



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 11:46 am GMT

PDB ID : 4PV1  
Title : Cytochrome B6F structure from *M. lamosus* with the quinone analog inhibitor stigmatellin  
Authors : Hasan, S.S.; Yamashita, E.; Cramer, W.A.  
Deposited on : 2014-03-14  
Resolution : 3.00 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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : recalc28949

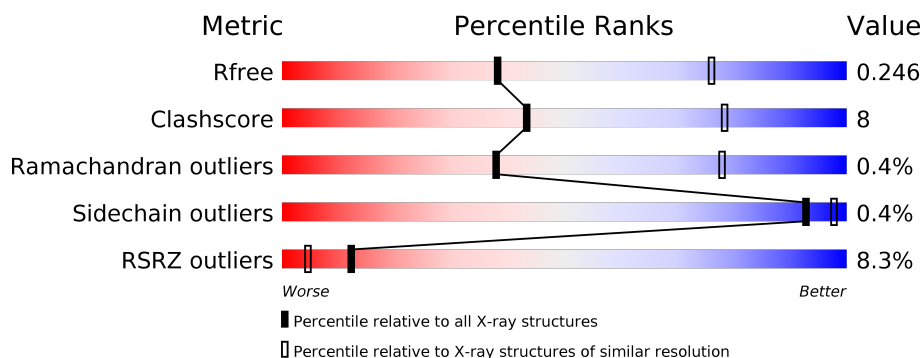
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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.



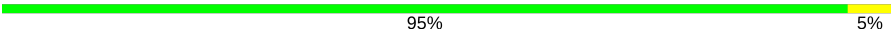

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	100719	1692 (3.00-3.00)
Clashscore	112137	2037 (3.00-3.00)
Ramachandran outliers	110173	1973 (3.00-3.00)
Sidechain outliers	110143	1976 (3.00-3.00)
RSRZ outliers	101464	1716 (3.00-3.00)

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>88%</div> <div>11%</div> <div>.</div> </div>
2	B	160	<div> <div>2%</div> <div>86%</div> <div>14%</div> <div>.</div> </div>
3	C	289	<div> <div>12%</div> <div>86%</div> <div>14%</div> </div>
4	D	179	<div> <div>21%</div> <div>72%</div> <div>17%</div> <div>12%</div> </div>
5	E	32	<div> <div>75%</div> <div>13%</div> <div>13%</div> </div>
6	F	35	<div> <div>6%</div> <div>83%</div> <div>6%</div> <div>11%</div> </div>

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Mol	Chain	Length	Quality of chain
7	G	37	 95% 5%
8	H	29	 90% 7%

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	UMQ	A	306	-	-	-	X
12	UMQ	A	307	-	-	-	X
12	UMQ	B	203	-	-	-	X
13	SMA	A	308	X	-	-	X
14	7PH	A	309	-	-	-	X
15	8K6	B	201	-	-	-	X
16	CLA	B	204	X	-	-	-
17	OPC	B	205	-	-	-	X
17	OPC	D	203	-	-	-	X
17	OPC	E	101	-	-	-	X
20	BCR	G	101	-	-	-	X
9	MYS	A	301	-	-	-	X

## 2 Entry composition

There are 21 unique types of molecules in this entry. The entry contains 8049 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 Cytochrome b6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	213	Total	C	N	O	S	5	0	0
			1698	1132	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	N	O	S	2	0	0
			1241	836	192	208	5			

- Molecule 3 is a protein called Apocytochrome f.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	288	Total	C	N	O	S	0	0	0
			2216	1415	369	424	8			

There is a discrepancy between the modelled and reference sequences:

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	158	Total	C	N	O	S	0	0	0
			1221	783	210	221	7			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	28	Total	C	N	O	0	0	0
			215	156	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	N	O	S	0	0	0
			234	160	34	39	1			

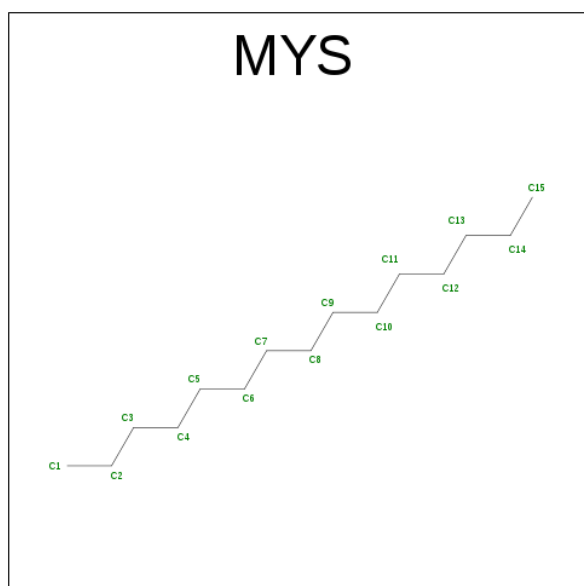
- Molecule 7 is a protein called Cytochrome b6-f complex subunit 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	37	Total	C	N	O	S	4	0	0
			283	188	44	50	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	28	Total	C	N	O	S	0	0	0
			222	151	35	35	1			

- Molecule 9 is PENTADECANE (three-letter code: MYS) (formula: C<sub>15</sub>H<sub>32</sub>).

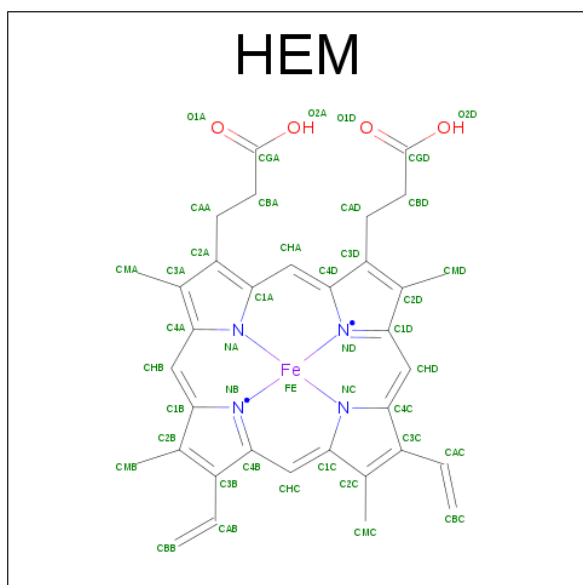


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	1	Total	C	0	0
			15	15		

- Molecule 10 is CADMIUM ION (three-letter code: CD) (formula: Cd).

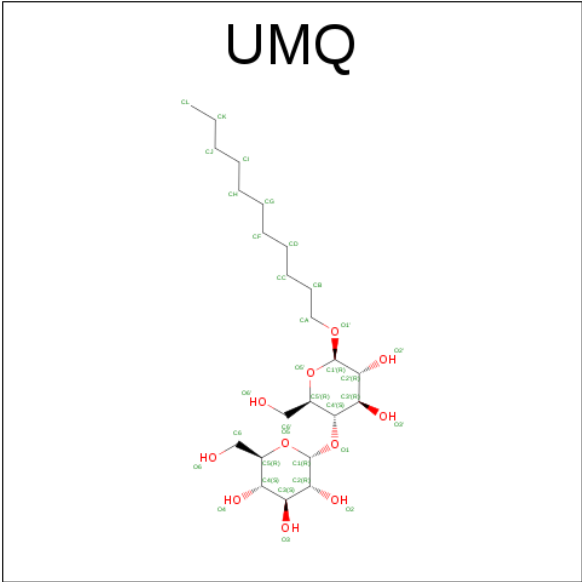
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	B	1	Total Cd 1 1	0	0
10	A	1	Total Cd 1 1	0	0

- Molecule 11 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).



