



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 05:05 PM GMT

PDB ID : 4H44  
Title : 2.70 Å 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 wwPDB X-ray Structure Validation Summary 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

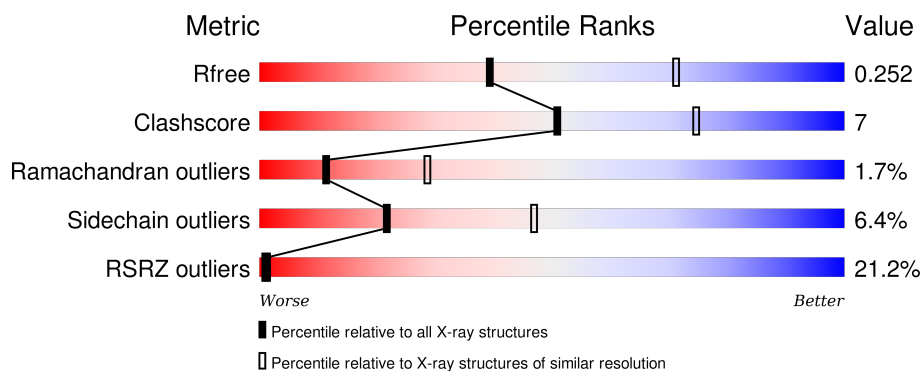
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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  $\geq 3$ , 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>14%</div> <div> <div>82%</div> <div>16%</div> <div>.</div> </div> </div>
2	B	160	<div> <div>18%</div> <div> <div>80%</div> <div>19%</div> <div>.</div> </div> </div>
3	C	289	<div> <div>20%</div> <div> <div>79%</div> <div>19%</div> <div>.</div> </div> </div>
4	D	179	<div> <div>40%</div> <div> <div>83%</div> <div>9%</div> <div>.</div> <div>7%</div> </div> </div>
5	E	31	<div> <div>13%</div> <div> <div>87%</div> <div>13%</div> </div> </div>

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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 [i](#)

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
1	A	215	Total	C	H	N	O	S	0	0	0
			3451	1144	1736	272	288	11			

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

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

- Molecule 3 is a protein called Apocytochrome f.

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

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

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

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

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

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

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

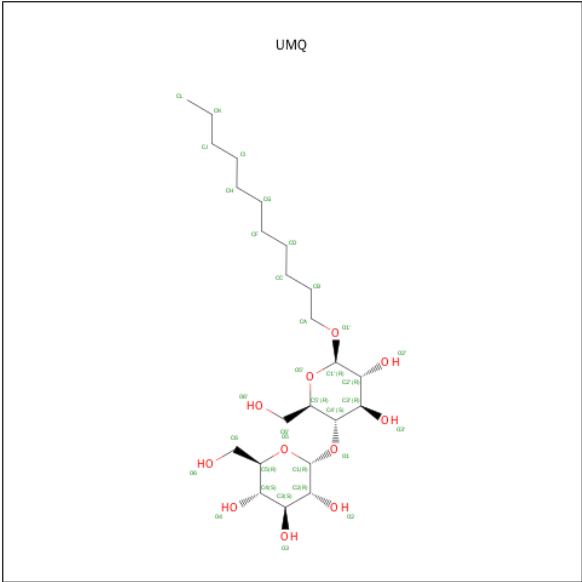
- | Mol | Chain | Residues | Atoms |     |     |    |    | ZeroOcc | AltConf | Trace |   |
|-----|-------|----------|-------|-----|-----|----|----|---------|---------|-------|---|
| 7   | G     | 37       | Total | C   | H   | N  | O  | S       | 0       | 0     | 0 |
|     |       |          | 584 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

- | 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       |         |       |   |

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- Chemical structure of HEM (Heme) showing a central iron atom coordinated by four nitrogen atoms in a porphyrin-like ring. The structure includes various side chains and a central iron atom labeled 'Fe'.

