Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 05:49 AM GMT

PDB ID	:	2UXL
Title	:	X-RAY HIGH RESOLUTION STRUCTURE OF THE PHOTOSYNTHETIC REACTION CENTER FROM RB. SPHAEROIDES AT PH 10 IN THE NEUTRAL STATE, 2ND DATASET
Authors	:	Koepke, J.; Diehm, R.; Fritzsch, G.
Deposited on	:	2007-03-28
Resolution	:	2.88 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

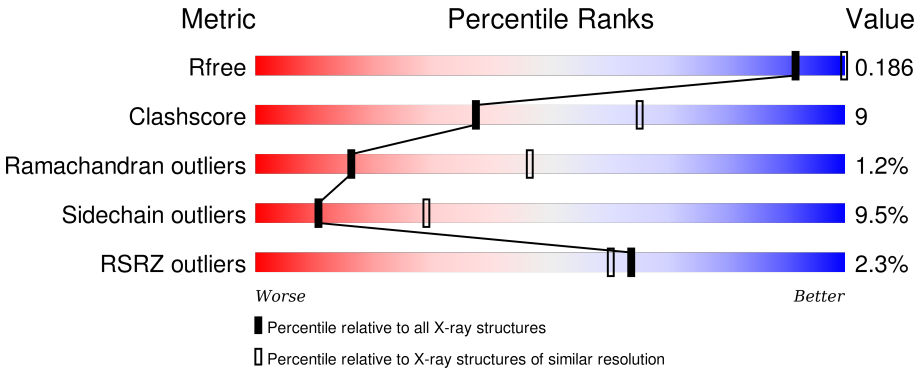
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.88 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1945 (2.90-2.86)
Clashscore	102246	2202 (2.90-2.86)
Ramachandran outliers	100387	2149 (2.90-2.86)
Sidechain outliers	100360	2152 (2.90-2.86)
RSRZ outliers	91569	1950 (2.90-2.86)

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 <=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	2% 70% 19% • 7%
2	L	281	2% 81% 16% •
3	M	307	3% 75% 20% • ••

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
11	U10	M	1310	-	-	-	X
12	SPO	M	1311	-	-	-	X
4	GOL	H	1251	-	-	-	X
4	GOL	H	1252	-	-	-	X
4	GOL	L	1287	-	-	-	X
5	BCL	L	1282	X	-	-	-
5	BCL	L	1285	X	-	-	-
5	BCL	M	1303	X	-	-	-
5	BCL	M	1304	X	-	-	-
6	BPH	M	1309	-	-	-	X
7	UQ2	L	1284[A]	-	-	-	X
7	UQ2	L	1284[B]	-	-	X	X
8	HTO	L	1286	-	-	-	X
9	LDA	M	1305	-	-	-	X
9	LDA	M	1306	-	-	-	X
9	LDA	M	1307	-	-	-	X

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 7302 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			

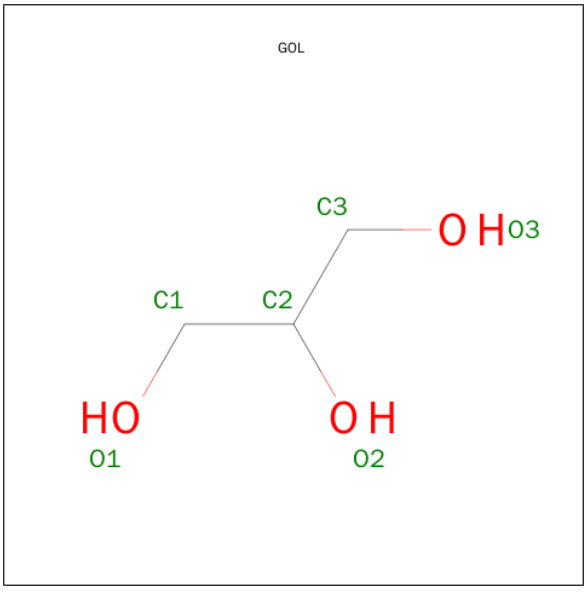
- Molecule 2 is a protein called REACTION CENTER PROTEIN L CHAIN.

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.

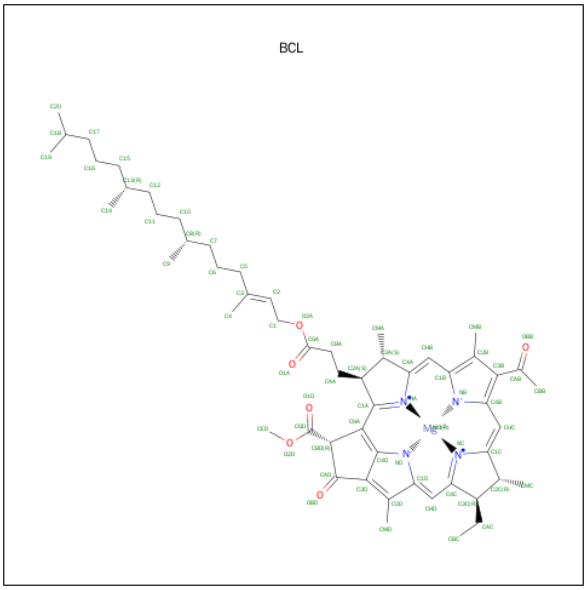
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	M	303	Total	C	N	O	S	0	0	1
			2409	1607	395	397	10			

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



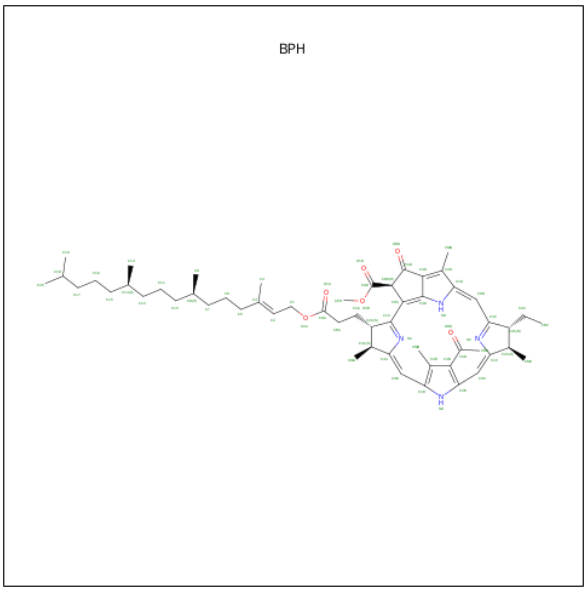
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	H	1	Total C O 6 3 3	0	0
4	H	1	Total C O 6 3 3	0	0
4	H	1	Total C O 6 3 3	0	0
4	L	1	Total C O 6 3 3	0	0

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



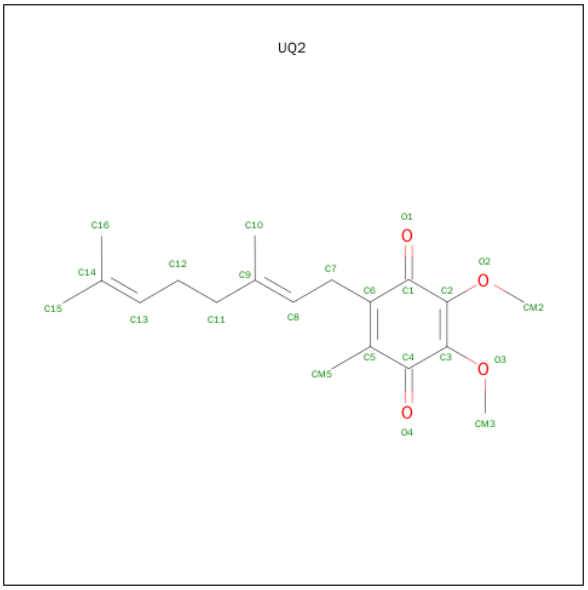
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	L	1	Total C Mg N O 66 55 1 4 6	0	0
5	L	1	Total C Mg N O 66 55 1 4 6	0	0
5	M	1	Total C Mg N O 66 55 1 4 6	0	0
5	M	1	Total C Mg N O 66 55 1 4 6	0	0

