



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 4, 2017 – 08:18 PM EDT

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 : unknown
Resolution : 3.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030345
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0

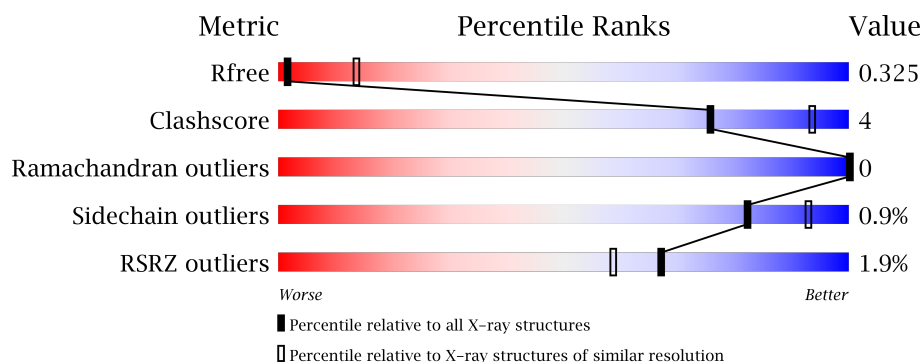
1 Overall quality at a glance

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}	100719	1195 (3.60-3.40)
Clashscore	112137	1322 (3.60-3.40)
Ramachandran outliers	110173	1283 (3.60-3.40)
Sidechain outliers	110143	1284 (3.60-3.40)
RSRZ outliers	101464	1226 (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	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: -10px; left: 0; width: 100%;"></div> <div style="position: absolute; top: 0; left: 0; width: 100%; height: 10px;"> <div style="width: 2%; height: 10px; background-color: red;"></div> <div style="width: 92%; height: 10px; background-color: green;"></div> <div style="width: 7%; height: 10px; background-color: yellow;"></div> <div style="width: 1%; height: 10px; background-color: grey;"></div> </div> </div> </div>
2	B	274	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: 0; left: 0; width: 100%; height: 10px;"> <div style="width: 92%; height: 10px; background-color: green;"></div> <div style="width: 8%; height: 10px; background-color: yellow;"></div> </div> </div> </div>
3	C	324	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: -10px; left: 0; width: 100%;"></div> <div style="position: absolute; top: 0; left: 0; width: 100%; height: 10px;"> <div style="width: 2%; height: 10px; background-color: red;"></div> <div style="width: 94%; height: 10px; background-color: green;"></div> <div style="width: 5%; height: 10px; background-color: yellow;"></div> </div> </div> </div>

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Ideal geometry (proteins) : Engh & Huber (2001)
 Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
 Validation Pipeline (wwPDB-VP) : rb-20030345

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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	405	-	-	-	X
13	OTP	C	406	-	-	-	X
14	PO4	C	408	-	-	-	X
6	DGA	A	405	-	-	-	X
9	MPG	B	305	-	-	-	X
9	MPG	B	306	-	-	-	X
9	MPG	C	407	-	-	-	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			

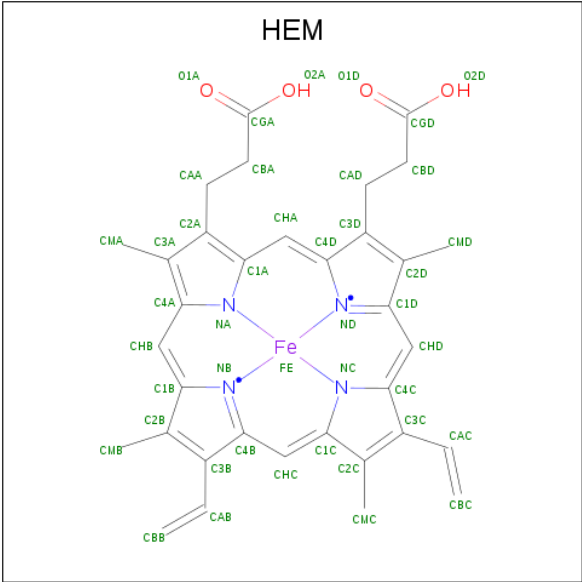
- Molecule 3 is a protein called REACTION CENTER PROTEIN M CHAIN.

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.

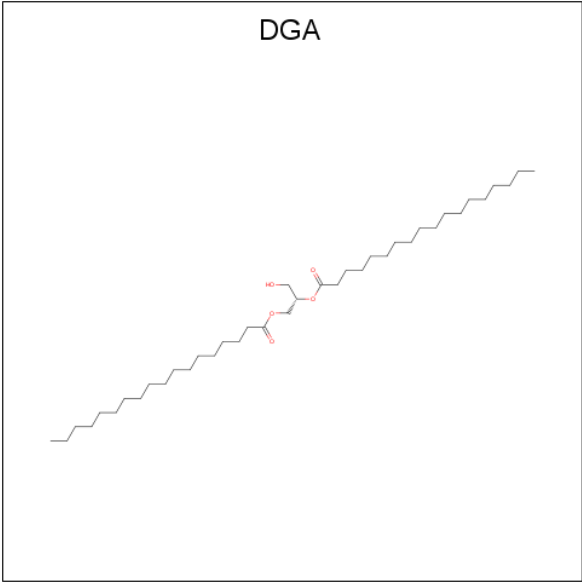
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	243	Total	C	N	O	S	0	0	0
			1771	1140	297	332	2			

- Molecule 5 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



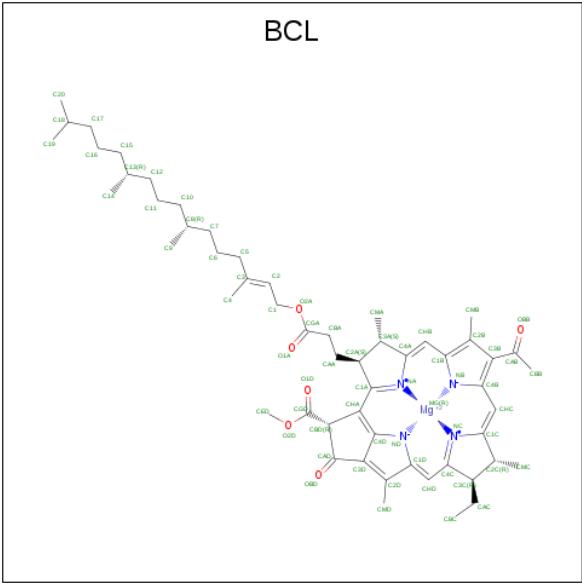
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
5	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
5	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
5	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 6 is DIACYL GLYCEROL (three-letter code: DGA) (formula: C₃₉H₇₆O₅).



