wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 08:02 AM GMT

PDB ID	:	3D38
Title	:	Crystal structure of new trigonal form of photosynthetic reaction center from Blastochloris viridis. Crystals grown in microfluidics by detergent capture.
Authors	:	Li, L.; Nachtergaele, S.H.M.; Seddon, A.M.; Tereshko, V.; Ponomarenko, N.; Ismagilov, R.F.; Accelerated Technologies Center for Gene to 3D Structure (ATCG3D)
Deposited on	:	2008-05-09
Resolution	:	3.21 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
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

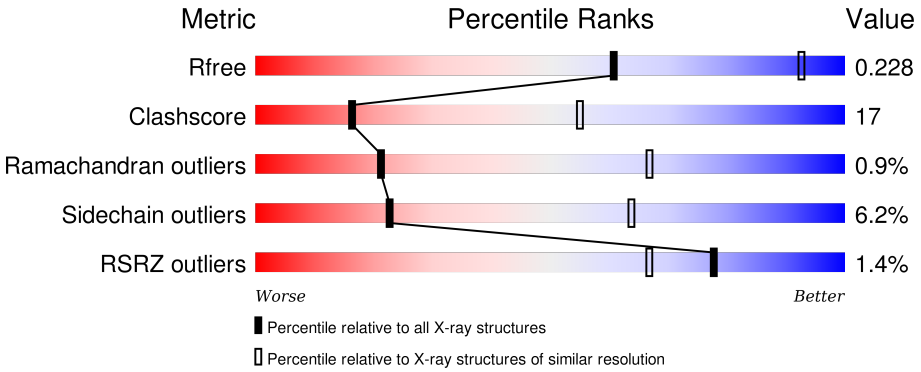
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.21 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	1095 (3.26-3.18)
Clashscore	102246	1046 (3.24-3.20)
Ramachandran outliers	100387	1026 (3.24-3.20)
Sidechain outliers	100360	1025 (3.24-3.20)
RSRZ outliers	91569	1100 (3.26-3.18)

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

Mol	Chain	Length	Quality of chain
1	C	336	2% 73% 24%
2	H	258	% 67% 26%
3	L	273	% 72% 26%
4	M	323	% 72% 25%

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
11	BPB	M	402	-	-	-	X
12	UQ1	L	502	-	-	-	X
12	UQ1	L	503	-	-	-	X
14	NS5	M	600	-	-	-	X
5	SO4	C	811	-	-	-	X
5	SO4	C	813	-	-	-	X
5	SO4	H	807	-	-	-	X
8	HTO	C	706	-	-	-	X
8	HTO	C	707	-	-	-	X
8	HTO	H	705	-	-	-	X
9	LDA	L	702	-	-	-	X
9	LDA	M	704	-	-	-	X

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 10311 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 Photosynthetic reaction center cytochrome c subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	332	Total	C	N	O	S	0	0	0
			2598	1637	465	478	18			

- Molecule 2 is a protein called Reaction center protein H chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	250	Total	C	N	O	S	0	0	0
			1958	1251	335	370	2			

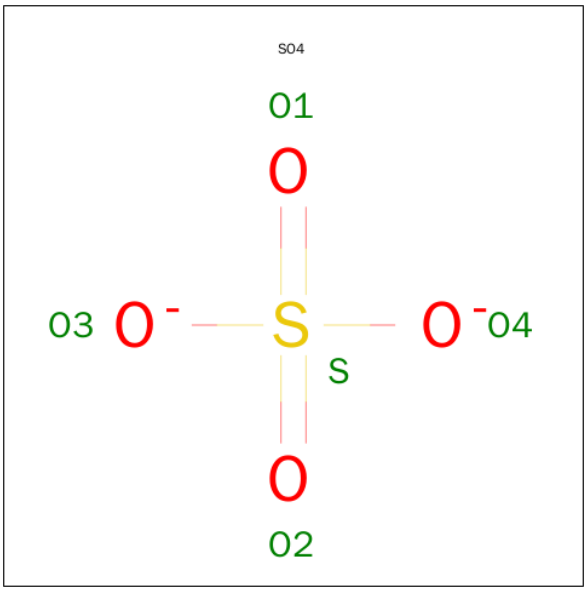
- Molecule 3 is a protein called Reaction center protein L chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	273	Total	C	N	O	S	0	0	0
			2171	1459	350	355	7			

- Molecule 4 is a protein called Reaction center protein M chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	M	323	Total	C	N	O	S	0	0	0
			2555	1702	419	423	11			

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	1	Total O S 5 4 1	0	0
5	C	1	Total O S 5 4 1	0	0
5	C	1	Total O S 5 4 1	0	0
5	C	1	Total O S 5 4 1	0	0
5	C	1	Total O S 5 4 1	0	0
5	C	1	Total O S 5 4 1	0	0
5	C	1	Total O S 5 4 1	0	0
5	H	1	Total O S 5 4 1	0	0
5	H	1	Total O S 5 4 1	0	0
5	H	1	Total O S 5 4 1	0	0
5	H	1	Total O S 5 4 1	0	0
5	M	1	Total O S 5 4 1	0	0
5	M	1	Total O S 5 4 1	0	0
5	M	1	Total O S 5 4 1	0	0

