



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:50 AM GMT

PDB ID : 2UX4
Title : X-RAY HIGH RESOLUTION STRUCTURE OF THE PHOTOSYNTHETIC
REACTION CENTER FROM RB. SPHAEROIDES AT PH 9 IN THE
CHARGE-SEPARATED STATE, 2ND DATASET
Authors : Koepke, J.; Diehm, R.; Fritzsche, G.
Deposited on : 2007-03-26
Resolution : 2.51 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

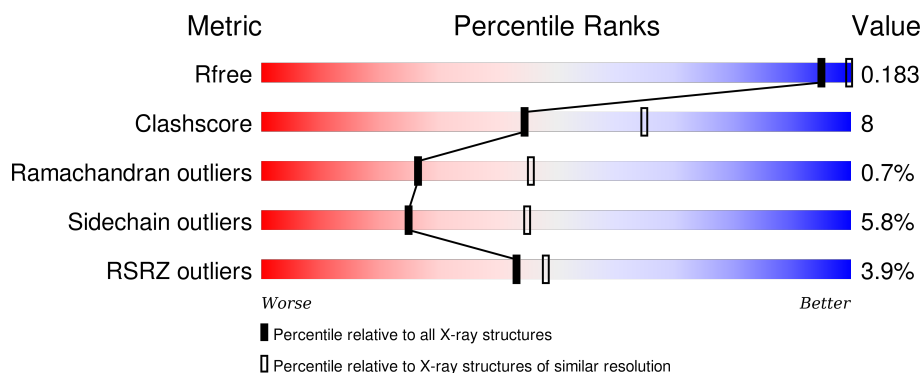
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.51 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	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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>83%</div> <div>8%</div> <div>7%</div> </div>
2	L	281	<div> <div>3%</div> <div>86%</div> <div>12%</div> <div></div> </div>
3	M	307	<div> <div>5%</div> <div>81%</div> <div>16%</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	1290	-	-	-	X
13	SPO	M	1313	-	-	-	X
14	CDL	M	1314	-	-	-	X
4	GOL	H	1251	-	-	-	X
4	GOL	L	1292	-	-	-	X
5	BCL	L	1282	X	-	-	-
5	BCL	L	1288	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	M	1305	-	-	-	X
6	LDA	M	1306	-	-	-	X
6	LDA	M	1307	-	-	-	X
6	LDA	M	1308	-	-	-	X
6	LDA	M	1309	-	-	-	X
8	UQ2	L	1287[A]	-	-	-	X
8	UQ2	L	1287[B]	-	-	-	X

2 Entry composition [i](#)

There are 15 unique types of molecules in this entry. The entry contains 7671 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.

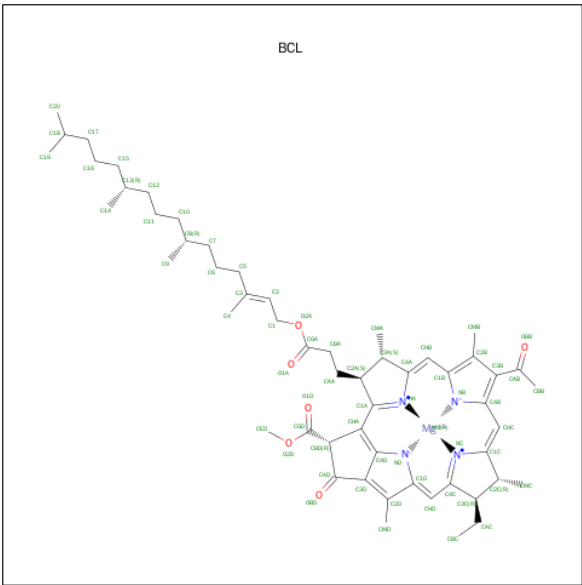
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	M	303	Total	C	N	O	S	0	0	1
			2409	1607	395	397	10			

- 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		

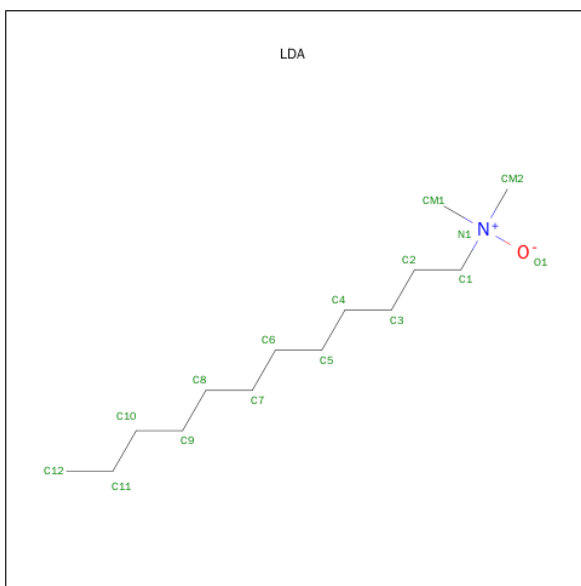
- Molecule 5 is BACTERIOCHLOROPHYLL A (three-letter code: BCL) (formula: C₅₅H₇₄MgN₄O₆).



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

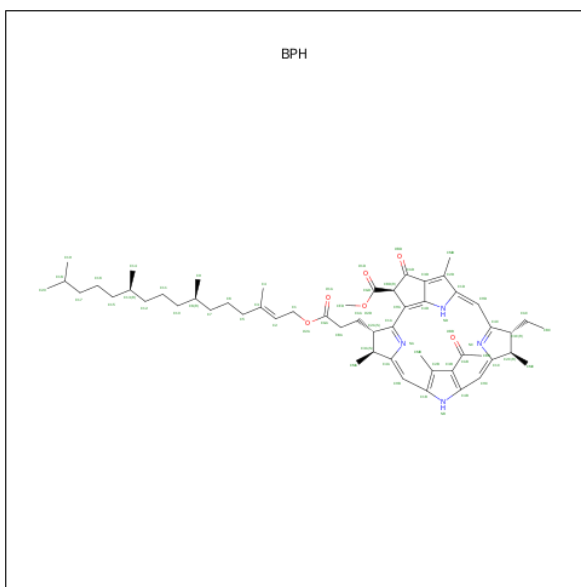
- Molecule 6 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula:

C₁₄H₃₁NO).



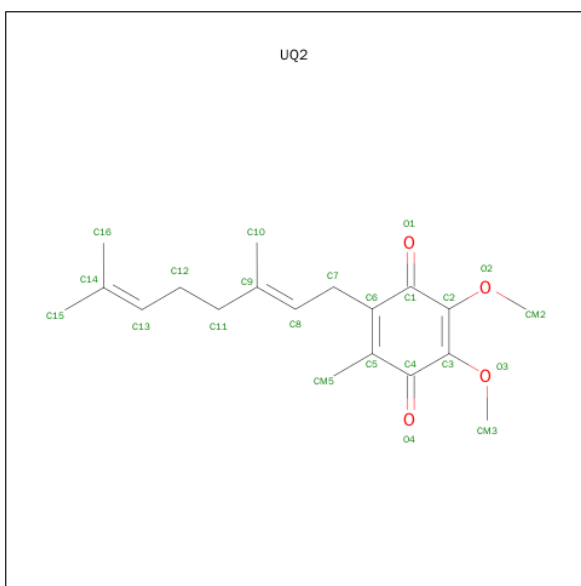
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	L	1	Total	C	N	O	0	0
			16	14	1	1		
6	L	1	Total	C	N	O	0	0
			16	14	1	1		
6	L	1	Total	C	N	O	0	0
			16	14	1	1		
6	M	1	Total	C	N	O	0	0
			16	14	1	1		
6	M	1	Total	C	N	O	0	0
			16	14	1	1		
6	M	1	Total	C	N	O	0	0
			16	14	1	1		
6	M	1	Total	C	N	O	0	0
			16	14	1	1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

