



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 11:56 PM GMT

PDB ID : 5PRC  
Title : PHOTOSYNTHETIC REACTION CENTER FROM RHODOPSEUDOMONAS VIRIDIS (ATRAZINE COMPLEX)  
Authors : Lancaster, C.R.D.; Michel, H.  
Deposited on : 1997-08-01  
Resolution : 2.35 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

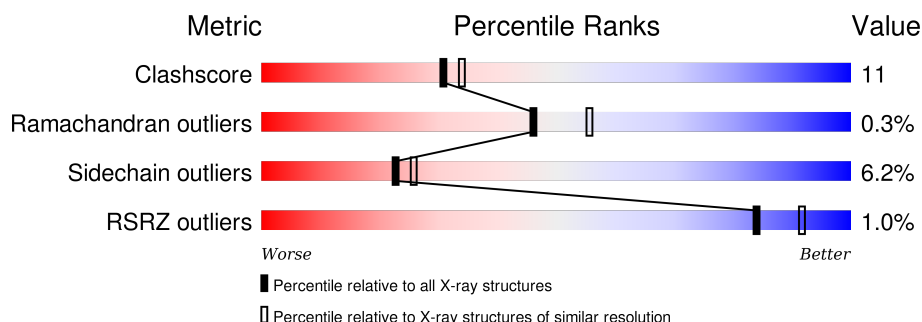
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.35 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))
Clashscore	102246	1456 (2.38-2.34)
Ramachandran outliers	100387	1435 (2.38-2.34)
Sidechain outliers	100360	1436 (2.38-2.34)
RSRZ outliers	91569	1358 (2.38-2.34)

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. 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  $\leq 5\%$ . 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	<div> <div>2%</div> <div>78%</div> <div>18%</div> <div>••</div> </div>
2	L	273	<div> <div>82%</div> <div>16%</div> <div>•</div> </div>
3	M	323	<div> <div>72%</div> <div>24%</div> <div>•</div> </div>
4	H	258	<div> <div>2%</div> <div>74%</div> <div>24%</div> <div>•</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
11	NS5	M	600	-	-	-	X
13	LDA	H	703	-	-	-	X
13	LDA	L	702	-	-	-	X
13	LDA	M	704	-	-	-	X
13	LDA	M	706	-	-	-	X
8	BPB	L	402	X	-	-	-

## 2 Entry composition [i](#)

There are 14 unique types of molecules in this entry. The entry contains 10501 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	332	Total	C	N	O	S	50	1	0
			2607	1642	467	480	18			

- Molecule 2 is a protein called PHOTOSYNTHETIC REACTION CENTER.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	273	Total	C	N	O	S	15	0	0
			2171	1459	350	355	7			

- Molecule 3 is a protein called PHOTOSYNTHETIC REACTION CENTER.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	M	323	Total	C	N	O	S	19	2	0
			2577	1720	421	425	11			

- Molecule 4 is a protein called PHOTOSYNTHETIC REACTION CENTER.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	258	Total	C	N	O	S	122	0	0
			2018	1292	344	380	2			

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

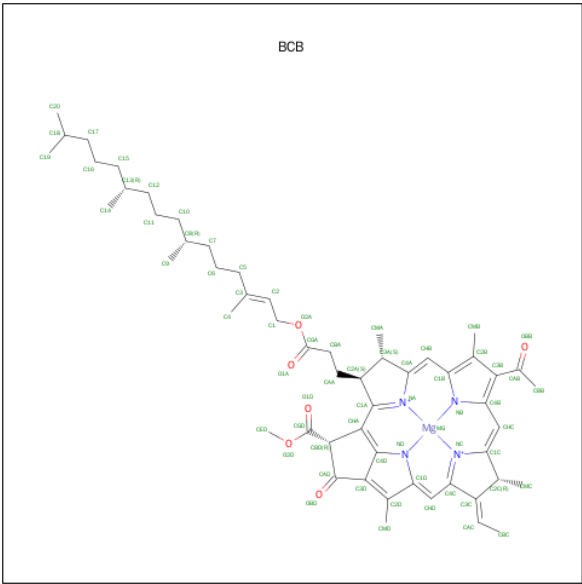
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	M	1	Total	Fe	0	0
			1	1		

