



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 03:37 AM GMT

PDB ID : 2UXM
Title : X-RAY HIGH RESOLUTION STRUCTURE OF THE PHOTOSYNTHETIC
REACTION CENTER FROM RB. SPHAEROIDES AT PH 10 IN THE
CHARGE-SEPARATED STATE, 2ND DATASET
Authors : Koepke, J.; Diehm, R.; Fritzsche, G.
Deposited on : 2007-03-28
Resolution : 2.70 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

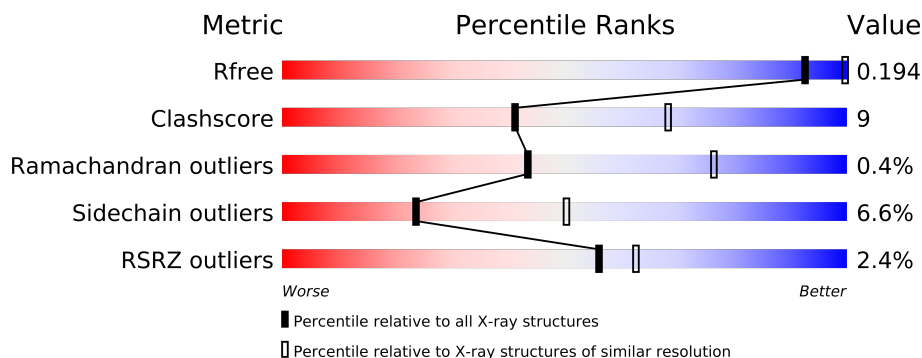
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.70 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}	66092	1557 (2.70-2.70)
Clashscore	79885	1939 (2.70-2.70)
Ramachandran outliers	78287	1905 (2.70-2.70)
Sidechain outliers	78261	1905 (2.70-2.70)
RSRZ outliers	66119	1559 (2.70-2.70)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	H	260	
2	L	281	
3	M	307	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
10	GOL	L	1290	-	X
10	GOL	M	1317	-	X
5	LDA	L	1284	-	X
5	LDA	M	1305	-	X
5	LDA	M	1306	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
5	LDA	M	1308	-	X
5	LDA	M	1309	-	X
5	LDA	M	1310	-	X
5	LDA	M	1311	-	X
5	LDA	M	1312	-	X
6	BPH	M	1314	-	X
7	UQ2	L	1286[A]	-	X
7	UQ2	L	1286[B]	-	X
8	PO4	L	1287	-	X
9	HTO	L	1288	-	X

2 Entry composition i

There are 14 unique types of molecules in this entry. The entry contains 7442 atoms, of which 0 are hydrogen and 0 are deuterium.

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 REACTION CENTER PROTEIN H CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	241	Total	C	N	O	S	0	3	1
			1846	1181	319	337	9			

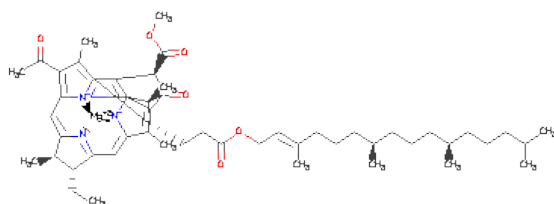
- Molecule 2 is a protein called REACTION CENTER PROTEIN L CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	281	Total	C	N	O	S	0	0	0
			2232	1507	355	362	8			

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

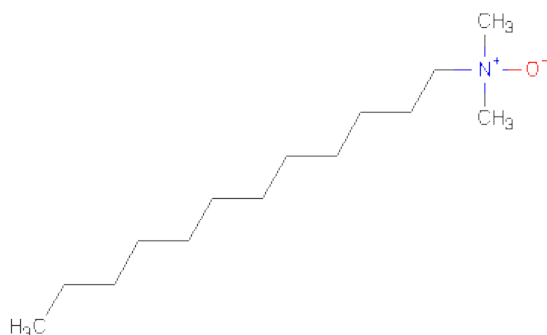
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	M	303	Total	C	N	O	S	0	0	1
			2409	1607	395	397	10			

- Molecule 4 is BACTERIOCHLOROPHYLL A (three-letter code: BCL) (formula: $C_{55}H_{74}MgN_4O_6$).



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

- Molecule 5 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula: $C_{14}H_{31}NO$).



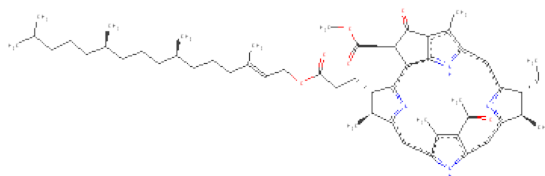
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	L	1	Total	C	N	O	0	0
			16	14	1	1		
5	M	1	Total	C	N	O	0	0
			16	14	1	1		
5	M	1	Total	C	N	O	0	0
			16	14	1	1		
5	M	1	Total	C	N	O	0	0
			16	14	1	1		
5	M	1	Total	C	N	O	0	0
			16	14	1	1		
5	M	1	Total	C	N	O	0	0
			16	14	1	1		

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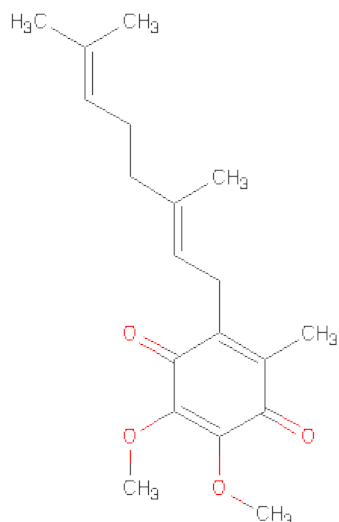
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	M	1	Total	C	N	O	0	0
			16	14	1	1		
5	M	1	Total	C	N	O	0	0
			16	14	1	1		

- Molecule 6 is BACTERIOPHEOPHYTIN A (three-letter code: BPH) (formula: $C_{55}H_{76}N_4O_6$).



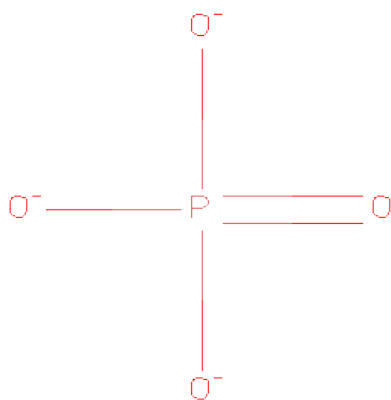
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	L	1	Total	C	N	O	0	0
			65	55	4	6		
6	M	1	Total	C	N	O	0	0
			65	55	4	6		

- Molecule 7 is UBIQUINONE-2 (three-letter code: UQ2) (formula: $C_{19}H_{26}O_4$).