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



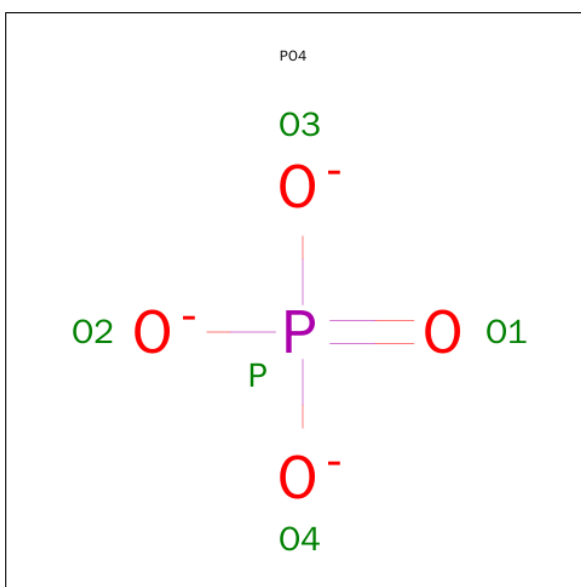
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	L	1	Total	C	N	O	0	0
			65	55	4	6		
7	M	1	Total	C	N	O	0	0
			65	55	4	6		

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



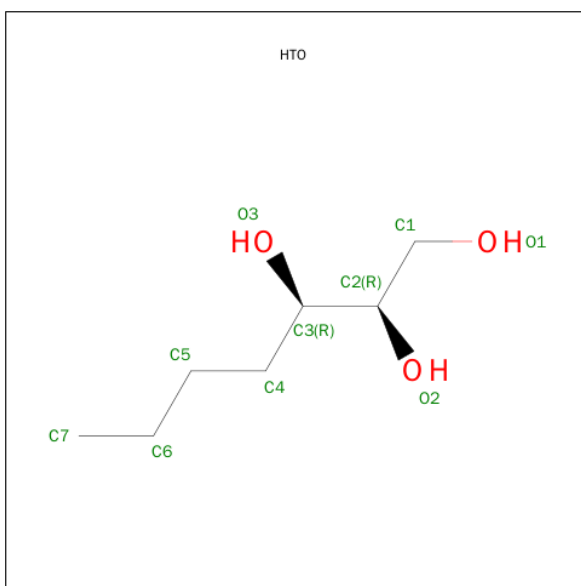
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	L	1	Total	C	O	0	1
			46	38	8		

- 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: $C_7H_{16}O_3$).

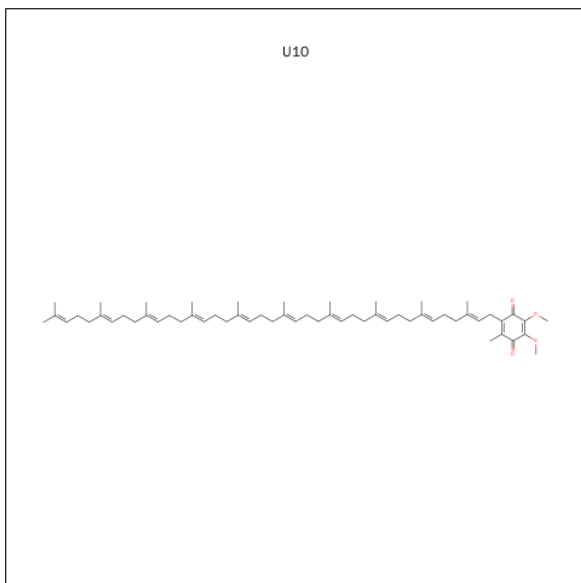


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	L	1	Total	C	O	0	0
			10	7	3		

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

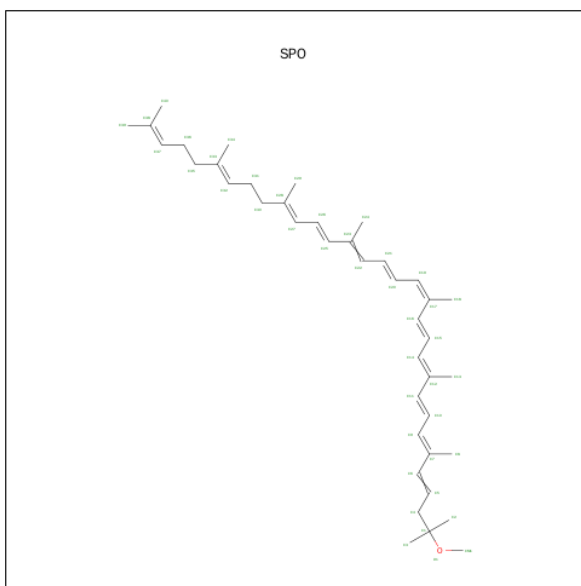
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	M	1	Total	Fe	0	0
			1	1		

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



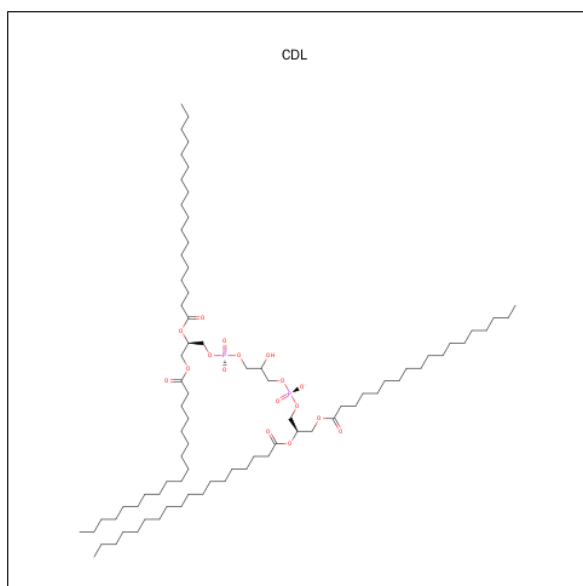
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	M	1	Total	C	O	0	0
			48	44	4		

- 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		

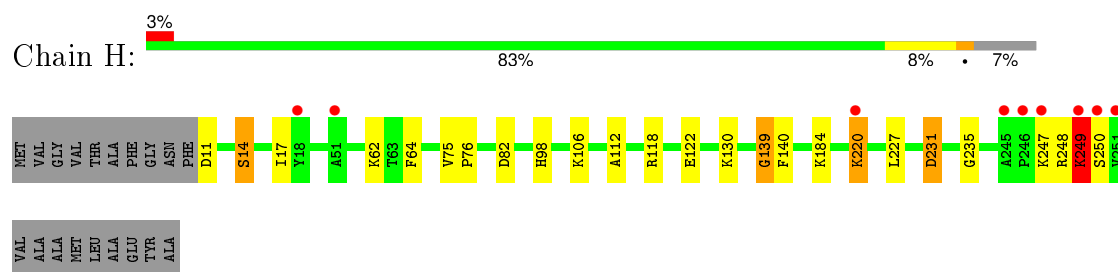
- Molecule 15 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	H	149	Total	O	0	0
			149	149		
15	L	111	Total	O	0	0
			111	111		
15	M	111	Total	O	0	0
			111	111		

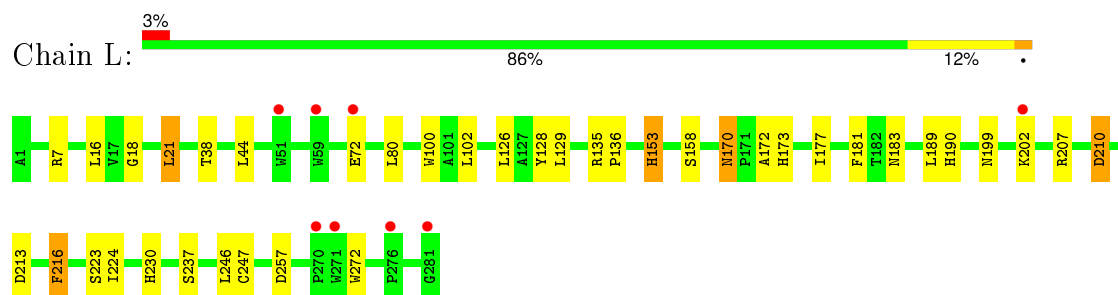
3 Residue-property plots [i](#)

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.