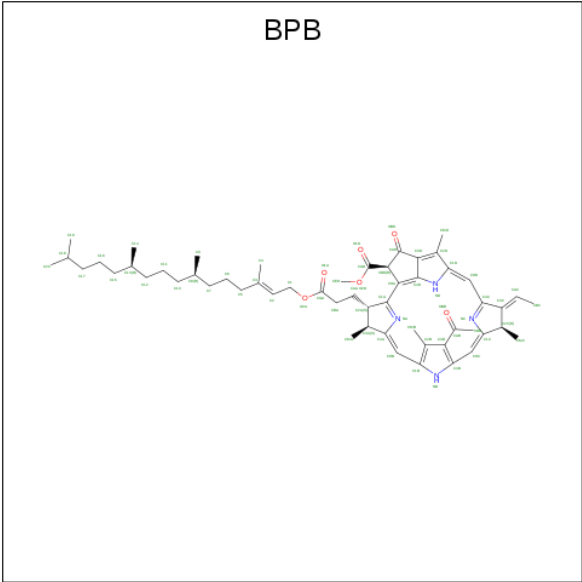
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			37	33	4		

- Molecule 7 is BACTERIOCHLOROPHYLL A (three-letter code: BCL) (formula: C₅₅H₇₄MgN₄O₆).



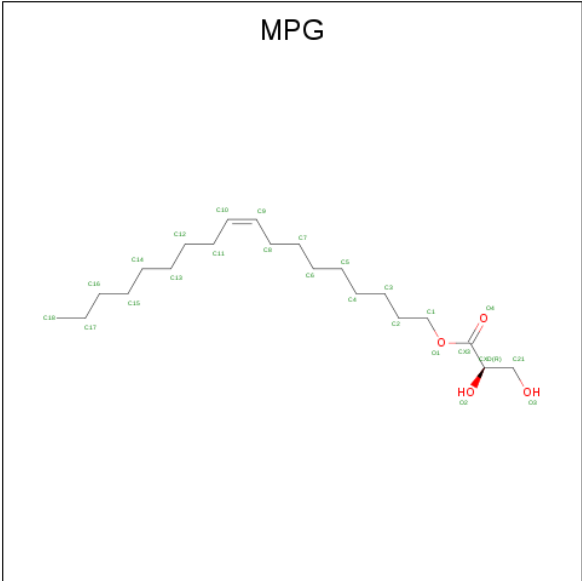
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	B	1	Total	C	Mg	N	O	0	0
			65	54	1	4	6		
7	B	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
7	B	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
7	C	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

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



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

- Molecule 9 is [(Z)-octadec-9-enyl] (2R)-2,3-bis(oxidanyl)propanoate (three-letter code: MPG) (formula: C₂₁H₄₀O₄).



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

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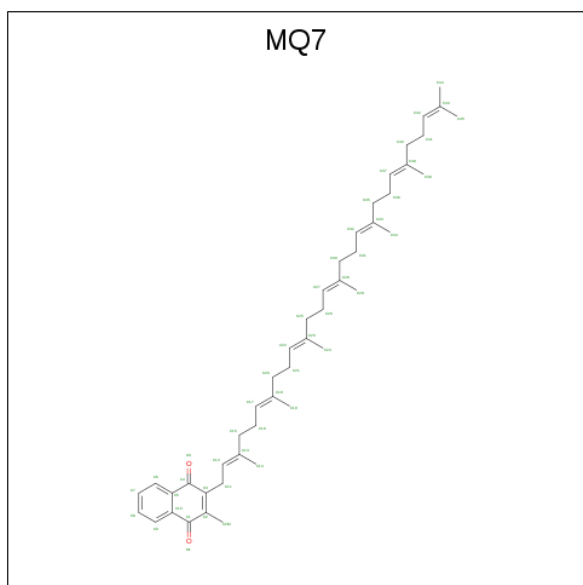
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	B	1	Total C O 25 21 4	0	0
9	C	1	Total C 17 17	0	0

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

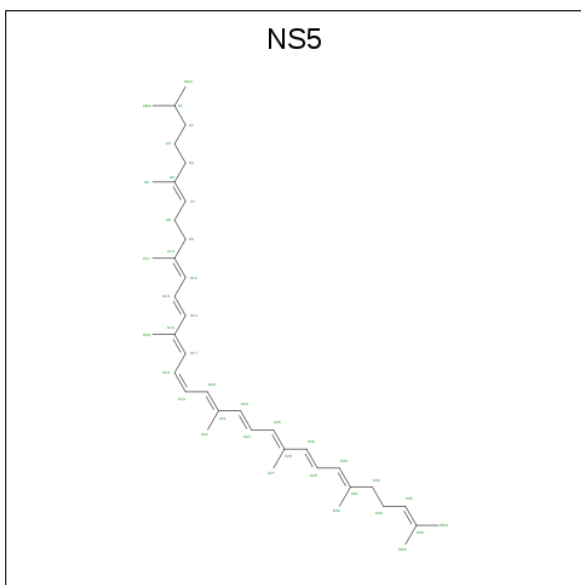
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	C	1	Total Fe 1 1	0	0

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



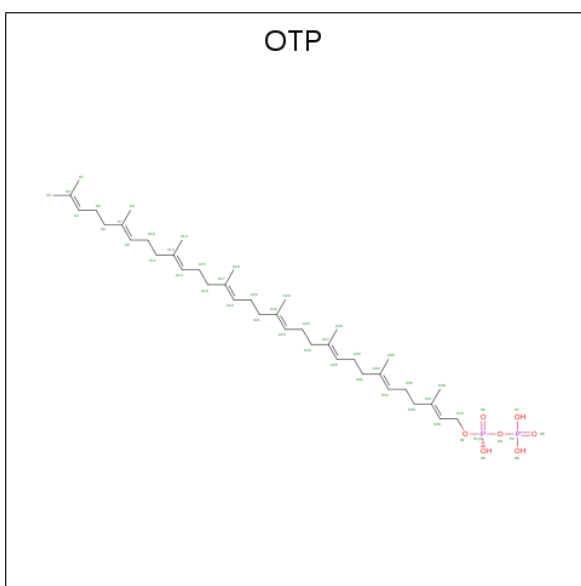
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	C	1	Total C O 48 46 2	0	0

