1	12.1	78 CA	19.6 23.3	6.4		92 OG1	27.4 18.	7 15.9	112	105 N 105 CA	10.3 8.8 17.5 9.1 8.1 18.0
	64 CB		1.8	76 CB 78 CG1	20.4 23.7	7.7		92 CG2	26.5 2C.	6 14.6		105 CB 105 CG1	9.3 6.5 18.0
	64 DE2	8.0 8.3 1	2.6	78 CG2	19.5 23.6	8.9		92 D	25.2 17.	6 16.7 9 17.9		105 CG2	8.7 5.8 15.8 8.8 6.2 19.4
	64 C	10.3 12.4 1	0.5	78 C 78 O	20.5 24.0	5.2	PHE			4 16.3		105 CD1	9.1 6.3 15.4
ALA	64 O 65 N	11.4 11.9 1 9.9 12.4	9.2 LE	U 79 N	20.9 25.2 20.6 23.3	5.3 4.1		93 CA 93 CB	25.8 15. 25.5 15.	3 17.2 8 18.6		105 C 105 O	8.6 8.6 19.4 7.6 8.5 19.8
	65 CA	10.9 11.9	8.1	79 CA	21.2 23.8	2.9		93 CG	24.3 15.	2 19.3	ALA	106 N	9.8 9.0 20.0
	65 CB 65 C	10.1 11.7 11.9 13.0	6.8 7.9	79 CB 79 CG	22.6 23.3 23.6 23.6	2.8 3.9		93 CB1	23.1 15. 22.0 15.	9 19.3 5 19.9		106 CA 106 CB	9.7 9.5 21.4
	65 0	13.0 12.8	7.5	79 CD1	24.3 22.4	4.4		93 CZ	21.9 14.	2 20 . 4		106 C	8.6 10.6 21.5
AS H	66 R		8.2 8.1	79 CD2 79 C	24.6 24.6 20.1 23.2	3.3 2.0		93 CE2 93 CD2	23.0 13. 24.3 14.	5 20.4 C 19.8	TYR	106 O	7.4 10.3 21.6 9.1 11.9 21.4
	66 CB	11.4 16.7	7.8	79 0	19.5 23.9	1.1		93 C	24.8 14.	2 16.7		107 CA	8.1 13.0 21.5
	66 CG 66 OD1	11.6 17.2 12.4 16.9	6.4 GI 5.6	U 80 N 80 CA	19.9 21.9 18.9 21.2	2.2 1.3	LYS	93 O 94 N	23.6 14. 25.2 13.	2 17.2 4 15.8		107 CB 107 CG	8.9 14.3 21.5 10.1 14.4 20.5
	66 MD2	10.5 18.0	6.0	80 CB	16.7 19.7	1.8		94 CA	24.4 12.	4 15.2		107 CD1	9.7 14.3 19.1
	66 C 66 O		9.3	80 CG	19.7 18.7	1.3		94 CB 94 CG		5 14.3		107 CE1 107 CZ	10.7 14.4 18.1
LEU	67 N		9.2	80 CD 80 OZ1	19.2 17.2 18.4 16.8	1.3		94 CD	26.6 11. 27.5 12.	4 14.4		107 OH	12.0 14.4 18.5 13.0 14.4 17.5
	67 CA 67 CB		1.6	80 022	19.8 16.6	2.2		94 CE 94 NZ	28.9 12.	0 14.7		107 CE2	12.4 14.4 19.8
	67 CG	12.7 14.8 1	2.7	80 C	17.6 22.0	1.5		94 C	29,3 12,	5 16.0 3 15.9		107 CD2	11.4 14.4 20.8 7.2 13.1 20.3
	67 CB1	10.5 15.1 1			17.0 21.9	2.7		94 0	23.0 11.	6 17.0		107 0	6.0 13.4 20.4
	67 CD2	10.8 16.0 1	11.5	81 CE 81 CB	15.8 22.6 15.0 21.9	3.0 4.0	1.20	95 N 95 Ca		1 15.4	LEU	108 M 108 CA	7.7 12.7 19.1 6.9 12.7 17.9
	67 0	15.9 14.5 1	11.9	81 CG	15.2 20.4	W_ 1		95 CB	21.4 9.	5 16.5		108 CB	7.4 11.7 16.9
ALA	68 M 68 CA	14.5 13.1 1 15.6 12.0 1	0.9	81 CE	14.2 19.7	3.3		95 CG 95 CD1	21.4 1C. 20.0 1C.	5 17.6 9 18.1		108 CG 108 CD1	6.8 10.3 16.9 7.8 9.3 17.4
	68 CB	15.0 10.8 1	0.0	81 WZ	13.3 17.4	3.0		95 CD2	22.2 10.	0 18.8		108 CD2	5.6 10.3 17.7
	68 C 68 O	16.7 12.6 17.9 12.3 1	9.9	81 C 81 O	16.0 24.1 15.5 24.5	3. 5 4. 6		95 C 95 O	22.5 7. 21.7 8.	9 15.0 1 14.0		108 C 108 O	5.4 12.4 18.1 4.6 12.5 17.2
ALA	69 N	16.3 13.3	8.9 SE	3 85 N	16. 8 24.9	2.7	THR	96 N	23.0 6.	7 15.2	LYS	109 N	5.1 12.1 19.4
	69 CA 69 CB	17.3 13.9 16.6 14.6	7.9 6.8	82 CA 82 CB	17.0 26.3 17.8 26.3	3. 1 4. 4		96 CA 96 CB	22.9 5. 23.7 4.			109 CA 109 CB	3.7 11.8 19.8 3.3 10.4 19.3