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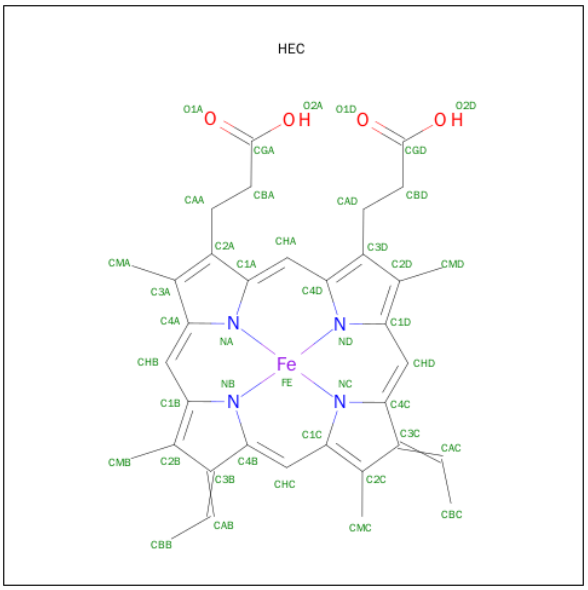
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	M	1	Total O S 5 4 1	0	0

- Molecule 6 is FE (II) ION (three-letter code: FE2) (formula: Fe).

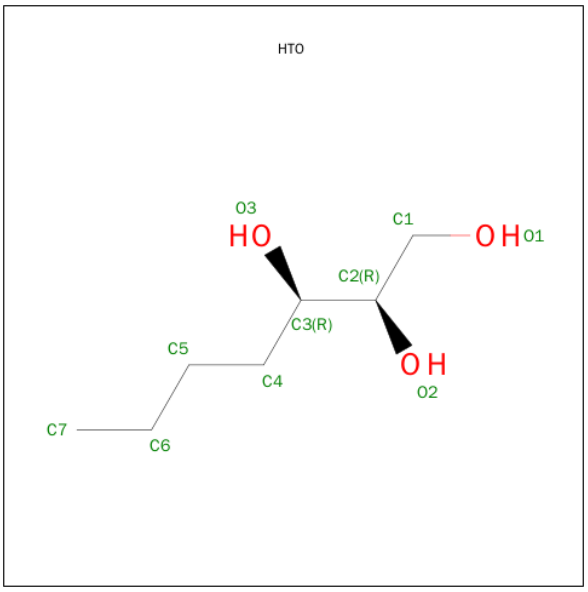
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	M	1	Total Fe 1 1	0	0

- Molecule 7 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



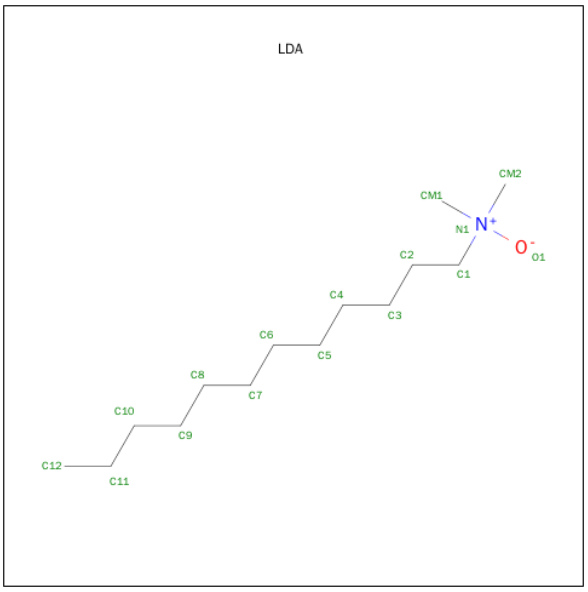
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	C	1	Total C Fe N O 43 34 1 4 4	0	0
7	C	1	Total C Fe N O 43 34 1 4 4	0	0
7	C	1	Total C Fe N O 43 34 1 4 4	0	0
7	C	1	Total C Fe N O 43 34 1 4 4	0	0

- Molecule 8 is HEPTANE-1,2,3-TRIOL (three-letter code: HTO) (formula: $C_7H_{16}O_3$).



