



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 03:24 PM GMT

PDB ID : 4CAS
Title : Serial femtosecond crystallography structure of a photosynthetic reaction center
Authors : Johansson, L.C.; Arnlund, D.; Katona, G.; White, T.A.; Barty, A.; DePonte, D.P.; Shoeman, R.L.; Wickstrand, C.; Sharma, A.; Williams, G.J.; Aquila, A.; Bogan, M.J.; Caleman, C.; Davidsson, J.; Doak, R.B.; Frank, M.; Fromme, R.; Galli, L.; Grotjohann, I.; Hunter, M.S.; Kassemeyer, S.; Kirian, R.A.; Kupitz, C.; Liang, M.; Lomb, L.; Malmerberg, E.; Martin, A.V.; Messerschmidt, M.; Nass, K.; Redecke, L.; Seibert, M.M.; Sjöhamn, J.; Steinbrener, J.; Stellato, F.; Wang, D.; Wahlgren, W.Y.; Weierstall, U.; Westenhoff, S.; Zatsepin, N.A.; Boutet, S.; Spence, J.C.H.; Schlichting, I.; Chapman, H.N.; Fromme, P.; Neutze, R.
Deposited on : 2013-10-09
Resolution : 3.50 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org

A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ 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)

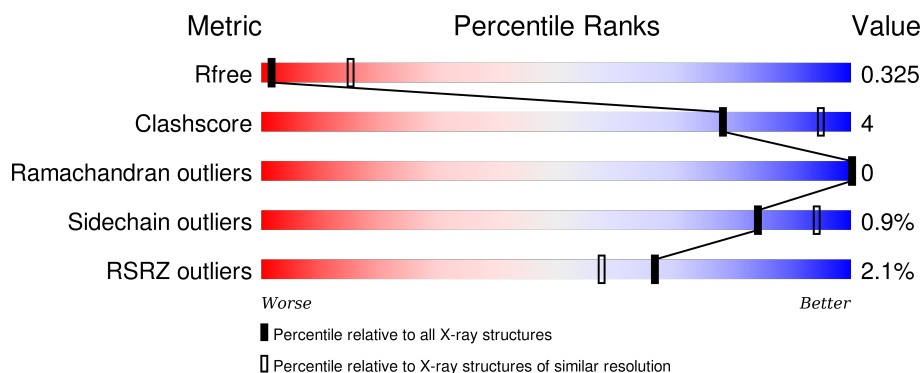
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION


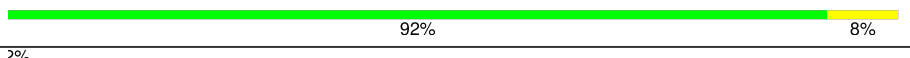
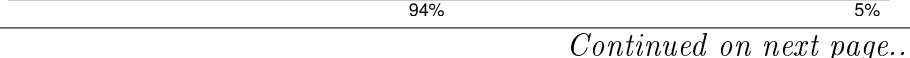
The reported resolution of this entry is 3.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1051 (3.60-3.40)
Clashscore	102246	1157 (3.60-3.40)
Ramachandran outliers	100387	1120 (3.60-3.40)
Sidechain outliers	100360	1121 (3.60-3.40)
RSRZ outliers	91569	1058 (3.60-3.40)


The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	A	356	 92% 7%
2	B	274	 92% 8%
3	C	324	 94% 5%

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Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

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Mol	Chain	Length	Quality of chain
4	D	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
12	NS5	C	1328	-	-	-	X
13	OTP	C	1329	-	-	-	X
14	PO4	C	1331	-	-	-	X
8	DGA	B	1278	-	-	-	X
9	MPG	B	1279	-	-	-	X
9	MPG	B	1280	-	-	-	X
9	MPG	C	1330	-	-	-	X

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 9890 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called PHOTOSYNTHETIC REACTION CENTER CYTOCHROME C SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	332	Total	C	N	O	S	0	0	0
			2598	1637	465	478	18			