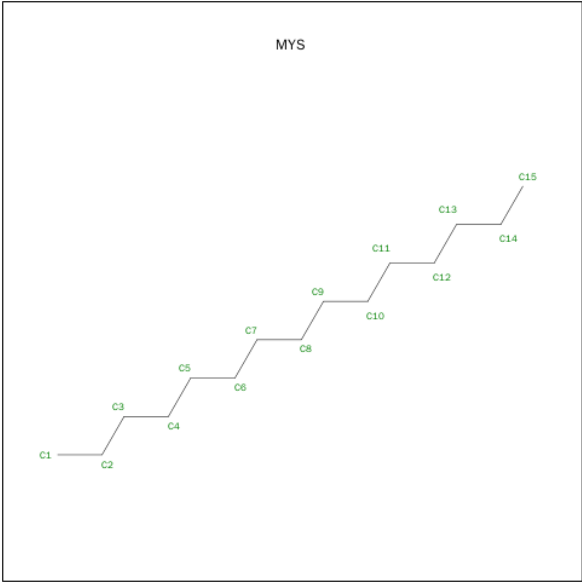
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
9	A	1	Total 73	C 34	Fe 1	H 30	N 4	O 4	0	0
9	A	1	Total 73	C 34	Fe 1	H 30	N 4	O 4	0	0
9	A	1	Total 73	C 34	Fe 1	H 30	N 4	O 4	0	0
9	C	1	Total 73	C 34	Fe 1	H 30	N 4	O 4	0	0

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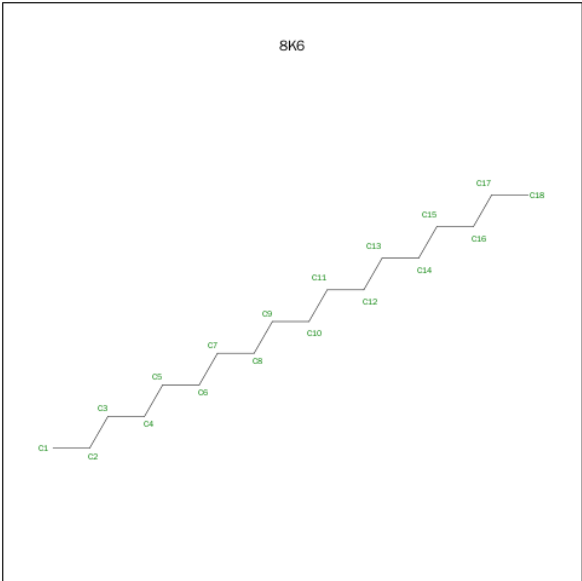
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	A	1	Total	C	H	O	0	0
			77	23	43	11		
10	A	1	Total	C	H	O	0	0
			77	23	43	11		
10	A	1	Total	C	H	O	0	0
			78	23	44	11		
10	A	1	Total	C	H	O	0	0
			77	23	43	11		
10	F	1	Total	C	H	O	0	0
			77	23	43	11		

- Molecule 11 is PENTADECANE (three-letter code: MYS) (formula: C<sub>15</sub>H<sub>32</sub>).



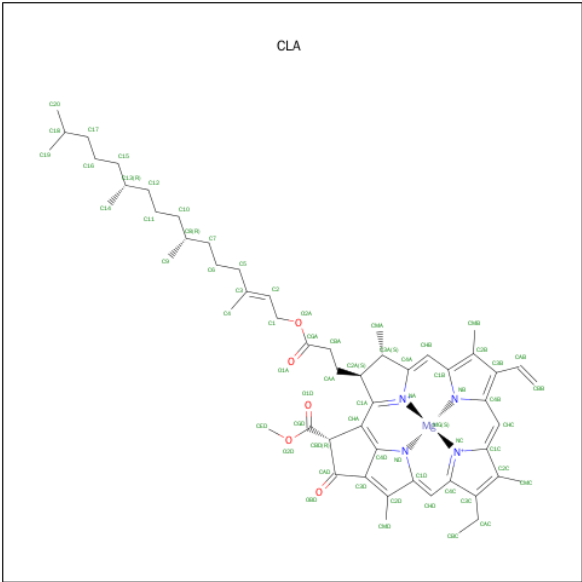
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	A	1	Total	C	H	0	0
			47	15	32		

- Molecule 12 is OCTADECANE (three-letter code: 8K6) (formula: C<sub>18</sub>H<sub>38</sub>).



