



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:49 AM GMT

PDB ID : 2UX3  
Title : X-RAY HIGH RESOLUTION STRUCTURE OF THE PHOTOSYNTHETIC  
REACTION CENTER FROM RB. SPHAEROIDES AT PH 9 IN THE NEU-  
TRAL STATE  
Authors : Koepke, J.; Diehm, R.; Fritzsche, G.  
Deposited on : 2007-03-26  
Resolution : 2.50 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](mailto: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

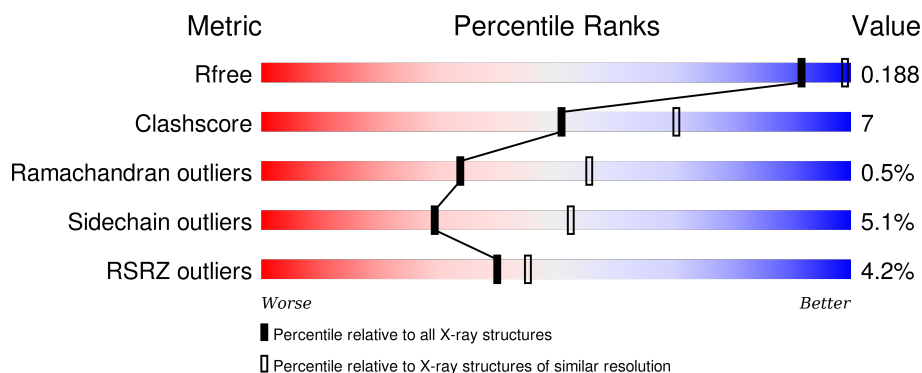
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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  $\geq 3$ , 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>82% 9% • 7%</div> </div>
2	L	281	<div> <div>4%</div> <div>84% 15% •</div> </div>
3	M	307	<div> <div>5%</div> <div>82% 16% ••</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	1288	-	-	-	X
14	CDL	M	1316	-	-	-	X
4	GOL	H	1251	-	-	-	X
4	GOL	L	1290	-	-	-	X
5	BCL	L	1282	X	-	-	-
5	BCL	L	1286	X	-	-	-
5	BCL	M	1303	X	-	-	-
5	BCL	M	1304	X	-	-	-
6	LDA	L	1283	-	-	-	X
6	LDA	L	1711	-	-	-	X
6	LDA	M	1305	-	-	-	X
6	LDA	M	1306	-	-	-	X
6	LDA	M	1309	-	-	-	X
6	LDA	M	1310	-	-	-	X
6	LDA	M	1311	-	-	-	X
8	UQ2	L	1285[A]	-	-	-	X
8	UQ2	L	1285[B]	-	-	-	X

## 2 Entry composition [i](#)

There are 15 unique types of molecules in this entry. The entry contains 7606 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.

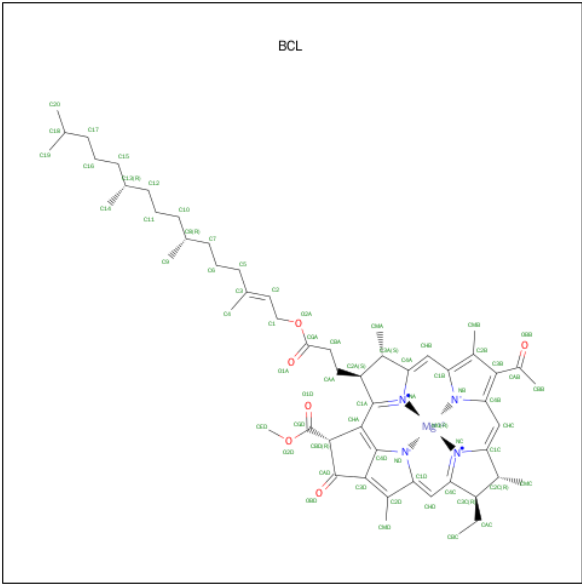
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	M	303	Total	C	N	O	S	0	1	1
			2419	1616	396	397	10			

