Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 05:05 PM GMT

PDB ID	:	4H44
Title	:	2.70 A Cytochrome b6f Complex Structure From Nostoc PCC 7120
Authors	:	Hasan, S.S.; Yamashita, E.; Baniulis, D.; Cramer, W.A.
Deposited on	:	2012-09-16
Resolution	:	2.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

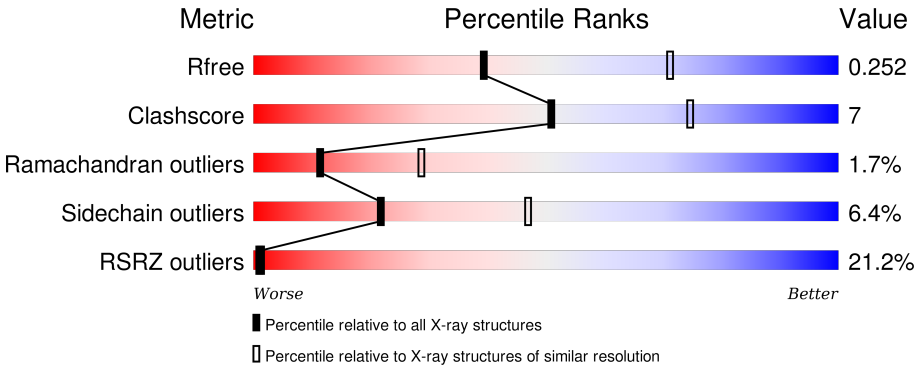
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.70 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

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	215	14% 82% 16% •
2	B	160	18% 80% 19% •
3	C	289	20% 79% 19% •
4	D	179	40% 83% 9% • 7%
5	E	31	13% 87% 13%

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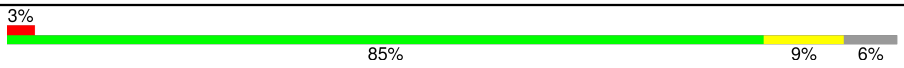
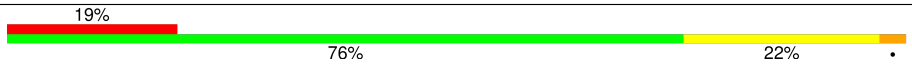
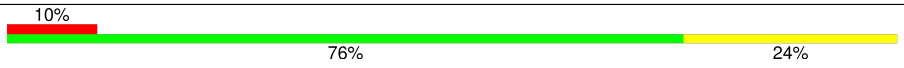
Mol	Chain	Length	Quality of chain
6	F	34	
7	G	37	
8	H	29	

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
10	UMQ	A	304	X	-	-	X
10	UMQ	A	305	X	-	-	-
10	UMQ	A	307	X	-	-	-
10	UMQ	A	309	X	-	-	-
10	UMQ	F	101	X	-	-	-
13	CLA	B	201	X	-	-	-
14	OPC	B	202	-	-	-	X
14	OPC	C	302	-	-	-	X

2 Entry composition

There are 21 unique types of molecules in this entry. The entry contains 16386 atoms, of which 8258 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 Cytochrome b6.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	215	3451	1144	1736	272	288	11	0	0	0

- Molecule 2 is a protein called Cytochrome b6-f complex subunit 4.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
2	B	160	2531	830	1292	195	208	6	0	0	0

- Molecule 3 is a protein called Apocytochrome f.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
3	C	289	4379	1396	2184	364	429	6	0	0	0

- Molecule 4 is a protein called Cytochrome b6-f complex iron-sulfur subunit 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
4	D	166	2459	791	1210	213	239	6	0	0	0

- Molecule 5 is a protein called Cytochrome b6-f complex subunit 6.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
5	E	31	484	157	257	35	34	1	0	0	0

- Molecule 6 is a protein called Cytochrome b6-f complex subunit 7.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
6	F	32	483	156	252	36	38	1	0	0	0

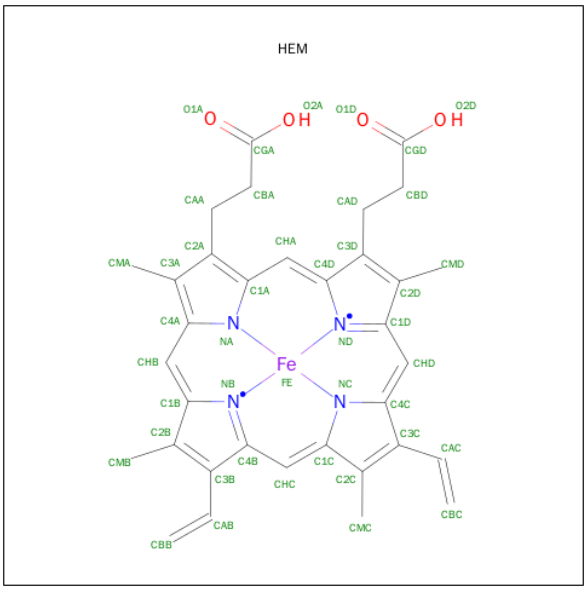
- Molecule 7 is a protein called Cytochrome b6-f complex subunit 5.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
7	G	37	Total	C	H	N	O	S	0	0	0
			584	188	303	44	48	1			

- Molecule 8 is a protein called Cytochrome b6-f complex subunit 8.

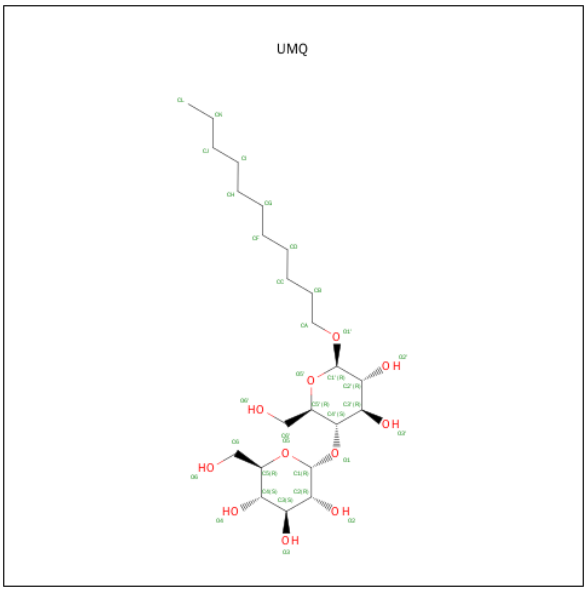
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
8	H	29	Total	C	H	N	O	S	0	0	0
			470	155	243	36	34	2			

- Molecule 9 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



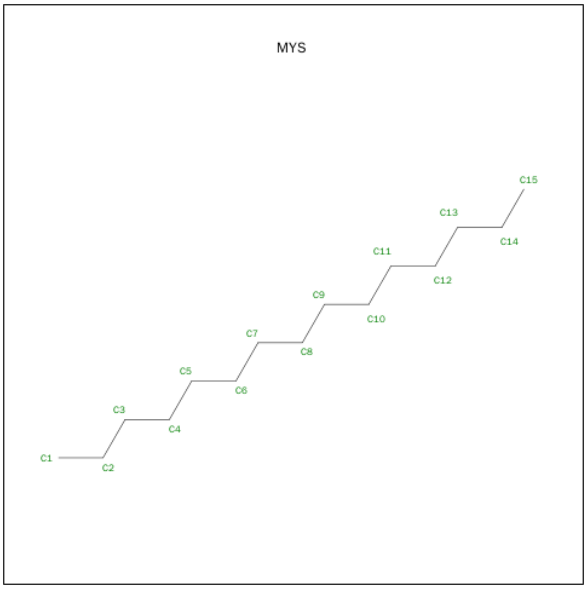
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
9	A	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		
9	A	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		
9	A	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		
9	C	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		

- Molecule 10 is UNDECYL-MALTOSIDE (three-letter code: UMQ) (formula: $C_{23}H_{44}O_{11}$).



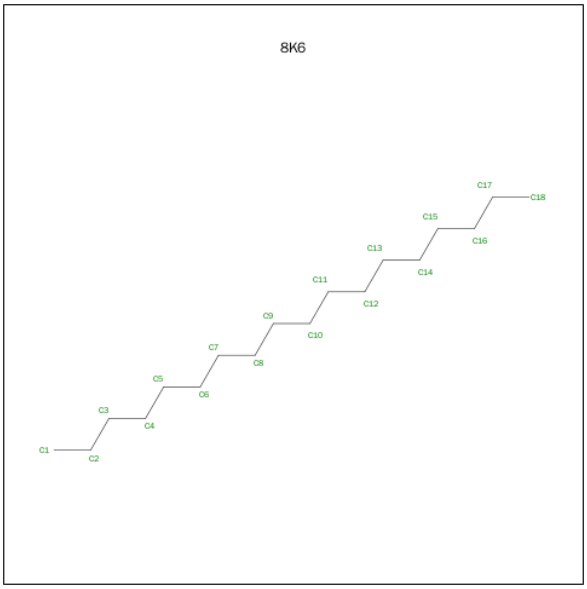
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	A	1	Total	C	H	O	0	0
			77	23	43	11		
10	A	1	Total	C	H	O	0	0
			77	23	43	11		
10	A	1	Total	C	H	O	0	0
			78	23	44	11		
10	A	1	Total	C	H	O	0	0
			77	23	43	11		
10	F	1	Total	C	H	O	0	0
			77	23	43	11		

- Molecule 11 is PENTADECANE (three-letter code: MYS) (formula: $C_{15}H_{32}$).



