



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 03:40 AM GMT

PDB ID : 2UXK
Title : X-RAY HIGH RESOLUTION STRUCTURE OF THE PHOTOSYNTHETIC
REACTION CENTER FROM RB. SPHAEROIDES AT PH 10 IN THE
CHARGE-SEPARATED STATE
Authors : Koepke, J.; Diehm, R.; Fritzsche, G.
Deposited on : 2007-03-28
Resolution : 2.31 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>

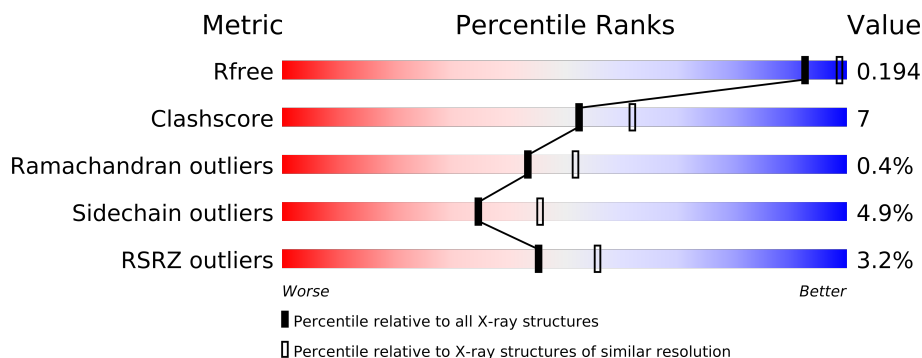
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.31 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	3293 (2.34-2.30)
Clashscore	79885	4097 (2.34-2.30)
Ramachandran outliers	78287	4055 (2.34-2.30)
Sidechain outliers	78261	4054 (2.34-2.30)
RSRZ outliers	66119	3294 (2.34-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	HTO	L	1291	-	X
14	CDL	M	1314	-	X
4	GOL	H	1251	-	X
4	GOL	H	1252	-	X
4	GOL	H	1253	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Geometry	Electron density
4	GOL	L	1293	-	X
4	GOL	M	1315	-	X
6	LDA	L	1283	-	X
6	LDA	L	1284	-	X
6	LDA	L	1285	-	X
6	LDA	L	1286	-	X
6	LDA	M	1305	-	X
6	LDA	M	1306	-	X
6	LDA	M	1307	-	X
6	LDA	M	1308	-	X
6	LDA	M	1309	-	X
8	UQ2	L	1288[A]	-	X
8	UQ2	L	1288[B]	-	X
9	PO4	L	1290	-	X

2 Entry composition i

There are 15 unique types of molecules in this entry. The entry contains 7701 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			

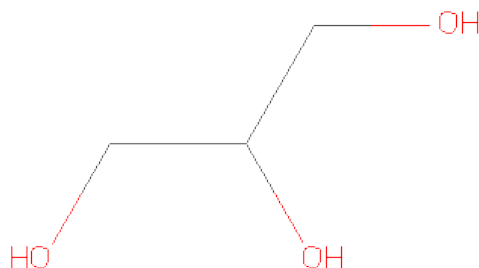
- Molecule 2 is a protein called REACTION CENTER PROTEIN L CHAIN.

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.

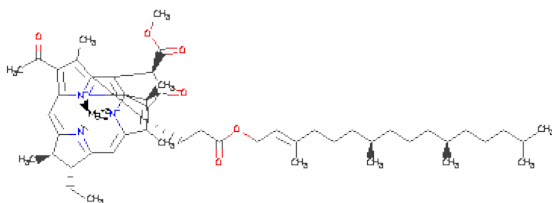
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	M	303	Total	C	N	O	S	0	0	1
			2409	1607	395	397	10			

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

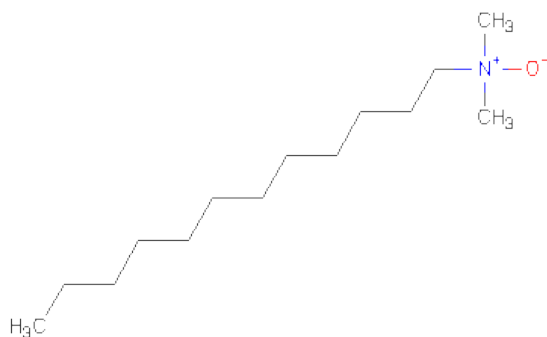
- Molecule 5 is BACTERIOCHLOROPHYLL A (three-letter code: BCL) (formula: $C_{55}H_{74}MgN_4O_6$).



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

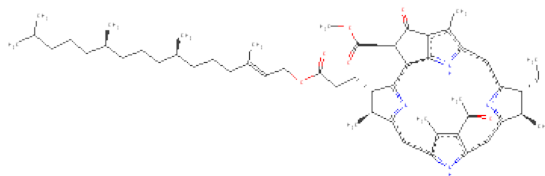
- Molecule 6 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula:

C₁₄H₃₁NO).



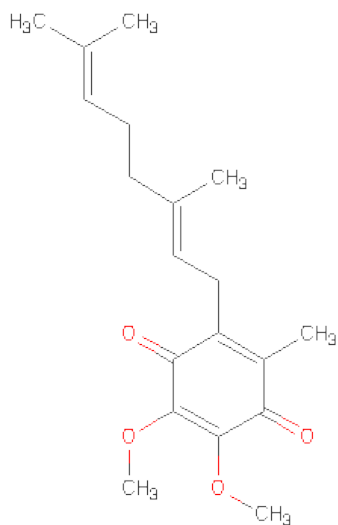
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	L	1	Total	C	N	O	0	0
			16	14	1	1		
6	L	1	Total	C	N	O	0	0
			16	14	1	1		
6	L	1	Total	C	N	O	0	0
			16	14	1	1		
6	L	1	Total	C	N	O	0	0
			16	14	1	1		
6	M	1	Total	C	N	O	0	0
			16	14	1	1		
6	M	1	Total	C	N	O	0	0
			16	14	1	1		
6	M	1	Total	C	N	O	0	0
			16	14	1	1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

- Molecule 7 is BACTERIOPHEOPHYTIN A (three-letter code: BPH) (formula: C₅₅H₇₆N₄O₆).



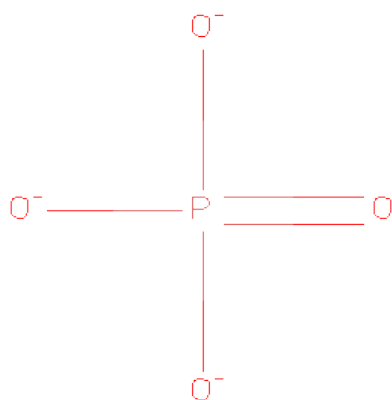
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	L	1	Total	C	N	O	0	0
			65	55	4	6		
7	M	1	Total	C	N	O	0	0
			65	55	4	6		

- Molecule 8 is UBIQUINONE-2 (three-letter code: UQ2) (formula: $C_{19}H_{26}O_4$).



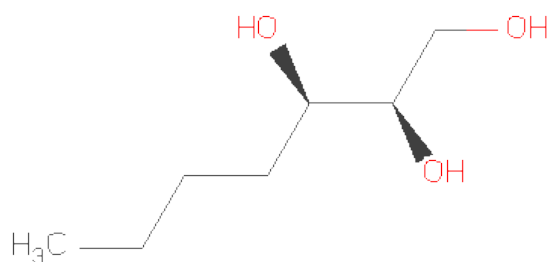
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	L	1	Total	C	O	0	1
			46	38	8		

- Molecule 9 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



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

- Molecule 10 is HEPTANE-1,2,3-TRIOL (three-letter code: HTO) (formula: C₇H₁₆O₃).