	69 C	18.1 14.9	8.7	82 OG	18.7 27.4	4.4		96 061	23.6 4.	5 16.4		109 CS	2.1 9.8 20.0
TYR	69 0 70 N	19.3 15.1 17.3 15.7	8.6 9.5	82 C 82 O	17.8 26.9 18.1 26.3	2.0		96 CG2 96 C	25.2 4. 21.4 5.	6 14.6 2 14.3		109 CD 109 CE	2.1 8.3 20.0 .8 7.8 19.3
	70 CA	18.0 16.8 1	10.2 G1	и 63 г.	16.C 28.2	2.1		96 O	20.6 5.	7 15.1		109 NZ	.7 6.3 19.4
	70 CB		11.0	83 CA 83 C	18.7 29.0	1.1	LYS	97 N 97 CA	21.0 4. 19.6 3.	4 13.3		109 C 109 O	3.4 11.9 21.3 2.2 12.2 21.6
	70 CD1	18.0 19.7 1	11.5	83 0	21.1 29.4	.8		97 CB	19.6 2.		THR	110 N	4.4 11.6 22.1
	70 C21 70 C2	18.6 20.7 1 18.6 20.4 1		P 84 N 84 CA	20.5 28.0 21.8 27.7	2. 5		97 CG 97 CD	20.1 2.	7 11.0		110 CA	4.2 11.7 23.5
	70 CZ	19.1 21.3 1	14.7	84 CB	22.3 26.4	2.4		97 CE	19.4 4.	2 9.1		110 CB 110 OG1	5.2 10.7 24.2 6.4 11.5 24.0
	70 CE2	17.9 19.3 1	14.3	84 CG 84 OD1	22.6 26.4	.9		97 NZ 97 C	18.7 5.	6 8.9		110 CG2	5.3 9.4 23.5
	70 CD2 70 C	19.0 16.3 1	11. 1	84 OD 2	22.6 27.4 23.0 25.4	. 2		97 C 97 O	18.8 3. 17.6 4.	1 14.4		110 C 110 O	4.3 13.1 23.9 3.5 13.7 24.7
	70 0	20.1 16.9 1		84 C	22.8 28.8	2. 4	AS P	98 X	19.4 3.	0 15.4	LBU	111 N	5.3 13.8 23.4
VAL	71 N 71 CA	18.8 15.1 1	12.7 PF	84 C C 85 N	23.6 28.6 22.5 3C.0	1.5		98 CA 98 CB	18.6 2. 19.6 2.	7 16.6 0 17.6		111 CA 111 CB	5.6 15.2 23.7 7.1 15.5 23.5
	71 CB	19.1 13.2 1	3.3	85 CA	23.4 31.2	2.4		98 CG	19.0 2.	0 19.0		111 CG	7.9 15.4 24.8
	71 CG1 71 CG2	20.2 12.1 1 18.3 13.5 1	14.5	85 CB 85 CG	22.6 32.4	3.0 4.0		98 OD 1 98 OD 2	18.6 . 18.9 3.	9 19.5 0 19.6		111 CD1 111 CD2	7.2 14.6 25.9 9.2 14.6 24.4
	71 C	21.0 14.2 1	11.9	85 CD	21.4 30.4	3. 6		98 C	18.1 4.	0 17.1		111 C	4.7 15.9 22.6
LYS	71 D 72 N	21.7 15.1 1	11.9	85 C 85 O	24. 6 31.0 25. 6 31.9	3.0 3.0	ASP	98 O 99 N	16.9 4. 18.9 4.	3 16.9 B 17.7	t ve	111 0 112 N	5.1 16.2 21.5 3.4 16.1 23.0
	72 CA	22.7 12.6 1	11.3 LY	S 86 K	25.0 29.7	3. 4	232	99 CA	18.5 6.	1 18.2	213	112 CA	2.5 16.8 22.1
	72 CB 72 CG	21.5 10.6 1	9.9 10.0	86 CB	26.3 29.4 27.3 30.6	4.0		99 CB	19.7 7. 20.5 6.	0 18.6		112 CB 112 CG	2.3 16.0 20.8 3.3 16.5 19.7
	72 CD	22.2 9.5	9.2	86 CG	26.2 30.6	5.2		99 OD1	20.3 5.	2 20.1		112 CD	2.9 18.0 19.3
	72 CE 72 N2	21.5 8.2	9.5 9.8	86 CD	28.7 32.0	5. 5		99 OD 2	21.5 6.	9 20.0		112 CE 112 NZ	1.6 18.0 18.4
	72 C	23.5 13.8 1	11.1	86 CE 86 N2	28.7 32.3 29.1 33.7	7.0		99 C 99 O	16.4 7.	9 17.3 1 17.5		112 C	1.2 16.6 18.0 1.2 16.8 22.9
151	72 O 73 H	24.6 13.9 1 23.1 14.7 1	0.2	86 C	25.7 28.9	5.3	C TO	100 W	18.2 7.	4 16.2		112 0 112 02	1.1 16.8 24.1 .1 16.9 22.1
	73 CA	23.9 15.9 1	0.0 AL	86 O A B7 N	26.4 28.6 24.4 28.8	6.3 5.3		100 CA 100 CB	18.1 0.	2 15.2 0 13.8			10.7 22.1
	73 CB 73 CG	24.5 15.8	8.5 8.6	87 CA	23.6 28.4	6.4		100 CG	17.1 8.	2 12.6			
		10 - 1	~. 4	87 CB	22.8 27.2	6.1		100 CD	16.6 9.	7 12.4			

