ATOMIC COORDINATES FOR FERRICYTOCHROME c_2 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

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Summary: Atomic coordinates and backbone torsion angles are tabulated for ferricytochrome c_2 of Rhodospirillum rubrum.

The three-dimensional structure of ferricytochrome 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 c (2-4).

Cytochrome 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 Nε2 nitrogen atom of histidine 18 and the Sδ 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 Sδ 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 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 Å 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).

Table I

			x	y	z
GLU	1	N	6.0	4.4	26.5
	1	CA	5.4	3.1	26.5
	1	CB	4.0	3.0	25.9
	1	CG	3.7	4.2	24.9
	1	CD	3.7	3.8	23.4
	1	OE1	4.7	3.3	22.9
	1	OE2	2.7	4.2	22.9
	1	C	6.3	2.2	25.6
	1	O	6.6	2.5	24.5
GLY	2	N	6.8	1.1	26.2
	2	CA	7.6	.1	25.5
	2	C	8.2	.8	24.3
	2	O	9.4	.8	24.0
ASP	3	N	7.3	1.3	23.5
	3	CA	7.8	2.0	22.2
	3	CB	6.5	2.3	21.3
	3	CG	6.6	1.4	20.1
	3	OD1	6.1	.3	20.0
	3	OD2	7.0	2.0	19.1
	3	C	8.5	3.3	22.5
	3	O	9.7	3.4	22.3
ALA	4	N	7.8	4.3	22.9
	4	CA	8.4	5.6	23.2
	4	CB	7.2	6.6	23.6
	4	C	9.3	5.5	24.4
	4	O	10.0	6.5	24.8
ALA	5	N	9.2	4.3	25.0
	5	CA	10.1	4.1	26.2
	5	CB	9.8	2.7	26.8
	5	C	11.5	4.2	25.9
	5	O	12.3	4.9	26.5
ALA	6	N	11.9	3.5	24.9
	6	CA	13.3	3.4	24.4
	6	CB	13.5	2.4	23.3
	6	C	13.7	4.8	23.8
	6	O	14.8	5.1	23.6
GLY	7	N	12.6	5.6	23.5
	7	CA	12.8	6.9	22.9
	7	C	13.4	7.8	23.9
	7	O	14.3	8.7	23.6
GLU	8	N	12.9	7.7	25.1
	8	CA	13.4	8.6	26.2
	8	CB	12.4	8.6	27.4
	8	CG	11.2	9.6	27.4
	8	CD	10.2	9.3	26.3
	8	OE1	9.7	8.2	26.1
	8	OE2	9.9	10.3	25.7
	8	C	14.8	8.3	26.7
	8	O	15.5	9.2	27.2
LYS	9	N	15.1	7.0	26.7
	9	CA	16.4	6.5	27.2
	9	CB	16.6	5.0	26.9
	9	CG	16.6	4.2	28.2
	9	CD	15.3	4.5	29.0
	9	CE	15.7	4.7	30.5
	9	NZ	14.7	4.0	31.4
	9	C	17.4	7.4	26.3
	9	O	18.2	8.1	26.9
VAL	10	N	17.1	7.4	25.0
	10	CA	18.0	8.1	24.1
	10	CB	17.6	7.8	22.6
	10	CG1	18.8	7.2	21.8
	10	CG2	16.4	7.0	22.6
	10	C	17.9	9.7	24.3
	10	O	18.9	10.4	24.2
SER	11	N	16.6	10.1	24.6
	11	CA	16.4	11.5	24.8
	11	CB	14.9	11.8	25.2
	11	OG	14.8	12.7	26.3
	11	C	17.3	12.1	25.9
	11	O	17.5	13.3	25.9
LYS	12	N	17.8	11.2	26.7
	12	CA	18.7	11.6	27.8
	12	CB	19.2	10.4	28.6
	12	CG	18.6	10.2	29.9
	12	CD	18.4	8.8	30.2
	12	CE	16.9	8.5	30.6
	12	NZ	16.8	7.7	31.8
	12	C	19.8	12.4	27.1
	12	O	20.3	13.5	27.6
LYS	13	N	20.2	12.0	26.0
	13	CA	21.3	12.6	25.2
	13	CB	21.8	11.8	24.1
	13	CG	22.6	10.6	24.5
	13	CD	23.1	9.8	23.3
	13	CE	22.2	8.6	23.0
	13	NZ	22.3	7.6	24.2
	13	C	21.0	14.0	24.6
	13	O	21.9	14.5	23.9
CYS	14	N	19.8	14.5	24.8
	14	CA	19.5	15.8	24.2
	14	CB	18.0	15.5	24.2
	14	SG	17.4	14.5	22.7
	14	C	19.3	16.9	25.3
	14	O	19.5	18.1	25.0
LEU	15	N	18.9	16.5	26.5
	15	CA	18.7	17.5	27.6
	15	CB	17.9	16.8	28.7
	15	CG	18.2	15.3	29.0
	15	CD1	19.6	15.2	29.6
	15	CD2	17.2	14.8	30.0
	15	C	20.1	17.9	28.0
	15	O	20.9	17.0	28.5
ALA	16	N	20.4	19.1	27.7
	16	CA	21.8	19.6	28.0
	16	CB	23.0	18.9	27.5
	16	C	21.6	20.9	27.2
	16	O	22.1	22.0	27.5
CYS	17	N	20.9	20.7	26.1
	17	CA	20.6	21.8	25.1
	17	CB	21.4	21.4	23.9
	17	SG	23.2	21.5	23.9
	17	C	19.1	22.0	25.2
	17	O	18.7	23.2	25.0
HIS	18	N	18.4	20.9	25.4
	18	CA	16.9	21.0	25.4
	18	CB	16.4	20.2	24.3
	18	CG	17.0	20.5	22.9
	18	ND1	16.6	21.5	22.1
	18	CE1	17.4	21.4	21.0
	18	NE2	18.2	20.4	21.1
	18	CD2	18.0	19.8	22.3
	18	C	16.2	20.6	26.7
	18	O	16.8	20.1	27.8
THR	19	N	14.9	20.8	26.6
	19	CA	14.1	20.4	27.8
	19	CB	13.9	21.6	28.7
