wwPDB X-ray Structure Validation Summary Report (i)

Jan 31, 2017 – 06:12 PM EST

PDB ID	:	5M7J
Title	:	Blastochloris viridis photosynthetic reaction center structure using best crystal approach
Authors	:	Sharma, A.S.; Johansson, L.; Dunevall, E.; Wahlgren, W.Y.; Neutze, R.; Katona, G.
Deposited on	:	2016-10-28
Resolution	:	3.50 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:

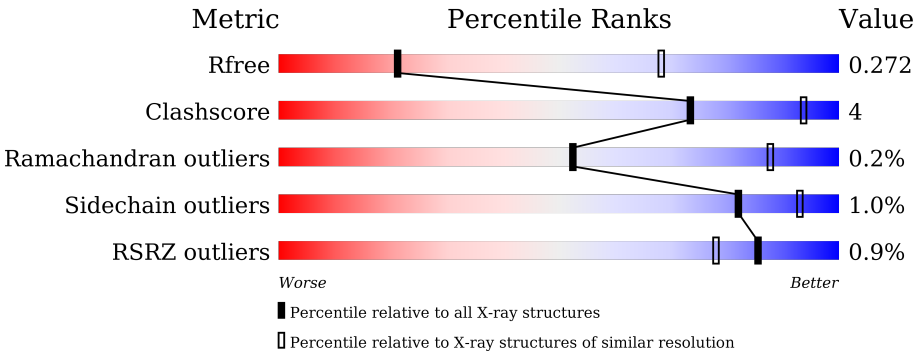
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20028442
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20028442

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 3.50 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	1051 (3.60-3.40)
Clashscore	102246	1157 (3.60-3.40)
Ramachandran outliers	100387	1120 (3.60-3.40)
Sidechain outliers	100360	1121 (3.60-3.40)
RSRZ outliers	91569	1058 (3.60-3.40)

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	A	356	84% 9% 7%
2	B	274	87% 13%
3	C	324	91% 8% .
4	D	258	4% 89% 5% 6%

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	PO4	C	407	-	-	-	X
6	DGA	A	405	-	-	-	X
9	MPG	B	305	-	-	-	X
9	MPG	B	306	-	-	-	X
9	MPG	C	406	-	-	-	X

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 9890 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	A	332	Total	C	N	O	S	0	0	0
			2598	1637	465	478	18			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	273	Total	C	N	O	S	0	2	0
			2170	1458	350	355	7			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	323	Total	C	N	O	S	0	0	0
			2546	1696	417	422	11			

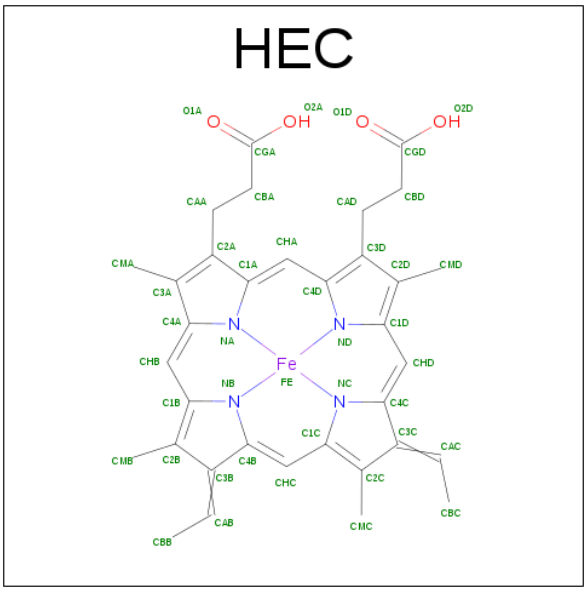
- Molecule 4 is a protein called Reaction center protein H chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	243	Total	C	N	O	S	0	0	0
			1771	1140	297	332	2			

There is a discrepancy between the modelled and reference sequences:

