



wwPDB X-ray Structure Validation Summary Report

Feb 26, 2014 – 07:13 PM 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 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/ValidationPDFNotes.html>

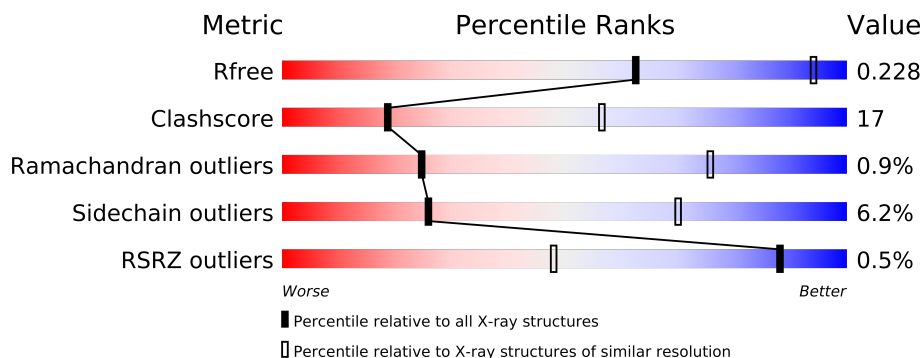
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

1 Overall quality at a glance

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}	66092	1205 (3.30-3.14)
Clashscore	79885	1072 (3.28-3.16)
Ramachandran outliers	78287	1052 (3.28-3.16)
Sidechain outliers	78261	1051 (3.28-3.16)
RSRZ outliers	66119	1206 (3.30-3.14)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	C	336	
2	H	258	
3	L	273	
4	M	323	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
11	BPB	M	402	-	X
12	UQ1	L	502	-	X
12	UQ1	L	503	-	X
13	MQ9	M	501	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
14	NS5	M	600	-	X
5	SO4	C	808	-	X
5	SO4	C	809	-	X
5	SO4	C	810	-	X
5	SO4	C	811	-	X
5	SO4	C	813	-	X
5	SO4	C	814	-	X
5	SO4	C	815	-	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 hydrogen and 0 are deuterium.

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: O₄S).



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

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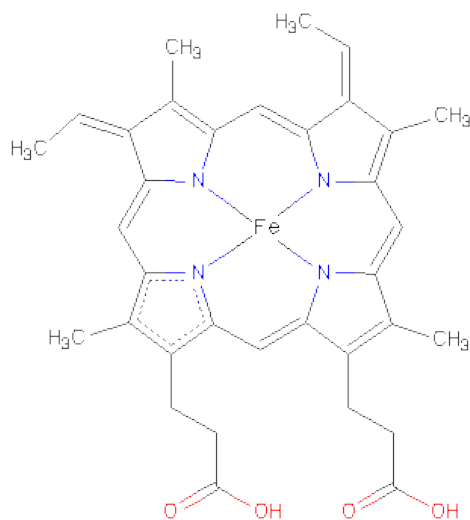
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	M	1	Total	O	S	0	0
			5	4	1		

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

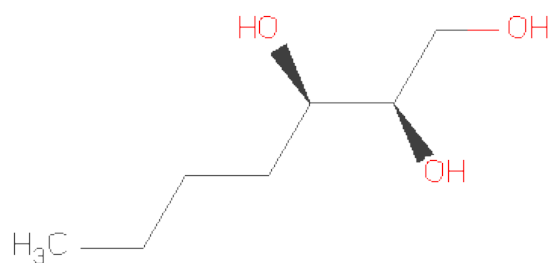
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	M	1	Total	Fe	0	0
			1	1		

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



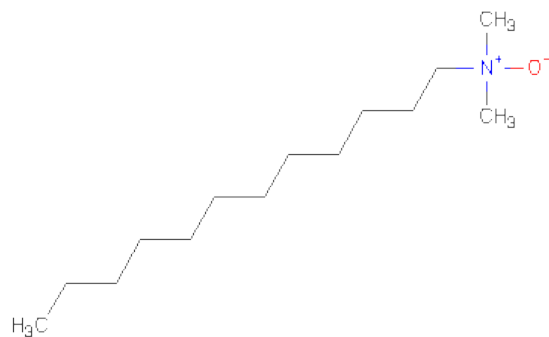
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
7	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
7	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
7	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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