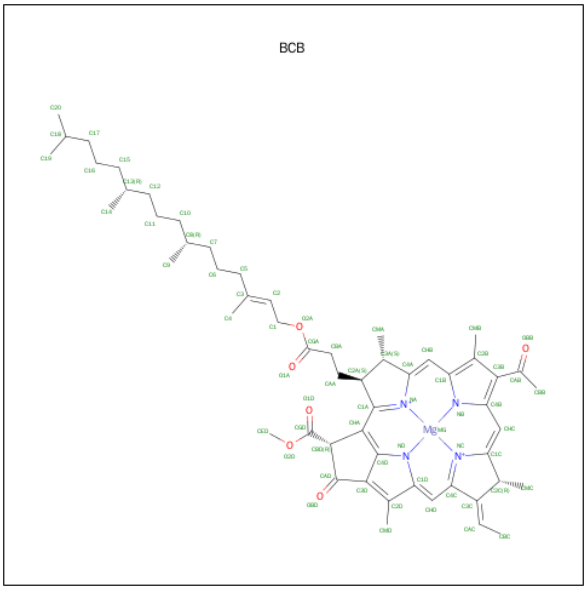
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	C	1	Total C O 10 7 3	0	0
8	C	1	Total C O 10 7 3	0	0
8	H	1	Total C O 10 7 3	0	0

- Molecule 9 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula: $C_{14}H_{31}NO$).



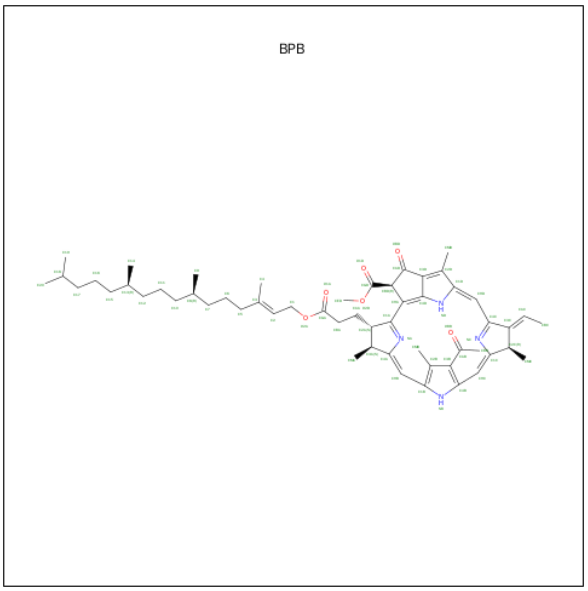
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	H	1	Total	C	N	O	0	0
			16	14	1	1		
9	H	1	Total	C	N	O	0	0
			16	14	1	1		
9	L	1	Total	C	N	O	0	0
			16	14	1	1		
9	M	1	Total	C	N	O	0	0
			16	14	1	1		

- Molecule 10 is BACTERIOCHLOROPHYLL B (three-letter code: BCB) (formula: $C_{55}H_{72}MgN_4O_6$).



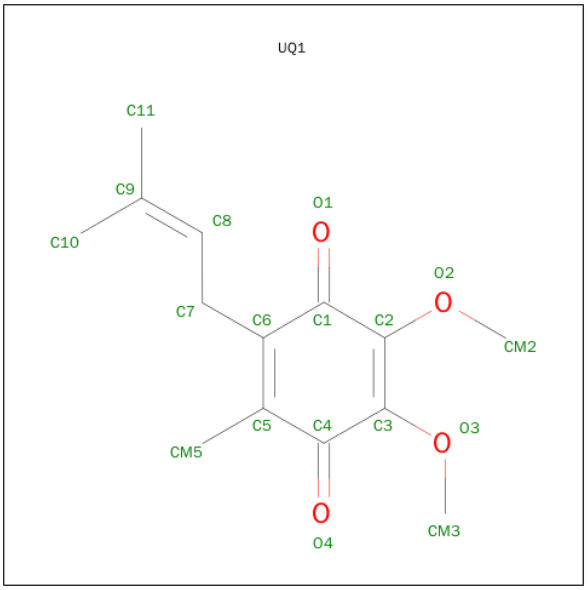
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
10	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
10	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
10	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

- Molecule 11 is BACTERIOPHEOPHYTIN B (three-letter code: BPB) (formula: $C_{55}H_{74}N_4O_6$).



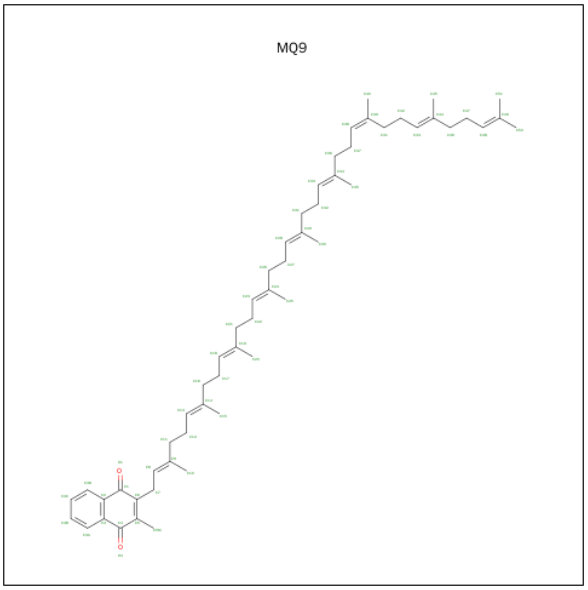
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	L	1	Total	C	N	O	0	0
			65	55	4	6		
11	M	1	Total	C	N	O	0	0
			65	55	4	6		

- Molecule 12 is UBIQUINONE-1 (three-letter code: UQ1) (formula: $C_{14}H_{18}O_4$).