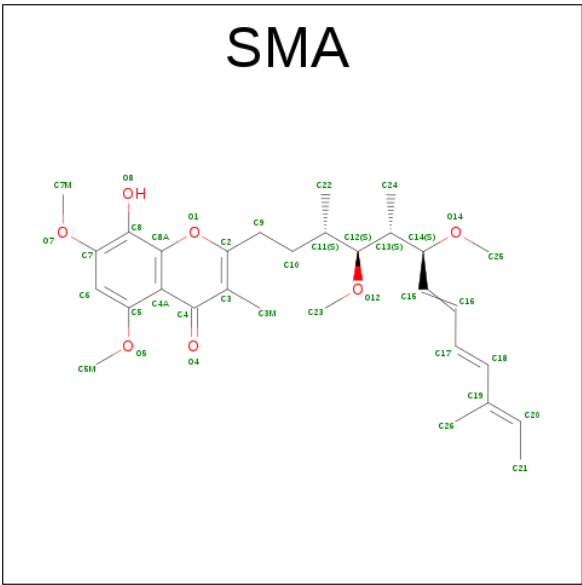
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	1	Total C Fe N O 43 34 1 4 4	0	0
11	A	1	Total C Fe N O 43 34 1 4 4	0	0
11	A	1	Total C Fe N O 43 34 1 4 4	0	0
11	C	1	Total C Fe N O 43 34 1 4 4	0	0

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



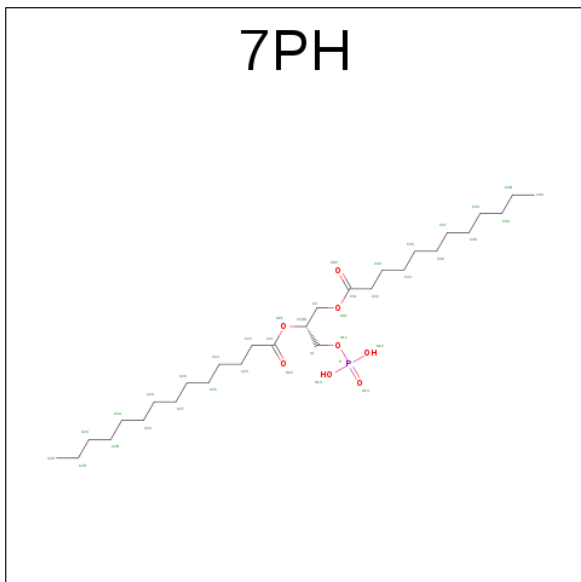
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	A	1	Total	C	O	6	0
			34	23	11		
12	A	1	Total	C	O	2	0
			34	23	11		
12	B	1	Total	C	O	0	0
			34	23	11		

- Molecule 13 is STIGMATELLIN A (three-letter code: SMA) (formula: C<sub>30</sub>H<sub>42</sub>O<sub>7</sub>).



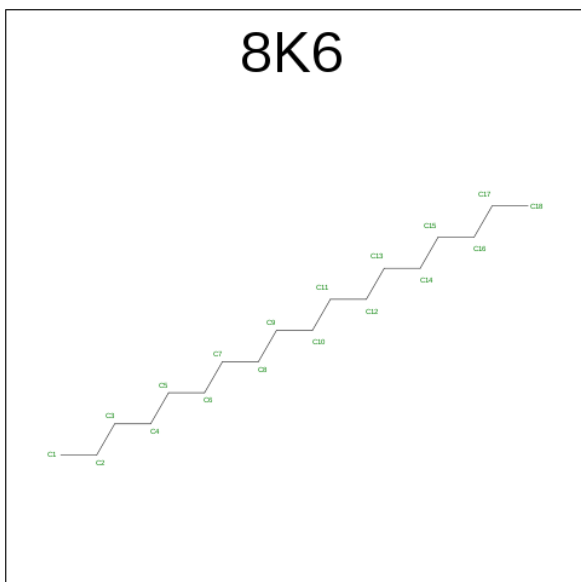
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
13	A	1	Total	C	O	3	0
			37	30	7		

- Molecule 14 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
14	A	1	Total	C	O	3	0
			32	27	5		

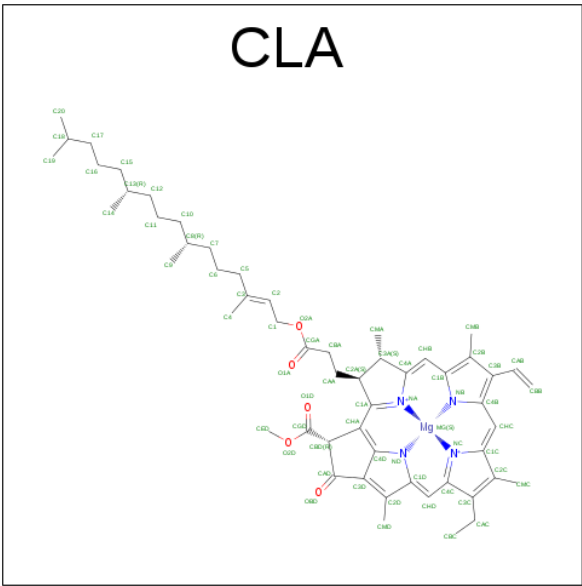
- Molecule 15 is OCTADECANE (three-letter code: 8K6) (formula:  $C_{18}H_{38}$ ).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	B	1	Total	C	0	0
			18	18		

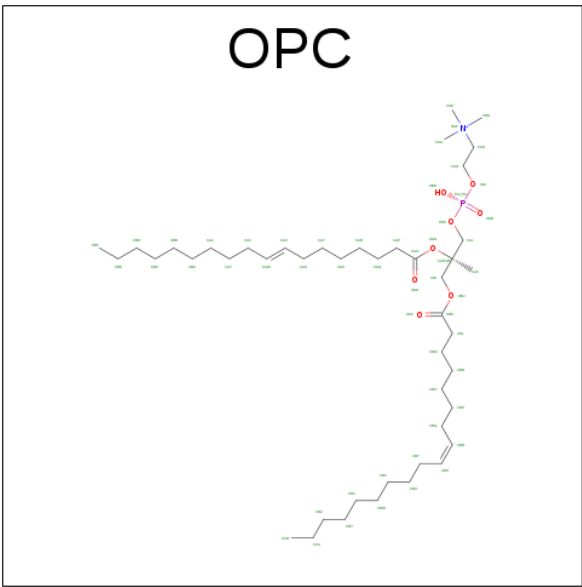


- Molecule 16 is CHLOROPHYLL A (three-letter code: CLA) (formula:  $C_{55}H_{72}MgN_4O_5$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
16	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

- Molecule 17 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:  $C_{45}H_{87}NO_8P$ ).



