



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:49 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 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 (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

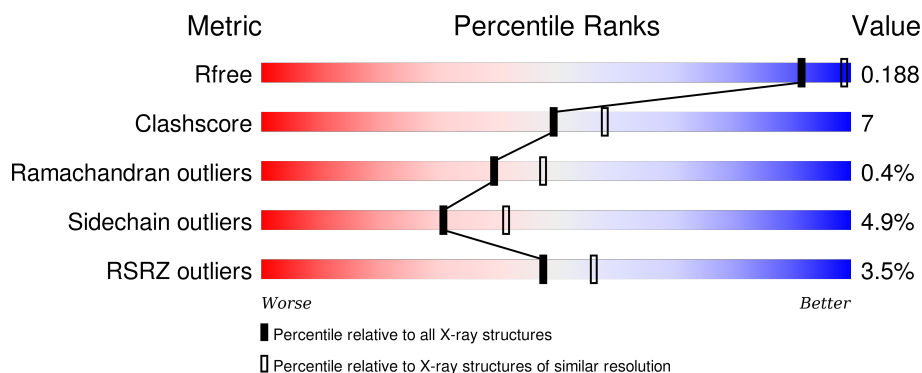
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

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}	91344	4425 (2.34-2.30)
Clashscore	102246	5057 (2.34-2.30)
Ramachandran outliers	100387	5008 (2.34-2.30)
Sidechain outliers	100360	5007 (2.34-2.30)
RSRZ outliers	91569	4432 (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. 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	
2	L	281	
3	M	307	

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	1291	-	-	-	X
13	SPO	M	1313	-	-	-	X
14	CDL	M	1314	-	-	-	X
4	GOL	H	1251	-	-	-	X
4	GOL	L	1293	-	-	-	X
5	BCL	L	1282	X	-	-	-
5	BCL	L	1289	X	-	-	-
5	BCL	M	1303	X	-	-	-
5	BCL	M	1304	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
8	UQ2	L	1288[A]	-	-	-	X
8	UQ2	L	1288[B]	-	-	-	X

2 Entry composition [i](#)

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

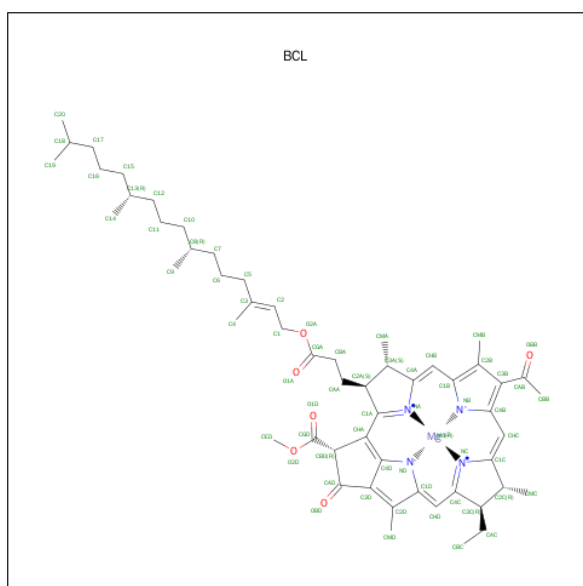
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	M	303	Total	C	N	O	S	0	0	1
			2409	1607	395	397	10			

- 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	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		

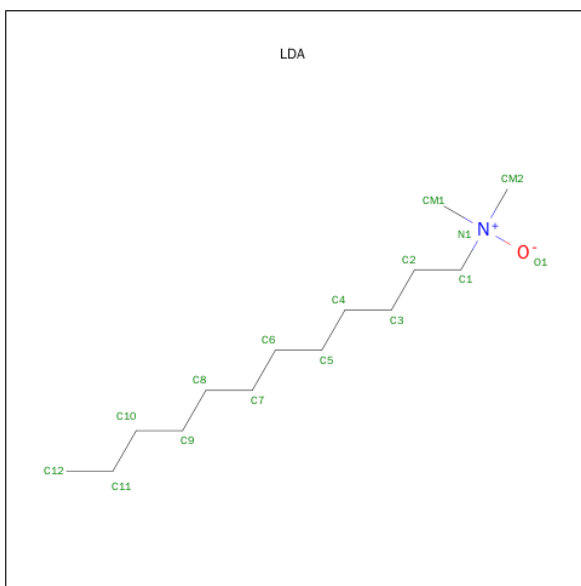
- Molecule 5 is BACTERIOCHLOROPHYLL A (three-letter code: BCL) (formula: $C_{55}H_{74}MgN_4O_6$).



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

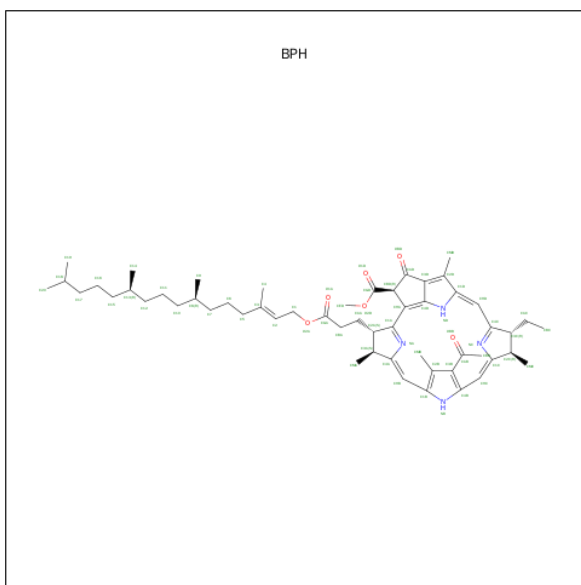
- Molecule 6 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula:

C₁₄H₃₁NO).