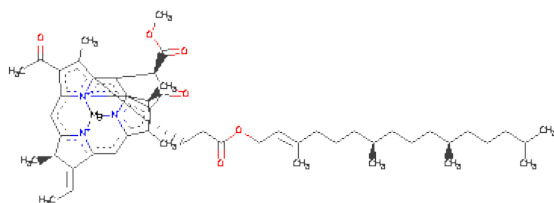
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	C	1	Total	C	O	0	0
			10	7	3		
8	C	1	Total	C	O	0	0
			10	7	3		
8	H	1	Total	C	O	0	0
			10	7	3		

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



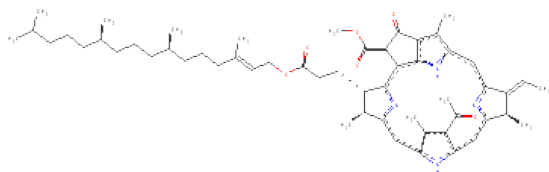
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	H	1	Total	C	N	O	0	0
			16	14	1	1		
9	H	1	Total	C	N	O	0	0
			16	14	1	1		
9	L	1	Total	C	N	O	0	0
			16	14	1	1		
9	M	1	Total	C	N	O	0	0
			16	14	1	1		

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



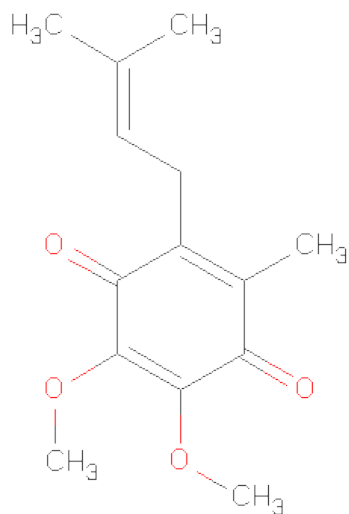
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
10	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
10	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
10	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

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



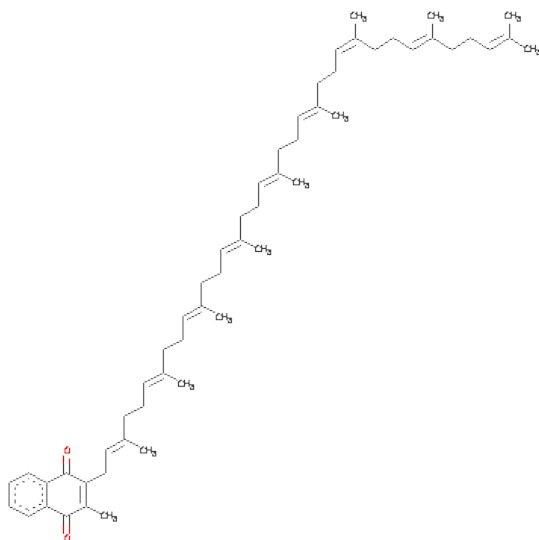
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	L	1	Total	C	N	O	0	0
			65	55	4	6		
11	M	1	Total	C	N	O	0	0
			65	55	4	6		

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



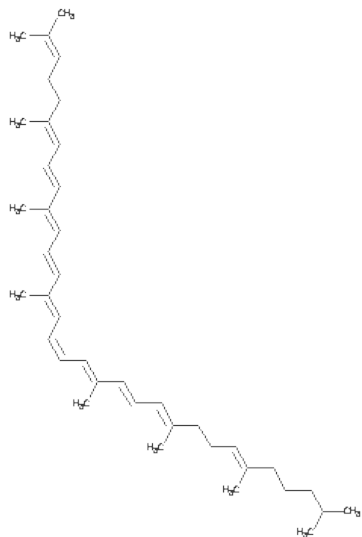
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	L	1	Total	C	O	0	0
			18	14	4		
12	L	1	Total	C	O	0	0
			18	14	4		

- 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	0	0
			58	56	2		

- 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	0	0
			40	40		

- Molecule 15 is water.