	19	OG1	12.7	22.3	28.2
	19	CG2	15.1	22.5	28.6
	19	C	12.8	19.9	27.0
	19	O	12.6	20.4	25.9
PHE	20	N	12.1	19.0	27.5
	20	CA	10.9	18.4	26.9
	20	CB	11.1	17.0	26.5
	20	CG	12.2	16.7	25.5
	20	CD1	13.5	16.5	26.0
	20	CE1	14.6	16.2	25.1
	20	CZ	14.3	16.1	23.8
	20	CE2	13.1	16.2	23.3
	20	CD2	12.0	16.6	24.2
	20	C	9.7	18.6	27.7
	20	O	8.6	18.1	27.5
ASP	21	N	9.9	19.4	28.8
	21	CA	8.6	19.6	29.7
	21	CB	9.4	19.7	31.2
	21	CG	10.4	18.7	31.8
	21	OD1	11.5	18.7	31.1
	21	OD2	10.0	17.8	32.1
	21	C	8.1	21.0	29.3
	21	O	8.6	22.0	29.5
GLN	22	N	6.9	20.8	28.7
	22	CA	6.2	22.0	28.3
	22	CB	4.8	21.5	28.0
	22	CG	3.8	22.7	28.0
	22	CD	2.3	22.3	27.9
	22	OE1	1.9	21.4	28.7
	22	NE2	1.6	22.8	27.0
	22	C	6.2	23.2	29.2
	22	O	5.6	23.1	30.3
GLY	23	N	6.9	24.2	28.8
	23	CA	7.0	25.4	29.6
	23	C	8.4	25.5	30.1
	23	O	8.9	26.5	30.7
GLY	24	N	9.1	24.4	29.9
	24	CA	10.5	24.3	30.4
	24	C	11.4	25.5	29.8
	24	O	10.9	26.2	28.9
ALA	25	N	12.5	25.7	30.5
	25	CA	13.4	26.8	30.1
	25	CB	14.6	26.8	31.0
	25	C	13.9	26.4	28.7
	25	O	13.6	25.4	28.1
ASN	26	N	14.6	27.3	28.1
	26	CA	15.3	27.1	26.8
	26	CB	15.3	28.4	26.0
	26	CG	14.0	29.6	25.3
	26	OD1	13.1	27.8	25.2
	26	ND2	13.7	29.9	24.9
	26	C	16.8	26.6	26.9
	26	O	17.0	25.4	26.6
LYS	27	N	17.6	27.4	27.4
	27	CA	19.0	27.1	27.6
	27	CB	19.2	26.0	28.7
	27	CG	18.0	25.9	29.6
	27	CD	17.9	24.4	30.1
	27	CE	18.8	23.5	29.3
	27	NZ	19.1	22.3	30.1
	27	C	19.7	26.4	26.4
	27	O	19.4	25.3	26.0
VAL	28	N	20.6	27.2	25.7
	28	CA	21.3	26.7	24.5
	28	CB	22.0	25.4	24.8
	28	CG1	23.0	25.0	23.8
	28	CG2	22.5	25.4	26.2
	28	C	20.2	26.6	23.4
	28	O	19.9	27.5	22.7
GLY	29	N	19.6	25.4	23.4
	29	CA	18.6	25.1	22.4
	29	C	17.1	25.3	22.9
	29	O	16.9	25.2	24.1
PRO	30	N	16.2	25.5	22.0
	30	CA	14.8	25.6	22.3
	30	CB	14.1	25.8	21.0
	30	CG	15.2	25.8	19.9
	30	CD	16.3	25.0	20.6
	30	C	14.3	24.3	22.9
	30	O	14.8	23.2	22.6
ASN	31	N	13.1	24.4	23.6
	31	CA	12.5	23.2	24.2
	31	CB	11.9	23.6	25.6
	31	CG	10.7	24.5	25.4
	31	OD1	10.6	25.7	25.3
	31	ND2	9.5	23.9	25.2
	31	C	11.5	22.7	23.2
	31	O	10.6	23.4	22.8
LEU	32	N	11.6	21.4	22.9
	32	CA	10.7	20.8	21.9
	32	CB	11.4	19.9	20.9
	32	CG	12.6	19.1	21.4
	32	CD1	13.2	18.3	20.3
	32	CD2	13.7	20.1	21.9
	32	C	9.6	19.9	22.5
	32	O	9.7	18.7	22.6
PHE	33	N	8.5	20.6	23.0
	33	CA	7.4	19.9	23.6
	33	CB	7.2	20.4	25.0
	33	CG	5.8	20.2	25.6
	33	CD1	5.7	19.2	26.6
	33	CE1	4.4	19.0	27.2
	33	CZ	3.3	19.8	26.8
	33	CE2	3.5	20.9	26.0
	33	CD2	4.8	21.0	25.3
	33	C	6.5	20.5	22.5
	33	O	6.6	21.6	22.1
GLY	34	N	5.6	19.6	22.0
	34	CA	4.7	20.0	20.9
	34	C	5.5	20.5	19.7
	34	O	5.1	21.5	19.0
VAL	35	N	6.6	19.8	19.4
	35	CA	7.5	20.2	18.3
	35	CB	8.9	20.1	18.7
	35	CG1	9.4	18.8	19.3
	35	CG2	9.9	20.6	17.6
	35	C	7.3	19.3	17.0
	35	O	7.5	19.7	15.9
PHE	36	N	6.9	18.1	17.3
	36	CA	6.7	17.1	16.2
	36	CB	5.4	16.3	16.5
	36	CG	5.3	15.1	15.6
	36	CD1	6.3	14.2	15.4
	36	CE1	6.3	13.1	14.6
	36	CZ	5.1	12.7	14.1
	36	CE2	4.0	13.5	14.3
	36	CD2	4.1	14.7	15.1
	36	C	6.5	17.9	14.9
	36	O	7.5	18.1	14.1
GLU	37	N	5.3	18.2	14.6
	37	CA	4.9	18.9	13.3
	37	CB	3.7	18.4	12.6
	37	CG	3.7	16.9	12.3
	37	CD	2.6	16.0	13.0
	37	OE1	1.6	16.5	13.4
	37	OE2	3.0	14.8	12.9
	37	C	4.7	20.4	13.6
	37	O	3.5	20.9	13.4
ASN	38	N	5.7	21.1	13.9
	38	CA	5.6	22.6	14.2
	38	CB	6.0	22.9	15.6
	38	CG	5.4	24.2	16.1
	38	OD1	5.7	24.8	17.1
	38	ND2	4.3	24.7	15.3
	38	C	6.6	23.2	13.2
	38	O	7.4	22.5	12.5
THR	39	N	6.5	24.5	13.1
	39	CA	7.4	25.3	12.1
	39	CB	7.2	26.8	12.4
	39	OG1	5.7	26.9	12.6
	39	CG2	7.6	27.6	11.2
	39	C	8.8	24.9	12.3
	39	O	9.2	24.0	13.2
ALA	40	N	9.7	25.4	11.5
	40	CA	11.1	25.1	11.6