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



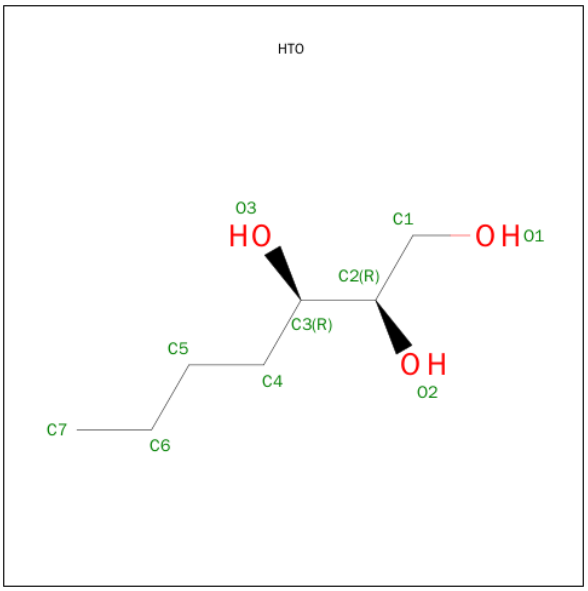
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	L	1	Total	C	N	O	0	0
			65	55	4	6		
6	M	1	Total	C	N	O	0	0
			65	55	4	6		

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



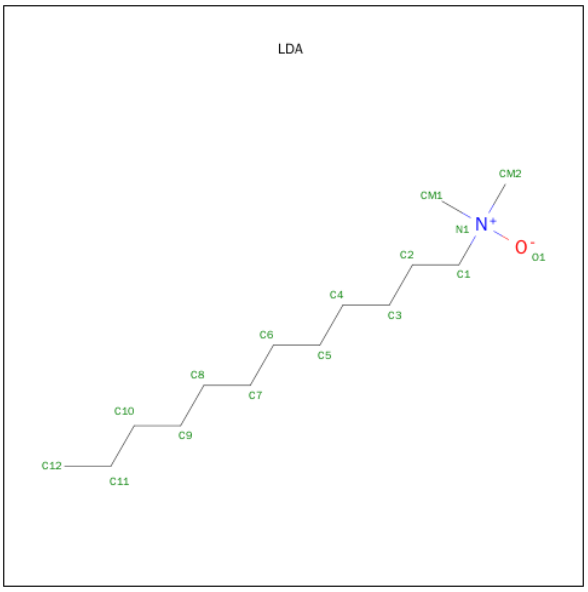
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	L	1	Total	C	O	0	1
			46	38	8		

- Molecule 8 is HEPTANE-1,2,3-TRIOL (three-letter code: HTO) (formula: $C_7H_{16}O_3$).



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

- Molecule 9 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula: $C_{14}H_{31}NO$).



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

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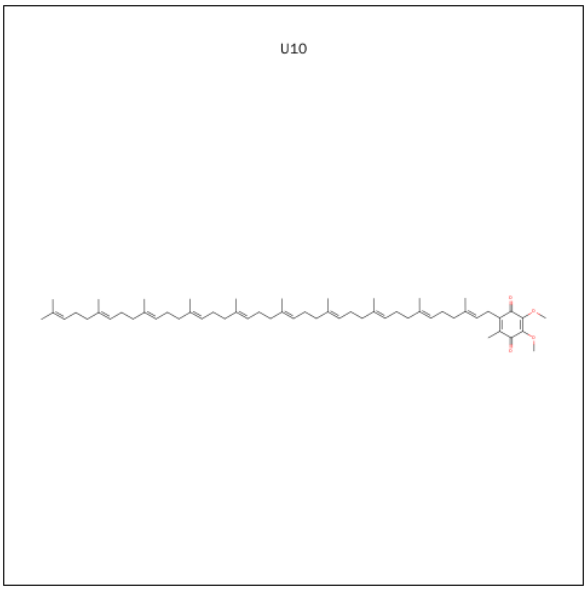
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	M	1	Total	C	N	O	0	0
			16	14	1	1		

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

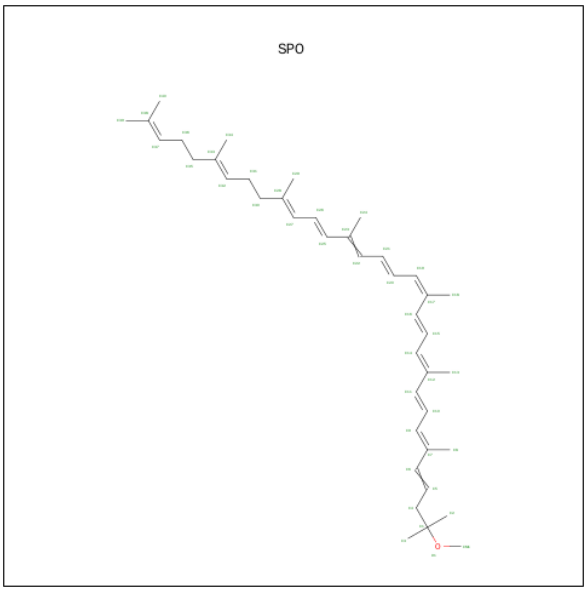
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	M	1	Total	Fe	0	0
			1	1		

- Molecule 11 is UBIQUINONE-10 (three-letter code: U10) (formula: $C_{59}H_{90}O_4$).



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

- Molecule 12 is SPHEROIDENE (three-letter code: SPO) (formula: $C_{41}H_{60}O$).



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

- Molecule 13 is water.

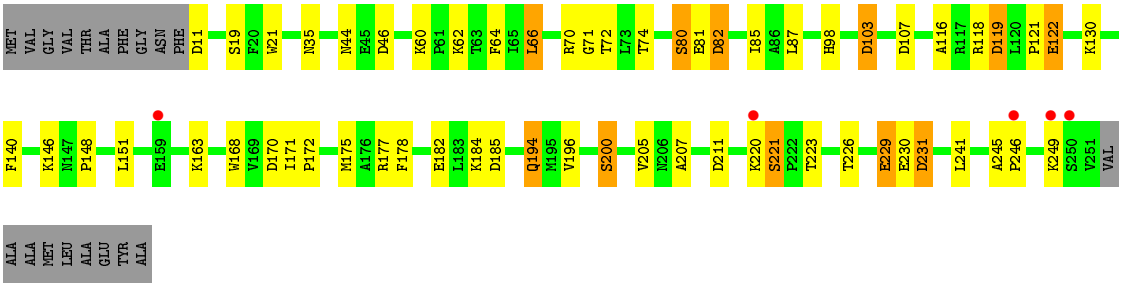
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	H	76	Total O 76 76	0	0
13	L	68	Total O 68 68	0	0
13	M	58	Total O 58 58	0	0