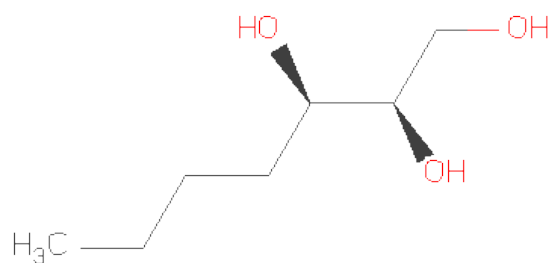
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	L	1	Total	C	O	0	1
			46	38	8		

- Molecule 8 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



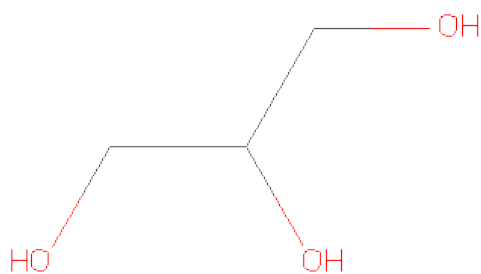
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	L	1	Total	O	P	0	0
			5	4	1		

- Molecule 9 is HEPTANE-1,2,3-TRIOL (three-letter code: HTO) (formula: $C_7H_{16}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	L	1	Total	C	O	0	0
			10	7	3		

- Molecule 10 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	L	1	Total	C	O	0	0
			6	3	3		
10	L	1	Total	C	O	0	0
			6	3	3		
10	M	1	Total	C	O	0	0
			6	3	3		

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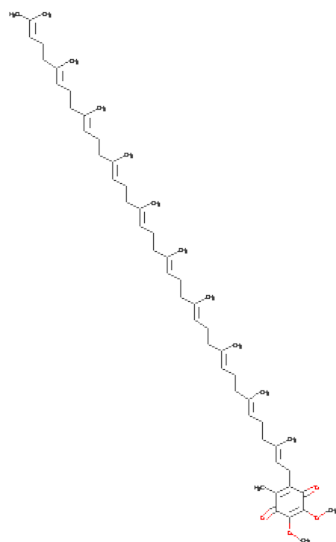
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	X	1	Total	C	O	0	0
			6	3	3		

- Molecule 11 is FE (III) ION (three-letter code: FE) (formula: Fe).

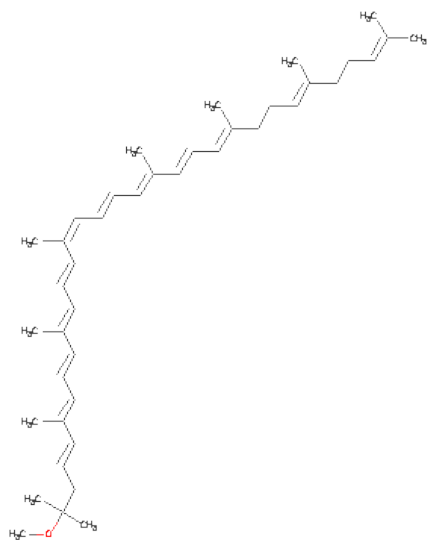
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	M	1	Total	Fe		0	0
			1	1			

- Molecule 12 is UBIQUINONE-10 (three-letter code: U10) (formula: C₅₉H₉₀O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	M	1	Total	C	O	0	0
			48	44	4		

- Molecule 13 is SPHEROIDENE (three-letter code: SPO) (formula: C₄₁H₆₀O).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
13	M	1	Total	C	O	0	0
			42	41	1		

- Molecule 14 is water.

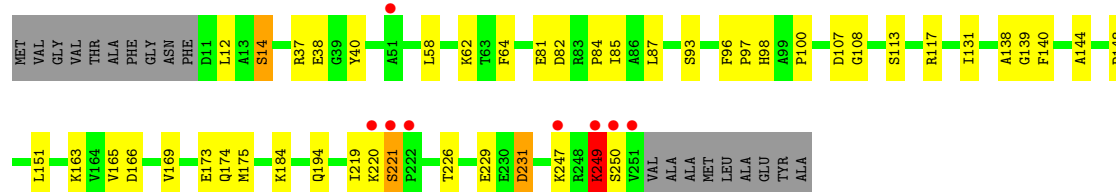
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	H	81	Total	O	0	0
			81	81		
14	L	87	Total	O	0	0
			87	87		
14	M	73	Total	O	0	0
			73	73		

3 Residue-property plots

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

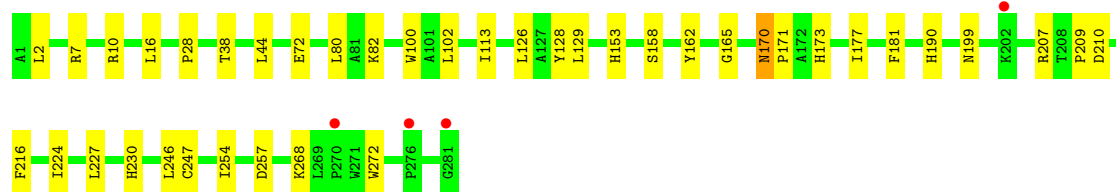
- Molecule 1: REACTION CENTER PROTEIN H CHAIN

Chain H: 



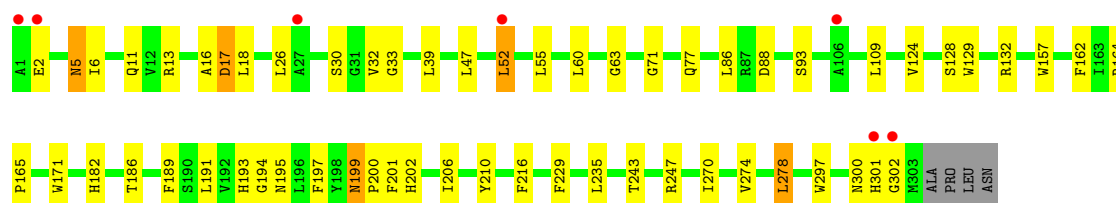
- Molecule 2: REACTION CENTER PROTEIN L CHAIN

Chain L: 



- Molecule 3: REACTION CENTER PROTEIN M CHAIN

Chain M: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	139.45Å 139.45Å 185.11Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	119.52 – 2.70 29.89 – 2.52	Depositor EDS
% Data completeness (in resolution range)	97.4 (119.52-2.70) 85.5 (29.89-2.52)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.37 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.186 , 0.221 0.192 , 0.194	Depositor DCC
R_{free} test set	3025 reflections (5.25%)	DCC
Wilson B-factor (Å ²)	41.9	Xtriage
Anisotropy	0.226	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 51.3	EDS
Estimated twinning fraction	0.023 for -h,-k,l	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 66734 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7442	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.91% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BCL, GOL, LDA, HTO, BPH, PO4, FE, SPO, U10, UQ2

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	H	0.70	0/1906	0.81	5/2591 (0.2%)
2	L	0.73	0/2320	0.72	1/3175 (0.0%)
3	M	0.68	0/2501	0.75	3/3415 (0.1%)
All	All	0.70	0/6727	0.76	9/9181 (0.1%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	231	ASP	CB-CG-OD2	5.91	123.62	118.30
1	H	82	ASP	CB-CG-OD2	5.32	123.09	118.30
2	L	257	ASP	CB-CG-OD2	5.32	123.08	118.30
1	H	107	ASP	CB-CG-OD2	5.24	123.02	118.30
3	M	17	ASP	CB-CG-OD2	5.19	122.97	118.30
3	M	88	ASP	CB-CG-OD2	5.12	122.91	118.30
1	H	250	SER	O-C-N	-5.09	114.55	122.70
1	H	166	ASP	CB-CG-OD2	5.07	122.86	118.30
3	M	86	LEU	CA-CB-CG	5.06	126.94	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the

chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	H	1846	0	1861	28	0
2	L	2232	0	2187	26	0
3	M	2409	0	2321	47	0
4	L	132	0	148	9	0
4	M	132	0	148	20	0
5	L	16	0	31	1	0
5	M	128	0	248	18	0
6	L	65	0	76	8	0
6	M	65	0	76	6	0
7	L	46	0	52	13	0
8	L	5	0	0	0	0
9	L	10	0	16	0	0
10	L	12	0	16	1	0
10	M	6	0	8	1	0
10	X	6	0	8	0	0
11	M	1	0	0	0	0
12	M	48	0	63	4	0
13	M	42	0	60	6	0
14	H	81	0	0	1	1
14	L	87	0	0	1	0
14	M	73	0	0	1	0
All	All	7442	0	7319	134	1

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 9.