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

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

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

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

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

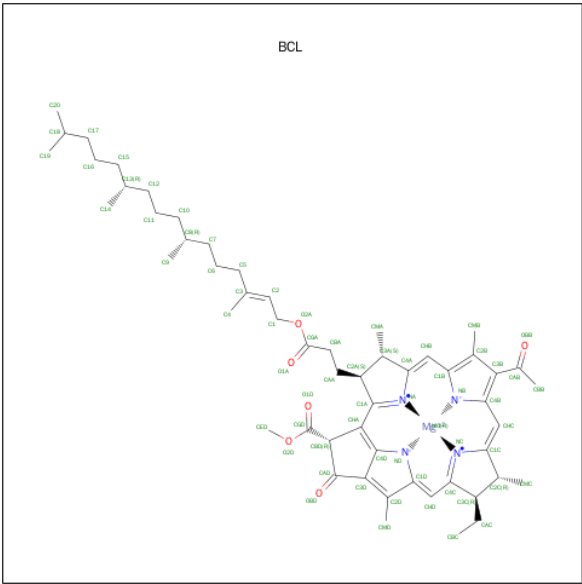
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	243	Total	C	N	O	S	0	0	0
			1771	1140	297	332	2			

- Molecule 5 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: C₃₄H₃₂FeN₄O₄).



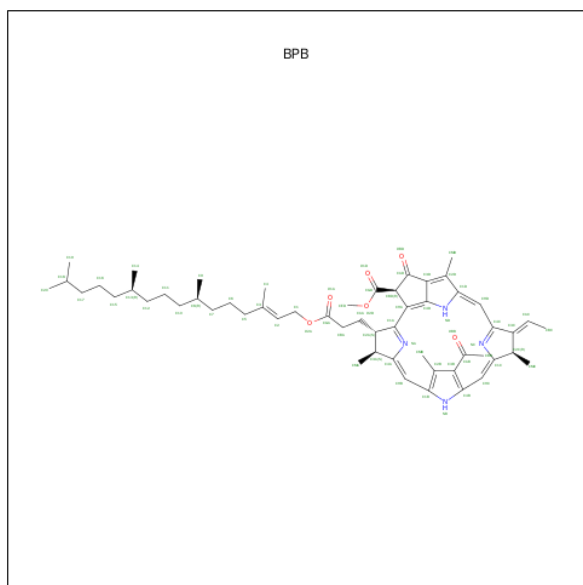
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
5	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
5	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
5	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 6 is BACTERIOCHLOROPHYLL A (three-letter code: BCL) (formula: $C_{55}H_{74}MgN_4O_6$).



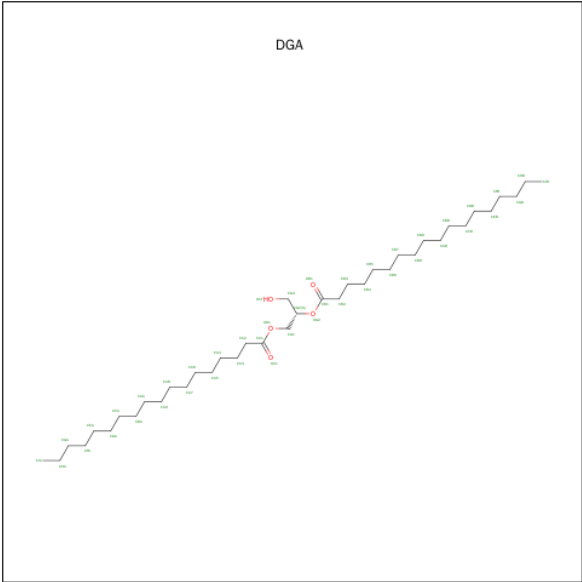
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	B	1	Total 65	C 54	Mg 1	N 4	O 6	0	0
6	B	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
6	B	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
6	C	1	Total 66	C 55	Mg 1	N 4	O 6	0	0

- Molecule 7 is BACTERIOPHEOPHYTIN B (three-letter code: BPB) (formula: $C_{55}H_{74}N_4O_6$).



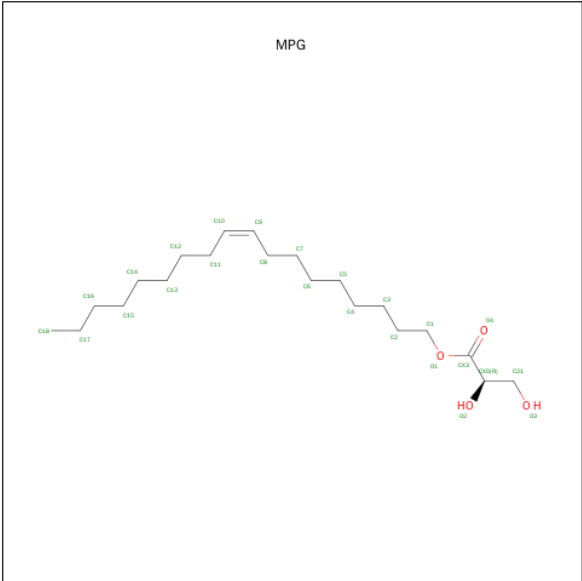
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	B	1	Total	C	N	O	0	0
			65	55	4	6		
7	C	1	Total	C	N	O	0	0
			61	51	4	6		

- Molecule 8 is DIACYL GLYCEROL (three-letter code: DGA) (formula: $C_{39}H_{76}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	C	O	0	0
			37	33	4		

- Molecule 9 is 1-MONOOLEOYL-RAC-GLYCEROL (three-letter code: MPG) (formula: C₂₁H₄₀O₄).