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



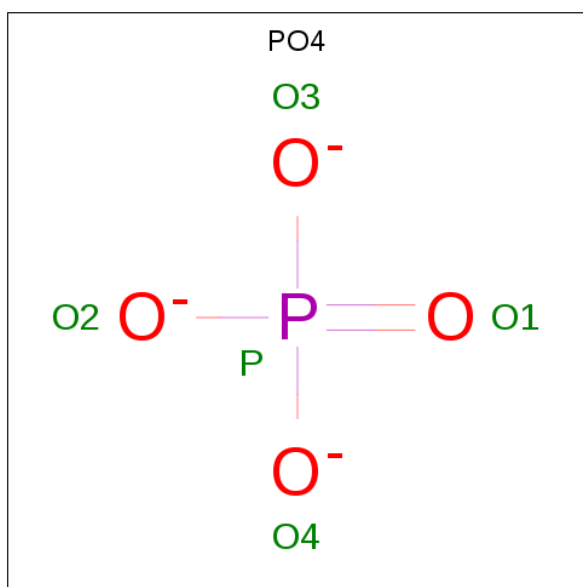
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	C	1	Total	C	0	0
			40	40		

- 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 the various outlier classes 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.

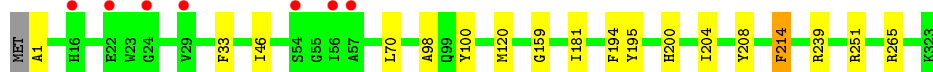
- Molecule 1: PHOTOSYNTHETIC REACTION CENTER CYTOCHROME C SUBUNIT



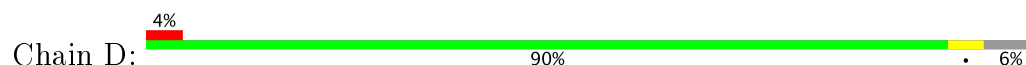
- Molecule 2: REACTION CENTER PROTEIN L CHAIN



- 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 , 77.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.32$, $\langle L^2 \rangle = 0.15$	Xtriage
Estimated twinning fraction	No twinning to report.	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, 0.333 respectively for untwinned datasets, and 0.375, 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	A	37	0	58	0	0
7	B	197	0	217	14	0
7	C	66	0	74	8	0
8	B	65	0	74	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	C	61	0	63	5	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.

All (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)
8:C:402:BPB:HBBB	8:C:402:BPB:HHC	1.62	0.81
8:B:304:BPB:HBBB	8:B:304:BPB:HHC	1.61	0.81
7:B:301:BCL:HHC	7:B:301:BCL:HBB2	1.75	0.68
2:B:181:PHE:HB3	8:C:402:BPB:HBBA	1.80	0.63
7:B:303:BCL:HMD2	7:C:401:BCL:HBB3	1.81	0.62
13:C:406:OTP:C29	13:C:406:OTP:H331	2.29	0.62
2:B:3:LEU:HG	3:C:251:ARG:NE	2.16	0.61
3:C:159:GLY:HA3	12:C:405:NS5:C11	2.34	0.58
2:B:39:ILE:HD12	11:C:404:MQ7:H452	1.86	0.58
2:B:124:PRO:HD3	8:B:304:BPB:HAC	1.86	0.58
3:C:159:GLY:HA3	12:C:405:NS5:H113	1.86	0.58
1:A:56:TYR:HB3	5:A:401:HEM:O2A	2.04	0.57
1:A:240:LEU:HD11	5:A:404:HEM:CHB	2.36	0.56
2:B:244:GLY:O	7:B:302:BCL:HED3	2.06	0.55
9:B:305:MPG:H21C	3:C:1:ALA:HA	1.87	0.55
5:A:401:HEM:HBC2	5:A:401:HEM:HMC2	1.89	0.55
5:A:404:HEM:HMB2	5:A:404:HEM:HBB2	1.90	0.54
3:C:195:TYR:CE2	7:C:401:BCL:HMC2	2.42	0.54
2:B:62:PHE:CZ	13:C:406:OTP:H333	2.43	0.54
2:B:3:LEU:HD11	3:C:251:ARG:HD2	1.89	0.53
2:B:168:HIS:CE1	7:B:302:BCL:HMC2	2.44	0.53
4:D:92:GLN:HA	4:D:101:LEU:HD23	1.93	0.51
8:C:402:BPB:CBB	8:C:402:BPB:HHC	2.38	0.50
13:C:406:OTP:C29	13:C:406:OTP:C33	2.89	0.50
8:B:304:BPB:HBB	3:C:208:TYR:CD2	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:16:LEU:HD13	2:B:106:GLU:HG2	1.93	0.50
7:B:302:BCL:HMB1	7:B:302:BCL:HBB3	1.94	0.49
2:B:148:TYR:CE1	8:B:304:BPB:H14B	2.47	0.49
5:A:403:HEM:HBC2	5:A:403:HEM:HMC2	1.95	0.48
2:B:181:PHE:CD2	8:C:402:BPB:HBB	2.48	0.48
2:B:39:ILE:CD1	11:C:404:MQ7:H452	2.44	0.48
2:B:42:ILE:CD1	8:B:304:BPB:H4A	2.45	0.47
7:B:303:BCL:HED3	13:C:406:OTP:H282	1.95	0.47
3:C:195:TYR:OH	7:C:401:BCL:OBB	2.16	0.47
7:B:302:BCL:H2C	7:C:401:BCL:H2C	1.98	0.46
7:B:301:BCL:CBB	7:B:301:BCL:HHC	2.43	0.46
2:B:259:TRP:N	2:B:260:PRO:CD	2.79	0.46
7:B:303:BCL:HMA1	7:B:303:BCL:H142	1.98	0.46
1:A:212:VAL:HG11	4:D:1:FME:CE	2.45	0.46
4:D:160:ALA:HB3	4:D:214:LEU:HD23	1.97	0.46
9:B:306:MPG:H52C	9:C:407:MPG:H182	1.98	0.46
3:C:120:MET:SD	7:C:401:BCL:H172	2.56	0.45
3:C:33:PHE:CE2	3:C:46:ILE:HD12	2.52	0.45
8:B:304:BPB:CBB	8:B:304:BPB:HHC	2.38	0.45
2:B:168:HIS:NE2	7:B:302:BCL:HMC2	2.31	0.45
5:A:404:HEM:CMB	5:A:404:HEM:HBB2	2.47	0.44
2:B:179:PHE:HA	2:B:182:VAL:HG12	1.99	0.44
5:A:401:HEM:HBB2	5:A:401:HEM:HMB2	2.00	0.44
7:B:303:BCL:HMB1	7:B:303:BCL:CBB	2.47	0.44
3:C:200:HIS:CE1	3:C:204:ILE:HD11	2.53	0.43
7:B:303:BCL:HMD2	7:C:401:BCL:CBB	2.48	0.42
2:B:42:ILE:HD11	8:B:304:BPB:H4A	2.00	0.42
2:B:195:LEU:HD21	3:C:265:ARG:HG3	2.00	0.42
2:B:151:LEU:HD21	13:C:406:OTP:H301	2.02	0.42
12:C:405:NS5:H18	12:C:405:NS5:H161	1.81	0.42
13:C:406:OTP:H29	13:C:406:OTP:C33	2.50	0.42
2:B:177:VAL:HG11	7:B:301:BCL:CMD	2.50	0.42
3:C:195:TYR:CZ	7:C:401:BCL:HMC2	2.55	0.41
3:C:70:LEU:HD21	12:C:405:NS5:H323	2.02	0.41
3:C:239:ARG:NH1	4:D:39:GLU:OE1	2.50	0.41
2:B:233:GLY:HA3	3:C:214:PHE:CE1	2.56	0.41
2:B:151:LEU:HD23	2:B:151:LEU:HA	1.90	0.41
7:B:303:BCL:HED3	13:C:406:OTP:C28	2.51	0.41
1:A:80:TRP:CD1	1:A:133:TYR:HB2	2.56	0.41
4:D:202:ASP:HB3	4:D:209:VAL:HB	2.01	0.41
7:C:401:BCL:HMB1	7:C:401:BCL:CBB	2.50	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:B:304:BPB:HBBA	3:C:208:TYR:HB3	2.04	0.40
3:C:181:ILE:HA	3:C:181:ILE:HD13	1.96	0.40
8:C:402:BPB:C9	12:C:405:NS5:HM32	2.51	0.40
3:C:98:ALA:HB3	3:C:100:TYR:CZ	2.56	0.40