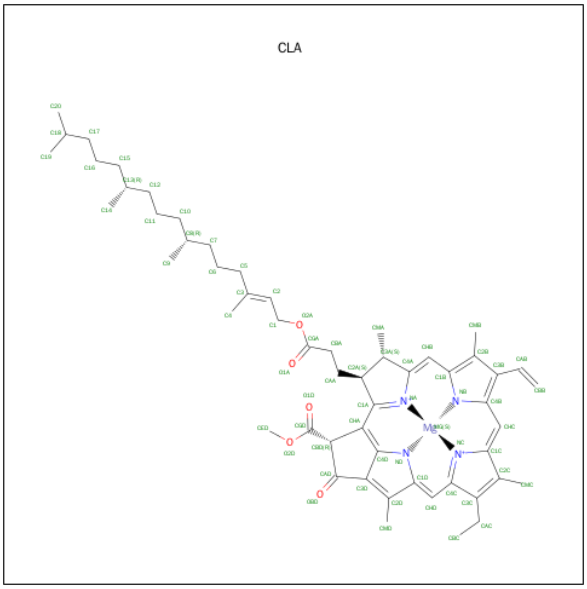
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	1	Total C H 47 15 32	0	0

- Molecule 12 is OCTADECANE (three-letter code: 8K6) (formula: $C_{18}H_{38}$).



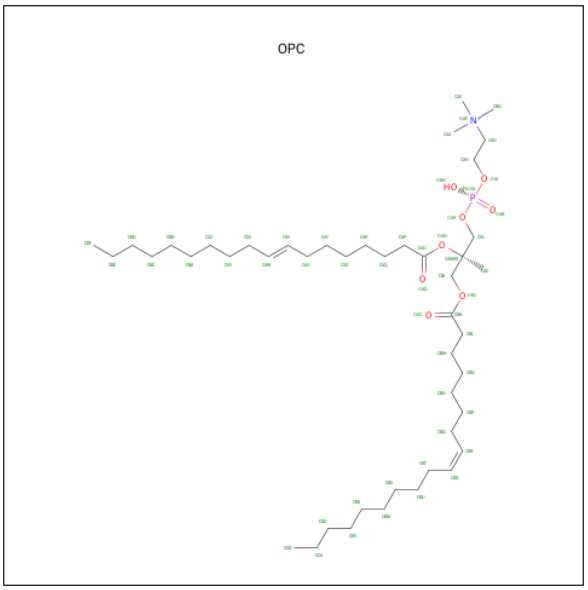
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	A	1	Total C H 56 18 38	0	0

- Molecule 13 is CHLOROPHYLL A (three-letter code: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



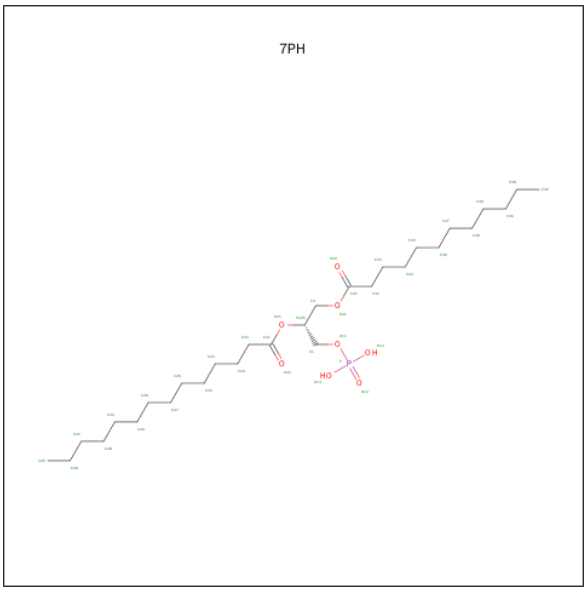
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
13	B	1	Total	C	H	Mg	N	O	0	0
			127	55	62	1	4	5		

- Molecule 14 is (7R,17E)-4-HYDROXY-N,N,N,7-TETRAMETHYL-7-[(8E)-OCTADEC-8-ENOYLOXY]-10-OXO-3,5,9-TRIOXA-4-PHOSPHAHEPTACOS-17-EN-1-AMINIUM 4-OXIDE (three-letter code: OPC) (formula: $C_{45}H_{87}NO_8P$).



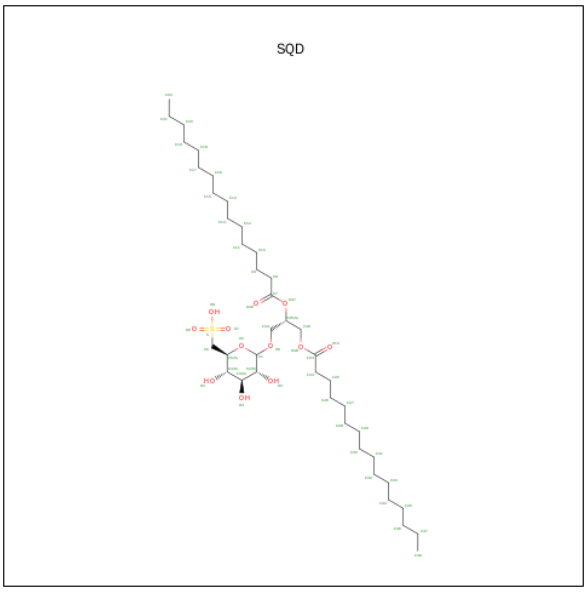
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
14	B	1	Total	C	H	N	O	P	0	0
			137	44	83	1	8	1		
14	C	1	Total	C	H	N	O	P	0	0
			137	44	83	1	8	1		

- Molecule 15 is (1R)-2-(DODECANOYLOXY)-1-[(PHOSPHONOOXY)METHYL]ETHYL TETRADECANOATE (three-letter code: 7PH) (formula: $C_{29}H_{57}O_8P$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
15	C	1	Total	C	H	O	0	0
			81	27	49	5		

- Molecule 16 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula: $C_{41}H_{78}O_{12}S$).

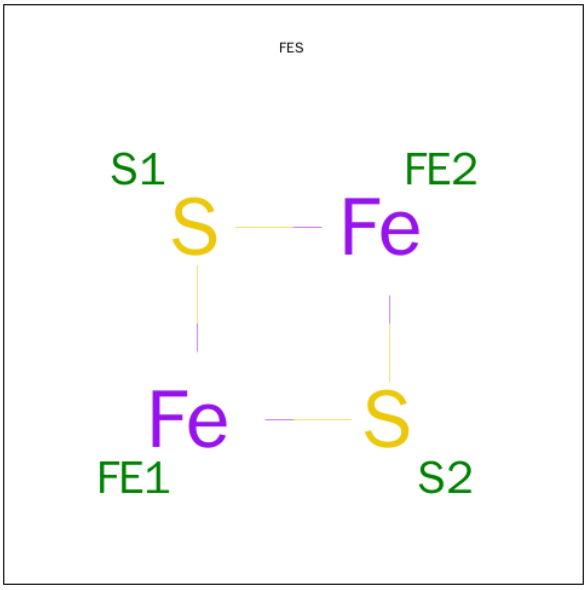


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
16	D	1	Total	C	H	O	S	0	0
			53	16	24	12	1		

- Molecule 17 is CADMIUM ION (three-letter code: CD) (formula: Cd).

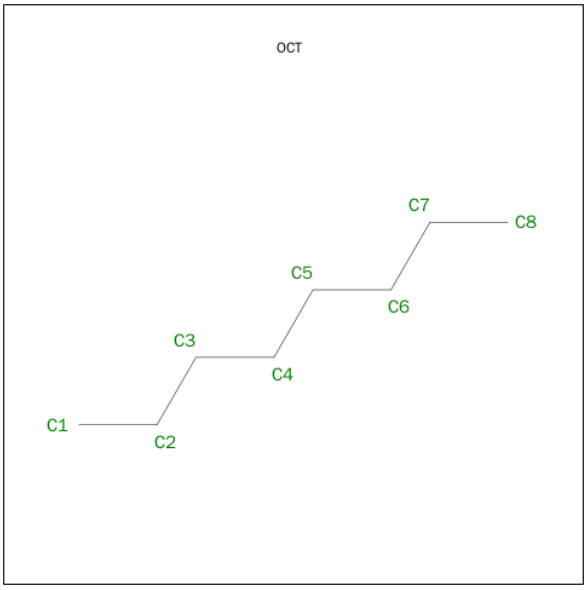
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	C	1	Total Cd 1 1	0	0