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

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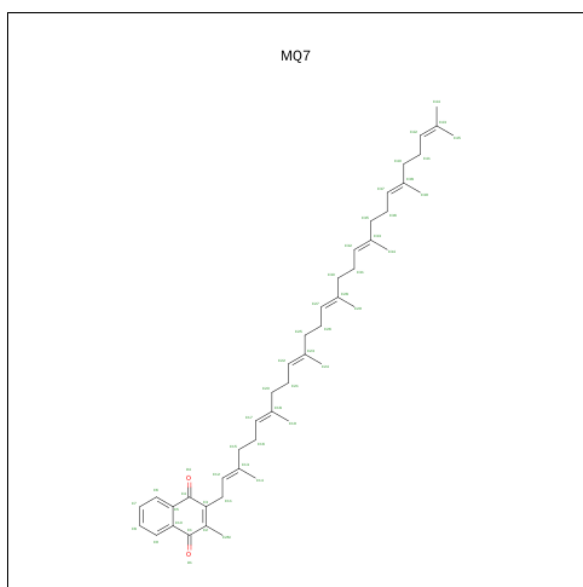
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	C	1	Total C 17 17	0	0

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

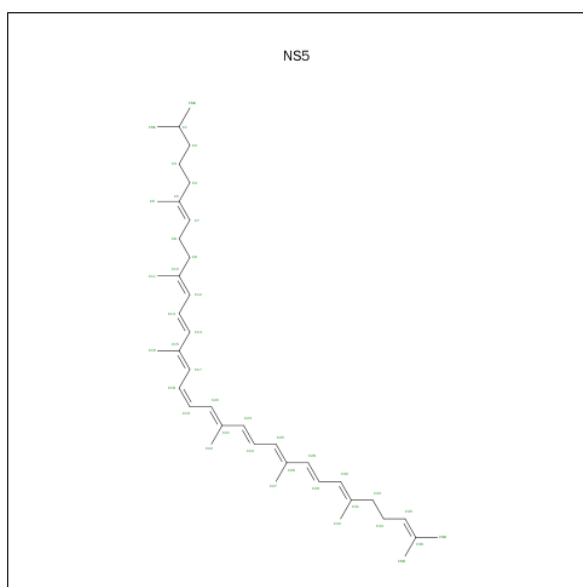
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	C	1	Total Fe 1 1	0	0

- Molecule 11 is MENAQUINONE-7 (three-letter code: MQ7) (formula: C₄₆H₆₄O₂).



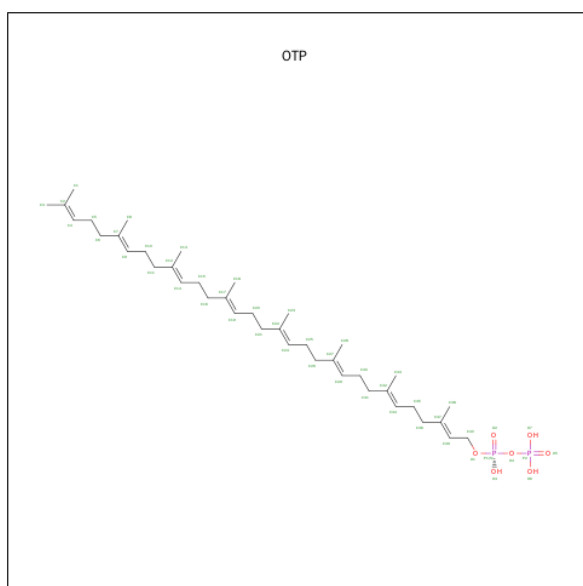
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	C	1	Total C O 48 46 2	0	0

- Molecule 12 is 15-CIS-1,2-DIHYDRONEUROSPORENE (three-letter code: NS5) (formula: C₄₀H₆₀).



