



# wwPDB X-ray Structure Validation Summary Report

Feb 28, 2014 – 11:39 PM GMT

PDB ID : 1R2C  
Title : PHOTOSYNTHETIC REACTION CENTER BLASTOCHLORIS VIRIDIS (ATCC)  
Authors : Baxter, R.H.; Ponomarenko, N.; Pahl, R.; Srajer, V.; Moffat, K.; Norris, J.R.  
Deposited on : 2003-09-26  
Resolution : 2.86 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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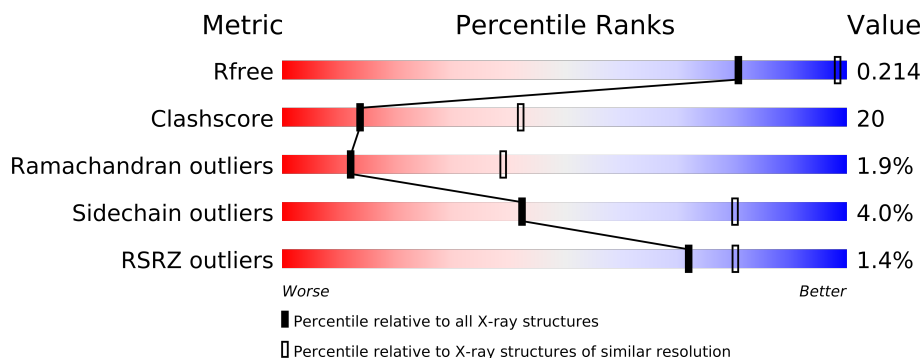
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 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 2.86 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	1524 (2.90-2.82)
Clashscore	79885	1879 (2.90-2.82)
Ramachandran outliers	78287	1824 (2.90-2.82)
Sidechain outliers	78261	1827 (2.90-2.82)
RSRZ outliers	66119	1526 (2.90-2.82)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	L	273	
3	M	323	
4	H	258	

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

Mol	Type	Chain	Res	Geometry	Electron density
10	MQ7	M	501	-	X
11	UQ2	L	502	-	X
12	NS5	M	600	-	X
13	LDA	H	703	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
13	LDA	M	702	-	X
13	LDA	M	704	-	X
13	LDA	M	706	-	X
9	BPB	M	401	-	X

## 2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 10140 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 precursor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	332	Total	C	N	O	S	41	0	0
			2602	1640	466	478	18			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	273	Total	C	N	O	S	10	0	0
			2171	1459	350	355	7			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	M	323	Total	C	N	O	S	15	0	0
			2555	1702	419	423	11			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	258	Total	C	N	O	S	98	0	0
			2018	1292	344	380	2			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	1	FME	MET	MODIFIED RESIDUE	UNP P06008

- Molecule 5 is FE (II) ION (three-letter code: FE2) (formula: Fe).

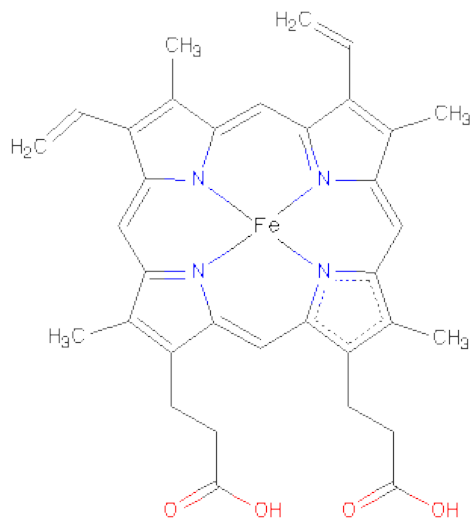
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	M	1	Total	Fe	0	0
			1	1		

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



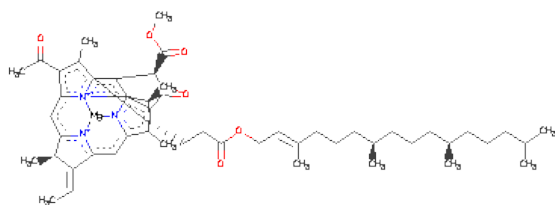
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	H	1	Total	O	S	0	0
			5	4	1		
6	M	1	Total	O	S	0	0
			5	4	1		
6	M	1	Total	O	S	0	0
			5	4	1		
6	M	1	Total	O	S	0	0
			5	4	1		

- Molecule 7 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: C<sub>34</sub>H<sub>32</sub>FeN<sub>4</sub>O<sub>4</sub>).



