



Full wwPDB X-ray Structure Validation Report ⓘ

Jul 3, 2017 – 04:20 PM EDT

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 : unknown
Resolution : 2.70 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20029824
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20029824

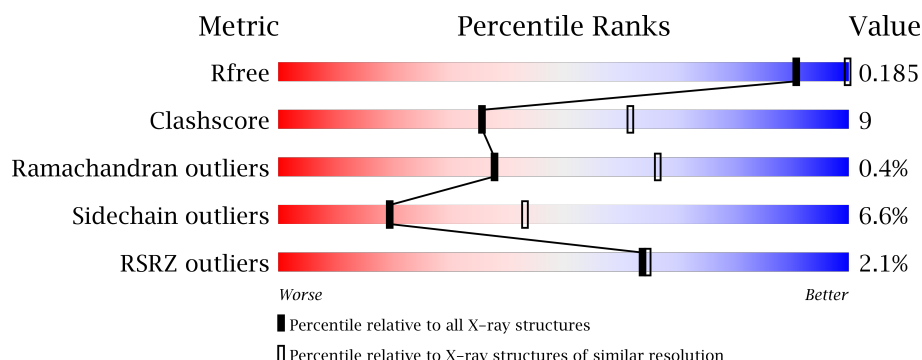
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	100719	2259 (2.70-2.70)
Clashscore	112137	2590 (2.70-2.70)
Ramachandran outliers	110173	2550 (2.70-2.70)
Sidechain outliers	110143	2550 (2.70-2.70)
RSRZ outliers	101464	2275 (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. 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	H	260	<div> <div>3%</div> <div> <div></div> <div>75%</div> <div>17%</div> <div>• 7%</div> </div> </div>
2	L	281	<div> <div>%</div> <div> <div></div> <div>86%</div> <div>14%</div> </div> </div>
3	M	307	<div> <div>2%</div> <div> <div></div> <div>79%</div> <div>18%</div> <div>••</div> </div> </div>

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
10	HTO	L	307	-	-	-	X
4	GOL	L	309	-	-	-	X
5	BCL	L	301	X	-	-	-
5	BCL	L	302	X	-	-	-
5	BCL	M	401	X	-	-	-
5	BCL	M	402	X	-	-	-
6	LDA	L	303	-	-	-	X
6	LDA	L	310	-	-	-	X
6	LDA	L	311	-	-	-	X
6	LDA	L	312	-	-	-	X
6	LDA	L	313	-	-	-	X
6	LDA	M	403	-	-	-	X
6	LDA	M	404	-	-	-	X
6	LDA	M	405	-	-	X	-
6	LDA	M	406	-	-	-	X
7	BPH	L	314	-	-	-	X
8	UQ2	L	305[A]	-	-	-	X
8	UQ2	L	305[B]	-	-	-	X
9	PO4	L	306	-	-	-	X

2 Entry composition [i](#)

There are 14 unique types of molecules in this entry. The entry contains 7442 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 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.

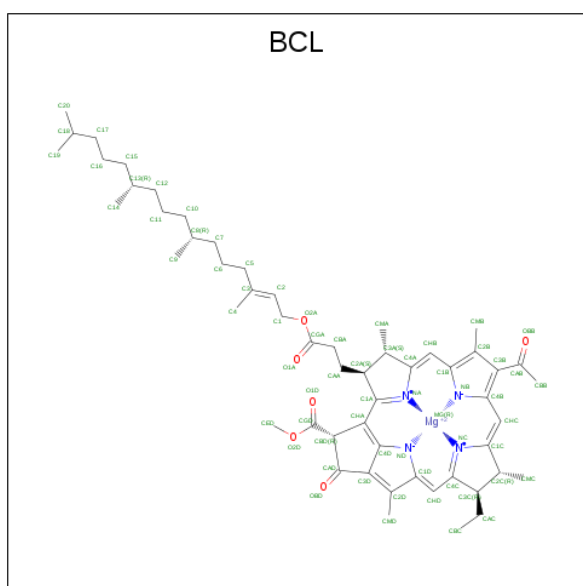
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	M	303	Total	C	N	O	S	0	0	1
			2409	1607	395	397	10			

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



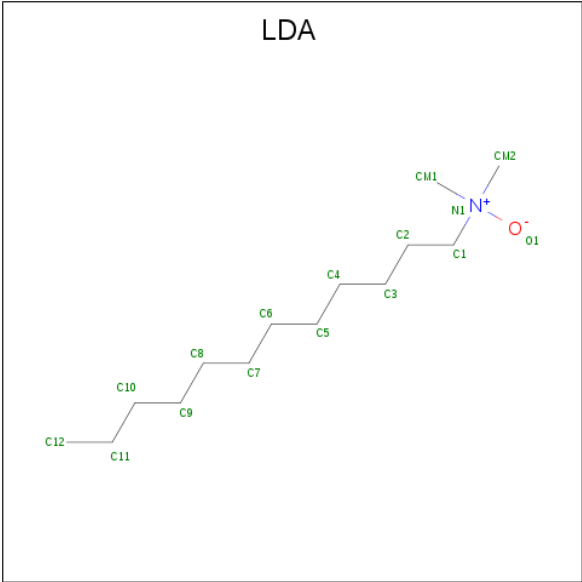
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	H	1	Total	C	O	0	0
			6	3	3		
4	L	1	Total	C	O	0	0
			6	3	3		
4	L	1	Total	C	O	0	0
			6	3	3		
4	L	1	Total	C	O	0	0
			6	3	3		

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



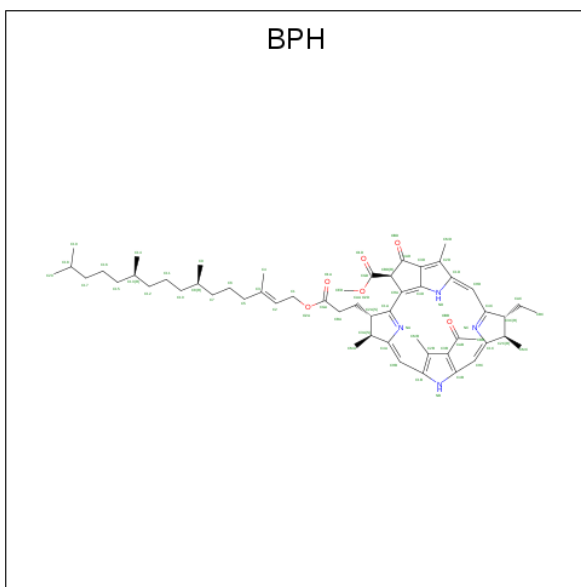
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
5	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
5	M	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
5	M	1	Total 66	C 55	Mg 1	N 4	O 6	0	0

- Molecule 6 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula: $C_{14}H_{31}NO$).



