



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 09:37 PM GMT

PDB ID : 1PRC
Title : CRYSTALLOGRAPHIC REFINEMENT AT 2.3 ANGSTROMS RESOLUTION AND REFINED MODEL OF THE PHOTOSYNTHETIC REACTION CENTER FROM RHODOPSEUDOMONAS VIRIDIS
Authors : Deisenhofer, J.; Epp, O.; Miki, K.; Huber, R.; Michel, H.
Deposited on : 1988-02-04
Resolution : 2.30 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 ⓘ symbol.

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

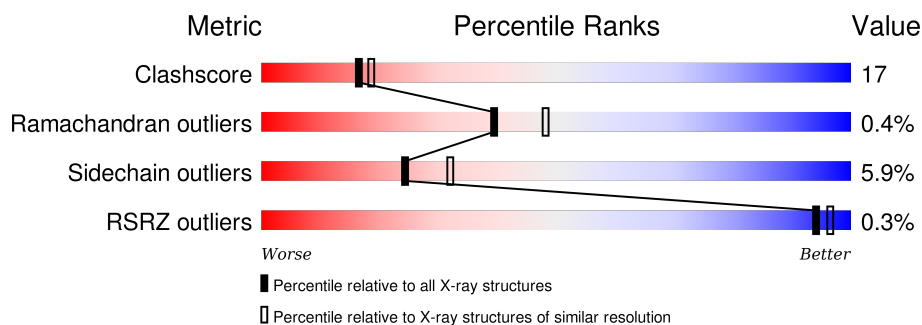
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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 $\leq 5\%$. 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	
2	L	273	
3	M	323	
4	H	258	

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	NS1	M	613	-	-	-	X
12	UQ1	L	614	-	-	X	X
13	LDA	H	616	-	-	-	X
6	SO4	H	622	-	-	-	X

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 10288 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	333	Total	C	N	O	S	54	0	1
			2603	1640	467	478	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	13	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	26	0	0
			2555	1702	419	423	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	106	0	0
			2018	1292	344	380	2			

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

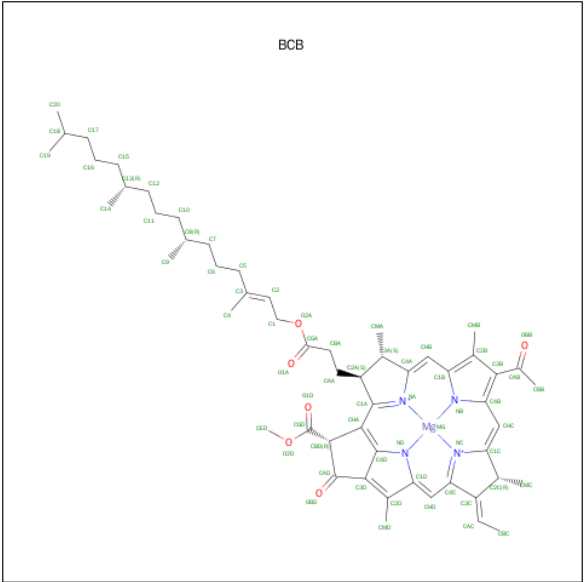
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	M	1	Total	Fe	0	0
			1	1		