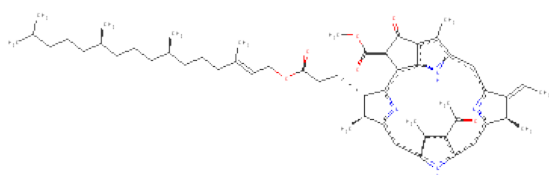
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
7	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
7	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
7	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 8 is BACTERIOCHLOROPHYLL B (three-letter code: BCB) (formula: C<sub>55</sub>H<sub>72</sub>MgN<sub>4</sub>O<sub>6</sub>).



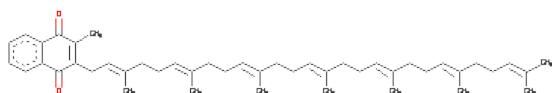
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	M	1	Total	C	Mg	N	O	15	0
			66	55	1	4	6		
8	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
8	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
8	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

- Molecule 9 is BACTERIOPHEOPHYTIN B (three-letter code: BPB) (formula:  $C_{55}H_{74}N_4O_6$ ).



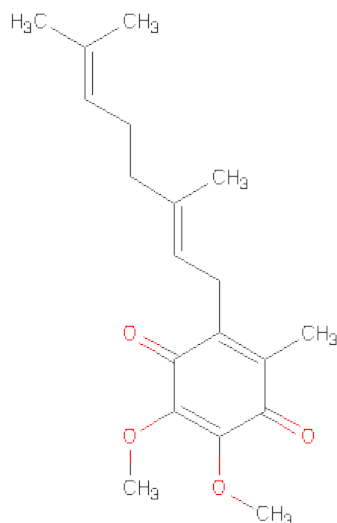
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	M	1	Total	C	N	O	0	0
			65	55	4	6		
9	L	1	Total	C	N	O	0	0
			65	55	4	6		

- Molecule 10 is MENAQUINONE-7 (three-letter code: MQ7) (formula:  $C_{46}H_{64}O_2$ ).



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

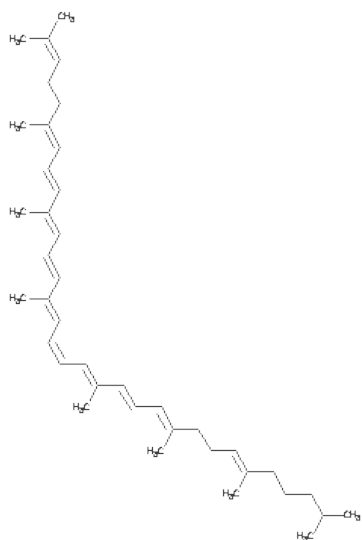
- Molecule 11 is UBIQUINONE-2 (three-letter code: UQ2) (formula:  $C_{19}H_{26}O_4$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	L	1	Total	C	O	0	0
			23	19	4		

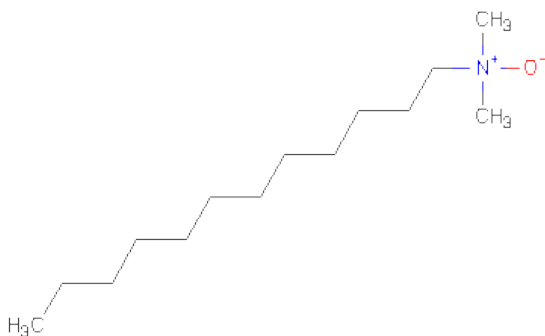
- Molecule 12 is 15-CIS-1,2-DIHYDRONEUROSPORENE (three-letter code: NS5) (formula:  $C_{40}H_{60}$ ).