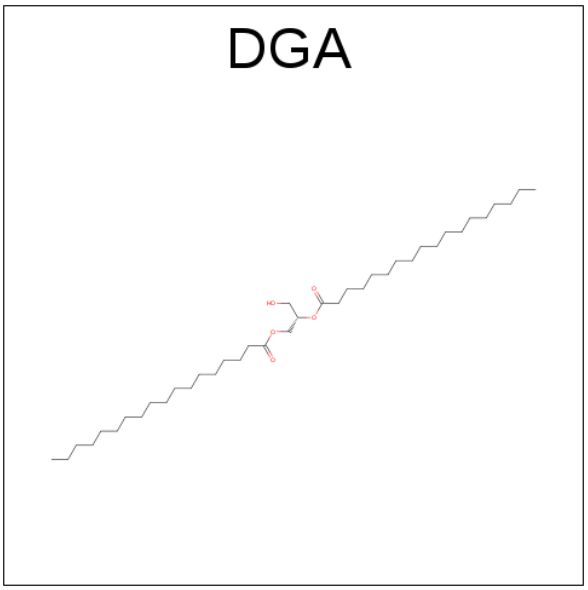
Chain	Residue	Modelled	Actual	Comment	Reference
D	1	FME	-	expression tag	UNP P06008

- Molecule 5 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



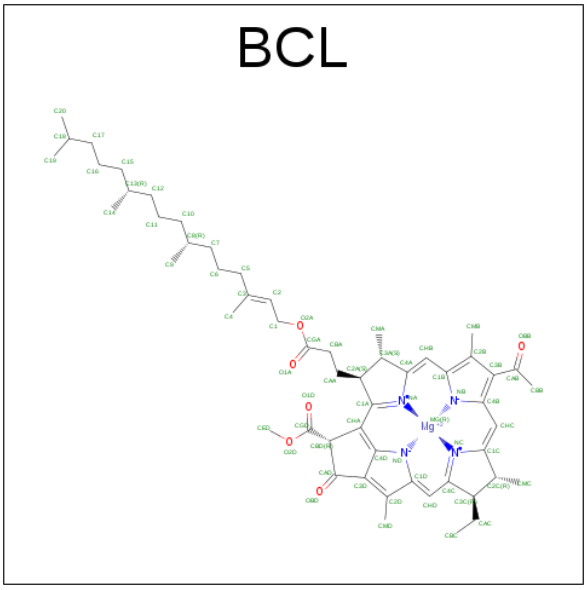
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
5	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
5	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
5	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 6 is DIACYL GLYCEROL (three-letter code: DGA) (formula: $C_{39}H_{76}O_5$).



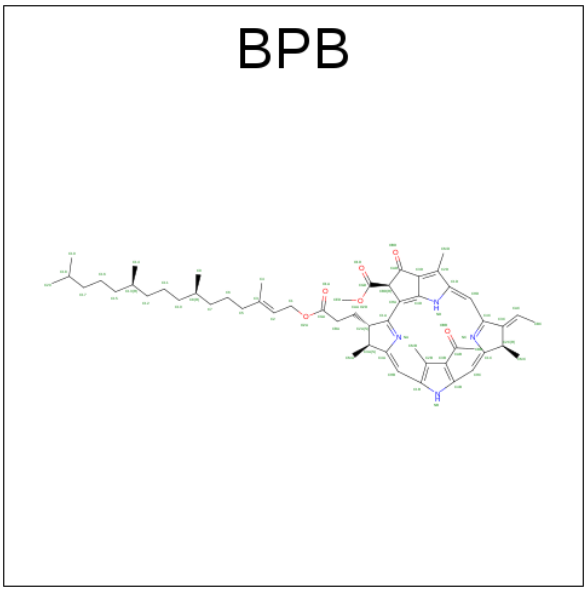
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			37	33	4		

- Molecule 7 is BACTERIOCHLOROPHYLL A (three-letter code: BCL) (formula: $C_{55}H_{74}MgN_4O_6$).



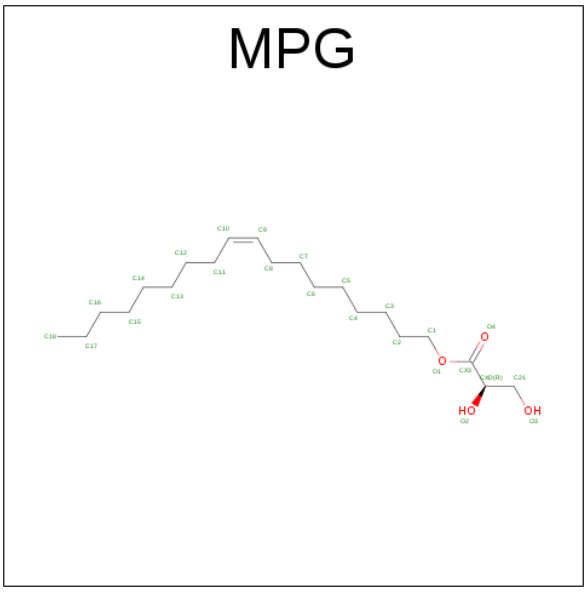
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	B	1	Total	C	Mg	N	O	14	0
			65	54	1	4	6		
7	B	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
7	B	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
7	C	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