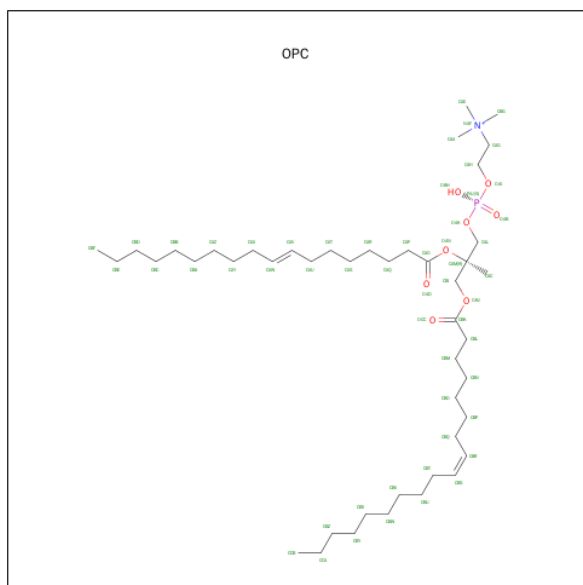
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	A	1	Total	C	H	0	0
			56	18	38		

- Molecule 13 is CHLOROPHYLL A (three-letter code: CLA) (formula: C<sub>55</sub>H<sub>72</sub>MgN<sub>4</sub>O<sub>5</sub>).



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

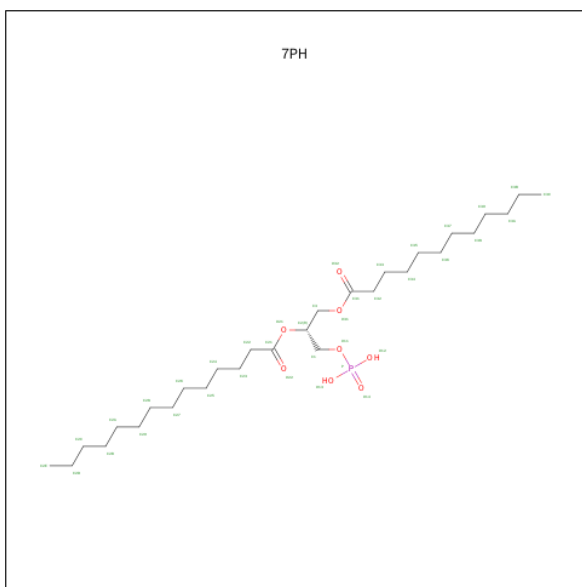
- Molecule 14 is (7R,17E)-4-HYDROXY-N,N,N,7-TETRAMETHYL-7-[(8E)-OCTADEC-8-ENOYLOXY]-10-OXO-3,5,9-TRIOXA-4-PHOSPHAHEPTACOS-17-EN-1-AMINIUM 4-OXIDE (three-letter code: OPC) (formula: C<sub>45</sub>H<sub>87</sub>NO<sub>8</sub>P).



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		

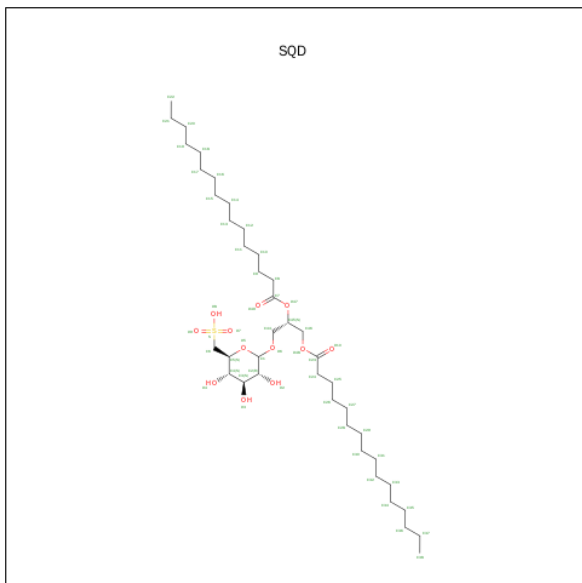
- Molecule 15 is (1R)-2-(DODECANOYLOXY)-1-[(PHOSPHONOOXY)METHYL]ETHYL TETRADECANOATE (three-letter code: 7PH) (formula: C<sub>29</sub>H<sub>57</sub>O<sub>8</sub>P).