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



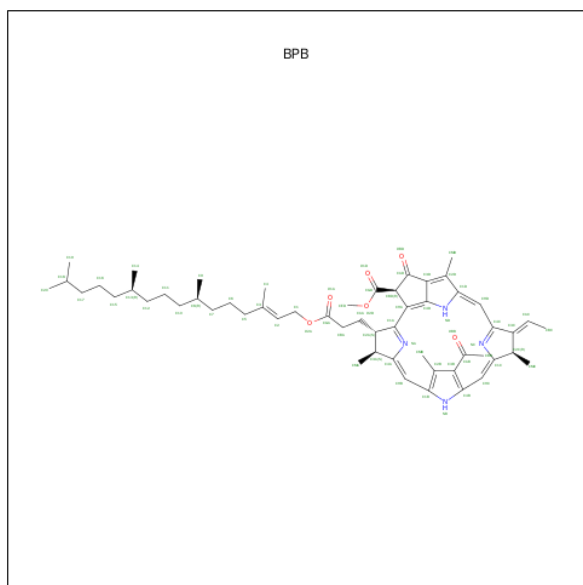
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	H	1	Total	O	S	0	0
			5	4	1		
6	M	1	Total	O	S	0	0
			5	4	1		
6	M	1	Total	O	S	0	0
			5	4	1		
6	M	1	Total	O	S	0	0
			5	4	1		

- Molecule 7 is BACTERIOCHLOROPHYLL B (three-letter code: BCB) (formula: C<sub>55</sub>H<sub>72</sub>MgN<sub>4</sub>O<sub>6</sub>).



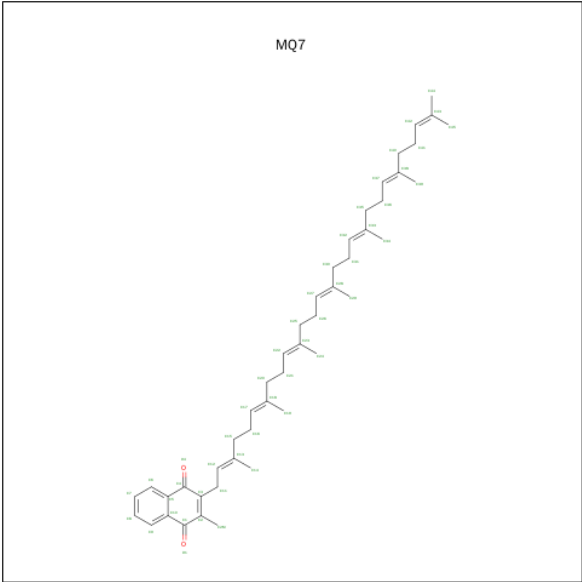
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	M	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
7	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
7	M	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
7	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0

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



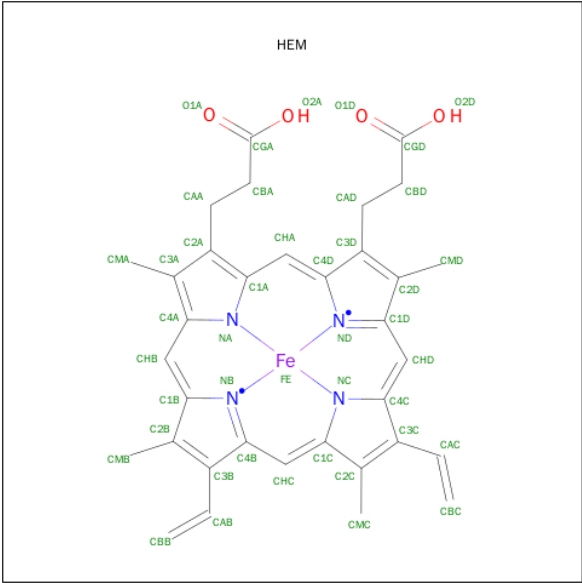
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	M	1	Total	C	N	O	7	0
			65	55	4	6		
8	L	1	Total	C	N	O	0	0
			65	55	4	6		

- 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 PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).



