



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:25 PM GMT

PDB ID : 4I7Z  
Title : Crystal structure of cytochrome b6f in DOPG, with disordered Rieske Iron-Sulfur Protein soluble domain  
Authors : Hasan, S.S.; Stofleth, J.T.; Yamashita, E.; Cramer, W.A.  
Deposited on : 2012-12-01  
Resolution : 2.80 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) 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

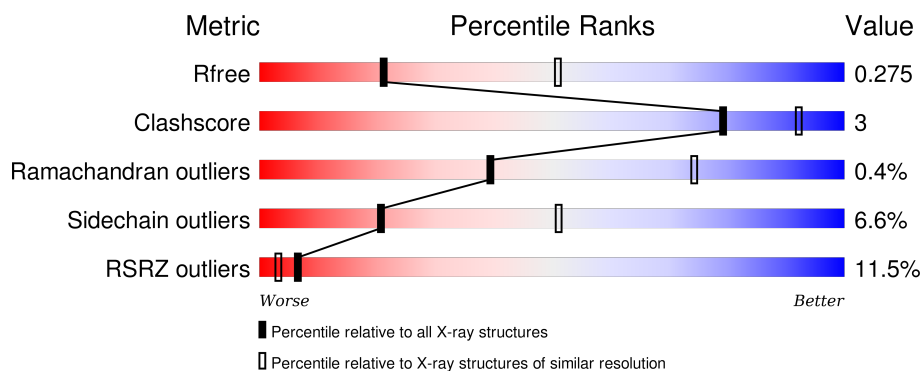
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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  $\geq 3$ , 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  $\leq 5\%$ . 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	<div> <div style="width: 89%;"></div> <div style="width: 10%;"></div> <div style="width: 1%;"></div> </div>
2	B	160	<div> <div style="width: 5%;"></div> <div style="width: 94%;"></div> <div style="width: 6%;"></div> </div>
3	C	289	<div> <div style="width: 23%;"></div> <div style="width: 88%;"></div> <div style="width: 11%;"></div> </div>
4	D	179	<div> <div style="width: 3%;"></div> <div style="width: 21%;"></div> <div style="width: 79%;"></div> </div>
5	E	32	<div> <div style="width: 9%;"></div> <div style="width: 84%;"></div> <div style="width: 13%;"></div> </div>

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Mol	Chain	Length	Quality of chain
6	F	35	
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	MYS	A	304	-	-	-	X
11	8K6	A	305	-	-	-	X
12	UMQ	A	306	X	-	-	X
12	UMQ	A	307	X	-	-	X
12	UMQ	A	308	X	-	-	-
13	CLA	B	201	X	-	-	-
15	OZ2	B	203	X	-	-	-
15	OZ2	C	303	-	-	-	X
16	1E2	D	201	X	-	-	-
17	BCR	G	101	-	-	-	X
18	OCT	F	101	-	-	-	X

## 2 Entry composition

There are 19 unique types of molecules in this entry. The entry contains 13828 atoms, of which 6869 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
1	A	213	Total	C	H	N	O	S	0	0	0
			3419	1132	1721	270	286	10			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	159	Total	C	H	N	O	S	0	0	0
			2538	836	1297	192	208	5			

- Molecule 3 is a protein called Apocytochrome f.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	C	288	Total	C	H	N	O	S	0	0	0
			4450	1415	2234	369	424	8			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	11	PRO	GLU	ENGINEERED MUTATION	UNP P83793

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	D	38	Total	C	H	N	O	S	0	0	0
			591	194	299	47	49	2			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
5	E	28	Total	C	H	N	O		0	0	0
			452	156	237	29	30				

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
6	F	31	Total	C	H	N	O	S	0	0	0
			482	160	248	34	39	1			

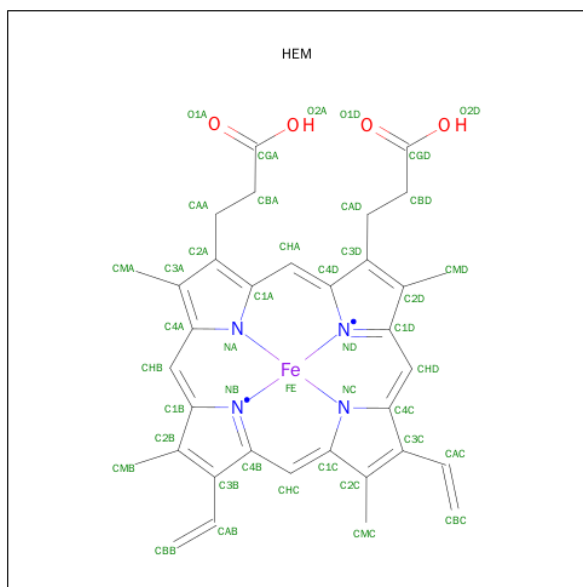
- Molecule 7 is a protein called Cytochrome b6-f complex subunit 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	35	Total	C	H	N	O	0	0	0
			536	178	268	42	48			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
8	H	28	Total	C	H	N	O	S	0	0	0
			449	151	227	35	35	1			

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



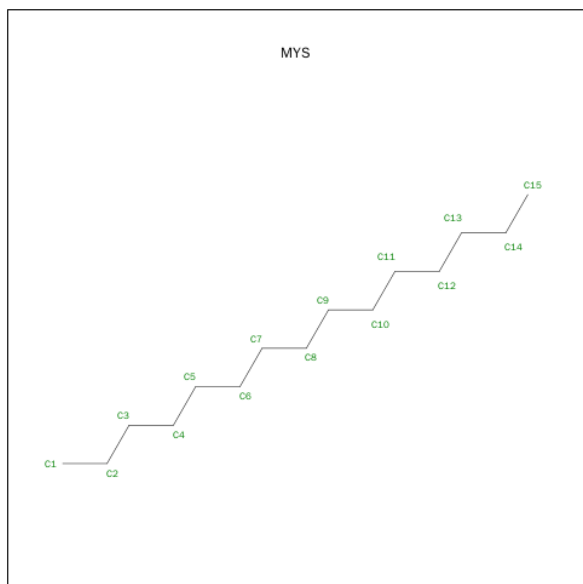
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
9	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
9	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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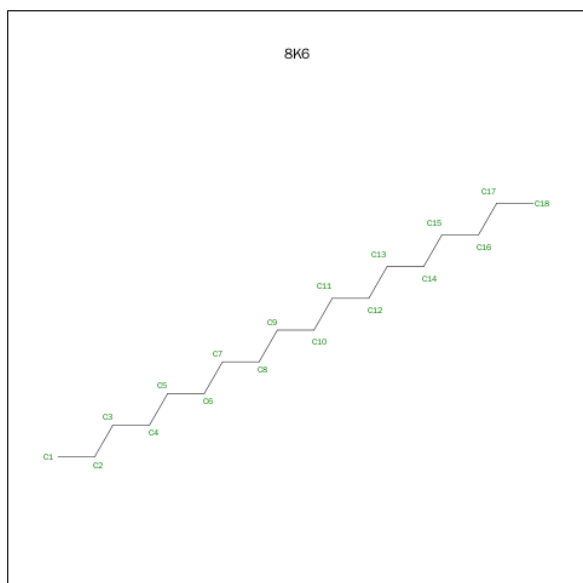
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	C	1	Total	C	Fe	N	O	
			43	34	1	4	4	
							0	0

- Molecule 10 is PENTADECANE (three-letter code: MYS) (formula:  $C_{15}H_{32}$ ).



