WORLDWIDE PDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 02:45 PM GMT

PDB ID : 4AC5
Title : Lipidic sponge phase crystal structure of the Bl. viridis reaction centre solved using serial femtosecond crystallography
Authors : Johansson, L.C.; Arnlund, D.; White, T.A.; Katona, G.; Deponte, D.P.; Weierstall, U.; Doak, R.B.; Shoeman, R.L.; Lomb, L.; Malmerberg, E.; Davidsson, J.; Nass, K.; Liang, M.; Andreasson, J.; Aquila, A.; Bajt, S.; Barthelmess, M.; Barty, A.; Bogan, M.J.; Bostedt, C.; Bozek, J.D.; Caleman, C.; Coffee, R.; Coppola, N.; Ekeberg, T.; Epp, S.W.; Erk, B.; Fleckenstein, H.; Foucar, L.; Graafsma, H.; Gumprecht, L.; Hajdu, J.; Hampton, C.Y.; Hartmann, R.; Hartmann, A.; Hauser, G.; Hirsemann, H.; Holl, P.; Hunter, M.S.; Kassemeyer, S.; Kimmel, N.; Kirian, R.A.; Maia, F.R.N.C.; Marchesini, S.; Martin, A.V.; Reich, C.; Rolles, D.; Rudek, B.; Rudenko, A.; Schlichting, I.; Schulz, J.; Seibert, M.M.; Sierra, R.; Soltau, H.; Starodub, D.; Stellato, F.; Stern, S.; Struder, L.; Timneanu, N.; Ullrich, J.; Wahlgren, W.Y.; Wang, X.; Weidenspointner, G.; Wunderer, C.; Fromme, P.; Chapman, H.N.; Spence, J.C.H.; Neutze, R.
Deposited on : 2011-12-14
Resolution : 8.20 Å(reported)

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

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 8.20 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.
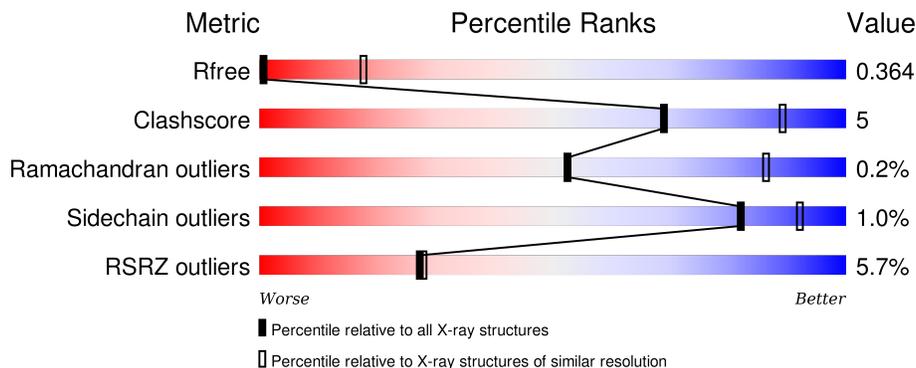
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1015 (11.50-3.66)
Clashscore	102246	1064 (11.50-3.70)
Ramachandran outliers	100387	1036 (11.50-3.66)
Sidechain outliers	100360	1006 (11.50-3.66)
RSRZ outliers	91569	1014 (11.50-3.66)

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	7% ... 84% ... 15% ...

Continued on next page...

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Mol	Chain	Length	Quality of chain
2	H	258	5% � 88% 6% 6%
3	L	274	5% � 89% 10%
4	M	324	6% ▀ ▀bar 89% 10%

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	NS5	M	1329	-	-	-	X
5	HEM	C	1334	-	-	-	X
6	BCB	L	1274	-	-	-	X
6	BCB	L	1275	-	-	-	X
6	BCB	M	1324	-	-	-	X
6	BCB	M	1325	-	-	-	X
7	BPB	L	1276	-	-	-	X
7	BPB	M	1326	-	-	-	X
9	MQ7	M	1328	-	-	-	X

2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 9835 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
			Total	C	N	O	S			
1	C	332	2590	1632	464	476	18	0	0	0

- Molecule 2 is a protein called REACTION CENTER PROTEIN H CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	H	243	1886	1209	326	349	2	0	0	0