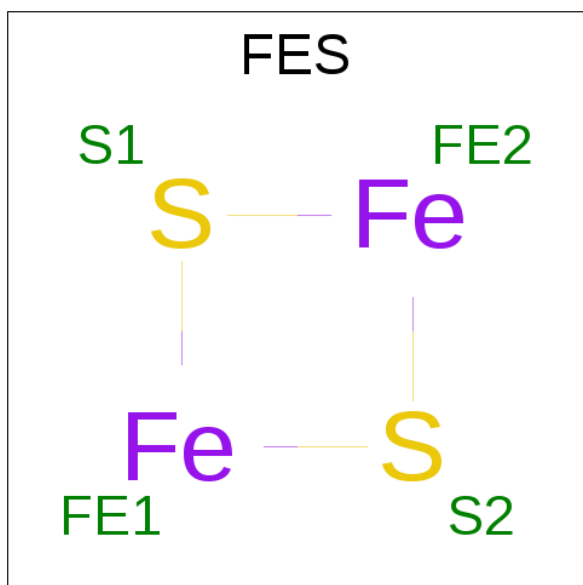
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
17	B	1	Total	C	N	O	P	0	0
			54	44	1	8	1		

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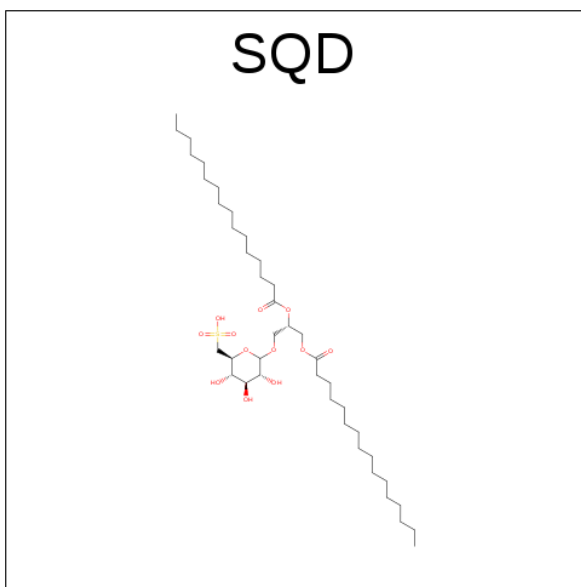
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
17	D	1	Total	C	N	O	P	1	0
			54	44	1	8	1		
17	E	1	Total	C	N	O	P	0	0
			54	44	1	8	1		

- Molecule 18 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe<sub>2</sub>S<sub>2</sub>).



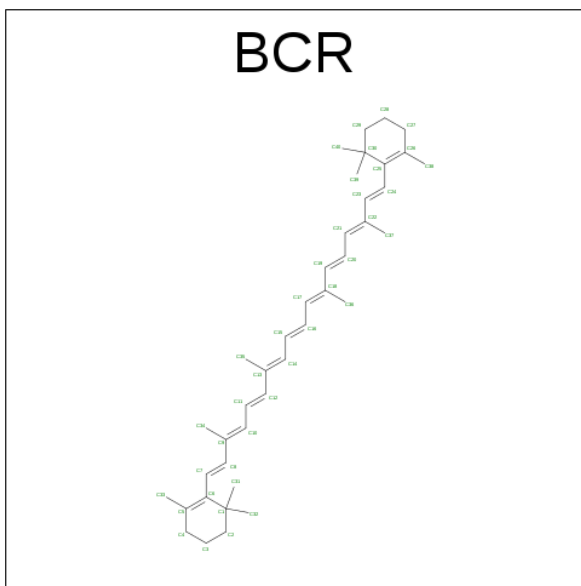
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
18	D	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 19 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula: C<sub>41</sub>H<sub>78</sub>O<sub>12</sub>S).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
19	D	1	Total	C	O	S	30	0
			54	41	12	1		

- 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	14	0
			40	40		


- Molecule 21 is water.

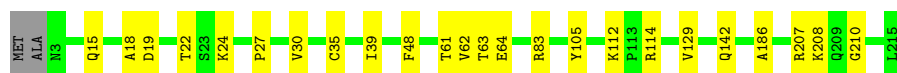
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
21	A	8	Total 8	O 8	0	0
21	B	5	Total 5	O 5	0	0
21	C	2	Total 2	O 2	0	0
21	G	1	Total 1	O 1	0	0

### 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 the various outlier classes 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

Chain A: 




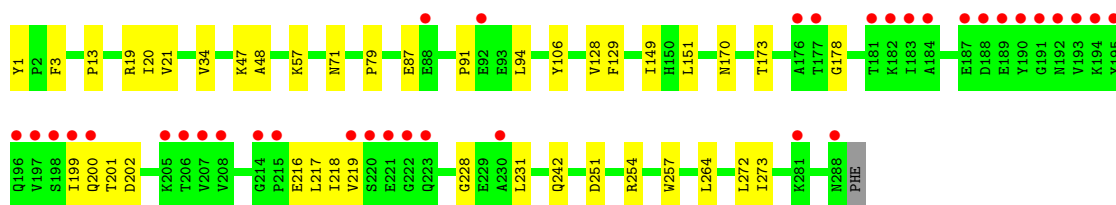
#### • Molecule 2: Cytochrome b6-f complex subunit 4

Chain B: 



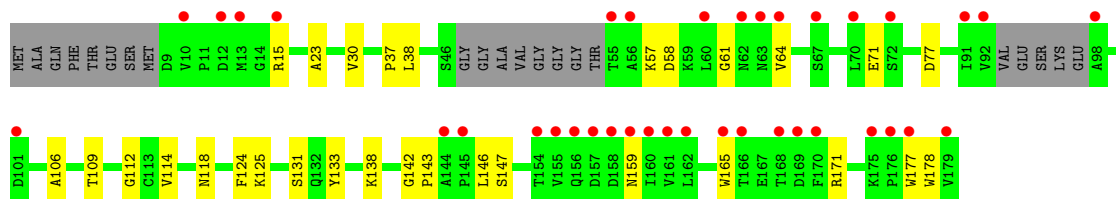
#### • Molecule 3: Apocytochrome f

Chain C: 



#### • Molecule 4: Cytochrome b6-f complex iron-sulfur subunit

Chain D: 



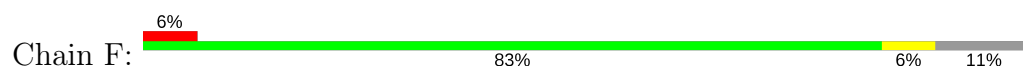
#### • Molecule 5: Cytochrome b6-f complex subunit 6

Chain E: 





- 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, $\alpha$ , $\beta$ , $\gamma$	159.09Å 159.09Å 361.32Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.34 – 3.00 48.34 – 3.00	Depositor EDS
% Data completeness (in resolution range)	91.2 (48.34-3.00) 83.4 (48.34-3.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.63 (at 3.01Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.8.4_1496)	Depositor
R, $R_{free}$	0.216 , 0.247 0.217 , 0.246	Depositor DCC
$R_{free}$ test set	2548 reflections (5.08%)	DCC
Wilson B-factor (Å <sup>2</sup> )	85.8	Xtriage
Anisotropy	0.219	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 78.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	8049	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	114.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.79% 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, 0.333 respectively for untwinned datasets, and 0.375, 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, BCR, FES, OPC, HEM, 8K6, SMA, 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	0.22	0/1750	0.37	0/2388
2	B	0.21	0/1280	0.37	0/1755
3	C	0.21	0/2264	0.39	0/3082
4	D	0.20	0/1252	0.37	0/1705
5	E	0.22	0/220	0.35	0/297
6	F	0.21	0/238	0.32	0/321
7	G	0.21	0/289	0.37	0/391
8	H	0.20	0/228	0.32	0/313
All	All	0.21	0/7521	0.37	0/10252

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

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	0	1719	25	1
2	B	1241	0	1296	17	0
3	C	2216	0	2232	24	1
4	D	1221	0	1206	19	0
5	E	215	0	237	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	F	234	0	248	2	0
7	G	283	0	289	1	0
8	H	222	0	227	2	0
9	A	15	0	32	3	0
10	A	1	0	0	0	0
10	B	1	0	0	0	0
11	A	129	0	90	11	0
11	C	43	0	30	3	0
12	A	68	0	87	10	0
12	B	34	0	44	10	0
13	A	37	0	41	7	0
14	A	32	0	45	3	0
15	B	18	0	38	0	0
16	B	65	0	72	5	0
17	B	54	0	83	5	0
17	D	54	0	83	4	0
17	E	54	0	83	12	0
18	D	4	0	0	0	0
19	D	54	0	78	1	0
20	G	40	0	56	1	0
21	A	8	0	0	0	0
21	B	5	0	0	1	0
21	C	2	0	0	0	0
21	G	1	0	0	0	0
All	All	8049	0	8316	124	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 8.