All (134) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
7:L:1286[A]:UQ2:H152	5:M:1309:LDA:H111	1.47	0.97
4:M:1304:BCL:HHC	4:M:1304:BCL:HBB3	1.50	0.91
7:L:1286[B]:UQ2:H162	5:M:1312:LDA:H121	1.56	0.87
2:L:72:GLU:HB3	14:L:2026:HOH:O	1.74	0.87
1:H:249:LYS:HE3	1:H:249:LYS:HA	1.59	0.84
5:M:1307:LDA:H81	5:M:1308:LDA:H62	1.59	0.83
3:M:197:PHE:HZ	4:M:1304:BCL:HBB2	1.42	0.83
3:M:197:PHE:CZ	4:M:1304:BCL:HBB2	2.14	0.82
6:L:1285:BPH:HHC	6:L:1285:BPH:HBB3	1.61	0.81
1:H:226:THR:OG1	1:H:229:GLU:HG3	1.80	0.81
6:L:1285:BPH:HHC	6:L:1285:BPH:CBB	2.13	0.78
1:H:148:PRO:HA	1:H:151:LEU:HD12	1.66	0.78

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:M:1304:BCL:CBB	4:M:1304:BCL:HHC	2.13	0.78
3:M:16:ALA:HB1	3:M:32:VAL:HG11	1.65	0.76
3:M:243:THR:O	3:M:247:ARG:HG3	1.86	0.76
5:M:1305:LDA:H92	5:M:1307:LDA:H121	1.66	0.75
2:L:28:PRO:HG3	5:M:1308:LDA:HM21	1.68	0.75
4:M:1304:BCL:H2	6:M:1314:BPH:HHC	1.68	0.73
3:M:33:GLY:HA2	5:M:1309:LDA:H11	1.69	0.73
6:L:1285:BPH:HBB2	3:M:210:TYR:HB3	1.70	0.73
2:L:199:ASN:HA	10:L:1289:GOL:H31	1.73	0.70
7:L:1286[B]:UQ2:H162	5:M:1312:LDA:C12	2.22	0.68
2:L:224:ILE:HG22	7:L:1286[B]:UQ2:H8	1.74	0.68
5:M:1305:LDA:H92	5:M:1307:LDA:C12	2.23	0.68
2:L:190:HIS:HA	7:L:1286[B]:UQ2:O4	1.94	0.68
2:L:170:ASN:C	2:L:170:ASN:HD22	1.97	0.67
5:M:1307:LDA:H21	14:M:2071:HOH:O	1.93	0.67
1:H:194:GLN:HG3	3:M:5:ASN:ND2	2.09	0.67
1:H:194:GLN:CG	3:M:5:ASN:ND2	2.58	0.67
2:L:181:PHE:HB3	6:M:1314:BPH:HBB2	1.78	0.65
3:M:199:ASN:C	3:M:199:ASN:HD22	2.00	0.65
4:M:1304:BCL:C2	6:M:1314:BPH:HHC	2.28	0.64
2:L:181:PHE:CD2	6:M:1314:BPH:HBB1	2.33	0.64
3:M:189:PHE:O	3:M:193:HIS:HD2	1.80	0.64
4:L:1282:BCL:H41	4:L:1283:BCL:HBB3	1.82	0.62
4:L:1282:BCL:HMB1	4:L:1282:BCL:CBB	2.31	0.61
3:M:55:LEU:HD22	3:M:128:SER:HB2	1.82	0.61
1:H:194:GLN:HG3	3:M:5:ASN:HD21	1.67	0.59
6:L:1285:BPH:CHC	6:L:1285:BPH:HBB3	2.33	0.58
3:M:194:GLY:O	3:M:195:ASN:HB3	2.04	0.57
7:L:1286[A]:UQ2:H153	3:M:47:LEU:HD11	1.86	0.57
5:M:1305:LDA:H11	10:M:1317:GOL:H11	1.86	0.56
3:M:300:ASN:C	3:M:302:GLY:H	2.09	0.56
4:L:1282:BCL:HMB2	4:M:1304:BCL:HHB	1.87	0.56
6:L:1285:BPH:CBB	3:M:210:TYR:HB3	2.36	0.55
3:M:197:PHE:HZ	4:M:1304:BCL:CBB	2.16	0.55
3:M:129:TRP:O	3:M:132:ARG:HB3	2.07	0.55
4:M:1304:BCL:CBB	4:M:1304:BCL:CHC	2.80	0.55
4:M:1303:BCL:HBB3	4:M:1303:BCL:HHC	1.88	0.55
6:L:1285:BPH:CHC	6:L:1285:BPH:CBB	2.86	0.54
2:L:209:PRO:HD3	3:M:235:LEU:HD12	1.90	0.53
3:M:16:ALA:HB1	3:M:32:VAL:CG1	2.36	0.53
4:L:1282:BCL:HMB1	4:L:1282:BCL:HBB2	1.89	0.53
1:H:194:GLN:HG2	3:M:5:ASN:ND2	2.23	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:M:1303:BCL:HBB2	13:M:1316:SPO:H243	1.90	0.53
12:M:1315:U10:H3M3	12:M:1315:U10:H4M2	1.91	0.52
2:L:224:ILE:CG2	7:L:1286[B]:UQ2:H8	2.38	0.52
3:M:270:ILE:O	3:M:274:VAL:HG13	2.09	0.52
1:H:117:ARG:NH1	14:H:2051:HOH:O	2.12	0.52
1:H:219:ILE:HD12	1:H:221:SER:O	2.10	0.52
3:M:189:PHE:O	3:M:193:HIS:CD2	2.63	0.51
2:L:181:PHE:HB3	6:M:1314:BPH:CBB	2.39	0.51
4:M:1303:BCL:H91	4:M:1303:BCL:H151	1.92	0.51
4:M:1303:BCL:CBB	13:M:1316:SPO:H243	2.41	0.50
12:M:1315:U10:H312	12:M:1315:U10:H352	1.94	0.50
1:H:81:GLU:HG3	1:H:85[B]:ILE:HD11	1.93	0.50
3:M:77:GLN:HE22	3:M:93:SER:H	1.59	0.50
1:H:140:PHE:HA	3:M:13:ARG:O	2.12	0.50
4:M:1304:BCL:HAA2	4:M:1304:BCL:HBD	1.93	0.49
3:M:202:HIS:CE1	3:M:206:ILE:HD11	2.47	0.49
1:H:96:PHE:HB3	1:H:97:PRO:CD	2.42	0.49
6:L:1285:BPH:HBB1	3:M:210:TYR:CD2	2.47	0.49
3:M:162:PHE:HB2	13:M:1316:SPO:H312	1.94	0.49
1:H:194:GLN:CG	3:M:5:ASN:HD21	2.23	0.49
1:H:37:ARG:O	1:H:38:GLU:HG2	2.13	0.48
2:L:224:ILE:H	7:L:1286[A]:UQ2:H2M3	1.78	0.48
4:M:1303:BCL:CBB	4:M:1303:BCL:HHC	2.45	0.47
3:M:71:GLY:HA3	13:M:1316:SPO:H6	1.97	0.46
3:M:186:THR:HG22	4:M:1304:BCL:HHD	1.96	0.46
3:M:157:TRP:HB2	4:M:1304:BCL:H71	1.96	0.46
7:L:1286[B]:UQ2:C16	5:M:1312:LDA:C12	2.93	0.46
4:L:1282:BCL:CMB	4:M:1304:BCL:HHB	2.46	0.46
3:M:164:ARG:HB3	3:M:165:PRO:HD3	1.98	0.46
1:H:108:GLY:O	1:H:113:SER:HA	2.16	0.46
5:M:1307:LDA:H31	5:M:1307:LDA:H61	1.68	0.45
4:L:1283:BCL:H161	4:L:1283:BCL:H142	1.78	0.45
1:H:163:LYS:HE2	1:H:165:VAL:HG12	1.99	0.45
1:H:87:LEU:HD23	1:H:100:PRO:HA	1.98	0.45
2:L:190:HIS:CE1	2:L:230:HIS:CE1	3.05	0.44
1:H:96:PHE:HB3	1:H:97:PRO:HD2	1.99	0.44
2:L:153:HIS:CD2	4:L:1283:BCL:NC	2.86	0.44
4:M:1303:BCL:H203	13:M:1316:SPO:H10	2.00	0.44
7:L:1286[B]:UQ2:H5M1	7:L:1286[B]:UQ2:H71	1.73	0.44
1:H:14:SER:OG	3:M:302:GLY:HA3	2.17	0.44
1:H:87:LEU:HD22	1:H:98:HIS:O	2.17	0.44
2:L:170:ASN:C	2:L:170:ASN:ND2	2.69	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:H:98:HIS:CD2	2:L:7:ARG:HH21	2.36	0.43
2:L:2:LEU:HD11	2:L:10:ARG:CZ	2.48	0.43
1:H:62:LYS:HE2	1:H:64:PHE:CZ	2.53	0.43
1:H:40:TYR:HB3	1:H:58:LEU:HD21	2.00	0.43
3:M:199:ASN:HD22	3:M:200:PRO:N	2.16	0.43
3:M:194:GLY:O	3:M:195:ASN:CB	2.66	0.43
3:M:274:VAL:O	3:M:278:LEU:HB2	2.19	0.43
2:L:173:HIS:CE1	2:L:177:ILE:HD11	2.54	0.43
5:L:1284:LDA:HM21	5:L:1284:LDA:H22	1.82	0.43
2:L:173:HIS:O	2:L:177:ILE:HG13	2.18	0.43
2:L:113:ILE:HG22	3:M:229:PHE:HE1	1.82	0.43
5:M:1307:LDA:HM22	5:M:1308:LDA:HM22	1.99	0.43
5:M:1307:LDA:H112	12:M:1315:U10:H202	2.00	0.42
1:H:84:PRO:O	1:H:85[A]:ILE:HD13	2.19	0.42
1:H:131:ILE:HA	1:H:169:VAL:O	2.19	0.42
3:M:199:ASN:ND2	3:M:199:ASN:C	2.72	0.42
3:M:26:LEU:HD12	3:M:26:LEU:H	1.84	0.42
4:L:1282:BCL:HHC	4:M:1304:BCL:CHC	2.49	0.42
7:L:1286[B]:UQ2:C16	5:M:1312:LDA:H121	2.37	0.42
5:M:1307:LDA:H22	5:M:1307:LDA:HM11	1.59	0.42
2:L:128:TYR:HD1	4:L:1283:BCL:HBB1	1.85	0.42
5:M:1307:LDA:H51	5:M:1307:LDA:H81	1.71	0.42
1:H:138:ALA:HA	1:H:139:GLY:HA2	1.85	0.42
1:H:144:ALA:HB3	3:M:11:GLN:HB2	2.01	0.42
2:L:162:TYR:HA	2:L:165:GLY:O	2.19	0.42
7:L:1286[A]:UQ2:H121	7:L:1286[A]:UQ2:H101	1.57	0.42
2:L:224:ILE:HD12	7:L:1286[A]:UQ2:H102	2.01	0.41
1:H:173:GLU:O	1:H:174:GLN:C	2.58	0.41
2:L:170:ASN:HD22	2:L:171:PRO:N	2.18	0.41
5:M:1307:LDA:H51	5:M:1308:LDA:H62	2.03	0.41
3:M:199:ASN:ND2	3:M:201:PHE:H	2.18	0.41
6:L:1285:BPH:HBB1	3:M:210:TYR:CG	2.56	0.40
3:M:63:GLY:HA3	6:M:1314:BPH:H5C1	2.03	0.40
2:L:38:THR:HG21	2:L:100:TRP:HE3	1.86	0.40
3:M:171:TRP:CZ3	13:M:1316:SPO:H343	2.56	0.40
12:M:1315:U10:H351	12:M:1315:U10:H372	1.78	0.40
2:L:227:LEU:HD21	3:M:5:ASN:OD1	2.21	0.40
3:M:297:TRP:CE2	3:M:302:GLY:HA2	2.57	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
14:H:2030:HOH:O	14:H:2030:HOH:O[4.555]	1.99	0.21