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



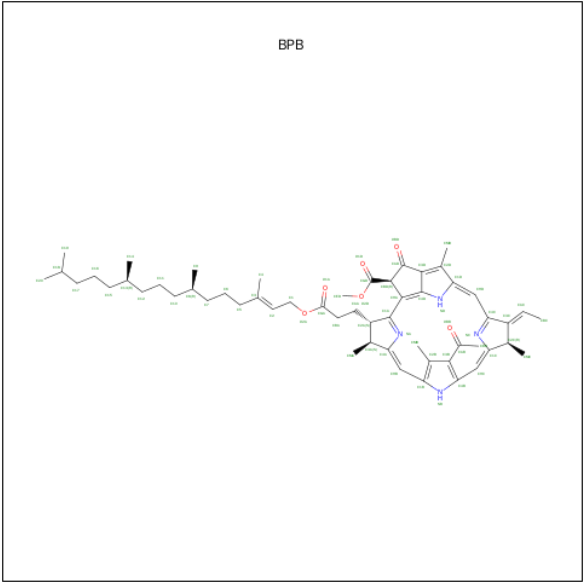
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	H	1	Total	O	S	0	0
			5	4	1		
6	M	1	Total	O	S	0	0
			5	4	1		
6	M	1	Total	O	S	0	0
			5	4	1		
6	M	1	Total	O	S	0	0
			5	4	1		
6	H	1	Total	O	S	0	0
			5	4	1		
6	H	1	Total	O	S	0	0
			5	4	1		

- Molecule 7 is BACTERIOCHLOROPHYLL B (three-letter code: BCB) (formula: $C_{55}H_{72}MgN_4O_6$).



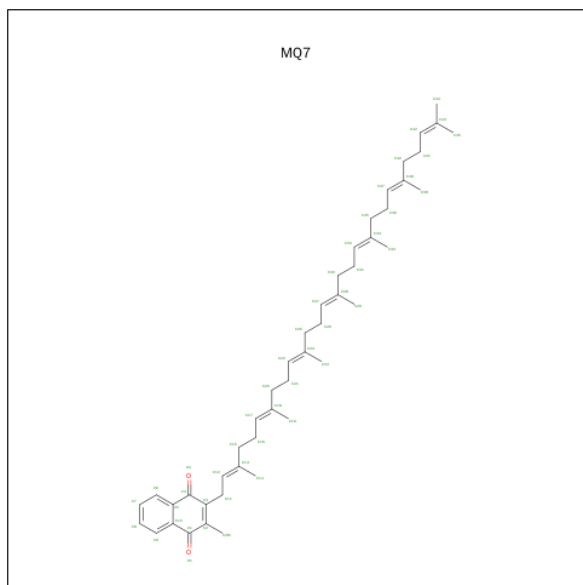
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	M	1	Total 66	C 55	Mg 1	N 4	O 6	13	0
7	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
7	M	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
7	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0

- Molecule 8 is BACTERIOPHEOPHYTIN B (three-letter code: BPB) (formula: C₅₅H₇₄N₄O₆).



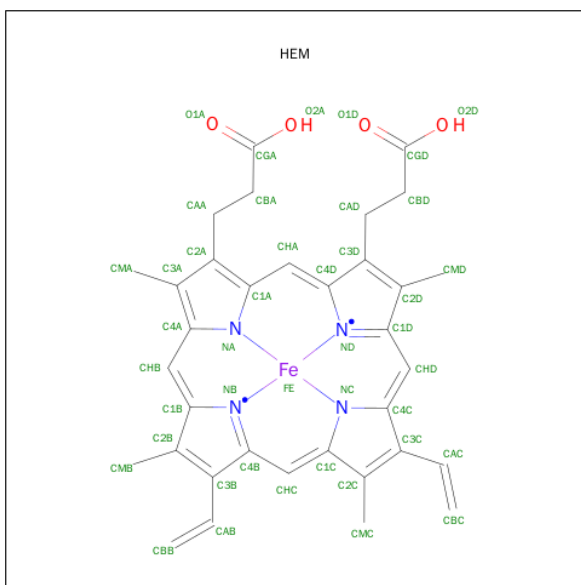
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	M	1	Total	C	N	O	7	0
			65	55	4	6		
8	L	1	Total	C	N	O	0	0
			65	55	4	6		

- Molecule 9 is MENAQUINONE-7 (three-letter code: MQ7) (formula: $C_{46}H_{64}O_2$).