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
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 [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	A	280/297 (94%)	279 (100%)	1 (0%)	93	97
2	B	218/219 (100%)	215 (99%)	3 (1%)	71	89

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	247/250 (99%)	245 (99%)	2 (1%)	85	94
4	D	167/212 (79%)	165 (99%)	2 (1%)	75	90
All	All	912/978 (93%)	904 (99%)	8 (1%)	82	93

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	TYR
2	B	160	PHE
2	B	249	ILE
2	B	272	TRP
3	C	194	PHE
3	C	214	PHE
4	D	185	LEU
4	D	236	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	37	GLN
1	A	302	GLN
2	B	183	ASN
2	B	239	ASN
3	C	200	HIS
4	D	8	GLN

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	9,9,10	0.74	0	7,9,11	3.44	4 (57%)

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	O-C-CA	-2.54	119.22	125.15
4	D	1	FME	CB-CA-C	-2.47	107.59	111.65
4	D	1	FME	CE-SD-CG	4.22	115.49	100.35

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	401	1	28,50,50	0.69	0	17,82,82	1.65	2 (11%)
5	HEM	A	402	1	28,50,50	0.72	0	17,82,82	1.77	4 (23%)
5	HEM	A	403	1	28,50,50	1.01	2 (7%)	17,82,82	1.44	3 (17%)
5	HEM	A	404	1	28,50,50	0.83	1 (3%)	17,82,82	1.37	4 (23%)
6	DGA	A	405	1	36,36,43	1.21	2 (5%)	38,38,45	1.28	3 (7%)
7	BCL	B	301	-	54,73,74	2.31	12 (22%)	63,113,115	2.21	18 (28%)
7	BCL	B	302	-	55,74,74	2.25	12 (21%)	65,115,115	2.15	22 (33%)
7	BCL	B	303	-	55,74,74	2.38	12 (21%)	65,115,115	1.97	17 (26%)
8	BPB	B	304	-	63,70,70	2.88	15 (23%)	67,101,101	2.14	18 (26%)
9	MPG	B	305	-	24,24,24	1.33	1 (4%)	23,25,25	1.17	2 (8%)
9	MPG	B	306	-	24,24,24	1.58	1 (4%)	23,25,25	0.93	2 (8%)
7	BCL	C	401	-	55,74,74	2.37	11 (20%)	65,115,115	1.95	18 (27%)
8	BPB	C	402	-	59,66,70	2.97	15 (25%)	62,96,101	2.18	13 (20%)
11	MQ7	C	404	-	49,49,49	1.45	2 (4%)	61,63,63	1.25	8 (13%)
12	NS5	C	405	-	39,39,39	2.22	7 (17%)	44,46,46	2.15	12 (27%)
13	OTP	C	406	-	40,40,48	1.51	2 (5%)	46,47,61	2.17	13 (28%)
9	MPG	C	407	-	16,16,24	0.41	0	15,15,25	0.66	0
14	PO4	C	408	-	4,4,4	0.74	0	6,6,6	0.54	0
14	PO4	C	409	-	4,4,4	0.63	0	6,6,6	0.59	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	401	1	-	0/6/54/54	0/0/8/8
5	HEM	A	402	1	-	0/6/54/54	0/0/8/8
5	HEM	A	403	1	-	0/6/54/54	0/0/8/8
5	HEM	A	404	1	-	0/6/54/54	0/0/8/8
6	DGA	A	405	1	-	0/37/37/45	0/0/0/0
7	BCL	B	301	-	-	0/36/136/137	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	BCL	B	302	-	-	0/37/137/137	0/0/9/9
7	BCL	B	303	-	-	0/37/137/137	0/0/9/9
8	BPB	B	304	-	-	0/47/105/105	0/1/6/6
9	MPG	B	305	-	-	0/25/25/25	0/0/0/0
9	MPG	B	306	-	-	0/25/25/25	0/0/0/0
7	BCL	C	401	-	-	0/37/137/137	0/0/9/9
8	BPB	C	402	-	-	0/43/101/105	0/1/6/6
11	MQ7	C	404	-	-	0/41/61/61	0/2/2/2
12	NS5	C	405	-	-	0/43/43/43	0/0/0/0
13	OTP	C	406	-	-	0/45/45/55	0/0/0/0
9	MPG	C	407	-	-	0/14/14/25	0/0/0/0
14	PO4	C	408	-	-	0/0/0/0	0/0/0/0
14	PO4	C	409	-	-	0/0/0/0	0/0/0/0