- Molecule 18 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



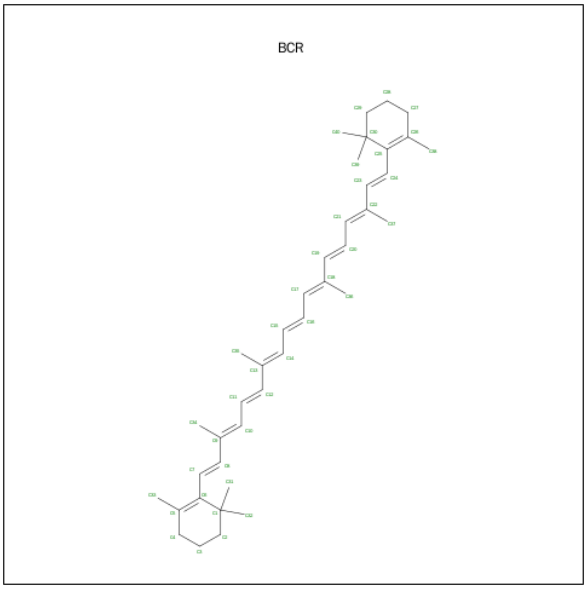
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	D	1	Total Fe S 4 2 2	0	0

- Molecule 19 is N-OCTANE (three-letter code: OCT) (formula: C_8H_{18}).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
19	F	1	Total C H 26 8 18	0	0

- Molecule 20 is BETA-CAROTENE (three-letter code: BCR) (formula: $C_{40}H_{56}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
20	G	1	Total C H 96 40 56	0	0

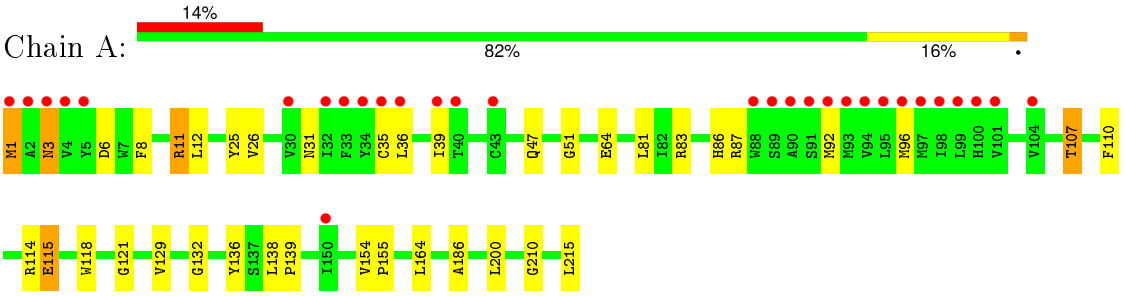
- Molecule 21 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
21	A	26	Total O 26 26	0	0
21	B	22	Total O 22 22	0	0
21	C	45	Total O 45 45	0	0
21	D	1	Total O 1 1	0	0
21	G	5	Total O 5 5	0	0
21	H	3	Total O 3 3	0	0

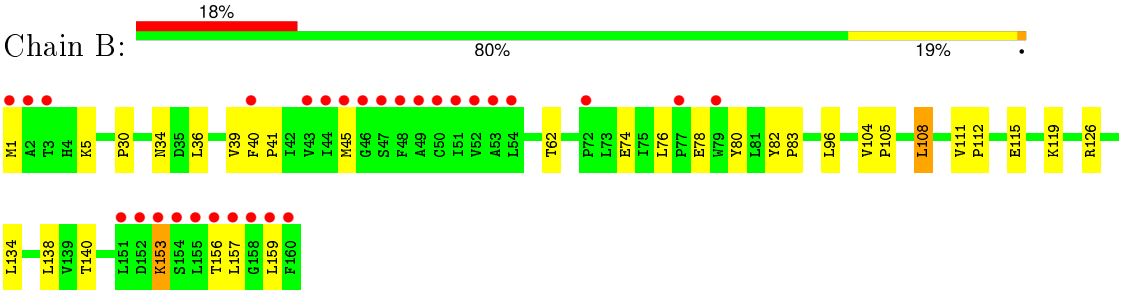
3 Residue-property plots (i)

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.

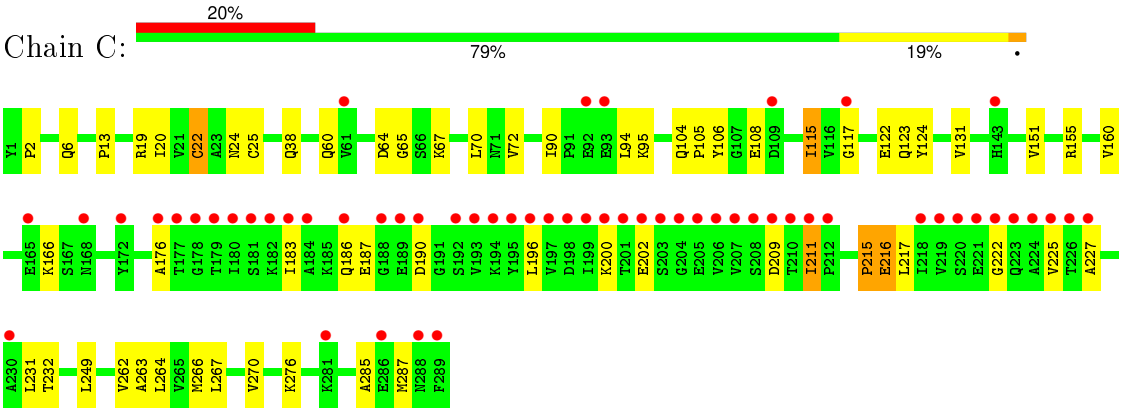
- Molecule 1: Cytochrome b6



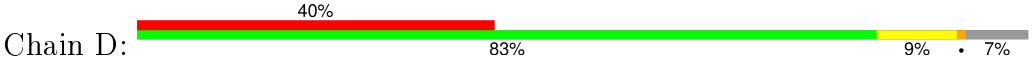
- Molecule 2: Cytochrome b6-f complex subunit 4

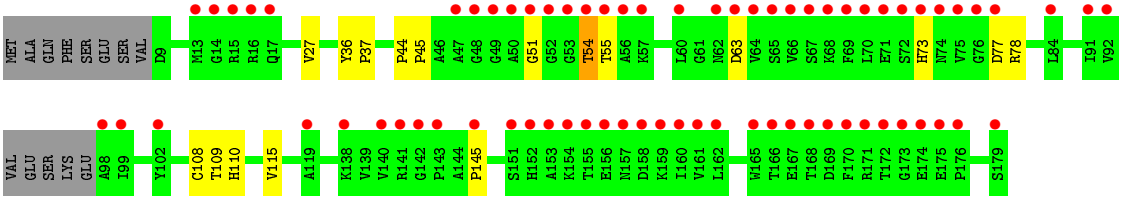


- Molecule 3: Apocytochrome f

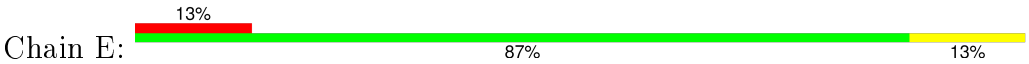


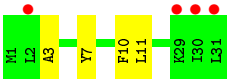
- Molecule 4: Cytochrome b6-f complex iron-sulfur subunit 1



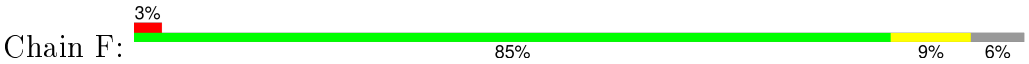


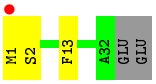
- Molecule 5: Cytochrome b6-f complex subunit 6





- Molecule 6: Cytochrome b6-f complex subunit 7





- Molecule 7: Cytochrome b6-f complex subunit 5

- Molecule 8: Cytochrome b6-f complex subunit 8

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α, β, γ	159.13Å 159.13Å 364.37Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	39.55 – 2.70 39.55 – 2.70	Depositor EDS
% Data completeness (in resolution range)	98.0 (39.55-2.70) 98.0 (39.55-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.39 (at 2.69Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, R_{free}	0.220 , 0.246 0.227 , 0.252	Depositor DCC
R_{free} test set	3731 reflections (5.31%)	DCC
Wilson B-factor (Å^2)	69.7	Xtriage
Anisotropy	0.071	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.41 , 71.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	0 of 74023 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	16386	wwPDB-VP
Average B, all atoms (Å^2)	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.58% of the height of the origin peak. No significant pseudotranslation is detected.*

[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: UMQ, MYS, CLA, CD, 7PH, FES, OPC, HEM, 8K6, OCT, 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	0.24	0/1768	0.39	0/2411
2	B	0.24	0/1278	0.45	1/1752 (0.1%)
3	C	0.22	0/2241	0.41	0/3053
4	D	0.21	0/1280	0.40	0/1745
5	E	0.25	0/230	0.36	0/309
6	F	0.25	0/234	0.35	0/315
7	G	0.25	0/286	0.41	0/387
8	H	0.26	0/233	0.42	0/319
All	All	0.23	0/7550	0.41	1/10291 (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})
2	B	39	VAL	CG1-CB-CG2	6.68	121.59	110.90

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	1715	1736	1734	30	1
2	B	1239	1292	1290	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	2195	2184	2183	31	0
4	D	1249	1210	1208	8	0
5	E	227	257	257	2	0
6	F	231	252	252	2	0
7	G	281	303	303	6	0
8	H	227	243	243	9	0
9	A	129	90	90	19	0
9	C	43	30	30	7	0
10	A	136	173	166	5	0
10	F	34	43	42	1	0
11	A	15	32	32	1	0
12	A	18	38	38	0	0
13	B	65	62	72	3	0
14	B	54	83	83	0	0
14	C	54	83	83	2	0
15	C	32	49	45	0	0
16	D	29	24	22	0	0
17	C	1	0	0	0	0
18	D	4	0	0	1	0
19	F	8	18	18	0	0
20	G	40	56	56	5	0
21	A	26	0	0	5	0
21	B	22	0	0	4	0
21	C	45	0	0	3	0
21	D	1	0	0	0	0
21	G	5	0	0	0	0
21	H	3	0	0	0	0
All	All	8128	8258	8247	112	1

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 7.