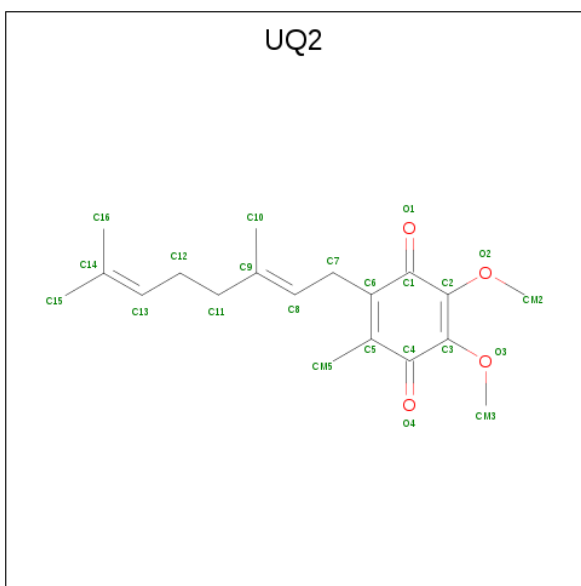
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	L	1	Total	C	N	O	0	0
			16	14	1	1		
6	L	1	Total	C	N	O	0	0
			16	14	1	1		
6	L	1	Total	C	N	O	0	0
			16	14	1	1		
6	L	1	Total	C	N	O	0	0
			16	14	1	1		
6	L	1	Total	C	N	O	0	0
			16	14	1	1		
6	M	1	Total	C	N	O	0	0
			16	14	1	1		
6	M	1	Total	C	N	O	0	0
			16	14	1	1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

- 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	L	1	Total	C	N	O	0	0
			65	55	4	6		

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



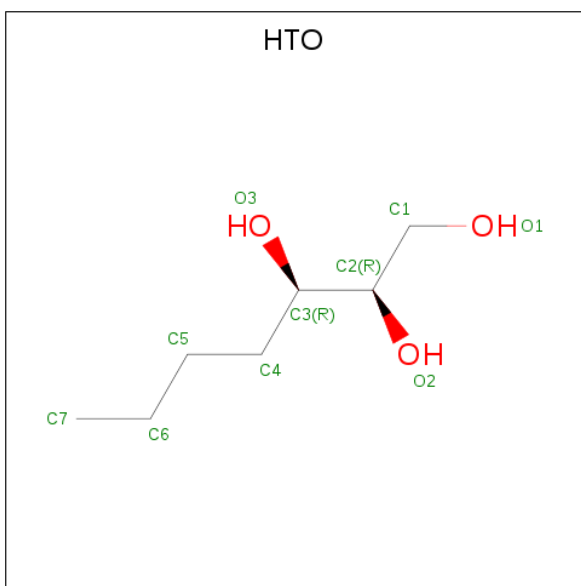
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	L	1	Total	C	O	0	1
			46	38	8		

- 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: $C_7H_{16}O_3$).

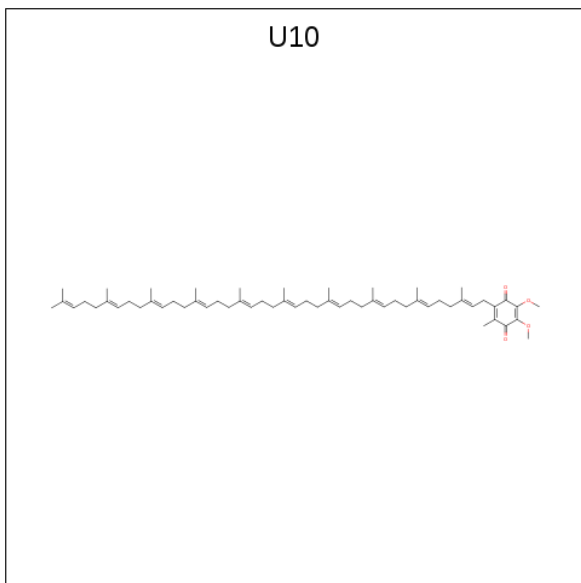


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	L	1	Total	C	O	0	0
			10	7	3		

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

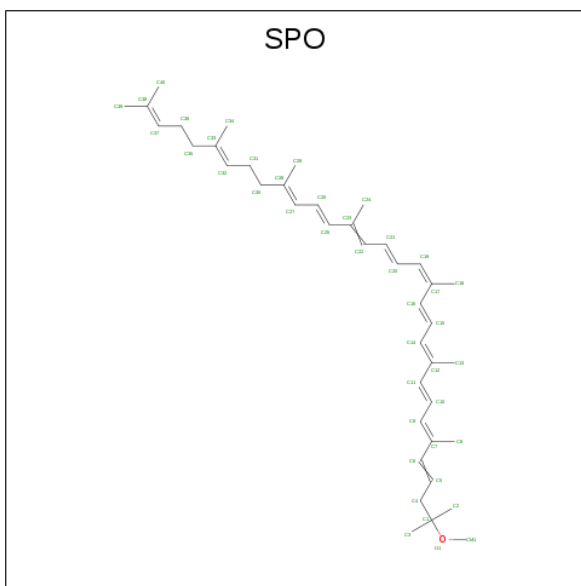
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	M	1	Total	Fe	0	0
			1	1		

- 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		

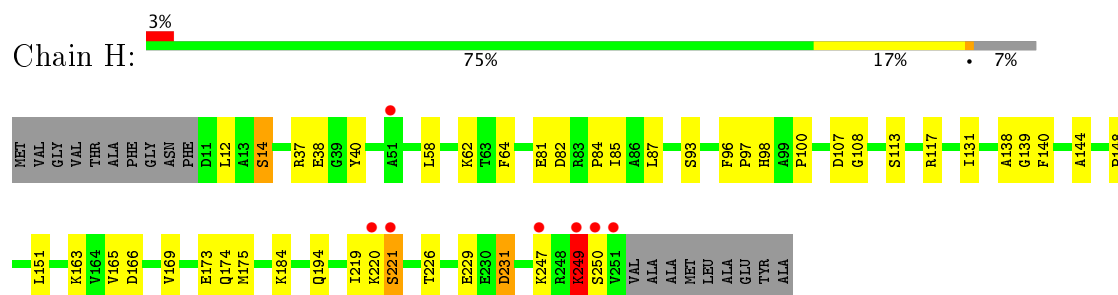
- Molecule 14 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	H	79	Total	O	0	0
			79	79		
14	L	91	Total	O	0	0
			91	91		
14	M	71	Total	O	0	0
			71	71		