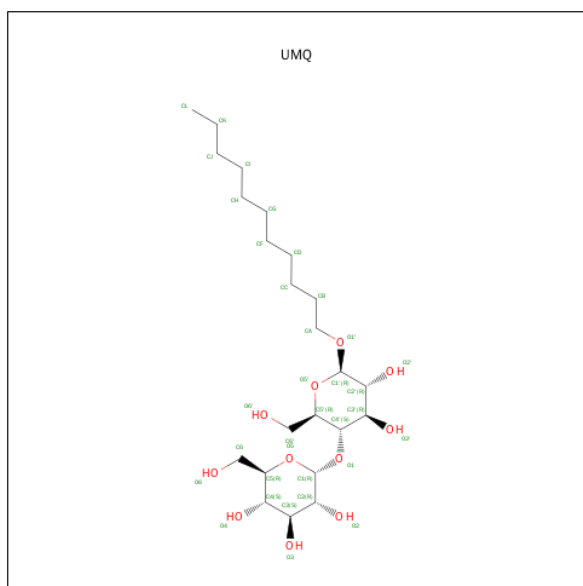
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	A	1	Total	C	H		
			47	15	32		
						0	0

- Molecule 11 is OCTADECANE (three-letter code: 8K6) (formula:  $C_{18}H_{38}$ ).



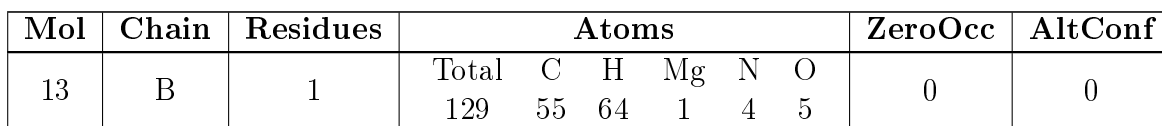
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	A	1	Total	C	H	0	0
			56	18	38		

- Molecule 12 is UNDECYL-MALTOSIDE (three-letter code: UMQ) (formula:  $C_{23}H_{44}O_{11}$ ).



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

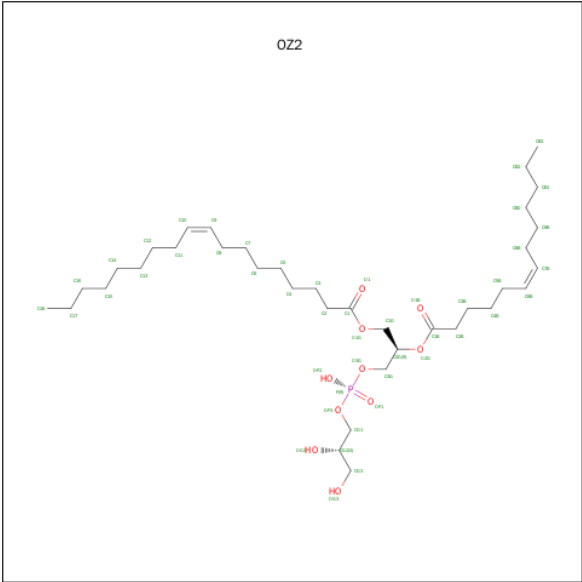
- Molecule 13 is CHLOROPHYLL A (three-letter code: CLA) (formula:  $C_{55}H_{72}MgN_4O_5$ ).



- | Mol | Chain | Residues | Atoms           | ZeroOcc | AltConf |
|-----|-------|----------|-----------------|---------|---------|
| 14  | B     | 1        | Total Cd<br>1 1 | 0       | 0       |
| 14  | A     | 1        | Total Cd<br>1 1 | 0       | 0       |
| 14  | C     | 1        | Total Cd<br>1 1 | 0       | 0       |

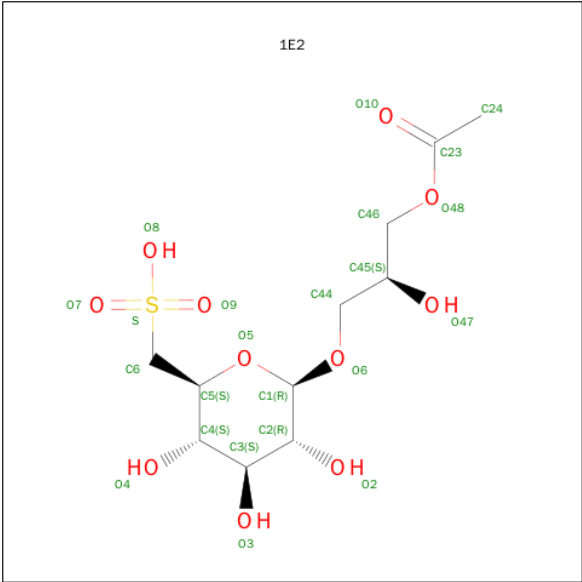
- Molecule 15 is (2R)-3-{[(R)-{[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-2-[(6Z)-TRIDEC-6-ENOYLOXY]PROPYL (9Z)-OCTADEC-9-ENOATE (three-letter code: OZ2) (formula: C<sub>37</sub>H<sub>69</sub>O<sub>10</sub>P).