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



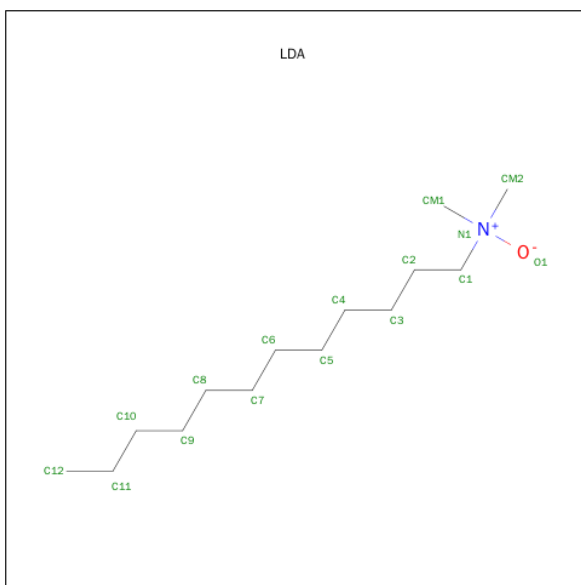
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	H	1	Total	C	O	0	0
			6	3	3		
4	H	1	Total	C	O	0	0
			6	3	3		
4	H	1	Total	C	O	0	0
			6	3	3		
4	H	1	Total	C	O	0	0
			6	3	3		
4	L	1	Total	C	O	0	0
			6	3	3		
4	L	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is BACTERIOCHLOROPHYLL A (three-letter code: BCL) (formula: C<sub>55</sub>H<sub>74</sub>MgN<sub>4</sub>O<sub>6</sub>).



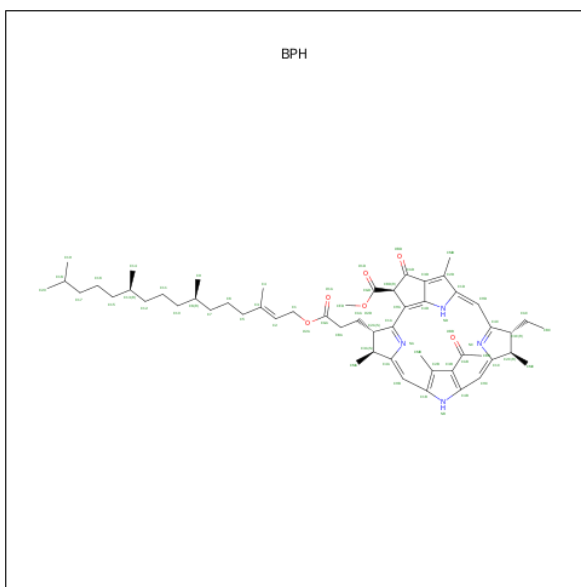
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
5	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
5	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
5	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

- Molecule 6 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula: C<sub>14</sub>H<sub>31</sub>NO).



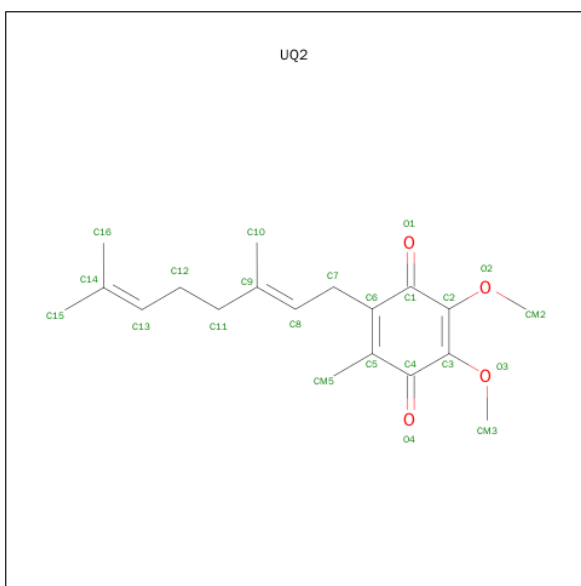
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	L	1	Total	C	N	O	0	0
			16	14	1	1		
6	L	1	Total	C	N	O	0	0
			16	14	1	1		
6	M	1	Total	C	N	O	0	0
			16	14	1	1		
6	M	1	Total	C	N	O	0	0
			16	14	1	1		
6	M	1	Total	C	N	O	0	0
			16	14	1	1		
6	M	1	Total	C	N	O	0	0
			16	14	1	1		
6	M	1	Total	C	N	O	0	0
			16	14	1	1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

- Molecule 7 is BACTERIOPHEOPHYTIN A (three-letter code: BPH) (formula: C<sub>55</sub>H<sub>76</sub>N<sub>4</sub>O<sub>6</sub>).