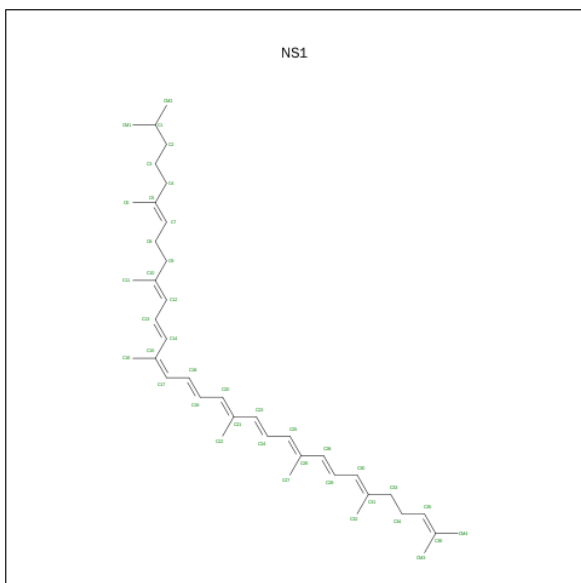
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	M	1	Total	C	O	4	0
			48	46	2		

- Molecule 10 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



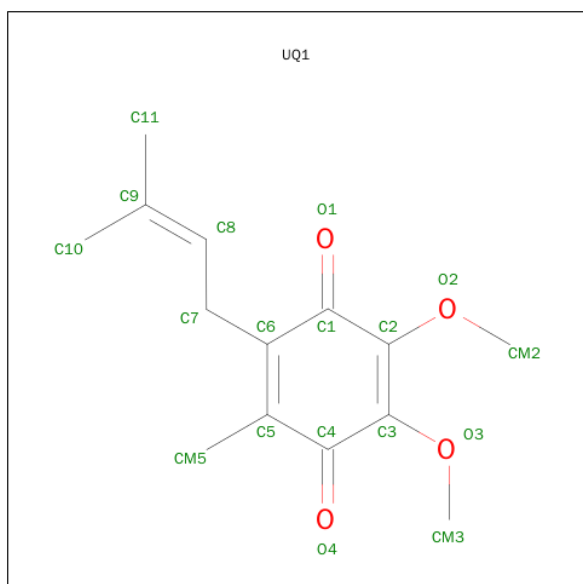
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
10	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
10	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
10	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 11 is 15-TRANS-1,2-DIHYDRONEUROSPORENE (three-letter code: NS1) (formula: C₄₀H₆₀).



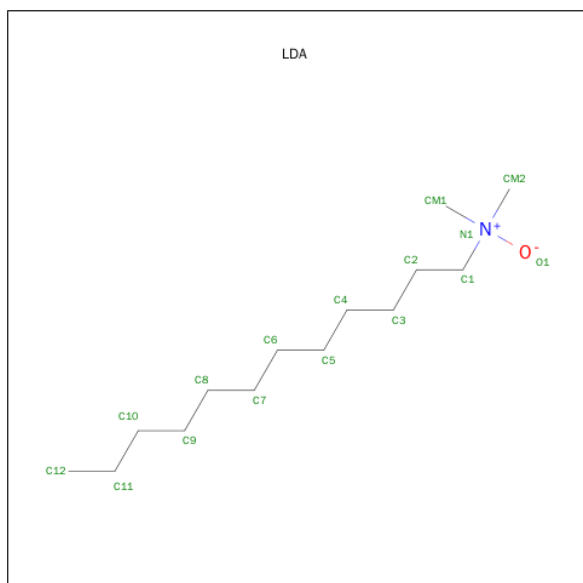
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	M	1	Total C 40 40	14	0

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



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

- 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	H	1	Total	C	N	O	6	0
			16	14	1	1		

