



# Full wwPDB X-ray Structure Validation 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 Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)

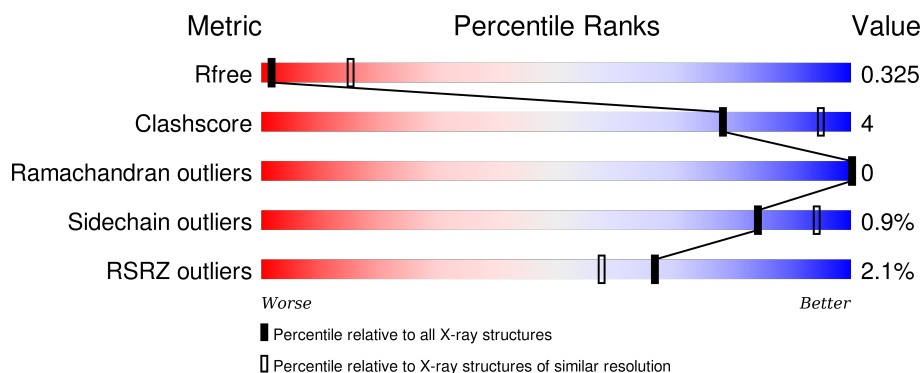
# 1 Overall quality at a glance

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	356	<div> <div style="width: 100%; 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: 3%; height: 10px; background-color: grey;"></div> <div style="position: absolute; left: 92%; top: -10px;">92%</div> <div style="position: absolute; left: 97%; top: -10px;">7%</div> </div>
2	B	274	<div> <div style="width: 92%; height: 10px; background-color: green;"></div> <div style="width: 8%; height: 10px; background-color: yellow;"></div> <div style="position: absolute; left: 92%; top: -10px;">92%</div> <div style="position: absolute; left: 98%; top: -10px;">8%</div> </div>
3	C	324	<div> <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 style="position: absolute; left: 2%; top: -10px;">2%</div> <div style="position: absolute; left: 94%; top: -10px;">94%</div> <div style="position: absolute; left: 99%; top: -10px;">5%</div> </div>

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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.

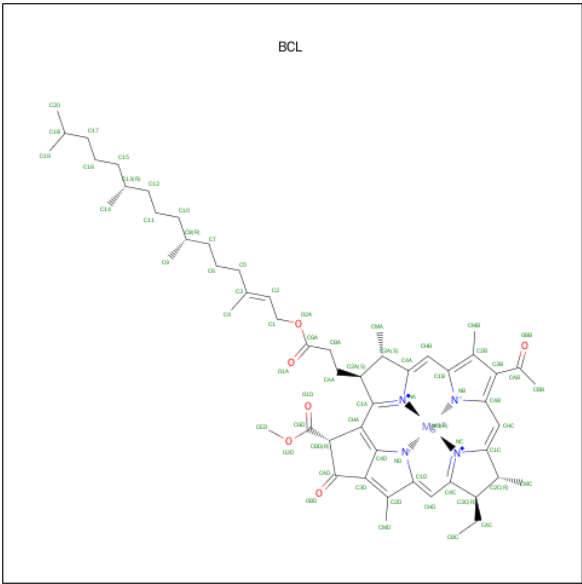
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	243	Total	C	N	O	S	0	0	0
			1771	1140	297	332	2			

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



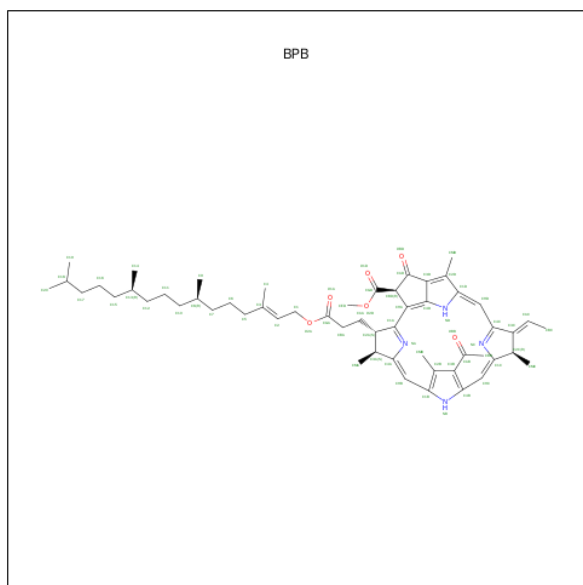
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
5	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
5	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
5	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 6 is BACTERIOCHLOROPHYLL A (three-letter code: BCL) (formula: C<sub>55</sub>H<sub>74</sub>MgN<sub>4</sub>O<sub>6</sub>).