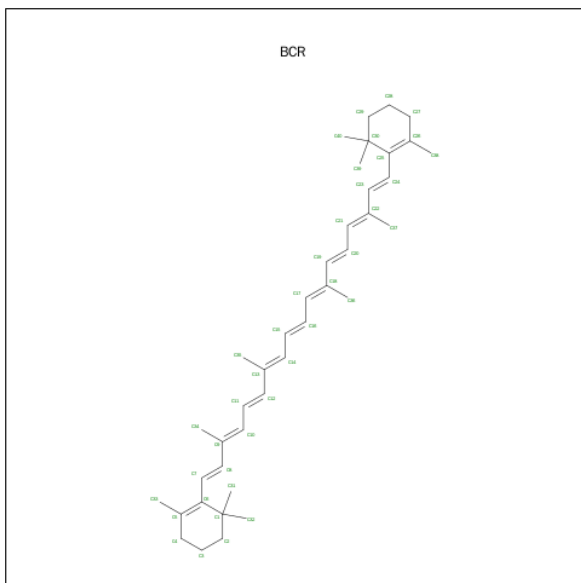
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
15	B	1	Total	C	O	P	0	0
			32	21	10	1		
15	C	1	Total	C	O	P	0	0
			38	27	10	1		
15	G	1	Total	C	O	P	0	0
			44	33	10	1		

- Molecule 16 is (2S)-3-(ACETYLOXY)-2-HYDROXYPROPYL 6-DEOXY-6-SULFO-BETA-D-GLUCOPYRANOSIDE (three-letter code: 1E2) (formula: C<sub>11</sub>H<sub>20</sub>O<sub>11</sub>S).



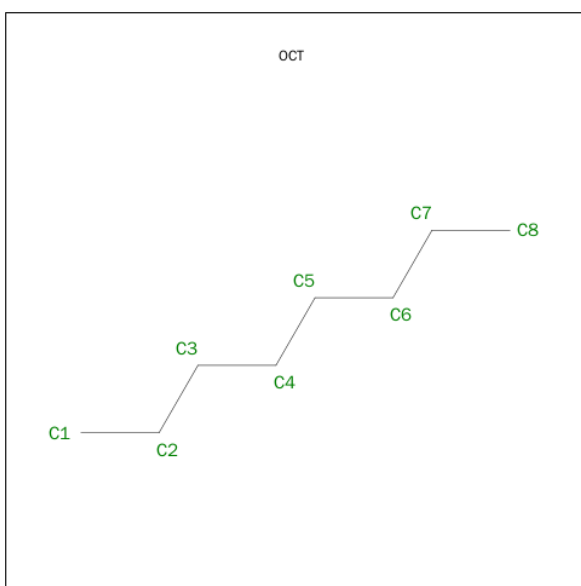
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
16	D	1	Total	C	O	S	0	0
			23	11	11	1		

- Molecule 17 is BETA-CAROTENE (three-letter code: BCR) (formula:  $C_{40}H_{56}$ ).



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

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



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

- Molecule 19 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
19	A	8	Total	O	0	0
			8	8		
19	B	4	Total	O	0	0
			4	4		
19	C	1	Total	O	0	0
			1	1		

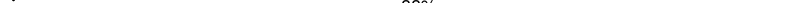


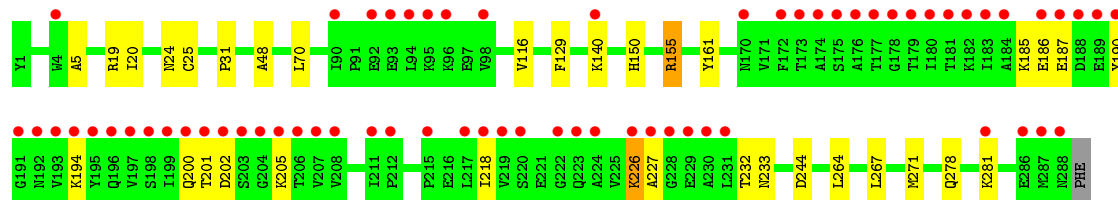
- Molecule 1: Cytochrome b6



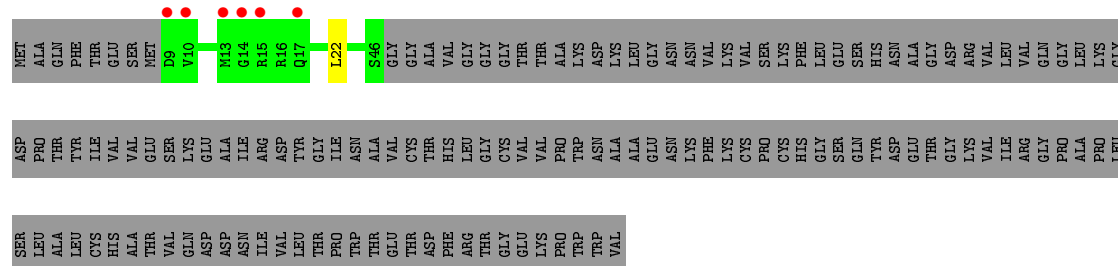
- Chain B:  5% 94% 6%



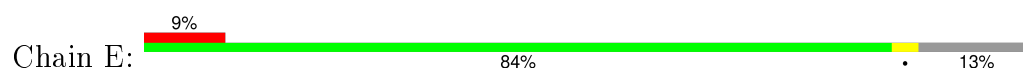
- Chain C:  23% 88% 11%



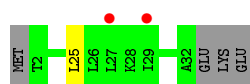
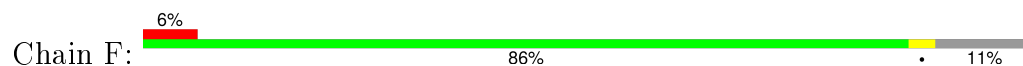
- Chain D:  3% 21% 79%



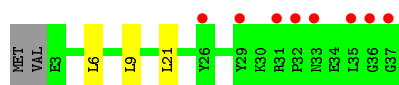
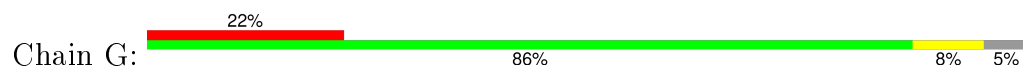
- Molecule 5: Cytochrome b6-f complex subunit 6



- 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

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	159.45Å 159.45Å 362.75Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.52 – 2.80 48.52 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.2 (48.52-2.80) 99.2 (48.52-2.80)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.14 (at 2.81Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, $R_{free}$	0.248 , 0.272 0.252 , 0.275	Depositor DCC
$R_{free}$ test set	3406 reflections (5.35%)	DCC
Wilson B-factor (Å <sup>2</sup> )	61.5	Xtriage
Anisotropy	0.189	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 66.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	3 of 67071 reflections (0.004%)	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	13828	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	102.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.15% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: UMQ, MYS, CLA, CD, 1E2, OZ2, HEM, 8K6, OCT, BCR

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	0.30	0/1750	0.45	0/2388
2	B	0.26	0/1280	0.41	0/1755
3	C	0.26	0/2264	0.44	0/3082
4	D	0.28	0/300	0.40	0/408
5	E	0.28	0/220	0.42	0/297
6	F	0.28	0/238	0.40	0/321
7	G	0.29	0/274	0.39	0/371
8	H	0.29	0/228	0.47	0/313
All	All	0.28	0/6554	0.43	0/8935

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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	1698	1721	1720	9	0
2	B	1241	1297	1296	3	0
3	C	2216	2234	2233	9	0
4	D	292	299	299	0	0
5	E	215	237	237	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	F	234	248	248	0	0
7	G	268	268	268	0	0
8	H	222	227	227	4	0
9	A	129	0	90	23	0
9	C	43	0	30	6	0
10	A	15	32	32	0	0
11	A	18	38	38	0	0
12	A	102	130	126	2	0
13	B	65	64	71	1	0
14	A	1	0	0	0	0
14	B	1	0	0	0	0
14	C	1	0	0	0	0
15	B	32	0	32	0	0
15	C	38	0	43	0	0
15	G	44	0	54	1	0
16	D	23	0	18	2	0
17	G	40	56	56	0	0
18	F	8	18	18	0	0
19	A	8	0	0	1	0
19	B	4	0	0	0	0
19	C	1	0	0	0	0
All	All	6959	6869	7136	49	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 3.