All (95) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	C	405	NS5	C9-C8	-5.24	1.35	1.53
8	C	402	BPB	C1A-NA	-4.95	1.26	1.36
8	B	304	BPB	C1A-NA	-4.40	1.28	1.36
8	B	304	BPB	C4C-NC	-4.26	1.27	1.36
8	C	402	BPB	C4C-NC	-4.05	1.27	1.36
7	C	401	BCL	C3C-C4C	-4.00	1.46	1.51
7	B	303	BCL	C2C-C3C	-3.42	1.44	1.54
5	A	403	HEM	C1B-NB	-3.42	1.32	1.36
7	B	301	BCL	C2C-C3C	-3.15	1.45	1.54
7	B	301	BCL	CAC-C3C	-3.11	1.47	1.54
8	C	402	BPB	C1C-NC	-3.07	1.32	1.38
8	B	304	BPB	C1C-NC	-3.01	1.32	1.38
7	C	401	BCL	C2C-C3C	-2.91	1.46	1.54
7	B	302	BCL	C2C-C3C	-2.82	1.46	1.54
7	B	303	BCL	C3C-C4C	-2.74	1.48	1.51
7	B	302	BCL	C3C-C4C	-2.72	1.48	1.51
7	B	303	BCL	CAC-C3C	-2.71	1.48	1.54
5	A	404	HEM	C1B-NB	-2.62	1.33	1.36
7	B	302	BCL	CAC-C3C	-2.56	1.48	1.54
7	C	401	BCL	CAC-C3C	-2.39	1.49	1.54
7	B	301	BCL	C3C-C4C	-2.31	1.48	1.51
8	B	304	BPB	C1D-ND	-2.19	1.33	1.38
5	A	403	HEM	C3B-C2B	-2.05	1.37	1.40
7	B	301	BCL	CHD-C4C	2.16	1.47	1.41
12	C	405	NS5	C28-C26	2.24	1.50	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	C	402	BPB	C4C-C3C	2.27	1.50	1.45
7	B	303	BCL	CHD-C4C	2.28	1.47	1.41
12	C	405	NS5	C14-C15	2.29	1.50	1.45
7	B	302	BCL	CHD-C4C	2.33	1.48	1.41
13	C	406	OTP	C40-C39	2.37	1.53	1.50
8	B	304	BPB	C4B-CHC	2.40	1.49	1.40
8	C	402	BPB	C1B-CHB	2.46	1.49	1.40
7	B	302	BCL	C1B-CHB	2.52	1.46	1.40
8	C	402	BPB	C4B-CHC	2.65	1.50	1.40
7	C	401	BCL	C1B-CHB	2.70	1.47	1.40
8	B	304	BPB	CHD-C4C	2.92	1.47	1.40
12	C	405	NS5	C29-C30	2.93	1.52	1.43
8	B	304	BPB	C1B-CHB	2.94	1.51	1.40
8	C	402	BPB	CHD-C4C	3.09	1.47	1.40
7	B	303	BCL	C1B-CHB	3.18	1.48	1.40
7	B	301	BCL	C4B-CHC	3.18	1.48	1.40
7	B	301	BCL	C1B-CHB	3.22	1.48	1.40
7	B	302	BCL	C3D-C2D	3.32	1.47	1.39
8	C	402	BPB	C3B-C2B	3.47	1.47	1.39
7	B	302	BCL	C4B-CHC	3.50	1.49	1.40
8	B	304	BPB	C3B-C2B	3.50	1.47	1.39
7	B	301	BCL	C3B-C2B	3.54	1.47	1.39
7	C	401	BCL	C4B-CHC	3.55	1.49	1.40
7	C	401	BCL	C3B-C2B	3.56	1.47	1.39
7	B	303	BCL	C3B-C2B	3.67	1.47	1.39
7	B	303	BCL	C4B-CHC	3.67	1.49	1.40
7	C	401	BCL	C3D-C2D	3.71	1.47	1.39
7	B	303	BCL	C3D-C2D	3.73	1.48	1.39
8	B	304	BPB	OBD-CAD	3.74	1.29	1.22
12	C	405	NS5	C12-C10	3.77	1.38	1.34
7	B	301	BCL	OBD-CAD	3.82	1.27	1.22
8	B	304	BPB	C3D-C2D	3.92	1.49	1.38
8	C	402	BPB	OBD-CAD	3.92	1.29	1.22
7	C	401	BCL	O2A-CGA	3.92	1.44	1.33
8	C	402	BPB	C3D-C2D	4.00	1.49	1.38
7	B	302	BCL	C3B-C2B	4.01	1.48	1.39
7	B	301	BCL	C3D-C2D	4.03	1.48	1.39
7	B	302	BCL	O2D-CGD	4.15	1.43	1.33
7	B	301	BCL	O2A-CGA	4.17	1.45	1.33
8	B	304	BPB	O2A-CGA	4.28	1.45	1.33
7	B	303	BCL	O2A-CGA	4.28	1.45	1.33
7	B	303	BCL	OBD-CAD	4.40	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	304	BPB	CHD-C1D	4.43	1.47	1.38
7	B	302	BCL	O2A-CGA	4.45	1.46	1.33
8	C	402	BPB	O2D-CGD	4.49	1.44	1.33
6	A	405	DGA	OG2-CB1	4.52	1.47	1.34
8	C	402	BPB	O2A-CGA	4.54	1.46	1.33
7	B	302	BCL	OBD-CAD	4.67	1.29	1.22
8	B	304	BPB	O2D-CGD	4.91	1.45	1.33
6	A	405	DGA	OG1-CA1	4.95	1.47	1.33
7	C	401	BCL	O2D-CGD	5.17	1.46	1.33
7	B	303	BCL	O2D-CGD	5.18	1.46	1.33
8	B	304	BPB	C3B-C4B	5.22	1.47	1.41
8	C	402	BPB	CHD-C1D	5.31	1.49	1.38
7	B	301	BCL	O2D-CGD	5.53	1.47	1.33
11	C	404	MQ7	C10-C5	5.60	1.50	1.40
8	C	402	BPB	C3B-C4B	5.87	1.48	1.41
7	C	401	BCL	OBD-CAD	6.04	1.31	1.22
9	B	305	MPG	O1-CX3	6.12	1.45	1.33
11	C	404	MQ7	C3-C2	6.67	1.50	1.35
9	B	306	MPG	O1-CX3	7.24	1.48	1.33
12	C	405	NS5	C29-C28	7.42	1.53	1.34
12	C	405	NS5	C35-C36	7.57	1.54	1.32
13	C	406	OTP	C39-C37	8.41	1.54	1.33
7	B	302	BCL	CHC-C1C	11.50	1.48	1.33
7	B	301	BCL	CHC-C1C	11.51	1.48	1.33
7	C	401	BCL	CHC-C1C	11.54	1.48	1.33
7	B	303	BCL	CHC-C1C	12.10	1.48	1.33
8	C	402	BPB	CAC-C3C	16.38	1.52	1.33
8	B	304	BPB	CAC-C3C	16.84	1.53	1.33