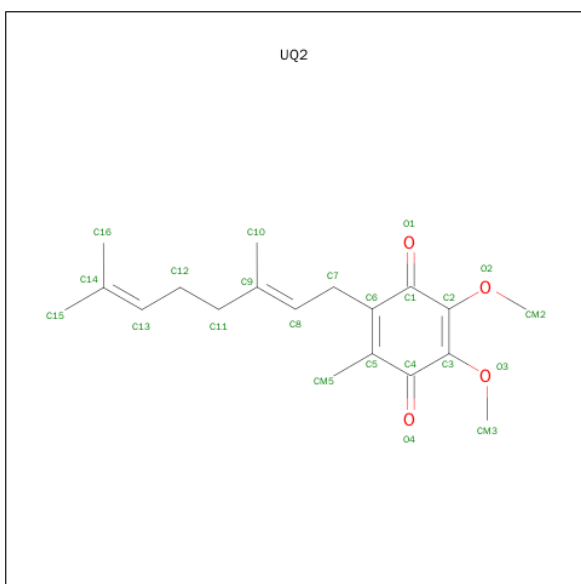
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	L	1	Total	C	N	O	0	0
			16	14	1	1		
6	L	1	Total	C	N	O	0	0
			16	14	1	1		
6	L	1	Total	C	N	O	0	0
			16	14	1	1		
6	L	1	Total	C	N	O	0	0
			16	14	1	1		
6	M	1	Total	C	N	O	0	0
			16	14	1	1		
6	M	1	Total	C	N	O	0	0
			16	14	1	1		
6	M	1	Total	C	N	O	0	0
			16	14	1	1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

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



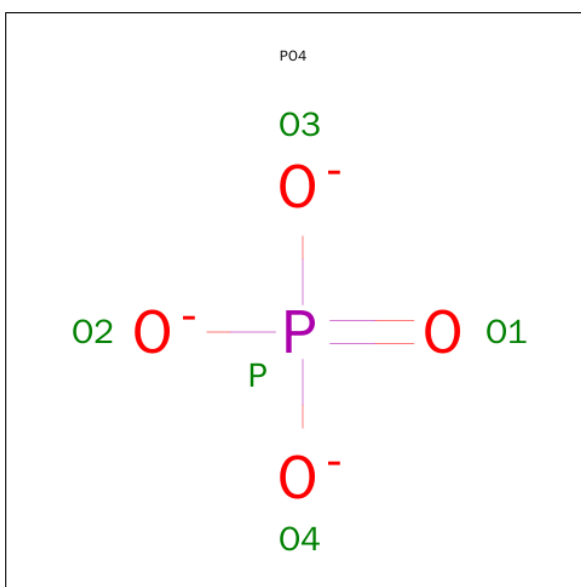
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	L	1	Total	C	N	O	0	0
			65	55	4	6		
7	M	1	Total	C	N	O	0	0
			65	55	4	6		

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



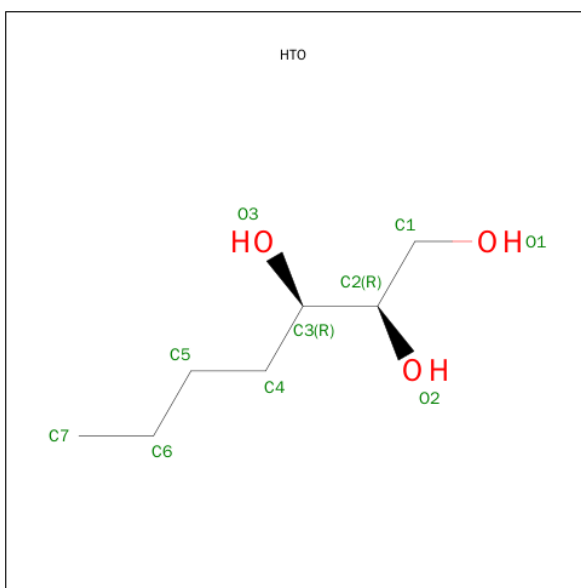
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	L	1	Total	C	O	0	1
			46	38	8		

- 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: $C_7H_{16}O_3$).

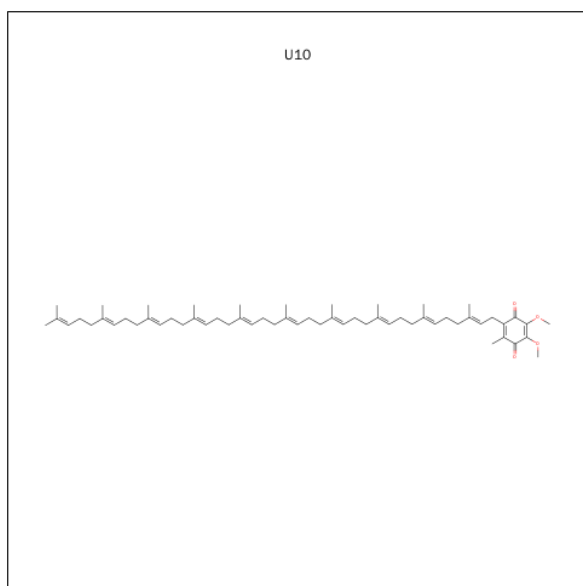


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	L	1	Total	C	O	0	0
			10	7	3		

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

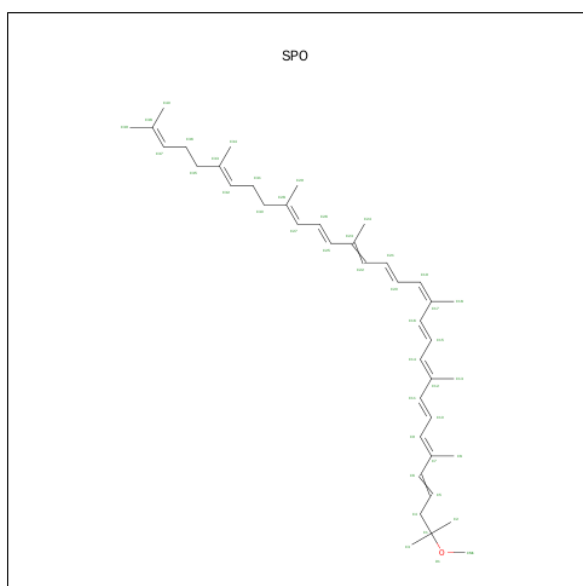
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	M	1	Total	Fe	0	0
			1	1		