All (49) 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)
9:A:303:HEM:HHA	9:A:303:HEM:HBD1	1.52	0.90
9:A:302:HEM:HBC2	9:A:302:HEM:HMC2	1.58	0.83
9:A:303:HEM:HMC1	9:A:303:HEM:HBC2	1.60	0.83
9:A:303:HEM:HBB2	9:A:303:HEM:HMB1	1.65	0.79
9:C:301:HEM:HMC1	9:C:301:HEM:HBC2	1.65	0.77
9:A:302:HEM:HMB1	9:A:302:HEM:HBB2	1.66	0.77
9:C:301:HEM:HBB2	9:C:301:HEM:HHC	1.68	0.76
9:A:301:HEM:HMC1	9:A:301:HEM:HBC2	1.67	0.76
12:A:306:UMQ:H11	12:A:306:UMQ:O3'	1.89	0.73
9:A:303:HEM:CMC	9:A:303:HEM:HBC2	2.25	0.66
9:A:301:HEM:HBB2	9:A:301:HEM:HMB1	1.77	0.66
13:B:201:CLA:HHC	13:B:201:CLA:HBB1	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:302:HEM:CMB	9:A:302:HEM:HBB2	2.27	0.64
9:A:301:HEM:CMC	9:A:301:HEM:HBC2	2.28	0.63
3:C:185:LYS:O	3:C:187:GLU:N	2.32	0.62
1:A:114:ARG:NH1	1:A:210:GLY:O	2.32	0.61
1:A:83:ARG:NH2	2:B:61:MET:O	2.34	0.61
3:C:25:CYS:SG	9:C:301:HEM:CAC	2.90	0.59
3:C:5:ALA:HB2	9:C:301:HEM:HBB2	1.85	0.59
1:A:83:ARG:NH1	9:A:301:HEM:O1D	2.35	0.59
9:C:301:HEM:HBC2	9:C:301:HEM:CMC	2.33	0.59
1:A:35:CYS:SG	9:A:303:HEM:CAB	2.91	0.59
9:A:302:HEM:HBC2	9:A:302:HEM:CMC	2.32	0.58
9:A:303:HEM:HBB2	9:A:303:HEM:CMB	2.34	0.58
1:A:35:CYS:HG	9:A:303:HEM:CAB	2.20	0.55
9:A:302:HEM:HBA1	9:A:302:HEM:HHA	1.89	0.54
15:G:102:OZ2:H11	8:H:15:PHE:CD1	2.42	0.54
9:A:302:HEM:HMA2	19:A:401:HOH:O	2.09	0.53
9:A:301:HEM:HBB2	9:A:301:HEM:CMB	2.40	0.51
3:C:150:HIS:ND1	3:C:244:ASP:OD1	2.43	0.48
8:H:23:VAL:HA	8:H:28:GLY:HA3	1.96	0.47
9:A:303:HEM:O1D	9:A:303:HEM:HBA1	2.14	0.47
3:C:31:PRO:O	3:C:155:ARG:NH2	2.44	0.46
1:A:15:GLN:NE2	1:A:19:ASP:OD1	2.49	0.45
1:A:54:MET:CE	9:A:301:HEM:HBA1	2.47	0.45
9:A:302:HEM:HMB1	9:A:302:HEM:CBB	2.43	0.44
8:H:29:LEU:HD12	8:H:29:LEU:N	2.33	0.44
3:C:19:ARG:NH1	3:C:24:ASN:OD1	2.48	0.43
9:A:301:HEM:HMC1	9:A:301:HEM:CBC	2.43	0.43
8:H:23:VAL:O	8:H:28:GLY:N	2.47	0.43
3:C:161:TYR:CE2	9:C:301:HEM:HBD2	2.54	0.42
16:D:201:1E2:H15	16:D:201:1E2:H4	1.75	0.42
2:B:82:TYR:HB2	2:B:83:PRO:HD3	2.01	0.42
1:A:138:LEU:N	1:A:139:PRO:CD	2.83	0.41
12:A:308:UMQ:HO61	16:D:201:1E2:H19	1.61	0.41
3:C:226:LYS:HG3	3:C:227:ALA:H	1.85	0.41
2:B:111:VAL:N	2:B:112:PRO:HD2	2.36	0.40
3:C:48:ALA:HB3	3:C:129:PHE:HB2	2.04	0.40
1:A:101:VAL:CG2	9:A:302:HEM:HMC3	2.51	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	211/215 (98%)	205 (97%)	6 (3%)	0	100	100
2	B	157/160 (98%)	152 (97%)	5 (3%)	0	100	100
3	C	286/289 (99%)	244 (85%)	39 (14%)	3 (1%)	19	52
4	D	36/179 (20%)	35 (97%)	1 (3%)	0	100	100
5	E	26/32 (81%)	25 (96%)	1 (4%)	0	100	100
6	F	29/35 (83%)	28 (97%)	1 (3%)	0	100	100
7	G	33/37 (89%)	30 (91%)	3 (9%)	0	100	100
8	H	26/29 (90%)	26 (100%)	0	0	100	100
All	All	804/976 (82%)	745 (93%)	56 (7%)	3 (0%)	39	74

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	186	GLU
3	C	205	LYS
3	C	20	ILE

### 5.3.2 Protein sidechains

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	183/184 (100%)	171 (93%)	12 (7%)	21	51
2	B	136/137 (99%)	132 (97%)	4 (3%)	50	83

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	242/243 (100%)	224 (93%)	18 (7%)	17	43
4	D	31/146 (21%)	30 (97%)	1 (3%)	46	80
5	E	21/25 (84%)	20 (95%)	1 (5%)	31	66
6	F	23/27 (85%)	22 (96%)	1 (4%)	35	70
7	G	26/28 (93%)	23 (88%)	3 (12%)	7	21
8	H	23/24 (96%)	18 (78%)	5 (22%)	1	3
All	All	685/814 (84%)	640 (93%)	45 (7%)	21	51