- Molecule 3 is a protein called REACTION CENTER PROTEIN L CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	L	273	2161	1452	350	352	7	0	0	0

- Molecule 4 is a protein called REACTION CENTER PROTEIN M CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	M	323	2548	1697	417	423	11	0	0	0

- Molecule 5 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).
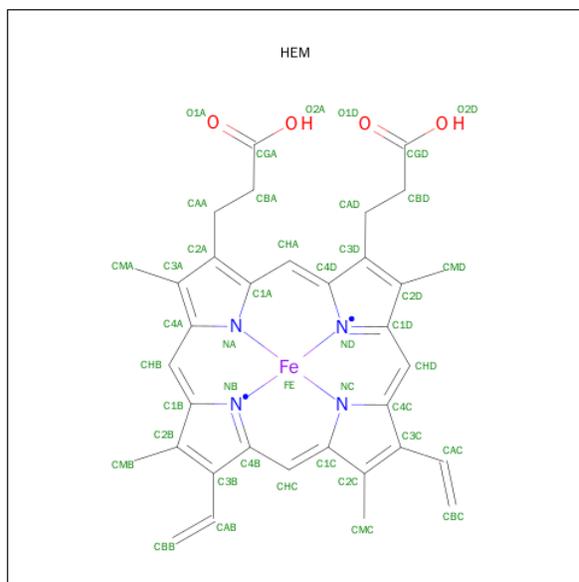
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
5	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
5	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
5	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 6 is BACTERIOCHLOROPHYLL B (three-letter code: BCB) (formula: $C_{55}H_{72}MgN_4O_6$).
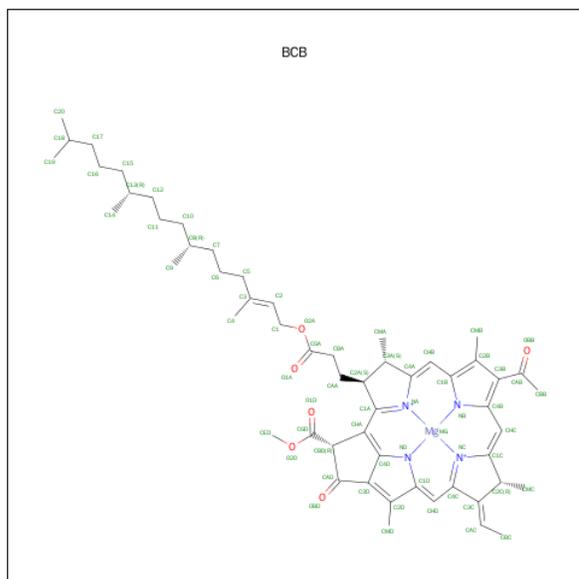
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
6	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
6	M	1	Total	C	Mg	N	O	0	0
			65	54	1	4	6		
6	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

- Molecule 7 is BACTERIOPHEOPHYTIN B (three-letter code: BPB) (formula: $C_{55}H_{74}N_4O_6$).
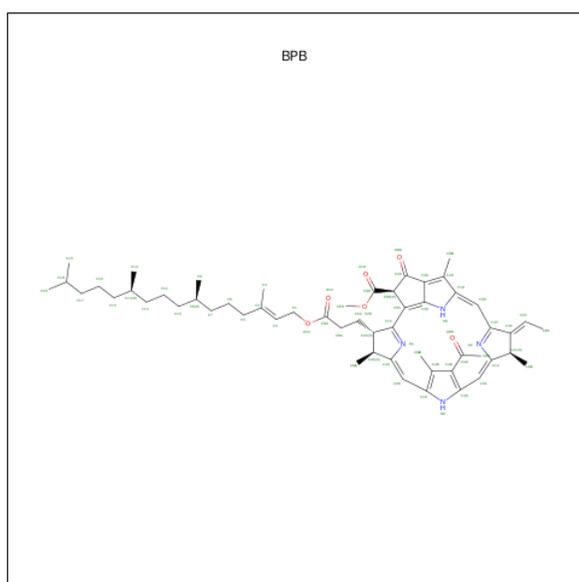
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	L	1	Total	C	N	O	0	0
			65	55	4	6		
7	M	1	Total	C	N	O	0	0
			61	51	4	6		

- Molecule 8 is FE (II) ION (three-letter code: FE2) (formula: Fe).