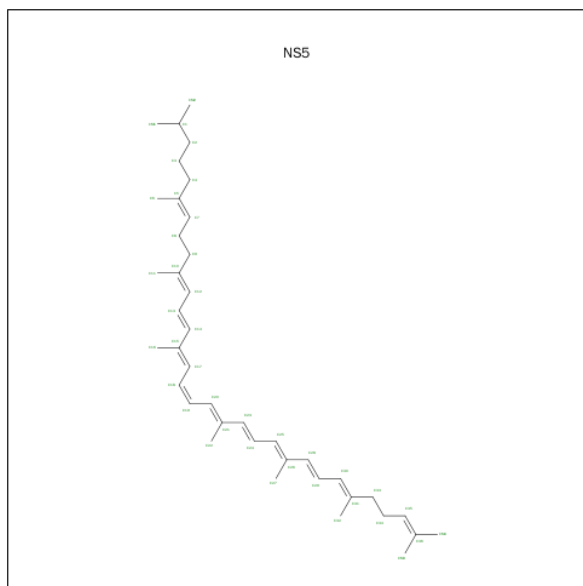
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
10	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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

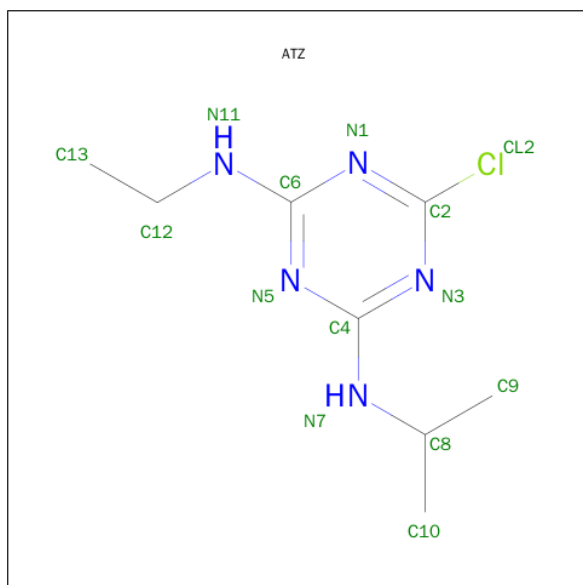
- Molecule 11 is 15-CIS-1,2-DIHYDRONEUROSPORENE (three-letter code: NS5) (formula: C<sub>40</sub>H<sub>60</sub>).



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

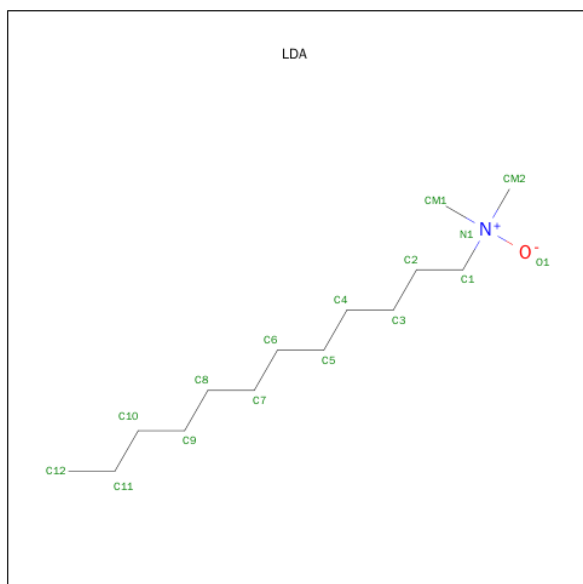
- Molecule 12 is 2-CHLORO-4-ISOPROPYLAMINO-6-ETHYLAMINO -1,3,5-TRIAZINE (three-letter code: ATZ) (formula: C<sub>8</sub>H<sub>14</sub>ClN<sub>5</sub>).





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
12	L	1	Total	C	Cl	N	0	0
			14	8	1	5		

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
13	H	1	Total	C	N	O	0	0
			16	14	1	1		
13	L	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	0	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	4	0
			16	14	1	1		

