wwPDB X-ray Structure Validation Summary Report (i)

Jan 31, 2016 – 09:43 PM GMT

PDB ID	:	1Q90
Title	:	Structure of the cytochrome b6f (plastohydroquinone : plastocyanin oxidoreductase) from Chlamydomonas reinhardtii
Authors	:	Stroebel, D.; Choquet, Y.; Popot, J.-L.; Picot, D.
Deposited on	:	2003-08-22
Resolution	:	3.10 Å(reported)

The following versions of software and data (see references (i)) were used in the production of this report:

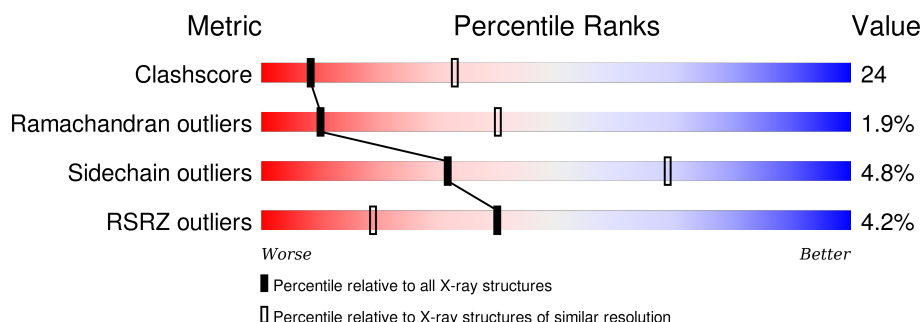|		
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.

Metric	Percentile Ranks	Value
Clashscore		24
Ramachandran outliers		1.9%
Sidechain outliers		4.8%
RSRZ outliers		4.2%

Worse   *Better*

▌ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	1222 (3.14-3.06)
Ramachandran outliers	100387	1174 (3.14-3.06)
Sidechain outliers	100360	1174 (3.14-3.06)
RSRZ outliers	91569	1119 (3.14-3.06)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	292	59% 37% •
2	B	215	57% 40% ••
3	C	127	24% 42% 53% 5% •
4	D	159	48% 45% 6% •
5	R	49	6% 57% 16% 6% 20%
6	G	37	65% 16% 19%
7	L	32	53% 34% 13%

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Mol	Chain	Length	Quality of chain
8	M	39	46% 33% 8% 13%
9	N	31	65% 35%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
12	CLA	D	910	X	-	-	-
13	BCR	B	904	-	-	-	X
14	TDS	D	920	-	-	-	X
16	LFA	B	960	-	-	-	X
17	LMG	D	953	-	-	-	X

2 Entry composition (i)

There are 18 unique types of molecules in this entry. The entry contains 7778 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Apocytochrome f.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	292	Total C N O S					0	0	0
			2266 1457 387 417 5							

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	287	HIS	-	EXPRESSION TAG	UNP P23577
A	288	HIS	-	EXPRESSION TAG	UNP P23577
A	289	HIS	-	EXPRESSION TAG	UNP P23577
A	290	HIS	-	EXPRESSION TAG	UNP P23577
A	291	HIS	-	EXPRESSION TAG	UNP P23577
A	292	HIS	-	EXPRESSION TAG	UNP P23577

- Molecule 2 is a protein called Cytochrome b6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	212	Total C N O S					0	0	0
			1681 1117 270 281 13							

- Molecule 3 is a protein called Cytochrome B6-F complex iron-sulfur subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	126	Total C N O S					0	0	0
			955 606 163 181 5							

- Molecule 4 is a protein called Cytochrome b6-f complex subunit 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	156	Total C N O S					0	0	0
			1201 807 185 204 5							

- Molecule 5 is a protein called Cytochrome B6-F complex iron-sulfur subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	R	39	Total	C	N	O	S	0	0	0
			283	184	46	51	2			

- Molecule 6 is a protein called Cytochrome b6f complex subunit petG.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	G	30	Total	C	N	O	S	0	0	0
			224	154	31	37	2			

- Molecule 7 is a protein called Cytochrome b6f complex subunit petL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	L	32	Total	C	N	O	S	0	0	0
			242	168	34	39	1			