- Molecule 8 is BACTERIOPHEOPHYTIN B (three-letter code: BPB) (formula: $C_{55}H_{74}N_4O_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	B	1	Total	C	N	O	0	0
			65	55	4	6		
8	C	1	Total	C	N	O	0	0
			61	51	4	6		

- Molecule 9 is [(Z)-octadec-9-enyl] (2R)-2,3-bis(oxidanyl)propanoate (three-letter code: MPG) (formula: $C_{21}H_{40}O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	B	1	Total	C	O	6	0
			25	21	4		

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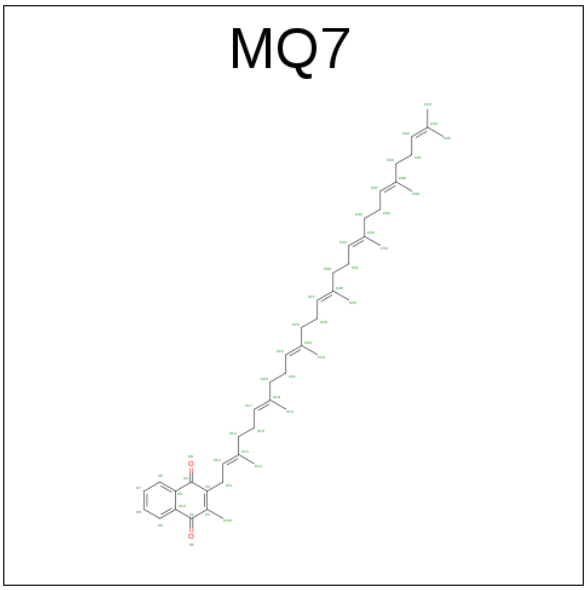
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	B	1	Total C O 25 21 4	0	0
9	C	1	Total C 17 17	0	0

- Molecule 10 is FE (II) ION (three-letter code: FE2) (formula: Fe).

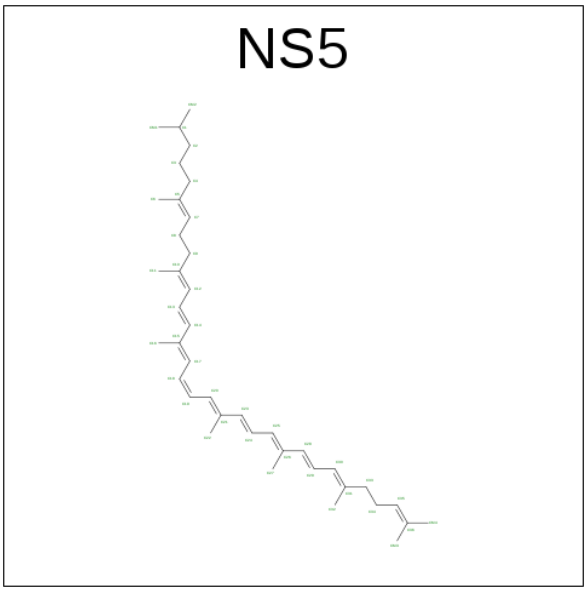
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	B	1	Total Fe 1 1	0	0

- Molecule 11 is MENAQUINONE-7 (three-letter code: MQ7) (formula: $C_{46}H_{64}O_2$).



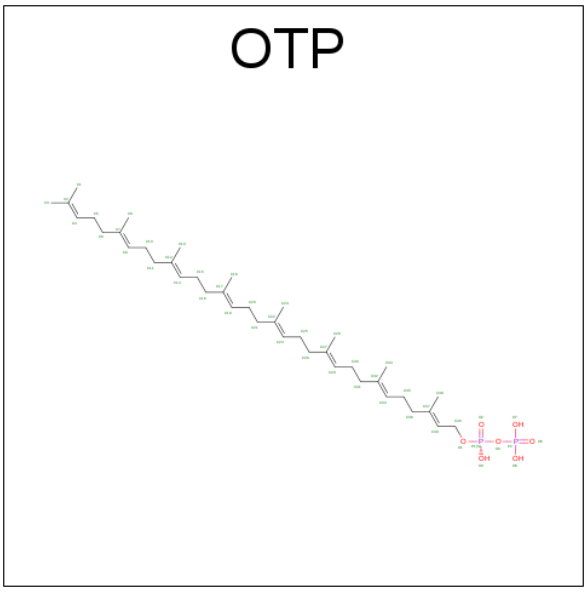
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	C	1	Total C O 48 46 2	0	0