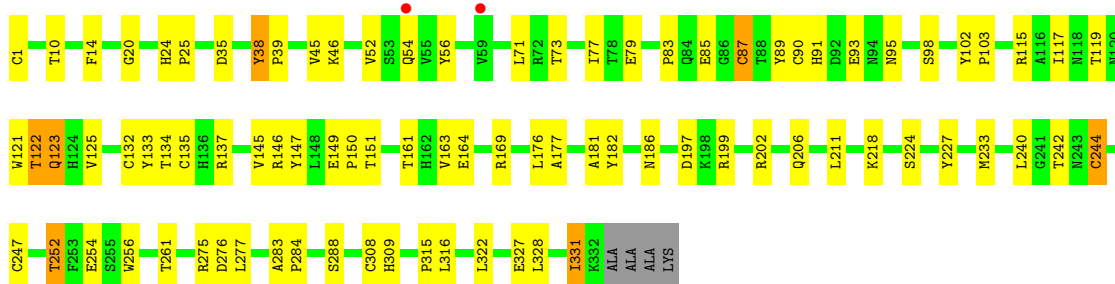
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	C	47	Total 47	O 47	0	0
15	H	28	Total 28	O 28	0	0
15	L	38	Total 38	O 38	0	0
15	M	46	Total 46	O 46	0	0

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 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.

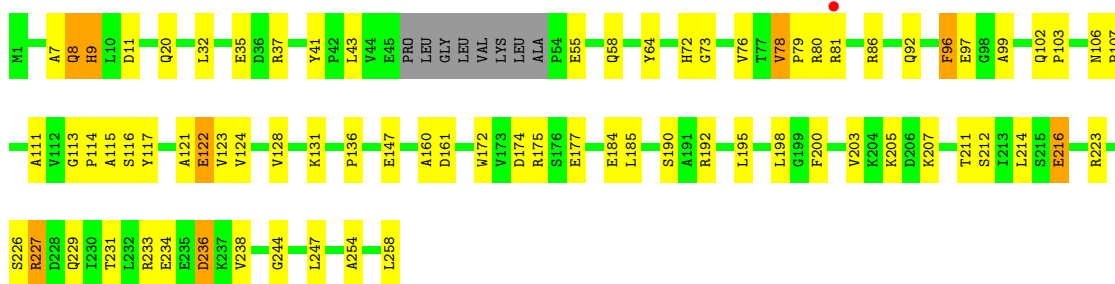
- Molecule 1: Photosynthetic reaction center cytochrome c subunit

Chain C: 



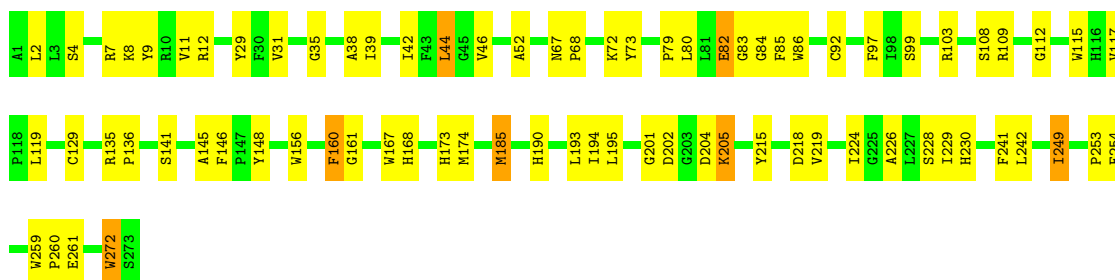
- Molecule 2: Reaction center protein H chain