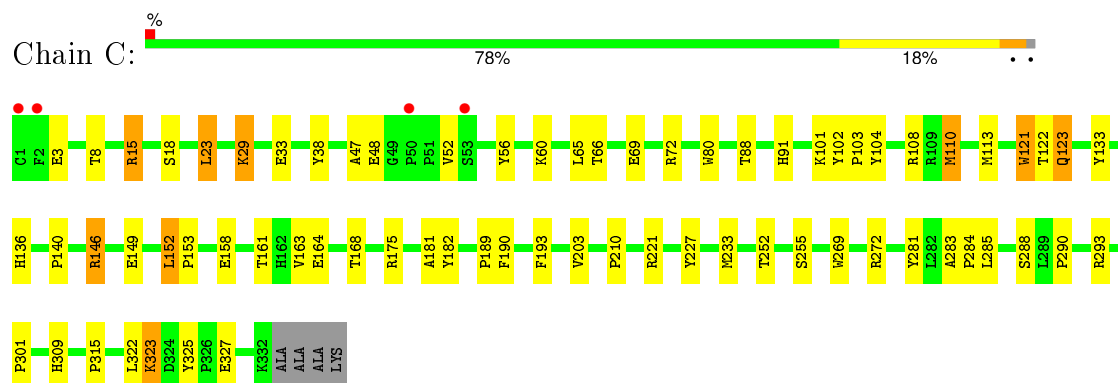
- Molecule 14 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	C	134	Total	O	0	0
			134	134		
14	H	81	Total	O	0	0
			81	81		
14	L	57	Total	O	0	0
			57	57		
14	M	71	Total	O	0	0
			71	71		

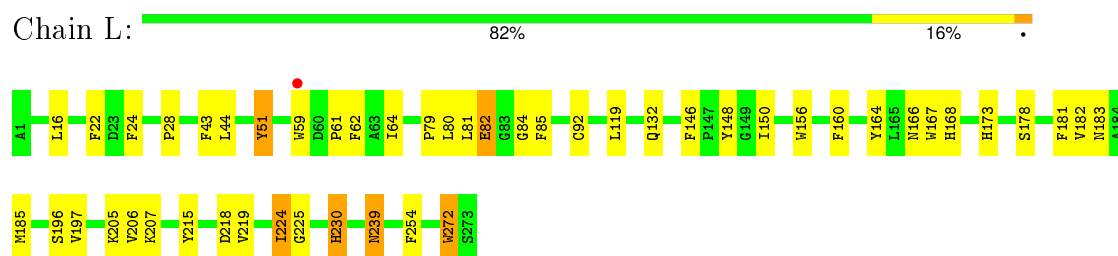
### 3 Residue-property plots [i](#)

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.

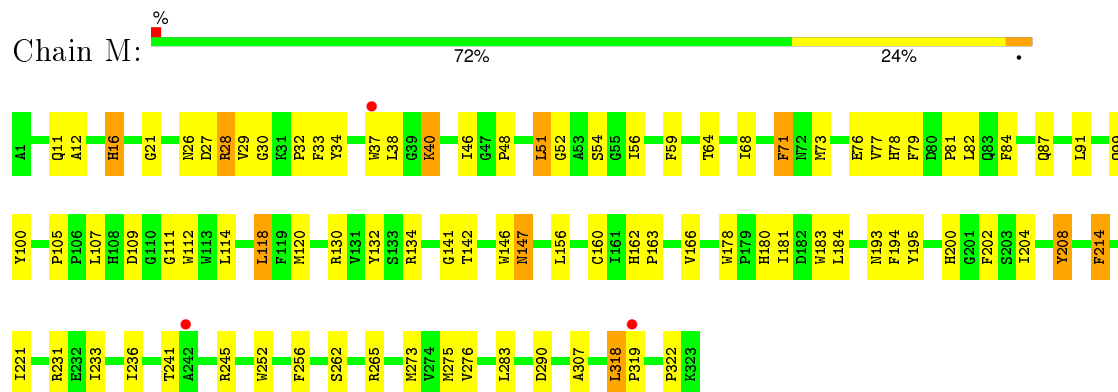
#### • Molecule 1: PHOTOSYNTHETIC REACTION CENTER