- Molecule 8 is a protein called Cytochrome b6f complex subunit PETM.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	M	34	Total	C	N	O	S	0	0	0
			247	162	37	46	2			

- Molecule 9 is a protein called Cytochrome b6f complex subunit PETN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	N	31	Total	C	N	O	S	0	0	0
			231	152	37	40	2			

- Molecule 10 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).
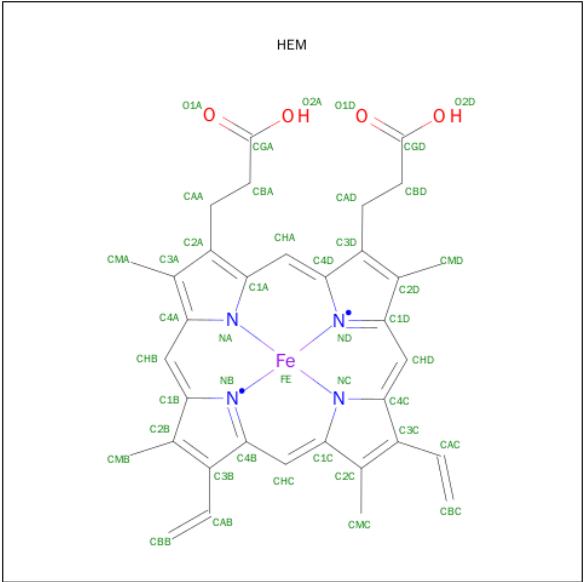
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
10	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
10	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
10	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

• Molecule 11 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).
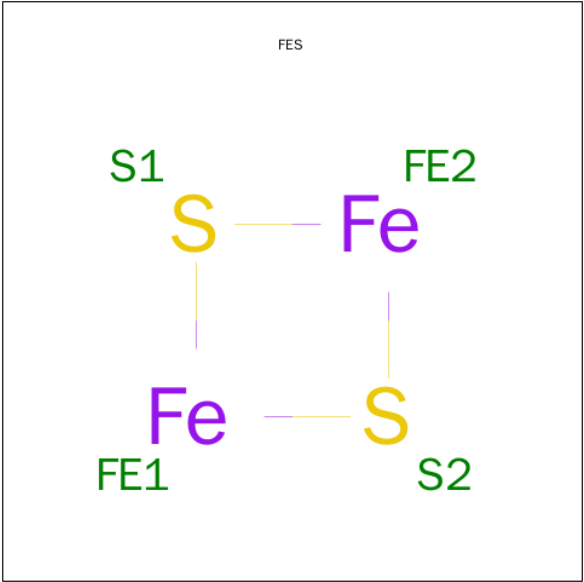
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
11	C	1	4	2	2	0	0

- Molecule 12 is CHLOROPHYLL A (three-letter code: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).
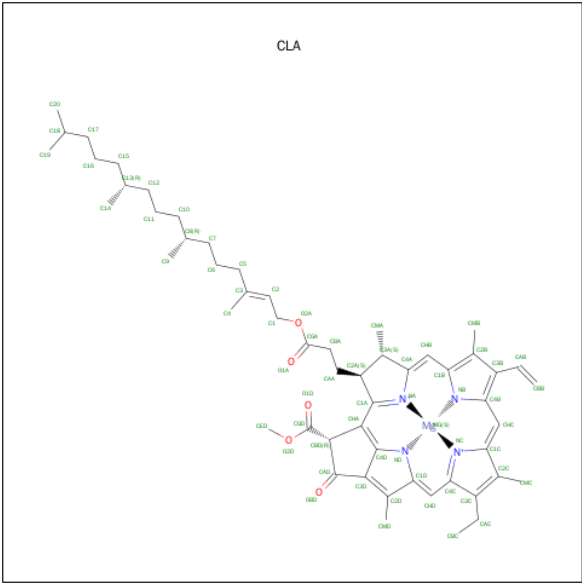
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Mg	N	O		
12	D	1	65	55	1	4	5	0	0