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



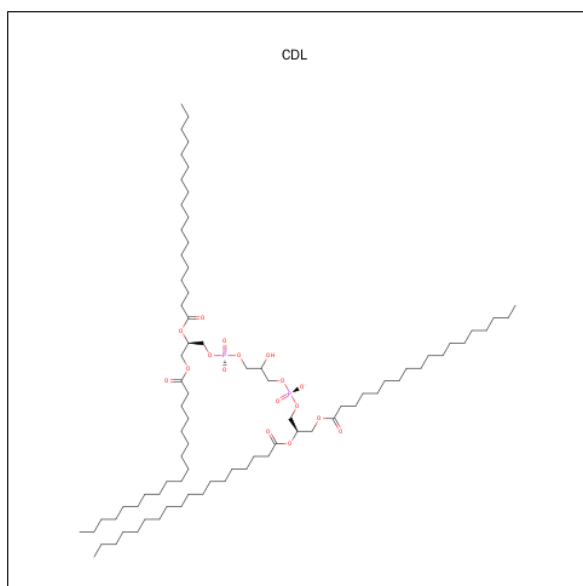
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	M	1	Total	C	O	0	0
			48	44	4		

- 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 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		

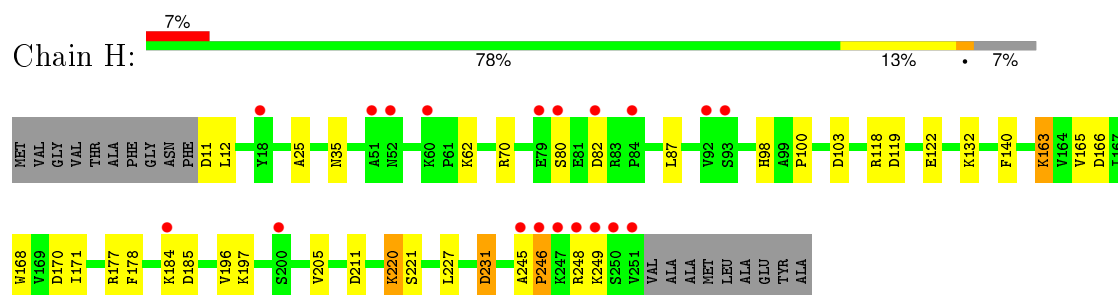
- Molecule 15 is water.

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		

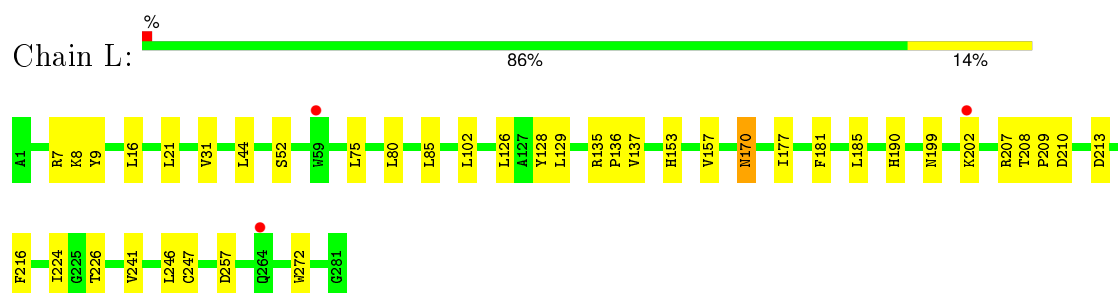
3 Residue-property plots [i](#)

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.

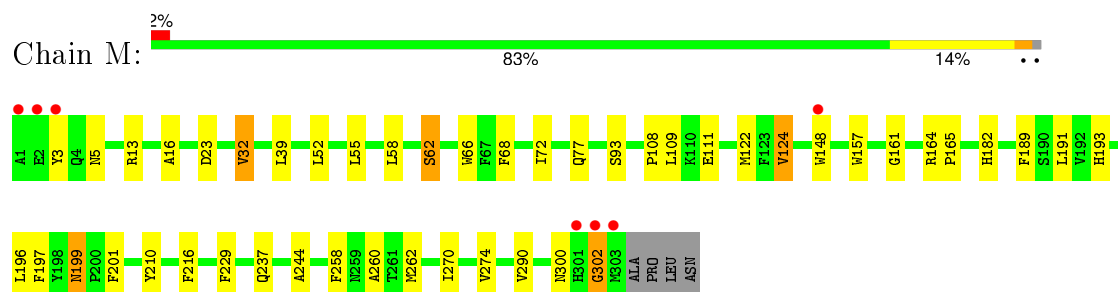
• Molecule 1: REACTION CENTER PROTEIN H CHAIN



• 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 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) 88.7 (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 0.191 , 0.188	Depositor DCC
R_{free} test set	4942 reflections (5.51%)	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 , 52.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	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.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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 7.