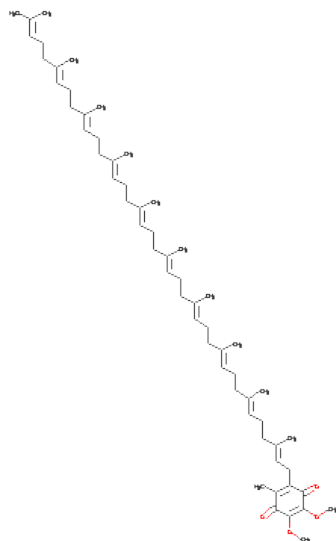


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	L	1	Total	C	O	0	0
			10	7	3		

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

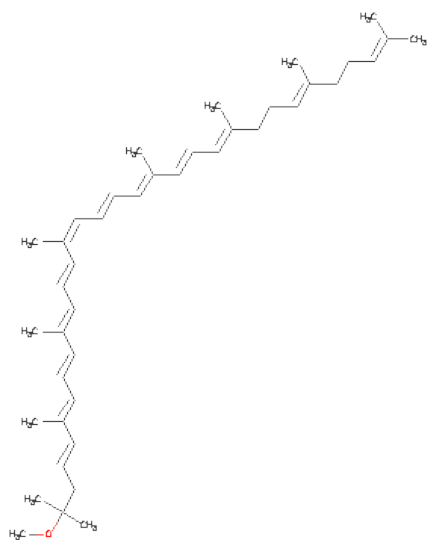
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	M	1	Total	Fe	0	0
			1	1		

- Molecule 12 is UBIQUINONE-10 (three-letter code: U10) (formula: $C_{59}H_{90}O_4$).



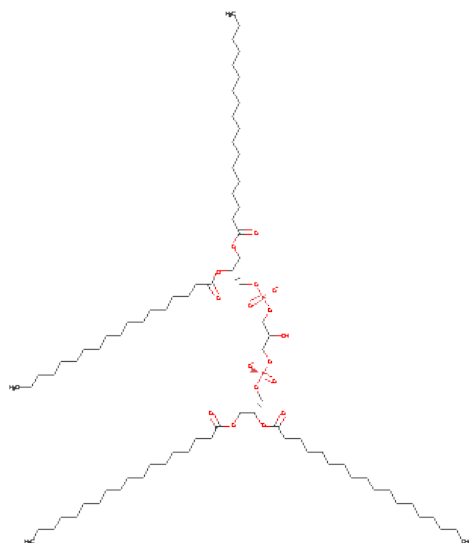
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	M	1	Total	C	O	0	0
			48	44	4		

- Molecule 13 is SPHEROIDENE (three-letter code: SPO) (formula: $C_{41}H_{60}O$).



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

- Molecule 14 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
14	M	1	Total	C	O	P	0	0
			81	62	17	2		

- Molecule 15 is water.

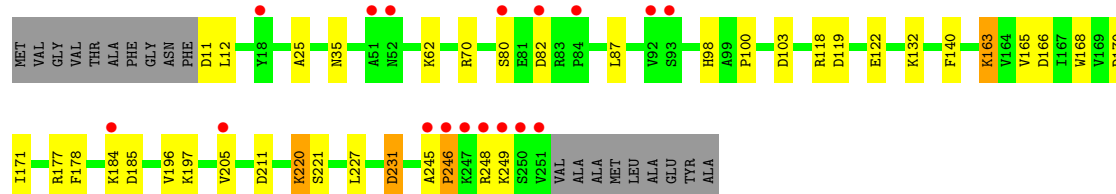
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	H	127	Total	O	0	0
			127	127		
15	L	127	Total	O	0	0
			127	127		
15	M	147	Total	O	0	0
			147	147		

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: 



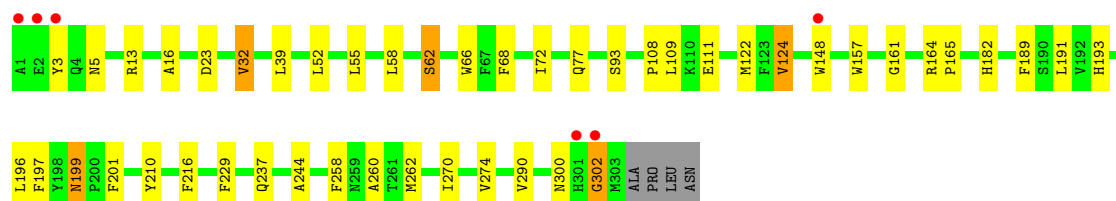
• Molecule 2: REACTION CENTER PROTEIN L CHAIN

Chain L: 



• Molecule 3: REACTION CENTER PROTEIN M CHAIN

Chain M: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	140.02Å 140.02Å 235.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	119.52 – 2.31 19.95 – 2.20	Depositor EDS
% Data completeness (in resolution range)	95.6 (119.52-2.31) 88.8 (19.95-2.20)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.38 (at 2.19Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.190 , 0.219 0.197 , 0.194	Depositor DCC
R_{free} test set	5299 reflections (5.27%)	DCC
Wilson B-factor (Å ²)	36.7	Xtriage
Anisotropy	0.038	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 53.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	0 of 112185 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7701	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.58% 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, CDL, BPH, PO4, HTO, 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	0.51	0/1906	0.74	8/2591 (0.3%)
2	L	0.57	0/2320	0.64	1/3175 (0.0%)
3	M	0.57	0/2501	0.64	2/3415 (0.1%)
All	All	0.55	0/6727	0.67	11/9181 (0.1%)

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	11	ASP	CB-CG-OD2	6.89	124.50	118.30
1	H	82	ASP	CB-CG-OD2	6.51	124.16	118.30
3	M	23	ASP	CB-CG-OD2	6.06	123.76	118.30
1	H	166	ASP	CB-CG-OD2	6.06	123.75	118.30
3	M	302	GLY	O-C-N	-5.88	113.30	122.70
1	H	211	ASP	CB-CG-OD2	5.77	123.49	118.30
1	H	231	ASP	CB-CG-OD2	5.72	123.44	118.30
1	H	185	ASP	CB-CG-OD2	5.30	123.07	118.30
1	H	103	ASP	CB-CG-OD2	5.25	123.03	118.30
2	L	213	ASP	CB-CG-OD2	5.22	123.00	118.30
1	H	119	ASP	CB-CG-OD2	5.10	122.89	118.30

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	18	0
2	L	2232	0	2187	23	0
3	M	2409	0	2321	32	0
4	H	24	0	32	3	0
4	L	12	0	16	1	0
4	M	6	0	8	2	0
5	L	132	0	148	6	0
5	M	132	0	148	15	0
6	L	64	0	124	3	0
6	M	80	0	155	7	0
7	L	65	0	76	7	0
7	M	65	0	76	11	0
8	L	46	0	52	4	0
9	L	5	0	0	0	0
10	L	10	0	16	0	0
11	M	1	0	0	0	0
12	M	48	0	63	1	0
13	M	42	0	60	2	0
14	M	81	0	86	3	0
15	H	127	0	0	2	0
15	L	127	0	0	3	0
15	M	147	0	0	0	0
All	All	7701	0	7429	105	0

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 7.