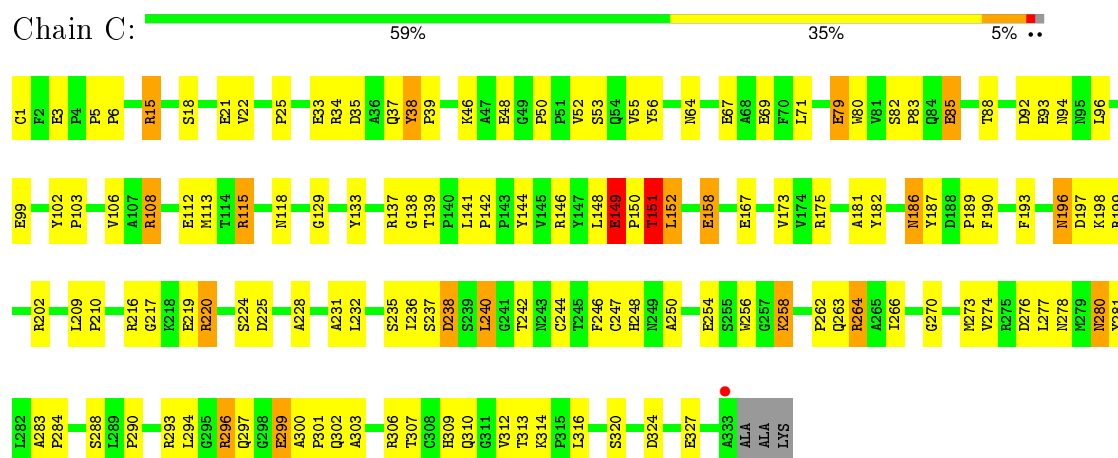
- Molecule 14 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	C	66	Total	O	0	0
			66	66		
14	H	41	Total	O	0	0
			41	41		
14	L	39	Total	O	0	0
			39	39		
14	M	55	Total	O	0	0
			55	55		

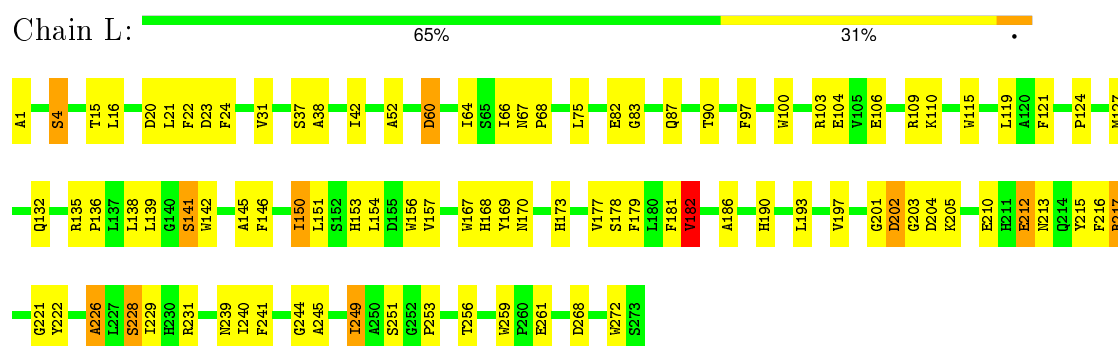
3 Residue-property plots

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.

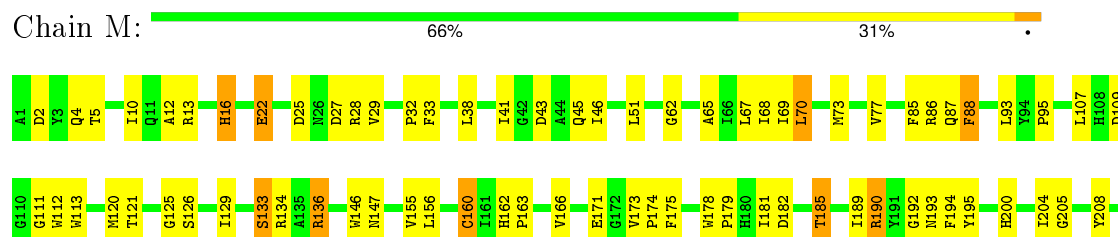
• Molecule 1: PHOTOSYNTHETIC REACTION CENTER