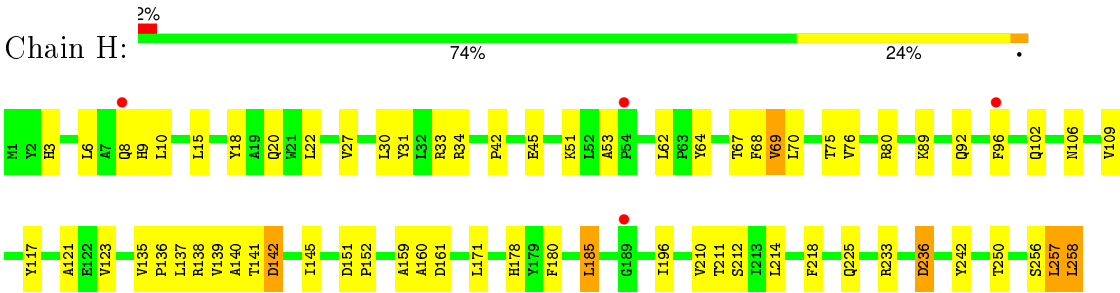


#### • Molecule 2: PHOTOSYNTHETIC REACTION CENTER



#### • Molecule 3: PHOTOSYNTHETIC REACTION CENTER





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	223.50 Å   223.50 Å   113.60 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	10.00 – 2.35 29.64 – 2.30	Depositor EDS
% Data completeness (in resolution range)	78.5 (10.00-2.35) 76.5 (29.64-2.30)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.85 (at 2.31 Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, $R_{free}$	0.190 ,   0.236 0.181 ,   (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	29.5	Xtriage
Anisotropy	0.086	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 101.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 96950 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	10501	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.65% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  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: LDA, BPB, BCB, FE2, SO4, MQ7, HEM, FME, ATZ, 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	0.52	0/2674	0.62	0/3645
2	L	0.54	0/2259	0.58	0/3084
3	M	0.55	0/2683	0.61	1/3669 (0.0%)
4	H	0.53	0/2055	0.69	2/2807 (0.1%)
All	All	0.53	0/9671	0.62	3/13205 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	6
2	L	0	4
3	M	0	2
4	H	0	3
All	All	0	15

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	53	ALA	CB-CA-C	-10.63	94.16	110.10
3	M	318	LEU	O-C-N	6.16	132.81	121.10
4	H	45	GLU	CB-CA-C	-5.25	99.89	110.40

There are no chirality outliers.

5 of 15 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	121	TRP	Mainchain
1	C	15	ARG	Sidechain
1	C	190	PHE	Sidechain
1	C	227	TYR	Sidechain
1	C	272	ARG	Sidechain

## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2607	0	2575	41	0
2	L	2171	0	2098	41	0
3	M	2577	0	2468	74	0
4	H	2018	0	2020	42	0
5	M	1	0	0	0	0
6	H	5	0	0	0	0
6	M	15	0	0	1	0
7	L	132	0	144	10	0
7	M	132	0	144	20	0
8	L	65	0	74	9	0
8	M	65	0	74	10	0
9	M	48	0	64	1	0
10	C	172	0	120	3	0
11	M	40	0	60	6	0
12	L	14	0	14	2	0
13	H	32	0	62	2	0
13	L	32	0	62	4	0
13	M	32	0	62	2	0
14	C	134	0	0	1	0
14	H	81	0	0	1	0
14	L	57	0	0	0	0
14	M	71	0	0	2	0
All	All	10501	0	10041	214	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 11.

The worst 5 of 214 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)
8:L:402:BPB:HBBB	8:L:402:BPB:HHC	1.32	1.09
1:C:52:VAL:HB	1:C:56:TYR:HD2	1.31	0.92
1:C:152:LEU:HD22	1:C:175:ARG:HA	1.53	0.91
8:L:402:BPB:HBBA	3:M:208:TYR:HB3	1.60	0.83
8:L:402:BPB:HHC	8:L:402:BPB:CBB	2.12	0.78

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	331/336 (98%)	313 (95%)	18 (5%)	0	100	100
2	L	271/273 (99%)	257 (95%)	14 (5%)	0	100	100
3	M	323/323 (100%)	309 (96%)	11 (3%)	3 (1%)	21	22
4	H	256/258 (99%)	237 (93%)	19 (7%)	0	100	100
All	All	1181/1190 (99%)	1116 (94%)	62 (5%)	3 (0%)	46	55

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	M	51	LEU
3	M	322	PRO
3	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	281/282 (100%)	264 (94%)	17 (6%)	24	28
2	L	218/218 (100%)	210 (96%)	8 (4%)	41	53
3	M	251/249 (101%)	236 (94%)	15 (6%)	24	28
4	H	212/212 (100%)	192 (91%)	20 (9%)	11	10
All	All	962/961 (100%)	902 (94%)	60 (6%)	23	26

5 of 60 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	M	27	ASP
3	M	118	LEU
4	H	236	ASP
3	M	40	LYS
3	M	156	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	58	ASN
2	L	183	ASN
2	L	239	ASN
3	M	147	ASN

### 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	H	1	4	8,9,10	0.55	0	6,9,11	4.19	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	-	0/6/9/11	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(°)	Ideal(°)
4	H	1	FME	O1-CN-N	-7.71	113.65	124.76
4	H	1	FME	CA-N-CN	-6.20	113.28	122.82
4	H	1	FME	O-C-CA	-2.27	119.43	125.44