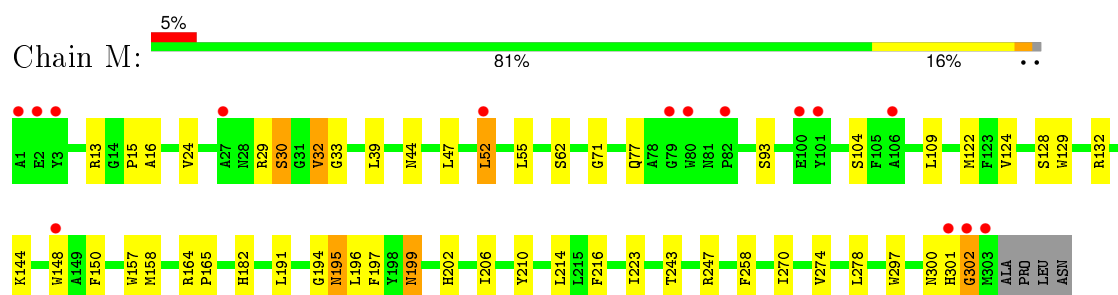
• Molecule 1: REACTION CENTER PROTEIN H CHAIN



• 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 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	139.58Å 139.58Å 184.96Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.51 29.45 – 2.51	Depositor EDS
% Data completeness (in resolution range)	97.6 (50.00-2.51) 90.9 (29.45-2.51)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.81 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.190 , 0.211 0.184 , 0.183	Depositor DCC
R_{free} test set	3493 reflections (5.67%)	DCC
Wilson B-factor (Å ²)	38.1	Xtriage
Anisotropy	0.301	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 53.2	EDS
Estimated twinning fraction	0.022 for -h,-k,l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 69781 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7671	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.82% 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	0.53	0/1906	0.74	4/2591 (0.2%)
2	L	0.56	0/2320	0.64	2/3175 (0.1%)
3	M	0.54	0/2501	0.63	0/3415
All	All	0.54	0/6727	0.66	6/9181 (0.1%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	L	213	ASP	CB-CG-OD2	6.87	124.49	118.30
1	H	82	ASP	CB-CG-OD2	6.09	123.78	118.30
1	H	11	ASP	CB-CG-OD2	5.91	123.62	118.30
1	H	139	GLY	N-CA-C	-5.89	98.37	113.10
1	H	231	ASP	CB-CG-OD2	5.67	123.40	118.30
2	L	257	ASP	CB-CG-OD2	5.36	123.12	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	16	0
2	L	2232	0	2187	26	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	M	2409	0	2321	37	0
4	H	24	0	32	1	0
4	L	12	0	16	1	0
4	M	6	0	8	2	0
5	L	132	0	148	7	0
5	M	132	0	148	24	0
6	L	48	0	93	7	0
6	M	96	0	186	10	0
7	L	65	0	76	7	0
7	M	65	0	76	12	0
8	L	46	0	52	6	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	0	0
13	M	42	0	60	4	0
14	M	81	0	82	2	0
15	H	149	0	0	3	0
15	L	111	0	0	1	0
15	M	111	0	0	1	0
All	All	7671	0	7425	116	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 8.