All (112) 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:126:ARG:NH1	21:B:319:HOH:O	2.04	0.90
3:C:25:CYS:SG	9:C:301:HEM:CAC	2.65	0.84
1:A:35:CYS:SG	9:A:303:HEM:CAB	2.70	0.80
9:A:303:HEM:O1A	21:A:425:HOH:O	2.03	0.77
1:A:3:ASN:ND2	1:A:6:ASP:OD2	2.20	0.75
10:A:307:UMQ:H51	2:B:36:LEU:HD21	1.71	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:47:GLN:O	21:A:422:HOH:O	2.06	0.72
2:B:140:THR:OG1	21:B:318:HOH:O	2.08	0.71
7:G:23:TYR:CE1	20:G:101:BCR:H23C	2.25	0.71
3:C:151:VAL:O	21:C:417:HOH:O	2.07	0.70
13:B:201:CLA:HHC	13:B:201:CLA:HBB1	1.75	0.67
3:C:22:CYS:SG	9:C:301:HEM:CAB	2.83	0.67
9:C:301:HEM:HBB2	9:C:301:HEM:HMB1	1.76	0.67
1:A:83:ARG:NH1	9:A:301:HEM:O1D	2.28	0.66
2:B:115:GLU:OE1	21:B:319:HOH:O	2.15	0.64
1:A:114:ARG:NH1	1:A:210:GLY:O	2.31	0.64
9:A:303:HEM:HHD	9:A:303:HEM:HBC2	1.80	0.64
1:A:35:CYS:SG	9:A:303:HEM:CBB	2.86	0.63
1:A:35:CYS:HG	9:A:303:HEM:CAB	2.11	0.63
3:C:25:CYS:SG	9:C:301:HEM:CBC	2.87	0.62
3:C:64:ASP:OD2	3:C:65:GLY:N	2.34	0.61
3:C:262:VAL:HG13	8:H:14:VAL:HG13	1.81	0.61
1:A:39:ILE:HD11	20:G:101:BCR:H312	1.84	0.59
3:C:270:VAL:HA	8:H:21:MET:HE2	1.84	0.59
9:A:303:HEM:HHA	9:A:303:HEM:HBD1	1.86	0.58
3:C:263:ALA:HA	3:C:266:MET:HE2	1.86	0.58
2:B:45:MET:HE3	4:D:27:VAL:HG13	1.85	0.58
3:C:262:VAL:HG13	8:H:14:VAL:CG1	2.34	0.57
1:A:1:MET:SD	1:A:1:MET:N	2.78	0.56
3:C:215:PRO:O	3:C:216:GLU:HB3	2.05	0.56
1:A:86:HIS:CE1	9:A:301:HEM:C4D	2.94	0.54
1:A:86:HIS:CD2	21:A:422:HOH:O	2.59	0.54
6:F:13:PHE:CD1	7:G:16:VAL:HG13	2.43	0.54
3:C:270:VAL:HA	8:H:21:MET:CE	2.39	0.53
1:A:215:LEU:O	21:A:406:HOH:O	2.19	0.53
5:E:7:TYR:CZ	5:E:11:LEU:HD11	2.43	0.53
3:C:215:PRO:O	3:C:216:GLU:CB	2.55	0.53
8:H:28:GLY:O	8:H:29:LEU:HB2	2.09	0.52
9:A:301:HEM:HMC1	9:A:301:HEM:HBC2	1.92	0.52
2:B:104:VAL:HB	2:B:105:PRO:CD	2.40	0.52
4:D:36:TYR:HB3	4:D:37:PRO:HD3	1.92	0.52
1:A:138:LEU:N	1:A:139:PRO:CD	2.74	0.51
2:B:36:LEU:O	2:B:40:PHE:HB2	2.11	0.51
7:G:20:GLY:N	20:G:101:BCR:H363	2.26	0.51
8:H:17:TRP:O	8:H:21:MET:HG2	2.11	0.51
14:C:302:OPC:HAR1	5:E:3:ALA:HB1	1.93	0.51
3:C:183:ILE:HG22	3:C:183:ILE:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:303:HEM:C2A	10:A:307:UMQ:H62	2.45	0.50
9:A:303:HEM:CBA	10:A:307:UMQ:H41	2.42	0.50
3:C:160:VAL:O	9:C:301:HEM:HMD1	2.10	0.50
4:D:108:CYS:SG	4:D:115:VAL:HG22	2.51	0.50
9:A:303:HEM:HMB1	9:A:303:HEM:HBB2	1.94	0.50
1:A:136:TYR:CE1	2:B:78:GLU:CG	2.94	0.50
7:G:13:LEU:HA	7:G:16:VAL:HG23	1.93	0.49
13:B:201:CLA:CBB	13:B:201:CLA:HHC	2.40	0.49
9:A:302:HEM:HMB1	9:A:302:HEM:HBB2	1.95	0.49
2:B:30:PRO:O	2:B:34:ASN:HB2	2.13	0.49
9:A:301:HEM:HBB2	9:A:301:HEM:HMB1	1.93	0.49
3:C:19:ARG:NH1	3:C:24:ASN:OD1	2.46	0.49
9:A:302:HEM:HBC2	9:A:302:HEM:HMC1	1.95	0.48
9:C:301:HEM:HBC2	9:C:301:HEM:HMC2	1.95	0.48
1:A:86:HIS:HE1	9:A:301:HEM:C4D	2.16	0.48
3:C:22:CYS:SG	9:C:301:HEM:CBB	3.02	0.47
1:A:31:ASN:HA	8:H:29:LEU:HD13	1.96	0.47
2:B:45:MET:CE	4:D:27:VAL:HG13	2.45	0.47
4:D:73:HIS:ND1	4:D:73:HIS:O	2.48	0.47
1:A:92:MET:O	1:A:96:MET:HG2	2.15	0.47
1:A:186:ALA:HB2	11:A:306:MYS:H81	1.96	0.46
1:A:107:THR:O	1:A:107:THR:HG23	2.14	0.46
4:D:77:ASP:N	4:D:77:ASP:OD2	2.47	0.46
1:A:35:CYS:SG	9:A:303:HEM:C3B	3.07	0.46
2:B:104:VAL:HB	2:B:105:PRO:HD3	1.96	0.46
3:C:115:ILE:HG21	21:C:413:HOH:O	2.16	0.46
2:B:82:TYR:HB2	2:B:83:PRO:HD3	1.97	0.45
2:B:153:LYS:O	2:B:157:LEU:N	2.50	0.45
2:B:111:VAL:N	2:B:112:PRO:HD2	2.32	0.45
3:C:72:VAL:HG21	3:C:124:TYR:O	2.17	0.45
3:C:211:ILE:O	3:C:211:ILE:HG13	2.15	0.45
1:A:154:VAL:N	1:A:155:PRO:CD	2.80	0.44
3:C:2:PRO:HG2	3:C:117:GLY:HA2	1.98	0.44
3:C:38:GLN:N	14:C:302:OPC:OAB	2.50	0.44
1:A:136:TYR:CE1	2:B:78:GLU:HG2	2.53	0.44
1:A:8:PHE:O	1:A:12:LEU:HB2	2.18	0.44
3:C:231:LEU:HD12	3:C:232:THR:HG23	1.99	0.44
7:G:12:GLY:O	7:G:16:VAL:HG22	2.18	0.43
3:C:13:PRO:HB3	3:C:106:TYR:CE1	2.53	0.43
20:G:101:BCR:C32	8:H:19:ILE:HD13	2.48	0.43
3:C:217:LEU:HD23	3:C:232:THR:HG22	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:B:308:HOH:O	3:C:276:LYS:NZ	2.52	0.43
3:C:186:GLN:OE1	3:C:187:GLU:N	2.52	0.43
1:A:118:TRP:CE3	9:A:302:HEM:HAC	2.54	0.43
1:A:51:GLY:HA3	21:A:422:HOH:O	2.19	0.43
3:C:6:GLN:NE2	21:C:413:HOH:O	2.51	0.42
3:C:266:MET:SD	8:H:13:VAL:HG12	2.59	0.42
1:A:121:GLY:O	9:A:302:HEM:HMC3	2.19	0.42
4:D:110:HIS:HB3	18:D:202:FES:S2	2.59	0.42
10:A:307:UMQ:H31	2:B:36:LEU:HD11	2.01	0.42
3:C:90:ILE:O	3:C:95:LYS:NZ	2.49	0.42
1:A:129:VAL:HG21	13:B:201:CLA:H11	2.02	0.42
3:C:176:ALA:HA	3:C:227:ALA:HB2	2.02	0.42
2:B:119:LYS:HG2	2:B:119:LYS:O	2.20	0.42
1:A:25:TYR:CZ	2:B:5:LYS:HD3	2.55	0.41
1:A:132:GLY:HA3	2:B:80:TYR:OH	2.20	0.41
7:G:23:TYR:CD2	20:G:101:BCR:H19C	2.56	0.41
10:A:307:UMQ:O3'	10:A:307:UMQ:O2	2.29	0.41
1:A:110:PHE:HB3	1:A:118:TRP:CE3	2.56	0.41
2:B:108:LEU:HA	2:B:108:LEU:HD13	1.94	0.41
2:B:82:TYR:N	2:B:83:PRO:CD	2.84	0.41
2:B:40:PHE:HB2	2:B:41:PRO:HD3	2.02	0.40
3:C:104:GLN:HA	3:C:105:PRO:HD3	1.97	0.40
4:D:44:PRO:HA	4:D:45:PRO:HD3	1.98	0.40
6:F:1:MET:O	10:F:101:UMQ:O6'	2.20	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11:ARG:NH1	1:A:115:GLU:OE1[12_565]	2.04	0.16