All (105) 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)
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:M:1311:BPH:CBB	7:M:1311:BPH:HHC	2.20	0.71
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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 [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%)	234 (97%)	6 (2%)	2 (1%)	24	27
2	L	279/281 (99%)	276 (99%)	2 (1%)	1 (0%)	39	48
3	M	301/307 (98%)	291 (97%)	10 (3%)	0	100	100
All	All	822/848 (97%)	801 (97%)	18 (2%)	3 (0%)	39	48

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%)	43	58
2	L	220/220 (100%)	205 (93%)	15 (7%)	20	25
3	M	236/240 (98%)	225 (95%)	11 (5%)	32	43
All	All	654/668 (98%)	621 (95%)	33 (5%)	31	41

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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	M	62	SER
3	M	109	LEU
3	M	124	VAL
3	M	182	HIS
3	M	191	LEU
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 [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 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	0.46	0	5,5,5	0.67	0
4	GOL	H	1252	-	5,5,5	0.40	0	5,5,5	0.40	0
4	GOL	H	1253	-	5,5,5	0.37	0	5,5,5	0.15	0
4	GOL	H	1254	-	5,5,5	0.38	0	5,5,5	0.25	0
5	BCL	L	1282	2	53,74,74	2.04	6 (11%)	57,115,115	2.03	10 (17%)
6	LDA	L	1283	-	15,15,15	3.77	2 (13%)	16,17,17	0.48	0
6	LDA	L	1284	-	15,15,15	3.86	2 (13%)	16,17,17	0.58	0
6	LDA	L	1285	-	15,15,15	3.56	1 (6%)	16,17,17	0.67	0
6	LDA	L	1286	-	15,15,15	3.63	2 (13%)	16,17,17	0.61	0
7	BPH	L	1287	-	64,70,70	3.03	17 (26%)	73,101,101	1.82	16 (21%)
8	UQ2	L	1288[A]	-	23,23,23	2.78	7 (30%)	28,31,31	1.08	3 (10%)
8	UQ2	L	1288[B]	-	23,23,23	2.69	7 (30%)	28,31,31	1.56	7 (25%)
5	BCL	L	1289	2	53,74,74	2.14	5 (9%)	57,115,115	1.86	11 (19%)
9	PO4	L	1290	-	4,4,4	0.47	0	6,6,6	0.27	0
10	HTO	L	1291	-	9,9,9	0.32	0	8,10,10	0.65	0
4	GOL	L	1292	-	5,5,5	0.22	0	5,5,5	0.54	0
4	GOL	L	1293	-	5,5,5	0.38	0	5,5,5	0.27	0
5	BCL	M	1303	3	53,74,74	2.07	4 (7%)	57,115,115	1.90	11 (19%)
5	BCL	M	1304	3	53,74,74	2.15	5 (9%)	57,115,115	1.95	15 (26%)
6	LDA	M	1305	-	15,15,15	3.76	1 (6%)	16,17,17	0.83	1 (6%)
6	LDA	M	1306	-	15,15,15	3.76	2 (13%)	16,17,17	0.51	0
6	LDA	M	1307	-	15,15,15	3.63	2 (13%)	16,17,17	0.71	0
6	LDA	M	1308	-	15,15,15	3.87	2 (13%)	16,17,17	0.92	1 (6%)
6	LDA	M	1309	-	15,15,15	3.82	2 (13%)	16,17,17	0.59	0
7	BPH	M	1311	-	64,70,70	3.00	19 (29%)	73,101,101	1.63	14 (19%)
12	U10	M	1312	-	48,48,63	3.09	12 (25%)	58,61,79	1.56	13 (22%)
13	SPO	M	1313	-	40,41,41	4.01	12 (30%)	45,50,50	2.08	17 (37%)
14	CDL	M	1314	-	80,80,99	1.99	18 (22%)	82,92,111	3.10	12 (14%)
4	GOL	M	1315	-	5,5,5	0.30	0	5,5,5	0.39	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
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	0/37/137/137	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	-	-	0/54/105/105	0/1/6/6
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	0/37/137/137	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	1/37/137/137	0/0/9/9
5	BCL	M	1304	3	2/2/21/25	0/37/137/137	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	-	-	0/54/105/105	0/1/6/6
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	-	-	0/91/91/110	0/0/0/0
4	GOL	M	1315	-	-	0/4/4/4	0/0/0/0