Chain H: 



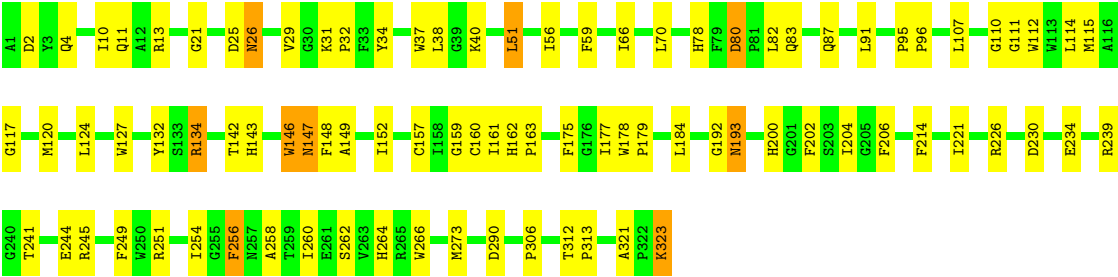
- Molecule 3: Reaction center protein L chain

Chain L: 



- Molecule 4: Reaction center protein M chain

Chain M: 



4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ ¹	2.78 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.4.0073	Depositor
R, R_{free}	0.192 , 0.224 0.197 , 0.228	Depositor DCC
R_{free} test set	3145 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 , 38.4	EDS
Estimated twinning fraction	0.028 for -h,-k,l	Xtriage
L-test for twinning	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	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.*

¹Intensities estimated from amplitudes.

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(°)	Ideal(°)
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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2598	0	2573	82	0
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

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 17.

The worst 5 of 337 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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

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	C	330/336 (98%)	294 (89%)	35 (11%)	1 (0%)	50	91
2	H	246/258 (95%)	220 (89%)	22 (9%)	4 (2%)	14	63
3	L	271/273 (99%)	246 (91%)	24 (9%)	1 (0%)	43	88
4	M	321/323 (99%)	290 (90%)	26 (8%)	5 (2%)	14	63
All	All	1168/1190 (98%)	1050 (90%)	107 (9%)	11 (1%)	25	76

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 ⓘ

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%)	34	78
2	H	205/212 (97%)	188 (92%)	17 (8%)	16	55
3	L	218/218 (100%)	203 (93%)	15 (7%)	22	65
4	M	249/249 (100%)	236 (95%)	13 (5%)	32	76
All	All	952/961 (99%)	893 (94%)	59 (6%)	26	70

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 ⓘ

There are no RNA chains in this entry.

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

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	9,9,10	5.92	1 (11%)	6,9,11	3.72	2 (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
2	FME	H	1	2	-	1/7/9/11	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	1	FME	O-C	17.57	1.23	1.11

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	1	FME	CA-N-CN	-8.59	108.76	122.97
2	H	1	FME	CE-SD-CG	2.24	108.62	100.27