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	213/215 (99%)	206 (97%)	6 (3%)	1 (0%)	34 63
2	B	158/160 (99%)	149 (94%)	8 (5%)	1 (1%)	30 59
3	C	287/289 (99%)	252 (88%)	27 (9%)	8 (3%)	6 15
4	D	162/179 (90%)	136 (84%)	22 (14%)	4 (2%)	7 18
5	E	29/31 (94%)	28 (97%)	1 (3%)	0	100 100
6	F	30/34 (88%)	28 (93%)	1 (3%)	1 (3%)	5 11
7	G	35/37 (95%)	34 (97%)	0	1 (3%)	6 14
8	H	27/29 (93%)	27 (100%)	0	0	100 100
All	All	941/974 (97%)	860 (91%)	65 (7%)	16 (2%)	11 29

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	190	ASP
3	C	216	GLU
4	D	78	ARG
3	C	200	LYS
3	C	222	GLY
3	C	287	MET
4	D	145	PRO
7	G	36	GLY
1	A	3	ASN
3	C	202	GLU
3	C	285	ALA
4	D	54	THR
2	B	74	GLU
3	C	215	PRO
6	F	2	SER
4	D	51	GLY

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	184/184 (100%)	173 (94%)	11 (6%)	24 50
2	B	134/134 (100%)	124 (92%)	10 (8%)	17 38
3	C	238/238 (100%)	218 (92%)	20 (8%)	14 30
4	D	133/145 (92%)	129 (97%)	4 (3%)	48 79
5	E	21/21 (100%)	20 (95%)	1 (5%)	31 62
6	F	22/24 (92%)	22 (100%)	0	100 100
7	G	29/29 (100%)	25 (86%)	4 (14%)	4 10
8	H	24/24 (100%)	24 (100%)	0	100 100
All	All	785/799 (98%)	735 (94%)	50 (6%)	22 47

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	11	ARG
1	A	26	VAL
1	A	36	LEU
1	A	64	GLU
1	A	81	LEU
1	A	87	ARG
1	A	107	THR
1	A	115	GLU
1	A	164	LEU
1	A	200	LEU
2	B	1	MET
2	B	62	THR
2	B	76	LEU
2	B	96	LEU
2	B	108	LEU
2	B	134	LEU
2	B	138	LEU
2	B	153	LYS
2	B	156	THR
2	B	159	LEU
3	C	20	ILE
3	C	22	CYS
3	C	60	GLN
3	C	67	LYS
3	C	70	LEU
3	C	94	LEU

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Mol	Chain	Res	Type
3	C	108	GLU
3	C	115	ILE
3	C	122	GLU
3	C	123	GLN
3	C	131	VAL
3	C	155	ARG
3	C	166	LYS
3	C	196	LEU
3	C	209	ASP
3	C	211	ILE
3	C	225	VAL
3	C	249	LEU
3	C	264	LEU
3	C	267	LEU
4	D	54	THR
4	D	55	THR
4	D	63	ASP
4	D	109	THR
5	E	10	PHE
7	G	6	LEU
7	G	16	VAL
7	G	21	LEU
7	G	27	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	86	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 20 ligands modelled in this entry, 1 is monoatomic - leaving 19 for Mogul analysis.

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	$\#\|Z\| > 2$
9	HEM	A	301	1	30,50,50	2.29	9 (30%)	24,82,82	2.36	7 (29%)
9	HEM	A	302	1	30,50,50	2.21	9 (30%)	24,82,82	2.34	7 (29%)
9	HEM	A	303	-	30,50,50	2.25	11 (36%)	24,82,82	2.25	7 (29%)
10	UMQ	A	304	-	35,35,35	1.29	6 (17%)	46,46,46	2.10	10 (21%)
10	UMQ	A	305	-	35,35,35	1.35	6 (17%)	46,46,46	2.22	8 (17%)
11	MYS	A	306	-	14,14,14	0.29	0	13,13,13	0.81	0
10	UMQ	A	307	-	35,35,35	1.29	4 (11%)	46,46,46	2.09	13 (28%)
12	8K6	A	308	-	17,17,17	0.19	0	16,16,16	0.52	0
10	UMQ	A	309	-	35,35,35	1.28	5 (14%)	46,46,46	2.07	11 (23%)
13	CLA	B	201	21	55,73,73	0.95	3 (5%)	61,113,113	1.19	7 (11%)
14	OPC	B	202	-	53,53,54	0.96	4 (7%)	57,61,64	1.03	1 (1%)
9	HEM	C	301	3	30,50,50	2.19	7 (23%)	24,82,82	2.39	8 (33%)
14	OPC	C	302	-	53,53,54	0.98	4 (7%)	57,61,64	1.01	2 (3%)
15	7PH	C	303	-	31,31,37	0.93	2 (6%)	33,33,42	1.18	3 (9%)
16	SQD	D	201	-	28,29,54	2.05	9 (32%)	36,40,65	7.92	8 (22%)
18	FES	D	202	4	0,4,4	0.00	-	0,4,4	0.00	-
10	UMQ	F	101	-	35,35,35	1.31	6 (17%)	46,46,46	2.05	13 (28%)
19	OCT	F	102	-	7,7,7	0.25	0	6,6,6	0.68	0
20	BCR	G	101	-	41,41,41	2.24	22 (53%)	56,56,56	2.20	19 (33%)

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
9	HEM	A	301	1	-	0/10/54/54	0/0/8/8
9	HEM	A	302	1	-	0/10/54/54	0/0/8/8

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	HEM	A	303	-	-	0/10/54/54	0/0/8/8
10	UMQ	A	304	-	2/2/10/10	0/20/60/60	0/2/2/2
10	UMQ	A	305	-	2/2/10/10	0/20/60/60	0/2/2/2
11	MYS	A	306	-	-	0/12/12/12	0/0/0/0
10	UMQ	A	307	-	2/2/10/10	0/20/60/60	0/2/2/2
12	8K6	A	308	-	-	0/15/15/15	0/0/0/0
10	UMQ	A	309	-	2/2/10/10	0/20/60/60	0/2/2/2
13	CLA	B	201	21	3/3/22/25	0/37/135/135	0/0/9/9
14	OPC	B	202	-	-	0/57/57/60	0/0/0/0
9	HEM	C	301	3	-	0/10/54/54	0/0/8/8
14	OPC	C	302	-	-	0/57/57/60	0/0/0/0
15	7PH	C	303	-	-	0/33/33/39	0/0/0/0
16	SQD	D	201	-	-	0/23/43/69	0/1/1/1
18	FES	D	202	4	-	0/0/4/4	0/1/1/1
10	UMQ	F	101	-	2/2/10/10	0/20/60/60	0/2/2/2
19	OCT	F	102	-	-	0/5/5/5	0/0/0/0
20	BCR	G	101	-	-	0/29/63/63	0/2/2/2