	40	CB	11.8	25.6	10.3
	40	C	11.7	25.9	12.7
	40	O	12.7	25.5	13.3
ALA	41	N	11.1	27.1	13.0
	41	CA	11.6	27.9	14.1
	41	CB	11.5	29.4	13.7
	41	C	10.5	27.8	15.2
	41	O	9.9	28.7	15.7
HIS	42	N	10.3	26.5	15.6
	42	CA	9.4	26.2	16.7
	42	CB	10.0	25.3	17.7
	42	CG	9.1	24.5	18.6
	42	ND1	9.5	23.9	19.8
	42	CE1	8.5	23.3	20.3
	42	NE2	7.4	23.6	19.6
	42	CD2	7.8	24.3	18.5
	42	C	8.8	27.5	17.4
	42	O	8.3	28.4	16.7
LYS	43	N	8.9	27.5	18.7
	43	CA	8.4	28.6	19.5
	43	CB	8.4	28.3	20.9
	43	CG	8.9	26.9	21.3
	43	CD	8.4	26.5	22.7
	43	CE	7.7	25.1	22.6
	43	NZ	6.2	25.4	22.3
	43	C	9.1	29.9	19.4
	43	O	10.4	30.0	19.4
ASP	44	N	8.4	31.0	19.3
	44	CA	8.9	32.3	19.3
	44	CB	7.9	33.3	18.8
	44	CG	6.5	32.7	18.6
	44	OD1	6.3	32.0	17.6
	44	OD2	5.8	32.8	19.5
	44	C	9.6	33.1	20.4
	44	O	9.7	34.4	20.4
ASN	45	N	10.0	32.4	21.4
	45	CA	10.6	33.0	22.6
	45	CB	9.9	32.5	23.9
	45	CG	10.2	31.1	24.2
	45	OD1	10.8	30.6	25.1
	45	ND2	9.6	30.2	23.3
	45	C	12.1	32.6	22.6
	45	O	12.8	32.7	23.6
TYR	46	N	12.5	32.2	21.4
	46	CA	13.9	31.7	21.3
	46	CB	14.0	30.2	21.0
	46	CG	15.4	29.6	21.0
	46	CD1	16.0	29.4	22.3
	46	CE1	17.4	28.9	22.3
	46	CZ	18.0	28.7	21.1
	46	OH	19.3	28.2	21.1
	46	CE2	17.4	28.9	19.8
	46	CD2	16.1	29.4	19.8
	46	C	14.6	32.5	20.1
	46	O	14.0	33.0	19.2
ALA	47	N	15.9	32.5	20.2
	47	CA	16.7	33.2	19.2
	47	CB	18.0	33.8	19.8
	47	C	17.3	32.2	18.1
	47	O	18.4	31.8	18.2
TYR	48	N	16.4	31.9	17.2
	48	CA	16.8	30.9	16.2
	48	CB	15.5	30.5	15.4
	48	CG	14.7	29.4	16.1
	48	CD1	14.6	28.1	15.5
	48	CE1	13.8	27.1	16.2
	48	CZ	13.1	27.4	17.3
	48	OH	12.4	26.4	17.9
	48	CE2	13.2	28.7	17.9
	48	CD2	14.0	29.7	17.3
	48	C	17.8	31.5	15.2
	48	O	18.2	32.6	15.3
SER	49	N	18.2	30.6	14.3
	49	CA	19.2	31.1	13.3
	49	CB	20.3	30.0	13.1
	49	OG	21.1	29.9	14.3
	49	C	18.5	31.3	12.0
	49	O	17.7	30.5	11.5
GLU	50	N	18.8	32.5	11.4
	50	CA	18.2	32.8	10.1
	50	CB	19.2	33.5	9.1
	50	CG	18.8	33.6	7.7
	50	CD	19.4	34.9	6.9
	50	OE1	19.6	35.9	7.4
	50	OE2	19.6	34.5	5.7
	50	C	17.6	31.6	9.4
	50	O	16.5	31.5	9.0
SER	51	N	18.5	30.6	9.2
	51	CA	18.1	29.4	8.5
	51	CB	19.3	28.7	7.9
	51	OG	20.5	28.7	8.8
	51	C	17.5	28.4	9.5
	51	O	18.0	27.3	9.8
TYR	52	N	16.3	28.8	10.0
	52	CA	15.6	28.0	11.0
	52	CB	16.3	28.0	12.3
	52	CG	17.1	26.8	12.6
	52	CD1	16.4	25.6	13.0
	52	CE1	17.2	24.4	13.3
	52	CZ	18.5	24.5	13.3
	52	OH	19.3	23.4	13.6
	52	CE2	19.2	25.6	12.9
	52	CD2	18.5	26.8	12.6
	52	C	14.2	28.6	10.9
	52	O	13.2	28.0	10.7
THR	53	N	14.2	30.0	10.9
	53	CA	12.9	30.7	10.9
	53	CB	13.1	32.0	11.8
	53	OG1	12.7	33.0	10.9
	53	CG2	14.5	32.1	12.3
	53	C	12.6	31.1	9.4
	53	O	12.4	32.3	9.2
GLU	54	N	12.5	30.2	8.6
	54	CA	12.2	30.4	7.2
	54	CB	13.3	30.4	6.2
	54	CG	14.8	30.3	6.8
	54	CD	15.7	31.1	5.8
	54	OE1	15.4	32.0	5.1
	54	OE2	16.8	30.5	5.8
	54	C	10.9	29.5	6.9
	54	O	10.0	29.9	6.2
MET	55	N	11.0	28.4	7.5
	55	CA	9.9	27.4	7.3
	55	CB	9.5	26.8	8.7
	55	CG	8.8	27.8	9.6
	55	SD	9.9	29.2	9.9
	55	CE	9.0	29.9	11.3
	55	C	8.6	28.0	6.7
	55	O	7.7	27.3	6.2
LYS	56	N	8.6	29.3	6.7
	56	CA	7.4	30.0	6.1
	56	CB	7.4	31.5	6.5
	56	CG	8.7	32.1	6.8
	56	CD	8.7	33.1	7.9
	56	CE	10.0	33.9	8.1
	56	NZ	9.8	34.9	9.1
	56	C	7.6	29.9	4.6
	56	O	6.7	29.6	3.8
ALA	57	N	8.8	30.2	4.1
	57	CA	9.1	30.1	2.7
	57	CB	10.4	30.9	2.2
	57	C	9.5	28.6	2.7
	57	O	10.5	28.2	3.2
LYS	58	N	8.6	27.9	2.1
	58	CA	8.8	26.4	2.1
	58	CB	10.2	26.0	2.4
	58	CG	11.2	27.0	1.8
	58	CD	12.6	26.2	1.7
	58	CE	13.1	26.4	.3
	58	NZ	14.4	25.6	.1
	58	C	7.8	25.7	3.0
	58	O	7.2	24.7	2.7
GLY	59	N	7.8	26.2	4.3
	59	CA	6.9	25.6	5.3
	59	C	7.6	24.5	6.1
	59	O	7.0	23.9	6.9
LEU	60	N	8.9	24.4	5.8
	60	CA	9.7	23.3	6.4