All (159) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	C	402	BPB	CBC-CAC-C3C	-7.40	110.69	127.00
8	B	304	BPB	CBC-CAC-C3C	-7.35	110.81	127.00
8	C	402	BPB	C2C-C3C-C4C	-6.32	101.23	107.35
8	B	304	BPB	C2C-C3C-C4C	-6.12	101.43	107.35
7	B	301	BCL	C3C-C2C-C1C	-6.06	92.09	101.87
12	C	405	NS5	C29-C28-C26	-5.95	109.70	126.42
13	C	406	OTP	C38-C37-C36	-4.65	107.21	115.29
7	B	302	BCL	C3C-C2C-C1C	-4.63	94.39	101.87
13	C	406	OTP	C38-C37-C39	-4.62	111.36	123.69
7	B	303	BCL	C3C-C2C-C1C	-4.59	94.46	101.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	C	405	NS5	C34-C35-C36	-4.40	112.08	127.80
7	B	302	BCL	OBD-CAD-C3D	-4.34	120.04	128.03
13	C	406	OTP	C36-C37-C39	-4.18	112.54	121.10
5	A	402	HEM	CBA-CAA-C2A	-4.10	104.64	112.48
7	C	401	BCL	OBD-CAD-C3D	-4.10	120.47	128.03
8	C	402	BPB	CMD-C2D-C3D	-4.08	117.98	127.86
9	B	305	MPG	O1-CX3-O4	-4.07	116.20	124.11
7	B	301	BCL	OBD-CAD-C3D	-3.95	120.76	128.03
5	A	401	HEM	CBA-CAA-C2A	-3.94	104.95	112.48
7	B	302	BCL	CMD-C2D-C3D	-3.92	117.62	124.89
8	B	304	BPB	CMD-C2D-C3D	-3.92	118.38	127.86
12	C	405	NS5	C19-C20-C21	-3.90	121.74	127.31
7	C	401	BCL	C3C-C2C-C1C	-3.86	95.64	101.87
12	C	405	NS5	C24-C25-C26	-3.74	121.98	127.31
12	C	405	NS5	C18-C17-C15	-3.73	121.98	127.31
12	C	405	NS5	CM3-C36-C35	-3.72	111.43	122.65
7	B	303	BCL	CMD-C2D-C3D	-3.68	118.07	124.89
7	B	303	BCL	OBD-CAD-C3D	-3.65	121.30	128.03
13	C	406	OTP	C18-C17-C19	-3.59	114.10	123.69
11	C	404	MQ7	C21-C22-C23	-3.57	118.70	127.68
7	C	401	BCL	O2D-CGD-O1D	-3.54	116.70	123.82
12	C	405	NS5	CM4-C36-C35	-3.49	112.11	122.65
8	B	304	BPB	CHD-C4C-C3C	-3.22	120.05	125.26
13	C	406	OTP	C21-C22-C24	-3.20	114.55	121.10
8	B	304	BPB	OBD-CAD-C3D	-3.15	120.69	128.43
7	B	302	BCL	O2D-CGD-O1D	-3.07	117.64	123.82
7	B	301	BCL	C1D-CHD-C4C	-3.01	121.43	125.92
7	B	302	BCL	C1-C2-C3	-3.01	120.41	125.96
8	C	402	BPB	O2D-CGD-O1D	-3.01	117.76	123.82
7	C	401	BCL	C1D-CHD-C4C	-2.97	121.49	125.92
7	B	301	BCL	O1D-CGD-CBD	-2.93	119.33	124.60
7	C	401	BCL	CMD-C2D-C3D	-2.93	119.47	124.89
7	B	302	BCL	C1D-CHD-C4C	-2.86	121.65	125.92
8	B	304	BPB	C1-C2-C3	-2.86	120.69	125.96
5	A	401	HEM	CBD-CAD-C3D	-2.82	107.09	112.47
8	B	304	BPB	O1D-CGD-CBD	-2.79	119.59	124.60
7	B	301	BCL	CMD-C2D-C3D	-2.74	119.81	124.89
7	B	301	BCL	C2A-C1A-CHA	-2.66	119.20	123.92
7	B	301	BCL	C1B-CHB-C4A	-2.65	124.88	130.12
5	A	402	HEM	CMA-C3A-C4A	-2.62	124.44	128.46
13	C	406	OTP	C30-C29-C27	-2.61	121.11	127.68
8	B	304	BPB	O2A-CGA-O1A	-2.52	117.30	123.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	403	HEM	C4C-C3C-C2C	-2.52	105.14	106.90
11	C	404	MQ7	C11-C12-C13	-2.47	122.57	126.71
7	B	302	BCL	C2A-C1A-CHA	-2.41	119.64	123.92
11	C	404	MQ7	C20-C18-C17	-2.41	116.17	121.10
7	B	302	BCL	C1B-CHB-C4A	-2.41	125.35	130.12
7	B	303	BCL	C2A-C1A-CHA	-2.40	119.66	123.92
7	C	401	BCL	O2A-CGA-O1A	-2.40	117.59	123.55
5	A	403	HEM	C1D-C2D-C3D	-2.39	105.33	107.00
7	B	303	BCL	C1D-CHD-C4C	-2.31	122.48	125.92
12	C	405	NS5	C30-C29-C28	-2.29	116.21	123.23
5	A	404	HEM	CMA-C3A-C4A	-2.28	124.96	128.46
13	C	406	OTP	C10-C9-C7	-2.25	122.04	127.68
9	B	306	MPG	O4-CX3-CXD	-2.22	118.23	123.60
7	B	301	BCL	OBD-CAD-CBD	-2.18	122.65	125.94
11	C	404	MQ7	C2M-C2-C3	-2.16	119.81	124.20
7	B	302	BCL	CHC-C1C-NC	-2.15	121.53	124.51
7	B	301	BCL	CHC-C1C-NC	-2.15	121.54	124.51
7	C	401	BCL	C1B-CHB-C4A	-2.15	125.86	130.12
7	B	303	BCL	C4B-CHC-C1C	-2.13	125.90	130.12
7	B	303	BCL	OBD-CAD-CBD	-2.11	122.76	125.94
5	A	402	HEM	CMD-C2D-C1D	-2.09	125.24	128.46
7	B	303	BCL	O1D-CGD-CBD	-2.09	120.85	124.60
7	B	302	BCL	C7-C6-C5	-2.06	107.40	113.11
8	C	402	BPB	OBD-CAD-C3D	-2.05	123.39	128.43
11	C	404	MQ7	C11-C3-C2	-2.04	119.45	123.47
12	C	405	NS5	C13-C14-C15	-2.03	120.73	126.42