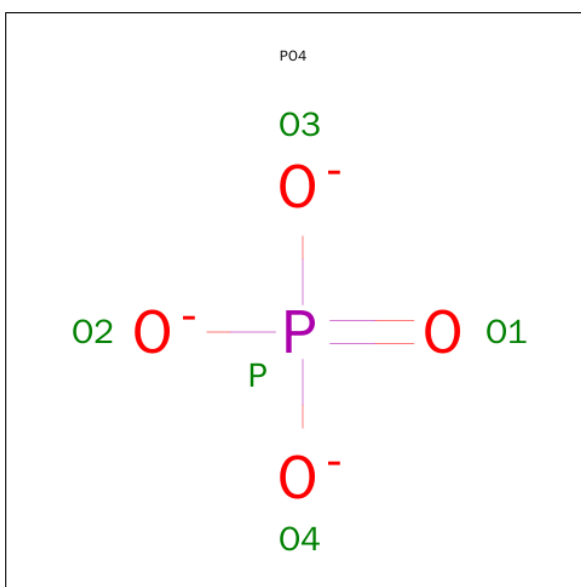
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	L	1	Total	C	N	O	0	0
			65	55	4	6		
7	M	1	Total	C	N	O	0	0
			65	55	4	6		

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



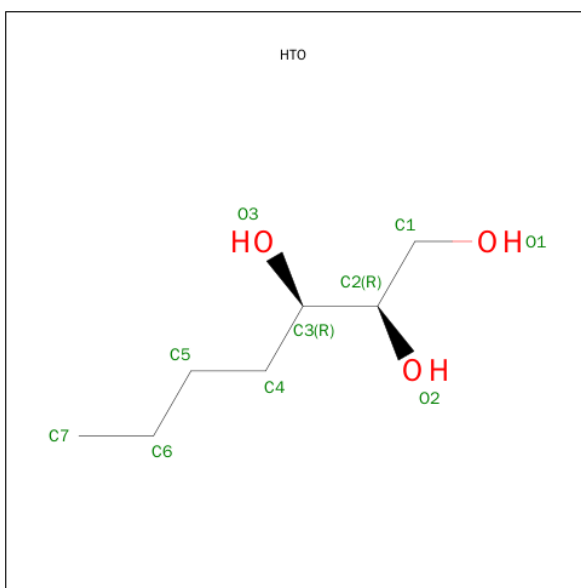
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	L	1	Total	C	O	0	1
			46	38	8		

- 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<sub>7</sub>H<sub>16</sub>O<sub>3</sub>).



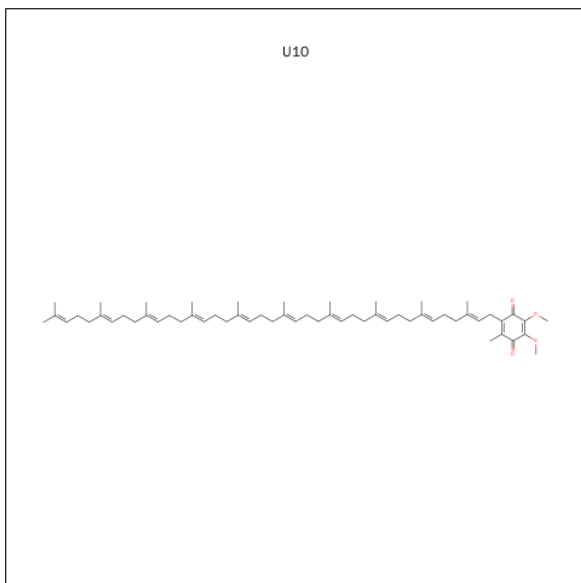
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	L	1	Total	C	O	0	0
			10	7	3		

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



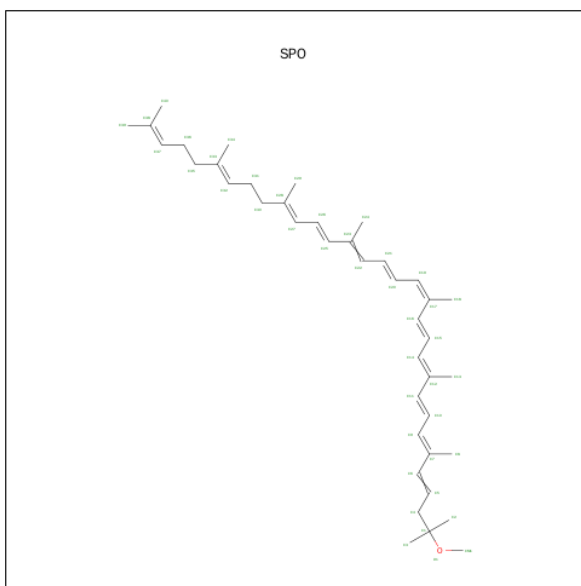
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	M	1	Total	Fe	0	0
			1	1		