Table I (continued)

			x	y	z
LEU	60	CB	11.1	23.9	6.8
	60	CG	12.2	22.9	7.0
	60	CD1	12.0	22.2	8.4
	60	CD2	12.2	21.8	5.9
	60	C	8.8	23.0	7.6
	60	O	8.4	23.8	8.4
THR	61	N	8.6	21.7	7.8
	61	CA	7.8	21.2	8.9
	61	CB	6.3	21.1	8.4
	61	OG1	5.6	21.8	9.4
	61	CG2	5.8	19.7	8.3
	61	C	8.4	19.8	9.3
	61	O	8.9	19.0	8.5
TRP	62	N	8.4	19.5	10.6
	62	CA	8.9	18.3	11.1
	62	CB	9.4	18.5	12.6
	62	CG	10.4	19.7	12.8
	62	CD1	10.1	20.9	13.4
	62	NE1	11.3	21.7	13.4
	62	CE2	12.2	21.0	12.8
	62	CZ2	13.5	21.5	12.6
	62	CH2	14.3	20.6	12.0
	62	CZ3	13.8	19.4	11.5
	62	CE3	12.5	18.9	11.7
	62	CD2	11.7	19.8	12.4
	62	C	8.0	17.0	11.1
	62	O	7.5	16.6	12.2
THR	63	N	7.7	16.5	10.0
	63	CA	6.8	15.4	9.8
	63	CB	6.5	15.2	8.3
	63	OG1	7.8	14.9	7.7
	63	CG2	5.9	16.4	7.7
	63	C	7.4	14.0	10.4
	63	O	6.7	13.0	10.4
GLU	64	N	8.6	14.1	10.9
	64	CA	9.2	12.9	11.4
	64	CB	8.2	11.8	11.7
	64	CG	8.8	10.4	12.1
	64	CD	7.8	9.2	11.8
	64	OE1	7.1	9.2	10.9
	64	OE2	8.0	8.3	12.6
	64	C	10.3	12.4	10.5
	64	O	11.4	11.9	10.9
ALA	65	N	9.9	12.4	9.2
	65	CA	10.9	11.9	8.1
	65	CB	10.1	11.7	6.8
	65	C	11.9	13.0	7.9
	65	O	13.0	12.8	7.5
ASN	66	N	11.4	14.2	8.2
	66	CA	12.3	15.4	8.1
	66	CB	11.4	16.7	7.8
	66	CG	11.6	17.2	6.4
	66	OD1	12.4	16.9	5.6
	66	ND2	10.5	18.0	6.0
	66	C	13.2	15.6	9.3
	66	O	14.1	16.2	9.2
LEU	67	N	12.8	15.1	10.4
	67	CA	13.6	15.2	11.6
	67	CB	12.7	14.8	12.8
	67	CG	11.2	14.9	12.7
	67	CD1	10.5	15.1	14.0
	67	CD2	10.8	16.0	11.7
	67	C	14.8	14.2	11.5
	67	O	15.9	14.5	11.9
ALA	68	N	14.5	13.1	10.9
	68	CA	15.6	12.0	10.8
	68	CB	15.0	10.8	10.0
	68	C	16.7	12.6	9.9
	68	O	17.9	12.3	10.2
ALA	69	N	16.3	13.3	8.9
	69	CA	17.3	13.9	7.9
	69	CB	16.6	14.6	6.8
	69	C	18.1	14.9	8.7
	69	O	19.3	15.1	8.6
TYR	70	N	17.3	15.7	9.5
	70	CA	18.0	16.8	10.2
	70	CB	16.9	17.5	11.0
	70	CG	17.4	18.6	12.0
	70	CD1	18.0	19.7	11.5
	70	CE1	18.6	20.7	12.5
	70	CZ	18.6	20.4	13.8
	70	OH	19.1	21.3	14.7
	70	CE2	17.9	19.3	14.3
	70	CD2	17.4	18.3	13.4
	70	C	19.0	16.3	11.1
	70	O	20.1	16.9	11.3
VAL	71	N	18.8	15.1	11.8
	71	CA	19.7	14.5	12.7
	71	CB	19.1	13.2	13.3
	71	CG1	20.2	12.1	13.5
	71	CG2	18.3	13.5	14.5
	71	C	21.0	14.2	11.9
	71	O	21.7	15.1	11.4
LYS	72	N	21.4	13.0	11.9
	72	CA	22.7	12.6	11.3
	72	CB	22.4	11.9	9.9
	72	CG	21.5	10.6	10.0
	72	CD	22.2	9.5	9.2
	72	CE	21.5	8.2	9.5
	72	NZ	22.5	7.1	9.8
	72	C	23.5	13.8	11.1
	72	O	24.6	13.9	11.7
ASN	73	N	23.1	14.7	10.2
	73	CA	23.9	15.9	10.0
	73	CB	24.5	15.8	8.5
	73	CG	26.0	16.1	8.6
	73	OD1	26.8	15.3	8.2
	73	ND2	26.4	17.3	9.0
	73	C	23.0	17.1	10.1
	73	O	22.2	17.5	9.1
PRO	74	N	23.0	17.8	11.2
	74	CA	22.2	19.0	11.5
	74	CB	21.9	18.9	12.9
	74	CG	23.3	18.4	13.5
	74	CD	24.0	18.1	12.2
	74	C	22.4	20.1	10.4
	74	O	21.4	20.6	9.9
LYS	75	N	23.6	20.4	10.1
	75	CA	23.9	21.4	9.1
	75	CB	25.4	21.7	9.1
	75	CG	26.3	20.8	9.8
	75	CD	27.7	21.3	10.1
	75	CE	27.8	22.1	11.4
	75	NZ	26.5	21.9	12.2
	75	C	23.5	21.0	7.7
	75	O	23.3	21.8	6.8
ALA	76	N	23.3	19.7	7.6
	76	CA	22.8	19.1	6.3
	76	CB	23.4	17.7	6.0
	76	C	21.3	19.0	6.4
	76	O	20.8	18.2	7.2
PHE	77	N	20.6	19.7	5.5
	77	CA	19.1	19.7	5.5
	77	CB	18.7	18.8	6.7
	77	CG	17.3	19.2	7.3
	77	CD1	17.2	20.4	7.9
	77	CE1	16.0	20.8	8.5
	77	CZ	14.9	20.0	8.3
	77	CE2	15.0	18.9	7.6
	77	CD2	16.2	18.4	7.1