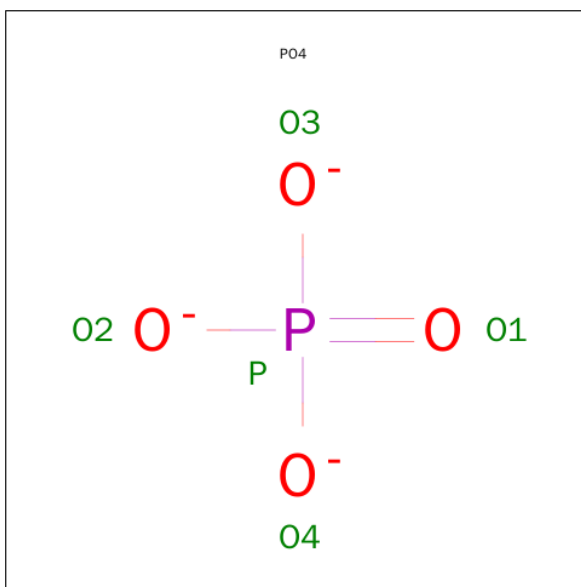
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	C	1	Total	C	0	0
			40	40		

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



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

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



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

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: PHOTOSYNTHETIC REACTION CENTER CYTOCHROME C SUBUNIT



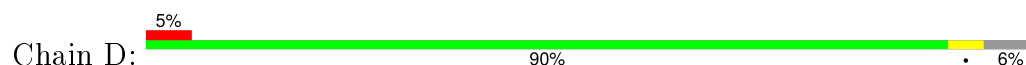
- Molecule 2: REACTION CENTER PROTEIN L CHAIN



- Molecule 3: REACTION CENTER PROTEIN M CHAIN



- Molecule 4: REACTION CENTER PROTEIN H CHAIN



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	57.90 Å 84.80 Å 384.30 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.64 – 3.50 49.59 – 3.50	Depositor EDS
% Data completeness (in resolution range)	99.1 (49.64-3.50) 99.2 (49.59-3.50)	Depositor EDS
R_{merge}	0.00	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.00 (at 3.48 Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.295 , 0.329 0.296 , 0.325	Depositor DCC
R_{free} test set	1262 reflections (5.38%)	DCC
Wilson B-factor (Å ²)	73.5	Xtriage
Anisotropy	0.134	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 77.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.32$, $\langle L^2 \rangle = 0.15$	Xtriage
Outliers	0 of 24721 reflections	Xtriage
F_o, F_c correlation	0.73	EDS
Total number of atoms	9890	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.64% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: BCL, MPG, BPB, PO4, DGA, FE2, MQ7, OTP, 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	A	0.56	0/2665	0.67	0/3633
2	B	0.50	0/2263	0.58	0/3089
3	C	0.52	0/2650	0.58	0/3629
4	D	0.43	0/1804	0.55	0/2485
All	All	0.51	0/9382	0.60	0/12836

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [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	A	2598	0	2567	4	0
2	B	2170	0	2100	22	0
3	C	2546	0	2430	19	0
4	D	1771	0	1656	5	0
5	A	172	0	120	7	0
6	B	197	0	217	14	0
6	C	66	0	74	8	0
7	B	65	0	74	8	0
7	C	61	0	63	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	B	37	0	58	0	0
9	B	50	0	80	2	0
9	C	17	0	31	1	0
10	C	1	0	0	0	0
11	C	48	0	64	2	0
12	C	40	0	60	5	0
13	C	41	0	65	7	0
14	C	10	0	0	0	0
All	All	9890	0	9659	70	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

The worst 5 of 70 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:C:1325:BPB:HBBB	7:C:1325:BPB:HHC	1.62	0.81
7:B:1277:BPB:HHC	7:B:1277:BPB:HBBB	1.61	0.81
6:B:1274:BCL:HHC	6:B:1274:BCL:HBB2	1.75	0.68
2:B:181:PHE:HB3	7:C:1325:BPB:HBBA	1.80	0.63
6:B:1276:BCL:HMD2	6:C:1324:BCL:HBB3	1.81	0.62

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	330/356 (93%)	323 (98%)	7 (2%)	0	100	100
2	B	273/274 (100%)	266 (97%)	7 (3%)	0	100	100
3	C	321/324 (99%)	312 (97%)	9 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	D	239/258 (93%)	233 (98%)	6 (2%)	0	100	100
All	All	1163/1212 (96%)	1134 (98%)	29 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	A	280/297 (94%)	279 (100%)	1 (0%)	93	98
2	B	218/219 (100%)	215 (99%)	3 (1%)	74	91
3	C	247/250 (99%)	245 (99%)	2 (1%)	86	95
4	D	167/212 (79%)	165 (99%)	2 (1%)	78	92
All	All	912/978 (93%)	904 (99%)	8 (1%)	84	94