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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	H	242/260 (93%)	233 (96%)	8 (3%)	1 (0%)	43	76
2	L	279/281 (99%)	266 (95%)	13 (5%)	0	100	100
3	M	301/307 (98%)	282 (94%)	17 (6%)	2 (1%)	30	62
All	All	822/848 (97%)	781 (95%)	38 (5%)	3 (0%)	43	76

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	249	LYS
3	M	52	LEU
3	M	301	HIS

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	H	198/208 (95%)	187 (94%)	11 (6%)	30	59
2	L	220/220 (100%)	203 (92%)	17 (8%)	18	40
3	M	236/240 (98%)	220 (93%)	16 (7%)	22	48
All	All	654/668 (98%)	610 (93%)	44 (7%)	24	49

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	12	LEU
1	H	14	SER
1	H	93	SER
1	H	175	MET
1	H	184	LYS
1	H	220[A]	LYS
1	H	220[B]	LYS
1	H	221	SER
1	H	231	ASP
1	H	247	LYS
1	H	249	LYS
2	L	16	LEU
2	L	44	LEU
2	L	80	LEU
2	L	82	LYS
2	L	102	LEU
2	L	126	LEU
2	L	129	LEU
2	L	158	SER
2	L	170	ASN
2	L	207	ARG
2	L	210	ASP
2	L	216	PHE
2	L	246	LEU
2	L	247	CYS
2	L	254	ILE
2	L	268	LYS
2	L	272	TRP
3	M	2	GLU
3	M	5	ASN
3	M	6	ILE
3	M	17	ASP
3	M	18	LEU
3	M	30	SER
3	M	39	LEU
3	M	52	LEU
3	M	60	LEU
3	M	109	LEU
3	M	124	VAL
3	M	182	HIS
3	M	191	LEU
3	M	199	ASN
3	M	216	PHE