All (128) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	M	1308	LDA	O1-N1	-14.75	1.25	1.39
6	L	1284	LDA	O1-N1	-14.61	1.25	1.39
6	M	1309	LDA	O1-N1	-14.53	1.25	1.39
6	L	1283	LDA	O1-N1	-14.31	1.25	1.39
6	M	1305	LDA	O1-N1	-14.25	1.26	1.39
6	M	1306	LDA	O1-N1	-14.24	1.26	1.39
6	L	1286	LDA	O1-N1	-13.80	1.26	1.39
6	M	1307	LDA	O1-N1	-13.76	1.26	1.39
6	L	1285	LDA	O1-N1	-13.58	1.26	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	M	1314	CDL	C32-C31	-6.55	1.27	1.52
14	M	1314	CDL	C11-CA5	-6.54	1.31	1.50
8	L	1288[B]	UQ2	O2-C2	-5.32	1.23	1.37
7	L	1287	BPH	C3D-C4D	-5.10	1.34	1.41
12	M	1312	U10	O3-C3	-4.78	1.24	1.37
7	M	1311	BPH	C3D-C4D	-4.60	1.35	1.41
8	L	1288[A]	UQ2	O3-C3	-4.52	1.25	1.37
8	L	1288[B]	UQ2	O3-C3	-4.43	1.25	1.37
8	L	1288[A]	UQ2	O2-C2	-4.42	1.25	1.37
14	M	1314	CDL	C16-C15	-4.40	1.26	1.51
14	M	1314	CDL	C17-C16	-4.35	1.26	1.51
12	M	1312	U10	O4-C4	-4.15	1.26	1.37
7	M	1311	BPH	C3D-CAD	-3.99	1.38	1.46
7	L	1287	BPH	C3D-CAD	-3.84	1.39	1.46
14	M	1314	CDL	C13-C12	-3.68	1.30	1.51
8	L	1288[B]	UQ2	C3-C4	-3.55	1.38	1.48
7	M	1311	BPH	C1B-C2B	-3.45	1.38	1.45
14	M	1314	CDL	C19-C18	-3.36	1.32	1.51
5	M	1303	BCL	O2D-CGD	-3.23	1.24	1.33
14	M	1314	CDL	C20-C19	-3.23	1.32	1.51
14	M	1314	CDL	C34-C33	-3.21	1.33	1.51
14	M	1314	CDL	C33-C32	-3.14	1.33	1.51
14	M	1314	CDL	C37-C36	-3.07	1.33	1.51
14	M	1314	CDL	C79-C78	-3.04	1.33	1.51
14	M	1314	CDL	C80-C79	-2.99	1.34	1.51
14	M	1314	CDL	C22-C21	-2.92	1.34	1.51
7	M	1311	BPH	O2D-CGD	-2.84	1.25	1.33
7	L	1287	BPH	C1B-C2B	-2.80	1.39	1.45
5	L	1289	BCL	O2D-CGD	-2.71	1.26	1.33
5	M	1304	BCL	O2D-CGD	-2.70	1.26	1.33
8	L	1288[A]	UQ2	C2-C1	-2.70	1.41	1.48
12	M	1312	U10	C4-C5	-2.69	1.41	1.48
8	L	1288[B]	UQ2	C2-C1	-2.67	1.41	1.48
8	L	1288[A]	UQ2	C3-C4	-2.63	1.41	1.48
5	L	1282	BCL	O2D-CGD	-2.58	1.26	1.33
6	M	1306	LDA	C1-N1	-2.50	1.46	1.51
6	L	1284	LDA	C1-N1	-2.49	1.46	1.51
12	M	1312	U10	C3-C2	-2.46	1.41	1.48
6	M	1307	LDA	C1-N1	-2.45	1.46	1.51
5	L	1282	BCL	O2A-CGA	-2.41	1.26	1.33
6	L	1283	LDA	C1-N1	-2.38	1.47	1.51
7	L	1287	BPH	O2D-CGD	-2.38	1.27	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	M	1311	BPH	O2A-CGA	-2.32	1.26	1.33
6	L	1286	LDA	C1-N1	-2.26	1.47	1.51
8	L	1288[B]	UQ2	C6-C1	-2.26	1.39	1.46
6	M	1308	LDA	C1-N1	-2.20	1.47	1.51
5	M	1304	BCL	O2A-CGA	-2.17	1.26	1.33
7	L	1287	BPH	O2A-CGA	-2.17	1.26	1.33
6	M	1309	LDA	C1-N1	-2.15	1.47	1.51
5	L	1289	BCL	O2A-CGA	-2.10	1.26	1.33
7	M	1311	BPH	C1A-NA	-2.02	1.33	1.37
7	M	1311	BPH	C1C-NC	-2.01	1.33	1.37
14	M	1314	CDL	C12-C11	-2.01	1.44	1.52
5	L	1282	BCL	O1D-CGD	2.26	1.26	1.21
12	M	1312	U10	C6-C1	2.28	1.40	1.35
7	L	1287	BPH	C1D-CHD	2.45	1.49	1.40
8	L	1288[A]	UQ2	C6-C5	2.63	1.41	1.35
7	M	1311	BPH	C1D-CHD	2.92	1.51	1.40
5	M	1304	BCL	C2-C3	3.35	1.39	1.33
7	L	1287	BPH	CHB-C4A	3.36	1.46	1.40
5	L	1282	BCL	C2-C3	3.48	1.39	1.33
7	L	1287	BPH	C3D-C2D	3.56	1.48	1.40
7	M	1311	BPH	CHC-C4B	3.66	1.49	1.40
7	M	1311	BPH	CHB-C4A	3.67	1.47	1.40
13	M	1313	SPO	C21-C20	3.70	1.45	1.35
7	L	1287	BPH	CHD-C4C	3.70	1.47	1.38
7	M	1311	BPH	C3D-C2D	3.77	1.49	1.40
7	L	1287	BPH	CHC-C4B	3.94	1.50	1.40
5	L	1289	BCL	C2-C3	4.07	1.40	1.33
13	M	1313	SPO	C15-C16	4.20	1.45	1.34
13	M	1313	SPO	C10-C11	4.21	1.45	1.34
7	M	1311	BPH	CHD-C4C	4.23	1.48	1.38
5	M	1303	BCL	C2-C3	4.34	1.41	1.33
14	M	1314	CDL	OB6-CB5	4.44	1.47	1.34
14	M	1314	CDL	OA6-CA5	4.46	1.47	1.34
14	M	1314	CDL	OB8-CB7	4.51	1.46	1.33
14	M	1314	CDL	OA8-CA7	4.57	1.47	1.33
13	M	1313	SPO	C26-C25	4.65	1.46	1.34
8	L	1288[B]	UQ2	C13-C14	4.98	1.47	1.32
7	M	1311	BPH	CHC-C1C	5.01	1.46	1.36
13	M	1313	SPO	C6-C5	5.05	1.46	1.31
12	M	1312	U10	C38-C39	5.13	1.48	1.32
8	L	1288[A]	UQ2	C13-C14	5.17	1.48	1.32
5	L	1282	BCL	O1A-CGA	5.55	1.39	1.22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	L	1287	BPH	CHC-C1C	5.60	1.47	1.36
13	M	1313	SPO	C37-C38	5.70	1.49	1.32
7	M	1311	BPH	CHB-C1B	5.81	1.50	1.38
5	M	1303	BCL	O1A-CGA	5.82	1.40	1.22
5	M	1304	BCL	O1A-CGA	5.84	1.40	1.22
5	L	1289	BCL	O1A-CGA	5.89	1.40	1.22
7	L	1287	BPH	CHB-C1B	5.93	1.50	1.38
7	L	1287	BPH	O1A-CGA	6.00	1.40	1.22
7	M	1311	BPH	O1A-CGA	6.25	1.41	1.22
7	L	1287	BPH	O1D-CGD	7.35	1.39	1.21
7	L	1287	BPH	C2-C3	7.38	1.47	1.33
12	M	1312	U10	C23-C24	7.42	1.47	1.33
12	M	1312	U10	C8-C9	7.47	1.47	1.33
8	L	1288[B]	UQ2	C8-C9	7.59	1.47	1.33
12	M	1312	U10	C13-C14	7.64	1.48	1.33
12	M	1312	U10	C28-C29	7.65	1.48	1.33
7	M	1311	BPH	C2-C3	7.74	1.48	1.33
7	M	1311	BPH	O1D-CGD	7.92	1.41	1.21
13	M	1313	SPO	C32-C33	7.93	1.48	1.33
12	M	1312	U10	C18-C19	7.97	1.48	1.33
12	M	1312	U10	C33-C34	8.01	1.48	1.33
13	M	1313	SPO	C14-C12	8.03	1.46	1.35
7	M	1311	BPH	OBB-CAB	8.29	1.41	1.23
13	M	1313	SPO	C9-C7	8.43	1.46	1.35
8	L	1288[A]	UQ2	C8-C9	8.51	1.49	1.33
13	M	1313	SPO	C22-C23	8.72	1.47	1.35
13	M	1313	SPO	C19-C17	9.15	1.47	1.35
7	L	1287	BPH	OBB-CAB	9.99	1.45	1.23
7	M	1311	BPH	OBD-CAD	11.37	1.39	1.22
5	M	1303	BCL	OBD-CAD	11.55	1.40	1.22
7	L	1287	BPH	OBD-CAD	11.60	1.40	1.22
5	L	1282	BCL	OBD-CAD	11.67	1.40	1.22
13	M	1313	SPO	C27-C28	12.14	1.47	1.34
5	L	1289	BCL	OBD-CAD	12.57	1.41	1.22
5	M	1304	BCL	OBD-CAD	12.75	1.41	1.22