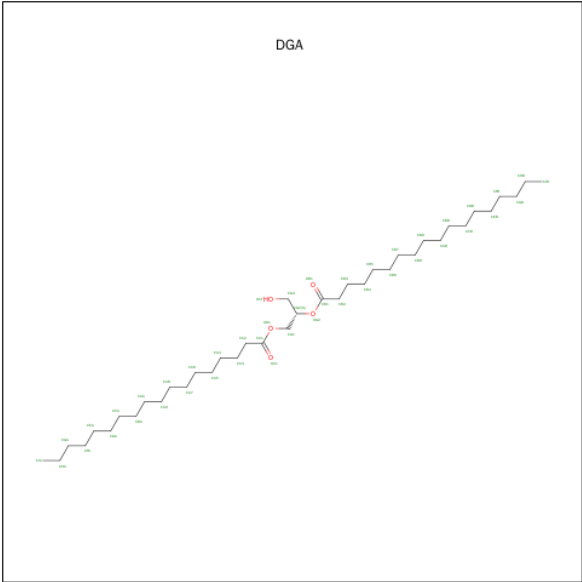
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	B	1	Total 65	C 54	Mg 1	N 4	O 6	0	0
6	B	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
6	B	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
6	C	1	Total 66	C 55	Mg 1	N 4	O 6	0	0

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



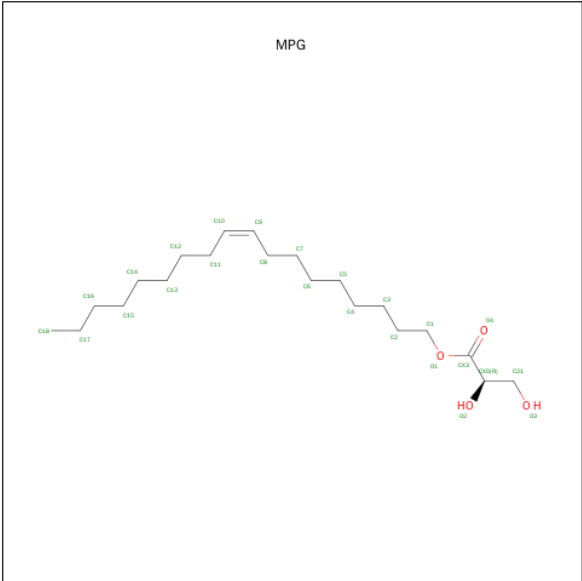
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	B	1	Total	C	N	O	0	0
			65	55	4	6		
7	C	1	Total	C	N	O	0	0
			61	51	4	6		

- 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: C<sub>21</sub>H<sub>40</sub>O<sub>4</sub>).



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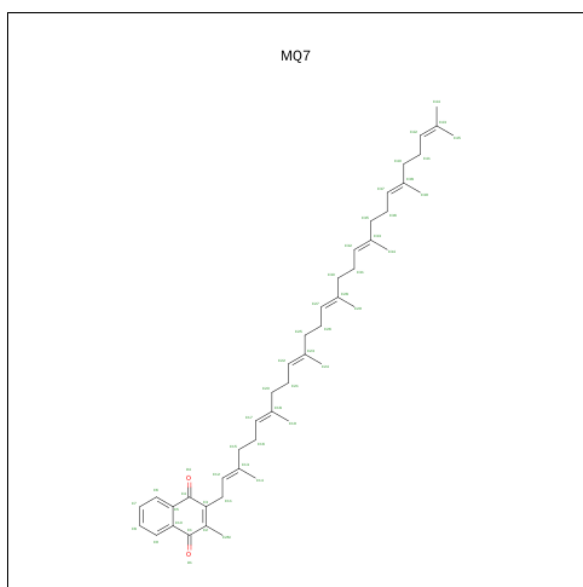
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	C	1	Total C 17 17	0	0

- 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

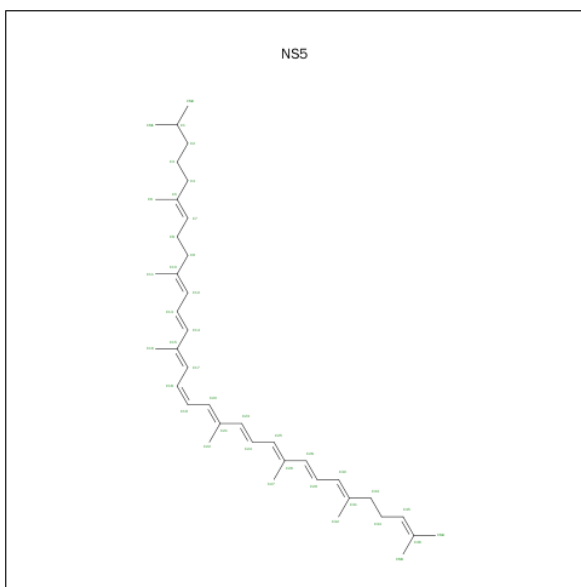
- Molecule 11 is MENAQUINONE-7 (three-letter code: MQ7) (formula: C<sub>46</sub>H<sub>64</sub>O<sub>2</sub>).



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

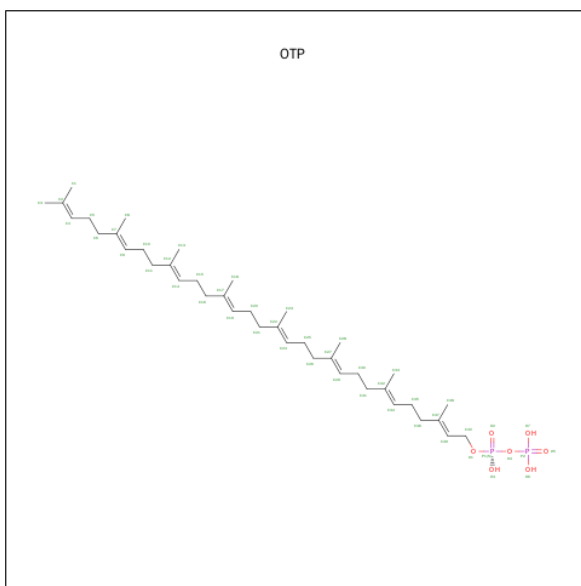
- Molecule 12 is 15-CIS-1,2-DIHYDRONEUROSPORENE (three-letter code: NS5) (formula: C<sub>40</sub>H<sub>60</sub>).