5 of 8 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	272	TRP
4	D	236	ASP
3	C	214	PHE
2	B	249	ILE
3	C	194	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	183	ASN
4	D	8	GLN
2	B	239	ASN
1	A	302	GLN
3	C	200	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	FME	D	1	4	8,9,10	0.74	0	6,9,11	3.77	4 (66%)

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

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

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	1	FME	CA-N-CN	-6.92	112.18	122.82
4	D	1	FME	O1-CN-N	-3.18	120.17	124.76
4	D	1	FME	O-C-CA	-2.36	119.22	125.44
4	D	1	FME	CE-SD-CG	4.43	115.49	100.37

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 20 ligands modelled in this entry, 1 is monoatomic - leaving 19 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
5	HEM	A	1333	1	30,50,50	2.15	6 (20%)	24,82,82	2.42	10 (41%)
5	HEM	A	1334	1	30,50,50	2.05	7 (23%)	24,82,82	2.52	10 (41%)
5	HEM	A	1335	1	30,50,50	2.15	8 (26%)	24,82,82	2.35	11 (45%)
5	HEM	A	1336	1	30,50,50	2.16	8 (26%)	24,82,82	2.35	10 (41%)
6	BCL	B	1274	-	52,73,74	1.67	11 (21%)	55,113,115	2.15	15 (27%)
6	BCL	B	1275	2	53,74,74	1.60	11 (20%)	57,115,115	2.09	18 (31%)
6	BCL	B	1276	2	53,74,74	1.70	11 (20%)	57,115,115	1.93	14 (24%)
7	BPB	B	1277	-	63,70,70	2.94	16 (25%)	63,101,101	2.27	15 (23%)
8	DGA	B	1278	1	36,36,43	1.18	2 (5%)	38,38,45	1.27	3 (7%)
9	MPG	B	1279	-	22,23,24	1.32	1 (4%)	20,23,25	1.81	3 (15%)
9	MPG	B	1280	-	22,23,24	1.56	1 (4%)	20,23,25	1.37	2 (10%)
6	BCL	C	1324	-	53,74,74	1.76	10 (18%)	57,115,115	1.98	16 (28%)
7	BPB	C	1325	-	59,66,70	3.01	16 (27%)	58,96,101	2.29	14 (24%)
11	MQ7	C	1327	-	49,49,49	1.50	3 (6%)	62,63,63	1.30	10 (16%)
12	NS5	C	1328	-	39,39,39	2.18	7 (17%)	44,46,46	2.13	12 (27%)
13	OTP	C	1329	-	40,40,48	1.86	2 (5%)	47,47,61	2.78	18 (38%)
9	MPG	C	1330	-	16,16,24	0.41	0	15,15,25	0.69	0
14	PO4	C	1331	-	4,4,4	0.41	0	6,6,6	0.27	0
14	PO4	C	1332	-	4,4,4	0.26	0	6,6,6	0.28	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	HEM	A	1333	1	-	0/10/54/54	0/0/8/8
5	HEM	A	1334	1	-	0/10/54/54	0/0/8/8
5	HEM	A	1335	1	-	0/10/54/54	0/0/8/8
5	HEM	A	1336	1	-	0/10/54/54	0/0/8/8
6	BCL	B	1274	-	-	0/36/136/137	0/0/9/9
6	BCL	B	1275	2	-	0/37/137/137	0/0/9/9
6	BCL	B	1276	2	-	0/37/137/137	0/0/9/9
7	BPB	B	1277	-	-	0/46/105/105	0/1/6/6
8	DGA	B	1278	1	-	0/37/37/45	0/0/0/0
9	MPG	B	1279	-	-	0/25/22/25	0/0/0/0
9	MPG	B	1280	-	-	0/25/22/25	0/0/0/0
6	BCL	C	1324	-	-	0/37/137/137	0/0/9/9
7	BPB	C	1325	-	-	0/42/101/105	0/1/6/6
11	MQ7	C	1327	-	-	0/41/61/61	0/2/2/2
12	NS5	C	1328	-	-	0/43/43/43	0/0/0/0
13	OTP	C	1329	-	-	0/45/45/55	0/0/0/0
9	MPG	C	1330	-	-	0/14/14/25	0/0/0/0
14	PO4	C	1331	-	-	0/0/0/0	0/0/0/0
14	PO4	C	1332	-	-	0/0/0/0	0/0/0/0