All (107) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	C	301	HEM	C3B-C4B	-7.32	1.45	1.51
9	A	301	HEM	C3B-C4B	-7.31	1.45	1.51
9	A	303	HEM	C3B-C4B	-7.25	1.45	1.51
9	A	302	HEM	C3B-C4B	-7.23	1.45	1.51
16	D	201	SQD	C6-S	-5.34	1.70	1.77
9	A	301	HEM	C3D-C4D	-5.26	1.44	1.51
9	C	301	HEM	C3D-C4D	-5.15	1.45	1.51
9	A	302	HEM	C3D-C4D	-5.00	1.45	1.51
16	D	201	SQD	O47-C45	-4.67	1.34	1.46
9	A	303	HEM	C3D-C4D	-4.45	1.45	1.51
9	A	303	HEM	C2C-C1C	-4.05	1.44	1.52
9	C	301	HEM	C2C-C1C	-3.76	1.45	1.52
9	A	301	HEM	C2C-C1C	-3.75	1.45	1.52
9	A	302	HEM	C2C-C1C	-3.69	1.45	1.52
16	D	201	SQD	C3-C2	-3.43	1.43	1.52
10	A	307	UMQ	C4-C5	-3.41	1.45	1.53
10	A	305	UMQ	C4-C5	-3.30	1.46	1.53
15	C	303	7PH	O21-C2	-3.26	1.38	1.46
10	A	304	UMQ	C4-C5	-3.08	1.46	1.53
10	A	309	UMQ	C4-C5	-2.97	1.46	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	C	303	7PH	O31-C3	-2.87	1.38	1.45
10	F	101	UMQ	C4-C5	-2.78	1.47	1.53
10	A	307	UMQ	C3-C4	-2.76	1.45	1.52
10	F	101	UMQ	O2'-C2'	-2.69	1.36	1.43
10	A	304	UMQ	C3-C4	-2.68	1.45	1.52
10	A	305	UMQ	O2'-C2'	-2.65	1.36	1.43
10	A	309	UMQ	O2'-C2'	-2.65	1.36	1.43
10	A	307	UMQ	O2'-C2'	-2.61	1.36	1.43
10	A	305	UMQ	C3-C4	-2.57	1.45	1.52
10	F	101	UMQ	O5'-C5'	-2.57	1.37	1.44
10	A	304	UMQ	O3'-C3'	-2.48	1.37	1.43
20	G	101	BCR	C32-C1	-2.48	1.48	1.53
13	B	201	CLA	CMB-C2B	-2.45	1.46	1.51
10	A	305	UMQ	O3'-C3'	-2.43	1.37	1.43
16	D	201	SQD	C1-C2	-2.42	1.45	1.52
10	A	309	UMQ	O3'-C3'	-2.40	1.37	1.43
10	A	309	UMQ	C3-C4	-2.39	1.46	1.52
10	F	101	UMQ	O3'-C3'	-2.39	1.37	1.43
14	B	202	OPC	OBJ-CBI	-2.33	1.39	1.45
10	F	101	UMQ	C3-C4	-2.32	1.46	1.52
16	D	201	SQD	O4-C4	-2.31	1.37	1.43
10	A	304	UMQ	O2'-C2'	-2.31	1.37	1.43
13	B	201	CLA	CMD-C2D	-2.29	1.46	1.51
10	A	309	UMQ	O5'-C5'	-2.29	1.38	1.44
10	A	304	UMQ	O1-C1	-2.25	1.35	1.41
20	G	101	BCR	C40-C30	-2.22	1.49	1.53
10	A	305	UMQ	O5'-C5'	-2.21	1.38	1.44
16	D	201	SQD	C4-C3	-2.20	1.46	1.52
14	C	302	OPC	OBJ-CBI	-2.18	1.40	1.45
10	A	307	UMQ	O3'-C3'	-2.15	1.37	1.43
9	A	303	HEM	C2D-C1D	-2.15	1.44	1.51
10	F	101	UMQ	O1-C1	-2.12	1.35	1.41
9	A	301	HEM	C2D-C1D	-2.08	1.45	1.51
9	C	301	HEM	C2D-C1D	-2.05	1.45	1.51
10	A	305	UMQ	O1-C1	-2.05	1.36	1.41
20	G	101	BCR	C39-C30	-2.05	1.49	1.53
9	A	302	HEM	C2B-C1B	-2.04	1.45	1.51
20	G	101	BCR	C31-C1	-2.03	1.49	1.53
10	A	304	UMQ	O5'-C5'	-2.01	1.39	1.44
20	G	101	BCR	C8-C7	2.04	1.39	1.33
9	A	302	HEM	C1C-NC	2.06	1.38	1.36
14	B	202	OPC	CAV-CAW	2.09	1.43	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	301	HEM	C4C-NC	2.11	1.38	1.36
9	A	303	HEM	C1C-NC	2.12	1.38	1.36
9	A	303	HEM	FE-NB	2.13	2.08	1.97
14	C	302	OPC	CAV-CAW	2.13	1.44	1.31
20	G	101	BCR	C11-C12	2.13	1.40	1.34
9	C	301	HEM	C3C-CAC	2.14	1.55	1.51
9	A	302	HEM	C3B-CAB	2.14	1.55	1.51
9	C	301	HEM	C3B-CAB	2.15	1.55	1.51
20	G	101	BCR	C20-C19	2.18	1.40	1.34
9	A	302	HEM	C3C-CAC	2.19	1.55	1.51
9	A	303	HEM	C3B-CAB	2.20	1.55	1.51
14	B	202	OPC	OBJ-CBK	2.22	1.40	1.33
16	D	201	SQD	O5-C5	2.23	1.49	1.44
9	A	301	HEM	C3B-CAB	2.26	1.55	1.51
9	A	301	HEM	C3C-CAC	2.30	1.55	1.51
9	A	303	HEM	C3C-CAC	2.34	1.55	1.51
20	G	101	BCR	C24-C23	2.35	1.39	1.33
9	A	303	HEM	C4C-NC	2.39	1.39	1.36
20	G	101	BCR	C10-C9	2.51	1.39	1.35
14	C	302	OPC	OBJ-CBK	2.52	1.40	1.33
16	D	201	SQD	O47-C7	2.56	1.41	1.35
13	B	201	CLA	CHC-C1C	2.58	1.43	1.35
20	G	101	BCR	C5-C6	2.61	1.38	1.34
9	A	303	HEM	FE-ND	2.64	2.11	1.97
9	A	302	HEM	FE-ND	2.67	2.11	1.97
9	C	301	HEM	FE-NC	2.84	2.07	1.95
9	A	302	HEM	FE-NC	2.95	2.07	1.95
20	G	101	BCR	C11-C10	3.05	1.53	1.43
20	G	101	BCR	C8-C9	3.06	1.52	1.45
20	G	101	BCR	C19-C18	3.06	1.52	1.45
20	G	101	BCR	C12-C13	3.07	1.52	1.45
16	D	201	SQD	O48-C23	3.07	1.42	1.33
20	G	101	BCR	C15-C14	3.11	1.53	1.43
20	G	101	BCR	C16-C17	3.12	1.53	1.43
20	G	101	BCR	C14-C13	3.14	1.39	1.35
14	B	202	OPC	OAN-CAO	3.16	1.43	1.34
9	A	301	HEM	FE-NC	3.21	2.08	1.95
20	G	101	BCR	C23-C22	3.24	1.53	1.45
9	A	303	HEM	FE-NC	3.24	2.08	1.95
14	C	302	OPC	OAN-CAO	3.26	1.44	1.34
20	G	101	BCR	C21-C22	3.30	1.40	1.35
20	G	101	BCR	C20-C21	3.30	1.54	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	G	101	BCR	C26-C25	3.39	1.39	1.34
20	G	101	BCR	C17-C18	3.43	1.40	1.35
9	A	301	HEM	FE-ND	3.52	2.16	1.97