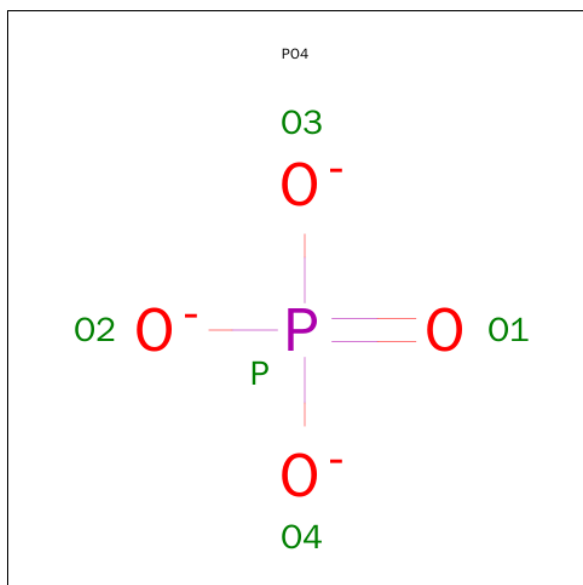
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	C	1	Total	C	0	0
			40	40		

- 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



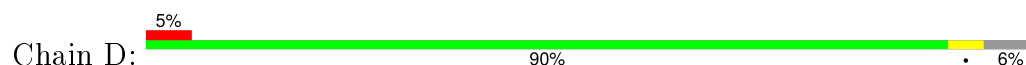
- Molecule 2: REACTION CENTER PROTEIN L CHAIN



- 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, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	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 <sup>2</sup> )	73.5	Xtriage
Anisotropy	0.134	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 77.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.32$ , $\langle L^2 \rangle = 0.15$	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 <sup>2</sup> )	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.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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.

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)
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
13:C:1329:OTP:C29	13:C:1329: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:1328:NS5:C11	2.34	0.58
2:B:39:ILE:HD12	11:C:1327:MQ7:H452	1.86	0.58
2:B:124:PRO:HD3	7:B:1277:BPB:HAC	1.86	0.58
3:C:159:GLY:HA3	12:C:1328:NS5:H113	1.86	0.58
1:A:56:TYR:HB3	5:A:1333:HEM:O2A	2.04	0.57
1:A:240:LEU:HD11	5:A:1336:HEM:CHB	2.36	0.56
2:B:244:GLY:O	6:B:1275:BCL:HED3	2.06	0.55
9:B:1279:MPG:H22	3:C:1:ALA:HA	1.87	0.55
5:A:1333:HEM:HMC2	5:A:1333:HEM:HBC2	1.89	0.55
5:A:1336:HEM:HMB2	5:A:1336:HEM:HBB2	1.90	0.54
3:C:195:TYR:CE2	6:C:1324:BCL:HMC2	2.42	0.54
2:B:62:PHE:CZ	13:C:1329: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	6:B:1275:BCL:HMC2	2.44	0.53
4:D:92:GLN:HA	4:D:101:LEU:HD23	1.93	0.51
7:C:1325:BPB:CBB	7:C:1325:BPB:HHC	2.38	0.50
13:C:1329:OTP:C29	13:C:1329:OTP:C33	2.89	0.50
7:B:1277: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
6:B:1275:BCL:HBB3	6:B:1275:BCL:HMB1	1.94	0.49
2:B:148:TYR:CE1	7:B:1277:BPB:H14B	2.47	0.49
5:A:1335:HEM:HMC2	5:A:1335:HEM:HBC2	1.95	0.48
2:B:181:PHE:CD2	7:C:1325:BPB:HBB	2.48	0.48
2:B:39:ILE:CD1	11:C:1327:MQ7:H452	2.44	0.48
2:B:42:ILE:CD1	7:B:1277:BPB:H4A	2.45	0.47
6:B:1276:BCL:HED3	13:C:1329:OTP:H282	1.95	0.47
3:C:195:TYR:OH	6:C:1324:BCL:OBB	2.16	0.47
6:B:1275:BCL:H2C	6:C:1324:BCL:H2C	1.98	0.46
6:B:1274:BCL:CBB	6:B:1274:BCL:HHC	2.43	0.46
6:B:1276:BCL:H142	6:B:1276:BCL:HMA1	1.98	0.46
2:B:259:TRP:N	2:B:260:PRO:CD	2.79	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:1280:MPG:H51	9:C:1330:MPG:H182	1.98	0.46
3:C:120:MET:SD	6:C:1324:BCL:H172	2.56	0.45
3:C:33:PHE:CE2	3:C:46:ILE:HD12	2.52	0.45
7:B:1277:BPB:HHC	7:B:1277:BPB:CBB	2.38	0.45
2:B:168:HIS:NE2	6:B:1275:BCL:HMC2	2.31	0.45
5:A:1336:HEM:CMB	5:A:1336:HEM:HBB2	2.47	0.44
2:B:179:PHE:HA	2:B:182:VAL:HG12	1.99	0.44
5:A:1333:HEM:HBB2	5:A:1333:HEM:HMB2	2.00	0.44
6:B:1276:BCL:CBB	6:B:1276:BCL:HMB1	2.47	0.44
3:C:200:HIS:CE1	3:C:204:ILE:HD11	2.53	0.43
6:B:1276:BCL:HMD2	6:C:1324:BCL:CBB	2.48	0.42
2:B:42:ILE:HD11	7:B:1277: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:1329:OTP:H301	2.02	0.42
12:C:1328:NS5:H161	12:C:1328:NS5:H18	1.81	0.42
13:C:1329:OTP:H29	13:C:1329:OTP:C33	2.50	0.42
2:B:177:VAL:HG11	6:B:1274:BCL:CMD	2.50	0.42
3:C:195:TYR:CZ	6:C:1324:BCL:HMC2	2.55	0.41
3:C:70:LEU:HD21	12:C:1328: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
6:B:1276:BCL:HED3	13:C:1329: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
6:C:1324:BCL:HMB1	6:C:1324:BCL:CBB	2.50	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:C:1325:BPB:C9	12:C:1328:NS5:HM32	2.51	0.40
7:B:1277:BPB:HBBA	3:C:208:TYR:HB3	2.04	0.40
3:C:98:ALA:HB3	3:C:100:TYR:CZ	2.56	0.40
3:C:181:ILE:HA	3:C:181:ILE:HD13	1.96	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	98
2	B	218/219 (100%)	215 (99%)	3 (1%)	74	91