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	ARG
1	A	12	LEU
1	A	14	ILE
1	A	63	THR
1	A	75	GLU
1	A	81	LEU
1	A	87	ARG
1	A	95	LEU
1	A	103	ARG
1	A	148	VAL
1	A	164	LEU
1	A	200	LEU
2	B	13	LYS
2	B	35	ASP
2	B	75	ILE
2	B	96	LEU
3	C	70	LEU
3	C	116	VAL
3	C	140	LYS
3	C	155	ARG
3	C	190	TYR
3	C	194	LYS
3	C	200	GLN
3	C	201	THR
3	C	202	ASP
3	C	218	ILE
3	C	226	LYS
3	C	232	THR
3	C	233	ASN

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Mol	Chain	Res	Type
3	C	264	LEU
3	C	267	LEU
3	C	271	MET
3	C	278	GLN
3	C	281	LYS
4	D	22	LEU
5	E	11	PHE
6	F	25	LEU
7	G	6	LEU
7	G	9	LEU
7	G	21	LEU
8	H	2	GLU
8	H	6	LEU
8	H	14	VAL
8	H	21	MET
8	H	29	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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](#)

Of 19 ligands modelled in this entry, 3 are monoatomic - leaving 16 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	2.21	9 (30%)	24,82,82	2.35	9 (37%)
9	HEM	A	302	1	30,50,50	2.19	7 (23%)	24,82,82	2.25	7 (29%)
9	HEM	A	303	19	30,50,50	2.21	9 (30%)	24,82,82	2.26	9 (37%)
10	MYS	A	304	-	14,14,14	0.30	0	13,13,13	0.79	0
11	8K6	A	305	-	17,17,17	0.19	0	16,16,16	0.50	0
12	UMQ	A	306	-	35,35,35	1.23	5 (14%)	46,46,46	2.38	11 (23%)
12	UMQ	A	307	-	35,35,35	1.29	5 (14%)	46,46,46	2.58	11 (23%)
12	UMQ	A	308	-	35,35,35	1.29	6 (17%)	46,46,46	2.02	9 (19%)
13	CLA	B	201	19	55,73,73	0.95	3 (5%)	61,113,113	1.29	8 (13%)
15	OZ2	B	203	-	31,31,47	1.22	3 (9%)	31,37,53	1.56	4 (12%)
9	HEM	C	301	3	30,50,50	2.12	7 (23%)	24,82,82	2.36	11 (45%)
15	OZ2	C	303	-	37,37,47	1.22	4 (10%)	37,43,53	1.29	3 (8%)
16	1E2	D	201	-	22,23,23	2.03	2 (9%)	29,33,33	3.63	8 (27%)
18	OCT	F	101	-	7,7,7	0.24	0	6,6,6	0.64	0
17	BCR	G	101	-	41,41,41	2.15	19 (46%)	56,56,56	2.29	22 (39%)
15	OZ2	G	102	-	43,43,47	1.15	4 (9%)	43,49,53	1.22	2 (4%)

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
9	HEM	A	303	19	-	0/10/54/54	0/0/8/8
10	MYS	A	304	-	-	0/12/12/12	0/0/0/0
11	8K6	A	305	-	-	0/15/15/15	0/0/0/0
12	UMQ	A	306	-	3/3/10/10	0/20/60/60	0/2/2/2
12	UMQ	A	307	-	3/3/10/10	0/20/60/60	0/2/2/2
12	UMQ	A	308	-	2/2/10/10	0/20/60/60	0/2/2/2
13	CLA	B	201	19	3/3/22/25	0/37/135/135	0/0/9/9
15	OZ2	B	203	-	1/1/5/9	0/35/35/52	0/0/0/0
9	HEM	C	301	3	-	0/10/54/54	0/0/8/8
15	OZ2	C	303	-	-	0/42/42/52	0/0/0/0
16	1E2	D	201	-	1/1/8/8	0/15/35/35	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	OCT	F	101	-	-	0/5/5/5	0/0/0/0
17	BCR	G	101	-	-	0/29/63/63	0/2/2/2
15	OZ2	G	102	-	-	0/48/48/52	0/0/0/0