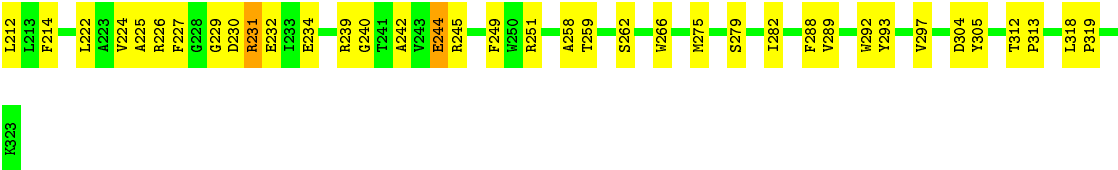


• Molecule 2: PHOTOSYNTHETIC REACTION CENTER

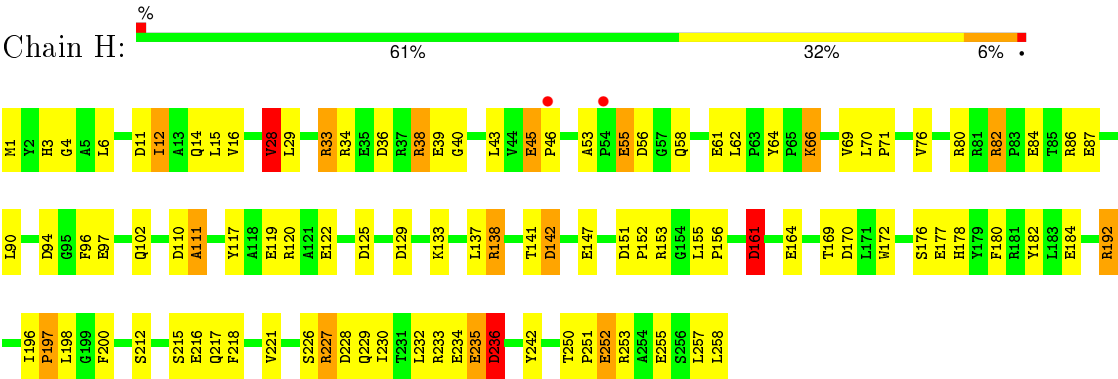


• Molecule 3: PHOTOSYNTHETIC REACTION CENTER





● Molecule 4: PHOTOSYNTHETIC REACTION CENTER



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	223.50 Å 223.50 Å 113.60 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.99 – 2.30 19.99 – 2.30	Depositor EDS
% Data completeness (in resolution range)	(Not available) (19.99-2.30) 75.5 (19.99-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$	-	Xtriage
Refinement program	TNT	Depositor
R, R_{free}	0.193 , (Not available) 0.186 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	22.4	Xtriage
Anisotropy	0.098	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 64.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ¹	$\langle L \rangle = 0.32$, $\langle L^2 \rangle = 0.15$	Xtriage
Outliers	0 of 95762 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	10288	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.96% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Theoretical 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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: LDA, BPB, BCB, FE, MQ7, HEM, UQ1, NS1, FME, SO4

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	1.07	17/2670 (0.6%)	1.56	36/3639 (1.0%)
2	L	1.01	5/2259 (0.2%)	1.42	18/3084 (0.6%)
3	M	0.96	3/2659 (0.1%)	1.46	26/3637 (0.7%)
4	H	1.13	18/2055 (0.9%)	1.65	32/2807 (1.1%)
All	All	1.04	43/9643 (0.4%)	1.52	112/13167 (0.9%)

The worst 5 of 43 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	255	GLU	CD-OE2	9.06	1.35	1.25
1	C	299	GLU	CD-OE2	8.31	1.34	1.25
3	M	244	GLU	CD-OE2	8.03	1.34	1.25
2	L	261	GLU	CD-OE2	7.64	1.34	1.25
1	C	21	GLU	CD-OE2	7.48	1.33	1.25