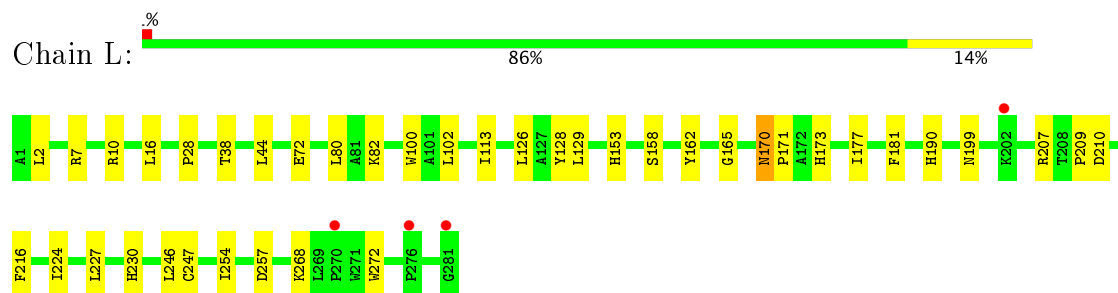
3 Residue-property plots [i](#)

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

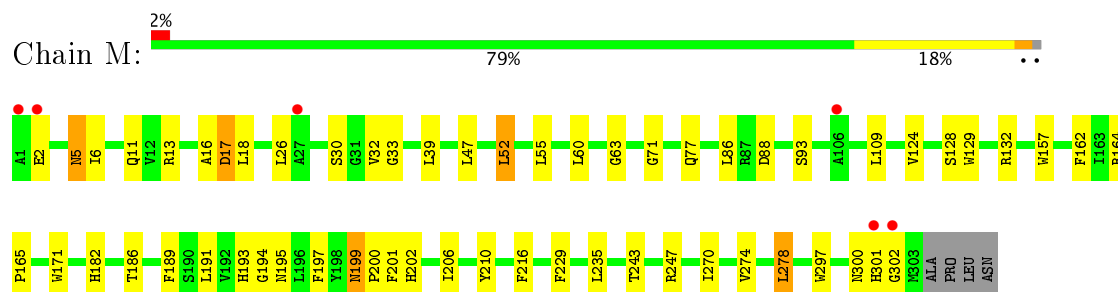
• Molecule 1: REACTION CENTER PROTEIN H CHAIN



• Molecule 2: REACTION CENTER PROTEIN L CHAIN



• Molecule 3: REACTION CENTER PROTEIN M CHAIN



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 0.182 , 0.185	Depositor DCC
R_{free} test set	2630 reflections (5.31%)	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 , 63.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.023 for -h,-k,l	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.

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

5 Model quality

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($^{\circ}$)	Ideal($^{\circ}$)
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 Too-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 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	H	1846	0	1861	28	0
2	L	2232	0	2187	26	0
3	M	2409	0	2321	47	0
4	H	6	0	8	0	0
4	L	18	0	24	2	0
5	L	132	0	148	9	0
5	M	132	0	148	20	0
6	L	80	0	155	11	0
6	M	64	0	124	11	0
7	L	130	0	152	14	0
8	L	46	0	52	13	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	4	0
13	M	42	0	60	6	0
14	H	79	0	0	1	1
14	L	91	0	0	2	0
14	M	71	0	0	0	0
All	All	7442	0	7319	134	1

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 9.