All (83) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	301	HEM	C3B-C4B	-7.50	1.45	1.51
9	A	303	HEM	C3B-C4B	-7.38	1.45	1.51
9	A	302	HEM	C3B-C4B	-7.17	1.45	1.51
9	C	301	HEM	C3B-C4B	-6.72	1.45	1.51
16	D	201	1E2	O47-C45	-6.45	1.24	1.43
9	A	301	HEM	C3D-C4D	-5.47	1.44	1.51
16	D	201	1E2	C6-S	-5.35	1.70	1.77
9	C	301	HEM	C3D-C4D	-5.17	1.44	1.51
9	A	302	HEM	C3D-C4D	-5.11	1.45	1.51
9	A	302	HEM	C2C-C1C	-4.14	1.44	1.52
9	A	303	HEM	C3D-C4D	-4.12	1.46	1.51
9	A	303	HEM	C2C-C1C	-3.76	1.45	1.52
9	C	301	HEM	C2C-C1C	-3.72	1.45	1.52
9	A	301	HEM	C2C-C1C	-3.59	1.45	1.52
15	B	203	OZ2	O2G-C2G	-3.35	1.38	1.46
15	C	303	OZ2	O2G-C2G	-3.25	1.38	1.46
12	A	307	UMQ	C4-C5	-3.06	1.46	1.53
15	G	102	OZ2	O2G-C2G	-2.87	1.39	1.46
15	C	303	OZ2	O1G-C1G	-2.79	1.38	1.45
15	B	203	OZ2	O1G-C1G	-2.77	1.38	1.45
12	A	308	UMQ	C4-C5	-2.73	1.47	1.53
12	A	307	UMQ	O2'-C2'	-2.67	1.36	1.43
12	A	308	UMQ	O5'-C5'	-2.67	1.37	1.44
12	A	306	UMQ	O5'-C5'	-2.58	1.37	1.44
17	G	101	BCR	C32-C1	-2.57	1.48	1.53
12	A	306	UMQ	O2'-C2'	-2.52	1.36	1.43
12	A	308	UMQ	O2'-C2'	-2.51	1.37	1.43
12	A	307	UMQ	O3'-C3'	-2.45	1.37	1.43
12	A	306	UMQ	C4-C5	-2.43	1.47	1.53
12	A	308	UMQ	C3-C4	-2.43	1.46	1.52
12	A	306	UMQ	C3-C4	-2.42	1.46	1.52
12	A	306	UMQ	O3'-C3'	-2.40	1.37	1.43
12	A	307	UMQ	C3-C4	-2.39	1.46	1.52
13	B	201	CLA	CMD-C2D	-2.38	1.46	1.51
12	A	308	UMQ	O3'-C3'	-2.37	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	B	201	CLA	CMB-C2B	-2.36	1.46	1.51
12	A	307	UMQ	O5'-C5'	-2.24	1.38	1.44
9	A	303	HEM	C2D-C1D	-2.18	1.44	1.51
9	A	301	HEM	C2B-C1B	-2.17	1.44	1.51
9	C	301	HEM	C2B-C1B	-2.14	1.44	1.51
12	A	308	UMQ	C4'-C5'	-2.14	1.47	1.52
9	A	302	HEM	C2D-C1D	-2.07	1.45	1.51
9	A	301	HEM	C2D-C1D	-2.04	1.45	1.51
17	G	101	BCR	C24-C25	2.00	1.53	1.45
17	G	101	BCR	C11-C12	2.01	1.39	1.34
9	A	302	HEM	C3C-CAC	2.06	1.55	1.51
9	A	301	HEM	C1C-NC	2.07	1.38	1.36
9	A	301	HEM	C3B-CAB	2.09	1.55	1.51
9	A	301	HEM	C3C-CAC	2.09	1.55	1.51
17	G	101	BCR	C20-C19	2.10	1.40	1.34
9	C	301	HEM	C4C-NC	2.11	1.38	1.36
9	A	302	HEM	C1C-NC	2.15	1.38	1.36
9	A	301	HEM	FE-NC	2.16	2.04	1.95
9	A	303	HEM	FE-NB	2.16	2.08	1.97
9	A	303	HEM	C1C-NC	2.19	1.38	1.36
17	G	101	BCR	C10-C9	2.20	1.38	1.35
9	A	303	HEM	C3B-CAB	2.23	1.55	1.51
9	C	301	HEM	C1C-NC	2.29	1.38	1.36
17	G	101	BCR	C5-C6	2.29	1.38	1.34
15	G	102	OZ2	O1G-C1	2.38	1.40	1.33
17	G	101	BCR	C24-C23	2.39	1.40	1.33
13	B	201	CLA	CHC-C1C	2.47	1.43	1.35
9	A	303	HEM	FE-ND	2.68	2.11	1.97
17	G	101	BCR	C14-C13	2.69	1.39	1.35
9	C	301	HEM	FE-NB	2.72	2.11	1.97
17	G	101	BCR	C12-C13	2.77	1.52	1.45
9	A	302	HEM	FE-NC	2.80	2.06	1.95
17	G	101	BCR	C19-C18	2.81	1.52	1.45
17	G	101	BCR	C11-C10	2.96	1.53	1.43
17	G	101	BCR	C16-C17	2.99	1.53	1.43
17	G	101	BCR	C8-C9	2.99	1.52	1.45
15	C	303	OZ2	C10-C9	3.00	1.49	1.28
17	G	101	BCR	C15-C14	3.08	1.53	1.43
15	C	303	OZ2	C7B-C6B	3.12	1.49	1.31
15	B	203	OZ2	C10-C9	3.17	1.50	1.31
17	G	101	BCR	C23-C22	3.24	1.53	1.45
17	G	101	BCR	C20-C21	3.27	1.53	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	G	101	BCR	C21-C22	3.33	1.40	1.35
17	G	101	BCR	C17-C18	3.38	1.40	1.35
9	A	303	HEM	FE-NC	3.41	2.09	1.95
15	G	102	OZ2	C7B-C6B	3.52	1.52	1.31
15	G	102	OZ2	C10-C9	3.67	1.52	1.31
17	G	101	BCR	C26-C25	3.77	1.40	1.34