The worst 5 of 120 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1333	HEM	C2D-C3D	-6.78	1.34	1.54
5	A	1336	HEM	C2D-C3D	-6.24	1.35	1.54
5	A	1335	HEM	C2D-C3D	-6.08	1.36	1.54
5	A	1333	HEM	C2C-C1C	-6.03	1.41	1.52
5	A	1334	HEM	C2D-C3D	-5.81	1.37	1.54

The worst 5 of 181 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	C	1329	OTP	C40-C39-C37	-8.38	112.70	126.39
7	C	1325	BPB	CBC-CAC-C3C	-7.10	110.69	127.07
7	B	1277	BPB	CBC-CAC-C3C	-7.05	110.81	127.07
7	C	1325	BPB	C2C-C3C-C4C	-6.58	101.23	107.24
7	B	1277	BPB	C2C-C3C-C4C	-6.36	101.43	107.24

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

15 monomers are involved in 52 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1333	HEM	3	0
5	A	1335	HEM	1	0
5	A	1336	HEM	3	0
6	B	1274	BCL	3	0
6	B	1275	BCL	5	0
6	B	1276	BCL	6	0
7	B	1277	BPB	8	0
9	B	1279	MPG	1	0
9	B	1280	MPG	1	0
6	C	1324	BCL	8	0
7	C	1325	BPB	5	0
11	C	1327	MQ7	2	0
12	C	1328	NS5	5	0
13	C	1329	OTP	7	0
9	C	1330	MPG	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	A	332/356 (93%)	-0.08	3 (0%) 85 78	21, 38, 56, 78	0
2	B	273/274 (99%)	-0.06	1 (0%) 93 90	27, 55, 89, 113	0
3	C	323/324 (99%)	0.04	8 (2%) 61 50	28, 56, 88, 109	0
4	D	242/258 (93%)	0.51	13 (5%) 29 23	63, 92, 115, 136	0
All	All	1170/1212 (96%)	0.08	25 (2%) 67 58	21, 54, 101, 136	0

The worst 5 of 25 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	85	THR	4.6
2	B	202	ASP	3.5
3	C	54	SER	3.4
4	D	159	ALA	3.0
4	D	144	SER	2.9

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	D	1	10/11	0.86	0.38	-	64,69,72,73	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
8	DGA	B	1278	37/44	0.72	0.41	5.44	53,77,94,103	0
12	NS5	C	1328	40/40	0.71	0.48	4.45	50,79,103,106	0
9	MPG	B	1280	25/25	0.68	0.47	4.43	67,77,97,98	0
13	OTP	C	1329	41/49	0.81	0.38	4.38	48,60,78,84	0
9	MPG	B	1279	25/25	0.73	0.45	3.55	80,101,116,120	0
6	BCL	B	1274	65/66	0.92	0.27	1.99	32,43,164,175	0
9	MPG	C	1330	17/25	0.64	0.46	0.71	60,84,100,103	0
14	PO4	C	1331	5/5	0.91	0.49	0.63	93,95,102,104	0
7	BPB	C	1325	61/65	0.89	0.31	0.60	51,68,83,88	0
11	MQ7	C	1327	48/48	0.89	0.29	0.41	32,42,66,70	0
6	BCL	B	1275	66/66	0.94	0.23	0.35	27,33,42,50	0
6	BCL	B	1276	66/66	0.95	0.23	0.08	18,27,47,48	0
5	HEM	A	1333	43/43	0.95	0.29	-0.06	23,31,34,35	0
7	BPB	B	1277	65/65	0.94	0.23	-0.09	27,35,47,60	0
6	BCL	C	1324	66/66	0.94	0.23	-0.24	29,37,54,66	0
5	HEM	A	1336	43/43	0.95	0.21	-0.68	32,37,53,58	0
5	HEM	A	1334	43/43	0.96	0.23	-0.70	23,25,29,35	0
5	HEM	A	1335	43/43	0.96	0.20	-1.05	22,25,27,30	0
10	FE2	C	1326	1/1	0.98	0.05	-3.20	48,48,48,48	0
14	PO4	C	1332	5/5	0.92	0.27	-	66,68,71,71	0

6.5 Other polymers [i](#)

There are no such residues in this entry.