3 Residue-property plots (i)

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

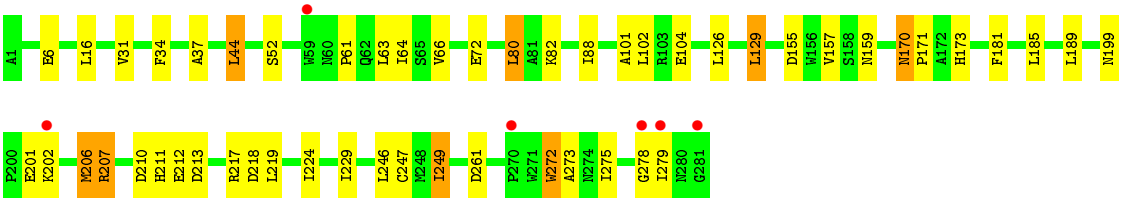
- Molecule 1: REACTION CENTER PROTEIN H CHAIN

Chain H:



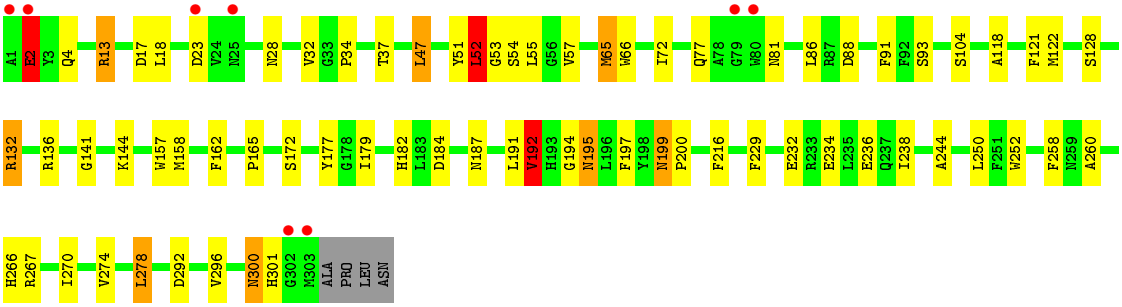
- Molecule 2: REACTION CENTER PROTEIN L CHAIN

Chain L:



- Molecule 3: REACTION CENTER PROTEIN M CHAIN

Chain M:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	139.00Å 139.00Å 183.55Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	119.52 – 2.88 42.91 – 2.88	Depositor EDS
% Data completeness (in resolution range)	81.2 (119.52-2.88) 77.9 (42.91-2.88)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.41 (at 2.86Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.176 , 0.220 0.179 , 0.186	Depositor DCC
R_{free} test set	1905 reflections (5.48%)	DCC
Wilson B-factor (Å^2)	54.3	Xtriage
Anisotropy	0.037	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 66.3	EDS
Estimated twinning fraction	0.029 for -h,-k,l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Outliers	0 of 38278 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	7302	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 2.68% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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, 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	0.83	2/1906 (0.1%)	0.92	7/2591 (0.3%)
2	L	0.80	0/2320	0.82	4/3175 (0.1%)
3	M	0.78	0/2501	0.81	5/3415 (0.1%)
All	All	0.80	2/6727 (0.0%)	0.85	16/9181 (0.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	122	GLU	CG-CD	5.70	1.60	1.51
1	H	194	GLN	CG-CD	5.07	1.62	1.51