	77	C	18.9	21.2	5.7
	77	O	17.9	21.7	5.2
VAL	78	N	19.9	21.9	6.2
	78	CA	19.8	23.3	6.4
	78	CB	20.4	23.7	7.7
	78	CG1	21.1	25.1	7.7
	78	CG2	19.5	23.6	8.9
	78	C	20.5	24.0	5.2
	78	O	20.9	25.2	5.3
LEU	79	N	20.6	23.3	4.1
	79	CA	21.2	23.8	2.9
	79	CB	22.6	23.3	2.8
	79	CG	23.6	23.6	3.9
	79	CD1	24.3	22.4	4.4
	79	CD2	24.6	24.6	3.3
	79	C	20.1	23.2	2.0
	79	O	19.5	23.9	1.1
GLU	80	N	19.9	21.9	2.2
	80	CA	18.9	21.2	1.3
	80	CB	18.7	19.7	1.8
	80	CG	19.7	18.7	1.3
	80	CD	19.2	17.2	1.3
	80	OE1	18.4	16.8	.5
	80	OE2	19.8	16.6	2.2
	80	C	17.6	22.0	1.5
	80	O	17.2	22.7	.6
LYS	81	N	17.0	21.9	2.7
	81	CA	15.8	22.6	3.0
	81	CB	15.0	21.9	4.0
	81	CG	15.2	20.4	4.1
	81	CD	14.2	19.7	3.3
	81	CE	14.5	18.2	3.2
	81	NZ	13.3	17.4	3.0
	81	C	16.0	24.1	3.5
	81	O	15.5	24.5	4.6
SER	82	N	16.8	24.9	2.7
	82	CA	17.0	26.3	3.1
	82	CB	17.8	26.3	4.4
	82	OG	18.7	27.4	4.4
	82	C	17.8	26.9	2.0
	82	O	18.1	26.3	.9
GLY	83	N	18.0	28.2	2.1
	83	CA	18.7	29.0	1.1
	83	C	20.2	28.8	1.4
	83	O	21.1	29.4	.8
ASP	84	N	20.5	28.0	2.5
	84	CA	21.8	27.7	2.9
	84	CB	22.3	26.4	2.4
	84	CG	22.6	26.4	.9
	84	OD1	22.6	27.4	.2
	84	OD2	23.0	25.4	.4
	84	C	22.8	28.8	2.4
	84	O	23.6	28.6	1.5
PRO	85	N	22.5	30.0	2.9
	85	CA	23.4	31.2	2.4
	85	CB	22.6	32.4	3.0
	85	CG	21.5	31.9	4.0
	85	CD	21.4	30.4	3.6
	85	C	24.8	31.0	3.0
	85	O	25.6	31.9	3.0
LYS	86	N	25.0	29.7	3.4
	86	CA	26.3	29.4	4.0
	86	CB	27.3	30.6	4.0
	86	CG	28.2	30.6	5.2
	86	CD	28.7	32.0	5.5
	86	CE	28.7	32.3	7.0
	86	NZ	29.1	33.7	7.3
	86	C	25.7	28.9	5.3
	86	O	26.4	28.6	6.3
ALA	87	N	24.4	28.8	5.3
	87	CA	23.6	28.4	6.4
	87	CB	22.8	27.2	6.1
ALA	87	C	24.7	27.9	7.4
	87	O	25.6	27.2	7.1
LYS	88	N	24.5	28.4	8.7
	88	CA	25.5	28.0	9.8
	88	CB	26.4	29.1	10.0
	88	CG	25.9	30.3	10.9
	88	CD	26.9	30.7	11.9
	88	CE	26.3	31.8	12.8
	88	NZ	25.1	31.3	13.5
	88	C	24.6	27.7	11.0
	88	O	23.7	28.5	11.4
SER	89	N	24.7	26.5	11.5
	89	CA	24.0	26.1	12.7
	89	CB	23.0	25.0	12.3
	89	OG	22.9	24.0	13.4
	89	C	24.8	25.7	13.9
	89	O	25.9	25.1	13.7
LYS	90	N	24.3	25.9	15.1
	90	CA	25.0	25.5	16.3
	90	CB	25.0	26.7	17.3
	90	CG	25.7	27.9	16.8
	90	CD	24.9	29.2	17.2
	90	CE	23.4	29.0	17.2
	90	NZ	22.7	30.2	17.5
	90	C	24.5	24.4	17.1
	90	O	24.0	24.5	18.3
MET	91	N	24.7	23.2	16.6
	91	CA	24.3	21.9	17.3
	91	CB	22.8	21.7	17.0
	91	CG	22.4	20.2	17.4
	91	SD	20.6	20.0	17.4
	91	CE	20.6	18.2	17.2
	91	C	25.1	20.8	16.8
	91	O	26.3	20.8	16.9
THR	92	N	24.4	19.8	16.1
	92	CA	25.1	18.6	15.6
	92	CB	26.4	19.1	15.0
	92	OG1	27.4	18.7	15.9
	92	CG2	26.5	20.6	14.8
	92	C	25.3	17.6	16.7
	92	O	25.2	17.9	17.9
PHE	93	N	25.6	16.4	16.3
	93	CA	25.8	15.3	17.2
	93	CB	25.5	15.8	18.6
	93	CG	24.3	15.2	19.3
	93	CD1	23.1	15.9	19.3
	93	CE1	22.0	15.5	19.9
	93	CZ	21.9	14.2	20.4
	93	CE2	23.0	13.5	20.4
	93	CD2	24.3	14.0	19.8
	93	C	24.8	14.2	16.7
	93	O	23.6	14.2	17.2
LYS	94	N	25.2	13.4	15.8
	94	CA	24.4	12.4	15.2
	94	CB	25.1	11.5	14.3
	94	CG	26.6	11.2	14.7
	94	CD	27.5	12.4	14.4
	94	CE	28.9	12.0	14.7
	94	NZ	29.3	12.5	16.0
	94	C	23.6	11.3	15.9
	94	O	23.0	11.6	17.0
LEU	95	N	23.5	10.1	15.4
	95	CA	22.7	9.0	15.9
	95	CB	21.4	9.5	16.5
	95	CG	21.4	10.5	17.6
	95	CD1	20.0	10.9	18.1
	95	CD2	22.2	10.0	18.8
	95	C	22.5	7.9	15.0
	95	O	21.7	8.1	14.0
THR	96	N	23.0	6.7	15.2