All (124) 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)
12:B:203:UMQ:O5'	12:B:203:UMQ:C5'	1.63	1.46
1:A:35:CYS:SG	11:A:305:HEM:CAB	2.04	1.44
12:B:203:UMQ:O5'	12:B:203:UMQ:C1'	1.69	1.41
12:A:307:UMQ:O5'	12:A:307:UMQ:C1'	1.69	1.40
1:A:35:CYS:SG	11:A:305:HEM:CBB	2.18	1.31
12:B:203:UMQ:C5'	12:B:203:UMQ:C1'	2.48	0.91
12:A:307:UMQ:C5'	12:A:307:UMQ:C1'	2.48	0.91
1:A:35:CYS:SG	11:A:305:HEM:C3B	2.64	0.91
9:A:301:MYS:H52	9:A:301:MYS:H101	1.52	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:83:ARG:NH1	11:A:303:HEM:O2D	2.04	0.89
17:E:101:OPC:HBI1	17:E:101:OPC:HAQ1	1.57	0.85
1:A:114:ARG:NH1	1:A:210:GLY:O	2.10	0.85
1:A:186:ALA:HB2	9:A:301:MYS:H81	1.61	0.83
1:A:208:LYS:NZ	12:A:306:UMQ:H61	1.98	0.79
2:B:78:GLU:OE2	2:B:80:TYR:OH	2.03	0.76
4:D:165:TRP:HB3	4:D:178:TRP:HE1	1.50	0.74
3:C:251:ASP:HB3	3:C:254:ARG:HD3	1.67	0.74
1:A:24:LYS:HG3	13:A:308:SMA:H4	1.71	0.73
11:A:303:HEM:HHC	11:A:303:HEM:HBB2	1.70	0.73
11:C:301:HEM:HBB2	11:C:301:HEM:HHC	1.75	0.69
1:A:208:LYS:HZ2	12:A:306:UMQ:H61	1.59	0.68
17:E:101:OPC:HBF2	6:F:14:GLY:HA3	1.76	0.67
5:E:5:ALA:HA	17:E:101:OPC:HAW	1.78	0.66
1:A:22:THR:HG21	12:B:203:UMQ:H2'1	1.78	0.66
4:D:57:LYS:HB3	4:D:61:GLY:HA2	1.79	0.65
14:A:309:7PH:H2CA	4:D:37:PRO:HG2	1.79	0.64
11:A:304:HEM:HMC2	11:A:304:HEM:HBC2	1.80	0.64
3:C:178:GLY:HA3	3:C:199:ILE:HG23	1.80	0.63
3:C:91:PRO:HG2	3:C:94:LEU:HB2	1.80	0.63
9:A:301:MYS:C5	9:A:301:MYS:H101	2.28	0.62
13:A:308:SMA:H36	13:A:308:SMA:H14	1.82	0.61
12:A:306:UMQ:O5'	12:A:306:UMQ:C6'	2.48	0.61
17:E:101:OPC:HBW1	8:H:15:PHE:CD1	2.35	0.61
4:D:131:SER:HA	4:D:142:GLY:HA3	1.82	0.60
4:D:124:PHE:HB2	4:D:133:TYR:HB2	1.83	0.60
1:A:39:ILE:HD11	20:G:101:BCR:H312	1.83	0.59
1:A:142:GLN:NE2	2:B:70:ALA:O	2.36	0.58
3:C:19:ARG:O	3:C:242:GLN:NE2	2.35	0.58
4:D:38:LEU:HD21	17:D:203:OPC:HAL2	1.85	0.58
1:A:142:GLN:HG3	2:B:72:PRO:HG3	1.86	0.57
5:E:8:TYR:CE2	17:E:101:OPC:HAZ1	2.39	0.56
4:D:109:THR:HG21	4:D:146:LEU:HB2	1.87	0.56
3:C:57:LYS:HB3	3:C:57:LYS:NZ	2.20	0.56
1:A:207:ARG:NH1	13:A:308:SMA:O4	2.38	0.56
11:A:305:HEM:HHA	11:A:305:HEM:HBD1	1.88	0.56
3:C:48:ALA:HB3	3:C:129:PHE:HB2	1.88	0.56
1:A:105:TYR:O	2:B:126:ARG:NH2	2.34	0.55
1:A:129:VAL:HG21	16:B:204:CLA:H43	1.88	0.55
3:C:79:PRO:HD3	3:C:149:ILE:HG12	1.87	0.55
11:A:305:HEM:HMC1	11:A:305:HEM:HBC2	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:272:LEU:HD23	4:D:23:ALA:HB1	1.89	0.54
17:E:101:OPC:HBI1	17:E:101:OPC:CAQ	2.35	0.54
11:A:303:HEM:HMC1	11:A:303:HEM:HBC2	1.90	0.54
2:B:17:LYS:NZ	2:B:26:TYR:OH	2.40	0.53
4:D:118:ASN:HD22	4:D:125:LYS:HD3	1.74	0.53
11:C:301:HEM:HBC2	11:C:301:HEM:HMC2	1.89	0.53
11:A:305:HEM:HMB1	11:A:305:HEM:HBB2	1.90	0.53
3:C:34:VAL:HB	3:C:151:LEU:HD22	1.90	0.53
1:A:61:THR:HG22	1:A:63:THR:H	1.73	0.53
17:D:203:OPC:HBI2	17:D:203:OPC:HBO1	1.90	0.53
16:B:204:CLA:HAC1	17:B:205:OPC:HBW1	1.91	0.52
2:B:84:VAL:HG13	2:B:101:MET:HG2	1.92	0.51
1:A:15:GLN:NE2	1:A:19:ASP:OD1	2.44	0.51
12:B:203:UMQ:O5'	12:B:203:UMQ:C6'	2.48	0.51
13:A:308:SMA:C25	12:B:203:UMQ:HL1	2.41	0.51
4:D:138:LYS:HD2	4:D:171:ARG:HG3	1.93	0.50
2:B:86:GLN:HE22	2:B:89:ARG:HH21	1.58	0.50
4:D:77:ASP:N	4:D:77:ASP:OD1	2.44	0.50
11:A:304:HEM:HBB2	11:A:304:HEM:HMB1	1.94	0.50
16:B:204:CLA:OBD	21:B:305:HOH:O	2.19	0.50
3:C:200:GLN:HG3	3:C:201:THR:H	1.77	0.49
3:C:47:LYS:HG3	3:C:128:VAL:HG13	1.94	0.49
4:D:106:ALA:HB1	4:D:114:VAL:HG13	1.94	0.49
17:B:205:OPC:HAS1	17:B:205:OPC:HBL2	1.94	0.49
1:A:18:ALA:HB2	12:A:307:UMQ:HD2	1.95	0.48
14:A:309:7PH:H24A	3:C:254:ARG:HA	1.95	0.48
1:A:208:LYS:HZ3	12:A:306:UMQ:H61	1.76	0.48
12:A:306:UMQ:O5'	12:A:306:UMQ:C4'	2.62	0.48
4:D:146:LEU:HD13	4:D:177:TRP:CG	2.49	0.48
3:C:231:LEU:H	3:C:231:LEU:HD23	1.79	0.47
1:A:27:PRO:HG2	1:A:30:VAL:HG23	1.95	0.47
3:C:173:THR:HB	3:C:228:GLY:HA2	1.95	0.47
2:B:50:CYS:HB3	17:E:101:OPC:HBX1	1.95	0.47
13:A:308:SMA:H43	12:B:203:UMQ:CL	2.45	0.47
4:D:131:SER:HB3	4:D:143:PRO:HD2	1.97	0.47
1:A:61:THR:HB	1:A:64:GLU:HB2	1.97	0.46
2:B:118:ASN:HD21	2:B:120:PHE:HB2	1.80	0.46
3:C:201:THR:OG1	3:C:202:ASP:N	2.48	0.46
17:E:101:OPC:HBN1	6:F:11:LEU:HD12	1.96	0.46
3:C:216:GLU:HG3	3:C:217:LEU:H	1.81	0.46
4:D:58:ASP:HB3	4:D:64:VAL:HG22	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:B:204:CLA:HBB2	17:B:205:OPC:HBM2	1.98	0.46
14:A:309:7PH:H26	3:C:257:TRP:HB2	1.97	0.45
2:B:115:GLU:HG2	17:B:205:OPC:HBI2	1.99	0.45
3:C:218:ILE:HD12	3:C:219:VAL:HG23	1.98	0.45
13:A:308:SMA:H43	12:B:203:UMQ:HL2	1.99	0.45
3:C:71:ASN:HB2	11:C:301:HEM:CGA	2.48	0.44
1:A:142:GLN:OE1	2:B:67:ASP:N	2.47	0.44
17:E:101:OPC:HBP2	17:E:101:OPC:HBS	1.68	0.44
17:E:101:OPC:HAZ2	17:E:101:OPC:HBC1	1.58	0.44
3:C:218:ILE:H	3:C:218:ILE:HG13	1.67	0.44
17:D:203:OPC:HAH2	17:D:203:OPC:HAA2	1.72	0.44
12:B:203:UMQ:HF1	12:B:203:UMQ:HI1	1.76	0.43
17:E:101:OPC:HAH1	17:E:101:OPC:HAE2	1.63	0.43
2:B:118:ASN:ND2	2:B:120:PHE:HB2	2.34	0.43
3:C:13:PRO:HB3	3:C:106:TYR:CE1	2.54	0.43
16:B:204:CLA:CBB	17:B:205:OPC:HBM2	2.50	0.42
17:E:101:OPC:HBP1	7:G:5:LEU:HD11	2.00	0.42
12:A:306:UMQ:H2'1	12:A:306:UMQ:HA2	1.67	0.42
12:A:306:UMQ:O5'	12:A:306:UMQ:C2'	2.67	0.42
3:C:170:ASN:OD1	3:C:170:ASN:N	2.51	0.42
13:A:308:SMA:H40	12:B:203:UMQ:HL1	2.02	0.42
2:B:33:PRO:HG3	19:D:202:SQD:H4	2.02	0.41
2:B:45:MET:HE1	4:D:30:VAL:HG21	2.01	0.41
4:D:15:ARG:HH12	5:E:29:ILE:HG22	1.85	0.41
2:B:86:GLN:OE1	2:B:90:SER:OG	2.39	0.41
3:C:1:TYR:HB3	3:C:3:PHE:CE1	2.56	0.40
4:D:64:VAL:N	4:D:159:ASN:OD1	2.54	0.40
1:A:48:PHE:HE2	17:D:203:OPC:HAQ2	1.87	0.40
1:A:62:VAL:HG23	1:A:63:THR:HG23	2.03	0.40
2:B:32:TRP:HA	2:B:33:PRO:HA	1.81	0.40
4:D:138:LYS:HA	4:D:147:SER:HB3	2.03	0.40
2:B:82:TYR:HB2	2:B:83:PRO:HD3	2.04	0.40
3:C:273:ILE:HD12	8:H:25:GLY:HA3	2.03	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:112:LYS:NZ	3:C:87:GLU:OE1[8_665]	2.19	0.01