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	M	52	LEU	CA-CB-CG	8.47	134.77	115.30
2	L	261	ASP	CB-CG-OD2	7.19	124.77	118.30
1	H	107	ASP	CB-CG-OD2	5.88	123.59	118.30
3	M	23	ASP	CB-CG-OD2	5.83	123.55	118.30
1	H	103	ASP	CB-CG-OD2	5.79	123.51	118.30
1	H	211	ASP	CB-CG-OD2	5.79	123.51	118.30
2	L	155	ASP	CB-CG-OD2	5.75	123.48	118.30
2	L	218	ASP	CB-CG-OD2	5.74	123.47	118.30
1	H	82	ASP	CB-CG-OD2	5.74	123.47	118.30
1	H	231	ASP	CB-CG-OD2	5.73	123.45	118.30
3	M	184	ASP	CB-CG-OD2	5.71	123.44	118.30
1	H	119	ASP	CB-CG-OD2	5.30	123.07	118.30
1	H	185	ASP	CB-CG-OD2	5.23	123.01	118.30
2	L	210	ASP	CB-CG-OD2	5.22	123.00	118.30
3	M	292	ASP	CB-CA-C	-5.16	100.08	110.40
3	M	88	ASP	CB-CG-OD2	5.15	122.94	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	H	1846	0	1861	32	0
2	L	2232	0	2187	35	0
3	M	2409	0	2321	41	0
4	H	18	0	24	3	0
4	L	6	0	8	2	0
5	L	132	0	148	3	0
5	M	132	0	148	13	0
6	L	65	0	76	8	0
6	M	65	0	76	11	0
7	L	46	0	52	14	0
8	L	10	0	16	0	0
9	M	48	0	93	3	0
10	M	1	0	0	0	0
11	M	48	0	63	1	0
12	M	42	0	60	1	0
13	H	76	0	0	3	0
13	L	68	0	0	1	0
13	M	58	0	0	2	0
All	All	7302	0	7133	133	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (133) 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)
6:L:1283:BPH:HHC	6:L:1283:BPH:CBB	1.94	0.97
6:M:1309:BPH:CBB	6:M:1309:BPH:HHC	1.94	0.95
5:M:1303:BCL:H151	5:M:1303:BCL:H91	1.53	0.89
7:L:1284[B]:UQ2:H5M1	7:L:1284[B]:UQ2:C8	2.02	0.88
3:M:197:PHE:HZ	5:M:1304:BCL:HBB2	1.39	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:229:PHE:HB2	3:M:244:ALA:HB2	1.55	0.85
6:L:1283:BPH:HHC	6:L:1283:BPH:HBB2	1.60	0.83
2:L:224:ILE:HG22	7:L:1284[B]:UQ2:C8	2.14	0.78
6:M:1309:BPH:HHC	6:M:1309:BPH:HBB3	1.64	0.78
6:M:1309:BPH:HHD	6:M:1309:BPH:HBC3	1.66	0.78
5:M:1303:BCL:HBC1	5:M:1304:BCL:HAA2	1.66	0.77
9:M:1305:LDA:H101	9:M:1306:LDA:H121	1.65	0.77
3:M:197:PHE:CZ	5:M:1304:BCL:HBB2	2.20	0.77
1:H:122:GLU:HG3	3:M:236:GLU:OE1	1.86	0.74
6:L:1283:BPH:CHC	6:L:1283:BPH:CBB	2.67	0.73
6:L:1283:BPH:HHC	6:L:1283:BPH:HBB3	1.70	0.72
1:H:148:PRO:HA	1:H:151:LEU:HD12	1.72	0.71
6:M:1309:BPH:HBB2	6:M:1309:BPH:HHC	1.73	0.69
3:M:194:GLY:O	3:M:195:ASN:HB3	1.93	0.69
2:L:229:ILE:HG12	7:L:1284[B]:UQ2:H5M2	1.75	0.69
1:H:62:LYS:HE2	1:H:64:PHE:CZ	2.29	0.68
2:L:170:ASN:C	2:L:170:ASN:HD22	1.98	0.67
9:M:1305:LDA:C10	9:M:1306:LDA:H121	2.26	0.66
6:M:1309:BPH:CHC	6:M:1309:BPH:CBB	2.74	0.65
2:L:212:GLU:HB3	7:L:1284[B]:UQ2:H2M3	1.79	0.65
1:H:80:SER:O	13:H:2025:HOH:O	2.15	0.64
1:H:177:ARG:NH2	3:M:232:GLU:OE2	2.31	0.63
3:M:187:ASN:HD22	5:M:1304:BCL:HBC1	1.65	0.62
2:L:88:ILE:HD11	4:L:1287:GOL:H31	1.83	0.60
2:L:157:VAL:HG21	5:L:1282:BCL:HHD	1.83	0.59
1:H:118[B]:ARG:HH11	1:H:119:ASP:H	1.49	0.59
2:L:278:GLY:HA2	3:M:77:GLN:O	2.03	0.59
6:L:1283:BPH:CHC	6:L:1283:BPH:HBB3	2.32	0.58
1:H:62:LYS:HD2	4:H:1251:GOL:H31	1.84	0.57
5:L:1282:BCL:HBB3	5:L:1285:BCL:H41	1.86	0.57
1:H:66:LEU:HG	1:H:71:GLY:O	2.03	0.57
3:M:77:GLN:HE22	3:M:93:SER:H	1.53	0.57
3:M:65:MET:HB3	3:M:121:PHE:CD2	2.40	0.57
2:L:272:TRP:HA	2:L:275:ILE:HD12	1.87	0.56
1:H:87:LEU:HD13	1:H:98:HIS:HB2	1.89	0.55
5:M:1303:BCL:HBB3	5:M:1304:BCL:H41	1.89	0.54
3:M:199:ASN:HD22	3:M:199:ASN:C	2.09	0.54
3:M:53:GLY:O	3:M:57:VAL:HG23	2.07	0.54
1:H:246:PRO:O	1:H:249:LYS:HB2	2.06	0.54
1:H:207:ALA:HA	1:H:241:LEU:HD23	1.90	0.54
5:M:1304:BCL:C2	6:M:1309:BPH:HBB3	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:101:ALA:O	2:L:104:GLU:HB2	2.10	0.52
2:L:212:GLU:CB	7:L:1284[B]:UQ2:H2M3	2.39	0.52
1:H:81:GLU:HG3	1:H:85[B]:ILE:HD11	1.92	0.52
6:M:1309:BPH:CHC	6:M:1309:BPH:HBB3	2.35	0.52
1:H:146:LYS:HE2	1:H:200:SER:O	2.10	0.51
1:H:140:PHE:HA	3:M:13:ARG:O	2.10	0.51
3:M:234:GLU:O	3:M:238:ILE:HG13	2.11	0.51
3:M:296:VAL:O	3:M:300:ASN:ND2	2.44	0.50
2:L:229:ILE:HD13	7:L:1284[B]:UQ2:H111	1.93	0.50
1:H:62:LYS:O	1:H:74:THR:HA	2.12	0.49
5:L:1285:BCL:HBB3	5:L:1285:BCL:HMB1	1.93	0.49
1:H:171:ILE:N	1:H:172:PRO:HD2	2.28	0.49
2:L:189:LEU:HD12	7:L:1284[B]:UQ2:H163	1.94	0.49
3:M:270:ILE:O	3:M:274:VAL:HG13	2.13	0.49
3:M:28:ASN:HB2	3:M:51:TYR:CE2	2.47	0.49
3:M:300:ASN:N	3:M:300:ASN:ND2	2.61	0.48
3:M:194:GLY:O	3:M:195:ASN:CB	2.61	0.48
1:H:81:GLU:O	1:H:82:ASP:HB2	2.14	0.48
1:H:70:ARG:NH2	1:H:121:PRO:O	2.46	0.48
1:H:196:VAL:HG12	1:H:205:VAL:HG22	1.96	0.48
1:H:35:ASN:OD1	3:M:260:ALA:HB1	2.13	0.48
2:L:213:ASP:HB3	2:L:217:ARG:NH1	2.29	0.48
3:M:300:ASN:N	3:M:300:ASN:HD22	2.12	0.47
6:M:1309:BPH:H2	6:M:1309:BPH:H6C2	1.72	0.47
2:L:80:LEU:HD13	4:L:1287:GOL:H11	1.97	0.47
3:M:192:VAL:O	3:M:192:VAL:HG13	2.15	0.47
2:L:275:ILE:HG21	3:M:81:ASN:ND2	2.30	0.46
2:L:212:GLU:OE2	7:L:1284[B]:UQ2:O3	2.33	0.46
1:H:21:TRP:CE2	4:H:1253:GOL:H11	2.51	0.46
6:L:1283:BPH:HBC2	6:L:1283:BPH:HHD	1.96	0.46
5:M:1304:BCL:CBB	5:M:1304:BCL:HHC	2.46	0.46
3:M:66:TRP:HD1	3:M:118:ALA:O	1.99	0.46
6:M:1309:BPH:CHD	6:M:1309:BPH:HBC3	2.43	0.46
7:L:1284[A]:UQ2:H5M1	7:L:1284[A]:UQ2:H71	1.74	0.46
2:L:34:PHE:HA	2:L:37:ALA:HB3	1.98	0.46
4:H:1252:GOL:H31	2:L:199:ASN:HA	1.99	0.45
6:L:1283:BPH:HBC2	6:L:1283:BPH:CHD	2.47	0.45
7:L:1284[B]:UQ2:H2M2	7:L:1284[B]:UQ2:O1	2.16	0.45
2:L:170:ASN:HD22	2:L:171:PRO:N	2.14	0.45
1:H:44:ASN:HB2	1:H:46:ASP:OD1	2.16	0.45
3:M:162:PHE:C	3:M:165:PRO:HD2	2.36	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:1304:BCL:H2	6:M:1309:BPH:HBB3	1.98	0.44
1:H:168:TRP:HB2	1:H:178:PHE:HB2	1.99	0.44
2:L:61:PRO:HA	2:L:64:ILE:HD12	1.99	0.44
3:M:2:GLU:H	3:M:4:GLN:HE21	1.65	0.44
6:L:1283:BPH:HED3	3:M:252:TRP:CZ3	2.53	0.44
1:H:130:LYS:HE3	1:H:170:ASP:OD2	2.18	0.44
3:M:252:TRP:CD1	11:M:1310:U10:C6	3.00	0.44
1:H:148:PRO:HA	1:H:151:LEU:CD1	2.44	0.43
1:H:194:GLN:NE2	13:H:2062:HOH:O	2.15	0.43
3:M:177:TYR:HD2	12:M:1311:SPO:H19	1.83	0.43
1:H:226:THR:OG1	1:H:229:GLU:HB2	2.18	0.43
1:H:118[B]:ARG:NH1	1:H:119:ASP:H	2.16	0.43
5:M:1303:BCL:HMB1	5:M:1303:BCL:OBB	2.18	0.43
3:M:157:TRP:CE3	3:M:158:MET:HG2	2.53	0.43
3:M:278:LEU:HA	3:M:278:LEU:HD23	1.89	0.43
2:L:229:ILE:HD13	7:L:1284[B]:UQ2:H8	2.01	0.43
2:L:219:LEU:O	3:M:132:ARG:NH1	2.52	0.42
7:L:1284[B]:UQ2:H101	7:L:1284[B]:UQ2:H122	1.77	0.42
2:L:207:ARG:HG3	2:L:211:HIS:CD2	2.54	0.42
2:L:44:LEU:HD23	2:L:44:LEU:HA	1.95	0.42
5:M:1303:BCL:H102	5:M:1303:BCL:H13	1.74	0.42
5:M:1304:BCL:CBB	5:M:1304:BCL:CHC	2.97	0.42
1:H:249:LYS:N	13:H:2076:HOH:O	2.52	0.42
5:M:1303:BCL:H162	5:M:1303:BCL:H141	1.75	0.42
3:M:66:TRP:CZ2	3:M:122:MET:CE	3.03	0.42
2:L:201:GLU:OE2	3:M:141:GLY:HA2	2.19	0.42
2:L:129:LEU:HD12	2:L:129:LEU:HA	1.82	0.42
3:M:199:ASN:HA	3:M:200:PRO:HD2	1.95	0.42
2:L:159:ASN:HD22	2:L:159:ASN:HA	1.70	0.42
9:M:1307:LDA:HM13	13:M:2013:HOH:O	2.19	0.42
7:L:1284[B]:UQ2:H5M1	7:L:1284[B]:UQ2:H8	1.96	0.41
2:L:170:ASN:C	2:L:170:ASN:ND2	2.70	0.41
2:L:249:ILE:HA	2:L:249:ILE:HD13	1.87	0.41
2:L:170:ASN:HB3	2:L:173:HIS:CB	2.50	0.41
1:H:175:MET:HE3	13:M:2005:HOH:O	2.20	0.41
2:L:170:ASN:HA	2:L:171:PRO:HD2	1.91	0.41
1:H:220[B]:LYS:NZ	1:H:221:SER:HB3	2.35	0.41
3:M:234:GLU:OE2	3:M:266:HIS:HE1	2.02	0.41
13:L:2058:HOH:O	3:M:136:ARG:HD3	2.21	0.41
2:L:279:ILE:HG21	3:M:91:PHE:HB3	2.03	0.41
2:L:224:ILE:HG22	7:L:1284[B]:UQ2:H8	1.96	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:55:LEU:HD22	3:M:128:SER:HB2	2.03	0.40
2:L:181:PHE:CD2	6:M:1309:BPH:HBB1	2.55	0.40
3:M:34:PRO:O	3:M:47:LEU:HB2	2.20	0.40
2:L:6:GLU:HA	3:M:250:LEU:HD11	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	242/260 (93%)	226 (93%)	14 (6%)	2 (1%)	24	58
2	L	279/281 (99%)	265 (95%)	11 (4%)	3 (1%)	17	49
3	M	301/307 (98%)	277 (92%)	19 (6%)	5 (2%)	11	36
All	All	822/848 (97%)	768 (93%)	44 (5%)	10 (1%)	16	46