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	M	1	Total	C		11	0
			40	40			

- Molecule 13 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula:  $C_{14}H_{31}NO$ ).



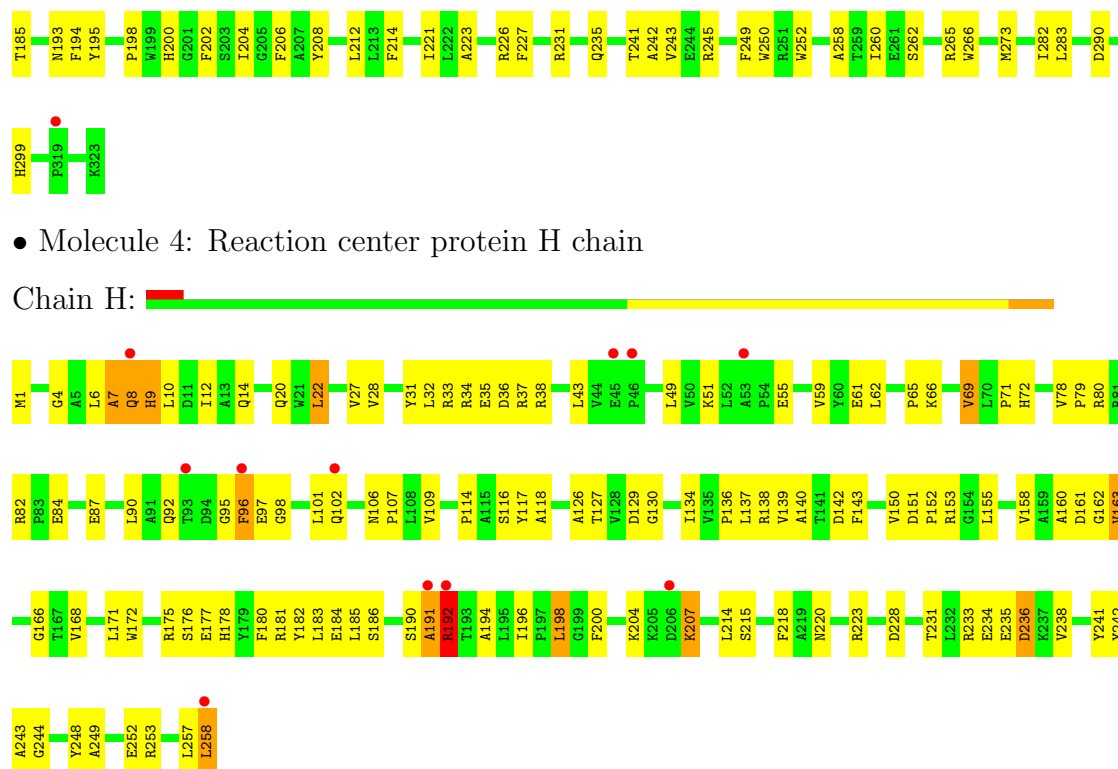
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
13	M	1	Total	C	N	O	0	0
			16	14	1	1		
13	M	1	Total	C	N	O	0	0
			16	14	1	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
13	H	1	Total	C	N	O	0	0
			16	14	1	1		
13	M	1	Total	C	N	O	3	0
			16	14	1	1		
13	L	1	Total	C	N	O	3	0
			16	14	1	1		
13	M	1	Total	C	N	O	0	0
			16	14	1	1		





• Molecule 4: Reaction center protein H chain

Chain H:

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	223.50Å 223.50Å 112.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.83 – 2.86 48.83 – 2.86	Depositor EDS
% Data completeness (in resolution range)	97.3 (48.83-2.86) 97.4 (48.83-2.86)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.90 (at 2.86Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.202 , 0.228 0.190 , 0.214	Depositor DCC
$R_{free}$ test set	6311 reflections (10.89%)	DCC
Wilson B-factor (Å <sup>2</sup> )	59.3	Xtriage
Anisotropy	0.312	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 32.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 64248 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	10140	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.10% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities 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, BCB, FE2, SO4, MQ7, HEM, FME, UQ2, 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	0.35	0/2669	0.62	1/3637 (0.0%)
2	L	0.41	0/2259	0.60	0/3084
3	M	0.42	0/2659	0.58	0/3637
4	H	0.35	0/2055	0.62	0/2807
All	All	0.38	0/9642	0.61	1/13165 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	249	ASN	N-CA-C	-6.50	93.44	111.00

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	2602	0	2579	74	0
2	L	2171	0	2098	90	0
3	M	2555	0	2452	112	0
4	H	2018	0	2020	113	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	M	1	0	0	0	0
6	H	5	0	0	0	0
6	M	15	0	0	0	0
7	C	172	0	120	7	0
8	L	132	0	144	22	0
8	M	132	0	143	29	0
9	L	65	0	74	12	0
9	M	65	0	74	22	0
10	M	48	0	64	0	0
11	L	23	0	26	4	0
12	M	40	0	60	5	0
13	H	16	0	31	4	0
13	L	16	0	31	2	0
13	M	64	0	124	11	0
All	All	10140	0	10040	393	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 20.

The worst 5 of 393 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:H:152:PRO:HA	4:H:155:LEU:HD12	1.31	1.05
9:M:401:BPB:H14	9:M:401:BPB:H17	1.39	1.03
3:M:32:PRO:HG3	3:M:48:PRO:HD3	1.39	1.02
8:L:302:BCB:HBA1	8:L:302:BCB:HBD	1.46	0.94
9:L:402:BPB:HBBA	3:M:208:TYR:HB3	1.47	0.94

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%)	299 (91%)	30 (9%)	1 (0%)	50 84

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	L	271/273 (99%)	251 (93%)	17 (6%)	3 (1%)	21	57
3	M	321/323 (99%)	299 (93%)	19 (6%)	3 (1%)	25	62
4	H	256/258 (99%)	216 (84%)	25 (10%)	15 (6%)	2	6
All	All	1178/1190 (99%)	1065 (90%)	91 (8%)	22 (2%)	12	39

5 of 22 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	L	57	PRO
4	H	7	ALA
4	H	8	GLN
4	H	9	HIS
4	H	96	PHE

### 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	281/282 (100%)	276 (98%)	5 (2%)	71	94
2	L	218/218 (100%)	209 (96%)	9 (4%)	41	79
3	M	249/249 (100%)	239 (96%)	10 (4%)	42	80
4	H	212/212 (100%)	198 (93%)	14 (7%)	24	55
All	All	960/961 (100%)	922 (96%)	38 (4%)	42	80

5 of 38 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	M	51	LEU
3	M	194	PHE
4	H	236	ASP
3	M	178	TRP
3	M	214	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:



Mol	Chain	Res	Type
2	L	239	ASN
3	M	16	HIS
4	H	72	HIS
2	L	213	ASN
4	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	$\# Z  > 2$
4	FME	H	1	4	9,9,10	5.82	2 (22%)	6,9,11	3.40	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
4	FME	H	1	4	-	0/7/9/11	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	1	FME	O-C	17.19	1.23	1.11
4	H	1	FME	CA-C	2.56	1.53	1.48

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	1	FME	CA-N-CN	-6.79	111.74	122.97
4	H	1	FME	O1-CN-N	-3.39	114.75	125.12
4	H	1	FME	CE-SD-CG	-3.00	89.07	100.27