## 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%)	201 (95%)	10 (5%)	0	100	100
2	B	157/160 (98%)	150 (96%)	7 (4%)	0	100	100
3	C	286/289 (99%)	256 (90%)	28 (10%)	2 (1%)	25	67
4	D	152/179 (85%)	127 (84%)	23 (15%)	2 (1%)	14	51
5	E	26/32 (81%)	26 (100%)	0	0	100	100
6	F	29/35 (83%)	27 (93%)	2 (7%)	0	100	100
7	G	35/37 (95%)	33 (94%)	2 (6%)	0	100	100
8	H	26/29 (90%)	26 (100%)	0	0	100	100
All	All	922/976 (94%)	846 (92%)	72 (8%)	4 (0%)	38	78

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	71	GLU
4	D	112	GLY
3	C	20	ILE
3	C	21	VAL

### 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%)	183 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	136/137 (99%)	136 (100%)	0	100	100
3	C	242/243 (100%)	241 (100%)	1 (0%)	93	98
4	D	132/146 (90%)	132 (100%)	0	100	100
5	E	21/25 (84%)	20 (95%)	1 (5%)	30	69
6	F	23/27 (85%)	23 (100%)	0	100	100
7	G	28/28 (100%)	27 (96%)	1 (4%)	40	77
8	H	23/24 (96%)	23 (100%)	0	100	100
All	All	788/814 (97%)	785 (100%)	3 (0%)	93	98

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	264	LEU
5	E	11	PHE
7	G	35	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 20 ligands modelled in this entry, 2 are monoatomic - leaving 18 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	MYS	A	301	-	14,14,14	0.10	0	13,13,13	0.79	0
11	HEM	A	303	1	28,50,50	2.23	6 (21%)	17,82,82	1.37	1 (5%)
11	HEM	A	304	1	28,50,50	2.16	6 (21%)	17,82,82	1.49	5 (29%)
11	HEM	A	305	13,21	28,50,50	2.20	6 (21%)	17,82,82	1.39	2 (11%)
12	UMQ	A	306	-	35,35,35	3.76	17 (48%)	46,46,46	2.26	8 (17%)
12	UMQ	A	307	-	35,35,35	3.77	17 (48%)	46,46,46	2.21	7 (15%)
13	SMA	A	308	11	36,38,38	2.98	11 (30%)	44,52,52	2.18	10 (22%)
14	7PH	A	309	-	31,31,37	1.26	2 (6%)	33,33,42	1.22	2 (6%)
15	8K6	B	201	-	17,17,17	0.09	0	16,16,16	0.85	0
12	UMQ	B	203	-	35,35,35	3.78	17 (48%)	46,46,46	2.17	7 (15%)
16	CLA	B	204	21	56,73,73	1.10	4 (7%)	65,113,113	1.25	7 (10%)
17	OPC	B	205	-	53,53,54	1.04	2 (3%)	58,61,64	1.03	2 (3%)
11	HEM	C	301	3	28,50,50	2.24	6 (21%)	17,82,82	1.47	3 (17%)
18	FES	D	201	4	0,4,4	0.00	-	0,4,4	0.00	-
19	SQD	D	202	-	53,54,54	0.96	5 (9%)	63,65,65	1.68	10 (15%)
17	OPC	D	203	-	53,53,54	1.03	2 (3%)	58,61,64	1.02	2 (3%)
17	OPC	E	101	-	53,53,54	1.03	3 (5%)	58,61,64	1.04	2 (3%)
20	BCR	G	101	-	41,41,41	1.10	2 (4%)	56,56,56	1.16	4 (7%)