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	M	2	GLU
3	M	52	LEU
1	H	116	ALA
2	L	273	ALA
1	H	245	ALA
2	L	206	MET
2	L	31	VAL
3	M	195	ASN
3	M	179	ILE
3	M	192	VAL

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%)	182 (92%)	16 (8%)	15 38
2	L	220/220 (100%)	200 (91%)	20 (9%)	12 31
3	M	236/240 (98%)	210 (89%)	26 (11%)	8 21
All	All	654/668 (98%)	592 (90%)	62 (10%)	11 29

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	11	ASP
1	H	19	SER
1	H	60	LYS
1	H	66	LEU
1	H	72	THR
1	H	80	SER
1	H	103	ASP
1	H	163	LYS
1	H	182	GLU
1	H	184	LYS
1	H	200	SER
1	H	221	SER
1	H	223	THR
1	H	229	GLU
1	H	230	GLU
1	H	231	ASP
2	L	16	LEU
2	L	44	LEU
2	L	52	SER
2	L	63	LEU
2	L	66	VAL
2	L	72	GLU
2	L	80	LEU
2	L	82	LYS
2	L	102	LEU
2	L	126	LEU

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Mol	Chain	Res	Type
2	L	129	LEU
2	L	170	ASN
2	L	185	LEU
2	L	202	LYS
2	L	206	MET
2	L	207	ARG
2	L	246	LEU
2	L	247	CYS
2	L	249	ILE
2	L	272	TRP
3	M	2	GLU
3	M	13	ARG
3	M	17	ASP
3	M	18	LEU
3	M	32	VAL
3	M	37	THR
3	M	47	LEU
3	M	52	LEU
3	M	54	SER
3	M	65	MET
3	M	72	ILE
3	M	86	LEU
3	M	104	SER
3	M	132	ARG
3	M	144	LYS
3	M	172	SER
3	M	182	HIS
3	M	191	LEU
3	M	192	VAL
3	M	199	ASN
3	M	216	PHE
3	M	258	PHE
3	M	267	ARG
3	M	278	LEU
3	M	300	ASN
3	M	301	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	98	HIS
2	L	62	GLN

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Mol	Chain	Res	Type
2	L	159	ASN
2	L	170	ASN
2	L	264	GLN
3	M	4	GLN
3	M	77	GLN
3	M	187	ASN
3	M	193	HIS
3	M	199	ASN
3	M	300	ASN

5.3.3 RNA

There are no RNA molecules 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 19 ligands modelled in this entry, 1 is monoatomic - leaving 18 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	0.55	0	5,5,5	0.70	0
4	GOL	H	1252	-	5,5,5	0.22	0	5,5,5	0.55	0
4	GOL	H	1253	-	5,5,5	0.35	0	5,5,5	0.42	0
5	BCL	L	1282	2	53,74,74	2.23	6 (11%)	57,115,115	2.28	14 (24%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	BPH	L	1283	-	64,70,70	3.01	17 (26%)	73,101,101	1.84	18 (24%)
7	UQ2	L	1284[A]	-	23,23,23	2.90	8 (34%)	28,31,31	1.31	3 (10%)
7	UQ2	L	1284[B]	-	23,23,23	2.72	7 (30%)	28,31,31	1.39	5 (17%)
5	BCL	L	1285	2	53,74,74	2.01	8 (15%)	57,115,115	2.12	15 (26%)
8	HTO	L	1286	-	9,9,9	0.87	1 (11%)	8,10,10	1.39	2 (25%)
4	GOL	L	1287	-	5,5,5	0.38	0	5,5,5	0.44	0
5	BCL	M	1303	3	53,74,74	2.16	6 (11%)	57,115,115	2.00	14 (24%)
5	BCL	M	1304	3	53,74,74	2.07	6 (11%)	57,115,115	2.05	15 (26%)
9	LDA	M	1305	-	15,15,15	3.72	1 (6%)	16,17,17	1.30	2 (12%)
9	LDA	M	1306	-	15,15,15	3.51	2 (13%)	16,17,17	0.91	1 (6%)
9	LDA	M	1307	-	15,15,15	3.82	1 (6%)	16,17,17	0.65	0
6	BPH	M	1309	-	64,70,70	2.89	17 (26%)	73,101,101	2.08	15 (20%)
11	U10	M	1310	-	48,48,63	3.13	13 (27%)	58,61,79	1.81	11 (18%)
12	SPO	M	1311	-	40,41,41	4.24	12 (30%)	45,50,50	2.00	12 (26%)

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
4	GOL	H	1253	-	-	0/4/4/4	0/0/0/0
5	BCL	L	1282	2	2/2/21/25	0/37/137/137	0/0/9/9
6	BPH	L	1283	-	-	0/54/105/105	0/1/6/6
7	UQ2	L	1284[A]	-	-	0/15/39/39	0/1/1/1
7	UQ2	L	1284[B]	-	-	0/15/39/39	0/1/1/1
5	BCL	L	1285	2	2/2/21/25	0/37/137/137	0/0/9/9
8	HTO	L	1286	-	-	0/10/10/10	0/0/0/0
4	GOL	L	1287	-	-	0/4/4/4	0/0/0/0
5	BCL	M	1303	3	2/2/21/25	0/37/137/137	0/0/9/9
5	BCL	M	1304	3	2/2/21/25	0/37/137/137	0/0/9/9
9	LDA	M	1305	-	-	0/13/13/13	0/0/0/0
9	LDA	M	1306	-	-	0/13/13/13	0/0/0/0
9	LDA	M	1307	-	-	0/13/13/13	0/0/0/0
6	BPH	M	1309	-	-	0/54/105/105	0/1/6/6
11	U10	M	1310	-	-	0/45/69/87	0/1/1/1
12	SPO	M	1311	-	-	0/47/47/47	0/0/0/0