All (105) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:L:7:ARG:NH1	15:L:2003:HOH:O	1.84	0.84
6:M:1307:LDA:H52	6:M:1308:LDA:H42	1.64	0.80
5:M:1303:BCL:HBB3	5:M:1304:BCL:H41	1.67	0.77
3:M:197:PHE:HZ	5:M:1304:BCL:HBB2	1.50	0.77
5:M:1304:BCL:HHC	5:M:1304:BCL:HBB3	1.68	0.76
3:M:197:PHE:CZ	5:M:1304:BCL:HBB2	2.22	0.74
7:L:1287:BPH:CBB	7:L:1287:BPH:HHC	2.18	0.74
2:L:199:ASN:HA	4:L:1292:GOL:H31	1.68	0.73
7:M:1311:BPH:HBB3	7:M:1311:BPH:HHC	1.69	0.73
7:M:1311:BPH:CBB	7:M:1311:BPH:HHC	2.20	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
7:M:1311:BPH:HHD	7:M:1311:BPH:HBC3	1.74	0.69
3:M:270:ILE:O	3:M:274:VAL:HG13	1.93	0.69
2:L:181:PHE:HB3	7:M:1311:BPH:HBB2	1.75	0.68
3:M:77:GLN:HE22	3:M:93:SER:H	1.38	0.68
3:M:108:PRO:HG2	3:M:111:GLU:HB2	1.75	0.68
7:L:1287:BPH:HBB3	7:L:1287:BPH:HHC	1.77	0.67
3:M:189:PHE:O	3:M:193:HIS:HD2	1.78	0.67
2:L:135:ARG:HB3	2:L:136:PRO:HD3	1.77	0.66
3:M:62:SER:OG	3:M:124:VAL:HG22	1.96	0.66
3:M:157:TRP:HB2	5:M:1304:BCL:H71	1.78	0.66
3:M:68:PHE:O	3:M:72:ILE:HG12	1.97	0.65
2:L:181:PHE:CD2	7:M:1311:BPH:HBB1	2.33	0.64
5:M:1303:BCL:CBB	5:M:1303:BCL:HHC	2.28	0.63
1:H:62:LYS:HE3	4:H:1251:GOL:H11	1.81	0.63
4:H:1251:GOL:H31	15:H:2001:HOH:O	2.02	0.60
2:L:7:ARG:HD3	15:L:2003:HOH:O	2.02	0.59
3:M:300:ASN:C	3:M:302:GLY:H	2.06	0.59
2:L:170:ASN:C	2:L:170:ASN:HD22	2.06	0.59
3:M:148:TRP:HB3	14:M:1314:CDL:H741	1.84	0.58
3:M:199:ASN:HD22	3:M:199:ASN:C	2.06	0.58
1:H:25:ALA:HB1	4:H:1252:GOL:H12	1.87	0.57
7:M:1311:BPH:HBB3	7:M:1311:BPH:CHC	2.35	0.56
1:H:70:ARG:O	1:H:118[A]:ARG:NH1	2.36	0.56
2:L:181:PHE:HB3	7:M:1311:BPH:CBB	2.36	0.55
3:M:16:ALA:HB1	3:M:32:VAL:HG11	1.88	0.55
2:L:226:THR:HG22	8:L:1288[B]:UQ2:H3M3	1.88	0.55
3:M:237:GLN:HB2	3:M:262:MET:HG2	1.89	0.55
3:M:148:TRP:CD1	14:M:1314:CDL:HB62	2.42	0.54
1:H:35:ASN:OD1	3:M:260:ALA:HB1	2.08	0.54
1:H:70:ARG:HB3	1:H:118[A]:ARG:NH1	2.23	0.53
5:M:1303:BCL:HBB2	5:M:1303:BCL:HHC	1.90	0.53
7:L:1287:BPH:HBB3	7:L:1287:BPH:CHC	2.38	0.52
7:L:1287:BPH:HBB2	7:L:1287:BPH:HHC	1.92	0.52
3:M:229:PHE:HB2	3:M:244:ALA:HB2	1.92	0.52
1:H:80:SER:HB2	15:H:2038:HOH:O	2.10	0.51
7:L:1287:BPH:CBB	7:L:1287:BPH:CHC	2.86	0.51
1:H:87:LEU:HD23	1:H:100:PRO:HA	1.93	0.51
7:M:1311:BPH:CBB	7:M:1311:BPH:CHC	2.89	0.51
2:L:177:ILE:HG12	5:L:1289:BCL:HMB3	1.93	0.51
7:L:1287:BPH:HBB2	3:M:210:TYR:HB3	1.94	0.51
5:L:1289:BCL:HBB3	5:L:1289:BCL:HMB1	1.93	0.50
5:M:1304:BCL:CBB	5:M:1304:BCL:HHC	2.40	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:M:148:TRP:HD1	14:M:1314:CDL:HB62	1.77	0.49
3:M:197:PHE:HZ	5:M:1304:BCL:CBB	2.23	0.49
6:M:1305:LDA:H32	4:M:1315:GOL:H32	1.94	0.49
3:M:189:PHE:O	3:M:193:HIS:CD2	2.64	0.49
2:L:128:TYR:HD1	5:L:1282:BCL:HBB1	1.78	0.49
1:H:168:TRP:HB2	1:H:178:PHE:HB2	1.94	0.48
2:L:157:VAL:HG11	5:M:1304:BCL:HBB1	1.95	0.48
6:M:1305:LDA:H12	4:M:1315:GOL:H12	1.95	0.48
2:L:190:HIS:HA	8:L:1288[B]:UQ2:O4	2.14	0.47
3:M:66:TRP:CD1	3:M:122:MET:HB2	2.49	0.47
6:L:1285:LDA:H22	6:L:1285:LDA:HM21	1.54	0.47
5:L:1289:BCL:CBB	5:L:1289:BCL:HMB1	2.45	0.47
1:H:12:LEU:HD23	3:M:290:VAL:HG21	1.96	0.47
6:L:1285:LDA:H41	6:L:1285:LDA:HM11	1.97	0.46
5:L:1282:BCL:HBB3	5:L:1289:BCL:H41	1.97	0.45
3:M:196:LEU:HD12	5:M:1304:BCL:CHD	2.47	0.45
2:L:257:ASP:HB3	15:L:2114:HOH:O	2.16	0.45
6:L:1283:LDA:H22	6:L:1283:LDA:HM22	1.70	0.45
2:L:241:VAL:HG21	7:L:1287:BPH:HBC3	1.99	0.45
3:M:58:LEU:O	3:M:62:SER:HB2	2.17	0.45
1:H:132:LYS:HB2	1:H:171:ILE:HD11	1.98	0.45
12:M:1312:U10:H4M2	12:M:1312:U10:H3M3	1.98	0.45
2:L:208:THR:HB	2:L:209:PRO:HD2	1.99	0.44
1:H:122:GLU:HB2	1:H:227:LEU:HD21	1.99	0.44
2:L:224:ILE:H	8:L:1288[B]:UQ2:H103	1.82	0.44
2:L:153:HIS:CD2	5:L:1282:BCL:NC	2.86	0.43
3:M:161:GLY:HA3	13:M:1313:SPO:H292	2.00	0.43
1:H:98:HIS:CD2	2:L:7:ARG:HE	2.37	0.43
2:L:8:LYS:HE2	2:L:9:TYR:CE2	2.53	0.42
3:M:3:TYR:CZ	3:M:5:ASN:HA	2.54	0.42
3:M:300:ASN:C	3:M:302:GLY:N	2.72	0.42
1:H:220[B]:LYS:HG2	1:H:221:SER:N	2.33	0.42
1:H:196:VAL:HG12	1:H:205:VAL:HG22	2.02	0.42
5:M:1304:BCL:HAA2	5:M:1304:BCL:HBD	2.02	0.42
3:M:164:ARG:HB3	3:M:165:PRO:HD3	2.00	0.42
5:M:1304:BCL:CBB	5:M:1304:BCL:CHC	2.97	0.42
5:M:1304:BCL:H61	7:M:1311:BPH:C4B	2.49	0.42
6:M:1307:LDA:H12	6:M:1308:LDA:HM11	2.02	0.42
2:L:52:SER:HB2	2:L:85:LEU:HD13	2.01	0.42
2:L:185:LEU:HD13	7:M:1311:BPH:ND	2.35	0.41
3:M:199:ASN:HD21	3:M:201:PHE:HB2	1.85	0.41
1:H:245:ALA:N	1:H:246:PRO:HD2	2.35	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:L:75:LEU:HD21	2:L:137:VAL:HA	2.03	0.41
1:H:163:LYS:HE3	1:H:165:VAL:HG12	2.03	0.41
1:H:170:ASP:HB2	1:H:177:ARG:HG3	2.02	0.41
6:M:1307:LDA:H21	6:M:1308:LDA:HM21	2.03	0.41
13:M:1313:SPO:H19	13:M:1313:SPO:H22	1.82	0.41
7:M:1311:BPH:HBC3	7:M:1311:BPH:CHD	2.48	0.40
1:H:140:PHE:HA	3:M:13:ARG:O	2.21	0.40
5:M:1303:BCL:HBB3	5:M:1304:BCL:C4	2.45	0.40
3:M:258:PHE:CG	6:M:1307:LDA:H51	2.56	0.40
8:L:1288[A]:UQ2:H101	8:L:1288[A]:UQ2:H121	1.64	0.40
6:M:1307:LDA:H22	6:M:1307:LDA:HM11	1.86	0.40

There are no symmetry-related clashes.