- Molecule 13 is BETA-CAROTENE (three-letter code: BCR) (formula: $C_{40}H_{56}$).
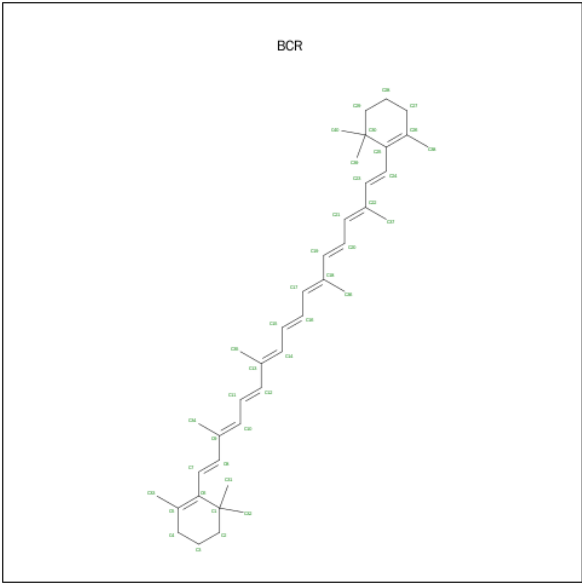
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	B	1	Total 27	C 27	0	0

- Molecule 14 is 8-HYDROXY-5,7-DIMETHOXY-3-METHYL-2-TRIDECYL-4H-CHROMEN-4-ONE (three-letter code: TDS) (formula: $C_{25}H_{38}O_5$).
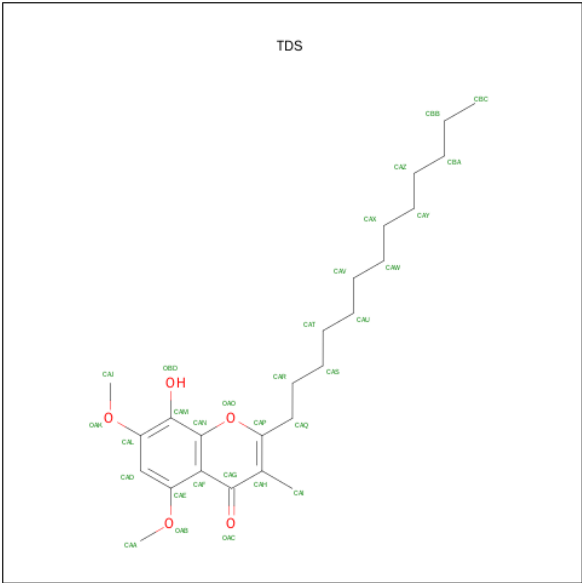
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
14	D	1	Total 30	C 25	O 5	0	0

- Molecule 15 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula: $C_{41}H_{78}O_{12}S$).
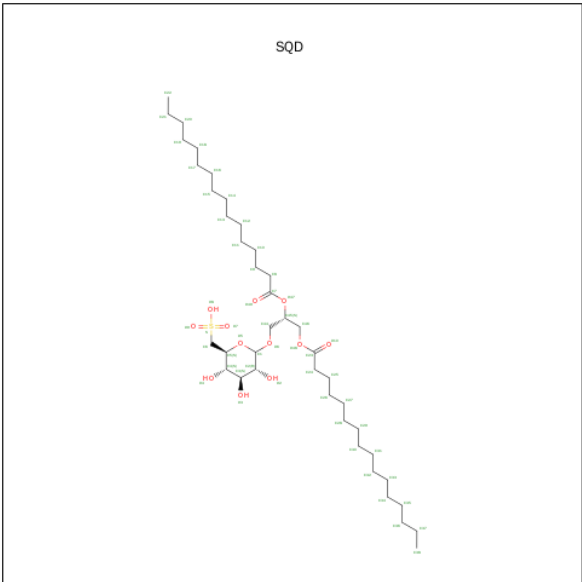
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	S		
15	R	1	33	20	12	1	0	0