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

- Molecule 9 is MENAQUINONE-7 (three-letter code: MQ7) (formula: $C_{46}H_{64}O_2$).
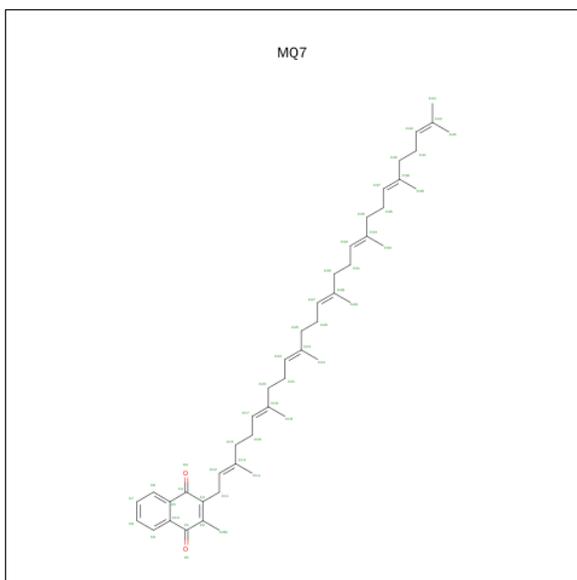
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	M	1	Total	C	O	0	0
			48	46	2		

- Molecule 10 is 15-CIS-1,2-DIHYDRONEUROSPORENE (three-letter code: NS5) (formula: $C_{40}H_{60}$).
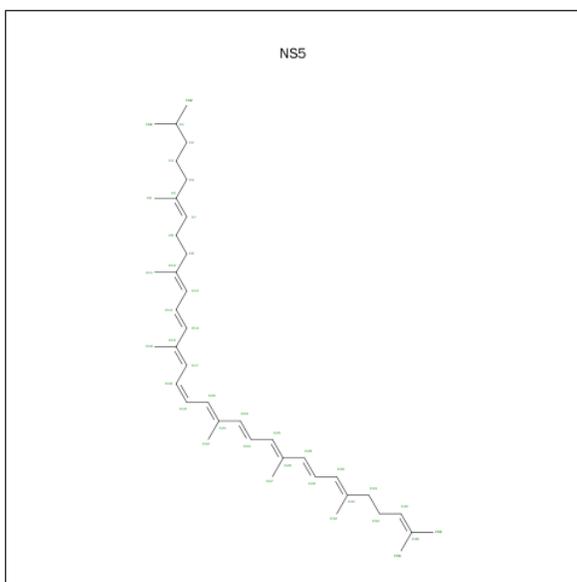
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	M	1	Total	C	0	0
			40	40		

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
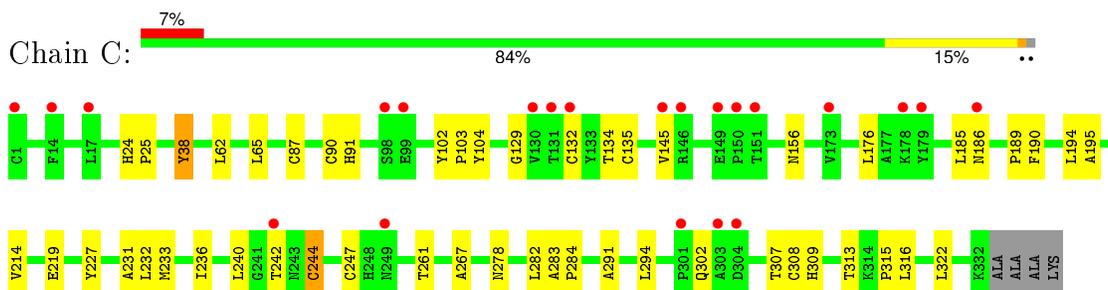
Chain C:

• Molecule 2: REACTION CENTER PROTEIN H CHAIN
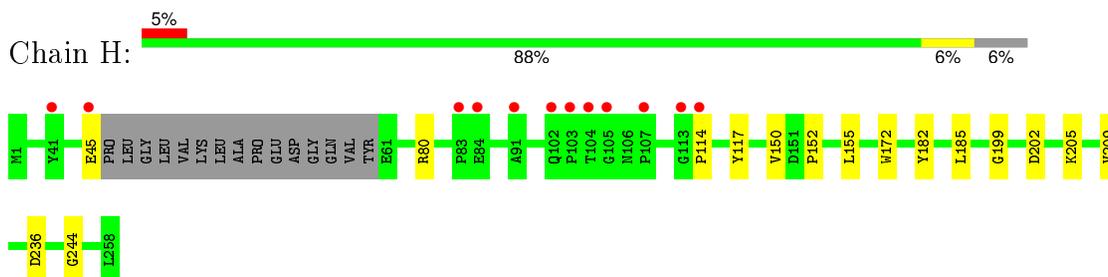
Chain H:

• Molecule 3: REACTION CENTER PROTEIN L CHAIN
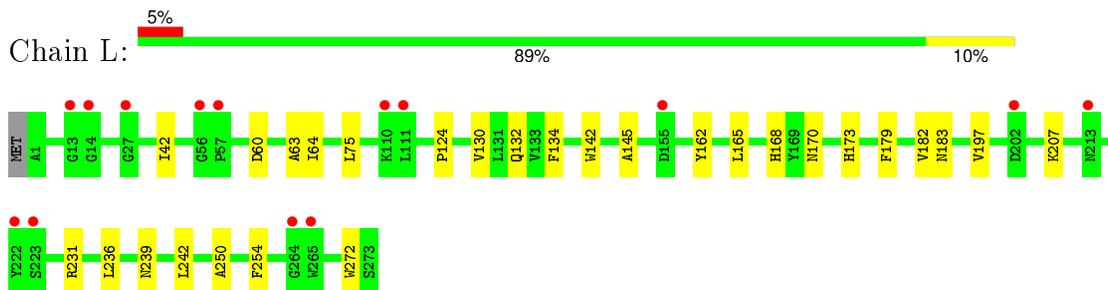
Chain L:

• Molecule 4: REACTION CENTER PROTEIN M CHAIN

Chain M:
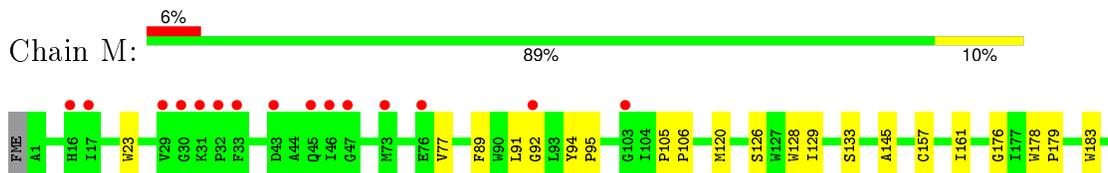
4 Data and refinement statistics (i)

| Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	57.50Å 84.60Å 375.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.10 – 8.20 56.84 – 8.20	Depositor EDS
% Data completeness (in resolution range)	96.9 (46.10-8.20) 97.3 (56.84-8.20)	Depositor EDS
R_{merge}	0.50	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	1.80 (at 8.36Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.351 , 0.384 0.341 , 0.364	Depositor DCC
R_{free} test set	94 reflections (4.97%)	DCC
Wilson B-factor (Å^2)	-2.7	Xtriage
Anisotropy	-13.102	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 214.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$<|L|> = 0.40, <L^2> = 0.23$	Xtriage
Outliers	0 of 1992 reflections	Xtriage
F_o,F_c correlation	0.67	EDS
Total number of atoms	9835	wwPDB-VP
Average B, all atoms (Å^2)	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.09% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: BPB, BCB, FE2, MQ7, HEM, 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	0.31	0/2657	0.46	0/3624
2	H	0.32	0/1919	0.46	0/2621
3	L	0.34	0/2248	0.42	0/3069
4	M	0.33	0/2652	0.40	0/3630
All	All	0.33	0/9476	0.44	0/12944

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 (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	C	2590	0	2561	34	0
2	H	1886	0	1880	8	0
3	L	2161	0	2089	16	0
4	M	2548	0	2432	22	0
5	C	172	0	120	10	0
6	L	132	0	144	12	0
6	M	131	0	140	5	0
7	L	65	0	74	4	0
7	M	61	0	63	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	M	1	0	0	0	0
9	M	48	0	64	0	0
10	M	40	0	60	3	0
All	All	9835	0	9627	90	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 5.