All (124) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	D	201	SQD	O9-S-C6	-28.96	82.53	106.94
16	D	201	SQD	O9-S-O7	-8.61	82.10	113.48
20	G	101	BCR	C16-C17-C18	-4.45	120.77	127.20
20	G	101	BCR	C38-C26-C25	-4.36	120.33	124.61
20	G	101	BCR	C15-C14-C13	-4.35	120.91	127.20
20	G	101	BCR	C20-C21-C22	-4.20	121.12	127.20
20	G	101	BCR	C33-C5-C6	-4.13	120.55	124.61
20	G	101	BCR	C7-C8-C9	-4.12	119.93	126.22
20	G	101	BCR	C11-C10-C9	-3.70	121.85	127.20
13	B	201	CLA	CMB-C2B-C1B	-3.13	123.19	128.36
20	G	101	BCR	C23-C24-C25	-3.07	118.10	127.32
10	A	305	UMQ	C1-O1-C4'	-2.94	110.34	118.01
20	G	101	BCR	C24-C23-C22	-2.90	121.80	126.22
20	G	101	BCR	C4-C5-C6	-2.86	119.14	122.78
9	A	303	HEM	CBA-CAA-C2A	-2.86	107.40	112.53
10	A	307	UMQ	C1-O1-C4'	-2.85	110.55	118.01
10	A	309	UMQ	C1-O1-C4'	-2.73	110.88	118.01
10	F	101	UMQ	C1'-O5'-C5'	-2.73	108.45	113.75
20	G	101	BCR	C34-C9-C10	-2.72	118.88	122.90
13	B	201	CLA	O2D-CGD-O1D	-2.70	118.21	123.79
20	G	101	BCR	C32-C1-C6	-2.51	106.36	110.30
10	F	101	UMQ	C1-O5-C5	-2.44	109.01	113.75
10	F	101	UMQ	C1-O1-C4'	-2.44	111.64	118.01
20	G	101	BCR	C8-C7-C6	-2.40	120.09	127.32
10	A	309	UMQ	C1-O5-C5	-2.39	109.10	113.75
20	G	101	BCR	C27-C26-C25	-2.25	119.92	122.78
15	C	303	7PH	O21-C21-O22	-2.20	117.77	123.67
10	A	305	UMQ	C1-O5-C5	-2.19	109.50	113.75
9	C	301	HEM	CAA-C2A-C1A	-2.16	124.67	127.01
10	F	101	UMQ	O5'-C1'-C2'	-2.16	105.85	110.28
20	G	101	BCR	C1-C6-C5	-2.12	119.54	122.66
9	A	301	HEM	CBD-CAD-C3D	-2.11	107.40	113.55
10	A	307	UMQ	C1'-C2'-C3'	-2.09	105.85	109.97
10	F	101	UMQ	C6'-C5'-C4'	-2.05	107.28	113.25
10	A	307	UMQ	C1'-O5'-C5'	2.01	117.65	113.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	A	303	HEM	C2D-C3D-C4D	2.06	104.98	101.50
10	A	304	UMQ	CA-O1'-C1'	2.15	117.71	113.94
13	B	201	CLA	CMD-C2D-C3D	2.16	129.31	125.09
16	D	201	SQD	O6-C44-C45	2.17	116.16	110.99
10	A	307	UMQ	O5-C5-C6	2.18	111.87	106.36
10	A	304	UMQ	O1'-C1'-C2'	2.18	110.80	108.04
10	A	309	UMQ	C3'-C4'-C5'	2.21	115.84	110.84
13	B	201	CLA	CHB-C4A-NA	2.22	127.58	124.51
15	C	303	7PH	O31-C31-C32	2.24	118.72	111.90
9	C	301	HEM	C3B-C4B-CHC	2.24	126.32	123.16
13	B	201	CLA	C4A-NA-C1A	2.25	109.26	106.36
13	B	201	CLA	O1D-CGD-CBD	2.26	127.86	124.62
10	F	101	UMQ	O5'-C5'-C4'	2.27	114.54	109.75
9	A	302	HEM	C3B-C4B-CHC	2.27	126.36	123.16
9	C	301	HEM	C2D-C3D-C4D	2.28	105.36	101.50
10	A	307	UMQ	O1'-C1'-C2'	2.35	111.01	108.04
10	A	304	UMQ	C6'-C5'-C4'	2.40	120.24	113.25
13	B	201	CLA	CMB-C2B-C3B	2.45	129.89	125.09
9	A	302	HEM	C2D-C3D-C4D	2.46	105.66	101.50
16	D	201	SQD	O48-C23-C24	2.55	119.68	111.90
10	F	101	UMQ	CA-O1'-C1'	2.63	118.54	113.94
9	A	301	HEM	C2D-C3D-C4D	2.63	105.97	101.50
14	C	302	OPC	OBJ-CBK-CBL	2.65	119.96	111.90
9	A	302	HEM	CMD-C2D-C3D	2.73	126.42	114.35
10	F	101	UMQ	C6-C5-C4	2.75	119.80	113.02
16	D	201	SQD	C44-O6-C1	2.82	119.74	113.82
9	A	303	HEM	CMD-C2D-C3D	2.83	126.88	114.35
20	G	101	BCR	C29-C30-C25	2.92	114.98	110.36
9	A	301	HEM	CMD-C2D-C3D	2.92	127.28	114.35
16	D	201	SQD	O48-C46-C45	2.92	116.56	108.69
10	A	307	UMQ	O5'-C5'-C4'	2.93	115.94	109.75
9	C	301	HEM	CMD-C2D-C3D	2.98	127.54	114.35
15	C	303	7PH	O21-C21-C22	3.13	118.33	111.53
10	A	309	UMQ	O5-C1-C2	3.17	116.78	110.28
20	G	101	BCR	C38-C26-C27	3.34	119.76	113.43
10	A	307	UMQ	C2'-C3'-C4'	3.42	117.12	109.60
10	A	305	UMQ	CA-O1'-C1'	3.61	120.25	113.94
20	G	101	BCR	C33-C5-C4	3.63	120.32	113.43
10	A	307	UMQ	O2-C2-C3	3.64	118.54	110.34
10	A	309	UMQ	C1-C2-C3	3.70	117.26	109.97
10	A	309	UMQ	O5'-C5'-C4'	3.79	117.75	109.75
9	A	303	HEM	CMC-C2C-C3C	3.88	126.22	116.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	A	303	HEM	CAD-C3D-C2D	3.93	124.50	113.22
9	A	301	HEM	CAD-C3D-C4D	3.94	126.38	112.47
10	A	307	UMQ	O2-C2-C1	3.95	118.68	110.02
10	A	305	UMQ	O5'-C1'-O1'	3.96	119.58	110.05
14	B	202	OPC	OAN-CAO-CAP	3.96	120.14	111.53
14	C	302	OPC	OAN-CAO-CAP	4.01	120.24	111.53
9	C	301	HEM	CAD-C3D-C4D	4.06	126.79	112.47
10	A	304	UMQ	C1'-C2'-C3'	4.14	118.13	109.97
10	A	307	UMQ	CA-O1'-C1'	4.14	121.18	113.94
20	G	101	BCR	C2-C1-C6	4.31	117.19	110.36
9	A	302	HEM	CAD-C3D-C4D	4.32	127.72	112.47
10	A	309	UMQ	O1-C1-O5	4.39	121.79	110.68
10	F	101	UMQ	O2-C2-C3	4.44	120.33	110.34
10	A	304	UMQ	O2'-C2'-C3'	4.47	120.40	110.34
10	F	101	UMQ	O2-C2-C1	4.50	119.89	110.02
10	F	101	UMQ	C1-C2-C3	4.57	118.98	109.97
9	A	302	HEM	CAD-C3D-C2D	4.66	126.61	113.22
10	F	101	UMQ	O5-C5-C6	4.73	118.32	106.36
10	A	304	UMQ	O5'-C5'-C4'	4.74	119.75	109.75
10	A	307	UMQ	O3'-C3'-C2'	4.76	121.04	110.34
10	A	304	UMQ	O1-C4'-C3'	4.76	119.45	107.17
10	A	305	UMQ	O5'-C5'-C6'	4.76	118.39	106.36
10	A	309	UMQ	O2-C2-C3	4.76	121.06	110.34
10	A	307	UMQ	O3'-C3'-C4'	4.79	121.20	109.87
10	A	304	UMQ	O5'-C5'-C6'	4.84	118.58	106.36
10	A	304	UMQ	O2'-C2'-C1'	4.86	120.67	110.02
10	A	309	UMQ	CA-O1'-C1'	4.87	122.46	113.94
16	D	201	SQD	O47-C7-C8	4.87	120.29	111.10
9	C	301	HEM	CMB-C2B-C3B	5.00	129.02	116.53
9	A	302	HEM	CMC-C2C-C3C	5.01	129.03	116.53
9	A	301	HEM	CAD-C3D-C2D	5.02	127.64	113.22
9	C	301	HEM	CMC-C2C-C3C	5.07	129.18	116.53
10	A	309	UMQ	O2-C2-C1	5.08	121.15	110.02
9	C	301	HEM	CAD-C3D-C2D	5.09	127.85	113.22
10	A	305	UMQ	O5'-C1'-C2'	5.09	120.72	110.28
9	A	301	HEM	CMC-C2C-C3C	5.10	129.26	116.53
9	A	303	HEM	CAD-C3D-C4D	5.11	130.50	112.47
9	A	303	HEM	CMB-C2B-C3B	5.21	129.53	116.53
9	A	301	HEM	CMB-C2B-C3B	5.22	129.55	116.53
9	A	302	HEM	CMB-C2B-C3B	5.26	129.67	116.53
10	A	304	UMQ	O1-C4'-C5'	5.30	123.26	109.32
10	A	309	UMQ	O1-C1-C2	5.40	121.24	108.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	A	305	UMQ	O5'-C5'-C4'	5.83	122.06	109.75
10	F	101	UMQ	O5-C5-C4	6.12	121.17	109.68
10	A	307	UMQ	C1-C2-C3	6.14	122.08	109.97
10	A	305	UMQ	O1'-C1'-C2'	9.13	119.57	108.04
16	D	201	SQD	O7-S-C6	35.56	136.92	106.94

All (13) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
10	F	101	UMQ	C5
10	F	101	UMQ	C2
10	A	309	UMQ	C2
10	A	309	UMQ	C1
10	A	307	UMQ	C2
10	A	307	UMQ	C3'
13	B	201	CLA	NC
13	B	201	CLA	ND
13	B	201	CLA	NA
10	A	304	UMQ	C5'
10	A	304	UMQ	C2'
10	A	305	UMQ	C5'
10	A	305	UMQ	C1'

There are no torsion outliers.

There are no ring outliers.