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%)	234 (97%)	6 (2%)	2 (1%)	27	30
2	L	279/281 (99%)	276 (99%)	2 (1%)	1 (0%)	43	52
3	M	301/307 (98%)	291 (97%)	10 (3%)	0	100	100
All	All	822/848 (97%)	801 (97%)	18 (2%)	3 (0%)	43	52

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	248	ARG
1	H	246	PRO
2	L	31	VAL

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%)	191 (96%)	7 (4%)	48	63
2	L	220/220 (100%)	205 (93%)	15 (7%)	22	28
3	M	236/240 (98%)	225 (95%)	11 (5%)	36	48
All	All	654/668 (98%)	621 (95%)	33 (5%)	35	45

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	163	LYS
1	H	184	LYS
1	H	197	LYS
1	H	220[A]	LYS
1	H	220[B]	LYS
1	H	231	ASP
1	H	249	LYS
2	L	16	LEU
2	L	21	LEU
2	L	44	LEU
2	L	80	LEU
2	L	102	LEU
2	L	126	LEU
2	L	129	LEU
2	L	170	ASN
2	L	202	LYS
2	L	207	ARG
2	L	210	ASP
2	L	216	PHE
2	L	246	LEU
2	L	247	CYS
2	L	272	TRP
3	M	32	VAL
3	M	39	LEU
3	M	52	LEU
3	M	55	LEU
3	M	62	SER
3	M	109	LEU
3	M	124	VAL
3	M	182	HIS
3	M	191	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	M	199	ASN
3	M	216	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) 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	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 30 ligands modelled in this entry, 1 is monoatomic - leaving 29 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	GOL	H	1251	-	5,5,5	0.43	0	5,5,5	0.74	0
4	GOL	H	1252	-	5,5,5	0.37	0	5,5,5	0.48	0
4	GOL	H	1253	-	5,5,5	0.36	0	5,5,5	0.20	0
4	GOL	H	1254	-	5,5,5	0.37	0	5,5,5	0.29	0
5	BCL	L	1282	2	74,74,74	2.00	13 (17%)	97,115,115	1.94	20 (20%)
6	LDA	L	1283	-	15,15,15	3.76	2 (13%)	17,17,17	0.58	0
6	LDA	L	1284	-	15,15,15	3.85	2 (13%)	17,17,17	0.81	1 (5%)
6	LDA	L	1285	-	15,15,15	3.56	1 (6%)	17,17,17	0.71	0
6	LDA	L	1286	-	15,15,15	3.63	2 (13%)	17,17,17	0.66	0
7	BPH	L	1287	-	70,70,70	2.95	17 (24%)	94,101,101	1.77	19 (20%)
8	UQ2	L	1288[A]	-	23,23,23	2.72	7 (30%)	31,31,31	1.14	3 (9%)
8	UQ2	L	1288[B]	-	23,23,23	2.65	7 (30%)	31,31,31	1.58	7 (22%)
5	BCL	L	1289	2	74,74,74	2.14	10 (13%)	97,115,115	2.07	23 (23%)
9	PO4	L	1290	-	4,4,4	0.29	0	6,6,6	0.31	0
10	HTO	L	1291	-	9,9,9	0.35	0	10,10,10	0.57	0
4	GOL	L	1292	-	5,5,5	0.21	0	5,5,5	0.57	0
4	GOL	L	1293	-	5,5,5	0.37	0	5,5,5	0.23	0
5	BCL	M	1303	3	74,74,74	2.08	10 (13%)	97,115,115	1.94	22 (22%)
5	BCL	M	1304	3	74,74,74	2.15	12 (16%)	97,115,115	1.93	27 (27%)
6	LDA	M	1305	-	15,15,15	3.75	1 (6%)	17,17,17	0.79	1 (5%)
6	LDA	M	1306	-	15,15,15	3.75	2 (13%)	17,17,17	0.63	0
6	LDA	M	1307	-	15,15,15	3.62	2 (13%)	17,17,17	0.76	0
6	LDA	M	1308	-	15,15,15	3.87	2 (13%)	17,17,17	0.84	0
6	LDA	M	1309	-	15,15,15	3.82	2 (13%)	17,17,17	0.59	0
7	BPH	M	1311	-	70,70,70	3.06	16 (22%)	94,101,101	1.68	18 (19%)
12	U10	M	1312	-	48,48,63	3.11	13 (27%)	59,61,79	1.57	12 (20%)
13	SPO	M	1313	-	41,41,41	3.98	12 (29%)	50,50,50	2.15	17 (34%)
14	CDL	M	1314	-	80,80,99	2.64	21 (26%)	92,92,111	2.87	13 (14%)
4	GOL	M	1315	-	5,5,5	0.29	0	5,5,5	0.45	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	GOL	H	1251	-	-	0/4/4/4	0/0/0/0
4	GOL	H	1252	-	-	0/4/4/4	0/0/0/0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	H	1253	-	-	0/4/4/4	0/0/0/0
4	GOL	H	1254	-	-	0/4/4/4	0/0/0/0
5	BCL	L	1282	2	2/2/21/25	0/41/137/137	0/0/9/9
6	LDA	L	1283	-	-	0/13/13/13	0/0/0/0
6	LDA	L	1284	-	-	0/13/13/13	0/0/0/0
6	LDA	L	1285	-	-	0/13/13/13	0/0/0/0
6	LDA	L	1286	-	-	0/13/13/13	0/0/0/0
7	BPH	L	1287	-	2/2/18/22	0/49/105/105	0/0/6/6
8	UQ2	L	1288[A]	-	-	0/15/39/39	0/1/1/1
8	UQ2	L	1288[B]	-	-	0/15/39/39	0/1/1/1
5	BCL	L	1289	2	2/2/21/25	0/41/137/137	0/0/9/9
9	PO4	L	1290	-	-	0/0/0/0	0/0/0/0
10	HTO	L	1291	-	-	0/10/10/10	0/0/0/0
4	GOL	L	1292	-	-	0/4/4/4	0/0/0/0
4	GOL	L	1293	-	-	0/4/4/4	0/0/0/0
5	BCL	M	1303	3	2/2/21/25	1/41/137/137	0/0/9/9
5	BCL	M	1304	3	2/2/21/25	0/41/137/137	0/0/9/9
6	LDA	M	1305	-	-	0/13/13/13	0/0/0/0
6	LDA	M	1306	-	-	0/13/13/13	0/0/0/0
6	LDA	M	1307	-	-	0/13/13/13	0/0/0/0
6	LDA	M	1308	-	-	0/13/13/13	0/0/0/0
6	LDA	M	1309	-	-	0/13/13/13	0/0/0/0
7	BPH	M	1311	-	2/2/18/22	0/49/105/105	0/0/6/6
12	U10	M	1312	-	-	0/45/69/87	0/1/1/1
13	SPO	M	1313	-	-	0/47/47/47	0/0/0/0
14	CDL	M	1314	-	1/1/9/9	0/91/91/110	0/0/0/0
4	GOL	M	1315	-	-	0/4/4/4	0/0/0/0