All (114) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	D	201	1E2	O9-S-C6	-10.38	98.19	106.94
16	D	201	1E2	O8-S-O9	-6.65	96.14	111.61
17	G	101	BCR	C33-C5-C6	-4.97	119.73	124.61
17	G	101	BCR	C24-C23-C22	-4.92	118.72	126.22
16	D	201	1E2	O9-S-O7	-4.74	96.20	113.48
17	G	101	BCR	C7-C8-C9	-4.58	119.23	126.22
17	G	101	BCR	C15-C14-C13	-4.53	120.66	127.20
17	G	101	BCR	C16-C17-C18	-4.39	120.85	127.20
17	G	101	BCR	C11-C10-C9	-4.29	121.00	127.20
17	G	101	BCR	C38-C26-C25	-3.90	120.78	124.61
17	G	101	BCR	C20-C21-C22	-3.45	122.22	127.20
13	B	201	CLA	CAA-CBA-CGA	-3.17	104.05	113.32
17	G	101	BCR	C23-C24-C25	-2.89	118.63	127.32
12	A	308	UMQ	C1-O1-C4'	-2.81	110.67	118.01
17	G	101	BCR	C32-C1-C6	-2.76	105.98	110.30
17	G	101	BCR	C34-C9-C10	-2.75	118.84	122.90
13	B	201	CLA	CMB-C2B-C1B	-2.70	123.91	128.36
12	A	307	UMQ	C1-O1-C4'	-2.65	111.09	118.01
17	G	101	BCR	C4-C5-C6	-2.63	119.42	122.78
9	C	301	HEM	C3B-CAB-CBB	-2.63	120.42	124.46
13	B	201	CLA	O2D-CGD-O1D	-2.63	118.36	123.79
15	B	203	OZ2	O2G-C1B-O1B	-2.38	118.16	122.92
16	D	201	1E2	O5-C1-C2	-2.36	105.44	110.28
17	G	101	BCR	C16-C15-C14	-2.31	118.27	123.39
9	A	303	HEM	CBA-CAA-C2A	-2.26	108.47	112.53
17	G	101	BCR	C27-C26-C25	-2.22	119.95	122.78
17	G	101	BCR	C8-C7-C6	-2.22	120.66	127.32
17	G	101	BCR	C20-C19-C18	-2.21	119.83	126.32
12	A	306	UMQ	C1'-O5'-C5'	-2.20	109.47	113.75
12	A	308	UMQ	C3'-C4'-C5'	-2.20	105.87	110.84
9	C	301	HEM	C3B-C4B-NB	-2.18	107.46	111.63
16	D	201	1E2	O5-C5-C4	-2.17	105.61	109.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	301	HEM	CAA-C2A-C1A	-2.16	124.66	127.01
9	C	301	HEM	CAA-C2A-C1A	-2.14	124.68	127.01
9	C	301	HEM	CMA-C3A-C4A	-2.14	124.82	128.36
17	G	101	BCR	C1-C6-C5	-2.09	119.59	122.66
9	A	302	HEM	C3B-CAB-CBB	-2.09	121.25	124.46
9	A	303	HEM	C3C-CAC-CBC	-2.08	121.26	124.46
17	G	101	BCR	C11-C12-C13	-2.08	120.21	126.32
9	A	301	HEM	CBD-CAD-C3D	-2.05	107.59	113.55
9	A	303	HEM	C2C-C1C-CHC	2.00	126.73	123.68
13	B	201	CLA	CMD-C2D-C3D	2.06	129.11	125.09
16	D	201	1E2	C3-C4-C5	2.09	113.83	110.20
9	A	301	HEM	C2D-C3D-C4D	2.14	105.13	101.50
13	B	201	CLA	CHB-C4A-NA	2.23	127.59	124.51
15	C	303	OZ2	O1G-C1-C2	2.26	118.79	111.90
9	A	302	HEM	C2D-C3D-C4D	2.31	105.41	101.50
9	A	301	HEM	C2C-C1C-CHC	2.32	127.21	123.68
9	C	301	HEM	C2D-C3D-C4D	2.38	105.54	101.50
17	G	101	BCR	C29-C30-C25	2.41	114.19	110.36
9	A	303	HEM	C2D-C3D-C4D	2.60	105.92	101.50
12	A	307	UMQ	C3'-C4'-C5'	2.61	116.75	110.84
13	B	201	CLA	C9-C8-C10	2.64	121.23	111.08
13	B	201	CLA	C4A-NA-C1A	2.69	109.83	106.36
9	A	303	HEM	CMD-C2D-C3D	2.69	126.24	114.35
13	B	201	CLA	O2D-CGD-CBD	2.72	115.03	111.30
9	C	301	HEM	CMD-C2D-C3D	2.75	126.50	114.35
12	A	308	UMQ	C6-C5-C4	2.84	120.01	113.02
12	A	306	UMQ	CA-O1'-C1'	2.91	119.03	113.94
9	A	301	HEM	CMD-C2D-C3D	2.92	127.28	114.35
15	B	203	OZ2	O1G-C1-C2	2.92	120.81	111.90
9	A	302	HEM	CMD-C2D-C3D	3.00	127.60	114.35
17	G	101	BCR	C38-C26-C27	3.08	119.27	113.43
15	G	102	OZ2	O1G-C1G-C2G	3.09	117.01	108.69
12	A	306	UMQ	C1-C2-C3	3.13	116.13	109.97
9	C	301	HEM	C3B-C4B-CHC	3.19	127.66	123.16
12	A	307	UMQ	O1-C1-O5	3.30	119.03	110.68
9	A	303	HEM	CAD-C3D-C2D	3.40	123.00	113.22
15	C	303	OZ2	O2G-C1B-C2B	3.44	119.00	111.53
12	A	306	UMQ	O1'-C1'-C2'	3.45	112.39	108.04
9	C	301	HEM	CMB-C2B-C3B	3.50	125.27	116.53
15	G	102	OZ2	O2G-C1B-C2B	3.55	119.25	111.53
15	C	303	OZ2	O1G-C1G-C2G	3.71	118.68	108.69
15	B	203	OZ2	O1G-C1G-C2G	3.78	118.86	108.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	301	HEM	CAD-C3D-C4D	3.87	126.14	112.47
17	G	101	BCR	C33-C5-C4	3.91	120.85	113.43
9	A	301	HEM	CMC-C2C-C3C	4.00	126.50	116.53
12	A	308	UMQ	CA-O1'-C1'	4.06	121.04	113.94
17	G	101	BCR	C2-C1-C6	4.09	116.84	110.36
16	D	201	1E2	O8-S-O7	4.16	121.30	111.61
12	A	306	UMQ	O5-C1-C2	4.19	118.87	110.28
9	C	301	HEM	CAD-C3D-C4D	4.20	127.29	112.47
9	A	302	HEM	CAD-C3D-C4D	4.21	127.30	112.47
9	A	302	HEM	CMB-C2B-C3B	4.21	127.05	116.53
12	A	307	UMQ	O5'-C5'-C6'	4.22	117.02	106.36
9	A	303	HEM	CMC-C2C-C3C	4.22	127.07	116.53
12	A	306	UMQ	O1-C1-O5	4.23	121.39	110.68
9	C	301	HEM	CMC-C2C-C3C	4.24	127.11	116.53
12	A	307	UMQ	O5'-C1'-C2'	4.33	119.16	110.28
9	A	303	HEM	CMB-C2B-C3B	4.35	127.38	116.53
15	B	203	OZ2	O2G-C1B-C2B	4.35	119.30	111.10
12	A	306	UMQ	O5-C5-C6	4.45	117.59	106.36
12	A	308	UMQ	C1-C2-C3	4.52	118.88	109.97
12	A	308	UMQ	O2-C2-C1	4.53	119.94	110.02
12	A	308	UMQ	O2-C2-C3	4.53	120.54	110.34
9	A	302	HEM	CMC-C2C-C3C	4.64	128.12	116.53
12	A	307	UMQ	O5'-C1'-O1'	4.66	121.28	110.05
12	A	306	UMQ	O1-C1-C2	4.67	119.48	108.10
12	A	307	UMQ	CA-O1'-C1'	4.71	122.18	113.94
12	A	308	UMQ	O5-C5-C6	4.74	118.34	106.36
9	C	301	HEM	CAD-C3D-C2D	4.85	127.16	113.22
9	A	302	HEM	CAD-C3D-C2D	4.89	127.28	113.22
12	A	307	UMQ	O5-C1-C2	4.91	120.35	110.28
9	A	301	HEM	CMB-C2B-C3B	4.95	128.89	116.53
12	A	306	UMQ	O2-C2-C3	5.04	121.68	110.34
12	A	307	UMQ	O1-C1-C2	5.09	120.49	108.10
9	A	303	HEM	CAD-C3D-C4D	5.28	131.08	112.47
12	A	306	UMQ	O2-C2-C1	5.32	121.67	110.02
9	A	301	HEM	CAD-C3D-C2D	5.39	128.73	113.22
12	A	308	UMQ	O5-C5-C4	6.01	120.97	109.68
12	A	307	UMQ	O5'-C5'-C4'	7.07	124.68	109.75
12	A	306	UMQ	O5-C5-C4	7.67	124.07	109.68
12	A	307	UMQ	O1'-C1'-C2'	8.99	119.39	108.04
16	D	201	1E2	O7-S-C6	12.56	117.53	106.94