- Molecule 12 is 15-cis-1,2-dihydroneurosporene (three-letter code: NS5) (formula: $C_{40}H_{60}$).



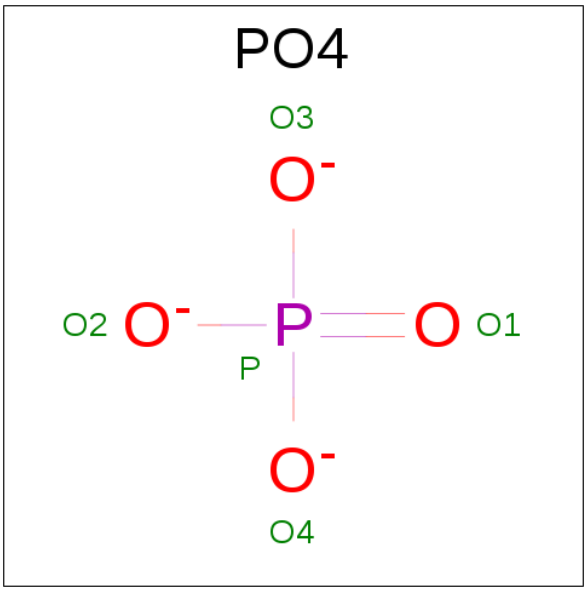
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	C	1	Total C 40 40	0	0

- Molecule 13 is (2E,6E,10E,14E,18E,22E,26E)-3,7,11,15,19,23,27,31-OCTAMETHYLD OTRIACONTA-2,6,10,14,18,22,26,30-OCTAENYL TRIHYDROGEN DIPHOSPHATE (three-letter code: OTP) (formula: $C_{40}H_{68}O_7P_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	C	1	Total C O 41 40 1	0	0

- Molecule 14 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



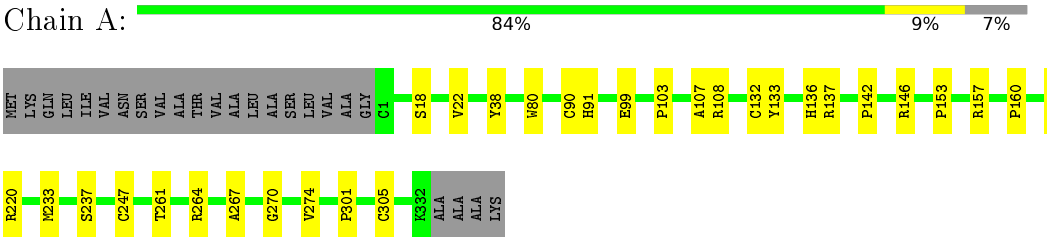
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	C	1	Total O P 5 4 1	0	0
14	C	1	Total O P 5 4 1	0	0

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.

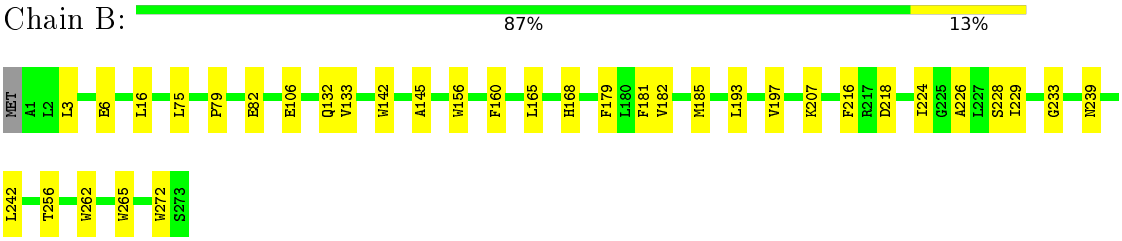
- Molecule 1: Photosynthetic reaction center cytochrome c subunit

Chain A:



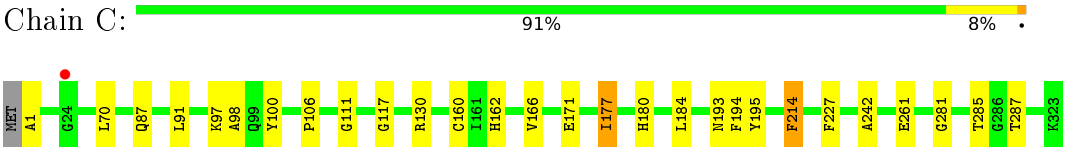
- Molecule 2: Reaction center protein L chain

Chain B:



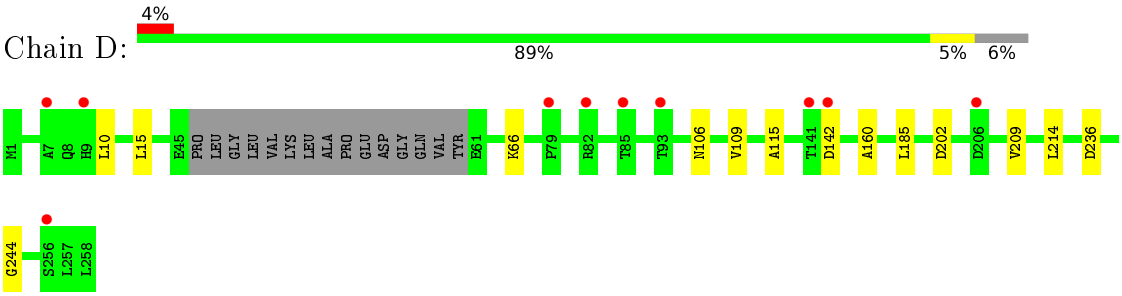
- Molecule 3: Reaction center protein M chain

Chain C:



- Molecule 4: Reaction center protein H chain

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	57.90Å 84.80Å 384.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	52.76 – 3.50 52.76 – 3.50	Depositor EDS
% Data completeness (in resolution range)	99.5 (52.76-3.50) 99.5 (52.76-3.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.77 (at 3.48Å)	Xtriage
Refinement program	PHENIX (1.10_2155: ???)	Depositor
R, R_{free}	0.253 , 0.273 0.252 , 0.272	Depositor DCC
R_{free} test set	1286 reflections (5.19%)	DCC
Wilson B-factor (Å^2)	68.7	Xtriage
Anisotropy	0.252	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 79.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.30$, $< L^2 > = 0.13$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.81	EDS
Total number of atoms	9890	wwPDB-VP
Average B, all atoms (Å^2)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.76% 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, 0.333 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: BCL, MPG, BPB, PO4, DGA, FE2, MQ7, HEC, OTP, 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	A	0.26	0/2665	0.45	0/3633
2	B	0.26	0/2263	0.42	0/3089
3	C	0.25	0/2650	0.39	0/3629
4	D	0.24	0/1804	0.44	0/2485
All	All	0.25	0/9382	0.43	0/12836

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	2598	0	2576	24	0
2	B	2170	0	2100	22	0
3	C	2546	0	2430	19	0
4	D	1771	0	1656	7	0
5	A	172	0	128	15	0
6	A	37	0	58	3	0
7	B	197	0	218	9	0
7	C	66	0	74	4	0
8	B	65	0	74	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	C	61	0	63	2	0
9	B	50	0	80	1	0
9	C	17	0	31	0	0
10	B	1	0	0	0	0
11	C	48	0	64	1	0
12	C	40	0	60	6	0
13	C	41	0	65	1	0
14	C	10	0	0	0	0
All	All	9890	0	9677	80	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 4.

The worst 5 of 80 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)
7:B:303:BCL:HMD2	7:C:401:BCL:HBB3	1.76	0.67
1:A:99:GLU:OE2	1:A:108:ARG:NH2	2.33	0.61
1:A:80:TRP:CD1	1:A:133:TYR:HB2	2.38	0.59
9:B:305:MPG:H21C	3:C:1:ALA:HA	1.85	0.59
1:A:220:ARG:NH2	3:C:171:GLU:OE2	2.35	0.58

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	A	330/356 (93%)	315 (96%)	15 (4%)	0	100 100
2	B	273/274 (100%)	263 (96%)	10 (4%)	0	100 100
3	C	321/324 (99%)	312 (97%)	7 (2%)	2 (1%)	30 75