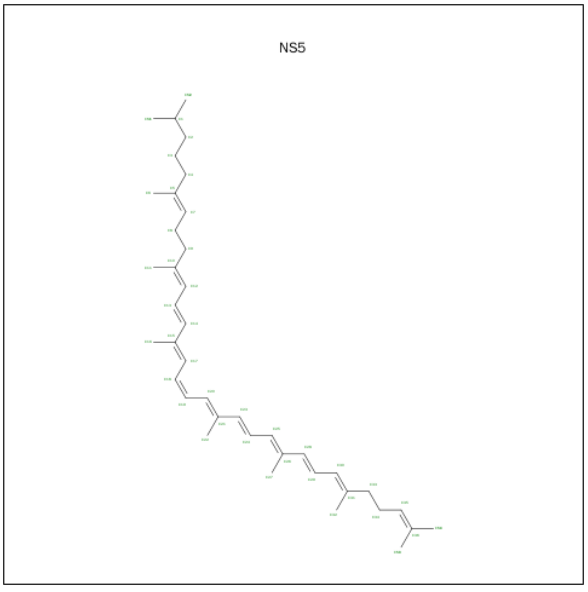
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	L	1	Total	C	O	0	0
			18	14	4		
12	L	1	Total	C	O	0	0
			18	14	4		

- Molecule 13 is MENAQUINONE-9 (three-letter code: MQ9) (formula: $C_{56}H_{80}O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	M	1	Total C O 58 56 2	0	0

- Molecule 14 is 15-CIS-1,2-DIHYDRONEUROSPORENE (three-letter code: NS5) (formula: $C_{40}H_{60}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	M	1	Total C 40 40	0	0

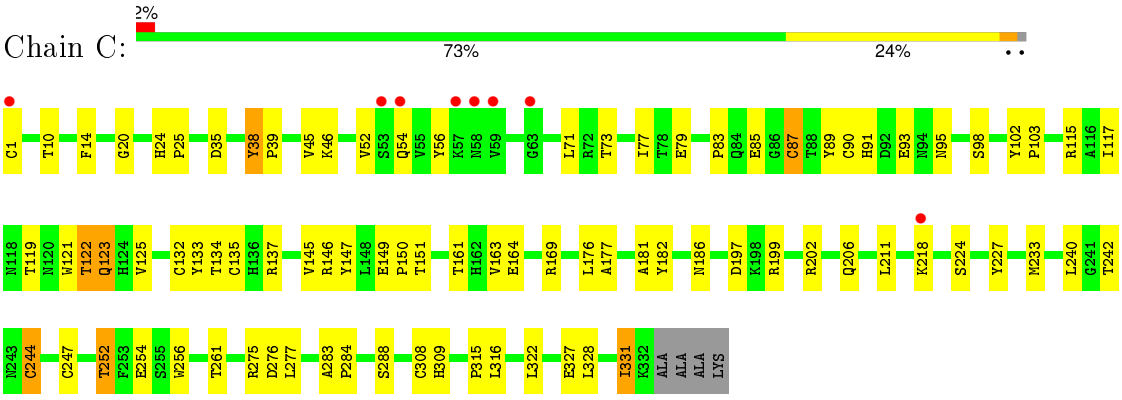
- Molecule 15 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	C	47	Total O 47 47	0	0
15	H	28	Total O 28 28	0	0
15	L	38	Total O 38 38	0	0
15	M	46	Total O 46 46	0	0

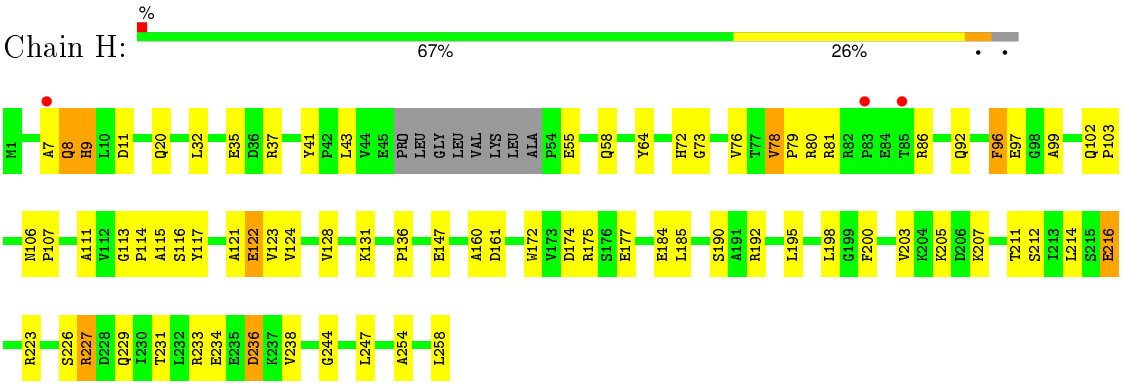
3 Residue-property plots (i)