All (131) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	1289	BCL	CMB-C2B-C1B	-6.95	116.87	128.36
5	L	1282	BCL	CMB-C2B-C1B	-6.59	117.45	128.36
5	M	1303	BCL	CMB-C2B-C1B	-6.22	118.07	128.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	M	1304	BCL	C1D-CHD-C4C	-5.72	117.34	126.07
5	M	1304	BCL	CMB-C2B-C1B	-5.41	119.41	128.36
7	L	1287	BPH	O1D-CGD-CBD	-5.14	117.25	124.62
13	M	1313	SPO	C10-C9-C7	-5.10	119.84	127.20
7	M	1311	BPH	CHC-C4B-NB	-4.90	115.57	124.91
5	M	1303	BCL	C1D-CHD-C4C	-4.37	119.39	126.07
5	L	1282	BCL	C1D-CHD-C4C	-4.29	119.51	126.07
13	M	1313	SPO	C21-C22-C23	-4.15	121.20	127.20
5	L	1289	BCL	CHB-C4A-NA	-4.00	118.97	124.51
5	L	1282	BCL	OBD-CAD-CBD	-3.82	120.18	125.94
7	L	1287	BPH	OBD-CAD-CBD	-3.69	120.36	125.94
13	M	1313	SPO	C20-C19-C17	-3.67	121.90	127.20
13	M	1313	SPO	C15-C14-C12	-3.56	122.06	127.20
7	M	1311	BPH	OBD-CAD-CBD	-3.24	121.04	125.94
13	M	1313	SPO	C4-C5-C6	-3.09	120.27	124.67
7	L	1287	BPH	OBD-CAD-C3D	-3.08	122.07	128.35
12	M	1312	U10	C22-C23-C24	-3.04	121.16	127.76
5	M	1303	BCL	O2D-CGD-O1D	-3.03	117.54	123.79
12	M	1312	U10	C17-C18-C19	-3.03	121.18	127.76
7	L	1287	BPH	CBB-CAB-C3B	-2.94	113.98	120.52
12	M	1312	U10	C30-C29-C28	-2.93	117.74	123.50
8	L	1288[B]	UQ2	CM5-C5-C6	-2.93	117.83	124.10
8	L	1288[B]	UQ2	C7-C8-C9	-2.91	121.76	126.70
7	M	1311	BPH	OBD-CAD-C3D	-2.91	122.41	128.35
7	M	1311	BPH	CMD-C2D-C3D	-2.82	119.57	125.09
7	L	1287	BPH	CHC-C4B-NB	-2.81	119.55	124.91
5	L	1282	BCL	O1D-CGD-CBD	-2.79	120.62	124.62
7	M	1311	BPH	O1D-CGD-CBD	-2.78	120.64	124.62
5	L	1289	BCL	C1D-CHD-C4C	-2.76	121.86	126.07
12	M	1312	U10	C27-C28-C29	-2.73	121.82	127.76
5	L	1289	BCL	CMD-C2D-C3D	-2.72	119.77	125.09
5	M	1304	BCL	C16-C15-C13	-2.67	106.63	115.49
5	M	1304	BCL	O2D-CGD-O1D	-2.65	118.31	123.79
12	M	1312	U10	C12-C13-C14	-2.59	122.14	127.76
13	M	1313	SPO	C8-C7-C9	-2.58	119.09	122.90
5	L	1282	BCL	O2D-CGD-O1D	-2.58	118.46	123.79
6	M	1305	LDA	CM2-N1-CM1	-2.56	105.94	108.83
7	L	1287	BPH	C1C-NC-C4C	-2.56	107.82	110.44
13	M	1313	SPO	C15-C16-C17	-2.56	118.80	126.32
7	M	1311	BPH	CAC-C3C-C2C	-2.55	107.72	114.13
13	M	1313	SPO	C21-C20-C19	-2.55	117.76	123.39
5	M	1303	BCL	OBD-CAD-CBD	-2.51	122.15	125.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	M	1311	BPH	O2D-CGD-O1D	-2.44	118.74	123.79
7	M	1311	BPH	C4-C3-C2	-2.39	118.82	123.50
5	M	1304	BCL	CHD-C4C-NC	-2.35	122.33	125.06
5	M	1304	BCL	CMD-C2D-C3D	-2.32	120.55	125.09
5	L	1289	BCL	O2D-CGD-O1D	-2.31	119.02	123.79
5	L	1289	BCL	O2A-CGA-O1A	-2.29	117.58	123.49
13	M	1313	SPO	C20-C21-C22	-2.29	118.33	123.39
13	M	1313	SPO	C14-C15-C16	-2.28	116.19	123.13
7	L	1287	BPH	C7-C6-C5	-2.23	106.48	113.06
5	L	1289	BCL	CHA-C1A-NA	-2.23	120.58	126.06
6	M	1308	LDA	O1-N1-C1	-2.22	107.77	110.27
8	L	1288[B]	UQ2	O4-C4-C3	-2.19	116.05	120.79
8	L	1288[A]	UQ2	C10-C9-C8	-2.18	119.23	123.50
8	L	1288[B]	UQ2	O1-C1-C6	-2.17	117.59	121.68
5	M	1303	BCL	CHA-C1A-NA	-2.16	120.73	126.06
5	M	1303	BCL	CHB-C4A-NA	-2.15	121.53	124.51
13	M	1313	SPO	C9-C10-C11	-2.13	116.65	123.13
13	M	1313	SPO	C11-C12-C14	-2.09	115.62	118.98
5	M	1304	BCL	CHC-C1C-NC	-2.07	121.65	124.51