1 16, 4	ERE 2C1 2.1.1 18.6 2.1.1 HERE 3CR 21.8 25.2 19.4 HERE 4CR 15.6 21.6 17.2 2.2 2.2 2.2.4 15.0 21.8 3CR 21.8 25.2 19.4 HERE 4CR 18.0 21.8 3CR 21.8 25.2 19.6 28.4 HERE 4CR 18.0 19.7 16.9 2.2 2.2 2.2.4 15.0 21.8 3CR 21.8 25.7 17.7 4CR 21.8 15.3 20.3 17.4 2.2 2.2 22.8 22.8 22.8 22.8 22.8 22.8
φψ φψ φψ φψ φ ψ GLU 1 0 125 GLY 24 -52 164 ALA 47 -98 78 TYR 70 -57 -42 PHE	
GLU 1 0 125 GLY 24 -52 164 ALA 47 -98 78 TYR 70 -57 -42 PHE	Table II
ALD ALD	-52 144 ALA 47 -98 78 TYR 70 -57 -42 PRE 93 126 87 -69 179 TYR 48 -65 177 VAL 71 58 -122 LTS 94 -52 -114 155 0 109 GLU 50 -20 -54 ASM 73 -130 97 THR 96 -60 116 115 66 -89 SYR 51 -84 65 PRO 74 -54 -99 LTS 97 -88 -44 156 66 -89 SYR 51 -84 65 PRO 74 -54 -99 LTS 97 -88 -44 156 66 -89 SYR 51 -84 65 PRO 74 -54 -99 LTS 97 -38 -44 156 66 -89 SYR 53 -90 55 ALA 76 -97 117 ASP 98 -51 -79 -79 126 GLU 50 TYR 57 -88 175 75 -66 -19 ASP 98 -51 -79 -92 126 GLU 54 -124 -36 PRE 77 128 -26 GLU 100 -25 -76 -91 17 ASP 99 -44 -72 -92 126 GLU 54 -724 -36 PRE 77 128 -26 GLU 100 -25 -76 -91 17 ASP 99 -44 -72 -91 17 ASP 99 -91