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

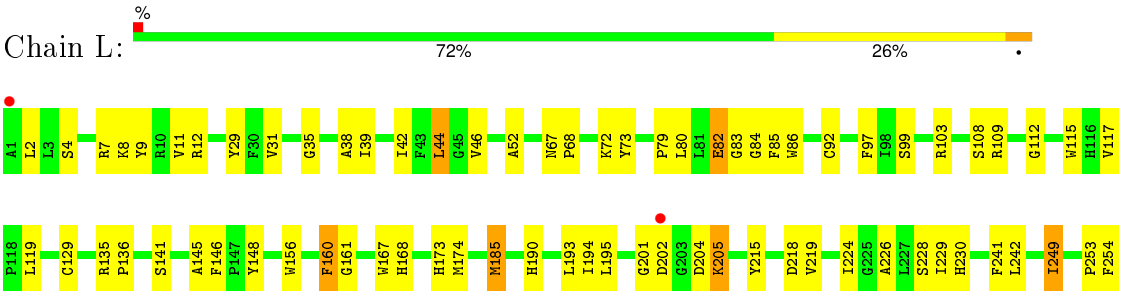
- Molecule 1: Photosynthetic reaction center cytochrome c subunit

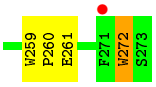


- Molecule 2: Reaction center protein H chain



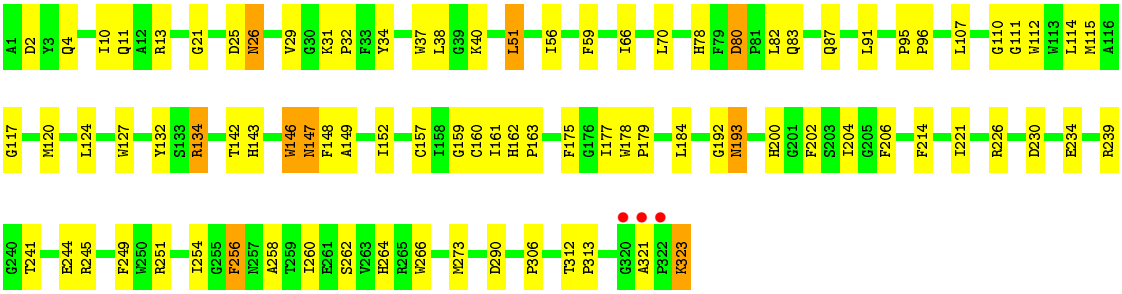
- Molecule 3: Reaction center protein L chain





• Molecule 4: Reaction center protein M chain

Chain M:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	241.17Å 241.17Å 113.39Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 3.21 47.92 – 3.21	Depositor EDS
% Data completeness (in resolution range)	99.6 (50.00-3.21) 99.6 (47.92-3.21)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.78 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.4.0073	Depositor
R, R_{free}	0.192 , 0.224 0.196 , 0.228	Depositor DCC
R_{free} test set	3141 reflections (5.34%)	DCC
Wilson B-factor (Å^2)	74.4	Xtriage
Anisotropy	0.053	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 68.8	EDS
Estimated twinning fraction	0.028 for -h,-k,l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Outliers	0 of 62022 reflections	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	10311	wwPDB-VP
Average B, all atoms (Å^2)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.40% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LDA, BPB, HTO, BCB, MQ9, FE2, SO4, HEC, UQ1, FME, NS5

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	C	0.53	1/2665 (0.0%)	0.64	0/3633
2	H	0.59	0/1993	0.68	0/2720
3	L	0.60	1/2259 (0.0%)	0.66	0/3084
4	M	0.57	0/2659	0.65	1/3637 (0.0%)
All	All	0.57	2/9576 (0.0%)	0.66	1/13074 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	87	CYS	CB-SG	-5.84	1.72	1.81
3	L	129	CYS	CB-SG	-5.38	1.73	1.81

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	M	70	LEU	CA-CB-CG	7.57	132.71	115.30

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	C	2598	0	2573	82	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	H	1958	0	1946	65	0
3	L	2171	0	2098	64	0
4	M	2555	0	2452	76	0
5	C	35	0	0	0	0
5	H	20	0	0	1	0
5	M	20	0	0	1	0
6	M	1	0	0	0	0
7	C	172	0	125	31	0
8	C	20	0	32	1	0
8	H	10	0	16	2	0
9	H	32	0	62	6	0
9	L	16	0	31	2	0
9	M	16	0	31	0	0
10	L	132	0	144	24	0
10	M	132	0	144	27	0
11	L	65	0	74	9	0
11	M	65	0	74	20	0
12	L	36	0	36	4	0
13	M	58	0	80	3	0
14	M	40	0	60	11	0
15	C	47	0	0	9	0
15	H	28	0	0	5	0
15	L	38	0	0	3	0
15	M	46	0	0	7	0
All	All	10311	0	9978	337	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 17.