	96	CA	22.9	5.6	14.4
	96	CB	23.7	4.4	14.9
	96	OG1	23.6	4.5	16.4
	96	CG2	25.2	4.6	14.6
	96	C	21.4	5.2	14.3
	96	O	20.6	5.7	15.1
LYS	97	N	21.0	4.4	13.3
	97	CA	19.6	3.9	13.2
	97	CB	19.6	2.6	12.4
	97	CG	20.1	2.7	11.0
	97	CD	20.1	4.1	10.4
	97	CE	19.4	4.2	9.1
	97	NZ	18.7	5.6	8.9
	97	C	18.8	3.7	14.4
	97	O	17.6	4.1	14.4
ASP	98	N	19.4	3.0	15.4
	98	CA	18.6	2.7	16.6
	98	CB	19.6	2.0	17.6
	98	CG	19.0	2.0	19.0
	98	OD1	18.6	.9	19.5
	98	OD2	18.9	3.0	19.6
	98	C	18.1	4.0	17.1
	98	O	16.9	4.3	16.9
ASP	99	N	18.9	4.8	17.7
	99	CA	18.5	6.1	18.2
	99	CB	19.7	7.0	18.6
	99	CG	20.5	6.3	19.6
	99	OD1	20.3	5.2	20.1
	99	OD2	21.5	6.9	20.0
	99	C	17.6	6.9	17.3
	99	O	16.4	7.1	17.5
GLU	100	N	18.2	7.4	16.2
	100	CA	17.5	8.2	15.2
	100	CB	18.1	8.0	13.8
	100	CG	17.1	8.2	12.6
	100	CD	16.6	9.7	12.4
GLU	100	OE1	15.9	10.2	13.2
	100	OE2	17.1	10.2	11.4
	100	C	16.0	7.9	15.2
	100	O	15.2	8.6	15.7
ILE	101	N	15.7	6.7	14.6
	101	CA	14.3	6.2	14.6
	101	CB	14.3	4.8	14.1
	101	CG1	15.5	4.3	13.3
	101	CG2	12.9	4.8	13.3
	101	CD1	15.2	3.5	12.0
	101	C	13.6	6.3	15.9
	101	O	12.4	6.7	16.0
GLU	102	N	14.3	5.9	16.9
	102	CA	13.8	5.9	18.3
	102	CB	14.7	5.2	19.3
	102	CG	14.1	4.3	20.4
	102	CD	14.4	2.8	20.2
	102	OE1	15.5	2.3	20.3
	102	OE2	13.3	2.2	20.0
	102	C	13.4	7.2	18.9
	102	O	12.3	7.4	19.5
ASN	103	N	14.3	8.2	18.7
	103	CA	14.0	9.5	19.3
	103	CB	15.3	10.4	19.0
	103	CG	16.4	10.1	19.9
	103	OD1	16.4	9.2	20.7
	103	ND2	17.6	10.9	19.6
	103	C	12.8	10.1	18.6
	103	O	11.8	10.5	19.4
VAL	104	N	12.7	10.1	17.3
	104	CA	11.6	10.6	16.6
	104	CB	11.7	10.4	15.1
	104	CG1	10.4	10.7	14.3
	104	CG2	13.0	11.0	14.6
	104	C	10.3	10.0	17.1
	104	O	9.2	10.7	17.2
ILE	105	N	10.3	8.8	17.5
	105	CA	9.1	8.1	18.0
	105	CB	9.3	6.5	18.0
	105	CG1	8.7	5.8	16.8
	105	CG2	8.8	6.2	19.4
	105	CD1	9.1	6.3	15.4
	105	C	8.8	8.6	19.4
	105	O	7.6	8.5	19.8
ALA	106	N	9.8	9.0	20.0
	106	CA	9.7	9.5	21.4
	106	CB	11.0	10.2	21.9
	106	C	8.6	10.6	21.5
	106	O	7.4	10.3	21.6
TYR	107	N	9.1	11.9	21.4
	107	CA	8.1	13.0	21.5
	107	CB	8.9	14.3	21.5
	107	CG	10.1	14.4	20.5
	107	CD1	9.7	14.3	19.1
	107	CE1	10.7	14.4	18.1
	107	CZ	12.0	14.4	18.5
	107	OH	13.0	14.4	17.5
	107	CE2	12.4	14.4	19.8
	107	CD2	11.4	14.4	20.8
	107	C	7.2	13.1	20.3
	107	O	6.0	13.4	20.4
LEU	108	N	7.7	12.7	19.1
	108	CA	6.9	12.7	17.9
	108	CB	7.4	11.7	16.9
	108	CG	6.8	10.3	16.9
	108	CD1	7.8	9.3	17.4
	108	CD2	5.6	10.3	17.7
	108	C	5.4	12.4	18.1
	108	O	4.6	12.5	17.2
LYS	109	N	5.1	12.1	19.4
	109	CA	3.7	11.8	19.8
	109	CB	3.3	10.4	19.3
	109	CG	2.1	9.8	20.0
	109	CD	2.1	8.3	20.0
	109	CE	.8	7.8	19.3
	109	NZ	.7	6.3	19.4
	109	C	3.4	11.9	21.3
	109	O	2.2	12.2	21.6
THR	110	N	4.4	11.6	22.1
	110	CA	4.2	11.7	23.5
	110	CB	5.2	10.7	24.2
	110	OG1	6.4	11.5	24.0
	110	CG2	5.3	9.4	23.5
	110	C	4.3	13.1	23.9
	110	O	3.5	13.7	24.7
LEU	111	N	5.3	13.8	23.4
	111	CA	5.6	15.2	23.7
	111	CB	7.1	15.5	23.5
	111	CG	7.9	15.4	24.8
	111	CD1	7.2	14.6	25.9
	111	CD2	9.2	14.6	24.4
	111	C	4.7	15.9	22.6
	111	O	5.1	16.2	21.5
LYS	112	N	3.4	16.1	23.0
	112	CA	2.5	16.8	22.1
	112	CB	2.3	16.0	20.8
	112	CG	3.3	16.5	19.7
	112	CD	2.9	18.0	19.3
	112	CE	1.6	18.0	18.4
	112	NZ	1.2	16.6	18.0
	112	C	1.2	16.8	22.9
	112	O	1.1	16.8	24.1
	112	O2	.1	16.9	22.1