All (154) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	M	1308	LDA	O1-N1	-14.74	1.25	1.39
6	L	1284	LDA	O1-N1	-14.60	1.25	1.39
6	M	1309	LDA	O1-N1	-14.52	1.25	1.39
6	L	1283	LDA	O1-N1	-14.30	1.25	1.39
7	M	1311	BPH	C1D-CHD	14.29	1.51	1.35
6	M	1305	LDA	O1-N1	-14.24	1.26	1.39
6	M	1306	LDA	O1-N1	-14.23	1.26	1.39
6	L	1286	LDA	O1-N1	-13.79	1.26	1.39
6	M	1307	LDA	O1-N1	-13.75	1.26	1.39
6	L	1285	LDA	O1-N1	-13.57	1.26	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	M	1304	BCL	OBD-CAD	13.40	1.41	1.22
5	L	1289	BCL	OBD-CAD	13.21	1.41	1.22
13	M	1313	SPO	C27-C28	12.71	1.47	1.34
7	L	1287	BPH	C1D-CHD	12.70	1.49	1.35
5	L	1282	BCL	OBD-CAD	12.26	1.40	1.22
7	L	1287	BPH	OBD-CAD	12.19	1.40	1.22
5	M	1303	BCL	OBD-CAD	12.14	1.40	1.22
7	M	1311	BPH	OBD-CAD	11.95	1.39	1.22
13	M	1313	SPO	C19-C17	9.19	1.47	1.35
13	M	1313	SPO	C22-C23	8.76	1.47	1.35
13	M	1313	SPO	C9-C7	8.47	1.46	1.35
8	L	1288[A]	UQ2	C8-C9	8.27	1.49	1.32
14	M	1314	CDL	C24-C23	-8.24	1.51	1.55
14	M	1314	CDL	C58-C57	-8.12	1.51	1.55
13	M	1313	SPO	C14-C12	8.07	1.46	1.35
14	M	1314	CDL	C84-C83	-7.99	1.52	1.55
7	M	1311	BPH	O1D-CGD	7.88	1.41	1.21
14	M	1314	CDL	C43-C42	-7.87	1.52	1.55
12	M	1312	U10	C33-C34	7.79	1.48	1.32
12	M	1312	U10	C18-C19	7.75	1.48	1.32
13	M	1313	SPO	C32-C33	7.71	1.48	1.32
7	M	1311	BPH	C2-C3	7.53	1.48	1.32
12	M	1312	U10	C28-C29	7.44	1.48	1.32
12	M	1312	U10	C13-C14	7.44	1.48	1.32
8	L	1288[B]	UQ2	C8-C9	7.38	1.47	1.32
7	L	1287	BPH	O1D-CGD	7.32	1.39	1.21
12	M	1312	U10	C8-C9	7.27	1.47	1.32
12	M	1312	U10	C23-C24	7.22	1.47	1.32
7	L	1287	BPH	C2-C3	7.18	1.47	1.32
12	M	1312	U10	C38-C39	6.86	1.48	1.34
7	L	1287	BPH	OBB-CAB	6.48	1.45	1.22
14	M	1314	CDL	C32-C31	-6.42	1.27	1.52
14	M	1314	CDL	C11-CA5	-6.33	1.31	1.50
7	M	1311	BPH	O1A-CGA	6.25	1.41	1.22
7	L	1287	BPH	O1A-CGA	6.01	1.40	1.22
5	L	1289	BCL	O1A-CGA	5.89	1.40	1.22
5	M	1304	BCL	O1A-CGA	5.85	1.40	1.22
5	M	1303	BCL	O1A-CGA	5.83	1.40	1.22
5	L	1282	BCL	O1A-CGA	5.55	1.39	1.22
7	L	1287	BPH	C4D-C3D	-5.47	1.34	1.41
8	L	1288[B]	UQ2	O2-C2	-5.40	1.23	1.36
7	M	1311	BPH	OBB-CAB	5.40	1.41	1.22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	L	1289	BCL	C4D-C3D	-5.36	1.35	1.41
13	M	1313	SPO	C37-C38	5.36	1.49	1.32
5	M	1303	BCL	C4D-C3D	-5.02	1.35	1.41
7	M	1311	BPH	C4D-C3D	-4.96	1.35	1.41
8	L	1288[A]	UQ2	C13-C14	4.86	1.48	1.32
12	M	1312	U10	O3-C3	-4.84	1.24	1.36
13	M	1313	SPO	C6-C5	4.81	1.46	1.31
8	L	1288[B]	UQ2	C13-C14	4.68	1.47	1.32
5	M	1304	BCL	C4D-C3D	-4.65	1.35	1.41
8	L	1288[A]	UQ2	O3-C3	-4.57	1.25	1.36
13	M	1313	SPO	C26-C25	4.49	1.46	1.34
8	L	1288[B]	UQ2	O3-C3	-4.47	1.25	1.36
8	L	1288[A]	UQ2	O2-C2	-4.47	1.25	1.36
14	M	1314	CDL	OA6-CA5	4.40	1.47	1.34
14	M	1314	CDL	OA8-CA7	4.40	1.47	1.33
14	M	1314	CDL	OB6-CB5	4.38	1.47	1.34
14	M	1314	CDL	OB8-CB7	4.34	1.46	1.33
5	L	1282	BCL	C4D-C3D	-4.25	1.36	1.41
5	M	1303	BCL	C2-C3	4.23	1.41	1.32
7	M	1311	BPH	C3D-CAD	-4.23	1.38	1.47
12	M	1312	U10	O4-C4	-4.18	1.26	1.36
14	M	1314	CDL	C16-C15	-4.15	1.26	1.51
14	M	1314	CDL	C17-C16	-4.10	1.26	1.51
7	L	1287	BPH	C3D-CAD	-4.07	1.39	1.47
5	M	1303	BCL	C1B-NB	4.07	1.39	1.34
13	M	1313	SPO	C10-C11	4.06	1.45	1.34
13	M	1313	SPO	C15-C16	4.05	1.45	1.34
5	L	1289	BCL	C2-C3	3.97	1.40	1.32
5	M	1304	BCL	C1B-NB	3.81	1.39	1.34
13	M	1313	SPO	C21-C20	3.76	1.45	1.35
8	L	1288[B]	UQ2	C3-C4	-3.50	1.38	1.48
5	M	1303	BCL	C3D-CAD	-3.49	1.40	1.47
14	M	1314	CDL	C13-C12	-3.47	1.30	1.51
5	M	1304	BCL	C4B-NB	3.46	1.38	1.34
5	L	1289	BCL	C3D-CAD	-3.43	1.40	1.47
5	L	1282	BCL	C2-C3	3.39	1.39	1.32
7	M	1311	BPH	CHD-C4C	3.36	1.48	1.41
5	M	1304	BCL	C2-C3	3.27	1.39	1.32
5	L	1289	BCL	C4B-NB	3.21	1.38	1.34
14	M	1314	CDL	C19-C18	-3.16	1.32	1.51
5	L	1289	BCL	C1B-NB	3.14	1.38	1.34
5	M	1303	BCL	O2D-CGD	-3.10	1.24	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	L	1282	BCL	C3D-CAD	-3.08	1.41	1.47
5	L	1289	BCL	C1A-NA	3.05	1.39	1.32
14	M	1314	CDL	C20-C19	-3.04	1.32	1.51
14	M	1314	CDL	C34-C33	-3.02	1.33	1.51
5	M	1303	BCL	C1C-NC	-2.96	1.32	1.39
14	M	1314	CDL	C33-C32	-2.95	1.33	1.51
5	L	1282	BCL	C1A-NA	2.93	1.38	1.32
7	M	1311	BPH	C3D-C2D	2.91	1.49	1.40
5	M	1304	BCL	C1C-NC	-2.90	1.32	1.39
5	M	1304	BCL	C3D-CAD	-2.90	1.41	1.47
14	M	1314	CDL	C37-C36	-2.88	1.33	1.51
14	M	1314	CDL	C79-C78	-2.86	1.33	1.51
14	M	1314	CDL	C80-C79	-2.81	1.34	1.51
7	L	1287	BPH	CHD-C4C	2.79	1.47	1.41
7	L	1287	BPH	C4D-ND	-2.78	1.34	1.38
5	L	1282	BCL	C1C-NC	-2.75	1.33	1.39
7	L	1287	BPH	C3D-C2D	2.75	1.48	1.40
14	M	1314	CDL	C22-C21	-2.74	1.34	1.51
7	M	1311	BPH	O2D-CGD	-2.72	1.25	1.33
8	L	1288[A]	UQ2	C2-C1	-2.66	1.41	1.48
12	M	1312	U10	C4-C5	-2.65	1.41	1.48
8	L	1288[B]	UQ2	C2-C1	-2.64	1.41	1.48
5	L	1282	BCL	C1B-NB	2.63	1.37	1.34
5	L	1289	BCL	O2D-CGD	-2.60	1.26	1.33
8	L	1288[A]	UQ2	C3-C4	-2.59	1.41	1.48
5	M	1304	BCL	O2D-CGD	-2.59	1.26	1.33
8	L	1288[A]	UQ2	C6-C5	2.58	1.41	1.35
7	M	1311	BPH	C1C-NC	-2.56	1.33	1.38
5	M	1303	BCL	C1A-NA	2.55	1.37	1.32
5	L	1282	BCL	O2D-CGD	-2.48	1.26	1.33
5	M	1304	BCL	C1A-NA	2.46	1.37	1.32
12	M	1312	U10	C3-C2	-2.43	1.41	1.48
6	M	1306	LDA	C1-N1	-2.38	1.46	1.51
6	L	1284	LDA	C1-N1	-2.37	1.46	1.51
7	L	1287	BPH	CHC-C1C	2.37	1.47	1.38
5	M	1304	BCL	CHD-C4C	2.36	1.46	1.39
5	L	1289	BCL	CHD-C4C	2.35	1.46	1.39
6	M	1307	LDA	C1-N1	-2.34	1.46	1.51
7	M	1311	BPH	C4A-NA	-2.31	1.33	1.38
5	L	1282	BCL	C4B-NB	2.31	1.37	1.34
7	M	1311	BPH	CHB-C4A	2.30	1.47	1.38
5	L	1282	BCL	O2A-CGA	-2.28	1.26	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	L	1287	BPH	O2D-CGD	-2.28	1.27	1.33
6	L	1283	LDA	C1-N1	-2.27	1.47	1.51
5	L	1282	BCL	O1D-CGD	2.27	1.26	1.21
8	L	1288[B]	UQ2	C6-C1	-2.25	1.39	1.46
12	M	1312	U10	C6-C1	2.25	1.40	1.35
7	L	1287	BPH	C1C-NC	-2.24	1.33	1.38
7	M	1311	BPH	O2A-CGA	-2.19	1.26	1.33
5	L	1282	BCL	CHD-C4C	2.18	1.46	1.39
7	L	1287	BPH	C4A-NA	-2.18	1.33	1.38
6	L	1286	LDA	C1-N1	-2.16	1.47	1.51
7	L	1287	BPH	CHB-C4A	2.16	1.46	1.38
12	M	1312	U10	C41-C39	2.12	1.52	1.40
6	M	1308	LDA	C1-N1	-2.10	1.47	1.51
7	M	1311	BPH	CHC-C1C	2.08	1.46	1.38
5	M	1303	BCL	CHD-C4C	2.06	1.45	1.39
6	M	1309	LDA	C1-N1	-2.05	1.47	1.51
5	M	1304	BCL	O2A-CGA	-2.05	1.26	1.33
7	L	1287	BPH	O2A-CGA	-2.05	1.26	1.33