The worst 5 of 337 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)
1:C:90:CYS:SG	7:C:401:HEC:HAC	1.31	1.69
1:C:132:CYS:SG	7:C:402:HEC:HAB	1.48	1.52
1:C:244:CYS:SG	7:C:403:HEC:HAB	1.54	1.47
1:C:132:CYS:SG	7:C:402:HEC:CAB	2.08	1.39
1:C:135:CYS:SG	7:C:402:HEC:CAC	2.12	1.37

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	330/336 (98%)	294 (89%)	35 (11%)	1 (0%)	46	84
2	H	246/258 (95%)	220 (89%)	22 (9%)	4 (2%)	12	54
3	L	271/273 (99%)	246 (91%)	24 (9%)	1 (0%)	39	80
4	M	321/323 (99%)	290 (90%)	26 (8%)	5 (2%)	12	54
All	All	1168/1190 (98%)	1050 (90%)	107 (9%)	11 (1%)	21	67

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	147	GLU
2	H	73	GLY
4	M	32	PRO
4	M	51	LEU
4	M	193	ASN

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	280/282 (99%)	266 (95%)	14 (5%)	30	71
2	H	205/212 (97%)	188 (92%)	17 (8%)	14	49
3	L	218/218 (100%)	203 (93%)	15 (7%)	19	59
4	M	249/249 (100%)	236 (95%)	13 (5%)	29	69
All	All	952/961 (99%)	893 (94%)	59 (6%)	23	64

5 of 59 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	H	216	GLU
3	L	7	ARG
4	M	214	PHE
2	H	223	ARG
2	H	236	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
2	H	106	ASN
2	H	225	GLN
4	M	4	GLN
2	H	58	GLN
2	H	102	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	FME	H	1	2	8,9,10	0.76	0	6,9,11	4.06	3 (50%)

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
2	FME	H	1	2	-	1/6/9/11	0/0/0/0

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	1	FME	CA-N-CN	-9.15	108.76	122.82
2	H	1	FME	O1-CN-N	-2.66	120.92	124.76
2	H	1	FME	CE-SD-CG	2.42	108.62	100.37

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	H	1	FME	O1-CN-N-CA

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 37 ligands modelled in this entry, 1 is monoatomic - leaving 36 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	$\#\|Z\| > 2$
7	HEC	C	401	1	24,50,50	2.12	2 (8%)	19,82,82	2.89	3 (15%)
7	HEC	C	402	1	24,50,50	1.91	2 (8%)	19,82,82	2.91	5 (26%)
7	HEC	C	403	1	24,50,50	1.87	3 (12%)	19,82,82	2.69	3 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
7	HEC	C	404	1	24,50,50	1.89	3 (12%)	19,82,82	2.87	6 (31%)
8	HTO	C	706	-	9,9,9	0.26	0	8,10,10	0.65	0
8	HTO	C	707	-	9,9,9	0.62	0	8,10,10	0.56	0
5	SO4	C	808	-	4,4,4	0.17	0	6,6,6	0.22	0
5	SO4	C	809	-	4,4,4	0.19	0	6,6,6	0.09	0
5	SO4	C	810	-	4,4,4	0.18	0	6,6,6	0.07	0
5	SO4	C	811	-	4,4,4	0.16	0	6,6,6	0.16	0
5	SO4	C	813	-	4,4,4	0.21	0	6,6,6	0.42	0
5	SO4	C	814	-	4,4,4	0.09	0	6,6,6	0.36	0
5	SO4	C	815	-	4,4,4	0.11	0	6,6,6	0.20	0
9	LDA	H	701	-	15,15,15	3.77	2 (13%)	16,17,17	0.79	1 (6%)
9	LDA	H	703	-	15,15,15	3.66	2 (13%)	16,17,17	1.16	2 (12%)
8	HTO	H	705	-	9,9,9	0.65	0	8,10,10	0.83	0
5	SO4	H	803	-	4,4,4	0.21	0	6,6,6	0.25	0
5	SO4	H	806	-	4,4,4	0.18	0	6,6,6	0.27	0
5	SO4	H	807	-	4,4,4	0.20	0	6,6,6	0.26	0
5	SO4	H	812	-	4,4,4	0.13	0	6,6,6	0.12	0
10	BCB	L	400	3	56,74,74	2.55	7 (12%)	57,115,115	1.66	12 (21%)
10	BCB	L	401	3	56,74,74	2.46	6 (10%)	57,115,115	1.83	9 (15%)
11	BPB	L	402	-	63,70,70	2.44	8 (12%)	63,101,101	2.87	18 (28%)
12	UQ1	L	502	-	18,18,18	1.80	2 (11%)	22,25,25	1.17	3 (13%)
12	UQ1	L	503	-	18,18,18	1.85	2 (11%)	22,25,25	1.07	1 (4%)
9	LDA	L	702	-	15,15,15	3.93	2 (13%)	16,17,17	0.68	0
10	BCB	M	400	4	56,74,74	2.50	7 (12%)	57,115,115	1.73	10 (17%)
10	BCB	M	401	4	56,74,74	2.67	7 (12%)	57,115,115	1.69	13 (22%)
11	BPB	M	402	-	63,70,70	2.39	9 (14%)	63,101,101	2.93	16 (25%)
13	MQ9	M	501	-	59,59,59	1.95	20 (33%)	74,75,75	1.64	20 (27%)
14	NS5	M	600	-	39,39,39	1.51	3 (7%)	44,46,46	1.91	12 (27%)
9	LDA	M	704	-	15,15,15	4.07	2 (13%)	16,17,17	1.34	2 (12%)
5	SO4	M	801	-	4,4,4	0.26	0	6,6,6	0.48	0
5	SO4	M	802	-	4,4,4	0.22	0	6,6,6	0.32	0
5	SO4	M	804	-	4,4,4	0.18	0	6,6,6	0.18	0
5	SO4	M	805	-	4,4,4	0.25	0	6,6,6	0.33	0