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 24 ligands modelled in this entry, 1 is monoatomic - leaving 23 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	HEM	C	1201	1	49,50,50	2.08	11 (22%)	46,82,82	1.26	4 (8%)
7	HEM	C	1202	1	49,50,50	1.96	11 (22%)	46,82,82	1.35	3 (6%)
7	HEM	C	1203	1	49,50,50	1.97	12 (24%)	46,82,82	1.32	6 (13%)
7	HEM	C	1204	1	49,50,50	2.25	13 (26%)	46,82,82	1.53	8 (17%)
13	LDA	H	703	-	15,15,15	4.87	3 (20%)	17,17,17	1.50	1 (5%)
6	SO4	H	801	-	4,4,4	0.79	0	6,6,6	0.35	0
8	BCB	L	302	2	74,74,74	1.72	13 (17%)	94,115,115	2.09	25 (26%)
8	BCB	L	304	2	74,74,74	1.72	14 (18%)	94,115,115	1.90	17 (18%)
9	BPB	L	402	-	70,70,70	1.74	11 (15%)	93,101,101	2.45	23 (24%)
11	UQ2	L	502	-	23,23,23	1.73	5 (21%)	31,31,31	1.26	3 (9%)
13	LDA	L	705	-	15,15,15	4.14	2 (13%)	17,17,17	2.65	1 (5%)
8	BCB	M	1301	3	74,74,74	1.71	12 (16%)	94,115,115	1.70	15 (15%)
8	BCB	M	1303	3	74,74,74	1.77	14 (18%)	94,115,115	1.75	19 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
9	BPB	M	401	-	70,70,70	1.80	12 (17%)	93,101,101	2.12	24 (25%)
10	MQ7	M	501	-	49,49,49	1.73	13 (26%)	63,63,63	1.55	8 (12%)
12	NS5	M	600	-	39,39,39	0.78	0	46,46,46	1.04	4 (8%)
13	LDA	M	701	-	15,15,15	4.71	3 (20%)	17,17,17	1.53	1 (5%)
13	LDA	M	702	-	15,15,15	4.27	1 (6%)	17,17,17	1.99	1 (5%)
13	LDA	M	704	-	15,15,15	4.81	4 (26%)	17,17,17	1.68	1 (5%)
13	LDA	M	706	-	15,15,15	4.61	2 (13%)	17,17,17	1.23	1 (5%)
6	SO4	M	802	-	4,4,4	1.13	0	6,6,6	0.42	0
6	SO4	M	803	-	4,4,4	1.04	0	6,6,6	0.07	0
6	SO4	M	804	-	4,4,4	1.11	0	6,6,6	0.27	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	HEM	C	1201	1	-	0/14/114/114	0/0/8/8
7	HEM	C	1202	1	-	0/14/114/114	0/0/8/8
7	HEM	C	1203	1	-	0/14/114/114	0/0/8/8
7	HEM	C	1204	1	-	0/14/114/114	0/0/8/8
13	LDA	H	703	-	-	0/13/13/13	0/0/0/0
6	SO4	H	801	-	-	0/0/0/0	0/0/0/0
8	BCB	L	302	2	-	0/41/137/137	0/0/9/9
8	BCB	L	304	2	1/1/21/26	0/41/137/137	0/0/9/9
9	BPB	L	402	-	-	0/52/105/105	0/0/6/6
11	UQ2	L	502	-	-	0/15/39/39	0/1/1/1
13	LDA	L	705	-	-	0/13/13/13	0/0/0/0
8	BCB	M	1301	3	-	0/41/137/137	0/0/9/9
8	BCB	M	1303	3	1/1/21/26	0/41/137/137	0/0/9/9
9	BPB	M	401	-	1/1/18/23	0/52/105/105	0/0/6/6
10	MQ7	M	501	-	-	0/41/61/61	0/0/2/2
12	NS5	M	600	-	-	0/43/43/43	0/0/0/0
13	LDA	M	701	-	-	0/13/13/13	0/0/0/0
13	LDA	M	702	-	-	0/13/13/13	0/0/0/0
13	LDA	M	704	-	-	0/13/13/13	0/0/0/0
13	LDA	M	706	-	-	0/13/13/13	0/0/0/0
6	SO4	M	802	-	-	0/0/0/0	0/0/0/0
6	SO4	M	803	-	-	0/0/0/0	0/0/0/0
6	SO4	M	804	-	-	0/0/0/0	0/0/0/0