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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

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	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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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

All (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
5	A	1334	HEM	C2C-C1C	-5.80	1.41	1.52
5	A	1336	HEM	C2C-C1C	-5.68	1.41	1.52
5	A	1335	HEM	C2C-C1C	-5.42	1.42	1.52
12	C	1328	NS5	C9-C8	-5.28	1.35	1.53
7	C	1325	BPB	C1A-NA	-4.95	1.26	1.36
5	A	1335	HEM	C3B-C4B	-4.89	1.47	1.51
7	B	1277	BPB	C1A-NA	-4.40	1.28	1.36
7	B	1277	BPB	C4C-NC	-4.23	1.27	1.37
7	C	1325	BPB	C4C-NC	-4.03	1.27	1.37
6	C	1324	BCL	C3C-C4C	-4.00	1.46	1.51
5	A	1336	HEM	C3B-C4B	-3.87	1.48	1.51
5	A	1334	HEM	C3D-C4D	-3.71	1.46	1.51
5	A	1333	HEM	C3D-C4D	-3.64	1.46	1.51
6	B	1276	BCL	C2C-C3C	-3.26	1.44	1.54
6	B	1274	BCL	CAC-C3C	-3.05	1.47	1.54
6	B	1274	BCL	C2C-C3C	-3.01	1.45	1.54
5	A	1335	HEM	C2B-C1B	-3.00	1.42	1.51
5	A	1336	HEM	C3D-C4D	-2.96	1.47	1.51
7	C	1325	BPB	C1C-NC	-2.93	1.32	1.38
5	A	1333	HEM	C2B-C1B	-2.90	1.42	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1334	HEM	C3B-C4B	-2.88	1.49	1.51
7	B	1277	BPB	C1C-NC	-2.87	1.32	1.38
6	C	1324	BCL	C2C-C3C	-2.79	1.46	1.54
6	B	1276	BCL	C3C-C4C	-2.74	1.48	1.51
6	B	1275	BCL	C3C-C4C	-2.72	1.48	1.51
6	B	1275	BCL	C2C-C3C	-2.70	1.46	1.54
6	B	1276	BCL	CAC-C3C	-2.66	1.48	1.54
6	B	1275	BCL	CAC-C3C	-2.51	1.48	1.54
5	A	1334	HEM	C2B-C1B	-2.51	1.43	1.51
5	A	1335	HEM	C3D-C4D	-2.38	1.48	1.51
6	C	1324	BCL	CAC-C3C	-2.34	1.49	1.54
6	B	1274	BCL	C3C-C4C	-2.31	1.48	1.51
7	B	1277	BPB	C1D-ND	-2.19	1.33	1.38
5	A	1336	HEM	C2B-C1B	-2.00	1.45	1.51
5	A	1335	HEM	CHC-C1C	2.00	1.41	1.36
6	B	1274	BCL	CHD-C4C	2.09	1.47	1.41
5	A	1334	HEM	FE-NB	2.14	2.08	1.97
5	A	1336	HEM	C1C-NC	2.16	1.38	1.36
12	C	1328	NS5	C28-C26	2.20	1.50	1.45
6	B	1276	BCL	CHD-C4C	2.21	1.47	1.41
12	C	1328	NS5	C14-C15	2.25	1.50	1.45
6	B	1275	BCL	CHD-C4C	2.26	1.48	1.41
5	A	1335	HEM	FE-NB	2.27	2.09	1.97
7	C	1325	BPB	C4C-C3C	2.30	1.50	1.45
5	A	1336	HEM	FE-NB	2.38	2.10	1.97
13	C	1329	OTP	C40-C39	2.38	1.53	1.50
7	B	1277	BPB	C4B-CHC	2.40	1.49	1.40
11	C	1327	MQ7	C12-C13	2.41	1.37	1.33
7	C	1325	BPB	C1B-CHB	2.46	1.49	1.40
6	B	1275	BCL	C1B-CHB	2.54	1.46	1.39
7	C	1325	BPB	C4B-CHC	2.65	1.50	1.40
6	C	1324	BCL	C1B-CHB	2.71	1.47	1.39