Table I (continued)

		x	y	z			x	y	z			x	y	z			x	y	z
HEME	FE	19.0	20.3	19.5	HEME	2C1	21.1	18.8	21.1	HEME	3CM	21.8	25.2	19.4	HEME	4C2	15.6	21.6	17.2
	N1	18.4	18.4	19.8		2C2	22.4	19.0	21.8		3C3	19.6	24.4	18.4		4CM	14.0	19.7	16.9
	1C1	17.3	17.8	19.4		2CM	23.1	18.0	22.5		3CA	19.2	25.7	17.7		4C3	15.3	20.3	17.4
	1C2	17.3	16.4	19.9		2C3	22.8	20.3	21.5		3CB	20.3	26.0	16.6		4CA	14.9	22.6	16.4
	1CM	16.2	15.4	19.6		2CA	24.0	20.9	22.0		3CC	19.9	27.4	16.4		4CB	13.8	22.3	16.6
	1C3	18.4	16.2	20.5		2CB	24.7	20.0	23.0		3O1	19.8	28.1	17.6		4CC	13.0	23.6	15.8
	1CA	18.8	14.9	21.2		2C4	21.7	20.9	20.8		3O2	20.8	28.1	15.5		4O1	12.5	24.7	16.3
	1CB	19.3	13.8	20.5		2C5	21.7	22.2	20.3		3C4	18.9	23.2	18.4		4O2	11.8	23.0	18.9
	1C4	19.1	17.4	20.5		N3	19.6	22.2	19.1		3C5	17.6	23.0	17.8		4C4	16.3	19.7	18.2
	1C5	20.4	17.6	21.1		3C1	20.7	22.8	19.6		N4	17.3	20.6	18.4		4C5	16.3	18.4	18.6
	N2	20.7	20.0	20.9		3C2	20.8	24.2	19.1		4C1	16.9	21.8	17.8					