5	A	404	HEM	CAA-CBA-CGA	-2.02	109.20	112.66
7	B	302	BCL	O2A-CGA-O1A	-2.01	118.55	123.55
5	A	403	HEM	CAA-CBA-CGA	-2.01	109.23	112.66
8	B	304	BPB	CED-O2D-CGD	2.02	120.70	115.97
7	B	303	BCL	CHB-C4A-NA	2.02	127.31	124.51
8	C	402	BPB	C3C-C4C-NC	2.05	113.05	109.60
8	B	304	BPB	CMB-C2B-C3B	2.07	128.74	124.89
8	B	304	BPB	C3D-C4D-ND	2.16	117.28	110.81
7	B	303	BCL	C1-O2A-CGA	2.19	122.02	116.77
7	B	302	BCL	CED-O2D-CGD	2.19	121.11	115.97
11	C	404	MQ7	C34-C33-C35	2.20	119.11	115.29
7	B	301	BCL	C1-O2A-CGA	2.22	122.10	116.77
7	C	401	BCL	O2A-CGA-CBA	2.23	118.40	111.90
7	C	401	BCL	C4-C3-C5	2.25	119.19	115.29
8	B	304	BPB	C4-C3-C5	2.28	119.24	115.29
5	A	402	HEM	C4A-C3A-C2A	2.28	108.58	107.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	404	HEM	C4A-C3A-C2A	2.32	108.61	107.00
5	A	404	HEM	CMC-C2C-C3C	2.32	129.20	124.89
7	B	301	BCL	C4-C3-C5	2.33	119.34	115.29
11	C	404	MQ7	C2M-C2-C1	2.35	120.17	116.23
12	C	405	NS5	C32-C31-C33	2.38	119.42	115.29
6	A	405	DGA	CG1-OG1-CA1	2.49	124.63	117.13
13	C	406	OTP	C13-C12-C11	2.52	119.66	115.29
8	C	402	BPB	O2A-CGA-CBA	2.53	119.25	111.90
7	B	302	BCL	CAA-C2A-C1A	2.54	120.31	111.97
7	C	401	BCL	CHB-C4A-NA	2.57	128.07	124.51
11	C	404	MQ7	C19-C18-C20	2.70	119.97	115.29
7	C	401	BCL	CAA-C2A-C1A	2.76	121.00	111.97
7	B	302	BCL	CBC-CAC-C3C	2.81	119.87	113.51
8	C	402	BPB	CAD-C3D-C2D	2.82	154.39	140.80
7	C	401	BCL	CAC-C3C-C4C	2.82	118.84	112.58
8	B	304	BPB	C3C-C4C-NC	2.87	114.44	109.60
7	B	301	BCL	CHB-C4A-NA	2.88	128.49	124.51
7	B	303	BCL	CED-O2D-CGD	2.88	122.73	115.97
7	C	401	BCL	CED-O2D-CGD	2.90	122.77	115.97
8	B	304	BPB	CAD-C3D-C2D	2.91	154.86	140.80
9	B	306	MPG	C1-O1-CX3	2.92	122.84	116.64
9	B	305	MPG	C1-O1-CX3	2.93	122.86	116.64
8	C	402	BPB	C4-C3-C5	2.94	120.39	115.29
7	B	301	BCL	CMB-C2B-C3B	2.94	130.35	124.89
13	C	406	OTP	C28-C27-C26	2.96	120.43	115.29
8	B	304	BPB	C2A-C1A-NA	3.02	110.39	107.83
7	B	302	BCL	C4-C3-C5	3.04	120.56	115.29
6	A	405	DGA	OG1-CA1-CA2	3.08	120.85	111.90
12	C	405	NS5	C6-C5-C4	3.17	120.78	115.29
7	B	303	BCL	CBC-CAC-C3C	3.19	120.73	113.51
8	C	402	BPB	C1-O2A-CGA	3.20	124.45	116.77
13	C	406	OTP	C18-C17-C16	3.26	120.95	115.29
7	C	401	BCL	CBC-CAC-C3C	3.30	120.98	113.51
7	B	301	BCL	CBC-CAC-C3C	3.32	121.04	113.51
7	B	302	BCL	O2D-CGD-CBD	3.50	117.55	111.30
7	B	303	BCL	CMB-C2B-C3B	3.59	131.55	124.89
7	B	302	BCL	CHB-C4A-NA	3.63	129.53	124.51
8	B	304	BPB	O2A-CGA-CBA	3.68	122.60	111.90
13	C	406	OTP	C33-C32-C31	3.70	121.71	115.29
7	B	302	BCL	CAC-C3C-C4C	3.76	120.93	112.58
7	C	401	BCL	C3D-CAD-CBD	3.82	113.00	107.60
7	B	302	BCL	O2A-CGA-CBA	3.85	123.12	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	302	BCL	CMB-C2B-C3B	3.89	132.11	124.89
12	C	405	NS5	C8-C9-C10	3.99	126.43	112.93
7	B	303	BCL	CAC-C3C-C4C	4.02	121.51	112.58
7	C	401	BCL	CMB-C2B-C3B	4.14	132.58	124.89
7	B	303	BCL	O2D-CGD-CBD	4.30	118.98	111.30
7	C	401	BCL	C2C-C3C-C4C	4.38	107.90	101.34
13	C	406	OTP	C23-C22-C21	4.52	123.14	115.29
7	B	301	BCL	O2D-CGD-CBD	4.54	119.41	111.30
13	C	406	OTP	C8-C7-C6	4.57	123.22	115.29
6	A	405	DGA	OG2-CB1-CB2	4.58	121.06	111.55
8	C	402	BPB	C2A-C1A-NA	4.75	111.86	107.83
8	B	304	BPB	O2D-CGD-CBD	5.13	120.47	111.30
7	B	302	BCL	C3D-CAD-CBD	5.32	115.11	107.60
7	C	401	BCL	O2D-CGD-CBD	5.50	121.13	111.30
8	C	402	BPB	O2D-CGD-CBD	5.53	121.18	111.30
7	B	301	BCL	CAC-C3C-C4C	5.58	124.97	112.58
7	B	302	BCL	C2C-C3C-C4C	5.74	109.94	101.34
7	B	303	BCL	C3D-CAD-CBD	5.90	115.94	107.60
8	C	402	BPB	CMD-C2D-C1D	6.05	134.47	125.04
8	B	304	BPB	CMD-C2D-C1D	6.29	134.84	125.04
7	B	303	BCL	C2C-C3C-C4C	6.29	110.76	101.34
7	B	301	BCL	C3D-CAD-CBD	6.35	116.57	107.60
7	B	301	BCL	C2C-C3C-C4C	7.00	111.82	101.34