5	A	1333	HEM	FE-NB	2.75	2.12	1.97
7	B	1277	BPB	CHD-C4C	2.83	1.47	1.40
12	C	1328	NS5	C29-C30	2.84	1.52	1.43
6	B	1275	BCL	C3D-C2D	2.90	1.47	1.40
7	B	1277	BPB	C1B-CHB	2.94	1.51	1.40
7	C	1325	BPB	CHD-C4C	2.98	1.47	1.40
7	C	1325	BPB	C3B-C2B	3.03	1.47	1.40
7	B	1277	BPB	C3B-C2B	3.06	1.47	1.40
6	B	1274	BCL	C3B-C2B	3.09	1.47	1.40
6	C	1324	BCL	C3B-C2B	3.11	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1333	HEM	FE-NC	3.12	2.08	1.95
6	B	1276	BCL	C1B-CHB	3.17	1.48	1.39
6	B	1274	BCL	C4B-CHC	3.17	1.48	1.39
6	B	1274	BCL	C1B-CHB	3.21	1.48	1.39
6	B	1276	BCL	C3B-C2B	3.21	1.47	1.40
6	C	1324	BCL	C3D-C2D	3.25	1.47	1.40
6	B	1276	BCL	C3D-C2D	3.27	1.48	1.40
5	A	1334	HEM	FE-NC	3.41	2.09	1.95
6	B	1275	BCL	C4B-CHC	3.48	1.49	1.39
6	B	1275	BCL	C3B-C2B	3.52	1.48	1.40
6	C	1324	BCL	C4B-CHC	3.53	1.49	1.39
6	B	1274	BCL	C3D-C2D	3.54	1.48	1.40
6	B	1274	BCL	OBD-CAD	3.61	1.27	1.22
6	B	1276	BCL	C4B-CHC	3.64	1.49	1.39
7	B	1277	BPB	OBD-CAD	3.68	1.29	1.22
5	A	1335	HEM	FE-NC	3.70	2.10	1.95
12	C	1328	NS5	C12-C10	3.71	1.38	1.34
5	A	1336	HEM	FE-NC	3.77	2.10	1.95
7	B	1277	BPB	C3D-C2D	3.82	1.49	1.38
6	C	1324	BCL	O2A-CGA	3.84	1.44	1.33
7	C	1325	BPB	OBD-CAD	3.85	1.29	1.22
7	C	1325	BPB	C3D-C2D	3.89	1.49	1.38
6	B	1274	BCL	O2A-CGA	4.08	1.45	1.33
6	B	1275	BCL	O2D-CGD	4.13	1.43	1.33
6	B	1276	BCL	OBD-CAD	4.16	1.28	1.22
7	B	1277	BPB	O2A-CGA	4.18	1.45	1.33
6	B	1276	BCL	O2A-CGA	4.19	1.45	1.33
6	B	1275	BCL	O2A-CGA	4.36	1.46	1.33
8	B	1278	DGA	OG2-CB1	4.38	1.47	1.34
6	B	1275	BCL	OBD-CAD	4.42	1.29	1.22
7	C	1325	BPB	O2A-CGA	4.45	1.46	1.33
7	B	1277	BPB	CHD-C1D	4.45	1.47	1.38
7	C	1325	BPB	O2D-CGD	4.46	1.44	1.33
8	B	1278	DGA	OG1-CA1	4.84	1.47	1.33
7	B	1277	BPB	O2D-CGD	4.87	1.45	1.33
7	B	1277	BPB	C3B-C4B	4.89	1.47	1.41
6	C	1324	BCL	O2D-CGD	5.14	1.46	1.33
6	B	1276	BCL	O2D-CGD	5.14	1.46	1.33
7	C	1325	BPB	CHD-C1D	5.35	1.49	1.38
6	B	1274	BCL	O2D-CGD	5.49	1.47	1.33
7	C	1325	BPB	C3B-C4B	5.51	1.48	1.41
6	C	1324	BCL	OBD-CAD	5.72	1.31	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	1279	MPG	O1-CX3	5.92	1.45	1.33
11	C	1327	MQ7	C10-C5	6.18	1.50	1.40
11	C	1327	MQ7	C3-C2	6.22	1.50	1.35
7	C	1325	BPB	C1A-CHA	6.96	1.49	1.36
9	B	1280	MPG	O1-CX3	7.00	1.48	1.33
12	C	1328	NS5	C35-C36	7.22	1.54	1.32
12	C	1328	NS5	C29-C28	7.31	1.53	1.34
7	B	1277	BPB	C1A-CHA	7.55	1.50	1.36
13	C	1329	OTP	C39-C37	10.73	1.54	1.33
7	C	1325	BPB	CAC-C3C	15.72	1.52	1.33
7	B	1277	BPB	CAC-C3C	16.16	1.53	1.33