Table II

		Φ	Ψ			Φ	Ψ			Φ	Ψ			Φ	Ψ			Φ	Ψ
GLU	1	0	125	GLY	24	-52	164	ALA	47	-98	78	TYR	70	-57	-42	PHE	93	126	87
GLY	2	16	-53	ALA	25	-69	179	TYR	48	-65	177	VAL	71	-58	-122	LYS	94	-52	-140
ASP	3	-70	-72	ASN	26	-100	-68	SER	49	-104	131	LYS	72	19	-67	LEU	95	164	115
ALA	4	-68	-7	LYS	27	50	109	GLU	50	-20	-54	ASN	73	-130	97	THR	96	-60	166
ALA	5	-63	-53	VAL	28	66	-89	SER	51	-84	65	PRO	74	-54	-49	LYS	97	-38	-44
ALA	6	-69	-15	GLY	29	-100	158	TYR	52	-163	-48	ILE	75	-66	-19	ASP	98	-51	-79
GLY	7	-71	-40	PRO	30	-67	160	THR	53	-90	55	ALA	76	-97	117	ASP	99	-44	-72
GLU	8	-74	-31	ASN	31	-92	126	GLU	54	-124	-36	PRE	77	128	-26	GLU	100	-25	-76
LYS	9	-56	-54	LEU	32	-101	82	MET	55	-13	-15	VAL	78	-94	22	ILE	101	-50	-41
VAL	10	-62	-40	PHE	33	-119	136	LYS	56	-76	-45	LEU	79	-137	-52	GLU	102	-66	-45
SER	11	-53	-23	GLY	34	59	40	ALA	57	-88	106	GLU	80	-53	-71	ASN	103	-59	-56
LYS	12	-53	-40	VAL	35	-102	-27	LYS	58	108	-46	LYS	81	-88	54	VAL	104	-50	-38
LYS	13	-69	4	PHE	36	-20	-90	GLY	59	87	6	SER	82	-173	178	ILE	105	-71	-27
CYS	14	-113	-29	GLU	37	-103	70	LEU	60	-16	130	GLY	83	-89	3	ALA	106	-55	-93
LEU	15	-74	114	ASN	38	-121	169	THR	61	-147	145	ASP	84	20	66	TYR	107	-67	-38
ALA	16	162	-73	THR	39	-49	178	THR	62	-86	72	PRO	85	-69	16	LEU	108	-31	-8
CYS	17	-117	-34	ALA	40	-79	-28	THR	63	-68	-2	LYS	86	123	8	LYS	109	-162	-30
HIS	18	-120	176	ALA	41	-107	55	GLU	64	104	-39	ALA	87	-6	133	THR	110	-83	-46
THR	19	-144	150	HIS	42	-8	-128	ALA	65	-81	-25	LYS	88	-138	126	LEU	111	-86	88
PHE	20	-120	10	LYS	43	-69	138	ASN	66	-84	-25	SER	89	-126	148	LYS	112	179	0
ASP	21	-93	105	ASP	44	-74	20	LEU	67	-73	-40	LYS	90	-106	70				
GLN	22	-41	110	ASN	45	-110	18	ALA	68	-60	-41	MET	91	-156	-117				
GLY	23	110	-11	TYR	46	-124	158	ALA	69	-68	-41	THR	92	84	163				

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

$$R = \frac{\Sigma||F_o|-|F_c||}{\Sigma|F_o|} = 44.5\%$$

The coordinates in Table I are given in Ångstrom 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 $P2_12_12_1$ with a = 32.3, b = 37.4, and c = 84.6 Å.

Table II gives the interpeptide dihedral angles, ϕ and ψ, according to

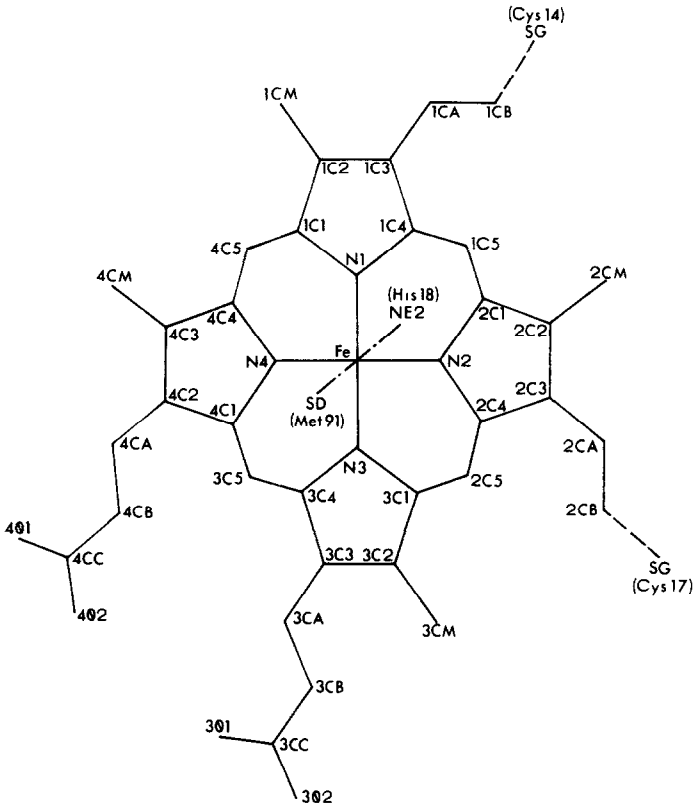
(Cys14)
SG
1CM
1CA
1CB
1C2
1C3
1C1
1C4
4C5
N1
1C5
4CM
2CM
(His18)
NE2
4C4
4C3
2C1
2C2
N4
Fe
N2
4C2
4C1
SD
(Met91)
2C4
2C3
4CA
2CA
N3
3C5
3C4
3C1
2C5
4CB
2CB
401
4CC
SG
(Cys17)
402
3C3
3C2
3CA
3CM
3CB
301
3CC
302

Fig. 1.

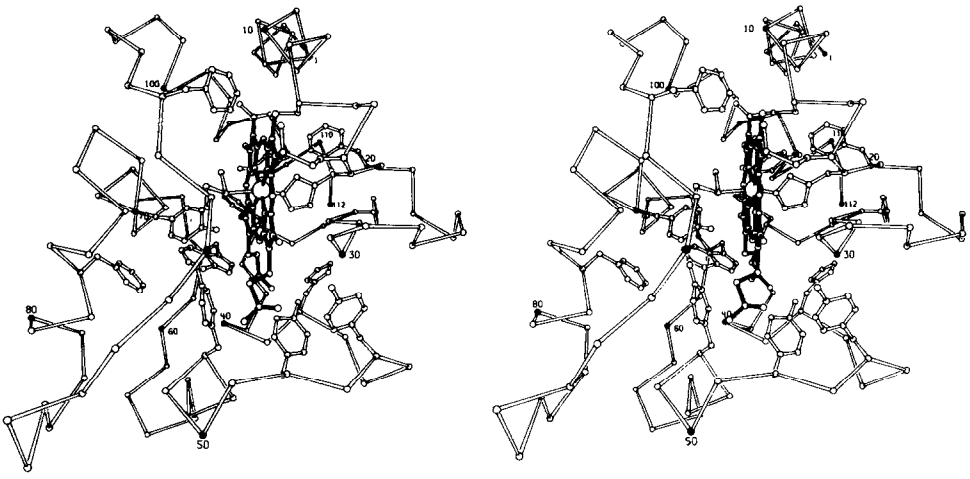

Fig. 2.

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 $\underline{c}_2$ molecule showing α-carbon positions, heme ligands, and aromatic residues.

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