All (116) 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)
1:H:248:ARG:HA	1:H:249:LYS:HB2	1.25	1.10
1:H:248:ARG:HA	1:H:249:LYS:CB	1.95	0.96
3:M:197:PHE:HZ	5:M:1304:BCL:HBB2	1.39	0.87
3:M:197:PHE:CZ	5:M:1304:BCL:HBB2	2.15	0.80
7:L:1286:BPH:HBB2	3:M:210:TYR:HB3	1.66	0.77
2:L:181:PHE:CD2	7:M:1311:BPH:HBB1	2.21	0.75
7:L:1286:BPH:HHC	7:L:1286:BPH:HBB3	1.67	0.75
2:L:224:ILE:HG22	8:L:1287[A]:UQ2:H8	1.72	0.72
3:M:16:ALA:HB1	3:M:32:VAL:HG11	1.73	0.71
1:H:248:ARG:CA	1:H:249:LYS:HB2	2.12	0.70
5:M:1303:BCL:HBB3	5:M:1304:BCL:H41	1.73	0.69
3:M:243:THR:O	3:M:247:ARG:HG3	1.94	0.68
7:L:1286:BPH:HHC	7:L:1286:BPH:CBB	2.23	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:1304:BCL:HHC	5:M:1304:BCL:HBB2	1.79	0.65
5:M:1303:BCL:CBB	5:M:1303:BCL:HHC	2.28	0.64
5:M:1303:BCL:HMA2	6:M:1309:LDA:H112	1.79	0.64
7:M:1311:BPH:HBB3	7:M:1311:BPH:HHC	1.78	0.63
5:M:1303:BCL:H203	13:M:1313:SPO:H10	1.81	0.62
3:M:300:ASN:C	3:M:302:GLY:H	2.02	0.62
1:H:220[B]:LYS:NZ	15:H:2135:HOH:O	2.34	0.61
1:H:62:LYS:HE2	1:H:64:PHE:CZ	2.36	0.60
6:M:1305:LDA:H12	4:M:1315:GOL:H12	1.83	0.60
2:L:189:LEU:CD2	7:M:1311:BPH:HMD2	2.32	0.60
1:H:98:HIS:CD2	2:L:7:ARG:HH21	2.19	0.59
6:M:1307:LDA:H52	6:M:1308:LDA:H62	1.84	0.59
3:M:77:GLN:HE22	3:M:93:SER:H	1.49	0.59
2:L:170:ASN:HD22	2:L:170:ASN:C	2.06	0.58
5:M:1304:BCL:CBB	5:M:1304:BCL:HHC	2.34	0.58
3:M:157:TRP:HB2	5:M:1304:BCL:H71	1.86	0.57
7:L:1286:BPH:HBB1	3:M:210:TYR:CD2	2.41	0.56
5:L:1282:BCL:HBB3	5:L:1288:BCL:H52	1.87	0.56
3:M:55:LEU:HD22	3:M:128:SER:HB2	1.88	0.55
4:H:1251:GOL:H32	15:H:2003:HOH:O	2.06	0.54
5:M:1304:BCL:CBB	5:M:1304:BCL:CHC	2.86	0.54
2:L:199:ASN:HA	4:L:1291:GOL:H31	1.91	0.53
1:H:140:PHE:HA	3:M:13:ARG:O	2.09	0.53
3:M:270:ILE:O	3:M:274:VAL:HG13	2.09	0.53
3:M:24:VAL:HG21	3:M:29:ARG:NH1	2.24	0.53
3:M:199:ASN:HD22	3:M:199:ASN:C	2.11	0.53
2:L:181:PHE:HB3	7:M:1311:BPH:HBB2	1.91	0.53
3:M:144:LYS:N	14:M:1314:CDL:OB3	2.38	0.53
3:M:62:SER:OG	3:M:124:VAL:HG22	2.09	0.52
1:H:248:ARG:CA	1:H:249:LYS:CB	2.78	0.52
1:H:112:ALA:HA	1:H:235:GLY:O	2.10	0.52
5:M:1304:BCL:HAA2	5:M:1304:BCL:HBD	1.90	0.52
6:M:1305:LDA:H32	4:M:1315:GOL:H32	1.91	0.52
3:M:202:HIS:CE1	3:M:206:ILE:HD11	2.45	0.52
1:H:98:HIS:HD2	2:L:7:ARG:HH21	1.57	0.52
6:L:1284:LDA:H11	3:M:33:GLY:HA2	1.91	0.51
5:M:1303:BCL:HBB2	5:M:1303:BCL:HHC	1.92	0.51
7:M:1311:BPH:CBB	7:M:1311:BPH:HHC	2.40	0.51
2:L:181:PHE:HB3	7:M:1311:BPH:CBB	2.40	0.51
3:M:194:GLY:O	3:M:195:ASN:HB3	2.10	0.51
2:L:190:HIS:HA	8:L:1287[A]:UQ2:O4	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:1288:BCL:HMB1	5:L:1288:BCL:CBB	2.41	0.51
7:L:1286:BPH:CHC	7:L:1286:BPH:HBB3	2.38	0.51
2:L:189:LEU:HD23	7:M:1311:BPH:HMD2	1.92	0.51
2:L:18:GLY:O	2:L:21:LEU:HB2	2.12	0.50
3:M:258:PHE:CG	6:M:1307:LDA:H51	2.46	0.50
2:L:210:ASP:OD1	2:L:210:ASP:N	2.45	0.49
6:L:1285:LDA:H42	6:M:1309:LDA:H81	1.94	0.49
6:M:1305:LDA:H101	6:M:1307:LDA:H121	1.95	0.49
5:L:1288:BCL:C1C	5:M:1304:BCL:HBB3	2.43	0.49
1:H:122:GLU:HB2	1:H:227:LEU:HD21	1.95	0.49
2:L:173:HIS:CE1	2:L:177:ILE:HD11	2.49	0.48
7:L:1286:BPH:ND	3:M:214:LEU:HD13	2.28	0.48
1:H:75:VAL:HA	1:H:76:PRO:C	2.35	0.47
1:H:14:SER:HA	1:H:17:ILE:HG22	1.97	0.47
2:L:230:HIS:CD2	3:M:223:ILE:HG13	2.50	0.47
7:M:1311:BPH:HBB3	7:M:1311:BPH:CHC	2.44	0.46
3:M:150:PHE:CD1	7:M:1311:BPH:C3D	2.98	0.46
5:L:1288:BCL:HMB2	5:M:1304:BCL:HHB	1.98	0.46
3:M:197:PHE:HZ	5:M:1304:BCL:CBB	2.19	0.46
2:L:128:TYR:HD1	5:L:1282:BCL:HBB1	1.81	0.45
6:L:1284:LDA:H62	3:M:47:LEU:HD12	1.99	0.44
2:L:153:HIS:CD2	5:L:1282:BCL:NC	2.85	0.44
7:L:1286:BPH:CHC	7:L:1286:BPH:CBB	2.94	0.44
3:M:297:TRP:CE2	3:M:302:GLY:HA2	2.53	0.44
2:L:135:ARG:HB3	2:L:136:PRO:HD3	1.99	0.44
3:M:197:PHE:CE1	5:M:1304:BCL:HHC	2.52	0.44
3:M:300:ASN:C	3:M:302:GLY:N	2.70	0.44
6:M:1307:LDA:H22	6:M:1307:LDA:HM11	1.54	0.44
6:M:1307:LDA:H41	6:M:1308:LDA:H42	1.99	0.44
2:L:189:LEU:HD13	2:L:216:PHE:HZ	1.81	0.44
5:M:1303:BCL:H101	5:M:1304:BCL:H171	2.00	0.43
3:M:196:LEU:HD12	5:M:1304:BCL:C1D	2.49	0.43
3:M:71:GLY:HA3	13:M:1313:SPO:H42	2.00	0.43
1:H:139:GLY:H	3:M:15:PRO:HD3	1.84	0.43
3:M:194:GLY:O	3:M:195:ASN:CB	2.67	0.42
1:H:130:LYS:HD2	15:L:2087:HOH:O	2.19	0.42
3:M:129:TRP:O	3:M:132:ARG:HB3	2.19	0.42
2:L:224:ILE:HD12	8:L:1287[B]:UQ2:H102	2.01	0.42
5:L:1282:BCL:HMB1	5:L:1288:BCL:H142	2.02	0.42
6:L:1285:LDA:H21	6:L:1285:LDA:HM21	1.90	0.42
3:M:157:TRP:CE3	3:M:158:MET:HG2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:164:ARG:HB3	3:M:165:PRO:HD3	2.02	0.42
2:L:38:THR:HG21	2:L:100:TRP:HE3	1.84	0.42
6:L:1285:LDA:H121	8:L:1287[A]:UQ2:H161	2.01	0.42
5:M:1303:BCL:H102	5:M:1303:BCL:H13	1.72	0.42
5:M:1303:BCL:HBB2	13:M:1313:SPO:H243	2.02	0.42
7:M:1311:BPH:H141	7:M:1311:BPH:H161	1.90	0.42
2:L:170:ASN:ND2	2:L:172:ALA:H	2.18	0.42
2:L:224:ILE:CG2	8:L:1287[A]:UQ2:H8	2.46	0.41
1:H:118[A]:ARG:HD3	15:M:2089:HOH:O	2.20	0.41
5:M:1303:BCL:CBB	13:M:1313:SPO:H243	2.51	0.41
5:M:1303:BCL:HBB3	5:M:1303:BCL:HHC	2.01	0.41
6:L:1285:LDA:H121	8:L:1287[A]:UQ2:C16	2.50	0.41
15:H:2003:HOH:O	14:M:1314:CDL:HA32	2.20	0.41
6:L:1283:LDA:H22	6:L:1283:LDA:HM11	1.86	0.41
3:M:122:MET:HE3	5:M:1304:BCL:H142	2.03	0.41
7:M:1311:BPH:H6C2	7:M:1311:BPH:H2	1.94	0.41
2:L:183:ASN:ND2	2:L:237:SER:HB3	2.36	0.41
6:M:1309:LDA:H21	6:M:1309:LDA:HM11	1.75	0.41
5:M:1303:BCL:CBB	5:M:1303:BCL:CHC	2.99	0.40
2:L:189:LEU:HD21	7:M:1311:BPH:HMD2	2.02	0.40
2:L:223:SER:O	3:M:44:ASN:HB2	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	242/260 (93%)	233 (96%)	8 (3%)	1 (0%)	39	61
2	L	279/281 (99%)	270 (97%)	9 (3%)	0	100	100
3	M	301/307 (98%)	287 (95%)	9 (3%)	5 (2%)	11	19
All	All	822/848 (97%)	790 (96%)	26 (3%)	6 (1%)	26	46

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	249	LYS
3	M	301	HIS
3	M	52	LEU
3	M	195	ASN
3	M	30	SER
3	M	302	GLY

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%)	189 (96%)	9 (4%)	34	59
2	L	220/220 (100%)	202 (92%)	18 (8%)	14	27
3	M	236/240 (98%)	224 (95%)	12 (5%)	29	52
All	All	654/668 (98%)	615 (94%)	39 (6%)	25	43