All (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
13	C	1329	OTP	C38-C37-C39	-6.18	111.36	123.50
12	C	1328	NS5	C29-C28-C26	-5.65	109.70	126.32
7	B	1277	BPB	C4D-C3D-C2D	-5.49	100.53	106.74
13	C	1329	OTP	C38-C37-C36	-5.36	107.21	115.41
7	C	1325	BPB	C4D-C3D-C2D	-5.07	101.01	106.74
13	C	1329	OTP	C18-C17-C19	-4.79	114.10	123.50
13	C	1329	OTP	C36-C37-C39	-4.49	112.54	121.05
5	A	1334	HEM	CBA-CAA-C2A	-4.40	104.64	112.53
7	C	1325	BPB	CMD-C2D-C3D	-4.32	117.98	128.04
5	A	1333	HEM	CBA-CAA-C2A	-4.23	104.95	112.53
11	C	1327	MQ7	C21-C22-C23	-4.17	118.70	127.76
7	B	1277	BPB	CMD-C2D-C3D	-4.15	118.38	128.04
6	B	1275	BCL	OBD-CAD-C3D	-4.08	120.04	128.35
12	C	1328	NS5	C34-C35-C36	-4.06	112.08	127.73
6	C	1324	BCL	OBD-CAD-C3D	-3.86	120.47	128.35
9	B	1279	MPG	O1-CX3-O11	-3.85	116.20	124.05
6	B	1275	BCL	CMD-C2D-C3D	-3.82	117.62	125.09
12	C	1328	NS5	C19-C20-C21	-3.78	121.74	127.20
6	B	1274	BCL	OBD-CAD-C3D	-3.72	120.76	128.35
6	B	1274	BCL	O1D-CGD-CBD	-3.69	119.33	124.62
12	C	1328	NS5	C24-C25-C26	-3.61	121.98	127.20
12	C	1328	NS5	C18-C17-C15	-3.61	121.98	127.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	1276	BCL	CMD-C2D-C3D	-3.59	118.07	125.09
7	B	1277	BPB	O1D-CGD-CBD	-3.51	119.59	124.62
12	C	1328	NS5	CM3-C36-C35	-3.48	111.43	122.61
6	B	1276	BCL	OBD-CAD-C3D	-3.46	121.30	128.35
6	C	1324	BCL	O2D-CGD-O1D	-3.43	116.70	123.79
13	C	1329	OTP	C21-C22-C24	-3.43	114.55	121.05
12	C	1328	NS5	CM4-C36-C35	-3.26	112.11	122.61
13	C	1329	OTP	C30-C29-C27	-3.06	121.11	127.76
6	B	1274	BCL	C1D-CHD-C4C	-3.04	121.43	126.07
6	C	1324	BCL	C1D-CHD-C4C	-3.00	121.49	126.07
6	B	1275	BCL	O2D-CGD-O1D	-2.98	117.64	123.79
7	C	1325	BPB	O2D-CGD-O1D	-2.92	117.76	123.79
6	B	1275	BCL	C1D-CHD-C4C	-2.89	121.65	126.07
6	C	1324	BCL	CMD-C2D-C3D	-2.87	119.47	125.09
7	B	1277	BPB	OBD-CAD-C3D	-2.84	120.69	128.37
6	B	1274	BCL	CMD-C2D-C3D	-2.70	119.81	125.09
6	B	1276	BCL	O1D-CGD-CBD	-2.63	120.85	124.62
13	C	1329	OTP	C10-C9-C7	-2.63	122.04	127.76
11	C	1327	MQ7	C20-C18-C17	-2.57	116.17	121.05
6	B	1274	BCL	C2A-C1A-CHA	-2.54	119.20	123.89
7	C	1325	BPB	O1D-CGD-CBD	-2.49	121.05	124.62
11	C	1327	MQ7	C11-C12-C13	-2.43	122.57	126.70
7	B	1277	BPB	O2A-CGA-O1A	-2.40	117.30	123.49
5	A	1334	HEM	C3B-C4B-NB	-2.38	107.07	111.63
5	A	1335	HEM	C3B-C4B-NB	-2.38	107.08	111.63
5	A	1334	HEM	CMA-C3A-C4A	-2.37	124.44	128.36
13	C	1329	OTP	C8-C7-C9	-2.37	118.84	123.50
6	B	1276	BCL	C1D-CHD-C4C	-2.35	122.48	126.07
5	A	1333	HEM	C3B-C4B-NB	-2.33	107.18	111.63
6	B	1275	BCL	C2A-C1A-CHA	-2.30	119.64	123.89
6	B	1276	BCL	C2A-C1A-CHA	-2.30	119.66	123.89
6	C	1324	BCL	O2A-CGA-O1A	-2.29	117.59	123.49
12	C	1328	NS5	C30-C29-C28	-2.27	116.21	123.13
5	A	1333	HEM	C1D-CHD-C4C	-2.27	122.03	125.82
11	C	1327	MQ7	C26-C27-C28	-2.25	122.87	127.76
5	A	1333	HEM	CBD-CAD-C3D	-2.22	107.09	113.55
6	B	1274	BCL	OBD-CAD-CBD	-2.18	122.65	125.94
6	B	1275	BCL	CHC-C1C-NC	-2.15	121.53	124.51
6	B	1274	BCL	CHC-C1C-NC	-2.15	121.54	124.51
5	A	1336	HEM	C1D-CHD-C4C	-2.12	122.28	125.82
6	B	1276	BCL	OBD-CAD-CBD	-2.11	122.76	125.94