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Mol	Chain	Res	Type
3	M	278	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	98	HIS
2	L	159	ASN
2	L	170	ASN
2	L	264	GLN
3	M	5	ASN
3	M	77	GLN
3	M	187	ASN
3	M	193	HIS
3	M	199	ASN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 26 ligands modelled in this entry, 1 is monoatomic - leaving 25 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
4	BCL	L	1282	2	74,74,74	2.08	10 (13%)	97,115,115	1.98	22 (22%)
4	BCL	L	1283	2	74,74,74	2.12	11 (14%)	97,115,115	2.26	30 (30%)
5	LDA	L	1284	-	15,15,15	3.62	1 (6%)	17,17,17	0.92	1 (5%)
6	BPH	L	1285	-	70,70,70	3.05	14 (20%)	94,101,101	1.80	17 (18%)
7	UQ2	L	1286[A]	-	23,23,23	2.79	7 (30%)	31,31,31	1.15	2 (6%)
7	UQ2	L	1286[B]	-	23,23,23	2.71	8 (34%)	31,31,31	1.50	4 (12%)
8	PO4	L	1287	-	4,4,4	0.25	0	6,6,6	0.31	0
9	HTO	L	1288	-	9,9,9	0.59	0	10,10,10	0.66	0
10	GOL	L	1289	-	5,5,5	0.29	0	5,5,5	0.64	0
10	GOL	L	1290	-	5,5,5	0.25	0	5,5,5	0.44	0
4	BCL	M	1303	3	74,74,74	2.18	11 (14%)	97,115,115	2.09	25 (25%)
4	BCL	M	1304	3	74,74,74	2.11	11 (14%)	97,115,115	2.18	27 (27%)
5	LDA	M	1305	-	15,15,15	3.56	1 (6%)	17,17,17	2.09	4 (23%)
5	LDA	M	1306	-	15,15,15	3.77	1 (6%)	17,17,17	0.61	0
5	LDA	M	1307	-	15,15,15	3.76	2 (13%)	17,17,17	0.97	1 (5%)
5	LDA	M	1308	-	15,15,15	3.84	1 (6%)	17,17,17	0.85	1 (5%)
5	LDA	M	1309	-	15,15,15	3.87	1 (6%)	17,17,17	0.66	0
5	LDA	M	1310	-	15,15,15	3.64	1 (6%)	17,17,17	0.68	0
5	LDA	M	1311	-	15,15,15	3.73	1 (6%)	17,17,17	0.98	1 (5%)
5	LDA	M	1312	-	15,15,15	3.93	2 (13%)	17,17,17	1.00	1 (5%)
6	BPH	M	1314	-	70,70,70	2.85	16 (22%)	94,101,101	1.88	19 (20%)
12	U10	M	1315	-	48,48,63	3.15	13 (27%)	59,61,79	1.74	11 (18%)
13	SPO	M	1316	-	41,41,41	4.20	12 (29%)	50,50,50	2.02	13 (26%)
10	GOL	M	1317	-	5,5,5	0.29	0	5,5,5	0.51	0
10	GOL	X	1007	-	5,5,5	0.33	0	5,5,5	0.40	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
4	BCL	L	1282	2	2/2/21/25	0/41/137/137	0/0/9/9
4	BCL	L	1283	2	2/2/21/25	0/41/137/137	0/0/9/9
5	LDA	L	1284	-	-	0/13/13/13	0/0/0/0
6	BPH	L	1285	-	2/2/18/22	0/49/105/105	0/0/6/6
7	UQ2	L	1286[A]	-	-	0/15/39/39	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	UQ2	L	1286[B]	-	-	0/15/39/39	0/1/1/1
8	PO4	L	1287	-	-	0/0/0/0	0/0/0/0
9	HTO	L	1288	-	-	0/10/10/10	0/0/0/0
10	GOL	L	1289	-	-	0/4/4/4	0/0/0/0
10	GOL	L	1290	-	-	0/4/4/4	0/0/0/0
4	BCL	M	1303	3	2/2/21/25	0/41/137/137	0/0/9/9
4	BCL	M	1304	3	2/2/21/25	0/41/137/137	0/0/9/9
5	LDA	M	1305	-	-	0/13/13/13	0/0/0/0
5	LDA	M	1306	-	-	0/13/13/13	0/0/0/0
5	LDA	M	1307	-	-	0/13/13/13	0/0/0/0
5	LDA	M	1308	-	-	0/13/13/13	0/0/0/0
5	LDA	M	1309	-	-	0/13/13/13	0/0/0/0
5	LDA	M	1310	-	-	0/13/13/13	0/0/0/0
5	LDA	M	1311	-	-	0/13/13/13	0/0/0/0
5	LDA	M	1312	-	-	0/13/13/13	0/0/0/0
6	BPH	M	1314	-	2/2/18/22	0/49/105/105	0/0/6/6
12	U10	M	1315	-	-	0/45/69/87	0/1/1/1
13	SPO	M	1316	-	-	0/47/47/47	0/0/0/0
10	GOL	M	1317	-	-	0/4/4/4	0/0/0/0
10	GOL	X	1007	-	-	0/4/4/4	0/0/0/0

All (124) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	M	1312	LDA	O1-N1	-14.99	1.25	1.39
5	M	1309	LDA	O1-N1	-14.81	1.25	1.39
5	M	1308	LDA	O1-N1	-14.64	1.25	1.39
6	L	1285	BPH	C1D-CHD	14.63	1.51	1.35
5	M	1306	LDA	O1-N1	-14.39	1.25	1.39
5	M	1311	LDA	O1-N1	-14.27	1.26	1.39
5	M	1307	LDA	O1-N1	-14.23	1.26	1.39
5	L	1284	LDA	O1-N1	-13.88	1.26	1.39
5	M	1310	LDA	O1-N1	-13.84	1.26	1.39
13	M	1316	SPO	C27-C28	13.55	1.48	1.34
5	M	1305	LDA	O1-N1	-13.43	1.26	1.39
6	M	1314	BPH	OBD-CAD	13.06	1.41	1.22
4	L	1283	BCL	OBD-CAD	12.95	1.41	1.22
4	M	1303	BCL	OBD-CAD	12.49	1.40	1.22
4	M	1304	BCL	OBD-CAD	12.40	1.40	1.22
6	L	1285	BPH	OBD-CAD	11.97	1.39	1.22
4	L	1282	BCL	OBD-CAD	11.88	1.39	1.22
6	M	1314	BPH	C1D-CHD	11.17	1.47	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	M	1316	SPO	C14-C12	9.56	1.48	1.35
13	M	1316	SPO	C9-C7	9.35	1.48	1.35
13	M	1316	SPO	C19-C17	9.10	1.47	1.35
13	M	1316	SPO	C22-C23	8.83	1.47	1.35
7	L	1286[A]	UQ2	C8-C9	8.30	1.49	1.32
12	M	1315	U10	C33-C34	8.23	1.49	1.32
7	L	1286[B]	UQ2	C8-C9	8.08	1.49	1.32
6	L	1285	BPH	O1D-CGD	7.98	1.41	1.21
12	M	1315	U10	C13-C14	7.84	1.48	1.32
13	M	1316	SPO	C32-C33	7.69	1.48	1.32
12	M	1315	U10	C23-C24	7.55	1.48	1.32
12	M	1315	U10	C28-C29	7.40	1.47	1.32
12	M	1315	U10	C8-C9	7.37	1.47	1.32
12	M	1315	U10	C18-C19	7.33	1.47	1.32
6	M	1314	BPH	O1D-CGD	7.20	1.39	1.21
6	M	1314	BPH	C2-C3	7.15	1.47	1.32
12	M	1315	U10	C38-C39	6.83	1.48	1.34
6	L	1285	BPH	C2-C3	6.79	1.46	1.32
6	L	1285	BPH	O1A-CGA	6.45	1.41	1.22
4	M	1303	BCL	O1A-CGA	6.31	1.41	1.22
6	M	1314	BPH	O1A-CGA	6.22	1.41	1.22
4	M	1304	BCL	O1A-CGA	6.19	1.41	1.22
6	L	1285	BPH	OBB-CAB	5.81	1.42	1.22
4	L	1283	BCL	O1A-CGA	5.72	1.39	1.22
13	M	1316	SPO	C37-C38	5.53	1.50	1.32
4	L	1282	BCL	O1A-CGA	5.50	1.39	1.22
4	M	1303	BCL	C4D-C3D	-5.49	1.34	1.41
4	M	1304	BCL	C4D-C3D	-5.39	1.35	1.41
6	M	1314	BPH	OBB-CAB	5.38	1.41	1.22
7	L	1286[B]	UQ2	C13-C14	5.34	1.49	1.32
4	L	1282	BCL	C4D-C3D	-5.23	1.35	1.41
13	M	1316	SPO	C6-C5	5.02	1.46	1.31
7	L	1286[B]	UQ2	O2-C2	-4.94	1.24	1.36
7	L	1286[A]	UQ2	O3-C3	-4.87	1.24	1.36
7	L	1286[A]	UQ2	C13-C14	4.87	1.48	1.32
4	L	1283	BCL	C4D-C3D	-4.74	1.35	1.41
4	M	1303	BCL	C3D-CAD	-4.72	1.37	1.47
7	L	1286[A]	UQ2	O2-C2	-4.72	1.24	1.36
12	M	1315	U10	O4-C4	-4.55	1.25	1.36
6	L	1285	BPH	C4D-C3D	-4.54	1.36	1.41
13	M	1316	SPO	C10-C11	4.48	1.46	1.34
13	M	1316	SPO	C15-C16	4.45	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	M	1316	SPO	C26-C25	4.39	1.46	1.34
6	L	1285	BPH	C3D-CAD	-4.31	1.38	1.47
6	M	1314	BPH	C4D-C3D	-4.19	1.36	1.41
12	M	1315	U10	O3-C3	-4.07	1.26	1.36
4	L	1282	BCL	C3D-CAD	-4.06	1.39	1.47
4	M	1303	BCL	C2-C3	4.01	1.41	1.32
4	M	1304	BCL	C3D-CAD	-3.97	1.39	1.47
7	L	1286[B]	UQ2	O3-C3	-3.96	1.26	1.36
4	L	1283	BCL	C3D-CAD	-3.84	1.39	1.47
4	L	1283	BCL	C2-C3	3.74	1.40	1.32
4	L	1282	BCL	C2-C3	3.68	1.40	1.32
4	M	1303	BCL	C1B-NB	3.67	1.39	1.34
6	M	1314	BPH	C3D-CAD	-3.65	1.39	1.47
4	M	1304	BCL	C2-C3	3.65	1.40	1.32
4	M	1304	BCL	C1A-NA	3.62	1.40	1.32
4	L	1282	BCL	C1A-NA	3.60	1.40	1.32
13	M	1316	SPO	C21-C20	3.60	1.45	1.35
4	L	1283	BCL	C4B-NB	3.34	1.38	1.34
4	L	1283	BCL	C1A-NA	3.32	1.39	1.32
6	M	1314	BPH	C3D-C2D	3.31	1.50	1.40
6	L	1285	BPH	C3D-C2D	3.21	1.50	1.40
4	M	1303	BCL	C4B-NB	3.19	1.38	1.34
4	L	1282	BCL	C1B-NB	3.18	1.38	1.34
4	L	1282	BCL	C4B-NB	3.16	1.38	1.34
4	L	1283	BCL	C1B-NB	3.12	1.38	1.34
6	L	1285	BPH	CHD-C4C	3.12	1.48	1.41
7	L	1286[A]	UQ2	C3-C4	-2.99	1.40	1.48
4	M	1303	BCL	O2D-CGD	-2.98	1.25	1.33
4	M	1304	BCL	C4B-NB	2.95	1.38	1.34
12	M	1315	U10	C6-C1	2.91	1.42	1.35
7	L	1286[B]	UQ2	C3-C4	-2.89	1.40	1.48
7	L	1286[A]	UQ2	C6-C5	2.83	1.42	1.35
5	M	1307	LDA	C1-N1	-2.78	1.46	1.51
4	L	1283	BCL	O2A-CGA	-2.76	1.24	1.33
4	L	1282	BCL	O2D-CGD	-2.76	1.25	1.33
6	M	1314	BPH	O2D-CGD	-2.74	1.25	1.33
7	L	1286[A]	UQ2	C2-C1	-2.66	1.41	1.48
4	M	1303	BCL	C1A-NA	2.66	1.38	1.32
12	M	1315	U10	C4-C5	-2.63	1.41	1.48
4	M	1304	BCL	C1C-NC	-2.57	1.33	1.39
4	M	1304	BCL	C1B-NB	2.51	1.37	1.34
4	L	1282	BCL	CHD-C4C	2.48	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	M	1314	BPH	O2A-CGA	-2.40	1.25	1.33
6	L	1285	BPH	C4A-NA	-2.40	1.33	1.38
6	M	1314	BPH	CHC-C1C	2.37	1.47	1.38
4	M	1303	BCL	CHD-C4C	2.30	1.46	1.39
6	M	1314	BPH	CHB-C4A	2.30	1.47	1.38
6	M	1314	BPH	CHD-C4C	2.29	1.46	1.41
6	L	1285	BPH	CHB-C4A	2.29	1.47	1.38
4	L	1283	BCL	O2D-CGD	-2.25	1.27	1.33
4	M	1304	BCL	CHD-C4C	2.24	1.46	1.39
7	L	1286[B]	UQ2	C2-C1	-2.24	1.42	1.48
7	L	1286[B]	UQ2	C6-C1	-2.23	1.39	1.46
4	M	1303	BCL	C1C-NC	-2.21	1.34	1.39
6	M	1314	BPH	C1C-NC	-2.17	1.33	1.38
4	L	1283	BCL	C1C-NC	-2.13	1.34	1.39
4	M	1304	BCL	O2D-CGD	-2.12	1.27	1.33
12	M	1315	U10	C41-C39	2.11	1.52	1.40
7	L	1286[B]	UQ2	C6-C5	2.11	1.40	1.35
5	M	1312	LDA	C1-N1	-2.07	1.47	1.51
6	L	1285	BPH	CHC-C1C	2.05	1.46	1.38
6	L	1285	BPH	O2D-CED	-2.03	1.40	1.45
6	M	1314	BPH	C4D-ND	-2.02	1.35	1.38
12	M	1315	U10	C3-C2	-2.02	1.43	1.48