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	14	SER
1	H	106	LYS
1	H	184	LYS
1	H	220[A]	LYS
1	H	220[B]	LYS
1	H	231	ASP
1	H	247	LYS
1	H	249	LYS
1	H	250	SER
2	L	16	LEU
2	L	21	LEU
2	L	44	LEU
2	L	72	GLU
2	L	80	LEU
2	L	102	LEU

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Mol	Chain	Res	Type
2	L	126	LEU
2	L	129	LEU
2	L	153	HIS
2	L	158	SER
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	30	SER
3	M	32	VAL
3	M	39	LEU
3	M	52	LEU
3	M	104	SER
3	M	109	LEU
3	M	148	TRP
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 (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	98	HIS
2	L	159	ASN
2	L	170	ASN
2	L	183	ASN
3	M	77	GLN
3	M	187	ASN
3	M	193	HIS
3	M	199	ASN

5.3.3 RNA ⓘ

There are no RNA 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 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	0.49	0	5,5,5	0.77	0
4	GOL	H	1252	-	5,5,5	0.35	0	5,5,5	0.20	0
4	GOL	H	1253	-	5,5,5	0.32	0	5,5,5	0.25	0
4	GOL	H	1254	-	5,5,5	0.35	0	5,5,5	0.24	0
5	BCL	L	1282	2	53,74,74	2.06	6 (11%)	57,115,115	2.07	14 (24%)
6	LDA	L	1283	-	15,15,15	3.76	2 (13%)	16,17,17	0.80	1 (6%)
6	LDA	L	1284	-	15,15,15	3.81	2 (13%)	16,17,17	0.54	0
6	LDA	L	1285	-	15,15,15	3.89	2 (13%)	16,17,17	0.93	1 (6%)
7	BPH	L	1286	-	64,70,70	3.00	17 (26%)	73,101,101	1.66	13 (17%)
8	UQ2	L	1287[A]	-	23,23,23	2.72	8 (34%)	28,31,31	1.50	6 (21%)
8	UQ2	L	1287[B]	-	23,23,23	2.81	7 (30%)	28,31,31	1.12	3 (10%)
5	BCL	L	1288	2	53,74,74	2.08	6 (11%)	57,115,115	1.84	12 (21%)
9	PO4	L	1289	-	4,4,4	0.41	0	6,6,6	0.27	0
10	HTO	L	1290	-	9,9,9	0.41	0	8,10,10	0.60	0
4	GOL	L	1291	-	5,5,5	0.27	0	5,5,5	0.52	0
4	GOL	L	1292	-	5,5,5	0.32	0	5,5,5	0.21	0
5	BCL	M	1303	3	53,74,74	2.13	5 (9%)	57,115,115	1.86	11 (19%)
5	BCL	M	1304	3	53,74,74	2.13	6 (11%)	57,115,115	1.97	13 (22%)
6	LDA	M	1305	-	15,15,15	3.88	1 (6%)	16,17,17	0.86	1 (6%)
6	LDA	M	1306	-	15,15,15	3.80	2 (13%)	16,17,17	0.82	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	LDA	M	1307	-	15,15,15	3.76	2 (13%)	16,17,17	0.76	0
6	LDA	M	1308	-	15,15,15	3.81	2 (13%)	16,17,17	0.70	0
6	LDA	M	1309	-	15,15,15	3.71	2 (13%)	16,17,17	0.70	0
7	BPH	M	1311	-	64,70,70	2.98	17 (26%)	73,101,101	1.79	13 (17%)
12	U10	M	1312	-	48,48,63	3.05	12 (25%)	58,61,79	1.77	13 (22%)
13	SPO	M	1313	-	40,41,41	4.15	12 (30%)	45,50,50	2.02	11 (24%)
14	CDL	M	1314	-	80,80,99	2.26	18 (22%)	82,92,111	4.00	14 (17%)
4	GOL	M	1315	-	5,5,5	0.29	0	5,5,5	0.30	0
6	LDA	M	1709	-	15,15,15	3.76	2 (13%)	16,17,17	0.60	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
7	BPH	L	1286	-	-	0/54/105/105	0/1/6/6
8	UQ2	L	1287[A]	-	-	0/15/39/39	0/1/1/1
8	UQ2	L	1287[B]	-	-	0/15/39/39	0/1/1/1
5	BCL	L	1288	2	2/2/21/25	0/37/137/137	0/0/9/9
9	PO4	L	1289	-	-	0/0/0/0	0/0/0/0
10	HTO	L	1290	-	-	0/10/10/10	0/0/0/0
4	GOL	L	1291	-	-	0/4/4/4	0/0/0/0
4	GOL	L	1292	-	-	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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
6	LDA	M	1709	-	-	0/13/13/13	0/0/0/0