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:  $C_{41}H_{78}O_{12}S$ ).

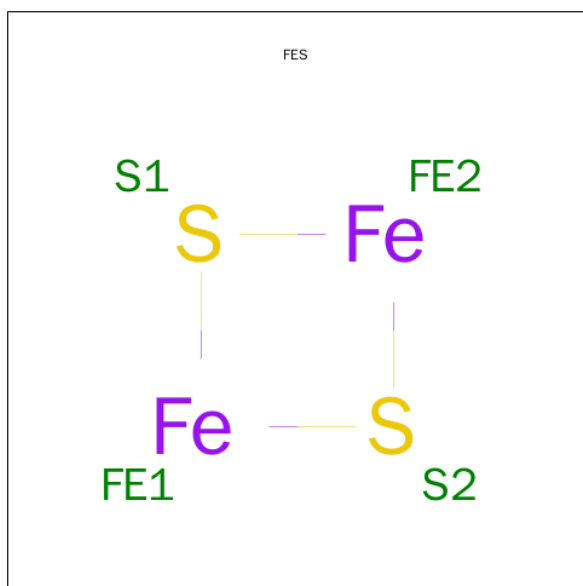


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
16	D	1	Total	C	H	O	S	0	0
			53	16	24	12	1		

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

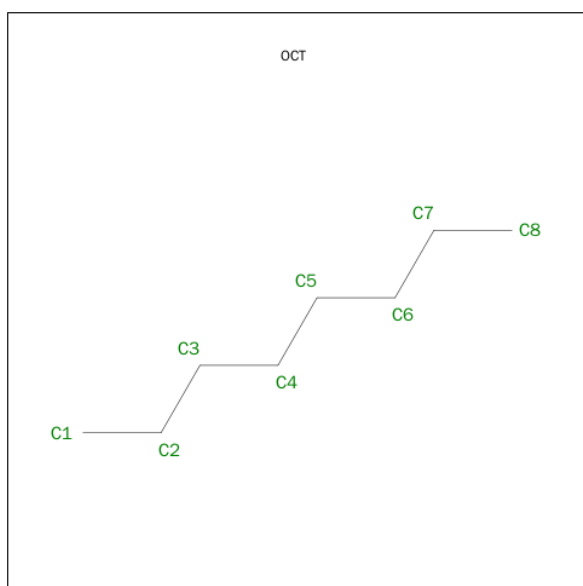
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	C	1	Total	Cd	0	0
			1	1		

- Molecule 18 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula:  $\text{Fe}_2\text{S}_2$ ).



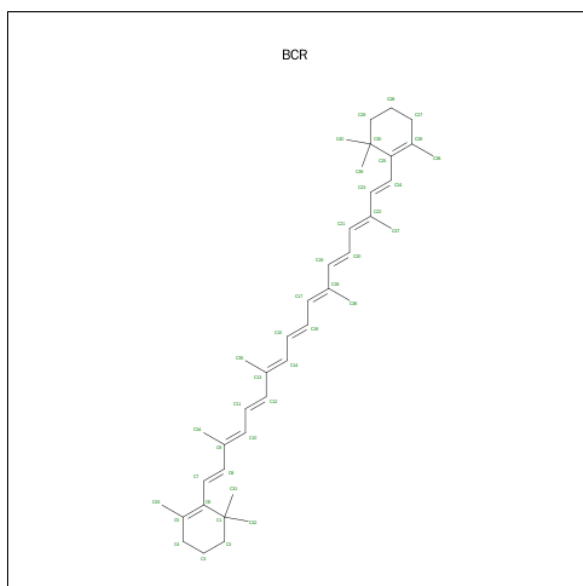
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
18	D	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 19 is N-OCTANE (three-letter code: OCT) (formula:  $\text{C}_8\text{H}_{18}$ ).