All (134) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:L:305[A]:UQ2:H152	6:L:311:LDA:H111	1.47	0.97
5:M:402:BCL:HHC	5:M:402:BCL:HBB3	1.50	0.91
8:L:305[B]:UQ2:H162	6:L:313:LDA:H121	1.56	0.87
2:L:72:GLU:HB3	14:L:416:HOH:O	1.74	0.87
1:H:249:LYS:HE3	1:H:249:LYS:HA	1.59	0.84
6:L:310:LDA:H62	6:M:405:LDA:H81	1.59	0.83
3:M:197:PHE:HZ	5:M:402:BCL:HBB2	1.42	0.83
3:M:197:PHE:CZ	5:M:402:BCL:HBB2	2.14	0.82
7:L:304:BPH:HBB3	7:L:304:BPH:HHC	1.61	0.81
1:H:226:THR:OG1	1:H:229:GLU:HG3	1.80	0.81
7:L:304:BPH:CBB	7:L:304:BPH:HHC	2.13	0.78
1:H:148:PRO:HA	1:H:151:LEU:HD12	1.66	0.78
5:M:402:BCL:CBB	5:M:402: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:M:403:LDA:H92	6:M:405:LDA:H121	1.66	0.75
2:L:28:PRO:HG3	6:L:310:LDA:HM21	1.68	0.75
7:L:314:BPH:HHC	5:M:402:BCL:H2	1.68	0.73
6:L:311:LDA:H11	3:M:33:GLY:HA2	1.69	0.73
7:L:304:BPH:HBB2	3:M:210:TYR:HB3	1.70	0.73
2:L:199:ASN:HA	4:L:308:GOL:H31	1.73	0.70
8:L:305[B]:UQ2:H162	6:L:313:LDA:C12	2.22	0.68
2:L:224:ILE:HG22	8:L:305[B]:UQ2:H8	1.74	0.68
6:M:403:LDA:H92	6:M:405:LDA:C12	2.23	0.68
2:L:190:HIS:HA	8:L:305[B]:UQ2:O4	1.94	0.68
2:L:170:ASN:C	2:L:170:ASN:HD22	1.97	0.67
14:L:460:HOH:O	6:M:405:LDA:H21	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	7:L:314:BPH:HBB2	1.78	0.65
3:M:199:ASN:HD22	3:M:199:ASN:C	2.00	0.65
7:L:314:BPH:HHC	5:M:402:BCL:C2	2.28	0.64
2:L:181:PHE:CD2	7:L:314:BPH:HBB1	2.33	0.64
3:M:189:PHE:O	3:M:193:HIS:HD2	1.80	0.64
5:L:301:BCL:H41	5:L:302:BCL:HBB3	1.82	0.62
5:L:301:BCL:CBB	5:L:301:BCL:HMB1	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
7:L:304:BPH:HBB3	7:L:304:BPH:CHC	2.33	0.58
3:M:194:GLY:O	3:M:195:ASN:HB3	2.04	0.57
8:L:305[A]:UQ2:H153	3:M:47:LEU:HD11	1.86	0.57
4:L:315:GOL:H11	6:M:403:LDA:H11	1.86	0.56
3:M:300:ASN:C	3:M:302:GLY:H	2.09	0.56
5:L:301:BCL:HMB2	5:M:402:BCL:HHB	1.87	0.56
7:L:304:BPH:CBB	3:M:210:TYR:HB3	2.36	0.55
3:M:197:PHE:HZ	5:M:402:BCL:CBB	2.16	0.55
3:M:129:TRP:O	3:M:132:ARG:HB3	2.07	0.55
5:M:402:BCL:CBB	5:M:402:BCL:CHC	2.80	0.55
5:M:401:BCL:HBB3	5:M:401:BCL:HHC	1.88	0.55
7:L:304:BPH:CHC	7:L:304: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
5:L:301:BCL:HBB2	5:L:301:BCL:HMB1	1.89	0.53
1:H:194:GLN:HG2	3:M:5:ASN:ND2	2.23	0.53
5:M:401:BCL:HBB2	13:M:409:SPO:H243	1.90	0.53
12:M:408:U10:H3M3	12:M:408:U10:H4M2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:224:ILE:CG2	8:L:305[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:401: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	7:L:314:BPH:CBB	2.39	0.51
5:M:401:BCL:H91	5:M:401:BCL:H151	1.92	0.51
5:M:401:BCL:CBB	13:M:409:SPO:H243	2.41	0.50
1:H:81:GLU:HG3	1:H:85[B]:ILE:HD11	1.93	0.50
12:M:408:U10:H352	12:M:408:U10:H312	1.94	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
5:M:402:BCL:HBD	5:M:402:BCL:HAA2	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
7:L:304:BPH:HBB1	3:M:210:TYR:CD2	2.47	0.49
3:M:162:PHE:HB2	13:M:409: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	8:L:305[A]:UQ2:H2M3	1.78	0.48
5:M:401:BCL:CBB	5:M:401:BCL:HHC	2.45	0.47
3:M:71:GLY:HA3	13:M:409:SPO:H6	1.97	0.46
3:M:186:THR:HG22	5:M:402:BCL:HHD	1.96	0.46
3:M:157:TRP:HB2	5:M:402:BCL:H71	1.96	0.46
8:L:305[B]:UQ2:C16	6:L:313:LDA:C12	2.93	0.46
5:L:301:BCL:CMB	5:M:402:BCL:HBB	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
6:M:405:LDA:H61	6:M:405:LDA:H31	1.68	0.45
1:H:87:LEU:HD23	1:H:100:PRO:HA	1.98	0.45
1:H:163:LYS:HE2	1:H:165:VAL:HG12	1.99	0.45
5:L:302:BCL:H142	5:L:302:BCL:H161	1.78	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	5:L:302:BCL:NC	2.86	0.44
5:M:401:BCL:H203	13:M:409:SPO:H10	2.00	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
8:L:305[B]:UQ2:H71	8:L:305[B]:UQ2:H5M1	1.73	0.44
2:L:170:ASN:C	2:L:170:ASN:ND2	2.69	0.44
1:H:62:LYS:HE2	1:H:64:PHE:CZ	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:2:LEU:HD11	2:L:10:ARG:CZ	2.48	0.43
1:H:98:HIS:CD2	2:L:7:ARG:HH21	2.36	0.43
1:H:40:TYR:HB3	1:H:58:LEU:HD21	2.00	0.43
3:M:194:GLY:O	3:M:195:ASN:CB	2.66	0.43
3:M:199:ASN:HD22	3:M:200:PRO:N	2.16	0.43
2:L:173:HIS:CE1	2:L:177:ILE:HD11	2.54	0.43
6:L:303:LDA:HM21	6:L:303:LDA:H22	1.82	0.43
3:M:274:VAL:O	3:M:278:LEU:HB2	2.19	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
6:L:310:LDA:HM22	6:M:405:LDA:HM22	1.99	0.43
1:H:131:ILE:HA	1:H:169:VAL:O	2.19	0.42
1:H:84:PRO:O	1:H:85[A]:ILE:HD13	2.19	0.42
6:M:405:LDA:H112	12:M:408:U10:H202	2.00	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
5:L:301:BCL:HHC	5:M:402:BCL:CHC	2.49	0.42
8:L:305[B]:UQ2:C16	6:L:313:LDA:H121	2.37	0.42
6:M:405:LDA:H22	6:M:405:LDA:HM11	1.59	0.42
1:H:138:ALA:HA	1:H:139:GLY:HA2	1.85	0.42
2:L:128:TYR:HD1	5:L:302:BCL:HBB1	1.85	0.42
2:L:162:TYR:HA	2:L:165:GLY:O	2.19	0.42
1:H:144:ALA:HB3	3:M:11:GLN:HB2	2.01	0.42
6:M:405:LDA:H81	6:M:405:LDA:H51	1.71	0.42
8:L:305[A]:UQ2:H101	8:L:305[A]:UQ2:H121	1.57	0.42
1:H:173:GLU:O	1:H:174:GLN:C	2.58	0.41
2:L:224:ILE:HD12	8:L:305[A]:UQ2:H102	2.01	0.41
2:L:170:ASN:HD22	2:L:171:PRO:N	2.18	0.41
6:L:310:LDA:H62	6:M:405:LDA:H51	2.03	0.41
3:M:199:ASN:ND2	3:M:201:PHE:H	2.18	0.41
7:L:304:BPH:HBB1	3:M:210:TYR:CG	2.56	0.40
7:L:314:BPH:H5C1	3:M:63:GLY:HA3	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:409:SPO:H343	2.56	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
12:M:408:U10:H372	12:M:408:U10:H351	1.78	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	Interatomic distance (Å)	Clash overlap (Å)
14:H:457:HOH:O	14:H:457:HOH:O[4_555]	1.99	0.21

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	H	242/260 (93%)	233 (96%)	8 (3%)	1 (0%)	38	66
2	L	279/281 (99%)	266 (95%)	13 (5%)	0	100	100
3	M	301/307 (98%)	282 (94%)	17 (6%)	2 (1%)	25	53
All	All	822/848 (97%)	781 (95%)	38 (5%)	3 (0%)	38	66

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 [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	H	198/208 (95%)	187 (94%)	11 (6%)	25	51
2	L	220/220 (100%)	203 (92%)	17 (8%)	15	34
3	M	236/240 (98%)	220 (93%)	16 (7%)	18	41

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	654/668 (98%)	610 (93%)	44 (7%)	19	42