- Molecule 16 is EICOSANE (three-letter code: LFA) (formula: $C_{20}H_{42}$).
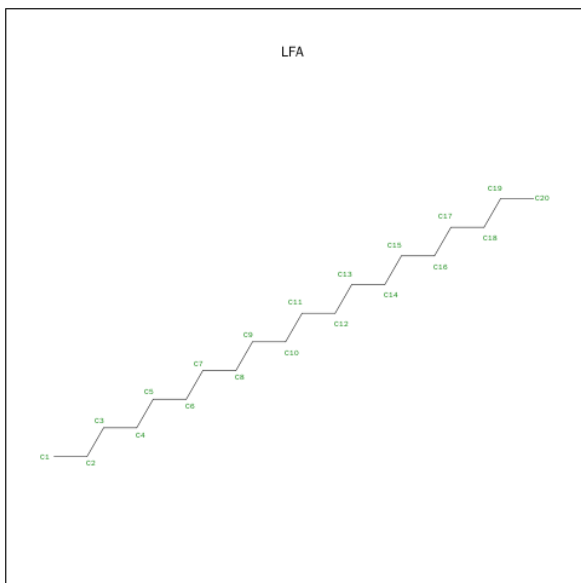
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	C		
16	B	1	20	20	0	0

- Molecule 17 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: $C_{45}H_{86}O_{10}$).
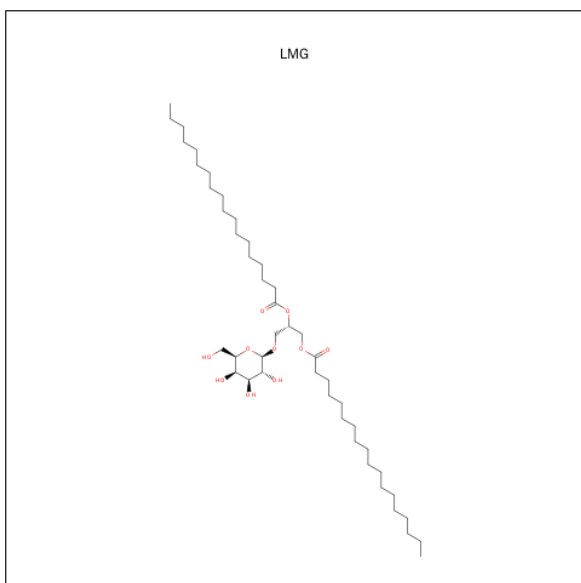
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
17	L	1	Total 42	C 32	O 10	0	0
17	D	1	Total 53	C 43	O 10	0	0

- Molecule 18 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
18	B	2	Total 2	O 2	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Apocytochrome f