All (179) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L	1283	BCL	CMB-C2B-C1B	-8.08	116.19	128.62
4	M	1304	BCL	CMB-C2B-C1B	-8.04	116.26	128.62
4	L	1282	BCL	C2D-C1D-ND	-7.92	103.43	109.41
6	M	1314	BPH	C3B-C2B-C1B	-7.76	102.37	107.01
4	M	1303	BCL	CMB-C2B-C1B	-7.10	117.70	128.62
4	L	1282	BCL	CMB-C2B-C1B	-6.85	118.08	128.62
6	L	1285	BPH	C3B-C2B-C1B	-6.60	103.06	107.01
4	M	1304	BCL	CMB-C2B-C3B	5.80	134.11	124.97
4	L	1283	BCL	O2D-CGD-CBD	5.77	123.08	111.33
12	M	1315	U10	C30-C29-C31	5.73	124.10	115.39
4	M	1304	BCL	C2D-C1D-ND	-5.72	105.09	109.41
5	M	1305	LDA	CM2-N1-CM1	-5.61	102.44	108.85
6	M	1314	BPH	O2D-CGD-CBD	5.61	122.75	111.33
4	L	1283	BCL	C2B-C1B-NB	-5.49	105.27	109.41
6	L	1285	BPH	O2D-CGD-CBD	5.48	122.49	111.33
4	L	1283	BCL	CMB-C2B-C3B	5.48	133.60	124.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	M	1314	BPH	OBD-CAD-CBD	-5.46	117.70	125.94
6	L	1285	BPH	CMD-C2D-C1D	5.43	134.61	125.81
4	M	1303	BCL	C3A-C4A-CHB	-5.35	113.22	124.33
4	M	1303	BCL	O2D-CGD-CBD	5.34	122.21	111.33
13	M	1316	SPO	C26-C27-C28	-5.32	122.82	127.91
6	M	1314	BPH	C1D-C2D-C3D	-5.28	102.36	106.89
4	L	1282	BCL	CMB-C2B-C3B	5.25	133.24	124.97
4	L	1282	BCL	C4D-ND-C1D	5.23	112.88	106.57
4	L	1283	BCL	CHB-C4A-NA	-5.10	118.53	124.58
4	M	1303	BCL	CMB-C2B-C3B	5.09	132.98	124.97
6	M	1314	BPH	OBD-CAD-C3D	-5.03	118.56	127.91
4	L	1283	BCL	C2D-C1D-ND	-4.90	105.71	109.41
4	M	1304	BCL	O2D-CGD-CBD	4.83	121.17	111.33
4	M	1304	BCL	C1D-CHD-C4C	-4.79	117.29	125.55
4	M	1303	BCL	C2D-C1D-ND	-4.63	105.92	109.41
4	M	1303	BCL	CHC-C1C-NC	-4.54	119.19	124.58
12	M	1315	U10	C17-C18-C19	-4.46	118.17	127.80
6	L	1285	BPH	C1D-C2D-C3D	-4.40	103.12	106.89
4	M	1304	BCL	CHD-C4C-NC	-4.36	119.56	125.86
13	M	1316	SPO	C20-C19-C17	-4.32	121.07	127.29
4	M	1304	BCL	CHC-C1C-NC	-4.31	119.47	124.58
4	M	1304	BCL	C2B-C1B-NB	-4.30	106.17	109.41
4	L	1283	BCL	C4B-CHC-C1C	-4.23	121.25	130.06
4	L	1282	BCL	C1D-CHD-C4C	-4.13	118.43	125.55
4	L	1283	BCL	CHC-C4B-NB	-4.11	117.71	124.58
5	M	1305	LDA	C2-C1-N1	4.08	120.83	113.80
4	M	1303	BCL	C1B-CHB-C4A	-4.05	121.64	130.06
13	M	1316	SPO	C10-C9-C7	-4.01	121.52	127.29
4	M	1303	BCL	C2B-C1B-NB	-3.97	106.42	109.41
4	L	1283	BCL	C4-C3-C5	3.86	121.26	115.39
4	L	1283	BCL	C1D-CHD-C4C	-3.79	119.02	125.55
6	L	1285	BPH	C1-C2-C3	-3.76	119.49	126.19
4	M	1304	BCL	C4D-ND-C1D	3.74	111.09	106.57
6	L	1285	BPH	O1D-CGD-CBD	-3.73	116.78	124.42
4	M	1303	BCL	CHB-C4A-NA	-3.72	120.16	124.58
4	M	1303	BCL	C1D-CHD-C4C	-3.71	119.14	125.55
4	L	1282	BCL	O2A-CGA-CBA	3.71	123.62	111.94
13	M	1316	SPO	C29-C28-C30	3.70	121.02	115.39
4	L	1283	BCL	C1C-NC-C4C	-3.70	103.30	107.79
4	M	1303	BCL	C4D-ND-C1D	3.66	110.99	106.57
4	L	1283	BCL	O2A-CGA-O1A	-3.66	113.44	123.43
4	M	1304	BCL	CMD-C2D-C1D	3.66	133.39	126.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L	1285	BPH	CED-O2D-CGD	3.62	124.64	116.02
4	M	1304	BCL	O2D-CGD-O1D	-3.61	116.46	123.79
4	L	1283	BCL	C4D-ND-C1D	3.55	110.86	106.57
6	M	1314	BPH	CMD-C2D-C3D	-3.47	119.50	124.97
4	M	1304	BCL	O2A-CGA-CBA	3.44	122.76	111.94
13	M	1316	SPO	C21-C22-C23	-3.42	122.36	127.29
4	L	1283	BCL	C2A-C3A-C4A	3.38	106.61	101.40
5	M	1305	LDA	O1-N1-C1	3.36	114.87	110.19
6	L	1285	BPH	C2B-C1B-NB	3.36	114.69	108.16
13	M	1316	SPO	C15-C14-C12	-3.34	122.48	127.29
4	M	1303	BCL	O2D-CGD-O1D	-3.34	117.01	123.79
6	M	1314	BPH	C2B-C1B-NB	3.32	114.62	108.16
4	M	1303	BCL	CMD-C2D-C1D	3.31	132.70	126.16
4	L	1283	BCL	CHA-C1A-NA	-3.30	119.44	126.22
7	L	1286[B]	UQ2	O1-C1-C6	-3.29	115.63	121.67
4	M	1304	BCL	C1B-CHB-C4A	-3.28	123.24	130.06
6	L	1285	BPH	OBD-CAD-C3D	-3.27	121.82	127.91
4	M	1303	BCL	O2A-C1-C2	3.26	115.62	108.55
6	L	1285	BPH	C3B-C4B-NB	3.26	110.78	107.10
12	M	1315	U10	C30-C29-C28	-3.24	117.10	123.52
13	M	1316	SPO	C24-C23-C25	3.18	123.24	118.09
6	L	1285	BPH	CMD-C2D-C3D	-3.16	119.98	124.97
13	M	1316	SPO	C34-C33-C35	3.17	120.20	115.39
6	M	1314	BPH	O2D-CGD-O1D	-3.14	117.42	123.79
4	M	1303	BCL	C4B-CHC-C1C	-3.14	123.53	130.06
4	M	1304	BCL	CHB-C1B-NB	-3.12	119.37	124.58
4	L	1283	BCL	CHD-C4C-NC	-3.08	121.42	125.86
7	L	1286[B]	UQ2	CM5-C5-C6	-3.07	118.10	124.20
4	L	1283	BCL	C1B-CHB-C4A	-3.06	123.69	130.06
4	M	1303	BCL	C1-O2A-CGA	3.06	125.54	116.98
4	M	1304	BCL	CMD-C2D-C3D	-3.05	120.16	124.97