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

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Mol	Chain	Res	Type
3	M	109	LEU
3	M	124	VAL
3	M	182	HIS
3	M	191	LEU
3	M	199	ASN
3	M	216	PHE
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 [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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	GOL	H	301	-	5,5,5	0.35	0	5,5,5	0.35	0
5	BCL	L	301	-	55,74,74	2.23	9 (16%)	65,115,115	1.89	14 (21%)
5	BCL	L	302	-	55,74,74	2.31	8 (14%)	65,115,115	2.35	19 (29%)
6	LDA	L	303	-	13,15,15	2.28	1 (7%)	14,17,17	0.84	0
7	BPH	L	304	-	65,70,70	2.92	16 (24%)	75,101,101	1.95	18 (24%)
8	UQ2	L	305[A]	-	23,23,23	2.69	7 (30%)	28,31,31	1.08	0
8	UQ2	L	305[B]	-	23,23,23	2.62	8 (34%)	28,31,31	1.49	5 (17%)
9	PO4	L	306	-	4,4,4	0.70	0	6,6,6	0.48	0
10	HTO	L	307	-	9,9,9	0.54	0	9,10,10	0.71	0
4	GOL	L	308	-	5,5,5	0.31	0	5,5,5	0.56	0
4	GOL	L	309	-	5,5,5	0.26	0	5,5,5	0.40	0
6	LDA	L	310	-	13,15,15	2.40	1 (7%)	14,17,17	0.71	0
6	LDA	L	311	-	13,15,15	2.41	1 (7%)	14,17,17	0.72	0
6	LDA	L	312	-	13,15,15	2.33	1 (7%)	14,17,17	0.56	0
6	LDA	L	313	-	13,15,15	2.45	1 (7%)	14,17,17	0.83	0
7	BPH	L	314	-	65,70,70	2.98	16 (24%)	75,101,101	1.90	16 (21%)
4	GOL	L	315	-	5,5,5	0.32	0	5,5,5	0.46	0
5	BCL	M	401	-	55,74,74	2.29	7 (12%)	65,115,115	2.08	18 (27%)
5	BCL	M	402	-	55,74,74	2.26	7 (12%)	65,115,115	2.27	20 (30%)
6	LDA	M	403	-	13,15,15	2.28	1 (7%)	14,17,17	1.49	2 (14%)
6	LDA	M	404	-	13,15,15	2.37	1 (7%)	14,17,17	0.64	0
6	LDA	M	405	-	13,15,15	2.38	2 (15%)	14,17,17	0.58	0
6	LDA	M	406	-	13,15,15	2.30	1 (7%)	14,17,17	0.70	0
12	U10	M	408	-	48,48,63	2.64	12 (25%)	58,61,79	1.55	11 (18%)
13	SPO	M	409	-	40,41,41	4.19	12 (30%)	49,50,50	1.95	12 (24%)

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	301	-	-	0/4/4/4	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	BCL	L	301	-	2/2/21/25	0/37/137/137	0/0/9/9
5	BCL	L	302	-	2/2/21/25	0/37/137/137	0/0/9/9
6	LDA	L	303	-	-	0/13/13/13	0/0/0/0
7	BPH	L	304	-	-	0/54/105/105	0/1/6/6
8	UQ2	L	305[A]	-	-	0/15/39/39	0/1/1/1
8	UQ2	L	305[B]	-	-	0/15/39/39	0/1/1/1
9	PO4	L	306	-	-	0/0/0/0	0/0/0/0
10	HTO	L	307	-	-	0/10/10/10	0/0/0/0
4	GOL	L	308	-	-	0/4/4/4	0/0/0/0
4	GOL	L	309	-	-	0/4/4/4	0/0/0/0
6	LDA	L	310	-	-	0/13/13/13	0/0/0/0
6	LDA	L	311	-	-	0/13/13/13	0/0/0/0
6	LDA	L	312	-	-	0/13/13/13	0/0/0/0
6	LDA	L	313	-	-	0/13/13/13	0/0/0/0
7	BPH	L	314	-	-	0/54/105/105	0/1/6/6
4	GOL	L	315	-	-	0/4/4/4	0/0/0/0
5	BCL	M	401	-	2/2/21/25	0/37/137/137	0/0/9/9
5	BCL	M	402	-	2/2/21/25	0/37/137/137	0/0/9/9
6	LDA	M	403	-	-	0/13/13/13	0/0/0/0
6	LDA	M	404	-	-	0/13/13/13	0/0/0/0
6	LDA	M	405	-	-	0/13/13/13	0/0/0/0
6	LDA	M	406	-	-	0/13/13/13	0/0/0/0
12	U10	M	408	-	-	0/45/69/87	0/1/1/1
13	SPO	M	409	-	-	0/47/47/47	0/0/0/0