Chain A:
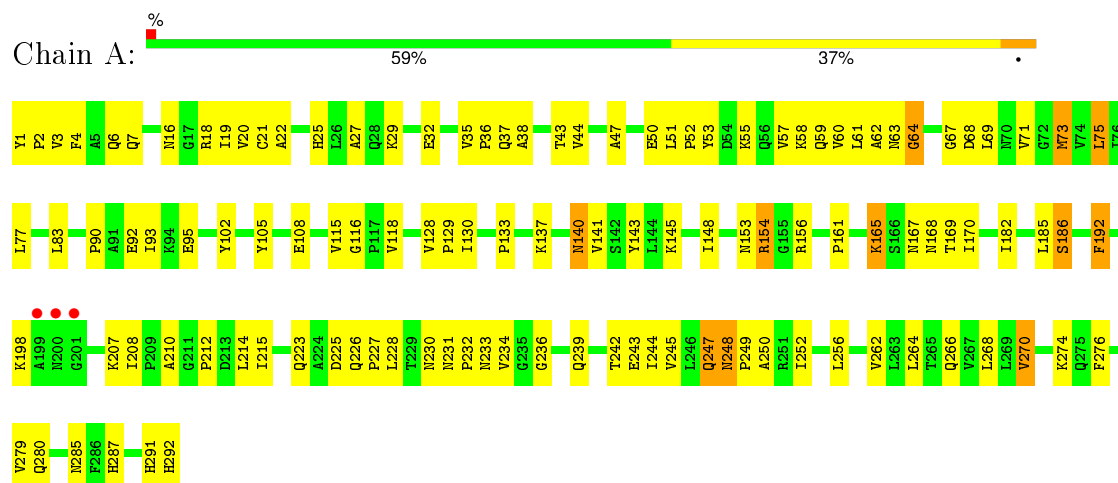
- Molecule 2: Cytochrome b6

Chain B:
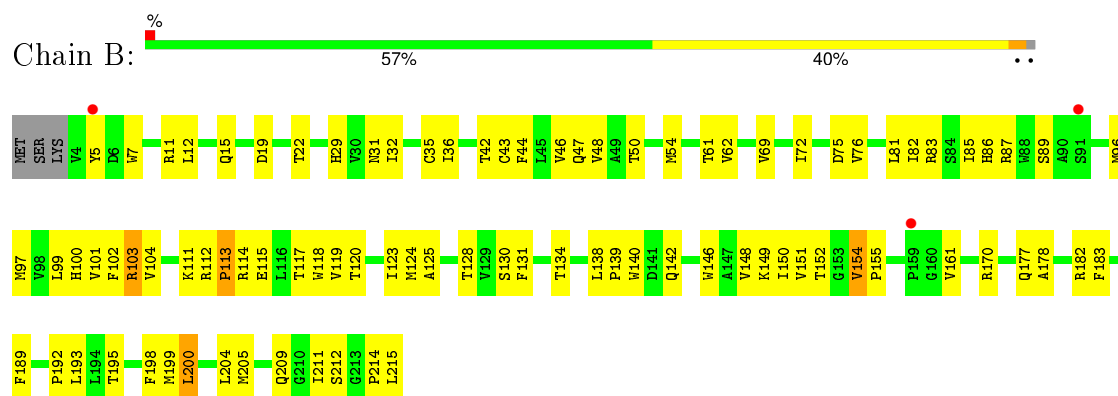
- Molecule 3: Cytochrome B6-F complex iron-sulfur subunit

Chain C:

K149 F150 K151 C152 P153 C154 H155 G156 S157 Q158 Y159 N160 K164 V165 V166 R167 L172 S173 L174 A175 L176 A177 H178 A182 E183 SER G185 L186 V187 T188 F189 S190 T191 W192 T195 D196 F197 R198 T199 G200 L201 E202 P203 W204 W205 A206
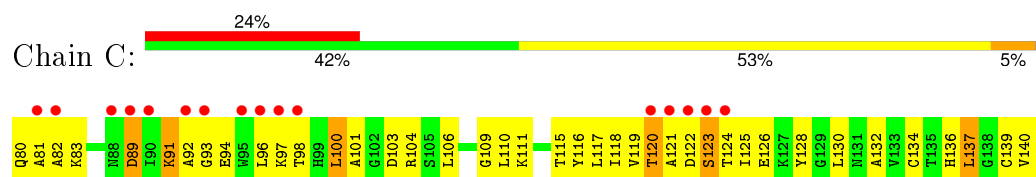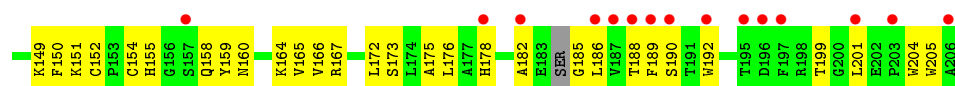
• Molecule 4: Cytochrome b6-f complex subunit 4

Chain D:

48%   45%   6% •

MET SER VAL T4 K5 D8 I9 S10 D11 P12 V13 L14 K15 A16 K17 L18 A19 H24 N25 T26 Y27 Q28 E29 P30 N34 I37 Y38 M39 F40 P41 V42 V43 I44 L45 G46 T47 I52 A61 A66 N67 L73 E74 I75 F81 Y82 P83 V84 F85 Q86 I87 L88

R89 V90 V91 P92 N93 K94 L95 L96 G97 V98 L99 L100 M101 A102 A103 V104 P105 A106 G107 L108 I109 T110 V111 I114 I117 N118 K119 F120 Q121 N122 P123 Y124 R125 R126 P127 I128 L132 L135 G136 T137 L138 V139 S147 P150 I151 D152 I153 S154 L155 G158 L159