4	L	1282	BCL	C2A-C3A-C4A	3.05	106.08	101.40
5	M	1305	LDA	O1-N1-CM2	-3.04	104.92	109.01
4	M	1303	BCL	C2A-C3A-C4A	3.02	106.04	101.40
6	M	1314	BPH	C3B-C4B-NB	2.99	110.48	107.10
7	L	1286[B]	UQ2	CM3-O3-C3	2.99	126.63	116.48
5	L	1284	LDA	O1-N1-C1	-2.98	106.03	110.19
4	M	1304	BCL	OBB-CAB-C3B	2.97	124.53	120.07
5	M	1307	LDA	C2-C1-N1	-2.96	108.70	113.80
5	M	1311	LDA	O1-N1-CM2	-2.95	105.04	109.01
4	L	1282	BCL	O2D-CGD-CBD	2.94	117.31	111.33
12	M	1315	U10	C27-C28-C29	-2.93	121.48	127.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L	1283	BCL	C3A-C4A-CHB	-2.92	118.26	124.33
5	M	1312	LDA	O1-N1-C1	-2.92	106.12	110.19
4	L	1283	BCL	O1D-CGD-CBD	-2.92	118.45	124.42
4	M	1303	BCL	C2C-C1C-CHC	-2.91	118.28	124.33
4	M	1303	BCL	O2A-CGA-CBA	2.91	121.08	111.94
4	M	1304	BCL	C4-C3-C5	2.87	119.75	115.39
13	M	1316	SPO	C4-C5-C6	-2.86	120.21	124.95
4	L	1282	BCL	C3A-C4A-CHB	-2.86	118.39	124.33
12	M	1315	U10	C10-C9-C11	2.86	119.73	115.39
6	M	1314	BPH	CMB-C2B-C1B	-2.80	124.38	128.65
6	M	1314	BPH	CMD-C2D-C1D	2.75	130.27	125.81
4	L	1282	BCL	CHC-C4B-NB	-2.75	119.99	124.58
13	M	1316	SPO	C20-C21-C22	-2.72	117.34	123.36
6	L	1285	BPH	O2A-CGA-CBA	2.72	120.49	111.94
4	M	1303	BCL	CAA-C2A-C3A	-2.70	106.66	113.04
12	M	1315	U10	C4M-O4-C4	2.70	125.64	116.48
7	L	1286[B]	UQ2	C10-C9-C11	2.67	119.45	115.39
4	L	1283	BCL	O2A-CGA-CBA	2.67	120.33	111.94
4	L	1282	BCL	CMA-C3A-C4A	-2.65	104.07	111.76
4	L	1282	BCL	C1-O2A-CGA	2.64	124.39	116.98
4	M	1303	BCL	CHA-C1A-NA	-2.64	120.79	126.22
4	L	1283	BCL	O2D-CGD-O1D	-2.63	118.44	123.79
6	M	1314	BPH	C4-C3-C5	2.63	119.38	115.39
6	L	1285	BPH	OBD-CAD-CBD	-2.61	122.00	125.94
4	M	1304	BCL	CED-O2D-CGD	2.61	122.22	116.02
12	M	1315	U10	C20-C19-C21	2.60	119.35	115.39
6	M	1314	BPH	CAA-C2A-C1A	-2.57	105.97	112.72
12	M	1315	U10	C12-C13-C14	-2.56	122.28	127.80
4	L	1283	BCL	CAA-CBA-CGA	2.56	121.51	113.27
6	L	1285	BPH	C1-O2A-CGA	2.54	124.09	116.98
4	L	1282	BCL	O2A-CGA-O1A	-2.53	116.52	123.43
4	L	1283	BCL	C2B-C1B-CHB	2.53	130.79	126.00
4	M	1304	BCL	CHB-C4A-NA	-2.52	121.59	124.58
4	L	1283	BCL	C5-C3-C2	-2.51	116.26	121.08
4	L	1282	BCL	CAA-C2A-C1A	-2.49	105.41	111.62
6	L	1285	BPH	C1B-NB-C4B	-2.49	103.01	108.72
4	L	1282	BCL	CED-O2D-CGD	2.48	121.91	116.02
4	M	1304	BCL	CHA-C1A-NA	-2.46	121.17	126.22
4	M	1303	BCL	C3C-C4C-CHD	-2.45	117.99	123.35
4	L	1282	BCL	CHA-C1A-NA	-2.43	121.23	126.22
12	M	1315	U10	C32-C33-C34	-2.42	122.58	127.80
12	M	1315	U10	C15-C14-C16	2.42	119.06	115.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	M	1314	BPH	C1-C2-C3	-2.39	121.93	126.19
4	M	1303	BCL	CBD-CHA-C1A	2.39	131.89	128.77
4	M	1304	BCL	C2A-C3A-C4A	2.36	105.03	101.40
4	M	1304	BCL	CGD-CBD-CHA	-2.34	103.01	110.96
4	L	1282	BCL	CMD-C2D-C1D	2.34	130.78	126.16
12	M	1315	U10	C22-C23-C24	-2.31	122.81	127.80
4	L	1283	BCL	CED-O2D-CGD	2.30	121.50	116.02
4	L	1282	BCL	C14-C13-C12	2.30	119.45	111.02
6	L	1285	BPH	C7-C6-C5	-2.30	106.25	113.01
13	M	1316	SPO	C5-C6-C7	-2.27	120.08	125.95
4	L	1283	BCL	C3C-C4C-CHD	-2.26	118.39	123.35
4	M	1303	BCL	C4A-NA-C1A	2.26	109.64	106.52
4	L	1283	BCL	CBD-CHA-C1A	2.26	131.72	128.77
4	M	1304	BCL	C16-C15-C13	-2.25	108.66	115.14
6	M	1314	BPH	O1D-CGD-CBD	-2.24	119.83	124.42
6	M	1314	BPH	C1B-NB-C4B	-2.24	103.58	108.72
6	M	1314	BPH	C2D-C1D-ND	2.23	113.92	106.38
13	M	1316	SPO	C27-C26-C25	-2.23	115.72	123.24
4	L	1283	BCL	CAA-C2A-C3A	-2.21	107.82	113.04
4	M	1304	BCL	C3C-C4C-CHD	-2.18	118.56	123.35
4	L	1282	BCL	C1C-NC-C4C	-2.18	105.14	107.79
7	L	1286[A]	UQ2	C10-C9-C8	-2.16	119.23	123.52
4	L	1282	BCL	O2A-C1-C2	2.17	113.24	108.55
4	M	1304	BCL	C2C-C1C-CHC	-2.16	119.83	124.33
4	L	1282	BCL	C2B-C1B-NB	-2.13	107.80	109.41
4	M	1304	BCL	C4-C3-C2	-2.12	119.31	123.52
4	L	1283	BCL	CHC-C1C-NC	-2.11	122.07	124.58
4	L	1282	BCL	C1B-CHB-C4A	-2.11	125.67	130.06
6	L	1285	BPH	CAC-C3C-C4C	2.10	118.46	112.68
4	L	1283	BCL	CMD-C2D-C1D	2.08	130.28	126.16
7	L	1286[A]	UQ2	CM2-O2-C2	2.08	123.56	116.48
6	M	1314	BPH	C4D-C3D-C2D	-2.07	104.86	107.37
5	M	1308	LDA	O1-N1-CM1	-2.07	106.22	109.01
4	M	1304	BCL	CGD-CBD-CAD	-2.06	103.97	110.96
6	M	1314	BPH	CED-O2D-CGD	2.05	120.89	116.02
4	M	1303	BCL	C1D-C2D-C3D	-2.03	105.12	106.78
13	M	1316	SPO	C14-C15-C16	-2.03	116.39	123.24