The worst 5 of 156 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	H	703	LDA	O1-N1	-18.37	1.22	1.39
13	M	704	LDA	O1-N1	-18.07	1.22	1.39
13	M	701	LDA	O1-N1	-17.72	1.22	1.39
13	M	706	LDA	O1-N1	-17.48	1.22	1.39
13	M	702	LDA	O1-N1	-16.30	1.24	1.39

The worst 5 of 165 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	L	705	LDA	C2-C1-N1	10.58	132.03	113.80
9	L	402	BPB	C1-C2-C3	10.48	144.81	126.19
9	M	401	BPB	C1-C2-C3	9.55	143.17	126.19
9	L	402	BPB	C5-C3-C2	8.43	137.31	121.08
13	M	702	LDA	C2-C1-N1	7.87	127.37	113.80

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
9	M	401	BPB	C13
8	M	1303	BCB	C13
8	L	304	BCB	C8

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, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	C	332/336 (98%)	-0.35	4 (1%) 75 83	23, 45, 67, 78	15 (4%)
2	L	273/273 (100%)	-0.51	1 (0%) 90 94	25, 43, 65, 76	6 (2%)
3	M	323/323 (100%)	-0.54	1 (0%) 91 95	25, 42, 68, 77	8 (2%)
4	H	252/258 (97%)	-0.07	11 (4%) 33 39	30, 56, 84, 93	19 (7%)
All	All	1180/1190 (99%)	-0.38	17 (1%) 72 80	23, 46, 71, 93	48 (4%)

The worst 5 of 17 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	H	8	GLN	4.6
4	H	46	PRO	4.2
4	H	258	LEU	4.1
4	H	191	ALA	3.6
4	H	93	THR	3.0

### 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<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	FME	H	1	10/11	0.27	2.37	53,55,63,65	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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
13	LDA	M	704	16/16	0.43	8.37	79,82,83,84	3
13	LDA	M	702	16/16	0.47	7.82	73,87,100,101	0
13	LDA	M	706	16/16	0.50	5.74	99,105,114,114	0
11	UQ2	L	502	23/23	0.24	4.89	48,49,50,50	23
13	LDA	H	703	16/16	0.37	3.56	74,79,85,85	0
12	NS5	M	600	40/40	0.22	3.56	39,58,67,68	11
9	BPB	M	401	65/65	0.22	2.88	37,45,94,95	0
10	MQ7	M	501	48/48	0.20	2.31	36,45,67,70	0
9	BPB	L	402	65/65	0.18	1.79	31,41,45,47	0
13	LDA	L	705	16/16	0.31	1.60	71,78,94,95	3
8	BCB	L	304	66/66	0.17	0.39	23,29,54,57	0
7	HEM	C	1203	43/43	0.15	0.34	26,33,41,44	0
8	BCB	M	1303	66/66	0.17	0.33	17,25,46,48	0
8	BCB	L	302	66/66	0.16	0.13	10,20,42,43	0
8	BCB	M	1301	66/66	0.17	0.07	33,43,59,63	15
13	LDA	M	701	16/16	0.17	0.07	48,50,52,52	0
6	SO4	M	803	5/5	0.13	-0.08	102,102,103,103	0
7	HEM	C	1204	43/43	0.13	-0.23	32,36,48,53	0
7	HEM	C	1201	43/43	0.13	-0.49	47,51,61,65	0
7	HEM	C	1202	43/43	0.13	-0.55	39,43,55,58	0
6	SO4	M	804	5/5	0.11	-0.72	81,82,82,83	0
6	SO4	H	801	5/5	0.12	-0.86	73,76,76,77	0
6	SO4	M	802	5/5	0.10	-1.69	57,59,61,61	0
5	FE2	M	500	1/1	0.05	-3.28	33,33,33,33	0

### 6.5 Other polymers ⓘ

There are no such residues in this entry.