12	M	1312	U10	C32-C33-C34	-2.07	123.27	127.76
5	M	1303	BCL	C11-C12-C13	-2.06	108.66	115.49
5	M	1304	BCL	OBD-CAD-CBD	-2.05	122.85	125.94
5	L	1282	BCL	CHD-C4C-NC	-2.04	122.70	125.06
5	M	1304	BCL	CAC-C3C-C4C	-2.03	108.07	112.58
5	M	1304	BCL	C4-C3-C2	-2.02	119.54	123.50
7	L	1287	BPH	CMD-C2D-C3D	-2.00	121.17	125.09
12	M	1312	U10	C41-C39-C40	2.05	119.69	114.64
7	L	1287	BPH	OBb-CAB-C3B	2.07	124.31	120.31
13	M	1313	SPO	C24-C23-C25	2.09	121.57	118.10
7	M	1311	BPH	O2A-CGA-CBA	2.10	118.30	111.90
7	L	1287	BPH	C2D-C1D-ND	2.11	113.74	110.29
8	L	1288[B]	UQ2	C16-C14-C15	2.17	119.97	114.64
7	M	1311	BPH	C4-C3-C5	2.22	118.80	115.41
8	L	1288[A]	UQ2	CM2-O2-C2	2.24	124.59	116.61
7	L	1287	BPH	CMB-C2B-C1B	2.25	128.73	125.06
12	M	1312	U10	C4M-O4-C4	2.35	124.99	116.61
5	M	1303	BCL	C4A-NA-C1A	2.36	109.41	106.36
7	L	1287	BPH	O2A-CGA-CBA	2.42	119.28	111.90
8	L	1288[B]	UQ2	C10-C9-C11	2.51	119.23	115.41
14	M	1314	CDL	C32-C31-CA7	2.51	123.45	113.59
8	L	1288[A]	UQ2	C10-C9-C11	2.58	119.35	115.41
14	M	1314	CDL	OA8-CA7-C31	2.65	119.97	111.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	1282	BCL	C4-C3-C5	2.71	119.55	115.41
7	M	1311	BPH	CED-O2D-CGD	2.73	122.39	115.99
13	M	1313	SPO	C13-C12-C11	2.73	122.64	118.10
12	M	1312	U10	C10-C9-C11	2.78	119.65	115.41
12	M	1312	U10	C35-C34-C36	2.78	119.65	115.41
12	M	1312	U10	C15-C14-C16	2.80	119.68	115.41
5	L	1289	BCL	CED-O2D-CGD	2.84	122.66	115.99
13	M	1313	SPO	C34-C33-C35	2.91	119.86	115.41
7	M	1311	BPH	C2B-C1B-NB	2.91	114.10	109.73
14	M	1314	CDL	OB8-CB7-C71	2.93	120.84	111.90
8	L	1288[B]	UQ2	CM3-O3-C3	2.96	127.12	116.61
5	L	1282	BCL	O2A-CGA-CBA	2.96	120.91	111.90
12	M	1312	U10	C25-C24-C26	2.98	119.95	115.41
5	M	1304	BCL	C4-C3-C5	3.16	120.24	115.41
5	M	1303	BCL	O2A-CGA-CBA	3.20	121.65	111.90
5	L	1289	BCL	O2A-CGA-CBA	3.25	121.82	111.90
13	M	1313	SPO	C8-C7-C6	3.26	123.52	118.10
5	M	1304	BCL	CED-O2D-CGD	3.35	123.84	115.99
7	L	1287	BPH	C2B-C1B-NB	3.46	114.91	109.73
5	M	1304	BCL	O2A-CGA-CBA	3.53	122.67	111.90
5	M	1304	BCL	CMB-C2B-C3B	3.56	132.04	125.09
7	M	1311	BPH	C3C-C4C-NC	3.64	111.58	107.93
13	M	1313	SPO	C29-C28-C30	3.76	121.15	115.41
5	L	1282	BCL	CMB-C2B-C3B	4.06	133.03	125.09
14	M	1314	CDL	OB6-CB5-C51	4.10	120.44	111.53
14	M	1314	CDL	OA6-CA5-C11	4.16	120.58	111.53
7	L	1287	BPH	CED-O2D-CGD	4.25	125.96	115.99
12	M	1312	U10	C30-C29-C31	4.26	121.92	115.41
5	L	1289	BCL	O2D-CGD-CBD	4.37	117.29	111.30
7	L	1287	BPH	C3C-C4C-NC	4.42	112.36	107.93
5	M	1303	BCL	CMB-C2B-C3B	4.43	133.76	125.09
5	L	1289	BCL	CMB-C2B-C3B	4.76	134.40	125.09
5	M	1304	BCL	O2D-CGD-CBD	5.69	119.10	111.30
14	M	1314	CDL	C20-C19-C18	6.44	147.81	114.53
5	M	1303	BCL	O2D-CGD-CBD	6.51	120.23	111.30
7	L	1287	BPH	O2D-CGD-CBD	6.73	120.54	111.30
14	M	1314	CDL	C34-C33-C32	6.76	149.42	114.53
7	M	1311	BPH	O2D-CGD-CBD	6.79	120.62	111.30
5	L	1282	BCL	O2D-CGD-CBD	7.01	120.92	111.30
14	M	1314	CDL	C35-C34-C33	7.50	153.26	114.53
14	M	1314	CDL	C13-C12-C11	7.74	141.69	113.29
14	M	1314	CDL	C12-C11-CA5	8.93	148.68	113.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	M	1314	CDL	C17-C16-C15	12.25	177.80	114.53
14	M	1314	CDL	C33-C32-C31	15.58	170.41	113.29