All (131) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	L	1285	LDA	O1-N1	-14.77	1.25	1.39
6	M	1305	LDA	O1-N1	-14.64	1.25	1.39
6	M	1306	LDA	O1-N1	-14.47	1.25	1.39
6	M	1308	LDA	O1-N1	-14.46	1.25	1.39
6	L	1284	LDA	O1-N1	-14.46	1.25	1.39
6	L	1283	LDA	O1-N1	-14.33	1.25	1.39
6	M	1709	LDA	O1-N1	-14.28	1.26	1.39
6	M	1307	LDA	O1-N1	-14.22	1.26	1.39
6	M	1309	LDA	O1-N1	-14.13	1.26	1.39
14	M	1314	CDL	C11-CA5	-7.19	1.29	1.50
14	M	1314	CDL	C32-C31	-6.63	1.26	1.52
14	M	1314	CDL	C12-C11	-5.65	1.30	1.52
14	M	1314	CDL	C34-C33	-5.63	1.19	1.51
14	M	1314	CDL	C33-C32	-5.58	1.19	1.51
8	L	1287[A]	UQ2	O2-C2	-4.94	1.24	1.37
8	L	1287[B]	UQ2	O2-C2	-4.81	1.24	1.37
8	L	1287[B]	UQ2	O3-C3	-4.76	1.24	1.37
12	M	1312	U10	O4-C4	-4.48	1.25	1.37
8	L	1287[A]	UQ2	O3-C3	-4.45	1.25	1.37
14	M	1314	CDL	C17-C16	-4.35	1.26	1.51
14	M	1314	CDL	C16-C15	-4.35	1.26	1.51
14	M	1314	CDL	C20-C19	-4.29	1.26	1.51
7	L	1286	BPH	C3D-CAD	-4.28	1.38	1.46
12	M	1312	U10	O3-C3	-4.26	1.25	1.37
14	M	1314	CDL	C19-C18	-4.23	1.27	1.51
7	L	1286	BPH	C3D-C4D	-3.84	1.36	1.41
7	M	1311	BPH	C3D-CAD	-3.81	1.39	1.46
14	M	1314	CDL	C13-C12	-3.64	1.30	1.51
8	L	1287[A]	UQ2	C3-C4	-3.29	1.39	1.48
12	M	1312	U10	C4-C5	-3.19	1.39	1.48
8	L	1287[B]	UQ2	C3-C4	-3.13	1.39	1.48
7	M	1311	BPH	C1B-C2B	-3.08	1.38	1.45
7	M	1311	BPH	C3D-C4D	-3.00	1.37	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	M	1314	CDL	C37-C36	-2.99	1.34	1.51
14	M	1314	CDL	C79-C78	-2.99	1.34	1.51
14	M	1314	CDL	C80-C79	-2.95	1.34	1.51
7	L	1286	BPH	O2D-CGD	-2.93	1.25	1.33
14	M	1314	CDL	C22-C21	-2.90	1.34	1.51
6	M	1307	LDA	C1-N1	-2.90	1.46	1.51
8	L	1287[B]	UQ2	C2-C1	-2.84	1.40	1.48
7	M	1311	BPH	O2D-CGD	-2.80	1.26	1.33
7	M	1311	BPH	O2A-CGA	-2.61	1.25	1.33
6	L	1284	LDA	C1-N1	-2.47	1.46	1.51
5	L	1282	BCL	O2A-CGA	-2.44	1.25	1.33
5	L	1288	BCL	O2D-CGD	-2.42	1.27	1.33
7	L	1286	BPH	C1B-C2B	-2.42	1.40	1.45
8	L	1287[A]	UQ2	C2-C1	-2.41	1.42	1.48
5	L	1282	BCL	O2D-CGD	-2.41	1.27	1.33
6	M	1709	LDA	C1-N1	-2.37	1.47	1.51
5	L	1282	BCL	C3D-CAD	-2.36	1.39	1.45
5	M	1303	BCL	O2D-CGD	-2.35	1.27	1.33
8	L	1287[A]	UQ2	C6-C1	-2.32	1.39	1.46
7	L	1286	BPH	O2A-CGA	-2.31	1.26	1.33
6	M	1306	LDA	C1-N1	-2.30	1.47	1.51
5	M	1304	BCL	C3D-CAD	-2.29	1.39	1.45
5	M	1304	BCL	O2A-CGA	-2.29	1.26	1.33
6	L	1285	LDA	C1-N1	-2.29	1.47	1.51
6	M	1308	LDA	C1-N1	-2.27	1.47	1.51
5	L	1288	BCL	C3D-CAD	-2.25	1.39	1.45
12	M	1312	U10	C3-C2	-2.22	1.42	1.48
5	L	1288	BCL	O2A-CGA	-2.20	1.26	1.33
5	M	1304	BCL	O2D-CGD	-2.19	1.27	1.33
6	L	1283	LDA	C1-N1	-2.11	1.47	1.51
6	M	1309	LDA	C1-N1	-2.09	1.47	1.51
8	L	1287[A]	UQ2	C6-C5	2.08	1.40	1.35
5	M	1303	BCL	O1D-CGD	2.26	1.26	1.21
7	L	1286	BPH	C1D-CHD	2.45	1.49	1.40
12	M	1312	U10	C6-C1	2.70	1.41	1.35
8	L	1287[B]	UQ2	C6-C5	2.74	1.41	1.35
7	M	1311	BPH	C1D-CHD	2.91	1.51	1.40
7	L	1286	BPH	CHC-C4B	3.37	1.48	1.40
7	L	1286	BPH	CHD-C4C	3.43	1.46	1.38
5	M	1304	BCL	C2-C3	3.45	1.39	1.33
7	M	1311	BPH	CHD-C4C	3.56	1.47	1.38
7	M	1311	BPH	C3D-C2D	3.63	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	M	1303	BCL	C2-C3	3.70	1.40	1.33
7	M	1311	BPH	CHB-C4A	3.72	1.47	1.40
7	L	1286	BPH	C3D-C2D	3.75	1.49	1.40
7	L	1286	BPH	CHB-C4A	3.80	1.47	1.40
13	M	1313	SPO	C21-C20	3.83	1.46	1.35
5	L	1282	BCL	C2-C3	3.93	1.40	1.33
7	M	1311	BPH	CHC-C4B	4.16	1.50	1.40
14	M	1314	CDL	OB8-CB7	4.21	1.46	1.33
14	M	1314	CDL	OA6-CA5	4.39	1.47	1.34
14	M	1314	CDL	OA8-CA7	4.45	1.46	1.33
13	M	1313	SPO	C26-C25	4.49	1.46	1.34
5	L	1288	BCL	C2-C3	4.51	1.41	1.33
13	M	1313	SPO	C10-C11	4.56	1.46	1.34
14	M	1314	CDL	OB6-CB5	4.65	1.48	1.34
13	M	1313	SPO	C15-C16	4.73	1.46	1.34
7	L	1286	BPH	CHC-C1C	4.79	1.45	1.36
8	L	1287[B]	UQ2	C13-C14	5.08	1.47	1.32
12	M	1312	U10	C38-C39	5.09	1.47	1.32
13	M	1313	SPO	C6-C5	5.21	1.46	1.31
8	L	1287[A]	UQ2	C13-C14	5.35	1.48	1.32
13	M	1313	SPO	C37-C38	5.38	1.48	1.32
7	M	1311	BPH	CHC-C1C	5.76	1.47	1.36
5	L	1282	BCL	O1A-CGA	5.83	1.40	1.22
5	L	1288	BCL	O1A-CGA	5.84	1.40	1.22
7	M	1311	BPH	O1A-CGA	6.01	1.40	1.22
5	M	1304	BCL	O1A-CGA	6.26	1.41	1.22
7	M	1311	BPH	CHB-C1B	6.29	1.50	1.38
5	M	1303	BCL	O1A-CGA	6.30	1.41	1.22
7	L	1286	BPH	O1A-CGA	6.34	1.41	1.22
7	L	1286	BPH	CHB-C1B	6.53	1.51	1.38
12	M	1312	U10	C28-C29	7.03	1.46	1.33
12	M	1312	U10	C23-C24	7.14	1.47	1.33
12	M	1312	U10	C8-C9	7.31	1.47	1.33
12	M	1312	U10	C18-C19	7.43	1.47	1.33
7	M	1311	BPH	C2-C3	7.66	1.48	1.33
13	M	1313	SPO	C32-C33	7.72	1.48	1.33
7	M	1311	BPH	O1D-CGD	7.74	1.40	1.21
7	L	1286	BPH	C2-C3	7.75	1.48	1.33
8	L	1287[A]	UQ2	C8-C9	7.78	1.48	1.33
7	M	1311	BPH	OBb-CAB	7.90	1.40	1.23
7	L	1286	BPH	O1D-CGD	8.00	1.41	1.21
12	M	1312	U10	C13-C14	8.14	1.48	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	M	1312	U10	C33-C34	8.22	1.49	1.33
8	L	1287[B]	UQ2	C8-C9	8.32	1.49	1.33
7	L	1286	BPH	OB-B-CAB	8.54	1.41	1.23
13	M	1313	SPO	C19-C17	8.95	1.47	1.35
13	M	1313	SPO	C14-C12	9.30	1.48	1.35
13	M	1313	SPO	C22-C23	9.34	1.48	1.35
13	M	1313	SPO	C9-C7	9.45	1.48	1.35
5	L	1288	BCL	OB-D-CAD	11.69	1.40	1.22
7	M	1311	BPH	OB-D-CAD	11.72	1.40	1.22
5	L	1282	BCL	OB-D-CAD	11.78	1.40	1.22
7	L	1286	BPH	OB-D-CAD	11.85	1.40	1.22
13	M	1313	SPO	C27-C28	11.99	1.47	1.34
5	M	1303	BCL	OB-D-CAD	12.20	1.41	1.22
5	M	1304	BCL	OB-D-CAD	12.26	1.41	1.22