5	A	1335	HEM	CAA-C2A-C1A	-2.11	124.72	127.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	C	1327	MQ7	C35-C33-C32	-2.10	117.06	121.05
5	A	1336	HEM	CMA-C3A-C4A	-2.06	124.96	128.36
5	A	1334	HEM	C1D-CHD-C4C	-2.05	122.39	125.82
13	C	1329	OTP	C15-C14-C12	-2.04	123.34	127.76
13	C	1329	OTP	C26-C25-C24	-2.03	106.38	111.69
11	C	1327	MQ7	C2M-C2-C3	-2.00	119.81	124.10
7	B	1277	BPB	CED-O2D-CGD	2.01	120.70	115.99
6	B	1276	BCL	CHB-C4A-NA	2.02	127.31	124.51
6	B	1275	BCL	OBB-CAB-C3B	2.03	123.22	120.00
11	C	1327	MQ7	C39-C38-C40	2.04	118.52	115.41
7	C	1325	BPB	C3C-C4C-NC	2.05	113.05	109.52
13	C	1329	OTP	C16-C17-C19	2.06	124.95	121.05
7	C	1325	BPB	C3D-C4D-ND	2.08	116.33	109.65
5	A	1335	HEM	CHC-C4B-NB	2.08	129.53	124.52
5	A	1335	HEM	C2C-C1C-CHC	2.12	126.90	123.68
7	C	1325	BPB	C2B-C1B-NB	2.13	113.78	110.29
6	C	1324	BCL	O2A-CGA-CBA	2.13	118.40	111.90
6	B	1275	BCL	CED-O2D-CGD	2.18	121.11	115.99
5	A	1336	HEM	CHD-C1D-ND	2.19	129.79	124.52
5	A	1336	HEM	CHC-C4B-NB	2.21	129.85	124.52
6	B	1275	BCL	CAA-C2A-C1A	2.22	120.31	112.47
5	A	1333	HEM	C2D-C3D-C4D	2.24	105.29	101.50
5	A	1334	HEM	C2D-C3D-C4D	2.25	105.31	101.50
5	A	1335	HEM	C3C-CAC-CBC	2.34	128.04	124.46
7	B	1277	BPB	C3D-C4D-ND	2.37	117.28	109.65
12	C	1328	NS5	C9-C8-C7	2.39	117.94	111.69
11	C	1327	MQ7	C2M-C2-C1	2.41	120.17	116.27
7	C	1325	BPB	O2A-CGA-CBA	2.41	119.25	111.90
6	C	1324	BCL	CAA-C2A-C1A	2.42	121.00	112.47
11	C	1327	MQ7	C34-C33-C35	2.42	119.11	115.41
6	C	1324	BCL	C4-C3-C5	2.47	119.19	115.41
5	A	1336	HEM	C2D-C3D-C4D	2.49	105.72	101.50
7	B	1277	BPB	C4-C3-C5	2.51	119.24	115.41
6	C	1324	BCL	CHB-C4A-NA	2.57	128.07	124.51
6	B	1274	BCL	C4-C3-C5	2.57	119.34	115.41
6	B	1275	BCL	CBC-CAC-C3C	2.58	119.87	113.57
12	C	1328	NS5	C32-C31-C33	2.62	119.42	115.41
6	B	1274	BCL	CMB-C2B-C3B	2.69	130.35	125.09
5	A	1333	HEM	CMD-C2D-C3D	2.71	126.33	114.35
5	A	1335	HEM	CMD-C2D-C3D	2.72	126.40	114.35
5	A	1336	HEM	CMD-C2D-C3D	2.77	126.59	114.35
8	B	1278	DGA	CG1-OG1-CA1	2.78	124.63	116.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	C	1329	OTP	C13-C12-C11	2.79	119.66	115.41
9	B	1280	MPG	C1-O1-CX3	2.79	122.84	116.59
9	B	1279	MPG	C1-O1-CX3	2.80	122.86	116.59
7	C	1325	BPB	CAD-C3D-C2D	2.82	154.39	140.80
6	C	1324	BCL	CAC-C3C-C4C	2.82	118.84	112.58
7	B	1277	BPB	C3C-C4C-NC	2.86	114.44	109.52
6	B	1276	BCL	CED-O2D-CGD	2.87	122.73	115.99
6	B	1274	BCL	CHB-C4A-NA	2.88	128.49	124.51
6	C	1324	BCL	CED-O2D-CGD	2.89	122.77	115.99
7	B	1277	BPB	CAD-C3D-C2D	2.91	154.86	140.80
6	B	1276	BCL	CBC-CAC-C3C	2.93	120.73	113.57
8	B	1278	DGA	OG1-CA1-CA2	2.94	120.85	111.90
11	C	1327	MQ7	C19-C18-C20	2.99	119.97	115.41
6	C	1324	BCL	CBC-CAC-C3C	3.03	120.98	113.57
6	B	1274	BCL	CBC-CAC-C3C	3.06	121.04	113.57
5	A	1334	HEM	CMD-C2D-C3D	3.10	128.05	114.35
5	A	1335	HEM	C2D-C3D-C4D	3.23	106.98	101.50
7	C	1325	BPB	C4-C3-C5	3.26	120.39	115.41
13	C	1329	OTP	C28-C27-C26	3.29	120.43	115.41
6	B	1276	BCL	CMB-C2B-C3B	3.30	131.55	125.09
6	B	1275	BCL	C4-C3-C5	3.38	120.56	115.41
7	B	1277	BPB	O2A-CGA-CBA	3.51	122.60	111.90
12	C	1328	NS5	C6-C5-C4	3.52	120.78	115.41