The worst 5 of 90 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)
6:M:1325:BCB:HAA1	6:M:1325:BCB:HBD	1.62	0.80
1:C:247:CYS:SG	5:C:1335:HEM:HAC	2.24	0.78
1:C:308:CYS:SG	5:C:1336:HEM:HAC	2.25	0.76
7:L:1276:BPB:HHC	7:L:1276:BPB:HBBB	1.69	0.73
3:L:239:ASN:HA	3:L:242:LEU:HB2	1.76	0.66

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%)	311 (94%)	19 (6%)	0	100	100
2	H	239/258 (93%)	229 (96%)	10 (4%)	0	100	100
3	L	271/274 (99%)	253 (93%)	17 (6%)	1 (0%)	39	80
4	M	321/324 (99%)	309 (96%)	11 (3%)	1 (0%)	46	83
All	All	1161/1192 (97%)	1102 (95%)	57 (5%)	2 (0%)	52	86

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	L	165	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	278/282 (99%)	274 (99%)	4 (1%)	74	89
2	H	194/212 (92%)	192 (99%)	2 (1%)	82	92
3	L	216/219 (99%)	215 (100%)	1 (0%)	92	96
4	M	247/249 (99%)	245 (99%)	2 (1%)	86	94
All	All	935/962 (97%)	926 (99%)	9 (1%)	82	92

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

Mol	Chain	Res	Type
2	H	45	GLU
4	M	214	PHE
3	L	272	TRP
1	C	244	CYS
2	H	185	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	278	ASN
4	M	72	ASN

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	0.65	0	6,9,11	3.95	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	-8.28	110.09	122.82
2	H	1	FME	O1-CN-N	-3.40	119.86	124.76
2	H	1	FME	CE-SD-CG	3.03	110.70	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 13 ligands modelled in this entry, 1 is monoatomic - leaving 12 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	HEM	C	1333	1	30,50,50	2.15	10 (33%)	24,82,82	2.31	10 (41%)
5	HEM	C	1334	1	30,50,50	2.17	7 (23%)	24,82,82	2.29	9 (37%)
5	HEM	C	1335	1	30,50,50	2.20	7 (23%)	24,82,82	2.28	8 (33%)
5	HEM	C	1336	1	30,50,50	2.21	8 (26%)	24,82,82	2.24	9 (37%)
6	BCB	L	1274	3	56,74,74	2.55	13 (23%)	57,115,115	2.16	16 (28%)
6	BCB	L	1275	-	56,74,74	2.53	13 (23%)	57,115,115	2.15	16 (28%)
7	BPB	L	1276	-	63,70,70	2.92	16 (25%)	63,101,101	2.32	16 (25%)
6	BCB	M	1324	-	55,73,74	2.54	13 (23%)	55,113,115	2.14	17 (30%)
6	BCB	M	1325	4	56,74,74	2.55	13 (23%)	57,115,115	2.21	17 (29%)
7	BPB	M	1326	-	59,66,70	3.01	16 (27%)	58,96,101	2.44	18 (31%)
9	MQ7	M	1328	-	49,49,49	1.36	2 (4%)	62,63,63	1.24	7 (11%)
10	NS5	M	1329	-	39,39,39	2.03	5 (12%)	44,46,46	2.41	14 (31%)

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	HEM	C	1333	1	-	0/10/54/54	0/0/8/8
5	HEM	C	1334	1	-	0/10/54/54	0/0/8/8
5	HEM	C	1335	1	-	0/10/54/54	0/0/8/8
5	HEM	C	1336	1	-	0/10/54/54	0/0/8/8
6	BCB	L	1274	3	-	1/37/137/137	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	BCB	L	1275	-	-	1/37/137/137	0/0/9/9
7	BPB	L	1276	-	-	1/46/105/105	0/1/6/6
6	BCB	M	1324	-	-	1/36/136/137	0/0/9/9
6	BCB	M	1325	4	-	1/37/137/137	0/0/9/9
7	BPB	M	1326	-	-	0/42/101/105	0/1/6/6
9	MQ7	M	1328	-	-	0/41/61/61	0/2/2/2
10	NS5	M	1329	-	-	0/43/43/43	0/0/0/0