The coordinates listed here derive from an intermediate stage of the crystallographic refinement including all 904 atoms of the protein molecule plus 120 water molecules (not listed). These coordinates (Table I) have been fitted to standard groups by a version of R. Diamond's model building program (9), and yield a structure with a crystallographic R factor

$$R = \frac{\Sigma ||F_0| - |F_C||}{\Sigma |F_0|} = 44.5\%$$

The coordinates in Table I are given in Angstrom units in a right-handed Cartesian system for convenience in model building. They may be converted to orthorhombic fractional crystallographic coordinates by the following transformation:

$$X_{cryst} = (310X + 6214)10^{-4}$$
 $Y_{cryst} = (268Y + 4781)10^{-4}$
 $Z_{cryst} = (118Z + 1972)10^{-4}$

where X, Y, and Z are the Cartesian coordinates given in Table I. Cytochrome \underline{c}_2 crystallized in space group $P2_1^2_1^2_1$ with a = 32.3, b = 37.4, and c = 84.6 Å. Table II gives the interpeptide dihedral angles, ϕ and ψ , according to

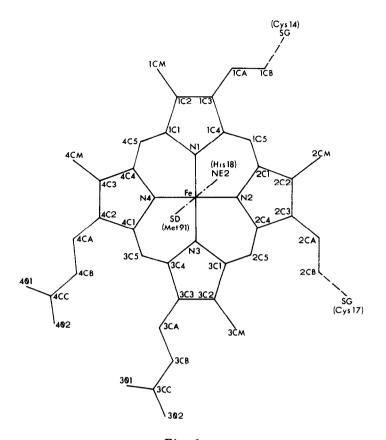


Fig. 1.

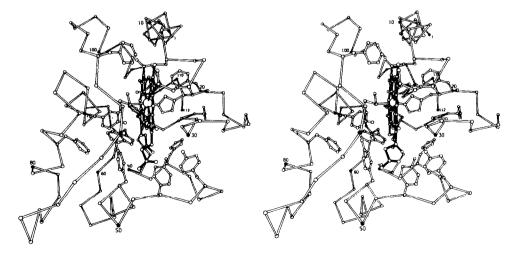


Fig. 2.

the IUPAC-IUB convention (10). Fig. 1 shows the convention for labeling atoms of the protoheme IX ring. Fig. 2 is a stereo drawing of the compolecule showing α -carbon positions, heme ligands, and aromatic residues.

This work was supported by research grants from the National Institutes of Health (GM 10928, GM 16717) and the National Science Foundation (GB 15684, GB 23054, GB 30828X) and by Public Health Service Research Career Development Awards to S.T.F. and R.A.A. from the National Institute of General Medical Sciences (GM 70-140, GM 15401).

REFERENCES

- 1. Salemme, F. R., Freer, S. T., Alden, R. A., Xuong, Ng. H., and Kraut, J. (1973) J. Biol. Chem. 248, 3910.
- Dickerson, R. E. (1972) Sci. Amer. 226, No. 4, 58-67.
 Timkovich, R., and Dickerson, R. E. (1973) J. Biol. Chem., in press.
- 4. Salemme, F. R., Kraut, J., and Kamen, M. D. (1973) J. Biol. Chem., submitted for publication.
- 5. Countryman, R., Collins, D. M., and Hoard, J. L. (1969) J. Am. Chem. Soc. 91, 5166-5167.
- 6. Salemme, F. R., and Fehr, D. G. (1972) J. Mol. Biol. 70, 697-700.
- 7. Richards, F. M. (1968) J. Mol. Biol. 37, 225-229.
- 8. Freer, S. T., Alden, R. A., Salemme, F. R., and Kraut, J. (1973) in preparation.
- 9. Diamond, R. (1966) Acta Cryst. 21, 253-259.
- 10. IUPAC-IUB Commission on Biochemical Nomenclature (1970) Biochemistry 9, 3471-3475.