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	MYS	A	301	-	-	0/12/12/12	0/0/0/0
11	HEM	A	303	1	-	0/6/54/54	0/0/8/8
11	HEM	A	304	1	-	0/6/54/54	0/0/8/8
11	HEM	A	305	13,21	-	0/6/54/54	0/0/8/8
12	UMQ	A	306	-	-	0/20/60/60	0/2/2/2
12	UMQ	A	307	-	-	0/20/60/60	0/2/2/2
13	SMA	A	308	11	1/1/5/10	1/33/34/34	0/2/2/2
14	7PH	A	309	-	-	0/33/33/39	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	8K6	B	201	-	-	0/15/15/15	0/0/0/0
12	UMQ	B	203	-	-	0/20/60/60	0/2/2/2
16	CLA	B	204	21	3/3/20/25	0/37/135/135	0/0/9/9
17	OPC	B	205	-	-	0/57/57/60	0/0/0/0
11	HEM	C	301	3	-	0/6/54/54	0/0/8/8
18	FES	D	201	4	-	0/0/4/4	0/1/1/1
19	SQD	D	202	-	-	0/49/69/69	0/1/1/1
17	OPC	D	203	-	-	0/57/57/60	0/0/0/0
17	OPC	E	101	-	-	0/57/57/60	0/0/0/0
20	BCR	G	101	-	-	0/29/63/63	0/2/2/2

All (106) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	A	306	UMQ	C6-C5	-5.77	1.32	1.51
12	A	307	UMQ	C6-C5	-5.76	1.32	1.51
12	B	203	UMQ	C6-C5	-5.73	1.32	1.51
11	C	301	HEM	C3B-C2B	-5.12	1.33	1.40
11	A	303	HEM	C3B-C2B	-4.91	1.33	1.40
12	B	203	UMQ	O1'-C1'	-4.68	1.31	1.40
12	A	307	UMQ	O1'-C1'	-4.66	1.32	1.40
12	A	307	UMQ	C3'-C4'	-4.66	1.39	1.52
12	A	306	UMQ	C3'-C4'	-4.65	1.39	1.52
12	B	203	UMQ	C3'-C4'	-4.64	1.39	1.52
12	A	306	UMQ	O1'-C1'	-4.54	1.32	1.40
12	B	203	UMQ	C3-C2	-4.32	1.41	1.52
12	A	306	UMQ	C3-C2	-4.30	1.41	1.52
12	A	307	UMQ	C3-C2	-4.29	1.41	1.52
11	A	304	HEM	C3B-C2B	-3.97	1.35	1.40
11	A	305	HEM	C3B-C2B	-3.97	1.35	1.40
11	A	305	HEM	C3C-C2C	-3.93	1.35	1.40
11	A	304	HEM	C3C-C2C	-3.92	1.35	1.40
11	C	301	HEM	C3C-C2C	-3.90	1.35	1.40
11	A	303	HEM	C3C-C2C	-3.85	1.35	1.40
12	A	307	UMQ	C3'-C2'	-3.69	1.43	1.52
12	A	306	UMQ	C3'-C2'	-3.62	1.43	1.52
12	B	203	UMQ	C3'-C2'	-3.59	1.43	1.52
20	G	101	BCR	C1-C6	-3.37	1.49	1.53
20	G	101	BCR	C30-C25	-3.12	1.49	1.53
12	A	307	UMQ	C6'-C5'	-2.93	1.41	1.51
12	B	203	UMQ	C6'-C5'	-2.92	1.41	1.51
12	A	306	UMQ	C6'-C5'	-2.92	1.41	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	B	203	UMQ	C1-C2	-2.61	1.45	1.52
12	A	306	UMQ	C1-C2	-2.58	1.45	1.52
12	A	307	UMQ	C1-C2	-2.57	1.45	1.52
16	B	204	CLA	CMB-C2B	-2.55	1.46	1.51
16	B	204	CLA	CMD-C2D	-2.30	1.46	1.51
13	A	308	SMA	C24-C13	-2.21	1.48	1.53
19	D	202	SQD	O2-C2	-2.15	1.38	1.43
19	D	202	SQD	O4-C4	-2.07	1.38	1.43
19	D	202	SQD	O3-C3	-2.05	1.38	1.43
17	E	101	OPC	CAG-NAF	-2.00	1.44	1.51
13	A	308	SMA	O4-C4	2.00	1.26	1.23
12	A	307	UMQ	O5-C1	2.08	1.47	1.41
12	A	306	UMQ	O5-C1	2.09	1.47	1.41
12	B	203	UMQ	O5-C1	2.14	1.47	1.41
11	C	301	HEM	C4D-ND	2.43	1.39	1.36
11	A	304	HEM	C4D-ND	2.47	1.39	1.36
12	A	306	UMQ	O2'-C2'	2.58	1.48	1.43
12	A	307	UMQ	O2'-C2'	2.61	1.49	1.43
12	B	203	UMQ	O2'-C2'	2.62	1.49	1.43
11	A	303	HEM	C4D-ND	2.63	1.39	1.36
16	B	204	CLA	CHC-C1C	2.68	1.43	1.35
11	A	305	HEM	C4D-ND	2.73	1.40	1.36
13	A	308	SMA	O5-C5	2.81	1.41	1.36
19	D	202	SQD	O47-C7	2.85	1.42	1.34
12	A	307	UMQ	O1-C4'	2.98	1.51	1.43
13	A	308	SMA	O7-C7	3.04	1.41	1.37
17	E	101	OPC	OAN-CAO	3.04	1.43	1.34
17	B	205	OPC	OAN-CAO	3.04	1.43	1.34
17	D	203	OPC	OAN-CAO	3.05	1.43	1.34
12	A	306	UMQ	O1-C4'	3.07	1.51	1.43
12	B	203	UMQ	O1-C4'	3.09	1.51	1.43
19	D	202	SQD	O48-C23	3.14	1.42	1.33
13	A	308	SMA	C9-C2	3.24	1.55	1.51
12	A	306	UMQ	O3-C3	3.42	1.50	1.43
12	A	307	UMQ	O3-C3	3.43	1.50	1.43
12	B	203	UMQ	O3-C3	3.44	1.50	1.43
12	A	307	UMQ	C4-C5	3.62	1.60	1.53
11	C	301	HEM	C3B-CAB	3.70	1.55	1.47
12	B	203	UMQ	C4-C5	3.71	1.60	1.53
17	D	203	OPC	OBJ-CBK	3.71	1.44	1.33
12	A	306	UMQ	C4-C5	3.71	1.60	1.53
17	E	101	OPC	OBJ-CBK	3.74	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	303	HEM	C3B-CAB	3.76	1.55	1.47
17	B	205	OPC	OBJ-CBK	3.78	1.44	1.33
11	A	304	HEM	C3B-CAB	3.86	1.55	1.47
11	A	305	HEM	C3B-CAB	3.92	1.55	1.47
11	A	304	HEM	C3C-CAC	3.94	1.55	1.47
14	A	309	7PH	O21-C21	3.95	1.45	1.34
13	A	308	SMA	C17-C16	3.97	1.55	1.44
16	B	204	CLA	CHB-C4A	3.98	1.38	1.33
11	A	303	HEM	C3C-CAC	4.01	1.55	1.47
11	C	301	HEM	C3C-CAC	4.01	1.55	1.47
11	A	305	HEM	C3C-CAC	4.05	1.55	1.47
14	A	309	7PH	O31-C31	4.24	1.45	1.33
13	A	308	SMA	C18-C19	4.41	1.55	1.45
12	A	307	UMQ	O2-C2	4.59	1.53	1.43
12	A	306	UMQ	O2-C2	4.59	1.53	1.43
12	B	203	UMQ	O2-C2	4.59	1.53	1.43
11	A	303	HEM	C3D-C2D	5.40	1.53	1.37
11	A	304	HEM	C3D-C2D	5.49	1.53	1.37
11	A	305	HEM	C3D-C2D	5.50	1.54	1.37
11	C	301	HEM	C3D-C2D	5.54	1.54	1.37
13	A	308	SMA	C3-C2	5.68	1.46	1.39
12	A	306	UMQ	O5-C5	5.91	1.58	1.44
12	A	307	UMQ	O5-C5	5.94	1.58	1.44
12	B	203	UMQ	O5-C5	5.98	1.58	1.44
13	A	308	SMA	C4-C4A	7.72	1.52	1.41
13	A	308	SMA	O1-C8A	7.73	1.48	1.36
12	A	307	UMQ	O5'-C5'	7.85	1.63	1.44
12	B	203	UMQ	O5'-C5'	7.87	1.63	1.44
12	A	306	UMQ	O5'-C5'	7.91	1.63	1.44
13	A	308	SMA	O1-C2	8.04	1.45	1.35
12	A	306	UMQ	O3'-C3'	8.62	1.62	1.43
12	A	307	UMQ	O3'-C3'	8.71	1.63	1.43
12	B	203	UMQ	O3'-C3'	8.71	1.63	1.43
12	A	306	UMQ	O5'-C1'	11.09	1.69	1.41
12	A	307	UMQ	O5'-C1'	11.10	1.69	1.41
12	B	203	UMQ	O5'-C1'	11.11	1.69	1.41