All (12) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	M	1303	BCL	C8

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Mol	Chain	Res	Type	Atom
4	M	1303	BCL	C13
4	L	1283	BCL	C8
4	L	1283	BCL	C13
6	L	1285	BPH	C8
6	L	1285	BPH	C13
4	M	1304	BCL	C8
4	M	1304	BCL	C13
6	M	1314	BPH	C8
6	M	1314	BPH	C13
4	L	1282	BCL	C8
4	L	1282	BCL	C13

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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	H	241/260 (92%)	-0.46	8 (3%)	44	49	38, 50, 63, 105	0
2	L	281/281 (100%)	-0.75	4 (1%)	72	77	32, 43, 69, 77	0
3	M	303/307 (98%)	-0.56	7 (2%)	57	64	31, 50, 75, 96	0
All	All	825/848 (97%)	-0.60	19 (2%)	56	64	31, 48, 71, 105	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	M	1	ALA	7.4
1	H	250	SER	7.1
1	H	251	VAL	7.0
1	H	249	LYS	3.9
3	M	302	GLY	3.8
1	H	220[A]	LYS	3.7
2	L	281	GLY	3.6
3	M	27	ALA	3.2
3	M	2	GLU	3.0
1	H	221	SER	2.7
1	H	247	LYS	2.5
3	M	106	ALA	2.3
3	M	301	HIS	2.3
1	H	51	ALA	2.2
3	M	52	LEU	2.2
2	L	202	LYS	2.2
2	L	270	PRO	2.0
1	H	222	PRO	2.0
2	L	276	PRO	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
5	LDA	M	1312	16/16	0.37	31.58	101,109,116,116	0
5	LDA	L	1284	16/16	0.46	27.00	61,96,114,115	0
5	LDA	M	1311	16/16	0.48	25.77	87,101,112,113	0
5	LDA	M	1308	16/16	0.43	15.99	91,99,110,110	0
7	UQ2	L	1286[A]	23/23	0.31	13.16	51,53,54,55	23
5	LDA	M	1309	16/16	0.45	11.32	111,117,128,129	0
7	UQ2	L	1286[B]	23/23	0.31	10.53	43,49,55,55	23
9	HTO	L	1288	10/10	0.30	6.90	77,81,82,82	0
5	LDA	M	1305	16/16	0.25	6.80	45,71,82,82	0
8	PO4	L	1287	5/5	0.61	6.78	156,156,157,157	0
10	GOL	M	1317	6/6	0.25	5.17	98,101,101,103	0
5	LDA	M	1310	16/16	0.61	5.09	100,116,126,126	0
5	LDA	M	1306	16/16	0.32	4.44	76,79,86,86	0
10	GOL	L	1290	6/6	0.24	2.45	81,81,82,82	0
6	BPH	M	1314	65/65	0.18	2.14	42,50,111,113	0
12	U10	M	1315	48/63	0.17	1.70	37,48,78,80	0
13	SPO	M	1316	42/42	0.18	1.67	44,60,78,81	0
10	GOL	L	1289	6/6	0.29	1.63	71,74,74,76	0
5	LDA	M	1307	16/16	0.19	1.40	65,67,78,79	0
4	BCL	M	1304	66/66	0.14	0.69	29,39,60,70	0
6	BPH	L	1285	65/65	0.12	0.68	26,32,41,43	0
4	BCL	M	1303	66/66	0.12	0.65	30,34,81,82	0
4	BCL	L	1282	66/66	0.12	0.45	30,36,47,52	0
4	BCL	L	1283	66/66	0.11	-0.36	30,37,58,62	0
11	FE	M	1313	1/1	0.04	-3.81	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
10	GOL	X	1007	6/6	0.33	-	96,97,98,98	0

6.5 Other polymers ⓘ

There are no such residues in this entry.