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	1335	HEM	C3B-C4B	-7.20	1.45	1.51
5	C	1336	HEM	C3B-C4B	-7.16	1.45	1.51
5	C	1334	HEM	C3B-C4B	-7.10	1.45	1.51
5	C	1333	HEM	C3B-C4B	-6.70	1.45	1.51
10	M	1329	NS5	C9-C8	-5.73	1.34	1.53

The worst 5 of 157 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	M	1326	BPB	CBC-CAC-C3C	-7.53	109.69	127.07
7	M	1326	BPB	C4D-C3D-C2D	-6.73	99.12	106.74
7	L	1276	BPB	C4D-C3D-C2D	-6.68	99.18	106.74
7	L	1276	BPB	CBC-CAC-C3C	-6.68	111.67	127.07
7	L	1276	BPB	C2C-C3C-C4C	-6.08	101.68	107.24

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	L	1276	BPB	CBC-CAC-C3C-C4C
6	L	1274	BCB	CBC-CAC-C3C-C4C
6	L	1275	BCB	CBC-CAC-C3C-C4C
6	M	1325	BCB	CBC-CAC-C3C-C2C
6	M	1324	BCB	CBC-CAC-C3C-C2C

There are no ring outliers.

10 monomers are involved in 34 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	1333	HEM	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	1334	HEM	2	0
5	C	1335	HEM	5	0
5	C	1336	HEM	2	0
6	L	1274	BCB	6	0
6	L	1275	BCB	7	0
7	L	1276	BPB	4	0
6	M	1325	BCB	5	0
7	M	1326	BPB	1	0
10	M	1329	NS5	3	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 (i)

6.1 Protein, DNA and RNA chains (i)

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%)	0.38	22 (6%)	22	23	12, 15, 19, 21	0
2	H	242/258 (93%)	0.25	12 (4%)	32	32	12, 16, 25, 26	0
3	L	273/274 (99%)	0.23	14 (5%)	32	32	10, 15, 21, 22	0
4	M	323/324 (99%)	0.25	19 (5%)	26	26	11, 15, 20, 20	0
All	All	1170/1192 (98%)	0.28	67 (5%)	27	28	10, 15, 21, 26	0

The worst 5 of 67 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	131	THR	5.2
1	C	186	ASN	4.7
2	H	84	GLU	4.6
2	H	83	PRO	4.5
3	L	223	SER	4.5

6.2 Non-standard residues in protein, DNA, RNA chains (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, 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	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	FME	H	1	10/11	0.71	0.38	-	18,18,18,18	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, 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	RSCC	RSR	LLDF	B-factors($Å^2$)	Q<0.9
6	BCB	L	1275	66/66	0.81	0.47	2.39	19,20,21,21	0
7	BPB	L	1276	65/65	0.90	0.46	1.99	2,2,4,4	0
9	MQ7	M	1328	48/48	0.86	0.58	1.90	9,9,10,10	0
10	NS5	M	1329	40/40	0.59	0.65	1.70	27,28,30,30	0
6	BCB	L	1274	66/66	0.90	0.42	1.63	29,29,30,30	0
7	BPB	M	1326	61/65	0.82	0.53	1.22	26,26,27,27	0
6	BCB	M	1325	66/66	0.87	0.45	1.02	12,12,15,15	0
5	HEM	C	1334	43/43	0.92	0.67	0.79	2,2,2,2	0
6	BCB	M	1324	65/66	0.76	0.45	0.68	16,16,16,17	0
8	FE2	M	1327	1/1	0.90	0.33	0.39	2,2,2,2	0
5	HEM	C	1336	43/43	0.91	0.38	0.11	2,2,2,2	0
5	HEM	C	1333	43/43	0.89	0.37	0.03	15,16,16,16	0
5	HEM	C	1335	43/43	0.93	0.33	-0.21	4,4,4,4	0

6.5 Other polymers (i)

There are no such residues in this entry.