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



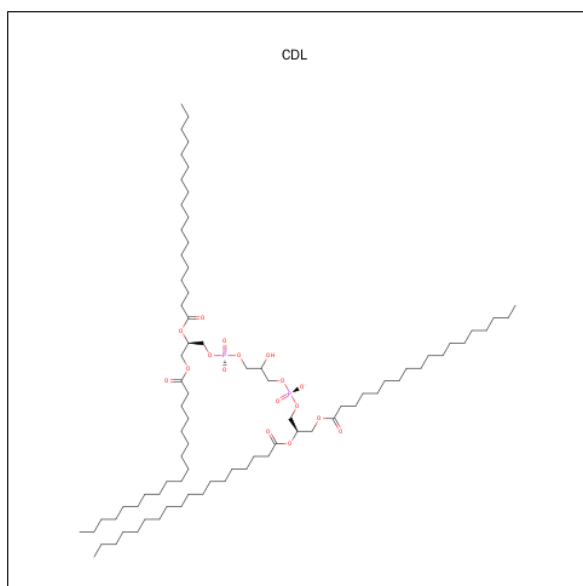
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	M	1	Total	C	O	0	0
			48	44	4		

- 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		

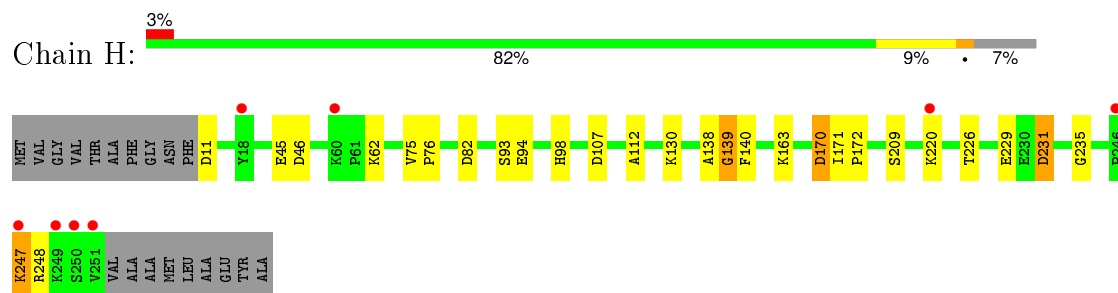
- Molecule 15 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	H	114	Total	O	0	0
			114	114		
15	L	92	Total	O	0	0
			92	92		
15	M	96	Total	O	0	0
			96	96		

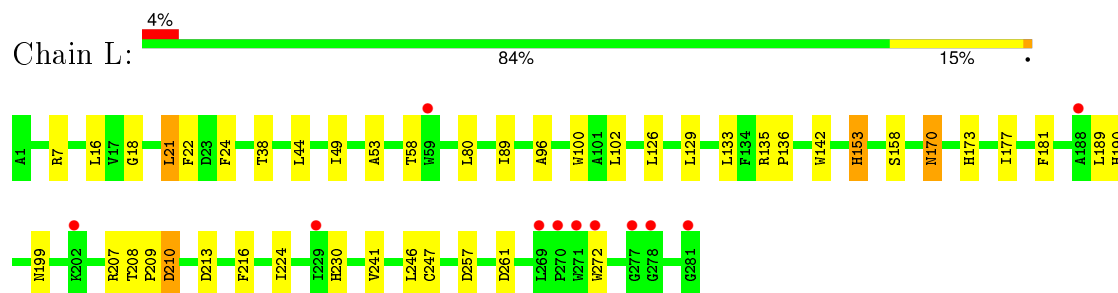
### 3 Residue-property plots [i](#)

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.

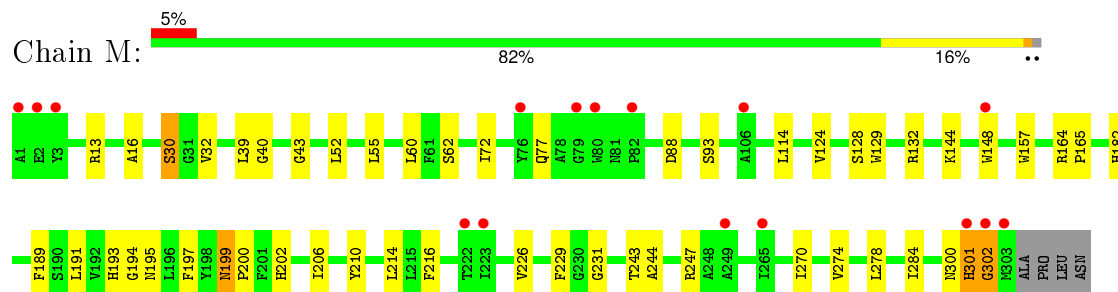
#### • Molecule 1: REACTION CENTER PROTEIN H CHAIN