The worst 5 of 112 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	38	ARG	NE-CZ-NH2	-18.45	111.08	120.30
3	M	245	ARG	NE-CZ-NH2	-11.45	114.57	120.30
3	M	25	ASP	CB-CG-OD2	-10.22	109.10	118.30
4	H	153	ARG	NE-CZ-NH2	-9.86	115.37	120.30
4	H	153	ARG	NE-CZ-NH1	9.74	125.17	120.30

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	C	2603	0	2579	81	0
2	L	2171	0	2098	83	0
3	M	2555	0	2452	78	0
4	H	2018	0	2020	58	0
5	M	1	0	0	0	0
6	H	15	0	0	0	0
6	M	20	0	0	0	0
7	L	132	0	144	22	0
7	M	132	0	144	22	0
8	L	65	0	74	8	0
8	M	65	0	74	11	0
9	M	48	0	64	1	0
10	C	172	0	120	14	0
11	M	40	0	59	4	0
12	L	18	0	18	10	0
13	H	16	0	31	2	0
13	M	16	0	31	1	0
14	C	66	0	0	5	0
14	H	41	0	0	1	0
14	L	39	0	0	3	0
14	M	55	0	0	3	0
All	All	10288	0	9908	321	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 17.

The worst 5 of 321 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)
3:M:120:MET:HE2	7:M:603:BCB:H172	1.41	1.00
3:M:136:ARG:HE	3:M:136:ARG:HA	1.31	0.93
1:C:152:LEU:HD22	1:C:175:ARG:HA	1.53	0.90
8:L:606:BPB:HHC	8:L:606:BPB:HBBB	1.52	0.90
7:L:602:BCB:H61	7:L:604:BCB:HBB3	1.55	0.88

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%)	306 (92%)	24 (7%)	1 (0%)	46	57
2	L	271/273 (99%)	252 (93%)	18 (7%)	1 (0%)	39	48
3	M	321/323 (99%)	300 (94%)	19 (6%)	2 (1%)	30	36
4	H	256/258 (99%)	239 (93%)	16 (6%)	1 (0%)	39	48
All	All	1179/1190 (99%)	1097 (93%)	77 (6%)	5 (0%)	39	48

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	M	22	GLU
4	H	53	ALA
3	M	88	PHE
1	C	250	ALA
2	L	31	VAL

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%)	261 (93%)	20 (7%)	18	23
2	L	218/218 (100%)	210 (96%)	8 (4%)	41	55
3	M	249/249 (100%)	235 (94%)	14 (6%)	26	35

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	H	212/212 (100%)	197 (93%)	15 (7%)	18	23
All	All	960/961 (100%)	903 (94%)	57 (6%)	24	32

5 of 57 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	L	228	SER
3	M	77	VAL
4	H	198	LEU
2	L	249	ILE
3	M	16	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
2	L	144	HIS
2	L	183	ASN
4	H	3	HIS
1	C	310	GLN
2	L	239	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	0.88	1 (12%)	6,9,11	3.46	2 (33%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	FME	H	1	4	-	1/6/9/11	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	1	FME	CA-N	-2.13	1.43	1.46

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	1	FME	O1-CN-N	-6.97	114.72	124.76
4	H	1	FME	CA-N-CN	-4.40	116.05	122.82