All (8) chirality outliers are listed below:

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

20 monomers are involved in 62 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	H	1251	GOL	2	0
4	H	1252	GOL	1	0
5	L	1282	BCL	3	0
6	L	1283	LDA	1	0
6	L	1285	LDA	2	0
7	L	1287	BPH	7	0
8	L	1288[A]	UQ2	1	0
8	L	1288[B]	UQ2	3	0
5	L	1289	BCL	4	0
4	L	1292	GOL	1	0
5	M	1303	BCL	4	0
5	M	1304	BCL	13	0
6	M	1305	LDA	2	0
6	M	1307	LDA	5	0
6	M	1308	LDA	3	0
7	M	1311	BPH	11	0
12	M	1312	U10	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	M	1313	SPO	2	0
14	M	1314	CDL	3	0
4	M	1315	GOL	2	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, 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%)	0.03	19 (7%) 15 22	39, 49, 63, 103	0
2	L	281/281 (100%)	-0.58	3 (1%) 82 87	31, 41, 53, 59	0
3	M	303/307 (98%)	-0.59	7 (2%) 64 72	32, 41, 54, 79	0
All	All	825/848 (97%)	-0.40	29 (3%) 48 56	31, 44, 58, 103	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	251	VAL	15.4
1	H	250	SER	13.7
1	H	247	LYS	8.1
3	M	1	ALA	6.9
1	H	246	PRO	6.0
1	H	249	LYS	5.7
3	M	302	GLY	5.5
1	H	248	ARG	5.5
3	M	301	HIS	5.4
1	H	92	VAL	4.2
1	H	245	ALA	4.0
3	M	2	GLU	3.9
2	L	59	TRP	3.6
3	M	3	TYR	3.6
1	H	18	TYR	3.5
3	M	148	TRP	3.2
1	H	51	ALA	2.7
1	H	84	PRO	2.7
1	H	79	GLU	2.5
1	H	82	ASP	2.3
1	H	93	SER	2.3
1	H	52	ASN	2.3
2	L	202	LYS	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	H	184	LYS	2.3
3	M	303	MET	2.3
1	H	200	SER	2.2
1	H	80	SER	2.2
1	H	60	LYS	2.1
2	L	264	GLN	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 [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	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
4	GOL	H	1251	6/6	0.55	0.40	51.58	69,72,73,74	0
6	LDA	L	1286	16/16	0.04	0.41	19.10	97,103,111,111	0
6	LDA	L	1285	16/16	0.35	0.31	14.92	76,86,98,98	0
6	LDA	L	1284	16/16	0.53	0.31	11.98	106,107,110,111	0
6	LDA	L	1283	16/16	0.06	0.48	11.38	80,97,107,108	0
6	LDA	M	1308	16/16	0.22	0.36	10.19	116,117,121,121	0
10	HTO	L	1291	10/10	0.78	0.26	9.98	72,76,77,78	0
6	LDA	M	1305	16/16	0.61	0.27	9.56	61,74,78,79	0
8	UQ2	L	1288[A]	23/23	0.90	0.20	8.38	28,38,56,57	23
14	CDL	M	1314	81/100	0.32	0.43	7.78	110,119,127,127	0
8	UQ2	L	1288[B]	23/23	0.90	0.20	6.95	36,40,47,47	23
6	LDA	M	1306	16/16	0.69	0.25	4.24	81,83,86,87	0
6	LDA	M	1307	16/16	0.78	0.21	4.19	71,75,79,79	0
4	GOL	L	1293	6/6	0.76	0.18	2.54	90,92,92,93	0
13	SPO	M	1313	42/42	0.87	0.17	2.01	38,44,62,66	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
12	U10	M	1312	48/63	0.90	0.13	1.40	36,49,77,78	0
5	BCL	L	1289	66/66	0.97	0.12	0.86	28,34,50,56	0
4	GOL	L	1292	6/6	0.86	0.18	0.85	62,65,66,68	0
7	BPH	M	1311	65/65	0.93	0.11	0.75	30,37,87,89	0
5	BCL	M	1304	66/66	0.96	0.11	0.74	27,33,48,55	0
5	BCL	M	1303	66/66	0.95	0.09	0.02	28,31,70,71	0
7	BPH	L	1287	65/65	0.97	0.10	-0.04	27,35,42,45	0
5	BCL	L	1282	66/66	0.97	0.07	-0.57	28,32,57,60	0
11	FE	M	1310	1/1	0.99	0.02	-5.65	34,34,34,34	0
4	GOL	H	1254	6/6	0.47	0.38	-	115,115,115,116	0
6	LDA	M	1309	16/16	-0.14	0.50	-	119,123,128,128	0
4	GOL	H	1253	6/6	0.55	0.35	-	108,108,109,109	0
4	GOL	M	1315	6/6	0.74	0.20	-	105,106,106,106	0
9	PO4	L	1290	5/5	0.79	0.34	-	170,170,171,171	0
4	GOL	H	1252	6/6	0.56	0.37	-	91,93,93,93	0

6.5 Other polymers [i](#)

There are no such residues in this entry.