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.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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	50,50,50	2.62	13 (26%)	56,82,82	1.83	10 (17%)
7	HEC	C	402	1	50,50,50	2.50	12 (24%)	56,82,82	1.95	13 (23%)
7	HEC	C	403	1	50,50,50	2.67	12 (24%)	56,82,82	1.75	9 (16%)
7	HEC	C	404	1	50,50,50	2.55	13 (26%)	56,82,82	1.88	15 (26%)
8	HTO	C	706	-	9,9,9	0.29	0	10,10,10	0.68	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	HTO	C	707	-	9,9,9	0.68	0	10,10,10	0.55	0
5	SO4	C	808	-	4,4,4	0.15	0	6,6,6	0.21	0
5	SO4	C	809	-	4,4,4	0.17	0	6,6,6	0.08	0
5	SO4	C	810	-	4,4,4	0.17	0	6,6,6	0.07	0
5	SO4	C	811	-	4,4,4	0.15	0	6,6,6	0.15	0
5	SO4	C	813	-	4,4,4	0.19	0	6,6,6	0.40	0
5	SO4	C	814	-	4,4,4	0.08	0	6,6,6	0.34	0
5	SO4	C	815	-	4,4,4	0.09	0	6,6,6	0.20	0
9	LDA	H	701	-	15,15,15	3.77	2 (13%)	17,17,17	0.93	2 (11%)
9	LDA	H	703	-	15,15,15	3.65	2 (13%)	17,17,17	1.82	3 (17%)
8	HTO	H	705	-	9,9,9	0.71	0	10,10,10	0.80	0
5	SO4	H	803	-	4,4,4	0.20	0	6,6,6	0.24	0
5	SO4	H	806	-	4,4,4	0.17	0	6,6,6	0.27	0
5	SO4	H	807	-	4,4,4	0.18	0	6,6,6	0.25	0
5	SO4	H	812	-	4,4,4	0.11	0	6,6,6	0.12	0
10	BCB	L	400	3	74,74,74	2.41	14 (18%)	94,115,115	1.68	23 (24%)
10	BCB	L	401	3	74,74,74	2.33	12 (16%)	94,115,115	1.63	19 (20%)
11	BPB	L	402	-	70,70,70	2.99	15 (21%)	93,101,101	3.03	29 (31%)
12	UQ1	L	502	-	18,18,18	1.75	2 (11%)	25,25,25	1.18	3 (12%)
12	UQ1	L	503	-	18,18,18	1.80	2 (11%)	25,25,25	1.10	2 (8%)
9	LDA	L	702	-	15,15,15	3.92	2 (13%)	17,17,17	0.86	1 (5%)
10	BCB	M	400	4	74,74,74	2.25	11 (14%)	94,115,115	1.57	16 (17%)
10	BCB	M	401	4	74,74,74	2.50	16 (21%)	94,115,115	1.65	25 (26%)
11	BPB	M	402	-	70,70,70	2.84	15 (21%)	93,101,101	3.12	26 (27%)
13	MQ9	M	501	-	59,59,59	1.90	18 (30%)	75,75,75	1.64	20 (26%)
14	NS5	M	600	-	39,39,39	1.46	3 (7%)	46,46,46	2.13	14 (30%)
9	LDA	M	704	-	15,15,15	4.06	2 (13%)	17,17,17	1.55	3 (17%)
5	SO4	M	801	-	4,4,4	0.26	0	6,6,6	0.48	0
5	SO4	M	802	-	4,4,4	0.21	0	6,6,6	0.30	0
5	SO4	M	804	-	4,4,4	0.16	0	6,6,6	0.18	0
5	SO4	M	805	-	4,4,4	0.24	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	-	0/10/54/54	0/0/8/8

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	HEC	C	402	1	-	0/10/54/54	0/0/8/8
7	HEC	C	403	1	-	0/10/54/54	0/0/8/8
7	HEC	C	404	1	-	0/10/54/54	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	-	0/41/137/137	0/0/9/9
10	BCB	L	401	3	-	0/41/137/137	0/0/9/9
11	BPB	L	402	-	-	0/52/105/105	0/0/6/6
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	-	0/41/137/137	0/0/9/9
10	BCB	M	401	4	-	0/41/137/137	0/0/9/9
11	BPB	M	402	-	-	0/52/105/105	0/0/6/6
13	MQ9	M	501	-	-	0/53/73/73	0/0/2/2
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 166 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	M	401	BCB	CAC-C3C	15.75	1.53	1.33
11	L	402	BPB	CAC-C3C	15.58	1.53	1.33
10	L	400	BCB	CAC-C3C	15.54	1.53	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	M	402	BPB	CAC-C3C	15.53	1.53	1.33
9	M	704	LDA	O1-N1	-15.41	1.24	1.39

The worst 5 of 233 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	M	402	BPB	C3D-C2D-C1D	-18.43	95.98	107.01
11	L	402	BPB	C3D-C2D-C1D	-17.70	96.42	107.01
11	M	402	BPB	C4D-C3D-C2D	16.14	126.29	107.04
11	L	402	BPB	C4D-C3D-C2D	15.44	125.45	107.04
7	C	402	HEC	CBB-CAB-C3B	-7.26	108.01	128.44