All (183) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	M	1314	CDL	C33-C32-C31	15.16	170.41	113.28
14	M	1314	CDL	C17-C16-C15	11.68	177.80	114.61
14	M	1314	CDL	C12-C11-CA5	8.97	148.68	113.51
5	L	1289	BCL	C2D-C1D-ND	-8.31	103.13	109.41
5	L	1289	BCL	CMB-C2B-C1B	-7.64	116.87	128.62
14	M	1314	CDL	C13-C12-C11	7.54	141.69	113.28
7	M	1311	BPH	C3B-C2B-C1B	-7.28	102.65	107.01
5	L	1282	BCL	CMB-C2B-C1B	-7.26	117.45	128.62
5	M	1304	BCL	C2D-C1D-ND	-7.19	103.99	109.41
7	L	1287	BPH	C3B-C2B-C1B	-7.16	102.72	107.01
14	M	1314	CDL	C35-C34-C33	7.14	153.26	114.61
5	M	1303	BCL	CMB-C2B-C1B	-6.86	118.07	128.62
14	M	1314	CDL	C34-C33-C32	6.43	149.42	114.61
5	M	1303	BCL	C2D-C1D-ND	-6.38	104.59	109.41
14	M	1314	CDL	C20-C19-C18	6.14	147.81	114.61
7	L	1287	BPH	C1D-C2D-C3D	-6.07	101.68	106.89
5	M	1304	BCL	CMB-C2B-C1B	-5.99	119.41	128.62
5	L	1289	BCL	CMB-C2B-C3B	5.98	134.40	124.97
13	M	1313	SPO	C26-C27-C28	-5.86	122.31	127.91
7	M	1311	BPH	C1D-C2D-C3D	-5.64	102.05	106.89

