

ATOMIC COORDINATES FOR FERRICYTOCHROME c_2 OF RHODOSPIRILLUM RUBRUM

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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 N ϵ 2 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 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 (continued)

HEHE			X	Y	Z	HEHE			X	Y	Z	HEHE			X	Y	Z
FR	19.0	20.3	19.5	2C1	21.1	18.8	21.1	HEHE	3C1	21.8	25.2	19.4	HEHE	4C2	15.6	21.6	17.2
N1	18.4	16.4	19.8	2C2	22.4	15.0	21.8	3C3	19.6	24.4	18.4	4C3	14.0	19.7	16.9		
IC1	17.3	17.8	19.4	2C3	23.1	18.0	22.5	3CA	19.2	25.7	17.7	4C3	15.3	20.3	17.4		
IC2	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		
ICM	18.2	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		
IC3	18.4	16.2	20.5	2CB	24.7	20.0	23.0	3OI	19.8	28.1	17.6	4CC	13.0	23.6	15.8		
ICA	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		
ICB	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	14.9		
IC4	19.1	17.4	20.5	M3	19.6	22.2	19.1	3C5	17.6	23.0	17.8	4C4	16.3	19.7	18.2		
IC5	20.4	17.6	21.1	3C1	20.7	22.8	19.6	H4	17.3	20.6	18.4	4C5	16.3	18.4	18.6		
M2	20.7	20.0	20.5	3C2	20.6	24.7	19.1	HC1	16.9	21.8	17.8						

Table II

		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	THR	48	-65	177	VAL	71	-58	-122	LYS	94	-52	-144
ASP	3	-70	-72	ASN	26	-100	-88	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	THR	52	-163	-48	LYS	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	PHE	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	-719	136	LYS	56	-78	-45	LEU	79	-137	-52	GLU	102	-86	-45
SER	11	-53	-23	GLY	34	59	40	ALA	57	-88	106	GLU	80	-53	-71	ASN	103	-59	-56
LYS	12	-53	-4	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	THR	107	-67	-38
ALA	16	162	-33	THR	39	-49	178	TRP	62	-86	72	PRO	85	-69	16	LEU	108	-31	-4
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	PHE	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	RET	91	-156	-117				
GLY	23	110	-11	THR	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

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

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:

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

where X, Y, and Z are the Cartesian coordinates given in Table I. Cytochrome c_2 crystallized in space group $P2_1^2 2_1^2$ with $a = 32.3$, $b = 37.4$, and $c = 84.6$ Å.

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

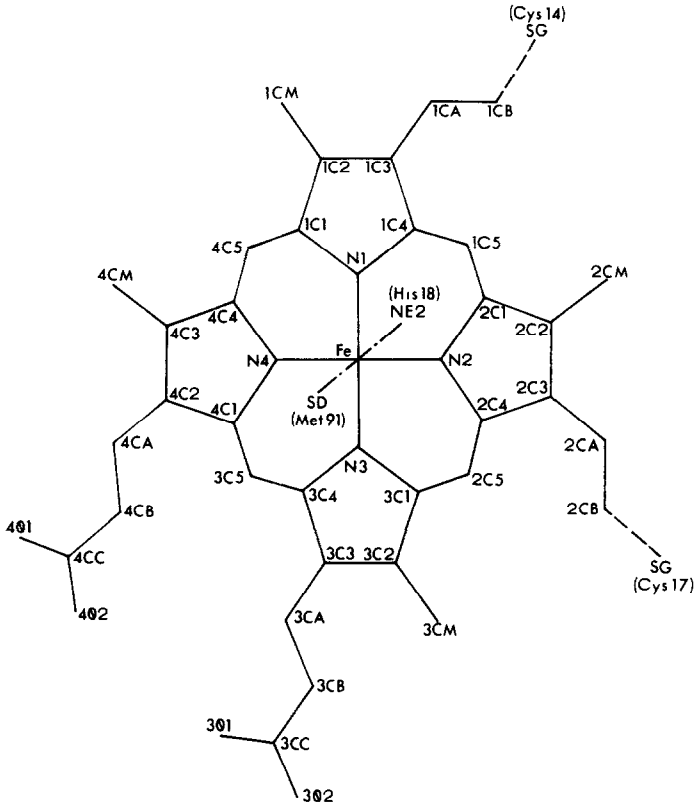


Fig. 1.

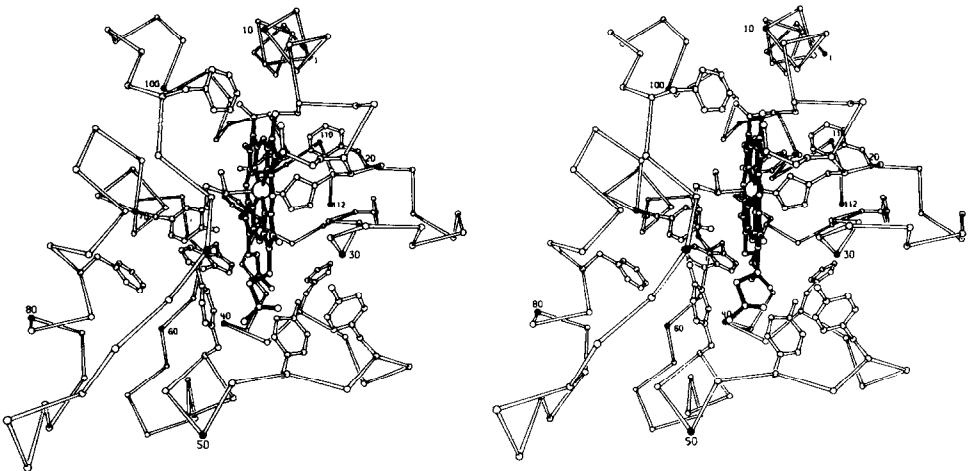


Fig. 2.

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 c_2 molecule showing α -carbon positions, heme ligands, and aromatic residues.

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