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

- 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	0	0
			96	40	56		

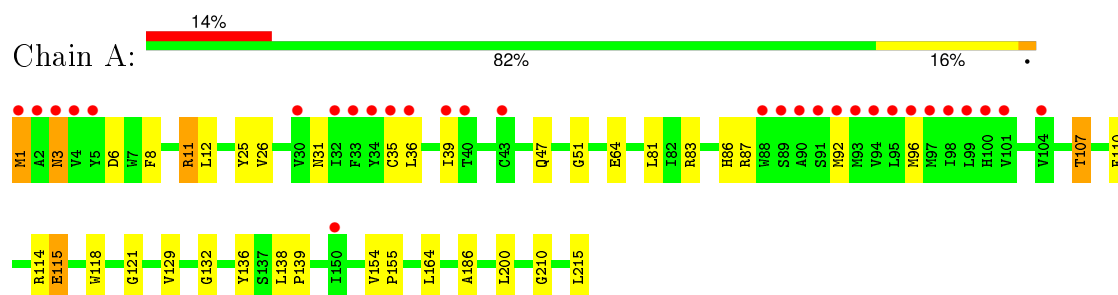
- Molecule 21 is water.

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

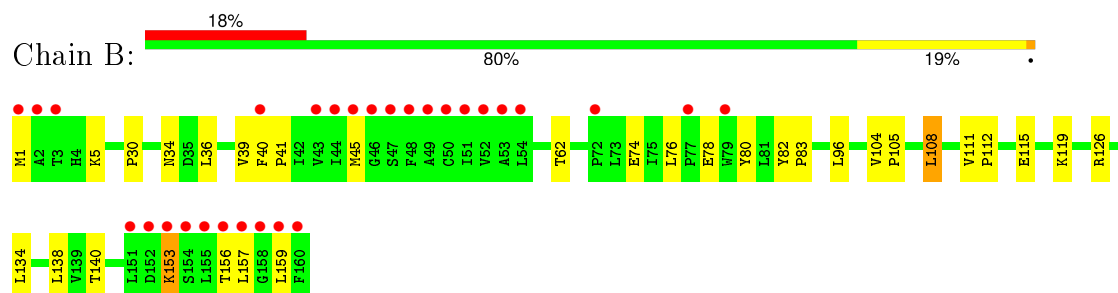
### 3 Residue-property plots [i](#)

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 ( $\text{RSRZ} > 2$ ). 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.