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th 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%)	-0.19	2 (0%) 86 43	46, 74, 113, 124	0
2	H	250/258 (96%)	-0.11	1 (0%) 90 54	50, 73, 99, 108	0
3	L	273/273 (100%)	-0.40	0 100 100	37, 54, 74, 85	0
4	M	323/323 (100%)	-0.37	0 100 100	42, 60, 89, 117	0
All	All	1178/1190 (98%)	-0.27	3 (0%) 88 60	37, 66, 102, 124	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	81	ARG	2.4
1	C	54	GLN	2.4
1	C	59	VAL	2.1

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, 95th 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	FME	H	1	10/11	0.41	2.92	104,105,115,117	0

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
5	SO4	C	808	5/5	0.42	47.80	104,104,104,104	5
8	HTO	C	706	10/10	0.74	12.87	56,57,58,58	10
9	LDA	M	704	16/16	0.45	11.25	68,70,73,73	16
8	HTO	H	705	10/10	0.56	7.44	56,59,61,61	10
5	SO4	C	811	5/5	0.47	5.28	76,76,76,77	5
12	UQ1	L	503	18/18	0.74	4.55	73,76,78,78	18
12	UQ1	L	502	18/18	0.33	4.37	63,65,66,66	18
8	HTO	C	707	10/10	0.37	3.32	44,48,49,49	10
9	LDA	L	702	16/16	0.30	3.22	67,73,79,80	0
14	NS5	M	600	40/40	0.29	3.19	65,71,100,101	4
5	SO4	C	809	5/5	0.47	3.01	109,110,110,110	5
5	SO4	C	815	5/5	0.24	2.79	40,40,41,41	5
13	MQ9	M	501	58/58	0.29	2.71	40,64,102,103	0
11	BPB	M	402	65/65	0.26	2.68	61,67,123,124	0
5	SO4	C	814	5/5	0.26	2.66	48,48,49,50	5
5	SO4	C	813	5/5	0.34	2.04	79,79,80,80	5
5	SO4	C	810	5/5	0.53	2.01	88,88,88,88	5
5	SO4	H	807	5/5	0.38	1.45	108,108,108,109	5
10	BCB	M	400	66/66	0.19	1.34	37,48,107,108	0
5	SO4	H	803	5/5	0.36	1.32	82,82,83,83	5
9	LDA	H	703	16/16	0.42	1.04	54,58,60,61	16
10	BCB	M	401	66/66	0.20	0.99	36,41,63,68	0
10	BCB	L	400	66/66	0.20	0.86	37,40,45,49	0
11	BPB	L	402	65/65	0.20	0.63	38,51,60,60	0
7	HEC	C	403	43/43	0.18	0.59	46,48,52,54	0
10	BCB	L	401	66/66	0.21	0.58	41,44,59,64	0
5	SO4	H	812	5/5	0.30	0.22	92,92,93,93	5
7	HEC	C	404	43/43	0.16	0.21	52,55,68,73	0
7	HEC	C	402	43/43	0.20	0.06	73,76,80,81	0
5	SO4	H	806	5/5	0.16	-0.08	72,72,73,73	5
5	SO4	M	804	5/5	0.15	-0.09	94,95,96,96	0
9	LDA	H	701	16/16	0.18	-0.14	54,57,68,68	0
7	HEC	C	401	43/43	0.26	-0.30	99,110,118,120	0
5	SO4	M	802	5/5	0.09	-1.17	89,89,90,90	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	SO4	M	805	5/5	0.10	-1.58	64,65,65,67	5
6	FE2	M	500	1/1	0.15	-1.71	50,50,50,50	0
5	SO4	M	801	5/5	0.10	-1.90	61,62,63,63	0

6.5 Other polymers ⓘ

There are no such residues in this entry.