• Molecule 5: Cytochrome B6-F complex iron-sulfur subunit

Chain R:

6%

57%   16% 6%   20%

ALA ALA S33 S34 E35 D38 M39 N40 K41 R42 N43 I44 M45 I48 L55 P56 F67 P71 SER SER GLY GLY GLY GLY GLY

• Molecule 6: Cytochrome b6f complex subunit petG

Chain G:

65%   16%   19%

M1 L13 V14 P15 V16 I21 Y26 L30 ARG GLY ASP LEU ALA THR TYR

• Molecule 7: Cytochrome b6f complex subunit petL

Chain L:

53%   34%   13%

M1 L2 T3 I4 L11 T18 I21 G24 L25 L26 K27 V28 V29 K30 L31 I32

• Molecule 8: Cytochrome b6f complex subunit PETM

Chain M:

46%   33% 8%   13%

GLY E62 F65 I66 T69 T72 M73 M76 L81 A82 I83 V86 R89 V90 E91 S92 L93 V94 E95 GLU GLY LYS ILE

• Molecule 9: Cytochrome b6f complex subunit PETN

Chain N:

65%   35%

G68 E69 P70 A71 I72 V73 Q74 F86 S89 W93 G94 R95 S96 G97 L98

4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	102.45Å 171.21Å 351.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.42 – 3.10 35.14 – 2.97	Depositor EDS
% Data completeness (in resolution range)	99.5 (34.42-3.10) 92.7 (35.14-2.97)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$<I/\sigma(I)>$ [1]	3.29 (at 2.95Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.222 , 0.261 0.219 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	62.5	Xtriage
Anisotropy	0.418	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 77.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$<|L|> = 0.50, <L^2> = 0.34$	Xtriage
Outliers	4 of 59045 reflections (0.007%)	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	7778	wwPDB-VP
Average B, all atoms (Å^2)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.58% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $<|L|>$, $<L^2>$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: LFA, CLA, FES, TDS, HEM, LMG, BCR, SQD

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$|Z|$ >5	RMSZ	#$|Z|$ >5
1	A	0.36	0/2318	0.64	0/3148
2	B	0.48	0/1732	0.64	0/2360
3	C	0.29	0/979	0.55	0/1333
4	D	0.38	0/1238	0.62	0/1698
5	R	0.46	0/289	0.94	1/393 (0.3%)
6	G	0.42	0/228	0.60	0/313
7	L	0.39	0/244	0.61	0/329
8	M	0.42	0/248	0.64	0/335
9	N	0.56	0/237	0.57	0/321
All	All	0.40	0/7513	0.63	1/10230 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	R	71	PRO	CA-N-CD	-13.91	92.03	111.50

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2266	0	2301	100	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1681	0	1692	103	0
3	C	955	0	922	67	0
4	D	1201	0	1256	87	0
5	R	283	0	291	13	0
6	G	224	0	248	9	0
7	L	242	0	286	12	0
8	M	247	0	263	19	0
9	N	231	0	230	19	0
10	A	43	0	30	2	0
10	B	129	0	90	5	0
11	C	4	0	0	1	0
12	D	65	0	72	5	0
13	B	27	0	35	3	0
14	D	30	0	38	2	0
15	R	33	0	29	1	0
16	B	20	0	42	2	0
17	D	53	0	79	3	0
17	L	42	0	54	4	0
18	B	2	0	0	0	0
All	All	7778	0	7958	381	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 24.

The worst 5 of 381 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:31:ASN:HA	9:N:98:LEU:HD22	1.24	1.18
3:C:178:HIS:HB2	3:C:190:SER:HB2	1.34	1.10
2:B:50:THR:HG23	2:B:86:HIS:HD1	1.07	1.07
1:A:59:GLN:HE22	1:A:156:ARG:HG3	1.27	1.00
2:B:142:GLN:NE2	4:D:67:ASN:H	1.63	0.96