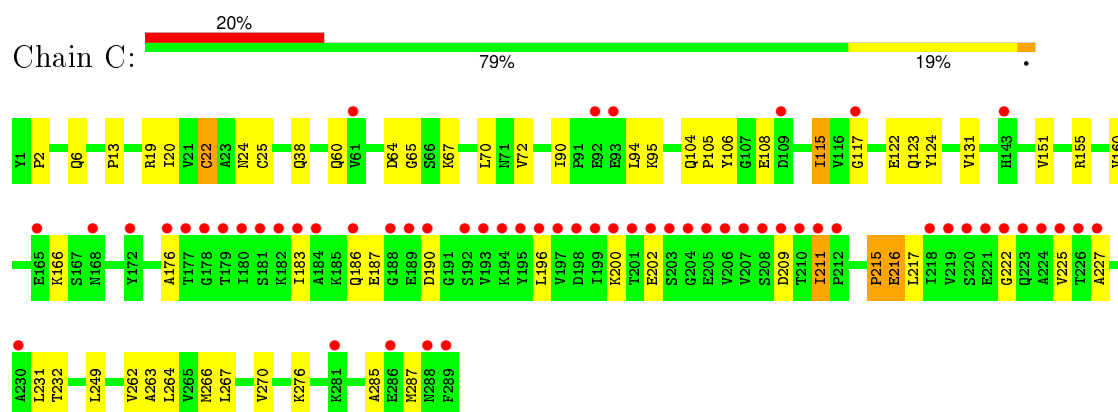
#### • Molecule 1: Cytochrome b6



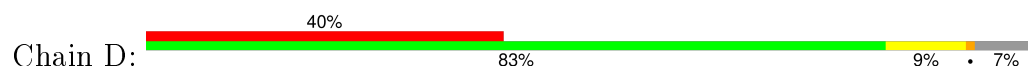
#### • Molecule 2: Cytochrome b6-f complex subunit 4

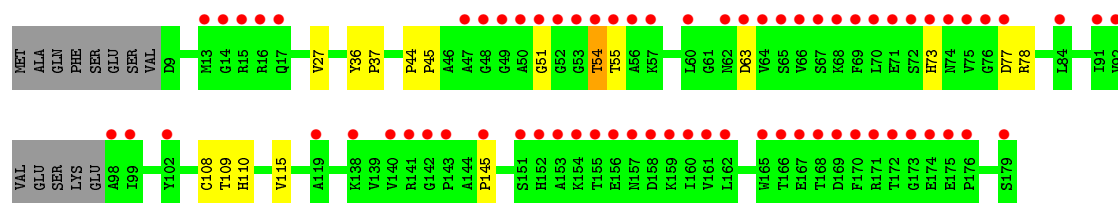


#### • Molecule 3: Apocytochrome f

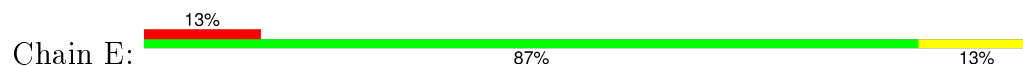


#### • Molecule 4: Cytochrome b6-f complex iron-sulfur subunit 1

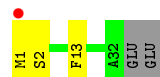
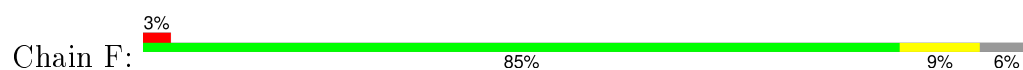




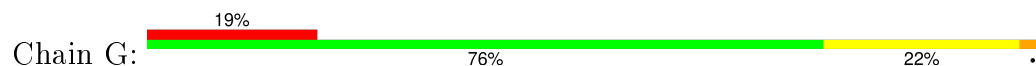
- Molecule 5: Cytochrome b6-f complex subunit 6



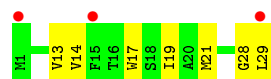
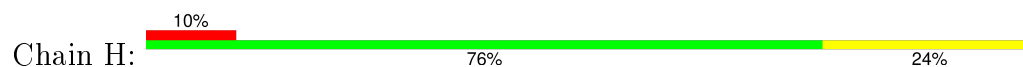
- Molecule 6: Cytochrome b6-f complex subunit 7



- Molecule 7: Cytochrome b6-f complex subunit 5



- Molecule 8: Cytochrome b6-f complex subunit 8



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	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 <sup>2</sup> )	69.7	Xtriage
Anisotropy	0.071	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.41 , 71.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	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 <sup>2</sup> )	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.*

<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, 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(°)	Ideal(°)
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 [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	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.

The worst 5 of 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



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

### 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	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

5 of 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

### 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	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

5 of 50 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	22	CYS
3	C	108	GLU
7	G	6	LEU
3	C	60	GLN
3	C	70	LEU

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 ⓘ

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
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

The worst 5 of 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

The worst 5 of 124 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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

5 of 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

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 [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	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

The worst 5 of 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

### 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 [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
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
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 [i](#)

There are no such residues in this entry.