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
4	D	239/258 (93%)	231 (97%)	8 (3%)	0	100 100
All	All	1163/1212 (96%)	1121 (96%)	40 (3%)	2 (0%)	52 88

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	193	ASN
3	C	177	ILE

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	A	280/297 (94%)	278 (99%)	2 (1%)	88 96
2	B	218/219 (100%)	215 (99%)	3 (1%)	74 91
3	C	247/250 (99%)	245 (99%)	2 (1%)	86 95
4	D	167/212 (79%)	165 (99%)	2 (1%)	78 92
All	All	912/978 (93%)	903 (99%)	9 (1%)	82 93

5 of 9 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	272	TRP
4	D	236	ASP
3	C	214	PHE
2	B	160	PHE
3	C	194	PHE

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

5.3.3 RNA

There are no RNA molecules 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	$\#\|Z\| > 2$
4	FME	D	1	4	8,9,10	0.86	0	5,9,11	0.99	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
4	FME	D	1	4	-	0/6/9/11	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

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	$\#\|Z\| > 2$
5	HEC	A	401	1	24,50,50	2.24	5 (20%)	19,82,82	1.78	5 (26%)
5	HEC	A	402	1	24,50,50	2.18	4 (16%)	19,82,82	2.01	7 (36%)
5	HEC	A	403	1	24,50,50	2.18	5 (20%)	19,82,82	1.95	5 (26%)
5	HEC	A	404	1	24,50,50	2.27	5 (20%)	19,82,82	1.62	4 (21%)
6	DGA	A	405	-	36,36,43	1.16	3 (8%)	38,38,45	3.07	6 (15%)
7	BCL	B	301	-	54,73,74	1.12	2 (3%)	53,113,115	1.17	4 (7%)
7	BCL	B	302	-	55,74,74	1.13	2 (3%)	55,115,115	1.36	8 (14%)
7	BCL	B	303	-	55,74,74	1.15	3 (5%)	55,115,115	1.23	6 (10%)
8	BPB	B	304	-	62,70,70	1.31	4 (6%)	64,101,101	1.58	9 (14%)
9	MPG	B	305	-	23,24,24	1.24	1 (4%)	20,25,25	1.88	2 (10%)
9	MPG	B	306	-	23,24,24	1.23	1 (4%)	20,25,25	1.51	1 (5%)
7	BCL	C	401	-	55,74,74	1.16	3 (5%)	55,115,115	1.32	9 (16%)
8	BPB	C	402	-	58,66,70	1.35	4 (6%)	58,96,101	1.52	9 (15%)
11	MQ7	C	403	-	49,49,49	1.59	8 (16%)	63,63,63	1.68	15 (23%)
12	NS5	C	404	-	39,39,39	2.30	18 (46%)	44,46,46	2.48	14 (31%)
13	OTP	C	405	-	40,40,48	0.63	0	47,47,61	2.14	19 (40%)
9	MPG	C	406	-	16,16,24	0.77	0	15,15,25	0.78	0
14	PO4	C	407	-	4,4,4	0.67	0	6,6,6	0.23	0
14	PO4	C	408	-	4,4,4	0.67	0	6,6,6	0.23	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
5	HEC	A	401	1	-	0/6/54/54	0/0/8/8
5	HEC	A	402	1	-	0/6/54/54	0/0/8/8

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	HEC	A	403	1	-	0/6/54/54	0/0/8/8
5	HEC	A	404	1	-	0/6/54/54	0/0/8/8
6	DGA	A	405	-	-	0/37/37/45	0/0/0/0
7	BCL	B	301	-	-	0/36/136/137	0/0/9/9
7	BCL	B	302	-	-	0/37/137/137	0/0/9/9
7	BCL	B	303	-	-	0/37/137/137	0/0/9/9
8	BPB	B	304	-	-	0/46/105/105	0/1/6/6
9	MPG	B	305	-	-	0/25/25/25	0/0/0/0
9	MPG	B	306	-	-	0/25/25/25	0/0/0/0
7	BCL	C	401	-	-	0/37/137/137	0/0/9/9
8	BPB	C	402	-	-	0/42/101/105	0/1/6/6
11	MQ7	C	403	-	-	0/41/61/61	0/2/2/2
12	NS5	C	404	-	-	0/43/43/43	0/0/0/0
13	OTP	C	405	-	-	0/45/45/55	0/0/0/0
9	MPG	C	406	-	-	0/14/14/25	0/0/0/0
14	PO4	C	407	-	-	0/0/0/0	0/0/0/0
14	PO4	C	408	-	-	0/0/0/0	0/0/0/0