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	290/292 (99%)	263 (91%)	21 (7%)	6 (2%)	9	37
2	B	210/215 (98%)	179 (85%)	29 (14%)	2 (1%)	19	58
3	C	122/127 (96%)	96 (79%)	22 (18%)	4 (3%)	5	26
4	D	154/159 (97%)	134 (87%)	15 (10%)	5 (3%)	5	26
5	R	37/49 (76%)	32 (86%)	5 (14%)	0	100	100
6	G	28/37 (76%)	24 (86%)	4 (14%)	0	100	100
7	L	30/32 (94%)	25 (83%)	5 (17%)	0	100	100
8	M	32/39 (82%)	31 (97%)	0	1 (3%)	5	27
9	N	29/31 (94%)	27 (93%)	2 (7%)	0	100	100
All	All	932/981 (95%)	811 (87%)	103 (11%)	18 (2%)	10	40

5 of 18 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	89	ASP
1	A	140	ASN
1	A	165	LYS
1	A	198	LYS
3	C	100	LEU

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	246/246 (100%)	233 (95%)	13 (5%)	28	64
2	B	179/182 (98%)	171 (96%)	8 (4%)	34	70
3	C	99/100 (99%)	96 (97%)	3 (3%)	48	81
4	D	131/134 (98%)	126 (96%)	5 (4%)	40	76
5	R	30/32 (94%)	27 (90%)	3 (10%)	9	34
6	G	25/30 (83%)	25 (100%)	0	100	100
7	L	27/27 (100%)	23 (85%)	4 (15%)	4	16
8	M	26/29 (90%)	24 (92%)	2 (8%)	16	50
9	N	24/24 (100%)	24 (100%)	0	100	100
All	All	787/804 (98%)	749 (95%)	38 (5%)	31	69

5 of 38 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	103	ARG
3	C	91	LYS
7	L	11	LEU
2	B	193	LEU
3	C	98	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 19 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	47	GLN
2	B	209	GLN
4	D	118	ASN
2	B	31	ASN
4	D	121	GLN

5.3.3   RNA (i)

There are no RNA molecules in this entry.

5.4   Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

12 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$|Z| > 2$	Counts	RMSZ	#$|Z| > 2$
10	HEM	A	900	1	30,50,50	2.52	9 (30%)	24,82,82	2.93	9 (37%)
10	HEM	B	901	2	30,50,50	2.14	6 (20%)	24,82,82	2.53	9 (37%)
10	HEM	B	902	2	30,50,50	1.93	5 (16%)	24,82,82	2.52	10 (41%)
10	HEM	B	903	18,2	30,50,50	2.37	10 (33%)	24,82,82	3.15	12 (50%)
13	BCR	B	904	-	27,27,41	1.54	4 (14%)	35,35,56	1.98	11 (31%)
16	LFA	B	960	-	19,19,19	0.42	0	18,18,18	0.60	0
11	FES	C	210	3	0,4,4	0.00	-	0,4,4	0.00	-
12	CLA	D	910	-	55,73,73	1.28	6 (10%)	61,113,113	1.56	9 (14%)
14	TDS	D	920	-	29,31,31	3.05	13 (44%)	29,40,40	2.37	8 (27%)
17	LMG	D	953	-	53,53,55	1.37	8 (15%)	61,61,63	1.42	6 (9%)
17	LMG	L	951	-	42,42,55	1.32	6 (14%)	50,50,63	1.45	5 (10%)
15	SQD	R	950	-	32,33,54	2.09	10 (31%)	40,44,65	3.30	12 (30%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	HEM	A	900	1	-	0/10/54/54	0/0/8/8
10	HEM	B	901	2	-	0/10/54/54	0/0/8/8
10	HEM	B	902	2	-	0/10/54/54	0/0/8/8
10	HEM	B	903	18,2	-	0/10/54/54	0/0/8/8
13	BCR	B	904	-	-	0/21/38/63	0/1/1/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	LFA	B	960	-	-	0/17/17/17	0/0/0/0
11	FES	C	210	3	-	0/0/4/4	0/1/1/1
12	CLA	D	910	-	4/4/20/25	0/37/135/135	0/0/9/9
14	TDS	D	920	-	-	1/16/17/17	0/2/2/2
17	LMG	D	953	-	-	0/48/68/70	0/1/1/1
17	LMG	L	951	-	-	0/37/57/70	0/1/1/1
15	SQD	R	950	-	-	0/28/48/69	0/1/1/1