All (112) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	L	313	LDA	O1-N1	-8.58	1.25	1.42
6	L	311	LDA	O1-N1	-8.49	1.25	1.42
6	L	310	LDA	O1-N1	-8.40	1.25	1.42
6	M	404	LDA	O1-N1	-8.28	1.25	1.42
6	L	312	LDA	O1-N1	-8.22	1.26	1.42
6	M	405	LDA	O1-N1	-8.20	1.26	1.42
6	L	303	LDA	O1-N1	-8.02	1.26	1.42
6	M	406	LDA	O1-N1	-8.01	1.26	1.42
6	M	403	LDA	O1-N1	-7.81	1.26	1.42
8	L	305[B]	UQ2	O2-C2	-5.08	1.24	1.36
8	L	305[A]	UQ2	O3-C3	-5.00	1.24	1.36
8	L	305[A]	UQ2	O2-C2	-4.85	1.24	1.36
12	M	408	U10	O4-C4	-4.67	1.25	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	L	304	BPH	C3D-C4D	-4.55	1.36	1.41
12	M	408	U10	O3-C3	-4.18	1.26	1.36
7	L	314	BPH	C3D-C4D	-4.18	1.36	1.41
8	L	305[B]	UQ2	O3-C3	-4.07	1.26	1.36
7	L	304	BPH	C3D-CAD	-3.74	1.38	1.47
7	L	314	BPH	C1B-C2B	-3.27	1.38	1.45
7	L	314	BPH	C3D-CAD	-3.17	1.39	1.47
5	M	401	BCL	O2D-CGD	-3.14	1.25	1.33
8	L	305[A]	UQ2	C3-C4	-3.04	1.40	1.48
5	L	302	BCL	O2A-CGA	-2.98	1.24	1.33
8	L	305[B]	UQ2	C3-C4	-2.95	1.40	1.48
5	M	401	BCL	C3D-CAD	-2.94	1.37	1.46
5	L	301	BCL	O2D-CGD	-2.91	1.25	1.33
7	L	314	BPH	O2D-CGD	-2.89	1.25	1.33
7	L	304	BPH	C1B-C2B	-2.73	1.39	1.45
8	L	305[A]	UQ2	C2-C1	-2.71	1.41	1.48
12	M	408	U10	C4-C5	-2.68	1.41	1.48
7	L	314	BPH	O2A-CGA	-2.59	1.25	1.33
5	L	301	BCL	C3D-CAD	-2.46	1.39	1.46
5	M	402	BCL	C3D-CAD	-2.40	1.39	1.46
5	L	302	BCL	O2D-CGD	-2.37	1.27	1.33
6	M	405	LDA	C1-N1	-2.33	1.46	1.51
5	L	302	BCL	C3D-CAD	-2.30	1.39	1.46
8	L	305[B]	UQ2	C2-C1	-2.29	1.42	1.48
8	L	305[B]	UQ2	C6-C1	-2.25	1.39	1.46
5	M	402	BCL	O2D-CGD	-2.24	1.27	1.33
7	L	304	BPH	O2D-CED	-2.10	1.40	1.45
12	M	408	U10	C3-C2	-2.07	1.43	1.48
5	L	301	BCL	O2A-CGA	-2.00	1.27	1.33
5	L	301	BCL	CHD-C4C	2.04	1.47	1.41
8	L	305[B]	UQ2	C6-C5	2.29	1.40	1.35
7	L	304	BPH	CHB-C4A	2.85	1.47	1.40
7	L	314	BPH	CHB-C4A	2.88	1.47	1.40
5	M	402	BCL	C2-C3	2.93	1.40	1.33
5	L	301	BCL	C2-C3	2.96	1.40	1.33
5	L	302	BCL	C2-C3	3.01	1.40	1.33
7	L	304	BPH	C1D-CHD	3.03	1.51	1.40
8	L	305[A]	UQ2	C6-C5	3.11	1.42	1.35
12	M	408	U10	C6-C1	3.20	1.42	1.35
7	L	314	BPH	CHD-C4C	3.21	1.46	1.38
5	M	401	BCL	C2-C3	3.22	1.41	1.33
7	L	304	BPH	CHC-C4B	3.46	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	M	401	BCL	CHC-C1C	3.59	1.38	1.33
13	M	409	SPO	C21-C20	3.62	1.45	1.35
5	L	301	BCL	CHB-C4A	3.69	1.38	1.33
7	L	304	BPH	CHD-C4C	3.94	1.48	1.38
5	L	302	BCL	CHC-C1C	3.95	1.38	1.33
5	M	402	BCL	CHB-C4A	4.35	1.39	1.33
7	L	314	BPH	CHC-C4B	4.51	1.51	1.40
13	M	409	SPO	C26-C25	4.61	1.46	1.34
13	M	409	SPO	C15-C16	4.68	1.46	1.34
13	M	409	SPO	C10-C11	4.71	1.46	1.34
7	L	304	BPH	C3D-C2D	4.71	1.50	1.39
5	M	402	BCL	CHC-C1C	4.79	1.39	1.33
5	M	401	BCL	CHB-C4A	4.82	1.39	1.33
7	L	314	BPH	C3D-C2D	4.84	1.50	1.39
7	L	304	BPH	CHC-C1C	5.01	1.46	1.36
12	M	408	U10	C38-C39	5.35	1.48	1.32
5	L	302	BCL	CHB-C4A	5.35	1.40	1.33
8	L	305[A]	UQ2	C13-C14	5.42	1.48	1.32
7	L	304	BPH	CHB-C1B	5.47	1.49	1.38
7	L	304	BPH	C2-C3	5.48	1.46	1.33
13	M	409	SPO	C6-C5	5.49	1.46	1.31
5	L	301	BCL	O1A-CGA	5.51	1.39	1.22
7	L	314	BPH	CHC-C1C	5.67	1.47	1.36
5	L	302	BCL	O1A-CGA	5.73	1.39	1.22
5	L	301	BCL	CHC-C1C	5.76	1.40	1.33
7	L	314	BPH	C2-C3	5.76	1.47	1.33
12	M	408	U10	C18-C19	5.90	1.47	1.33
12	M	408	U10	C8-C9	5.94	1.47	1.33
8	L	305[B]	UQ2	C13-C14	5.95	1.49	1.32
12	M	408	U10	C28-C29	5.96	1.47	1.33
7	L	314	BPH	CHB-C1B	6.01	1.50	1.38
12	M	408	U10	C23-C24	6.08	1.48	1.33
13	M	409	SPO	C37-C38	6.17	1.50	1.32
5	M	402	BCL	O1A-CGA	6.20	1.41	1.22
13	M	409	SPO	C32-C33	6.20	1.48	1.33
7	L	314	BPH	O1A-CGA	6.23	1.41	1.22
5	M	401	BCL	O1A-CGA	6.31	1.41	1.22
12	M	408	U10	C13-C14	6.32	1.48	1.33
7	L	304	BPH	O1A-CGA	6.46	1.41	1.22
8	L	305[B]	UQ2	C8-C9	6.52	1.49	1.33
12	M	408	U10	C33-C34	6.64	1.49	1.33
8	L	305[A]	UQ2	C8-C9	6.70	1.49	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	L	314	BPH	O1D-CGD	7.23	1.39	1.21
7	L	304	BPH	O1D-CGD	8.02	1.41	1.21
7	L	314	BPH	OBB-CAB	8.27	1.41	1.23
13	M	409	SPO	C22-C23	8.74	1.47	1.35
7	L	304	BPH	OBB-CAB	8.94	1.42	1.23
13	M	409	SPO	C19-C17	9.01	1.47	1.35
13	M	409	SPO	C9-C7	9.26	1.48	1.35
13	M	409	SPO	C14-C12	9.47	1.48	1.35
5	L	301	BCL	OBD-CAD	11.92	1.39	1.22
7	L	304	BPH	OBD-CAD	12.00	1.39	1.22
5	M	402	BCL	OBD-CAD	12.43	1.40	1.22
5	M	401	BCL	OBD-CAD	12.53	1.40	1.22
5	L	302	BCL	OBD-CAD	12.98	1.41	1.22
7	L	314	BPH	OBD-CAD	13.10	1.41	1.22
13	M	409	SPO	C27-C28	13.13	1.48	1.34