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
7	HEC	C	401	1	-	0/6/54/54	0/0/8/8
7	HEC	C	402	1	-	0/6/54/54	0/0/8/8
7	HEC	C	403	1	-	0/6/54/54	0/0/8/8
7	HEC	C	404	1	-	0/6/54/54	0/0/8/8
8	HTO	C	706	-	-	0/10/10/10	0/0/0/0
8	HTO	C	707	-	-	0/10/10/10	0/0/0/0
5	SO4	C	808	-	-	0/0/0/0	0/0/0/0
5	SO4	C	809	-	-	0/0/0/0	0/0/0/0
5	SO4	C	810	-	-	0/0/0/0	0/0/0/0
5	SO4	C	811	-	-	0/0/0/0	0/0/0/0
5	SO4	C	813	-	-	0/0/0/0	0/0/0/0
5	SO4	C	814	-	-	0/0/0/0	0/0/0/0
5	SO4	C	815	-	-	0/0/0/0	0/0/0/0
9	LDA	H	701	-	-	0/13/13/13	0/0/0/0
9	LDA	H	703	-	-	0/13/13/13	0/0/0/0
8	HTO	H	705	-	-	0/10/10/10	0/0/0/0
5	SO4	H	803	-	-	0/0/0/0	0/0/0/0
5	SO4	H	806	-	-	0/0/0/0	0/0/0/0
5	SO4	H	807	-	-	0/0/0/0	0/0/0/0
5	SO4	H	812	-	-	0/0/0/0	0/0/0/0
10	BCB	L	400	3	-	0/37/137/137	0/0/9/9
10	BCB	L	401	3	-	0/37/137/137	0/0/9/9
11	BPB	L	402	-	-	0/46/105/105	0/1/6/6
12	UQ1	L	502	-	-	0/9/33/33	0/1/1/1
12	UQ1	L	503	-	-	0/9/33/33	0/1/1/1
9	LDA	L	702	-	-	0/13/13/13	0/0/0/0
10	BCB	M	400	4	-	0/37/137/137	0/0/9/9
10	BCB	M	401	4	-	0/37/137/137	0/0/9/9
11	BPB	M	402	-	-	0/46/105/105	0/1/6/6
13	MQ9	M	501	-	-	0/53/73/73	0/2/2/2
14	NS5	M	600	-	-	0/43/43/43	0/0/0/0
9	LDA	M	704	-	-	0/13/13/13	0/0/0/0
5	SO4	M	801	-	-	0/0/0/0	0/0/0/0
5	SO4	M	802	-	-	0/0/0/0	0/0/0/0
5	SO4	M	804	-	-	0/0/0/0	0/0/0/0
5	SO4	M	805	-	-	0/0/0/0	0/0/0/0

The worst 5 of 89 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	M	704	LDA	O1-N1	-15.43	1.24	1.39
9	L	702	LDA	O1-N1	-14.96	1.25	1.39
9	H	701	LDA	O1-N1	-14.28	1.26	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	H	703	LDA	O1-N1	-13.49	1.26	1.39
7	C	401	HEC	C3B-C2B	-6.89	1.33	1.40

The worst 5 of 136 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	C	402	HEC	CBB-CAB-C3B	-8.70	108.01	127.35
7	C	401	HEC	CBC-CAC-C3C	-8.64	108.15	127.35
7	C	404	HEC	CBB-CAB-C3B	-7.79	110.03	127.35
7	C	403	HEC	CBB-CAB-C3B	-7.55	110.57	127.35
7	C	401	HEC	CBB-CAB-C3B	-7.38	110.94	127.35