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	H	1	FME	O1-CN-N-CA

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	H	1	FME	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 23 ligands modelled in this entry, 1 is monoatomic - leaving 22 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	609	1	30,50,50	4.25	9 (30%)	24,82,82	3.23	9 (37%)
10	HEM	C	610	1	30,50,50	4.20	11 (36%)	24,82,82	3.39	11 (45%)
10	HEM	C	611	1	30,50,50	3.76	11 (36%)	24,82,82	3.08	10 (41%)
10	HEM	C	612	1	30,50,50	3.54	11 (36%)	24,82,82	2.71	9 (37%)
13	LDA	H	616	-	15,15,15	4.75	4 (26%)	16,17,17	1.20	2 (12%)
6	SO4	H	617	-	4,4,4	1.45	0	6,6,6	0.21	0
6	SO4	H	622	-	4,4,4	1.62	1 (25%)	6,6,6	0.20	0
6	SO4	H	623	-	4,4,4	1.47	0	6,6,6	0.26	0
7	BCB	L	602	2	56,74,74	1.58	6 (10%)	57,115,115	1.76	15 (26%)
7	BCB	L	604	2	56,74,74	1.53	6 (10%)	57,115,115	1.50	13 (22%)
8	BPB	L	606	-	63,70,70	1.38	7 (11%)	63,101,101	1.56	14 (22%)
12	UQ1	L	614	-	18,18,18	0.77	1 (5%)	22,25,25	1.07	3 (13%)
7	BCB	M	601	3	56,74,74	1.31	5 (8%)	57,115,115	1.63	13 (22%)
7	BCB	M	603	3	56,74,74	1.80	16 (28%)	57,115,115	1.86	18 (31%)
8	BPB	M	605	-	63,70,70	1.30	6 (9%)	63,101,101	1.39	7 (11%)
9	MQ7	M	608	-	49,49,49	1.41	6 (12%)	62,63,63	2.37	22 (35%)
11	NS1	M	613	-	39,39,39	2.65	12 (30%)	44,46,46	2.12	16 (36%)
13	LDA	M	615	-	15,15,15	4.97	4 (26%)	16,17,17	3.15	5 (31%)
6	SO4	M	618	-	4,4,4	1.16	0	6,6,6	0.29	0
6	SO4	M	619	-	4,4,4	1.20	0	6,6,6	0.23	0
6	SO4	M	620	-	4,4,4	0.91	0	6,6,6	0.15	0
6	SO4	M	621	-	4,4,4	1.60	0	6,6,6	0.29	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
10	HEM	C	609	1	-	0/10/54/54	0/0/8/8
10	HEM	C	610	1	-	0/10/54/54	0/0/8/8
10	HEM	C	611	1	-	0/10/54/54	0/0/8/8
10	HEM	C	612	1	-	0/10/54/54	0/0/8/8
13	LDA	H	616	-	-	0/13/13/13	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	SO4	H	617	-	-	0/0/0/0	0/0/0/0
6	SO4	H	622	-	-	0/0/0/0	0/0/0/0
6	SO4	H	623	-	-	0/0/0/0	0/0/0/0
7	BCB	L	602	2	-	0/37/137/137	0/0/9/9
7	BCB	L	604	2	-	0/37/137/137	0/0/9/9
8	BPB	L	606	-	-	0/46/105/105	0/1/6/6
12	UQ1	L	614	-	-	0/9/33/33	0/1/1/1
7	BCB	M	601	3	-	0/37/137/137	0/0/9/9
7	BCB	M	603	3	-	0/37/137/137	0/0/9/9
8	BPB	M	605	-	-	0/46/105/105	0/1/6/6
9	MQ7	M	608	-	-	0/41/61/61	0/2/2/2
11	NS1	M	613	-	-	0/43/43/43	0/0/0/0
13	LDA	M	615	-	-	0/13/13/13	0/0/0/0
6	SO4	M	618	-	-	0/0/0/0	0/0/0/0
6	SO4	M	619	-	-	0/0/0/0	0/0/0/0
6	SO4	M	620	-	-	0/0/0/0	0/0/0/0
6	SO4	M	621	-	-	0/0/0/0	0/0/0/0

The worst 5 of 116 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	M	615	LDA	O1-N1	-18.58	1.21	1.39
13	H	616	LDA	O1-N1	-17.56	1.22	1.39
10	C	609	HEM	C3B-C4B	-16.79	1.36	1.51
10	C	610	HEM	C3B-C4B	-14.89	1.38	1.51
10	C	611	HEM	C3B-C4B	-13.04	1.40	1.51