All (13) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
15	B	203	OZ2	CG2
12	A	306	UMQ	C5
12	A	306	UMQ	C2
12	A	306	UMQ	C1
13	B	201	CLA	NC
13	B	201	CLA	ND
13	B	201	CLA	NA
12	A	307	UMQ	C5'
12	A	307	UMQ	C1'
12	A	307	UMQ	C1
16	D	201	1E2	C5
12	A	308	UMQ	C5
12	A	308	UMQ	C2

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 34 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	301	HEM	7	0
9	A	302	HEM	8	0
9	A	303	HEM	8	0
12	A	306	UMQ	1	0
12	A	308	UMQ	1	0
13	B	201	CLA	1	0
9	C	301	HEM	6	0
16	D	201	1E2	2	0
15	G	102	OZ2	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 ⓘ

### 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	213/215 (99%)	0.09	1 (0%) 91 88	47, 65, 96, 135	0
2	B	159/160 (99%)	0.23	8 (5%) 32 21	51, 85, 126, 184	0
3	C	288/289 (99%)	0.96	66 (22%) 1 1	58, 95, 219, 257	1 (0%)
4	D	38/179 (21%)	0.53	6 (15%) 3 1	51, 76, 168, 214	0
5	E	28/32 (87%)	0.25	3 (10%) 8 4	83, 95, 118, 139	0
6	F	31/35 (88%)	0.32	2 (6%) 22 13	72, 87, 125, 131	0
7	G	35/37 (94%)	1.11	8 (22%) 1 1	62, 84, 193, 242	0
8	H	28/29 (96%)	0.12	0 100 100	67, 76, 99, 122	0
All	All	820/976 (84%)	0.50	94 (11%) 6 3	47, 84, 185, 257	1 (0%)

All (94) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	206	THR	11.4
3	C	220	SER	9.8
3	C	219	VAL	9.4
7	G	35	LEU	7.4
7	G	36	GLY	7.2
3	C	207	VAL	7.1
3	C	190	TYR	7.1
3	C	287	MET	6.9
3	C	176	ALA	6.8
7	G	33	ASN	6.6
3	C	179	THR	5.9
4	D	10	VAL	5.6
3	C	208	VAL	5.6
3	C	191	GLY	5.1
3	C	199	ILE	5.1
3	C	224	ALA	5.1

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Mol	Chain	Res	Type	RSRZ
3	C	288	ASN	5.1
4	D	9	ASP	4.7
3	C	203	SER	4.5
3	C	195	TYR	4.3
3	C	192	ASN	4.2
3	C	92	GLU	4.2
3	C	201	THR	4.1
2	B	160	PHE	4.1
3	C	177	THR	4.0
3	C	204	GLY	4.0
3	C	200	GLN	3.9
3	C	181	THR	3.9
3	C	180	ILE	3.9
3	C	188	ASP	3.8
3	C	205	LYS	3.8
3	C	140	LYS	3.7
3	C	211	ILE	3.7
3	C	218	ILE	3.7
3	C	172	PHE	3.6
3	C	96	LYS	3.6
3	C	230	ALA	3.6
3	C	217	LEU	3.5
7	G	37	GLY	3.4
3	C	95	LYS	3.4
2	B	151	LEU	3.3
3	C	189	GLU	3.3
3	C	197	VAL	3.2
4	D	13	MET	3.1
3	C	193	VAL	3.1
3	C	187	GLU	3.1
3	C	173	THR	3.0
3	C	202	ASP	3.0
3	C	222	GLY	3.0
3	C	215	PRO	3.0
3	C	196	GLN	2.9
3	C	186	GLU	2.8
2	B	158	GLY	2.8
3	C	226	LYS	2.8
2	B	2	ALA	2.8
3	C	170	ASN	2.8
3	C	98	VAL	2.8
3	C	184	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
3	C	194	LYS	2.7
3	C	4	TRP	2.7
3	C	174	ALA	2.7
5	E	29	ILE	2.6
3	C	182	LYS	2.6
7	G	31	ARG	2.6
3	C	286	GLU	2.4
6	F	29	ILE	2.4
2	B	159	LEU	2.4
3	C	227	ALA	2.4
3	C	198	SER	2.4
4	D	15	ARG	2.4
3	C	178	GLY	2.4
3	C	175	SER	2.4
2	B	75	ILE	2.4
7	G	32	PRO	2.4
2	B	153	LYS	2.4
6	F	27	LEU	2.3
7	G	26	TYR	2.3
2	B	74	GLU	2.3
3	C	231	LEU	2.3
3	C	93	GLU	2.3
4	D	17	GLN	2.2
3	C	90	ILE	2.2
5	E	23	ILE	2.2
3	C	223	GLN	2.2
3	C	281	LYS	2.1
5	E	28	SER	2.1
3	C	228	GLY	2.1
3	C	212	PRO	2.1
3	C	229	GLU	2.1
4	D	14	GLY	2.1
3	C	94	LEU	2.0
3	C	183	ILE	2.0
1	A	15	GLN	2.0
7	G	29	TYR	2.0

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

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

### 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 6.4 Ligands ⓘ

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
11	8K6	A	305	18/18	0.72	0.45	10.73	96,120,123,123	0
18	OCT	F	101	8/8	0.79	0.47	4.40	102,123,135,135	0
12	UMQ	A	306	34/34	0.68	0.39	4.11	85,138,194,197	0
15	OZ2	C	303	38/48	0.75	0.34	2.92	54,108,185,186	0
10	MYS	A	304	15/15	0.85	0.26	2.70	77,94,102,102	0
17	BCR	G	101	40/40	0.86	0.33	2.43	68,95,177,180	0
9	HEM	A	302	43/43	0.98	0.27	1.84	51,64,74,79	0
15	OZ2	G	102	44/48	0.81	0.27	1.52	58,102,166,169	0
9	HEM	A	303	43/43	0.96	0.26	1.45	50,74,88,89	0
12	UMQ	A	307	34/34	0.81	0.47	1.42	115,144,174,177	0
12	UMQ	A	308	34/34	0.83	0.38	1.41	109,146,192,197	0
13	CLA	B	201	65/65	0.93	0.23	0.67	68,98,132,135	0
9	HEM	A	301	43/43	0.98	0.25	0.67	38,50,63,75	0
14	CD	B	202	1/1	0.98	0.22	0.05	124,124,124,124	0
9	HEM	C	301	43/43	0.97	0.20	-0.15	76,82,98,107	0
15	OZ2	B	203	32/48	0.93	0.17	-0.46	91,97,127,128	0
16	1E2	D	201	23/23	0.91	0.17	-1.04	104,110,123,134	0
14	CD	A	309	1/1	0.99	0.20	-	85,85,85,85	0
14	CD	C	302	1/1	0.95	0.17	-	142,142,142,142	0

### 6.5 Other polymers ⓘ

There are no such residues in this entry.