All (105) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	M	1307	LDA	O1-N1	-14.61	1.25	1.39
9	M	1305	LDA	O1-N1	-14.19	1.26	1.39
9	M	1306	LDA	O1-N1	-13.31	1.26	1.39
7	L	1284[A]	UQ2	O3-C3	-4.98	1.23	1.37
11	M	1310	U10	O3-C3	-4.46	1.25	1.37
7	L	1284[B]	UQ2	O2-C2	-4.45	1.25	1.37
7	L	1284[A]	UQ2	O2-C2	-4.39	1.25	1.37
7	L	1284[B]	UQ2	O3-C3	-4.27	1.25	1.37
11	M	1310	U10	O4-C4	-3.96	1.26	1.37
6	M	1309	BPH	C3D-C4D	-3.92	1.36	1.41
6	M	1309	BPH	O2D-CGD	-3.60	1.23	1.33
6	L	1283	BPH	C3D-CAD	-3.43	1.39	1.46
5	M	1303	BCL	O2D-CGD	-3.13	1.25	1.33
6	M	1309	BPH	C1B-C2B	-3.03	1.39	1.45
6	M	1309	BPH	C3D-CAD	-2.86	1.41	1.46
6	L	1283	BPH	O2D-CGD	-2.80	1.26	1.33
7	L	1284[A]	UQ2	C3-C4	-2.67	1.41	1.48
6	L	1283	BPH	C3D-C4D	-2.61	1.38	1.41
7	L	1284[B]	UQ2	C3-C4	-2.59	1.41	1.48
6	L	1283	BPH	C1C-NC	-2.48	1.31	1.37
6	M	1309	BPH	O2A-CGA	-2.47	1.25	1.33
11	M	1310	U10	C4-C5	-2.47	1.41	1.48
7	L	1284[A]	UQ2	C2-C1	-2.46	1.41	1.48
6	L	1283	BPH	C1B-C2B	-2.43	1.40	1.45
9	M	1306	LDA	C1-N1	-2.42	1.47	1.51
5	L	1285	BCL	O2A-CGA	-2.42	1.26	1.33
5	L	1282	BCL	O2D-CGD	-2.38	1.27	1.33
5	L	1285	BCL	C3D-CAD	-2.37	1.39	1.45
5	M	1304	BCL	O2A-CGA	-2.35	1.26	1.33
5	M	1304	BCL	O2D-CGD	-2.32	1.27	1.33
7	L	1284[B]	UQ2	C2-C1	-2.29	1.42	1.48
5	M	1303	BCL	C3D-CAD	-2.22	1.39	1.45
5	M	1303	BCL	C3C-C4C	-2.20	1.48	1.51
11	M	1310	U10	C3-C2	-2.19	1.42	1.48
5	L	1282	BCL	C3D-CAD	-2.17	1.39	1.45
5	L	1285	BCL	O2D-CGD	-2.11	1.27	1.33
5	L	1282	BCL	O2A-CGA	-2.10	1.26	1.33
5	M	1304	BCL	C3D-CAD	-2.09	1.39	1.45
11	M	1310	U10	C6-C5	-2.01	1.40	1.46
7	L	1284[A]	UQ2	C7-C6	2.02	1.55	1.51
11	M	1310	U10	C6-C1	2.07	1.40	1.35
8	L	1286	HTO	C4-C3	2.13	1.56	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	L	1285	BCL	O1D-CGD	2.25	1.26	1.21
5	L	1285	BCL	CHD-C4C	2.36	1.48	1.41
7	L	1284[B]	UQ2	C6-C5	2.58	1.41	1.35
6	L	1283	BPH	C1D-CHD	2.81	1.51	1.40
7	L	1284[A]	UQ2	C6-C5	2.92	1.42	1.35
6	M	1309	BPH	C1D-CHD	2.93	1.51	1.40
6	M	1309	BPH	CHB-C4A	3.01	1.46	1.40
5	M	1304	BCL	C2-C3	3.30	1.39	1.33
6	L	1283	BPH	CHB-C4A	3.31	1.46	1.40
6	L	1283	BPH	CHD-C4C	3.43	1.46	1.38
6	M	1309	BPH	CHD-C4C	3.49	1.47	1.38
6	M	1309	BPH	CHC-C4B	3.54	1.49	1.40
6	L	1283	BPH	CHC-C4B	3.61	1.49	1.40
6	M	1309	BPH	CHC-C1C	3.84	1.44	1.36
5	L	1282	BCL	C2-C3	4.01	1.40	1.33
6	L	1283	BPH	C3D-C2D	4.04	1.49	1.40
12	M	1311	SPO	C21-C20	4.18	1.47	1.35
6	L	1283	BPH	CHC-C1C	4.50	1.45	1.36
12	M	1311	SPO	C15-C16	4.54	1.46	1.34
6	M	1309	BPH	C3D-C2D	4.62	1.51	1.40
5	L	1285	BCL	C2-C3	4.64	1.42	1.33
5	M	1303	BCL	C2-C3	4.69	1.42	1.33
12	M	1311	SPO	C10-C11	4.98	1.47	1.34
12	M	1311	SPO	C26-C25	4.99	1.47	1.34
7	L	1284[B]	UQ2	C13-C14	5.42	1.48	1.32
12	M	1311	SPO	C37-C38	5.44	1.49	1.32
12	M	1311	SPO	C6-C5	5.49	1.47	1.31
6	L	1283	BPH	CHB-C1B	5.57	1.49	1.38
7	L	1284[A]	UQ2	C13-C14	5.60	1.49	1.32
5	M	1304	BCL	O1A-CGA	5.69	1.39	1.22
5	L	1285	BCL	O1A-CGA	5.75	1.39	1.22
6	M	1309	BPH	CHB-C1B	5.82	1.50	1.38
5	M	1303	BCL	O1A-CGA	5.95	1.40	1.22
11	M	1310	U10	C38-C39	6.02	1.50	1.32
5	L	1282	BCL	O1A-CGA	6.24	1.41	1.22
6	L	1283	BPH	O1A-CGA	6.36	1.41	1.22
6	M	1309	BPH	O1A-CGA	6.45	1.41	1.22
6	M	1309	BPH	C2-C3	7.16	1.47	1.33
11	M	1310	U10	C8-C9	7.20	1.47	1.33
11	M	1310	U10	C23-C24	7.26	1.47	1.33
11	M	1310	U10	C18-C19	7.53	1.47	1.33
6	L	1283	BPH	C2-C3	7.72	1.48	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	M	1310	U10	C13-C14	7.89	1.48	1.33
6	M	1309	BPH	O1D-CGD	8.09	1.41	1.21
12	M	1311	SPO	C32-C33	8.10	1.48	1.33
6	L	1283	BPH	O1D-CGD	8.15	1.41	1.21
11	M	1310	U10	C28-C29	8.18	1.49	1.33
7	L	1284[B]	UQ2	C8-C9	8.18	1.49	1.33
12	M	1311	SPO	C19-C17	8.26	1.46	1.35
6	L	1283	BPH	OBB-CAB	8.30	1.41	1.23
11	M	1310	U10	C33-C34	8.38	1.49	1.33
6	M	1309	BPH	OBB-CAB	8.50	1.41	1.23
7	L	1284[A]	UQ2	C8-C9	8.59	1.49	1.33
12	M	1311	SPO	C9-C7	9.01	1.47	1.35
12	M	1311	SPO	C22-C23	9.25	1.48	1.35
12	M	1311	SPO	C14-C12	9.36	1.48	1.35
6	M	1309	BPH	OBD-CAD	10.75	1.38	1.22
5	L	1285	BCL	OBD-CAD	10.86	1.38	1.22
5	M	1304	BCL	OBD-CAD	12.03	1.40	1.22
5	M	1303	BCL	OBD-CAD	12.14	1.40	1.22
6	L	1283	BPH	OBD-CAD	13.01	1.42	1.22
12	M	1311	SPO	C27-C28	13.05	1.48	1.34
5	L	1282	BCL	OBD-CAD	13.15	1.42	1.22