6	B	1275	BCL	CMB-C2B-C3B	3.59	132.11	125.09
6	B	1275	BCL	CHB-C4A-NA	3.63	129.53	124.51
13	C	1329	OTP	C18-C17-C16	3.63	120.95	115.41
6	B	1275	BCL	O2A-CGA-CBA	3.68	123.12	111.90
6	B	1275	BCL	CAC-C3C-C4C	3.76	120.93	112.58
5	A	1333	HEM	CMC-C2C-C3C	3.77	125.94	116.53
6	C	1324	BCL	C2C-C3C-C4C	3.78	107.90	101.50
6	C	1324	BCL	C3D-CAD-CBD	3.82	113.00	107.60
6	C	1324	BCL	CMB-C2B-C3B	3.83	132.58	125.09
6	B	1276	BCL	CAC-C3C-C4C	4.02	121.51	112.58
5	A	1334	HEM	CAD-C3D-C4D	4.02	126.66	112.47
13	C	1329	OTP	C33-C32-C31	4.12	121.71	115.41
5	A	1335	HEM	CMC-C2C-C3C	4.13	126.85	116.53
5	A	1336	HEM	CMB-C2B-C3B	4.18	126.97	116.53
12	C	1328	NS5	C8-C9-C10	4.21	126.43	112.71
5	A	1335	HEM	CAD-C3D-C2D	4.23	125.38	113.22
5	A	1336	HEM	CAD-C3D-C4D	4.27	127.53	112.47
5	A	1333	HEM	CAD-C3D-C4D	4.28	127.56	112.47
5	A	1335	HEM	CAD-C3D-C4D	4.29	127.61	112.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	1278	DGA	OG2-CB1-CB2	4.39	121.06	111.53
5	A	1335	HEM	CMB-C2B-C3B	4.46	127.67	116.53
6	B	1275	BCL	O2D-CGD-CBD	4.56	117.55	111.30
5	A	1334	HEM	CMC-C2C-C3C	4.57	127.94	116.53
5	A	1336	HEM	CAD-C3D-C2D	4.69	126.70	113.22
5	A	1333	HEM	CMB-C2B-C3B	4.74	128.37	116.53
5	A	1334	HEM	CMB-C2B-C3B	4.77	128.45	116.53
5	A	1333	HEM	CAD-C3D-C2D	4.84	127.14	113.22
9	B	1280	MPG	O1-CX3-CXD	4.86	120.65	111.79
6	B	1275	BCL	C2C-C3C-C4C	4.98	109.94	101.50
13	C	1329	OTP	C23-C22-C21	5.06	123.14	115.41
5	A	1336	HEM	CMC-C2C-C3C	5.08	129.20	116.53
13	C	1329	OTP	C8-C7-C6	5.11	123.22	115.41
5	A	1334	HEM	CAD-C3D-C2D	5.15	128.02	113.22
6	B	1275	BCL	C3D-CAD-CBD	5.32	115.11	107.60
6	B	1276	BCL	C2C-C3C-C4C	5.46	110.76	101.50
6	B	1274	BCL	CAC-C3C-C4C	5.58	124.97	112.58
6	B	1276	BCL	O2D-CGD-CBD	5.60	118.98	111.30
7	C	1325	BPB	CMD-C2D-C1D	5.78	134.47	125.06
6	B	1276	BCL	C3D-CAD-CBD	5.90	115.94	107.60
6	B	1274	BCL	O2D-CGD-CBD	5.91	119.41	111.30
7	B	1277	BPB	CMD-C2D-C1D	6.01	134.84	125.06
6	B	1274	BCL	C2C-C3C-C4C	6.09	111.82	101.50
9	B	1279	MPG	O1-CX3-CXD	6.23	123.14	111.79
6	B	1274	BCL	C3D-CAD-CBD	6.35	116.57	107.60
7	B	1277	BPB	O2D-CGD-CBD	6.68	120.47	111.30
6	C	1324	BCL	O2D-CGD-CBD	7.16	121.13	111.30
7	C	1325	BPB	O2D-CGD-CBD	7.20	121.18	111.30

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

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
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

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	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

All (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
4	D	206	ASP	2.7
4	D	61	GLU	2.5
3	C	24	GLY	2.4
3	C	22	GLU	2.4
4	D	93	THR	2.4
1	A	161	THR	2.3
4	D	155	LEU	2.3
4	D	7	ALA	2.3
4	D	154	GLY	2.2
4	D	167	THR	2.2
3	C	57	ALA	2.2
4	D	91	ALA	2.1
3	C	16	HIS	2.1
3	C	29	VAL	2.1
1	A	168	THR	2.1
3	C	56	ILE	2.0

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Mol	Chain	Res	Type	RSRZ
4	D	256	SER	2.0
3	C	37	TRP	2.0
4	D	110	ASP	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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
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.