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 [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

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
10	HEM	C	337	1	30,50,50	2.72	7 (23%)	24,82,82	3.30	9 (37%)
10	HEM	C	338	1	30,50,50	2.80	9 (30%)	24,82,82	2.96	9 (37%)
10	HEM	C	339	1	30,50,50	2.40	8 (26%)	24,82,82	3.23	10 (41%)
10	HEM	C	340	1	30,50,50	2.75	11 (36%)	24,82,82	2.78	9 (37%)
13	LDA	H	701	-	15,15,15	4.77	4 (26%)	16,17,17	0.65	0
13	LDA	H	703	-	15,15,15	4.73	3 (20%)	16,17,17	0.73	1 (6%)
6	SO4	H	801	-	4,4,4	1.25	0	6,6,6	0.68	0
7	BCB	L	302	2	56,74,74	1.53	7 (12%)	57,115,115	1.88	11 (19%)
7	BCB	L	304	2	56,74,74	1.52	9 (16%)	57,115,115	2.03	9 (15%)
8	BPB	L	402	-	63,70,70	1.33	9 (14%)	63,101,101	1.87	10 (15%)
12	ATZ	L	502	-	14,14,14	0.65	0	17,18,18	1.55	1 (5%)
13	LDA	L	702	-	15,15,15	4.99	4 (26%)	16,17,17	0.54	0
13	LDA	L	705	-	15,15,15	4.53	4 (26%)	16,17,17	0.75	0
8	BPB	M	401	-	63,70,70	1.51	7 (11%)	63,101,101	1.99	12 (19%)
9	MQ7	M	501	-	49,49,49	1.85	12 (24%)	62,63,63	1.61	13 (20%)
11	NS5	M	600	-	39,39,39	0.84	1 (2%)	44,46,46	1.34	6 (13%)
13	LDA	M	704	-	15,15,15	3.56	4 (26%)	16,17,17	0.54	0
13	LDA	M	706	-	15,15,15	4.44	4 (26%)	16,17,17	0.60	0
6	SO4	M	802	-	4,4,4	1.08	0	6,6,6	0.48	0
6	SO4	M	803	-	4,4,4	0.97	0	6,6,6	0.86	0
6	SO4	M	804	-	4,4,4	1.41	0	6,6,6	0.97	0
7	BCB	M	805	3	56,74,74	1.65	6 (10%)	57,115,115	2.05	9 (15%)
7	BCB	M	806	3	56,74,74	1.61	8 (14%)	57,115,115	2.15	15 (26%)

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
10	HEM	C	337	1	-	0/10/54/54	0/0/8/8
10	HEM	C	338	1	-	0/10/54/54	0/0/8/8
10	HEM	C	339	1	-	0/10/54/54	0/0/8/8
10	HEM	C	340	1	-	0/10/54/54	0/0/8/8
13	LDA	H	701	-	-	0/13/13/13	0/0/0/0
13	LDA	H	703	-	-	0/13/13/13	0/0/0/0
6	SO4	H	801	-	-	0/0/0/0	0/0/0/0
7	BCB	L	302	2	-	0/37/137/137	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	BCB	L	304	2	-	0/37/137/137	0/0/9/9
8	BPB	L	402	-	1/1/18/23	0/46/105/105	0/1/6/6
12	ATZ	L	502	-	-	0/7/7/7	0/1/1/1
13	LDA	L	702	-	-	0/13/13/13	0/0/0/0
13	LDA	L	705	-	-	0/13/13/13	0/0/0/0
8	BPB	M	401	-	-	0/46/105/105	0/1/6/6
9	MQ7	M	501	-	-	0/41/61/61	0/2/2/2
11	NS5	M	600	-	-	0/43/43/43	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
7	BCB	M	805	3	-	0/37/137/137	0/0/9/9
7	BCB	M	806	3	-	0/37/137/137	0/0/9/9

The worst 5 of 117 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	L	702	LDA	O1-N1	-18.52	1.21	1.39
13	H	703	LDA	O1-N1	-17.41	1.22	1.39
13	H	701	LDA	O1-N1	-17.17	1.23	1.39
13	L	705	LDA	O1-N1	-16.88	1.23	1.39
13	M	706	LDA	O1-N1	-16.60	1.23	1.39

The worst 5 of 124 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	C	337	HEM	C3B-CAB-CBB	-9.81	109.41	124.46
10	C	339	HEM	C3B-CAB-CBB	-8.86	110.86	124.46
10	C	338	HEM	C3B-CAB-CBB	-7.29	113.28	124.46
10	C	338	HEM	C3C-CAC-CBC	-7.27	113.30	124.46
10	C	340	HEM	C3B-CAB-CBB	-7.21	113.40	124.46

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
8	L	402	BPB	C13

There are no torsion outliers.