All (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	A	307	UMQ	C1'-O5'-C5'	-9.13	96.52	113.72
12	A	306	UMQ	C1'-O5'-C5'	-9.09	96.59	113.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	B	203	UMQ	C1'-O5'-C5'	-9.01	96.73	113.72
13	A	308	SMA	O7-C7-C8	-7.23	107.34	114.49
12	A	307	UMQ	O5-C5-C4	-4.32	101.70	109.66
12	A	306	UMQ	C1-O1-C4'	-4.26	107.61	118.00
12	A	306	UMQ	O5-C5-C4	-4.02	102.25	109.66
12	A	307	UMQ	C1-O1-C4'	-3.84	108.64	118.00
16	B	204	CLA	CMB-C2B-C1B	-3.74	122.71	128.46
19	D	202	SQD	O9-S-O7	-3.72	100.96	113.86
12	B	203	UMQ	O5-C5-C4	-3.67	102.90	109.66
13	A	308	SMA	C5M-O5-C5	-3.33	113.03	117.77
12	B	203	UMQ	C1-O1-C4'	-3.26	110.06	118.00
16	B	204	CLA	O2D-CGD-O1D	-2.98	117.82	123.82
19	D	202	SQD	C5-C6-S	-2.95	110.22	114.34
13	A	308	SMA	C9-C10-C11	-2.91	110.80	114.72
20	G	101	BCR	C33-C5-C6	-2.77	121.40	124.51
13	A	308	SMA	C14-C15-C16	-2.65	120.09	125.61
13	A	308	SMA	C7M-O7-C7	-2.65	113.73	117.54
11	A	304	HEM	C1D-C2D-C3D	-2.51	105.25	107.00
11	C	301	HEM	C1D-C2D-C3D	-2.36	105.35	107.00
16	B	204	CLA	C1B-CHB-C4A	-2.34	125.47	130.12
11	A	304	HEM	CBD-CAD-C3D	-2.25	108.18	112.47
13	A	308	SMA	C17-C18-C19	-2.24	120.12	126.42
12	A	306	UMQ	O3'-C3'-C2'	-2.13	105.72	110.36
12	B	203	UMQ	O3'-C3'-C2'	-2.10	105.78	110.36
11	A	303	HEM	C1D-C2D-C3D	-2.03	105.58	107.00
20	G	101	BCR	C7-C8-C9	-2.01	123.19	126.21
20	G	101	BCR	C24-C23-C22	-2.01	123.20	126.21
11	C	301	HEM	CMA-C3A-C4A	-2.00	125.39	128.46
12	A	307	UMQ	O3'-C3'-C2'	-2.00	106.00	110.36
12	A	307	UMQ	O5-C5-C6	2.01	111.22	106.41
11	A	304	HEM	CMB-C2B-C3B	2.03	128.66	124.89
11	A	304	HEM	C4A-C3A-C2A	2.06	108.43	107.00
11	C	301	HEM	CMC-C2C-C3C	2.09	128.78	124.89
19	D	202	SQD	O5-C5-C4	2.11	113.55	109.66
12	B	203	UMQ	C1-C2-C3	2.17	114.02	109.98
19	D	202	SQD	O6-C1-C2	2.22	111.85	108.23
11	A	305	HEM	CMB-C2B-C3B	2.24	129.04	124.89
12	A	306	UMQ	O5'-C1'-C2'	2.24	114.61	110.30
11	A	305	HEM	CMC-C2C-C3C	2.24	129.06	124.89
11	A	304	HEM	CMC-C2C-C3C	2.26	129.09	124.89
16	B	204	CLA	CMD-C2D-C3D	2.28	129.11	124.89
13	A	308	SMA	O12-C12-C11	2.32	111.34	107.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	B	203	UMQ	C3-C4-C5	2.40	114.44	110.22
16	B	204	CLA	CHB-C4A-NA	2.40	127.83	124.51
20	G	101	BCR	C27-C26-C25	2.41	126.28	122.74
19	D	202	SQD	O48-C23-C24	2.45	119.03	111.90
16	B	204	CLA	C4A-NA-C1A	2.48	109.53	106.45
14	A	309	7PH	O31-C31-C32	2.49	119.15	111.90
12	A	306	UMQ	C3-C4-C5	2.50	114.62	110.22
17	B	205	OPC	OBJ-CBK-CBL	2.62	119.53	111.90
19	D	202	SQD	C44-O6-C1	2.67	119.23	113.76
12	A	307	UMQ	C1-C2-C3	2.71	115.02	109.98
12	A	306	UMQ	C1-C2-C3	2.72	115.03	109.98
17	E	101	OPC	OBJ-CBK-CBL	2.79	120.02	111.90
17	D	203	OPC	OBJ-CBK-CBL	2.80	120.06	111.90
16	B	204	CLA	CMB-C2B-C3B	2.90	130.27	124.89
13	A	308	SMA	O1-C8A-C8	2.90	119.47	116.03
19	D	202	SQD	O8-S-C6	3.53	110.31	106.01
19	D	202	SQD	O47-C7-C8	3.80	119.45	111.55
17	D	203	OPC	OAN-CAO-CAP	3.83	119.51	111.55
17	E	101	OPC	OAN-CAO-CAP	3.87	119.58	111.55
14	A	309	7PH	O21-C21-C22	3.89	119.63	111.55
17	B	205	OPC	OAN-CAO-CAP	4.25	120.37	111.55
13	A	308	SMA	O7-C7-C6	4.76	132.20	124.17
19	D	202	SQD	O9-S-C6	5.36	111.40	106.83
19	D	202	SQD	O7-S-C6	5.58	111.60	106.83
13	A	308	SMA	O1-C2-C9	6.77	120.28	111.94
12	A	307	UMQ	C2'-C3'-C4'	7.22	124.57	109.61
12	A	306	UMQ	C2'-C3'-C4'	7.53	125.23	109.61
12	B	203	UMQ	C2'-C3'-C4'	7.65	125.47	109.61