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	M	1303	BCL	CMB-C2B-C3B	5.58	133.76	124.97
13	M	1313	SPO	C10-C9-C7	-5.17	119.84	127.29
5	L	1282	BCL	CMB-C2B-C3B	5.12	133.03	124.97
5	M	1304	BCL	C1D-CHD-C4C	-4.76	117.34	125.55
5	L	1289	BCL	CHB-C4A-NA	-4.73	118.97	124.58
5	L	1282	BCL	O2D-CGD-CBD	4.71	120.92	111.33
5	L	1282	BCL	C2D-C1D-ND	-4.64	105.91	109.41
5	L	1289	BCL	C4D-ND-C1D	4.57	112.08	106.57
7	M	1311	BPH	O2D-CGD-CBD	4.56	120.62	111.33
5	M	1303	BCL	C3A-C4A-CHB	-4.54	114.89	124.33
7	L	1287	BPH	O2D-CGD-CBD	4.52	120.54	111.33
5	M	1304	BCL	CMB-C2B-C3B	4.49	132.04	124.97
5	M	1303	BCL	O2D-CGD-CBD	4.37	120.23	111.33
5	L	1289	BCL	C3A-C4A-CHB	-4.35	115.29	124.33
12	M	1312	U10	C30-C29-C31	4.30	121.92	115.39
5	L	1282	BCL	C4B-CHC-C1C	-4.29	121.14	130.06
13	M	1313	SPO	C21-C22-C23	-4.23	121.20	127.29
7	L	1287	BPH	CED-O2D-CGD	4.18	125.96	116.02
14	M	1314	CDL	OA6-CA5-C11	4.12	120.58	111.56
14	M	1314	CDL	OB6-CB5-C51	4.06	120.44	111.56
5	M	1304	BCL	C4D-ND-C1D	3.95	111.34	106.57
5	L	1282	BCL	CHC-C4B-NB	-3.84	118.17	124.58
5	L	1282	BCL	OBD-CAD-CBD	-3.82	120.18	125.94
5	M	1304	BCL	O2D-CGD-CBD	3.82	119.10	111.33
5	M	1303	BCL	C4D-ND-C1D	3.81	111.17	106.57
13	M	1313	SPO	C29-C28-C30	3.79	121.15	115.39
5	M	1303	BCL	C1-O2A-CGA	3.78	127.56	116.98
13	M	1313	SPO	C20-C19-C17	-3.74	121.90	127.29
7	L	1287	BPH	OBD-CAD-CBD	-3.69	120.36	125.94
13	M	1313	SPO	C15-C14-C12	-3.63	122.06	127.29
5	M	1303	BCL	C1D-CHD-C4C	-3.57	119.39	125.55
5	L	1282	BCL	C1D-CHD-C4C	-3.50	119.51	125.55
7	L	1287	BPH	O1D-CGD-CBD	-3.50	117.25	124.42
7	L	1287	BPH	C2B-C1B-NB	3.47	114.91	108.16
7	M	1311	BPH	CMD-C2D-C3D	-3.42	119.57	124.97
5	M	1304	BCL	O2A-CGA-CBA	3.41	122.67	111.94
13	M	1313	SPO	C8-C7-C6	3.36	123.52	118.09
5	L	1289	BCL	CMD-C2D-C3D	-3.30	119.77	124.97
5	L	1282	BCL	C2B-C1B-NB	-3.29	106.93	109.41
5	M	1304	BCL	CED-O2D-CGD	3.29	123.84	116.02
5	L	1282	BCL	C3A-C4A-CHB	-3.28	117.50	124.33
7	M	1311	BPH	OBD-CAD-CBD	-3.24	121.04	125.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	L	1288[B]	UQ2	CM5-C5-C6	-3.21	117.83	124.20
5	M	1304	BCL	C4-C3-C5	3.19	120.24	115.39
5	L	1289	BCL	C4B-CHC-C1C	-3.14	123.52	130.06
5	L	1289	BCL	O2A-CGA-CBA	3.14	121.82	111.94
7	L	1287	BPH	OBD-CAD-C3D	-3.14	122.07	127.91
8	L	1288[B]	UQ2	CM3-O3-C3	3.13	127.12	116.48
7	L	1287	BPH	CMD-C2D-C1D	3.13	130.88	125.81
5	L	1282	BCL	C2A-C3A-C4A	3.11	106.19	101.40
5	M	1304	BCL	C1B-CHB-C4A	-3.10	123.61	130.06
5	M	1303	BCL	O2A-CGA-CBA	3.09	121.65	111.94
5	M	1303	BCL	O2D-CGD-O1D	-3.08	117.54	123.79
12	M	1312	U10	C22-C23-C24	-3.08	121.16	127.80
12	M	1312	U10	C17-C18-C19	-3.07	121.18	127.80
7	M	1311	BPH	CMD-C2D-C1D	3.05	130.76	125.81
7	M	1311	BPH	C2B-C1B-NB	3.05	114.10	108.16
12	M	1312	U10	C25-C24-C26	3.00	119.95	115.39
8	L	1288[B]	UQ2	C7-C8-C9	-2.96	121.76	126.76
7	M	1311	BPH	OBD-CAD-C3D	-2.95	122.41	127.91
5	M	1304	BCL	C16-C15-C13	-2.95	106.63	115.14
5	M	1303	BCL	C1B-CHB-C4A	-2.94	123.93	130.06
13	M	1313	SPO	C34-C33-C35	2.94	119.86	115.39
5	L	1289	BCL	O2D-CGD-CBD	2.92	117.29	111.33
12	M	1312	U10	C30-C29-C28	-2.92	117.74	123.52
5	M	1304	BCL	C4B-CHC-C1C	-2.86	124.11	130.06
5	L	1282	BCL	O2A-CGA-CBA	2.85	120.91	111.94
7	L	1287	BPH	C3B-C4B-NB	2.85	110.32	107.10
5	L	1289	BCL	CMD-C2D-C1D	2.84	131.77	126.16
5	M	1304	BCL	CMD-C2D-C1D	2.84	131.77	126.16
13	M	1313	SPO	C4-C5-C6	-2.83	120.27	124.95
14	M	1314	CDL	OB8-CB7-C71	2.83	120.84	111.94
7	L	1287	BPH	OBB-CAB-C3B	2.83	124.31	120.07
12	M	1312	U10	C15-C14-C16	2.82	119.68	115.39
5	L	1282	BCL	C4D-ND-C1D	2.82	109.97	106.57
13	M	1313	SPO	C13-C12-C11	2.81	122.64	118.09
5	M	1304	BCL	CMD-C2D-C3D	-2.81	120.55	124.97
12	M	1312	U10	C10-C9-C11	2.80	119.65	115.39
12	M	1312	U10	C35-C34-C36	2.80	119.65	115.39
5	L	1289	BCL	CED-O2D-CGD	2.79	122.66	116.02
12	M	1312	U10	C27-C28-C29	-2.77	121.82	127.80
5	M	1303	BCL	O2A-C1-C2	2.75	114.50	108.55
5	L	1289	BCL	CHA-C1A-NA	-2.75	120.58	126.22
5	L	1282	BCL	C4-C3-C5	2.73	119.55	115.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	M	1313	SPO	C8-C7-C9	-2.70	119.09	122.92
5	M	1304	BCL	O2D-CGD-O1D	-2.70	118.31	123.79
7	M	1311	BPH	CAC-C3C-C2C	-2.69	107.72	113.89
5	M	1304	BCL	C2C-C1C-CHC	-2.69	118.74	124.33
5	L	1289	BCL	C1-O2A-CGA	2.68	124.49	116.98
5	M	1303	BCL	CMD-C2D-C1D	2.68	131.45	126.16
7	M	1311	BPH	CED-O2D-CGD	2.68	122.39	116.02
5	M	1303	BCL	CHA-C1A-NA	-2.67	120.73	126.22
13	M	1313	SPO	C15-C16-C17	-2.66	118.80	126.38
12	M	1312	U10	C12-C13-C14	-2.62	122.14	127.80
5	L	1282	BCL	O2D-CGD-O1D	-2.62	118.46	123.79
5	L	1289	BCL	C2A-C3A-C4A	2.61	105.41	101.40
8	L	1288[A]	UQ2	C10-C9-C11	2.61	119.35	115.39
5	L	1289	BCL	CHC-C4B-NB	-2.59	120.26	124.58
5	M	1303	BCL	CHB-C4A-NA	-2.57	121.53	124.58
14	M	1314	CDL	OA8-CA7-C31	2.55	119.97	111.94
6	M	1305	LDA	CM2-N1-CM1	-2.55	105.94	108.85
7	M	1311	BPH	C4B-C3B-C2B	2.55	109.44	107.60
14	M	1314	CDL	C21-C22-C23	2.54	123.40	113.78
5	L	1282	BCL	C1B-CHB-C4A	-2.54	124.78	130.06
14	M	1314	CDL	C32-C31-CA7	2.53	123.45	113.51
5	L	1289	BCL	CMA-C3A-C4A	-2.53	104.41	111.76
13	M	1313	SPO	C21-C20-C19	-2.53	117.76	123.36
8	L	1288[B]	UQ2	C10-C9-C11	2.53	119.23	115.39
5	M	1303	BCL	OBD-CAD-CBD	-2.51	122.15	125.94
12	M	1312	U10	C4M-O4-C4	2.50	124.99	116.48
7	M	1311	BPH	O2D-CGD-O1D	-2.48	118.74	123.79
5	M	1304	BCL	CHC-C1C-NC	-2.47	121.65	124.58
5	M	1303	BCL	C2A-C3A-C4A	2.46	105.18	101.40
5	M	1304	BCL	C1C-NC-C4C	2.45	110.76	107.79
6	L	1284	LDA	C2-C1-N1	-2.44	109.59	113.80
5	M	1304	BCL	CHD-C4C-NC	-2.44	122.33	125.86
5	M	1304	BCL	C2B-C1B-NB	-2.43	107.58	109.41
7	L	1287	BPH	CMD-C2D-C3D	-2.41	121.17	124.97
7	M	1311	BPH	C1-O2A-CGA	2.40	123.72	116.98
5	M	1304	BCL	C3A-C4A-NA	2.40	113.87	110.95
5	L	1289	BCL	C2C-C1C-CHC	-2.40	119.34	124.33
8	L	1288[A]	UQ2	CM2-O2-C2	2.39	124.59	116.48
7	M	1311	BPH	CMB-C2B-C3B	2.38	128.72	124.97
7	M	1311	BPH	C4-C3-C2	-2.37	118.82	123.52
5	M	1303	BCL	CMA-C3A-C4A	-2.36	104.92	111.76
5	M	1303	BCL	CMD-C2D-C3D	-2.36	121.25	124.97