All (127) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	M	1309	BPH	OBD-CAD-CBD	-8.26	113.48	125.94
5	L	1285	BCL	CMB-C2B-C1B	-6.40	117.78	128.36
5	L	1282	BCL	CMB-C2B-C1B	-6.28	117.98	128.36
5	M	1304	BCL	CMB-C2B-C1B	-6.10	118.27	128.36
5	L	1282	BCL	C1D-CHD-C4C	-5.96	116.98	126.07
5	L	1285	BCL	CHB-C4A-NA	-5.69	116.64	124.51
5	M	1303	BCL	CMB-C2B-C1B	-5.40	119.43	128.36
5	M	1304	BCL	C1D-CHD-C4C	-5.22	118.10	126.07
12	M	1311	SPO	C21-C22-C23	-5.13	119.79	127.20
11	M	1310	U10	C32-C33-C34	-4.88	117.15	127.76
6	M	1309	BPH	O2D-CGD-O1D	-4.80	113.87	123.79
5	L	1282	BCL	CHD-C4C-NC	-4.68	119.62	125.06
12	M	1311	SPO	C20-C19-C17	-4.67	120.46	127.20
5	M	1303	BCL	O1D-CGD-CBD	-4.65	117.96	124.62
5	L	1285	BCL	C1D-CHD-C4C	-4.50	119.19	126.07
12	M	1311	SPO	C10-C9-C7	-4.47	120.74	127.20
6	L	1283	BPH	CMD-C2D-C3D	-4.45	116.38	125.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	M	1311	SPO	C15-C14-C12	-4.38	120.87	127.20
5	M	1303	BCL	C1D-CHD-C4C	-4.34	119.45	126.07
11	M	1310	U10	C17-C18-C19	-3.95	119.18	127.76
6	M	1309	BPH	CHC-C4B-NB	-3.92	117.45	124.91
6	L	1283	BPH	O1D-CGD-CBD	-3.80	119.18	124.62
5	L	1282	BCL	O1D-CGD-CBD	-3.79	119.19	124.62
6	M	1309	BPH	CMD-C2D-C3D	-3.64	117.97	125.09
11	M	1310	U10	C22-C23-C24	-3.63	119.87	127.76
6	M	1309	BPH	CAC-C3C-C2C	-3.34	105.74	114.13
5	L	1282	BCL	CHC-C1C-NC	-3.33	119.90	124.51
6	L	1283	BPH	OBD-CAD-CBD	-3.32	120.92	125.94
9	M	1305	LDA	O1-N1-CM1	-3.24	104.72	109.05
6	L	1283	BPH	OBD-CAD-C3D	-3.20	121.81	128.35
5	L	1285	BCL	CHA-C1A-NA	-3.12	118.38	126.06
5	M	1304	BCL	CMD-C2D-C3D	-3.10	119.02	125.09
5	M	1304	BCL	CHD-C4C-NC	-3.04	121.53	125.06
5	L	1282	BCL	O2D-CGD-O1D	-2.97	117.66	123.79
5	M	1303	BCL	CHB-C4A-NA	-2.94	120.44	124.51
6	L	1283	BPH	CHB-C1B-NB	-2.94	119.18	124.66
9	M	1305	LDA	O1-N1-CM2	-2.92	105.15	109.05
12	M	1311	SPO	C4-C5-C6	-2.88	120.56	124.67
6	M	1309	BPH	OBD-CAD-C3D	-2.81	122.63	128.35
5	M	1304	BCL	CHB-C4A-NA	-2.80	120.63	124.51
5	M	1303	BCL	OBB-CAB-C3B	-2.79	115.58	120.00
5	M	1303	BCL	CHA-C1A-NA	-2.79	119.19	126.06
11	M	1310	U10	C25-C24-C23	-2.77	118.07	123.50
11	M	1310	U10	C27-C28-C29	-2.65	122.01	127.76
5	M	1303	BCL	CAA-C2A-C3A	-2.60	105.73	113.22
6	M	1309	BPH	CMA-C3A-C4A	-2.59	104.56	113.01
5	M	1304	BCL	C3C-C4C-CHD	-2.57	117.59	123.33
5	L	1282	BCL	C11-C10-C8	-2.55	107.02	115.49
12	M	1311	SPO	C18-C17-C19	-2.55	119.14	122.90
5	L	1285	BCL	CMD-C2D-C3D	-2.53	120.13	125.09
12	M	1311	SPO	C8-C7-C9	-2.51	119.19	122.90
6	L	1283	BPH	C1C-NC-C4C	-2.50	107.87	110.44
6	L	1283	BPH	C1B-NB-C4B	-2.49	101.59	106.51
5	M	1304	BCL	CHA-C1A-NA	-2.49	119.94	126.06
5	M	1303	BCL	CHC-C1C-NC	-2.48	121.08	124.51
5	M	1304	BCL	C4-C3-C2	-2.46	118.67	123.50
7	L	1284[A]	UQ2	C5-C6-C1	-2.45	117.32	120.12
5	L	1285	BCL	CHC-C1C-NC	-2.45	121.13	124.51
5	M	1304	BCL	O1D-CGD-CBD	-2.42	121.16	124.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	L	1282	BCL	CMD-C2D-C3D	-2.39	120.41	125.09
5	L	1282	BCL	CHA-C1A-NA	-2.32	120.34	126.06
5	L	1285	BCL	OBB-CAB-C3B	-2.32	116.33	120.00
5	L	1285	BCL	O2D-CGD-O1D	-2.30	119.05	123.79
5	M	1304	BCL	O2A-CGA-O1A	-2.30	117.56	123.49
5	L	1285	BCL	O2A-CGA-O1A	-2.28	117.60	123.49
5	M	1304	BCL	CBA-CAA-C2A	-2.27	107.33	113.73
5	M	1303	BCL	C3C-C4C-CHD	-2.23	118.36	123.33
6	L	1283	BPH	CAA-C2A-C1A	-2.23	107.00	112.86
11	M	1310	U10	C7-C8-C9	-2.21	122.96	126.70
5	L	1285	BCL	C3C-C4C-CHD	-2.17	118.50	123.33
6	L	1283	BPH	C3B-C2B-C1B	-2.13	102.35	105.77
6	M	1309	BPH	O2A-CGA-O1A	-2.13	118.00	123.49
6	L	1283	BPH	CHC-C4B-NB	-2.10	120.91	124.91
11	M	1310	U10	C35-C34-C33	-2.10	119.38	123.50
6	M	1309	BPH	C4-C3-C2	-2.10	119.39	123.50
7	L	1284[B]	UQ2	C10-C9-C8	-2.02	119.55	123.50
5	M	1303	BCL	OBD-CAD-CBD	-2.01	122.90	125.94
5	M	1303	BCL	CHD-C4C-NC	2.00	127.38	125.06
12	M	1311	SPO	C8-C7-C6	2.01	121.43	118.10
6	M	1309	BPH	C3D-CAD-CBD	2.01	110.43	107.60
7	L	1284[B]	UQ2	O2-C2-C1	2.03	122.87	116.41
12	M	1311	SPO	O1-C1-C4	2.05	110.88	105.87
5	L	1282	BCL	O2A-CGA-CBA	2.10	118.28	111.90
12	M	1311	SPO	C40-C38-C39	2.10	119.79	114.64
9	M	1306	LDA	CM2-N1-CM1	2.12	111.23	108.83
5	L	1285	BCL	C4-C3-C5	2.16	118.70	115.41
11	M	1310	U10	C35-C34-C36	2.21	118.78	115.41
12	M	1311	SPO	C34-C33-C35	2.31	118.94	115.41
7	L	1284[B]	UQ2	CM3-O3-C3	2.39	125.11	116.61
6	L	1283	BPH	C2D-C1D-ND	2.39	114.21	110.29
7	L	1284[A]	UQ2	C10-C9-C11	2.41	119.09	115.41
6	M	1309	BPH	O2A-CGA-CBA	2.43	119.31	111.90
6	L	1283	BPH	CMB-C2B-C1B	2.46	129.07	125.06
5	L	1282	BCL	C4A-NA-C1A	2.50	109.59	106.36
7	L	1284[B]	UQ2	CM2-O2-C2	2.66	126.07	116.61
6	M	1309	BPH	C4-C3-C5	2.68	119.50	115.41
8	L	1286	HTO	C5-C4-C3	2.69	119.02	114.20
7	L	1284[A]	UQ2	C7-C6-C1	2.70	121.73	118.56
5	L	1282	BCL	C4-C3-C5	2.76	119.62	115.41
8	L	1286	HTO	O3-C3-C4	2.82	115.62	109.35
6	L	1283	BPH	O2A-CGA-CBA	2.85	120.59	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	M	1303	BCL	CMB-C2B-C3B	2.89	130.74	125.09
6	L	1283	BPH	C3C-C4C-NC	3.01	110.95	107.93
5	M	1303	BCL	O2A-CGA-CBA	3.05	121.18	111.90
7	L	1284[B]	UQ2	C10-C9-C11	3.19	120.28	115.41
12	M	1311	SPO	C29-C28-C30	3.22	120.33	115.41
5	M	1304	BCL	C4-C3-C5	3.46	120.69	115.41
5	M	1304	BCL	O2A-CGA-CBA	3.51	122.58	111.90
6	M	1309	BPH	C3C-C4C-NC	3.58	111.52	107.93
6	L	1283	BPH	CED-O2D-CGD	3.66	124.58	115.99
6	L	1283	BPH	C2B-C1B-NB	3.79	115.41	109.73
11	M	1310	U10	C30-C29-C31	3.83	121.25	115.41
6	M	1309	BPH	C2B-C1B-NB	3.87	115.53	109.73
5	L	1285	BCL	O2A-CGA-CBA	3.91	123.80	111.90
5	L	1282	BCL	CMB-C2B-C3B	3.96	132.84	125.09
5	L	1285	BCL	O2D-CGD-CBD	4.05	116.86	111.30
11	M	1310	U10	C25-C24-C26	4.20	121.83	115.41
6	L	1283	BPH	C4-C3-C5	4.21	121.84	115.41
5	L	1285	BCL	CMB-C2B-C3B	4.25	133.40	125.09
5	L	1285	BCL	CED-O2D-CGD	4.34	126.17	115.99
5	M	1304	BCL	CMB-C2B-C3B	4.44	133.78	125.09
11	M	1310	U10	C10-C9-C11	4.53	122.32	115.41
5	M	1304	BCL	O2D-CGD-CBD	5.09	118.29	111.30
6	L	1283	BPH	O2D-CGD-CBD	5.38	118.68	111.30
5	M	1303	BCL	O2D-CGD-CBD	7.92	122.17	111.30
6	M	1309	BPH	O2D-CGD-CBD	8.12	122.44	111.30
5	L	1282	BCL	O2D-CGD-CBD	8.64	123.15	111.30