11 monomers are involved in 42 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	301	HEM	5	0
9	A	302	HEM	4	0
9	A	303	HEM	10	0
11	A	306	MYS	1	0
10	A	307	UMQ	5	0
13	B	201	CLA	3	0
9	C	301	HEM	7	0
14	C	302	OPC	2	0
18	D	202	FES	1	0
10	F	101	UMQ	1	0
20	G	101	BCR	5	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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, 95^{th} 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	215/215 (100%)	0.73	30 (13%)	4 3	29, 43, 78, 165	0
2	B	160/160 (100%)	0.93	29 (18%)	2 1	40, 59, 103, 129	0
3	C	289/289 (100%)	1.23	58 (20%)	1 1	42, 66, 168, 188	0
4	D	166/179 (92%)	2.24	71 (42%)	0 0	34, 119, 168, 174	0
5	E	31/31 (100%)	0.49	4 (12%)	5 4	63, 74, 100, 115	0
6	F	32/34 (94%)	0.41	1 (3%)	52 52	55, 67, 106, 126	0
7	G	37/37 (100%)	1.22	7 (18%)	2 1	46, 58, 108, 114	0
8	H	29/29 (100%)	1.16	3 (10%)	9 6	49, 56, 66, 90	0
All	All	959/974 (98%)	1.19	203 (21%)	1 1	29, 63, 160, 188	0

All (203) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1	MET	11.7
4	D	70	LEU	11.2
3	C	204	GLY	11.2
2	B	160	PHE	10.1
4	D	160	ILE	10.1
3	C	199	ILE	9.8
2	B	1	MET	9.7
3	C	224	ALA	9.3
4	D	69	PHE	8.8
3	C	206	VAL	8.7
3	C	184	ALA	8.1
3	C	205	GLU	7.7
4	D	73	HIS	7.7
4	D	175	GLU	7.6
4	D	92	VAL	7.5
3	C	203	SER	7.2

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Mol	Chain	Res	Type	RSRZ
3	C	227	ALA	7.2
4	D	171	ARG	7.1
3	C	201	THR	7.0
3	C	196	LEU	6.9
1	A	2	ALA	6.8
4	D	72	SER	6.6
4	D	174	GLU	6.4
4	D	75	VAL	6.3
4	D	67	SER	6.2
4	D	159	LYS	6.2
4	D	155	THR	6.2
4	D	161	VAL	6.2
7	G	37	GLY	5.9
4	D	158	ASP	5.9
4	D	156	GLU	5.9
4	D	48	GLY	5.9
4	D	102	TYR	5.8
4	D	173	GLY	5.8
3	C	177	THR	5.8
4	D	56	ALA	5.7
4	D	140	VAL	5.7
6	F	1	MET	5.7
4	D	64	VAL	5.6
4	D	172	THR	5.5
4	D	63	ASP	5.5
3	C	207	VAL	5.5
4	D	91	ILE	5.5
3	C	176	ALA	5.4
4	D	157	ASN	5.3
4	D	66	VAL	5.3
3	C	197	VAL	5.2
3	C	226	THR	5.2
4	D	49	GLY	5.1
3	C	219	VAL	5.0
3	C	189	GLU	5.0
3	C	183	ILE	5.0
3	C	179	THR	4.9
3	C	193	VAL	4.9
4	D	179	SER	4.9
3	C	182	LYS	4.9
3	C	180	ILE	4.9
3	C	186	GLN	4.9

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Mol	Chain	Res	Type	RSRZ
2	B	2	ALA	4.9
4	D	170	PHE	4.9
4	D	141	ARG	4.8
3	C	181	SER	4.8
3	C	188	GLY	4.8
3	C	209	ASP	4.7
4	D	99	ILE	4.7
4	D	84	LEU	4.6
3	C	208	SER	4.5
4	D	54	THR	4.5
4	D	52	GLY	4.5
4	D	162	LEU	4.4
4	D	47	ALA	4.4
3	C	225	VAL	4.4
7	G	30	LYS	4.3
3	C	194	LYS	4.2
3	C	212	PRO	4.2
4	D	71	GLU	4.2
2	B	159	LEU	4.2
4	D	166	THR	4.2
3	C	143	HIS	4.1
4	D	50	ALA	4.1
2	B	151	LEU	4.1
2	B	50	CYS	4.1
3	C	192	SER	4.0
4	D	65	SER	4.0
3	C	190	ASP	4.0
4	D	57	LYS	4.0
3	C	220	SER	4.0
4	D	77	ASP	3.9
4	D	55	THR	3.9
5	E	29	LYS	3.9
4	D	76	GLY	3.9
1	A	35	CYS	3.9
5	E	31	LEU	3.8
4	D	51	GLY	3.8
3	C	195	TYR	3.8
4	D	169	ASP	3.8
4	D	62	ASN	3.7
3	C	202	GLU	3.7
2	B	153	LYS	3.7
2	B	155	LEU	3.7

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Mol	Chain	Res	Type	RSRZ
3	C	198	ASP	3.7
4	D	119	ALA	3.6
3	C	200	LYS	3.6
1	A	96	MET	3.6
1	A	95	LEU	3.5
3	C	289	PHE	3.5
3	C	222	GLY	3.5
4	D	68	LYS	3.5
3	C	218	ILE	3.5
4	D	168	THR	3.5
4	D	98	ALA	3.4
3	C	210	THR	3.4
1	A	92	MET	3.4
7	G	1	MET	3.4
4	D	53	GLY	3.3
2	B	47	SER	3.3
4	D	167	GLU	3.3
3	C	178	GLY	3.3
4	D	74	ASN	3.3
4	D	145	PRO	3.2
1	A	5	TYR	3.2
2	B	157	LEU	3.1
3	C	61	VAL	3.1
8	H	1	MET	3.1
3	C	281	LYS	3.1
4	D	165	TRP	3.0
1	A	91	SER	3.0
3	C	211	ILE	3.0
4	D	154	LYS	3.0
2	B	46	GLY	2.9
3	C	223	GLN	2.9
1	A	43	CYS	2.9
3	C	288	ASN	2.9
4	D	16	ARG	2.8
3	C	168	ASN	2.8
3	C	221	GLU	2.8
4	D	17	GLN	2.8
5	E	30	ILE	2.8
4	D	15	ARG	2.7
3	C	117	GLY	2.7
1	A	99	LEU	2.7
4	D	153	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
4	D	60	LEU	2.7
1	A	88	TRP	2.7
2	B	79	TRP	2.7
2	B	45	MET	2.7
2	B	51	ILE	2.6
2	B	54	LEU	2.6
5	E	2	LEU	2.6
1	A	4	VAL	2.6
2	B	154	SER	2.5
1	A	98	ILE	2.5
1	A	89	SER	2.5
3	C	93	GLU	2.5
4	D	176	PRO	2.5
1	A	32	ILE	2.5
2	B	156	THR	2.5
1	A	39	ILE	2.4
2	B	49	ALA	2.4
7	G	33	ASN	2.4
2	B	53	ALA	2.4
3	C	286	GLU	2.4
2	B	152	ASP	2.4
1	A	104	VAL	2.4
4	D	142	GLY	2.4
1	A	97	MET	2.4
7	G	35	LEU	2.4
1	A	101	VAL	2.4
3	C	165	GLU	2.3
2	B	40	PHE	2.3
1	A	93	MET	2.3
1	A	94	VAL	2.3
2	B	52	VAL	2.3
7	G	10	VAL	2.3
8	H	15	PHE	2.3
1	A	100	HIS	2.3
3	C	109	ASP	2.2
2	B	77	PRO	2.2
2	B	3	THR	2.2
1	A	34	TYR	2.2
3	C	172	TYR	2.2
1	A	150	ILE	2.2
4	D	13	MET	2.2
2	B	48	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
4	D	138	LYS	2.2
2	B	43	VAL	2.2
4	D	14	GLY	2.1
1	A	90	ALA	2.1
1	A	33	PHE	2.1
4	D	143	PRO	2.1
4	D	152	HIS	2.1
1	A	30	VAL	2.1
1	A	3	ASN	2.1
2	B	158	GLY	2.1
4	D	151	SER	2.1
2	B	72	PRO	2.1
7	G	26	TYR	2.1
3	C	230	ALA	2.1
2	B	44	ILE	2.1
1	A	36	LEU	2.0
8	H	29	LEU	2.0
1	A	40	THR	2.0
3	C	92	GLU	2.0

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.

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, 95^{th} 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
10	UMQ	A	304	34/34	0.67	0.53	4.35	78,129,162,173	0
14	OPC	B	202	54/55	0.90	0.36	4.20	52,93,137,149	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
15	7PH	C	303	32/38	0.70	0.30	1.99	49,72,135,154	0
10	UMQ	A	307	34/34	0.68	0.34	1.97	72,111,140,165	0
14	OPC	C	302	54/55	0.61	0.43	1.95	47,96,152,167	0
10	UMQ	F	101	34/34	0.64	0.36	1.32	63,128,205,215	0
19	OCT	F	102	8/8	0.82	0.25	1.02	61,76,90,99	0
10	UMQ	A	305	34/34	0.90	0.28	0.87	58,110,148,166	0
10	UMQ	A	309	34/34	0.59	0.39	0.70	57,121,187,208	0
13	CLA	B	201	65/65	0.91	0.27	0.68	47,73,127,132	0
11	MYS	A	306	15/15	0.84	0.23	0.68	50,68,96,98	0
20	BCR	G	101	40/40	0.67	0.36	0.63	40,73,127,138	0
9	HEM	A	301	43/43	0.97	0.25	0.43	29,39,55,66	0
9	HEM	A	302	43/43	0.98	0.28	0.38	23,42,53,56	0
9	HEM	C	301	43/43	0.97	0.22	0.17	34,61,83,89	0
9	HEM	A	303	43/43	0.97	0.26	0.09	40,60,72,79	0
16	SQD	D	201	29/54	0.92	0.21	-0.44	63,90,129,145	0
18	FES	D	202	4/4	0.94	0.13	-1.26	79,81,82,95	0
12	8K6	A	308	18/18	0.88	0.15	-1.67	50,71,84,87	0
17	CD	C	304	1/1	-0.76	0.99	-	206,206,206,206	0

6.5 Other polymers

There are no such residues in this entry.