The worst 5 of 167 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	C	610	HEM	C3C-CAC-CBC	-10.70	108.04	124.46
13	M	615	LDA	CM2-N1-CM1	-10.47	97.01	108.83
10	C	609	HEM	C3B-CAB-CBB	-9.65	109.66	124.46
9	M	608	MQ7	C11-C3-C4	-8.64	108.61	118.47
10	C	610	HEM	C3B-CAB-CBB	-7.46	113.01	124.46

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

15 monomers are involved in 87 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	C	609	HEM	4	0
10	C	610	HEM	2	0
10	C	611	HEM	6	0
10	C	612	HEM	2	0
13	H	616	LDA	2	0
7	L	602	BCB	16	0
7	L	604	BCB	11	0
8	L	606	BPB	8	0
12	L	614	UQ1	10	0
7	M	601	BCB	7	0
7	M	603	BCB	15	0
8	M	605	BPB	11	0
9	M	608	MQ7	1	0
11	M	613	NS1	4	0
13	M	615	LDA	1	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	333/336 (99%)	-0.99	1 (0%) 94 96	7, 21, 46, 73	17 (5%)
2	L	273/273 (100%)	-1.12	0 100 100	6, 16, 36, 53	6 (2%)
3	M	323/323 (100%)	-1.05	0 100 100	4, 18, 41, 58	8 (2%)
4	H	250/258 (96%)	-0.91	2 (0%) 87 90	8, 23, 51, 78	17 (6%)
All	All	1179/1190 (99%)	-1.02	3 (0%) 94 96	4, 19, 44, 78	48 (4%)

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	H	46	PRO	3.8
4	H	54	PRO	3.3
1	C	333	ALA	3.1

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
4	FME	H	1	10/11	0.98	0.06	-	21,32,41,45	0

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
12	UQ1	L	614	18/18	0.84	0.57	46.70	19,26,29,30	18
6	SO4	H	622	5/5	0.92	0.22	11.58	73,74,85,89	0
13	LDA	H	616	16/16	0.91	0.17	7.37	0,27,42,46	6
11	NS1	M	613	40/40	0.96	0.11	4.14	0,25,39,49	14
8	BPB	M	605	65/65	0.96	0.10	1.48	0,21,62,71	7
10	HEM	C	611	43/43	0.99	0.09	0.94	5,16,25,38	0
6	SO4	M	618	5/5	1.00	0.07	0.63	22,23,35,37	0
10	HEM	C	610	43/43	0.99	0.09	0.61	3,21,29,37	0
8	BPB	L	606	65/65	0.99	0.07	0.54	3,10,19,22	0
6	SO4	H	617	5/5	0.98	0.07	0.53	47,50,59,61	0
10	HEM	C	612	43/43	0.98	0.08	0.25	3,22,31,46	0
10	HEM	C	609	43/43	0.99	0.08	0.20	7,22,32,36	0
7	BCB	L	602	66/66	0.99	0.07	0.05	3,10,19,21	0
13	LDA	M	615	16/16	0.97	0.07	-0.17	17,25,36,37	0
9	MQ7	M	608	48/48	0.98	0.06	-0.49	0,10,20,32	4
7	BCB	L	604	66/66	0.98	0.06	-0.52	3,10,27,35	0
7	BCB	M	603	66/66	0.99	0.06	-0.62	3,10,20,21	0
7	BCB	M	601	66/66	0.98	0.06	-1.15	0,12,40,61	13
5	FE	M	607	1/1	1.00	0.04	-1.20	19,19,19,19	0
6	SO4	M	620	5/5	0.99	0.05	-1.25	31,34,40,41	0
6	SO4	H	623	5/5	0.94	0.13	-	58,59,62,64	5
6	SO4	M	619	5/5	0.99	0.11	-	39,43,50,59	0
6	SO4	M	621	5/5	0.97	0.20	-	68,78,81,82	0

6.5 Other polymers ⓘ

There are no such residues in this entry.