All (135) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	302	BCL	CMB-C2B-C1B	-7.98	116.19	128.46
5	M	402	BCL	CMB-C2B-C1B	-7.94	116.26	128.46
5	M	401	BCL	CMB-C2B-C1B	-7.00	117.70	128.46
5	L	301	BCL	CMB-C2B-C1B	-6.75	118.08	128.46
5	M	402	BCL	C1D-CHD-C4C	-5.79	117.29	125.92
7	L	314	BPH	OBD-CAD-CBD	-5.46	117.70	125.94
7	L	314	BPH	OBD-CAD-C3D	-5.14	118.56	128.03
5	L	301	BCL	C1D-CHD-C4C	-5.03	118.43	125.92
5	M	402	BCL	CHD-C4C-NC	-4.96	119.56	125.08
5	L	302	BCL	C1D-CHD-C4C	-4.63	119.02	125.92
5	M	401	BCL	C1D-CHD-C4C	-4.55	119.14	125.92
5	L	302	BCL	C4B-CHC-C1C	-4.48	121.25	130.12
6	M	403	LDA	CM2-N1-CM1	-4.47	102.44	110.99
13	M	409	SPO	C20-C19-C17	-4.37	121.07	127.31
7	L	304	BPH	O1D-CGD-CBD	-4.35	116.78	124.60
5	L	302	BCL	CHB-C4A-NA	-4.33	118.53	124.51
5	M	401	BCL	C1B-CHB-C4A	-4.28	121.64	130.12
5	L	302	BCL	O2A-CGA-O1A	-4.07	113.44	123.55
13	M	409	SPO	C10-C9-C7	-4.06	121.52	127.31
13	M	409	SPO	C5-C6-C7	-3.85	120.08	125.89
5	M	401	BCL	CHC-C1C-NC	-3.85	119.19	124.51
12	M	408	U10	C17-C18-C19	-3.79	118.17	127.68
5	M	402	BCL	O2D-CGD-O1D	-3.66	116.46	123.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	M	402	BCL	CHC-C1C-NC	-3.65	119.47	124.51
7	L	304	BPH	C1-C2-C3	-3.51	119.49	125.96
5	M	402	BCL	C1B-CHB-C4A	-3.47	123.24	130.12
13	M	409	SPO	C21-C22-C23	-3.47	122.36	127.31
5	L	302	BCL	O1D-CGD-CBD	-3.43	118.45	124.60
13	M	409	SPO	C15-C14-C12	-3.38	122.48	127.31
5	M	401	BCL	O2D-CGD-O1D	-3.38	117.01	123.82
7	L	304	BPH	OBD-CAD-C3D	-3.37	121.82	128.03
8	L	305[B]	UQ2	O1-C1-C6	-3.36	115.63	121.82
5	M	401	BCL	C4B-CHC-C1C	-3.32	123.53	130.12
5	L	302	BCL	CHD-C4C-NC	-3.29	121.42	125.08
5	L	302	BCL	C1B-CHB-C4A	-3.25	123.69	130.12
7	L	304	BPH	C1C-NC-C4C	-3.20	107.66	110.54
7	L	314	BPH	O2D-CGD-O1D	-3.18	117.42	123.82
5	M	401	BCL	CHB-C4A-NA	-3.14	120.16	124.51
13	M	409	SPO	C4-C5-C6	-3.03	120.21	124.57
8	L	305[B]	UQ2	CM5-C5-C6	-3.01	118.10	124.20
7	L	314	BPH	CMD-C2D-C3D	-2.91	119.50	124.89
5	L	302	BCL	CHA-C1A-NA	-2.90	119.44	126.18
13	M	409	SPO	C20-C21-C22	-2.87	117.34	123.46
5	L	301	BCL	CMA-C3A-C4A	-2.86	104.07	111.77
5	L	301	BCL	O2A-CGA-O1A	-2.83	116.52	123.55
5	L	302	BCL	O2D-CGD-O1D	-2.67	118.44	123.82
7	L	314	BPH	O1D-CGD-CBD	-2.66	119.83	124.60
7	L	304	BPH	CMD-C2D-C3D	-2.65	119.98	124.89
7	L	314	BPH	C1C-NC-C4C	-2.62	108.18	110.54
7	L	304	BPH	OBD-CAD-CBD	-2.61	122.00	125.94
5	M	402	BCL	CMD-C2D-C3D	-2.55	120.16	124.89
5	M	401	BCL	C3C-C4C-CHD	-2.54	117.99	123.34
7	L	304	BPH	CHC-C4B-NB	-2.52	120.12	124.97
7	L	304	BPH	C7-C6-C5	-2.47	106.25	113.11
12	M	408	U10	C30-C29-C28	-2.47	117.10	123.69
12	M	408	U10	C27-C28-C29	-2.47	121.48	127.68
13	M	409	SPO	C27-C26-C25	-2.45	115.72	123.23
7	L	314	BPH	CAA-C2A-C1A	-2.44	105.97	112.28
5	L	302	BCL	C5-C3-C2	-2.37	116.26	121.10
5	L	302	BCL	C3C-C4C-CHD	-2.35	118.39	123.34
7	L	314	BPH	C3B-C2B-C1B	-2.33	102.37	105.82
5	M	401	BCL	CHA-C1A-NA	-2.32	120.79	126.18
5	M	402	BCL	C3C-C4C-CHD	-2.27	118.56	123.34
5	L	301	BCL	C1B-CHB-C4A	-2.25	125.67	130.12
5	M	401	BCL	CAA-C2A-C3A	-2.24	106.66	112.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	M	409	SPO	C14-C15-C16	-2.23	116.39	123.23
7	L	314	BPH	C1-C2-C3	-2.18	121.93	125.96
5	M	402	BCL	CHA-C1A-NA	-2.16	121.17	126.18
5	M	402	BCL	C16-C15-C13	-2.15	108.66	115.73
12	M	408	U10	C12-C13-C14	-2.15	122.28	127.68
5	M	401	BCL	O1D-CGD-CBD	-2.14	120.75	124.60
5	L	301	BCL	CHA-C1A-NA	-2.13	121.23	126.18
5	M	402	BCL	CHB-C4A-NA	-2.11	121.59	124.51
5	M	401	BCL	CMA-C3A-C4A	-2.10	106.12	111.77
8	L	305[B]	UQ2	C2-C3-C4	-2.10	116.30	120.67
5	M	402	BCL	O2A-CGA-O1A	-2.07	118.42	123.55
12	M	408	U10	O5-C5-C6	-2.06	118.02	121.82
12	M	408	U10	C32-C33-C34	-2.03	122.58	127.68
5	M	402	BCL	C4B-CHC-C1C	-2.02	126.11	130.12
5	M	402	BCL	CGD-CBD-CAD	-2.01	103.97	110.71
5	L	301	BCL	CAA-C2A-C1A	-2.00	105.41	111.97
7	L	314	BPH	O2A-CGA-CBA	2.01	117.75	111.90
7	L	314	BPH	CED-O2D-CGD	2.10	120.89	115.97
12	M	408	U10	C15-C14-C16	2.18	119.06	115.29
5	L	301	BCL	C14-C13-C12	2.22	119.45	111.36
7	L	304	BPH	CAC-C3C-C4C	2.25	118.46	112.67
6	M	403	LDA	O1-N1-C1	2.28	114.87	109.27
7	L	304	BPH	C4A-NA-C1A	2.32	110.03	108.16
12	M	408	U10	C20-C19-C21	2.34	119.35	115.29
5	L	302	BCL	CED-O2D-CGD	2.36	121.50	115.97
7	L	314	BPH	C4-C3-C5	2.36	119.38	115.29
8	L	305[B]	UQ2	C10-C9-C11	2.40	119.45	115.29
5	M	402	BCL	OBB-CAB-C3B	2.40	124.53	119.95
5	L	301	BCL	CED-O2D-CGD	2.53	121.91	115.97
12	M	408	U10	C10-C9-C11	2.56	119.73	115.29
5	M	401	BCL	C4A-NA-C1A	2.57	109.64	106.45
5	M	402	BCL	C4-C3-C5	2.57	119.75	115.29
12	M	408	U10	C4M-O4-C4	2.57	125.64	116.44
5	M	401	BCL	C2A-C3A-C4A	2.58	106.04	101.87
5	L	301	BCL	C2A-C3A-C4A	2.61	106.08	101.87
7	L	304	BPH	CMB-C2B-C1B	2.66	129.18	125.04
5	M	402	BCL	CED-O2D-CGD	2.67	122.22	115.97
5	L	302	BCL	CAA-CBA-CGA	2.71	121.51	113.35
13	M	409	SPO	C34-C33-C35	2.83	120.20	115.29
8	L	305[B]	UQ2	CM3-O3-C3	2.85	126.63	116.44
5	L	302	BCL	O2A-CGA-CBA	2.90	120.33	111.90
5	L	302	BCL	C2A-C3A-C4A	2.93	106.61	101.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	L	304	BPH	O2A-CGA-CBA	2.95	120.49	111.90
7	L	304	BPH	C1-O2A-CGA	3.05	124.09	116.77
5	M	401	BCL	O2A-CGA-CBA	3.16	121.08	111.90
5	L	301	BCL	C1-O2A-CGA	3.17	124.39	116.77
13	M	409	SPO	C24-C23-C25	3.23	123.24	118.10
7	L	314	BPH	C2B-C1B-NB	3.24	114.62	109.82
7	L	304	BPH	C2B-C1B-NB	3.29	114.69	109.82
13	M	409	SPO	C29-C28-C30	3.30	121.02	115.29
5	L	301	BCL	O2D-CGD-CBD	3.37	117.31	111.30
5	L	302	BCL	C4-C3-C5	3.44	121.26	115.29
5	M	401	BCL	C1-O2A-CGA	3.66	125.54	116.77
7	L	304	BPH	CED-O2D-CGD	3.70	124.64	115.97
7	L	304	BPH	C3C-C4C-NC	3.72	111.47	107.97
5	M	402	BCL	O2A-CGA-CBA	3.73	122.76	111.90
5	L	301	BCL	O2A-CGA-CBA	4.03	123.62	111.90
5	M	401	BCL	CMB-C2B-C3B	4.36	132.98	124.89
5	L	301	BCL	CMB-C2B-C3B	4.50	133.24	124.89
5	L	302	BCL	CMB-C2B-C3B	4.69	133.60	124.89
7	L	314	BPH	C3C-C4C-NC	4.71	112.40	107.97
5	M	402	BCL	CMB-C2B-C3B	4.97	134.11	124.89
12	M	408	U10	C30-C29-C31	5.08	124.10	115.29
5	M	402	BCL	O2D-CGD-CBD	5.52	121.17	111.30
7	L	314	BPH	C4D-C3D-CAD	5.92	111.16	107.78
5	M	401	BCL	O2D-CGD-CBD	6.10	122.21	111.30
7	L	304	BPH	O2D-CGD-CBD	6.26	122.49	111.30
7	L	304	BPH	C4D-C3D-CAD	6.38	111.43	107.78
7	L	314	BPH	O2D-CGD-CBD	6.41	122.75	111.30
5	L	302	BCL	O2D-CGD-CBD	6.59	123.08	111.30