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
13	A	308	SMA	C12
16	B	204	CLA	NC
16	B	204	CLA	ND
16	B	204	CLA	NA

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	A	308	SMA	C17-C16-C15-C14

There are no ring outliers.

16 monomers are involved in 68 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	301	MYS	3	0
11	A	303	HEM	3	0
11	A	304	HEM	2	0
11	A	305	HEM	6	0
12	A	306	UMQ	7	0
12	A	307	UMQ	3	0
13	A	308	SMA	7	0
14	A	309	7PH	3	0
12	B	203	UMQ	10	0
16	B	204	CLA	5	0
17	B	205	OPC	5	0
11	C	301	HEM	3	0
19	D	202	SQD	1	0
17	D	203	OPC	4	0
17	E	101	OPC	12	0
20	G	101	BCR	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%)	-0.27	0 100 100	49, 74, 114, 157	5 (2%)
2	B	159/160 (99%)	-0.24	3 (1%) 67 37	60, 96, 139, 208	2 (1%)
3	C	288/289 (99%)	0.28	36 (12%) 4 2	67, 110, 237, 280	0
4	D	158/179 (88%)	0.98	37 (23%) 1 0	65, 170, 227, 287	0
5	E	28/32 (87%)	-0.55	0 100 100	92, 108, 131, 153	0
6	F	31/35 (88%)	0.19	2 (6%) 20 7	83, 100, 159, 177	0
7	G	37/37 (100%)	-0.02	0 100 100	74, 93, 202, 239	4 (10%)
8	H	28/29 (96%)	-0.22	0 100 100	77, 90, 128, 148	0
All	All	942/976 (96%)	0.13	78 (8%) 12 4	49, 100, 212, 287	11 (1%)

All (78) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	220	SER	7.0
3	C	192	ASN	6.1
6	F	32	ALA	5.9
4	D	56	ALA	5.7
4	D	159	ASN	5.5
4	D	179	VAL	5.1
4	D	91	ILE	5.0
4	D	166	THR	4.6
4	D	160	ILE	4.6
3	C	199	ILE	4.3
3	C	181	THR	4.2
4	D	157	ASP	4.2
3	C	219	VAL	4.1
3	C	183	ILE	4.0
4	D	175	LYS	4.0
4	D	92	VAL	4.0

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Mol	Chain	Res	Type	RSRZ
2	B	160	PHE	3.9
4	D	55	THR	3.9
4	D	162	LEU	3.8
4	D	156	GLN	3.7
3	C	189	GLU	3.7
4	D	158	ASP	3.6
3	C	182	LYS	3.6
4	D	170	PHE	3.5
3	C	190	TYR	3.4
3	C	206	THR	3.4
4	D	67	SER	3.4
4	D	101	ASP	3.4
3	C	188	ASP	3.3
4	D	161	VAL	3.2
3	C	198	SER	3.1
4	D	72	SER	3.1
4	D	176	PRO	3.1
3	C	207	VAL	3.1
4	D	169	ASP	3.1
3	C	177	THR	3.1
4	D	62	ASN	3.0
4	D	144	ALA	3.0
3	C	281	LYS	3.0
3	C	184	ALA	3.0
3	C	222	GLY	2.9
4	D	155	VAL	2.9
3	C	194	LYS	2.9
4	D	98	ALA	2.9
4	D	13	MET	2.8
3	C	197	VAL	2.7
4	D	15	ARG	2.7
6	F	31	GLY	2.7
4	D	70	LEU	2.7
4	D	168	THR	2.7
4	D	145	PRO	2.6
4	D	64	VAL	2.6
4	D	165	TRP	2.5
4	D	177	TRP	2.5
3	C	208	VAL	2.5
3	C	191	GLY	2.4
2	B	116	ASN	2.4
2	B	74	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
4	D	12	ASP	2.4
3	C	221	GLU	2.4
4	D	60	LEU	2.4
3	C	193	VAL	2.3
3	C	187	GLU	2.3
4	D	154	THR	2.3
3	C	200	GLN	2.2
3	C	176	ALA	2.2
3	C	195	TYR	2.2
3	C	88	GLU	2.2
3	C	205	LYS	2.1
3	C	230	ALA	2.1
3	C	92	GLU	2.1
3	C	288	ASN	2.1
3	C	215	PRO	2.1
3	C	196	GLN	2.0
3	C	214	GLY	2.0
3	C	223	GLN	2.0
4	D	10	VAL	2.0
4	D	63	ASN	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<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
15	8K6	B	201	18/18	0.77	0.43	6.95	74,93,107,115	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
12	UMQ	A	307	34/34	0.89	0.36	5.84	100,139,156,232	3
12	UMQ	A	306	34/34	0.73	0.41	5.43	72,128,148,161	7
14	7PH	A	309	32/38	0.81	0.39	5.31	53,85,112,116	4
9	MYS	A	301	15/15	0.89	0.34	4.88	50,68,85,86	0
17	OPC	D	203	54/55	0.71	0.41	4.48	67,125,194,215	1
13	SMA	A	308	37/37	0.87	0.35	4.14	77,110,157,166	12
17	OPC	B	205	54/55	0.90	0.34	3.77	80,118,150,151	0
12	UMQ	B	203	34/34	0.83	0.31	2.85	107,167,218,223	0
20	BCR	G	101	40/40	0.89	0.35	2.58	57,80,98,107	14
17	OPC	E	101	54/55	0.86	0.34	2.50	67,112,195,227	0
16	CLA	B	204	65/65	0.94	0.23	0.54	69,97,126,131	0
11	HEM	C	301	43/43	0.97	0.23	0.45	60,87,128,141	0
11	HEM	A	303	43/43	0.99	0.23	0.26	47,67,82,100	0
11	HEM	A	305	43/43	0.98	0.21	-0.15	71,96,110,126	0
10	CD	B	202	1/1	0.81	0.19	-0.41	231,231,231,231	0
11	HEM	A	304	43/43	0.99	0.21	-0.45	46,68,82,91	0
19	SQD	D	202	54/54	0.90	0.19	-0.58	104,125,149,154	30
18	FES	D	201	4/4	0.94	0.13	-0.99	151,161,163,260	0
10	CD	A	302	1/1	0.99	0.20	-	100,100,100,100	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.