There are no ring outliers.

17 monomers are involved in 63 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	C	338	HEM	2	0
10	C	339	HEM	1	0
13	H	703	LDA	2	0
7	L	302	BCB	5	0
7	L	304	BCB	5	0
8	L	402	BPB	9	0
12	L	502	ATZ	2	0
13	L	702	LDA	3	0
13	L	705	LDA	1	0
8	M	401	BPB	10	0
9	M	501	MQ7	1	0
11	M	600	NS5	6	0
13	M	704	LDA	1	0
13	M	706	LDA	1	0
6	M	804	SO4	1	0
7	M	805	BCB	9	0
7	M	806	BCB	13	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, 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%)	-0.66	4 (1%) 81 89	13, 30, 57, 82	18 (5%)
2	L	273/273 (100%)	-0.74	1 (0%) 93 97	11, 25, 49, 67	7 (2%)
3	M	323/323 (100%)	-0.55	3 (0%) 85 92	10, 28, 59, 72	10 (3%)
4	H	249/258 (96%)	-0.46	4 (1%) 74 84	16, 39, 70, 90	19 (7%)
All	All	1177/1190 (98%)	-0.61	12 (1%) 84 92	10, 30, 60, 90	54 (4%)

The worst 5 of 12 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	H	54	PRO	3.8
3	M	319	PRO	3.0
2	L	59	TRP	2.8
3	M	37	TRP	2.8
1	C	2	PHE	2.3

### 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, 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	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	FME	H	1	10/11	0.97	0.09	-	34,38,46,54	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	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
13	LDA	M	704	16/16	0.80	0.29	5.11	67,73,102,103	0
13	LDA	M	706	16/16	0.65	0.33	4.69	77,82,87,87	4
13	LDA	L	702	16/16	0.84	0.21	3.97	34,54,73,75	0
11	NS5	M	600	40/40	0.91	0.16	3.18	34,51,70,70	14
13	LDA	H	703	16/16	0.96	0.18	2.68	30,40,65,67	0
9	MQ7	M	501	48/48	0.94	0.13	0.73	12,18,46,48	0
7	BCB	M	806	66/66	0.99	0.12	0.66	6,16,31,36	0
10	HEM	C	338	43/43	0.98	0.13	0.52	15,30,38,47	0
10	HEM	C	340	43/43	0.99	0.10	0.45	10,23,36,53	0
6	SO4	M	802	5/5	0.99	0.09	0.40	37,41,47,51	0
7	BCB	L	304	66/66	0.99	0.12	0.38	8,17,29,44	0
13	LDA	L	705	16/16	0.86	0.16	0.33	62,70,78,79	3
7	BCB	M	805	66/66	0.95	0.10	0.32	8,27,61,62	0
13	LDA	H	701	16/16	0.97	0.12	0.23	18,28,36,37	0
6	SO4	H	801	5/5	0.98	0.08	0.19	62,65,65,66	0
8	BPB	L	402	65/65	0.98	0.08	0.17	2,17,22,26	0
8	BPB	M	401	65/65	0.96	0.10	0.11	14,32,81,82	7
12	ATZ	L	502	14/14	0.98	0.12	0.10	21,33,35,36	0
7	BCB	L	302	66/66	0.99	0.10	0.03	3,13,21,24	0
6	SO4	M	804	5/5	0.98	0.10	-0.25	45,49,53,54	0
10	HEM	C	339	43/43	0.99	0.08	-0.29	6,19,24,34	0
10	HEM	C	337	43/43	0.98	0.08	-0.54	25,31,44,49	0
5	FE2	M	500	1/1	0.99	0.08	-2.15	24,24,24,24	0
6	SO4	M	803	5/5	0.95	0.11	-	84,88,90,90	0

### 6.5 Other polymers ⓘ

There are no such residues in this entry.