All (127) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	1282	BCL	CMB-C2B-C1B	-7.12	116.58	128.36
5	M	1303	BCL	CMB-C2B-C1B	-6.94	116.88	128.36
5	M	1304	BCL	CMB-C2B-C1B	-6.86	117.01	128.36
5	L	1288	BCL	CMB-C2B-C1B	-6.76	117.18	128.36
13	M	1313	SPO	C4-C5-C6	-5.70	116.56	124.67
7	M	1311	BPH	CHC-C4B-NB	-5.39	114.64	124.91
5	M	1304	BCL	C1D-CHD-C4C	-4.71	118.88	126.07
7	M	1311	BPH	O1D-CGD-CBD	-4.57	118.07	124.62
13	M	1313	SPO	C10-C9-C7	-4.39	120.86	127.20
13	M	1313	SPO	C20-C19-C17	-4.25	121.05	127.20
7	M	1311	BPH	OB-D-CAD-CBD	-4.22	119.58	125.94
12	M	1312	U10	C27-C28-C29	-4.14	118.76	127.76
5	L	1282	BCL	C1D-CHD-C4C	-4.03	119.92	126.07
5	M	1303	BCL	C1D-CHD-C4C	-3.85	120.19	126.07
7	L	1286	BPH	OB-D-CAD-C3D	-3.84	120.52	128.35
5	L	1282	BCL	O1D-CGD-CBD	-3.68	119.35	124.62
7	L	1286	BPH	O1D-CGD-CBD	-3.47	119.65	124.62
5	L	1288	BCL	CMD-C2D-C3D	-3.40	118.44	125.09
12	M	1312	U10	C17-C18-C19	-3.34	120.51	127.76
12	M	1312	U10	C22-C23-C24	-3.28	120.63	127.76
7	M	1311	BPH	OB-D-CAD-C3D	-3.18	121.87	128.35
13	M	1313	SPO	C15-C14-C12	-3.16	122.64	127.20
12	M	1312	U10	C30-C29-C28	-3.15	117.31	123.50
7	M	1311	BPH	CMD-C2D-C3D	-2.91	119.40	125.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	M	1304	BCL	C3C-C4C-CHD	-2.90	116.87	123.33
5	M	1304	BCL	CMD-C2D-C3D	-2.85	119.51	125.09
5	M	1303	BCL	CHB-C4A-NA	-2.78	120.67	124.51
7	L	1286	BPH	C1C-NC-C4C	-2.75	107.62	110.44
8	L	1287[A]	UQ2	O1-C1-C6	-2.70	116.60	121.68
13	M	1313	SPO	C21-C22-C23	-2.66	123.35	127.20
13	M	1313	SPO	C31-C32-C33	-2.64	122.03	127.76
5	L	1282	BCL	CHB-C4A-NA	-2.60	120.91	124.51
5	L	1282	BCL	CHA-C1A-NA	-2.58	119.70	126.06
8	L	1287[A]	UQ2	CM5-C5-C6	-2.57	118.61	124.10
6	L	1285	LDA	O1-N1-C1	-2.54	107.42	110.27
7	M	1311	BPH	CBC-CAC-C3C	-2.52	107.41	113.57
5	M	1304	BCL	O2D-CGD-O1D	-2.48	118.67	123.79
5	L	1282	BCL	C3C-C4C-CHD	-2.45	117.87	123.33
6	M	1305	LDA	O1-N1-CM2	-2.41	105.83	109.05
5	M	1303	BCL	O2D-CGD-O1D	-2.38	118.87	123.79
5	M	1303	BCL	O1D-CGD-CBD	-2.38	121.22	124.62
7	M	1311	BPH	C3B-C2B-C1B	-2.35	102.00	105.77
5	M	1304	BCL	CAC-C3C-C4C	-2.33	107.40	112.58
5	L	1288	BCL	C1D-CHD-C4C	-2.33	122.51	126.07
5	M	1304	BCL	C16-C15-C13	-2.32	107.78	115.49
6	L	1283	LDA	O1-N1-C1	-2.28	107.70	110.27
7	L	1286	BPH	O2D-CGD-O1D	-2.27	119.11	123.79
6	M	1306	LDA	O1-N1-C1	-2.23	107.76	110.27
5	L	1282	BCL	O2D-CGD-O1D	-2.22	119.20	123.79
8	L	1287[A]	UQ2	C7-C8-C9	-2.22	122.94	126.70
8	L	1287[B]	UQ2	C10-C9-C8	-2.20	119.19	123.50
7	M	1311	BPH	C4D-C3D-C2D	-2.19	104.25	107.08
5	L	1288	BCL	C2A-C1A-CHA	-2.19	119.85	123.89
7	L	1286	BPH	CMD-C2D-C3D	-2.19	120.81	125.09
5	L	1282	BCL	O2A-CGA-O1A	-2.15	117.95	123.49
5	M	1304	BCL	CHD-C4C-NC	-2.13	122.59	125.06
5	L	1288	BCL	CHB-C4A-NA	-2.12	121.58	124.51
5	L	1288	BCL	O1D-CGD-CBD	-2.11	121.59	124.62
8	L	1287[A]	UQ2	C10-C9-C8	-2.10	119.37	123.50
5	M	1303	BCL	CHA-C1A-NA	-2.10	120.89	126.06
14	M	1314	CDL	OA8-CA7-OA9	-2.08	118.11	123.49
8	L	1287[B]	UQ2	C5-C6-C1	-2.07	117.76	120.12
7	L	1286	BPH	O2A-CGA-O1A	-2.05	118.19	123.49
5	L	1282	BCL	CMD-C2D-C3D	-2.05	121.09	125.09
12	M	1312	U10	C32-C33-C34	-2.04	123.33	127.76
14	M	1314	CDL	OB8-CB7-OB9	-2.03	118.26	123.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	M	1312	U10	C12-C13-C14	-2.00	123.41	127.76
7	L	1286	BPH	OBD-CAD-CBD	-2.00	122.92	125.94
8	L	1287[B]	UQ2	C10-C9-C11	2.01	118.48	115.41
5	M	1303	BCL	CED-O2D-CGD	2.03	120.74	115.99
13	M	1313	SPO	C13-C12-C11	2.11	121.62	118.10
5	L	1288	BCL	C4-C3-C5	2.14	118.67	115.41
12	M	1312	U10	C4M-O4-C4	2.17	124.33	116.61
5	M	1303	BCL	C4A-NA-C1A	2.17	109.17	106.36
7	M	1311	BPH	CED-O2D-CGD	2.20	121.15	115.99
5	L	1282	BCL	C4A-NA-C1A	2.23	109.24	106.36
13	M	1313	SPO	C40-C38-C39	2.25	120.17	114.64
5	L	1288	BCL	C4A-NA-C1A	2.29	109.32	106.36
13	M	1313	SPO	O1-C1-C4	2.36	111.65	105.87
14	M	1314	CDL	C32-C31-CA7	2.36	122.89	113.59
7	M	1311	BPH	O2A-CGA-CBA	2.39	119.18	111.90
7	L	1286	BPH	C4A-NA-C1A	2.42	110.37	108.21
8	L	1287[A]	UQ2	CM3-O3-C3	2.50	125.50	116.61
12	M	1312	U10	C15-C14-C16	2.52	119.25	115.41
5	M	1303	BCL	O2A-CGA-CBA	2.64	119.94	111.90
13	M	1313	SPO	C34-C33-C35	2.68	119.50	115.41
12	M	1312	U10	C20-C19-C21	2.69	119.52	115.41
5	L	1282	BCL	O2A-CGA-CBA	2.71	120.16	111.90
7	L	1286	BPH	C2B-C1B-NB	2.74	113.83	109.73
5	M	1304	BCL	C4-C3-C5	2.82	119.72	115.41
14	M	1314	CDL	OA8-CA7-C31	2.87	120.64	111.90
12	M	1312	U10	C25-C24-C26	2.90	119.83	115.41
7	L	1286	BPH	O2A-CGA-CBA	2.90	120.75	111.90
14	M	1314	CDL	OB8-CB7-C71	2.92	120.79	111.90
7	M	1311	BPH	C2B-C1B-NB	2.96	114.17	109.73
7	L	1286	BPH	CED-O2D-CGD	3.08	123.21	115.99
5	M	1304	BCL	O2A-CGA-CBA	3.10	121.36	111.90
5	L	1288	BCL	CED-O2D-CGD	3.11	123.28	115.99
12	M	1312	U10	C35-C34-C36	3.25	120.37	115.41
5	M	1304	BCL	CED-O2D-CGD	3.36	123.87	115.99
5	L	1288	BCL	O2A-CGA-CBA	3.39	122.22	111.90
5	L	1282	BCL	C4-C3-C5	3.42	120.64	115.41
14	M	1314	CDL	OB6-CB5-C51	3.61	119.37	111.53
8	L	1287[A]	UQ2	C10-C9-C11	3.66	120.99	115.41
13	M	1313	SPO	C29-C28-C30	3.78	121.17	115.41
7	M	1311	BPH	C3C-C4C-NC	4.07	112.00	107.93
5	L	1282	BCL	CMB-C2B-C3B	4.08	133.07	125.09
12	M	1312	U10	C10-C9-C11	4.10	121.67	115.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	M	1303	BCL	CMB-C2B-C3B	4.36	133.62	125.09
5	M	1304	BCL	CMB-C2B-C3B	4.39	133.68	125.09
5	L	1288	BCL	CMB-C2B-C3B	4.45	133.80	125.09
7	L	1286	BPH	C3C-C4C-NC	4.47	112.41	107.93
5	L	1288	BCL	O2D-CGD-CBD	5.09	118.28	111.30
14	M	1314	CDL	OA6-CA5-C11	5.22	122.88	111.53
12	M	1312	U10	C30-C29-C31	5.28	123.47	115.41
5	M	1304	BCL	O2D-CGD-CBD	5.63	119.02	111.30
5	M	1303	BCL	O2D-CGD-CBD	6.28	119.91	111.30
7	L	1286	BPH	O2D-CGD-CBD	7.22	121.21	111.30
7	M	1311	BPH	O2D-CGD-CBD	7.23	121.22	111.30
5	L	1282	BCL	O2D-CGD-CBD	7.38	121.43	111.30
14	M	1314	CDL	C12-C11-CA5	10.73	155.76	113.59
14	M	1314	CDL	C20-C19-C18	11.97	176.33	114.53
14	M	1314	CDL	C34-C33-C32	12.10	177.02	114.53
14	M	1314	CDL	C35-C34-C33	12.27	177.91	114.53
14	M	1314	CDL	C17-C16-C15	12.30	178.05	114.53
14	M	1314	CDL	C13-C12-C11	12.51	159.15	113.29
14	M	1314	CDL	C33-C32-C31	17.88	178.87	113.29