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	M	1303	BCL	CHC-C1C-NC	-2.35	121.79	124.58
5	L	1289	BCL	O2D-CGD-O1D	-2.35	119.02	123.79
5	L	1282	BCL	CHB-C4A-NA	-2.34	121.80	124.58
7	L	1287	BPH	O2A-CGA-CBA	2.33	119.28	111.94
5	L	1282	BCL	C1-C2-C3	-2.32	122.06	126.19
7	L	1287	BPH	C1B-NB-C4B	-2.30	103.45	108.72
13	M	1313	SPO	C20-C21-C22	-2.27	118.33	123.36
5	M	1303	BCL	C11-C12-C13	-2.25	108.66	115.14
5	M	1304	BCL	C3A-C4A-CHB	-2.25	119.66	124.33
7	M	1311	BPH	C4-C3-C5	2.24	118.80	115.39
5	L	1282	BCL	CHC-C1C-NC	-2.24	121.92	124.58
8	L	1288[B]	UQ2	O1-C1-C6	-2.22	117.59	121.67
7	L	1287	BPH	C7-C6-C5	-2.22	106.48	113.01
8	L	1288[B]	UQ2	O4-C4-C3	-2.22	116.05	120.96
5	L	1282	BCL	CHD-C4C-NC	-2.19	122.70	125.86
7	L	1287	BPH	CMB-C2B-C3B	2.19	128.41	124.97
7	L	1287	BPH	C2D-C1D-ND	2.18	113.74	106.38
5	L	1289	BCL	C1B-CHB-C4A	-2.18	125.52	130.06
13	M	1313	SPO	C11-C12-C14	-2.18	115.62	118.97
8	L	1288[A]	UQ2	C10-C9-C8	-2.17	119.23	123.52
7	L	1287	BPH	CBB-CAB-C3B	-2.16	113.98	120.30
13	M	1313	SPO	C24-C23-C25	2.15	121.57	118.09
5	M	1304	BCL	CHA-C1A-NA	-2.15	121.81	126.22
5	L	1289	BCL	O2A-CGA-O1A	-2.14	117.58	123.43
5	L	1289	BCL	C1D-CHD-C4C	-2.14	121.86	125.55
7	L	1287	BPH	C1-C2-C3	-2.13	122.40	126.19
12	M	1312	U10	C32-C33-C34	-2.10	123.27	127.80
8	L	1288[B]	UQ2	C16-C14-C15	2.10	119.97	114.62
5	M	1303	BCL	C4A-NA-C1A	2.09	109.41	106.52
13	M	1313	SPO	C14-C15-C16	-2.09	116.19	123.24
7	M	1311	BPH	C1-C2-C3	-2.07	122.51	126.19
5	M	1304	BCL	OBD-CAD-CBD	-2.05	122.85	125.94
5	M	1304	BCL	CAC-C3C-C4C	-2.03	108.07	112.58
5	M	1304	BCL	C3C-C4C-CHD	-2.03	118.91	123.35
7	M	1311	BPH	O2A-CGA-CBA	2.02	118.30	111.94
5	L	1289	BCL	CHC-C1C-NC	-2.02	122.18	124.58
5	M	1304	BCL	C4-C3-C2	-2.01	119.54	123.52

All (13) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	M	1303	BCL	C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
5	M	1303	BCL	C13
5	L	1282	BCL	C8
5	L	1282	BCL	C13
7	M	1311	BPH	C8
7	M	1311	BPH	C13
7	L	1287	BPH	C8
7	L	1287	BPH	C13
14	M	1314	CDL	CA4
5	L	1289	BCL	C8
5	L	1289	BCL	C13
5	M	1304	BCL	C8
5	M	1304	BCL	C13

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	M	1303	BCL	C1-C2-C3-C4

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%)	0.05	17 (7%) 16 23	39, 49, 63, 103	0
2	L	281/281 (100%)	-0.52	2 (0%) 84 91	31, 41, 53, 59	0
3	M	303/307 (98%)	-0.54	6 (1%) 62 72	32, 41, 54, 79	0
All	All	825/848 (97%)	-0.36	25 (3%) 45 59	31, 44, 58, 103	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	251	VAL	15.0
1	H	250	SER	14.3
1	H	247	LYS	7.7
3	M	1	ALA	7.1
1	H	249	LYS	6.5
1	H	246	PRO	6.2
1	H	248	ARG	5.8
3	M	302	GLY	5.3
3	M	301	HIS	5.3
1	H	245	ALA	4.3
1	H	92	VAL	4.2
3	M	2	GLU	4.2
2	L	59	TRP	3.4
3	M	3	TYR	3.3
3	M	148	TRP	3.2
1	H	18	TYR	3.2
1	H	51	ALA	2.8
1	H	84	PRO	2.7
1	H	82	ASP	2.4
1	H	52	ASN	2.3
1	H	93	SER	2.3
1	H	205	VAL	2.2
2	L	202	LYS	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	H	184	LYS	2.0
1	H	80	SER	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

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	RSR	LLDF	B-factors(Å ²)	Q<0.9
4	GOL	H	1251	6/6	0.37	31.71	69,72,73,74	0
4	GOL	H	1252	6/6	0.38	20.28	91,93,93,93	0
6	LDA	L	1286	16/16	0.42	17.95	97,103,111,111	0
4	GOL	H	1253	6/6	0.34	16.81	108,108,109,109	0
6	LDA	L	1285	16/16	0.32	14.51	76,86,98,98	0
6	LDA	M	1309	16/16	0.49	12.74	119,123,128,128	0
10	HTO	L	1291	10/10	0.30	12.54	72,76,77,78	0
6	LDA	M	1308	16/16	0.39	11.66	116,117,121,121	0
6	LDA	L	1284	16/16	0.31	10.34	106,107,110,111	0
6	LDA	L	1283	16/16	0.45	10.31	80,97,107,108	0
6	LDA	M	1305	16/16	0.26	9.08	61,74,78,79	0
14	CDL	M	1314	81/100	0.42	7.36	110,119,127,127	0
8	UQ2	L	1288[A]	23/23	0.19	6.87	28,38,56,57	23
8	UQ2	L	1288[B]	23/23	0.19	5.95	36,40,47,47	23
9	PO4	L	1290	5/5	0.37	4.85	170,170,171,171	0
6	LDA	M	1306	16/16	0.25	4.00	81,83,86,87	0
4	GOL	M	1315	6/6	0.20	3.59	105,106,106,106	0
6	LDA	M	1307	16/16	0.20	3.41	71,75,79,79	0
4	GOL	L	1293	6/6	0.19	3.19	90,92,92,93	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
13	SPO	M	1313	42/42	0.15	1.68	38,44,62,66	0
12	U10	M	1312	48/63	0.12	1.23	36,49,77,78	0
4	GOL	L	1292	6/6	0.19	1.02	62,65,66,68	0
5	BCL	L	1289	66/66	0.11	0.74	28,34,50,56	0
7	BPH	M	1311	65/65	0.11	0.63	30,37,87,89	0
5	BCL	M	1304	66/66	0.10	0.60	27,33,48,55	0
5	BCL	M	1303	66/66	0.09	-0.01	28,31,70,71	0
7	BPH	L	1287	65/65	0.09	-0.28	27,35,42,45	0
5	BCL	L	1282	66/66	0.07	-0.74	28,32,57,60	0
11	FE	M	1310	1/1	0.02	-4.36	34,34,34,34	0
4	GOL	H	1254	6/6	0.35	-	115,115,115,116	0

6.5 Other polymers ⓘ

There are no such residues in this entry.