#### • 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, $\alpha$ , $\beta$ , $\gamma$	139.45Å 139.45Å 184.58Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	119.52 – 2.50 36.90 – 2.50	Depositor EDS
% Data completeness (in resolution range)	92.1 (119.52-2.50) 86.6 (36.90-2.50)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.79 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, $R_{free}$	0.185 , 0.221 0.182 , 0.188	Depositor DCC
$R_{free}$ test set	2004 reflections (3.31%)	DCC
Wilson B-factor (Å <sup>2</sup> )	44.7	Xtriage
Anisotropy	0.190	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 49.3	EDS
Estimated twinning fraction	0.021 for -h,-k,l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 66473 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	7606	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.99% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BCL, GOL, LDA, CDL, BPH, PO4, HTO, FE, SPO, U10, UQ2

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	H	0.63	0/1906	0.78	7/2591 (0.3%)
2	L	0.66	0/2320	0.68	4/3175 (0.1%)
3	M	0.61	0/2517	0.68	2/3438 (0.1%)
All	All	0.63	0/6743	0.71	13/9204 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	M	0	1

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	82	ASP	CB-CG-OD2	7.62	125.16	118.30
1	H	11	ASP	CB-CG-OD2	7.00	124.60	118.30
2	L	213	ASP	CB-CG-OD2	6.80	124.42	118.30
1	H	139	GLY	N-CA-C	-5.99	98.13	113.10
2	L	210	ASP	CB-CG-OD1	5.96	123.67	118.30
1	H	231	ASP	CB-CG-OD2	5.63	123.36	118.30
3	M	88	ASP	CB-CG-OD2	5.47	123.23	118.30
2	L	257	ASP	CB-CG-OD2	5.43	123.19	118.30
1	H	107	ASP	CB-CG-OD2	5.38	123.14	118.30
2	L	261	ASP	CB-CG-OD2	5.14	122.92	118.30
1	H	170	ASP	CB-CG-OD2	5.13	122.92	118.30
1	H	46	ASP	CB-CG-OD2	5.09	122.88	118.30
3	M	302	GLY	O-C-N	-5.00	114.70	122.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	M	300	ASN	Peptide

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	H	1846	0	1861	13	0
2	L	2232	0	2187	28	0
3	M	2419	0	2327	28	0
4	H	24	0	32	1	0
4	L	12	0	16	1	0
5	L	132	0	148	8	0
5	M	132	0	148	18	0
6	L	32	0	62	2	0
6	M	112	0	217	2	0
7	L	65	0	76	9	0
7	M	65	0	76	14	0
8	L	46	0	52	8	0
9	L	5	0	0	0	0
10	L	10	0	16	2	0
11	M	1	0	0	0	0
12	M	48	0	63	2	0
13	M	42	0	60	3	0
14	M	81	0	82	3	0
15	H	114	0	0	0	1
15	L	92	0	0	0	0
15	M	96	0	0	0	0
All	All	7606	0	7423	101	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (101) 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:224:ILE:HG22	8:L:1285[A]:UQ2:H8	1.61	0.83
8:L:1285[A]:UQ2:H161	6:L:1711:LDA:H121	1.62	0.81
3:M:197:PHE:HZ	5:M:1304:BCL:HBB2	1.46	0.79
2:L:181:PHE:CD2	7:M:1313:BPH:HBB1	2.18	0.78
3:M:197:PHE:CZ	5:M:1304:BCL:HBB2	2.18	0.78
1:H:62:LYS:HE3	4:H:1251:GOL:H11	1.64	0.78
5:M:1303:BCL:H62	7:M:1313:BPH:HMB1	1.66	0.78
3:M:16:ALA:HB1	3:M:32:VAL:HG11	1.66	0.75
7:L:1284:BPH:HBB2	3:M:210:TYR:HB3	1.75	0.69
7:L:1284:BPH:HHC	7:L:1284:BPH:CBB	2.22	0.69
2:L:181:PHE:HB3	7:M:1313:BPH:HBB2	1.74	0.69
7:L:1284:BPH:HBB3	7:L:1284:BPH:HHC	1.76	0.66
7:M:1313:BPH:HHC	7:M:1313:BPH:HBB3	1.76	0.65
3:M:157:TRP:HB2	5:M:1304:BCL:H71	1.78	0.65
3:M:144:LYS:N	14:M:1316:CDL:OB3	2.26	0.65
2:L:170:ASN:C	2:L:170:ASN:HD22	2.01	0.64
3:M:77:GLN:HE22	3:M:93:SER:H	1.44	0.63
5:M:1303:BCL:HBB3	5:M:1304:BCL:H41	1.79	0.62
7:M:1313:BPH:HBC2	7:M:1313:BPH:HHD	1.80	0.62
2:L:199:ASN:HA	4:L:1289:GOL:H31	1.82	0.61
2:L:199:ASN:O	14:M:1316:CDL:HB22	2.00	0.60
5:M:1303:BCL:H62	7:M:1313:BPH:CMB	2.32	0.59
2:L:181:PHE:HB3	7:M:1313:BPH:CBB	2.33	0.59
1:H:140:PHE:HA	3:M:13:ARG:O	2.03	0.58
2:L:190:HIS:HA	8:L:1285[A]:UQ2:O4	2.04	0.58
5:M:1303:BCL:CBB	13:M:1315:SPO:H243	2.34	0.57
3:M:197:PHE:CE1	5:M:1304:BCL:HHC	2.40	0.57
8:L:1285[A]:UQ2:C16	6:L:1711:LDA:H121	2.34	0.56
6:M:1308:LDA:H71	12:M:1314:U10:H23	1.88	0.56
3:M:199:ASN:HD22	3:M:199:ASN:C	2.09	0.55
5:M:1304:BCL:HBB2	5:M:1304:BCL:HHC	1.90	0.54
3:M:62:SER:OG	3:M:124:VAL:HG22	2.07	0.54
3:M:189:PHE:O	3:M:193:HIS:HD2	1.90	0.53
5:M:1303:BCL:HBB2	13:M:1315:SPO:H243	1.90	0.52
5:L:1286:BCL:HMB1	5:L:1286:BCL:CBB	2.40	0.52
3:M:194:GLY:O	3:M:195:ASN:HB3	2.10	0.51
7:L:1284:BPH:HBB1	3:M:210:TYR:CD2	2.46	0.51
7:M:1313:BPH:HHC	7:M:1313:BPH:CBB	2.38	0.51
7:L:1284:BPH:CHC	7:L:1284:BPH:HBB3	2.40	0.51
5:M:1304:BCL:HAA2	5:M:1304:BCL:HBD	1.93	0.51
2:L:135:ARG:HB3	2:L:136:PRO:HD3	1.94	0.49
5:M:1304:BCL:CBB	5:M:1304:BCL:CHC	2.90	0.49