All (8) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	M	1304	BCL	C8
5	M	1304	BCL	C13
5	L	1282	BCL	C8
5	L	1282	BCL	C13
5	M	1303	BCL	C8
5	M	1303	BCL	C13
5	L	1285	BCL	C8
5	L	1285	BCL	C13

There are no torsion outliers.

There are no ring outliers.

17 monomers are involved in 57 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	H	1251	GOL	1	0
4	H	1252	GOL	1	0
4	H	1253	GOL	1	0
5	L	1282	BCL	2	0
6	L	1283	BPH	8	0
7	L	1284[A]	UQ2	1	0
7	L	1284[B]	UQ2	13	0
5	L	1285	BCL	2	0
4	L	1287	GOL	2	0
5	M	1303	BCL	6	0
5	M	1304	BCL	9	0
9	M	1305	LDA	2	0
9	M	1306	LDA	2	0
9	M	1307	LDA	1	0
6	M	1309	BPH	11	0
11	M	1310	U10	1	0
12	M	1311	SPO	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	5 (2%)	67	63	36, 51, 66, 102	0
2	L	281/281 (100%)	-0.66	6 (2%)	67	63	32, 44, 69, 84	0
3	M	303/307 (98%)	-0.45	8 (2%)	59	55	34, 51, 76, 104	0
All	All	825/848 (97%)	-0.52	19 (2%)	64	60	32, 49, 72, 104	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	M	1	ALA	4.2
2	L	281	GLY	3.6
1	H	249	LYS	3.5
1	H	220[A]	LYS	3.4
1	H	250	SER	3.3
3	M	302	GLY	3.0
2	L	279	ILE	3.0
3	M	79	GLY	3.0
3	M	303	MET	2.9
2	L	202	LYS	2.9
2	L	59	TRP	2.9
3	M	23	ASP	2.8
3	M	25	ASN	2.5
3	M	2	GLU	2.4
1	H	159	GLU	2.3
1	H	246	PRO	2.3
3	M	80	TRP	2.3
2	L	278	GLY	2.1
2	L	270	PRO	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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
4	GOL	H	1251	6/6	0.82	0.40	16.88	69,77,81,82	0
8	HTO	L	1286	10/10	0.88	0.48	13.85	71,83,83,84	0
7	UQ2	L	1284[A]	23/23	0.85	0.32	11.25	51,59,74,74	23
4	GOL	L	1287	6/6	0.86	0.48	9.74	85,86,86,87	0
7	UQ2	L	1284[B]	23/23	0.85	0.32	7.54	31,35,43,45	23
9	LDA	M	1307	16/16	0.84	0.31	6.24	98,102,114,115	0
9	LDA	M	1305	16/16	0.87	0.26	6.23	74,83,86,87	0
4	GOL	H	1252	6/6	0.87	0.41	4.35	81,84,85,87	0
9	LDA	M	1306	16/16	0.91	0.26	4.04	49,62,72,72	0
12	SPO	M	1311	42/42	0.96	0.26	3.10	47,59,82,85	0
6	BPH	M	1309	65/65	0.94	0.21	2.57	39,48,109,110	0
11	U10	M	1310	48/63	0.92	0.22	2.39	42,52,81,82	0
5	BCL	M	1304	66/66	0.98	0.16	1.21	32,40,59,68	0
6	BPH	L	1283	65/65	0.97	0.15	0.93	25,35,53,55	0
5	BCL	L	1285	66/66	0.98	0.14	0.59	30,37,55,60	0
5	BCL	M	1303	66/66	0.98	0.15	0.32	29,41,93,96	0
5	BCL	L	1282	66/66	0.98	0.13	0.15	31,40,64,75	0
10	FE	M	1308	1/1	0.99	0.07	-2.99	41,41,41,41	0
4	GOL	H	1253	6/6	0.68	0.47	-	113,114,115,116	0

6.5 Other polymers (i)

There are no such residues in this entry.