All (8) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	M	401	BCL	C8
5	M	401	BCL	C13
5	L	301	BCL	C8
5	L	301	BCL	C13
5	M	402	BCL	C8
5	M	402	BCL	C13
5	L	302	BCL	C8
5	L	302	BCL	C13

There are no torsion outliers.

There are no ring outliers.

18 monomers are involved in 72 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	L	301	BCL	6	0
5	L	302	BCL	4	0
6	L	303	LDA	1	0
7	L	304	BPH	8	0
8	L	305[A]	UQ2	5	0
8	L	305[B]	UQ2	8	0
4	L	308	GOL	1	0
6	L	310	LDA	4	0
6	L	311	LDA	2	0
6	L	313	LDA	4	0
7	L	314	BPH	6	0
4	L	315	GOL	1	0
5	M	401	BCL	6	0
5	M	402	BCL	14	0
6	M	403	LDA	3	0
6	M	405	LDA	10	0
12	M	408	U10	4	0
13	M	409	SPO	6	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	H	241/260 (92%)	-0.42	7 (2%)	52	52	38, 50, 63, 105	0
2	L	281/281 (100%)	-0.78	4 (1%)	75	76	32, 43, 69, 77	0
3	M	303/307 (98%)	-0.57	6 (1%)	65	66	31, 50, 75, 96	0
All	All	825/848 (97%)	-0.60	17 (2%)	64	65	31, 48, 71, 105	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	251	VAL	9.0
3	M	1	ALA	8.1
1	H	250	SER	7.8
3	M	302	GLY	4.6
1	H	220[A]	LYS	3.8
1	H	249	LYS	3.8
2	L	281	GLY	3.6
3	M	27	ALA	3.5
3	M	301	HIS	3.3
3	M	2	GLU	3.3
1	H	221	SER	2.7
3	M	106	ALA	2.4
2	L	270	PRO	2.3
2	L	276	PRO	2.2
2	L	202	LYS	2.2
1	H	51	ALA	2.2
1	H	247	LYS	2.1

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 ⓘ

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	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
6	LDA	L	312	16/16	0.28	0.50	26.72	87,101,112,113	0
6	LDA	L	303	16/16	0.45	0.52	21.09	61,96,114,115	0
6	LDA	L	313	16/16	0.54	0.34	18.50	101,109,116,116	0
6	LDA	L	310	16/16	0.50	0.44	18.48	91,99,110,110	0
6	LDA	L	311	16/16	0.37	0.47	12.45	111,117,128,129	0
8	UQ2	L	305[A]	23/23	0.84	0.30	9.46	51,53,54,55	23
6	LDA	M	403	16/16	0.80	0.26	8.77	45,71,82,82	0
8	UQ2	L	305[B]	23/23	0.84	0.30	8.18	43,49,55,55	23
9	PO4	L	306	5/5	0.68	0.61	6.41	156,156,157,157	0
6	LDA	M	406	16/16	0.26	0.59	6.26	100,116,126,126	0
10	HTO	L	307	10/10	0.74	0.28	4.62	77,81,82,82	0
4	GOL	L	309	6/6	0.88	0.26	4.13	81,81,82,82	0
6	LDA	M	404	16/16	0.84	0.34	4.09	76,79,86,86	0
7	BPH	L	314	65/65	0.91	0.17	2.20	42,50,111,113	0
6	LDA	M	405	16/16	0.89	0.21	1.87	65,67,78,79	0
13	SPO	M	409	42/42	0.89	0.19	1.72	44,60,78,81	0
4	GOL	L	308	6/6	0.85	0.30	1.71	71,74,74,76	0
12	U10	M	408	48/63	0.93	0.18	1.67	37,48,78,80	0
5	BCL	M	402	66/66	0.97	0.15	1.18	29,39,60,70	0
7	BPH	L	304	65/65	0.98	0.13	1.07	26,32,41,43	0
5	BCL	L	301	66/66	0.97	0.14	0.93	30,36,47,52	0
5	BCL	M	401	66/66	0.96	0.13	0.63	30,34,81,82	0
5	BCL	L	302	66/66	0.97	0.12	-0.06	30,37,58,62	0
11	FE	M	407	1/1	0.99	0.04	-3.72	37,37,37,37	0
4	GOL	L	315	6/6	0.67	0.26	-	98,101,101,103	0
4	GOL	H	301	6/6	0.86	0.31	-	96,97,98,98	0

6.5 Other polymers [i](#)

There are no such residues in this entry.