Continued on next page...

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:55:LEU:HD22	3:M:128:SER:HB2	1.95	0.48
5:L:1282:BCL:HBB3	5:L:1286:BCL:H52	1.95	0.47
2:L:133:LEU:HD13	10:L:1288:HTO:H62	1.95	0.47
8:L:1285[B]:UQ2:H8	8:L:1285[B]:UQ2:H5M1	1.96	0.47
7:L:1284:BPH:CHC	7:L:1284:BPH:CBB	2.91	0.47
3:M:243:THR:O	3:M:247:ARG:HG3	2.14	0.47
1:H:98:HIS:CD2	2:L:7:ARG:HH21	2.32	0.47
1:H:75:VAL:HA	1:H:76:PRO:C	2.36	0.47
2:L:224:ILE:CG2	8:L:1285[A]:UQ2:H8	2.40	0.46
3:M:164:ARG:HB3	3:M:165:PRO:HD3	1.98	0.46
7:M:1313:BPH:CHD	7:M:1313:BPH:HBC2	2.44	0.46
3:M:284:ILE:HG12	5:M:1304:BCL:HED3	1.97	0.46
1:H:209:SER:OG	1:H:247:LYS:HD3	2.16	0.46
3:M:229:PHE:HB2	3:M:244:ALA:HB2	1.98	0.46
2:L:38:THR:HG21	2:L:100:TRP:HE3	1.80	0.45
2:L:22:PHE:HA	2:L:24:PHE:CE2	2.52	0.45
3:M:129:TRP:O	3:M:132:ARG:HB3	2.16	0.45
6:M:1307:LDA:H112	12:M:1314:U10:H202	1.98	0.45
2:L:49:ILE:HG13	2:L:89:ILE:HD13	1.98	0.45
5:M:1304:BCL:CBB	5:M:1304:BCL:HHC	2.47	0.45
2:L:189:LEU:CD2	7:M:1313:BPH:HMD2	2.47	0.45
1:H:226:THR:OG1	1:H:229:GLU:HG3	2.17	0.45
1:H:45:GLU:HG3	1:H:94:GLU:OE1	2.16	0.45
5:L:1282:BCL:HHC	5:L:1282:BCL:HBB2	1.98	0.44
8:L:1285[A]:UQ2:H5M1	8:L:1285[A]:UQ2:H71	1.64	0.44
7:M:1313:BPH:HBB3	7:M:1313:BPH:CHC	2.47	0.44
2:L:96:ALA:HB1	7:L:1284:BPH:H2	2.00	0.44
2:L:241:VAL:HG21	7:L:1284:BPH:HBC3	2.00	0.44
5:M:1303:BCL:HBB1	13:M:1315:SPO:H243	2.00	0.43
1:H:98:HIS:HD2	2:L:7:ARG:HH21	1.67	0.43
1:H:171:ILE:N	1:H:172:PRO:HD2	2.33	0.43
5:L:1282:BCL:H161	5:L:1282:BCL:H122	1.64	0.43
5:M:1304:BCL:H61	7:M:1313:BPH:C4B	2.49	0.43
5:M:1303:BCL:H13	5:M:1303:BCL:H102	1.82	0.43
7:L:1284:BPH:ND	3:M:214:LEU:HD13	2.34	0.43
3:M:189:PHE:O	3:M:193:HIS:CD2	2.71	0.42
1:H:112:ALA:HA	1:H:235:GLY:O	2.19	0.42
2:L:190:HIS:CE1	2:L:230:HIS:CE1	3.07	0.42
1:H:138:ALA:HA	1:H:139:GLY:HA2	1.82	0.42
2:L:173:HIS:CE1	2:L:177:ILE:HD11	2.55	0.42
2:L:189:LEU:HD23	7:M:1313:BPH:HMD2	2.02	0.42