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

19 monomers are involved in 129 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	C	401	HEC	13	0
7	C	402	HEC	10	0
7	C	403	HEC	6	0
7	C	404	HEC	2	0
8	C	706	HTO	1	0
9	H	703	LDA	6	0
8	H	705	HTO	2	0
5	H	807	SO4	1	0
10	L	400	BCB	17	0
10	L	401	BCB	10	0
11	L	402	BPB	9	0
12	L	502	UQ1	4	0
9	L	702	LDA	2	0
10	M	400	BCB	11	0
10	M	401	BCB	17	0
11	M	402	BPB	20	0
13	M	501	MQ9	3	0
14	M	600	NS5	11	0
5	M	805	SO4	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^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	C	332/336 (98%)	-0.22	8 (2%)	62	50	46, 74, 113, 124	0
2	H	249/258 (96%)	-0.17	3 (1%)	81	71	50, 73, 99, 105	0
3	L	273/273 (100%)	-0.57	3 (1%)	82	73	37, 54, 74, 85	0
4	M	323/323 (100%)	-0.50	3 (0%)	85	79	42, 60, 89, 117	0
All	All	1177/1190 (98%)	-0.37	17 (1%)	78	67	37, 66, 102, 124	0

The worst 5 of 17 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	85	THR	3.8
1	C	59	VAL	3.7
1	C	54	GLN	3.0
1	C	53	SER	2.9
2	H	83	PRO	2.8

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	FME	H	1	10/11	0.77	0.37	-	104,105,115,117	0

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
8	HTO	C	706	10/10	0.88	0.71	11.55	56,57,58,58	10
9	LDA	M	704	16/16	0.91	0.41	11.44	68,70,73,73	16
8	HTO	H	705	10/10	0.55	0.59	7.00	56,59,61,61	10
12	UQ1	L	502	18/18	0.89	0.40	5.83	63,65,66,66	18
8	HTO	C	707	10/10	0.77	0.39	5.67	44,48,49,49	10
5	SO4	C	811	5/5	0.85	0.60	5.56	76,76,76,77	5
9	LDA	L	702	16/16	0.95	0.36	5.15	67,73,79,80	0
14	NS5	M	600	40/40	0.87	0.28	4.97	65,71,100,101	4
12	UQ1	L	503	18/18	0.62	0.59	3.92	73,76,78,78	18
11	BPB	M	402	65/65	0.89	0.28	3.04	61,67,123,124	0
5	SO4	C	813	5/5	0.82	0.43	2.34	79,79,80,80	5
5	SO4	H	807	5/5	0.81	0.42	2.22	108,108,108,109	5
13	MQ9	M	501	58/58	0.91	0.25	1.87	40,64,102,103	0
9	LDA	H	703	16/16	0.94	0.39	1.47	54,58,60,61	16
7	HEC	C	403	43/43	0.98	0.19	0.81	46,48,52,54	0
11	BPB	L	402	65/65	0.96	0.19	0.79	38,51,60,60	0
10	BCB	M	401	66/66	0.98	0.18	0.77	36,41,63,68	0
10	BCB	M	400	66/66	0.97	0.18	0.66	37,48,107,108	0
10	BCB	L	400	66/66	0.97	0.18	0.56	37,40,45,49	0
10	BCB	L	401	66/66	0.97	0.19	0.44	41,44,59,64	0
7	HEC	C	404	43/43	0.98	0.16	0.17	52,55,68,73	0
7	HEC	C	402	43/43	0.98	0.19	0.09	73,76,80,81	0
9	LDA	H	701	16/16	0.96	0.17	-0.03	54,57,68,68	0
7	HEC	C	401	43/43	0.96	0.27	-0.34	99,110,118,120	0
5	SO4	H	806	5/5	0.95	0.14	-0.57	72,72,73,73	5
5	SO4	M	802	5/5	0.99	0.09	-1.07	89,89,90,90	0
6	FE2	M	500	1/1	1.00	0.16	-1.74	50,50,50,50	0
5	SO4	C	814	5/5	0.92	0.37	-	48,48,49,50	5
5	SO4	M	801	5/5	0.96	0.11	-	61,62,63,63	0
5	SO4	C	808	5/5	0.47	0.40	-	104,104,104,104	5

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
5	SO4	M	804	5/5	0.95	0.18	-	94,95,96,96	0
5	SO4	H	803	5/5	0.76	0.34	-	82,82,83,83	5
5	SO4	C	810	5/5	0.80	0.42	-	88,88,88,88	5
5	SO4	C	809	5/5	0.48	0.54	-	109,110,110,110	5
5	SO4	C	815	5/5	0.92	0.25	-	40,40,41,41	5
5	SO4	M	805	5/5	0.96	0.09	-	64,65,65,67	5
5	SO4	H	812	5/5	0.76	0.33	-	92,92,93,93	5

6.5 Other polymers

There are no such residues in this entry.