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	401	HEM	3	0
5	A	403	HEM	1	0
5	A	404	HEM	3	0
7	B	301	BCL	3	0
7	B	302	BCL	5	0
7	B	303	BCL	6	0
8	B	304	BPB	8	0
9	B	305	MPG	1	0
9	B	306	MPG	1	0
7	C	401	BCL	8	0
8	C	402	BPB	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	C	404	MQ7	2	0
12	C	405	NS5	5	0
13	C	406	OTP	7	0
9	C	407	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

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, 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%)	-0.11	3 (0%) 84 77	21, 38, 56, 78	0
2	B	273/274 (99%)	-0.09	1 (0%) 92 89	27, 55, 89, 113	0
3	C	323/324 (99%)	0.01	7 (2%) 62 53	28, 56, 88, 109	0
4	D	242/258 (93%)	0.48	11 (4%) 34 27	63, 92, 115, 136	0
All	All	1170/1212 (96%)	0.05	22 (1%) 67 59	21, 54, 101, 136	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	85	THR	4.5
2	B	202	ASP	3.4
3	C	54	SER	3.3
4	D	159	ALA	3.0
4	D	144	SER	2.8
4	D	206	ASP	2.6
3	C	24	GLY	2.4
4	D	61	GLU	2.4
4	D	155	LEU	2.3
4	D	93	THR	2.3
1	A	161	THR	2.3
3	C	22	GLU	2.3
4	D	154	GLY	2.2
4	D	7	ALA	2.2
4	D	167	THR	2.2
3	C	57	ALA	2.2
3	C	16	HIS	2.2
4	D	91	ALA	2.1
3	C	29	VAL	2.1
3	C	56	ILE	2.1
1	A	168	THR	2.0
1	A	46	LYS	2.0

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
6	DGA	A	405	37/44	0.72	0.41	5.41	53,77,94,103	0
12	NS5	C	405	40/40	0.71	0.48	4.45	50,79,103,106	0
9	MPG	B	306	25/25	0.68	0.47	4.43	67,77,97,98	0
13	OTP	C	406	41/49	0.81	0.38	4.38	48,60,78,84	0
9	MPG	B	305	25/25	0.73	0.45	3.55	80,101,116,120	0
7	BCL	B	301	65/66	0.92	0.27	2.00	32,43,164,175	0
9	MPG	C	407	17/25	0.64	0.46	0.71	60,84,100,103	0
14	PO4	C	408	5/5	0.91	0.49	0.63	93,95,102,104	0
8	BPB	C	402	61/65	0.89	0.31	0.60	51,68,83,88	0
11	MQ7	C	404	48/48	0.89	0.29	0.41	32,42,66,70	0
7	BCL	B	302	66/66	0.94	0.23	0.35	27,33,42,50	0
7	BCL	B	303	66/66	0.95	0.23	0.08	18,27,47,48	0
5	HEM	A	401	43/43	0.95	0.29	-0.06	23,31,34,35	0
8	BPB	B	304	65/65	0.94	0.23	-0.09	27,35,47,60	0
7	BCL	C	401	66/66	0.94	0.23	-0.24	29,37,54,66	0
5	HEM	A	404	43/43	0.95	0.21	-0.68	32,37,53,58	0
5	HEM	A	402	43/43	0.96	0.23	-0.70	23,25,29,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	HEM	A	403	43/43	0.96	0.20	-1.05	22,25,27,30	0
10	FE2	C	403	1/1	0.98	0.05	-3.20	48,48,48,48	0
14	PO4	C	409	5/5	0.92	0.27	-	66,68,71,71	0

6.5 Other polymers [i](#)

There are no such residues in this entry.