*Continued on next page...*



Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:M:1313:BPH:H142	7:M:1313:BPH:H111	1.95	0.42
3:M:199:ASN:HD22	3:M:200:PRO:N	2.18	0.42
1:H:98:HIS:CD2	2:L:7:ARG:HE	2.37	0.42
3:M:40:GLY:HA2	3:M:43:GLY:O	2.20	0.42
1:H:130:LYS:HE3	1:H:170:ASP:OD2	2.19	0.42
8:L:1285[B]:UQ2:C8	8:L:1285[B]:UQ2:H5M1	2.50	0.41
3:M:202:HIS:CE1	3:M:206:ILE:HD11	2.55	0.41
2:L:53:ALA:HB1	2:L:58:THR:O	2.19	0.41
3:M:148[B]:TRP:CD1	14:M:1316:CDL:HB62	2.56	0.41
5:L:1282:BCL:O1A	5:L:1282:BCL:H43	2.21	0.41
3:M:226:VAL:HG23	3:M:231:GLY:HA3	2.03	0.41
5:L:1286:BCL:C1C	5:M:1304:BCL:HBB3	2.51	0.41
2:L:142:TRP:CZ2	10:L:1288:HTO:H3	2.54	0.41
3:M:270:ILE:O	3:M:274:VAL:HG13	2.21	0.41
2:L:18:GLY:O	2:L:21:LEU:HB2	2.20	0.40
2:L:153:HIS:CD2	5:L:1282:BCL:NC	2.89	0.40
2:L:208:THR:HB	2:L:209:PRO:HD2	2.04	0.40
5:L:1286:BCL:HBB3	5:L:1286:BCL:HMB1	2.03	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:H:2033:HOH:O	15:H:2033:HOH:O[4_555]	2.10	0.10

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	242/260 (93%)	234 (97%)	7 (3%)	1 (0%)	39	61
2	L	279/281 (99%)	270 (97%)	9 (3%)	0	100	100

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	M	302/307 (98%)	286 (95%)	13 (4%)	3 (1%)	19	34
All	All	823/848 (97%)	790 (96%)	29 (4%)	4 (0%)	34	55

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	M	301	HIS
1	H	248	ARG
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%)	192 (97%)	6 (3%)	48	76
2	L	220/220 (100%)	204 (93%)	16 (7%)	17	32
3	M	237/240 (99%)	225 (95%)	12 (5%)	29	52
All	All	655/668 (98%)	621 (95%)	34 (5%)	29	51

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	93	SER
1	H	163	LYS
1	H	220[A]	LYS
1	H	220[B]	LYS
1	H	231	ASP
1	H	247	LYS
2	L	16	LEU
2	L	21	LEU
2	L	44	LEU
2	L	80	LEU
2	L	102	LEU

*Continued on next page...*

*Continued from previous page...*

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	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	39	LEU
3	M	52	LEU
3	M	60	LEU
3	M	72	ILE
3	M	114	LEU
3	M	182	HIS
3	M	191	LEU
3	M	199	ASN
3	M	216	PHE
3	M	278	LEU
3	M	301	HIS