The worst 5 of 68 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	404	HEC	C3B-C2B	-5.76	1.34	1.40
5	A	401	HEC	C3B-C2B	-5.54	1.35	1.40
5	A	404	HEC	C3C-C2C	-5.50	1.35	1.40
5	A	401	HEC	C3C-C2C	-5.44	1.35	1.40
5	A	402	HEC	C3B-C2B	-5.38	1.35	1.40

The worst 5 of 123 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	405	DGA	OG2-CG2-CG3	-12.78	79.06	107.89
6	A	405	DGA	OG2-CG2-CG1	-10.09	83.03	105.90
12	C	404	NS5	C29-C30-C31	-8.71	117.00	127.69
12	C	404	NS5	C18-C17-C15	-6.22	118.18	127.22
8	B	304	BPB	C2C-C3C-C4C	-6.16	101.66	107.24

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

15 monomers are involved in 39 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	401	HEC	3	0
5	A	402	HEC	3	0
5	A	403	HEC	5	0
5	A	404	HEC	4	0
6	A	405	DGA	3	0
7	B	301	BCL	3	0
7	B	302	BCL	4	0
7	B	303	BCL	2	0
8	B	304	BPB	1	0
9	B	305	MPG	1	0
7	C	401	BCL	4	0
8	C	402	BPB	2	0
11	C	403	MQ7	1	0
12	C	404	NS5	6	0
13	C	405	OTP	1	0

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, 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	A	332/356 (93%)	-0.45	0 100 100	19, 37, 59, 79	0
2	B	273/274 (99%)	-0.37	0 100 100	24, 50, 84, 107	0
3	C	323/324 (99%)	-0.31	1 (0%) 94 91	23, 54, 82, 106	0
4	D	242/258 (93%)	0.18	10 (4%) 41 32	48, 90, 110, 142	0
All	All	1170/1212 (96%)	-0.26	11 (0%) 85 78	19, 52, 98, 142	0

The worst 5 of 11 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	24	GLY	3.2
4	D	206	ASP	2.8
4	D	141	THR	2.5
4	D	7	ALA	2.5
4	D	9	HIS	2.4

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
4	FME	D	1	10/11	0.92	0.44	-	45,61,73,80	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
9	MPG	B	306	25/25	0.74	0.42	3.74	54,74,89,101	0
9	MPG	B	305	25/25	0.76	0.34	2.88	54,81,92,93	6
6	DGA	A	405	37/44	0.74	0.38	2.43	43,71,89,91	0
12	NS5	C	404	40/40	0.84	0.33	1.91	31,61,90,94	0
7	BCL	B	302	66/66	0.95	0.20	1.91	25,36,45,56	0
13	OTP	C	405	41/49	0.87	0.30	1.88	37,59,79,90	0
14	PO4	C	407	5/5	0.88	0.46	1.55	90,90,98,107	0
5	HEC	A	403	43/43	0.97	0.20	1.44	17,26,32,35	0
9	MPG	C	406	17/25	0.70	0.57	1.39	61,79,106,107	0
11	MQ7	C	403	48/48	0.91	0.29	1.33	27,53,66,69	0
8	BPB	B	304	65/65	0.94	0.21	1.26	28,43,51,57	0
7	BCL	C	401	66/66	0.96	0.20	0.87	30,38,49,57	0
8	BPB	C	402	61/65	0.92	0.26	0.58	43,57,71,72	0
5	HEC	A	401	43/43	0.95	0.29	0.53	35,45,55,56	0
7	BCL	B	303	66/66	0.96	0.19	0.49	25,33,44,51	0
5	HEC	A	402	43/43	0.97	0.22	0.25	14,31,37,49	0
5	HEC	A	404	43/43	0.96	0.18	0.01	24,36,46,48	0
7	BCL	B	301	65/66	0.96	0.18	-0.10	30,45,152,159	14
10	FE2	B	307	1/1	0.94	0.12	-2.51	54,54,54,54	0
14	PO4	C	408	5/5	0.93	0.19	-	79,82,84,88	0

6.5 Other polymers (i)

There are no such residues in this entry.