The worst 5 of 77 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	903	HEM	C2D-C3D	-6.84	1.34	1.54
10	A	900	HEM	C2D-C3D	-6.83	1.34	1.54
10	B	901	HEM	C3B-C4B	-6.61	1.46	1.51
10	B	902	HEM	C3B-C4B	-5.95	1.46	1.51
10	A	900	HEM	C3B-C4B	-5.50	1.47	1.51

The worst 5 of 91 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	B	903	HEM	C3B-CAB-CBB	-6.99	113.73	124.46
10	A	900	HEM	C3B-CAB-CBB	-6.52	114.46	124.46
10	A	900	HEM	C3C-CAC-CBC	-5.96	115.32	124.46
10	B	903	HEM	C3C-CAC-CBC	-5.67	115.76	124.46
10	B	903	HEM	CBA-CAA-C2A	-4.12	105.15	112.53

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
12	D	910	CLA	C8
12	D	910	CLA	NC
12	D	910	CLA	ND
12	D	910	CLA	NA

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	D	920	TDS	CAH-CAP-CAQ-CAR

There are no ring outliers.

11 monomers are involved in 28 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	A	900	HEM	2	0
10	B	901	HEM	4	0
10	B	903	HEM	1	0
13	B	904	BCR	3	0
16	B	960	LFA	2	0
11	C	210	FES	1	0
12	D	910	CLA	5	0
14	D	920	TDS	2	0
17	D	953	LMG	3	0
17	L	951	LMG	4	0
15	R	950	SQD	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	292/292 (100%)	-0.14	3 (1%)	84	69	42, 66, 102, 131	3 (1%)
2	B	212/215 (98%)	-0.08	3 (1%)	78	60	29, 47, 76, 114	0
3	C	126/127 (99%)	1.04	31 (24%)	1	0	70, 121, 159, 180	0
4	D	156/159 (98%)	-0.18	0	100	100	37, 62, 96, 131	0
5	R	39/49 (79%)	-0.08	3 (7%)	16	5	37, 51, 135, 159	0
6	G	30/37 (81%)	-0.19	0	100	100	41, 54, 77, 97	0
7	L	32/32 (100%)	-0.30	0	100	100	46, 65, 86, 126	0
8	M	34/39 (87%)	-0.39	0	100	100	41, 57, 83, 130	0
9	N	31/31 (100%)	-0.34	0	100	100	36, 50, 68, 91	0
All	All	952/981 (97%)	0.00	40 (4%)	40	19	29, 62, 135, 180	3 (0%)

The worst 5 of 40 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	R	33	SER	4.2
3	C	186	LEU	3.9
3	C	93	GLY	3.6
3	C	196	ASP	3.6
3	C	81	ALA	3.4

6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

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6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
17	LMG	D	953	53/55	0.63	0.43	3.62	88,88,107,107	0
14	TDS	D	920	30/30	0.87	0.30	3.01	87,89,89,89	0
16	LFA	B	960	20/20	0.91	0.29	2.89	59,59,59,59	0
13	BCR	B	904	27/40	0.85	0.40	2.42	49,49,64,64	0
17	LMG	L	951	42/55	0.77	0.33	1.52	78,85,85,85	0
12	CLA	D	910	65/65	0.88	0.28	1.19	63,70,92,94	0
15	SQD	R	950	33/54	0.93	0.19	0.14	62,62,111,111	0
10	HEM	A	900	43/43	0.95	0.22	-0.15	63,67,77,80	0
10	HEM	B	901	43/43	0.97	0.21	-0.37	30,37,45,50	0
10	HEM	B	902	43/43	0.97	0.19	-0.46	35,43,48,50	0
10	HEM	B	903	43/43	0.95	0.21	-0.63	53,53,53,53	0
11	FES	C	210	4/4	0.99	0.09	-1.62	62,62,63,65	0

6.5 Other polymers (i)

There are no such residues in this entry.