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	1288	BCL	C8
5	L	1288	BCL	C13

There are no torsion outliers.

There are no ring outliers.

20 monomers are involved in 72 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	H	1251	GOL	1	0
5	L	1282	BCL	4	0
6	L	1283	LDA	1	0
6	L	1284	LDA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	L	1285	LDA	4	0
7	L	1286	BPH	7	0
8	L	1287[A]	UQ2	5	0
8	L	1287[B]	UQ2	1	0
5	L	1288	BCL	5	0
4	L	1291	GOL	1	0
5	M	1303	BCL	11	0
5	M	1304	BCL	15	0
6	M	1305	LDA	3	0
6	M	1307	LDA	5	0
6	M	1308	LDA	2	0
6	M	1309	LDA	3	0
7	M	1311	BPH	12	0
13	M	1313	SPO	4	0
14	M	1314	CDL	2	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%)	-0.35	9 (3%)	45	50	33, 43, 53, 85	0
2	L	281/281 (100%)	-0.49	8 (2%)	56	61	30, 39, 61, 68	0
3	M	303/307 (98%)	-0.33	15 (4%)	32	37	29, 44, 69, 76	0
All	All	825/848 (97%)	-0.39	32 (3%)	43	48	29, 42, 63, 85	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	250	SER	6.6
3	M	1	ALA	5.7
1	H	249	LYS	4.7
1	H	251	VAL	4.7
3	M	148	TRP	4.5
3	M	302	GLY	4.0
3	M	301	HIS	4.0
2	L	59	TRP	4.0
3	M	2	GLU	3.7
3	M	303	MET	3.6
3	M	52	LEU	3.3
1	H	247	LYS	3.0
2	L	281	GLY	2.9
3	M	106	ALA	2.9
2	L	271	TRP	2.8
3	M	80	TRP	2.8
2	L	270	PRO	2.7
2	L	72	GLU	2.7
1	H	245	ALA	2.6
1	H	51	ALA	2.6
3	M	27	ALA	2.6
3	M	100	GLU	2.5
3	M	3	TYR	2.4

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Mol	Chain	Res	Type	RSRZ
1	H	246	PRO	2.4
1	H	220[A]	LYS	2.3
2	L	202	LYS	2.3
2	L	276	PRO	2.2
1	H	18	TYR	2.2
3	M	79	GLY	2.2
3	M	101	TYR	2.1
3	M	82	PRO	2.1
2	L	51	TRP	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
6	LDA	L	1285	16/16	0.67	0.41	81.15	106,109,111,111	0
6	LDA	M	1309	16/16	0.12	0.55	23.00	94,102,110,110	0
6	LDA	M	1308	16/16	0.53	0.39	20.13	90,97,105,105	0
10	HTO	L	1290	10/10	0.74	0.36	10.78	74,77,77,78	0
6	LDA	L	1283	16/16	0.27	0.48	9.55	86,103,111,111	0
4	GOL	H	1251	6/6	0.83	0.23	9.00	65,68,70,71	0
6	LDA	M	1305	16/16	0.80	0.28	8.47	50,63,70,71	0
6	LDA	L	1284	16/16	0.59	0.32	8.26	98,102,109,109	0
8	UQ2	L	1287[B]	23/23	0.84	0.31	6.00	40,43,47,48	23
8	UQ2	L	1287[A]	23/23	0.84	0.31	5.82	39,42,51,52	23
6	LDA	M	1306	16/16	0.80	0.33	5.02	72,74,84,84	0
14	CDL	M	1314	81/100	0.50	0.50	4.78	96,107,120,121	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
6	LDA	M	1307	16/16	0.80	0.24	2.91	64,68,77,77	0
13	SPO	M	1313	42/42	0.86	0.21	2.82	38,51,68,71	0
4	GOL	L	1292	6/6	0.80	0.25	2.26	85,87,87,87	0
7	BPH	M	1311	65/65	0.91	0.17	1.67	35,42,94,95	0
12	U10	M	1312	48/63	0.93	0.15	1.47	30,39,68,69	0
5	BCL	M	1304	66/66	0.97	0.16	1.01	25,31,53,59	0
5	BCL	M	1303	66/66	0.96	0.14	0.82	26,31,80,81	0
7	BPH	L	1286	65/65	0.98	0.13	0.75	25,30,39,40	0
9	PO4	L	1289	5/5	0.95	0.26	0.69	103,103,103,103	0
4	GOL	L	1291	6/6	0.90	0.18	0.58	47,52,53,54	0
5	BCL	L	1288	66/66	0.97	0.13	0.39	25,30,48,52	0
5	BCL	L	1282	66/66	0.97	0.12	-0.08	30,34,51,54	0
11	FE	M	1310	1/1	0.99	0.02	-3.81	32,32,32,32	0
4	GOL	H	1253	6/6	0.74	0.41	-	102,103,104,104	0
4	GOL	M	1315	6/6	0.80	0.22	-	85,86,86,87	0
6	LDA	M	1709	16/16	0.40	0.49	-	92,100,107,107	0
4	GOL	H	1254	6/6	0.79	0.21	-	102,102,103,103	0
4	GOL	H	1252	6/6	0.88	0.31	-	88,89,89,89	0

6.5 Other polymers [i](#)

There are no such residues in this entry.