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 29 ligands modelled in this entry, 1 is monoatomic - leaving 28 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	0.53	0	5,5,5	0.65	0
4	GOL	H	1252	-	5,5,5	0.37	0	5,5,5	0.33	0
4	GOL	H	1253	-	5,5,5	0.32	0	5,5,5	0.32	0
4	GOL	H	1254	-	5,5,5	0.31	0	5,5,5	0.30	0
5	BCL	L	1282	2	53,74,74	2.14	6 (11%)	57,115,115	2.13	13 (22%)
6	LDA	L	1283	-	15,15,15	3.76	1 (6%)	16,17,17	0.75	0
7	BPH	L	1284	-	64,70,70	2.97	17 (26%)	73,101,101	1.81	13 (17%)
8	UQ2	L	1285[A]	-	23,23,23	2.69	8 (34%)	28,31,31	1.68	6 (21%)
8	UQ2	L	1285[B]	-	23,23,23	2.79	7 (30%)	28,31,31	1.17	3 (10%)
5	BCL	L	1286	2	53,74,74	2.08	5 (9%)	57,115,115	1.92	12 (21%)
9	PO4	L	1287	-	4,4,4	0.44	0	6,6,6	0.27	0
10	HTO	L	1288	-	9,9,9	0.38	0	8,10,10	0.88	0
4	GOL	L	1289	-	5,5,5	0.32	0	5,5,5	0.33	0
4	GOL	L	1290	-	5,5,5	0.33	0	5,5,5	0.27	0
6	LDA	L	1711	-	15,15,15	3.95	2 (13%)	16,17,17	0.94	1 (6%)
5	BCL	M	1303	3	53,74,74	2.10	6 (11%)	57,115,115	1.86	10 (17%)
5	BCL	M	1304	3	53,74,74	2.09	6 (11%)	57,115,115	1.95	14 (24%)
6	LDA	M	1305	-	15,15,15	3.70	1 (6%)	16,17,17	1.10	2 (12%)
6	LDA	M	1306	-	15,15,15	3.71	2 (13%)	16,17,17	0.57	0
6	LDA	M	1307	-	15,15,15	3.77	2 (13%)	16,17,17	0.84	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	LDA	M	1308	-	15,15,15	3.79	2 (13%)	16,17,17	0.64	0
6	LDA	M	1309	-	15,15,15	3.84	2 (13%)	16,17,17	0.50	0
6	LDA	M	1310	-	15,15,15	3.78	2 (13%)	16,17,17	0.58	0
6	LDA	M	1311	-	15,15,15	3.74	2 (13%)	16,17,17	0.72	0
7	BPH	M	1313	-	64,70,70	3.01	17 (26%)	73,101,101	1.82	14 (19%)
12	U10	M	1314	-	48,48,63	3.08	12 (25%)	58,61,79	1.72	16 (27%)
13	SPO	M	1315	-	40,41,41	4.15	12 (30%)	45,50,50	2.05	13 (28%)
14	CDL	M	1316	-	80,80,99	2.31	18 (22%)	82,92,111	3.80	16 (19%)

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
7	BPH	L	1284	-	-	0/54/105/105	0/1/6/6
8	UQ2	L	1285[A]	-	-	0/15/39/39	0/1/1/1
8	UQ2	L	1285[B]	-	-	0/15/39/39	0/1/1/1
5	BCL	L	1286	2	2/2/21/25	0/37/137/137	0/0/9/9
9	PO4	L	1287	-	-	0/0/0/0	0/0/0/0
10	HTO	L	1288	-	-	0/10/10/10	0/0/0/0
4	GOL	L	1289	-	-	0/4/4/4	0/0/0/0
4	GOL	L	1290	-	-	0/4/4/4	0/0/0/0
6	LDA	L	1711	-	-	0/13/13/13	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
6	LDA	M	1310	-	-	0/13/13/13	0/0/0/0
6	LDA	M	1311	-	-	0/13/13/13	0/0/0/0
7	BPH	M	1313	-	-	0/54/105/105	0/1/6/6

Continued on next page...

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	U10	M	1314	-	-	0/45/69/87	0/1/1/1
13	SPO	M	1315	-	-	0/47/47/47	0/0/0/0
14	CDL	M	1316	-	-	0/91/91/110	0/0/0/0

All (130) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	L	1711	LDA	O1-N1	-15.02	1.25	1.39
6	M	1309	LDA	O1-N1	-14.59	1.25	1.39
6	M	1308	LDA	O1-N1	-14.38	1.25	1.39
6	L	1283	LDA	O1-N1	-14.36	1.25	1.39
6	M	1310	LDA	O1-N1	-14.34	1.25	1.39
6	M	1307	LDA	O1-N1	-14.24	1.26	1.39
6	M	1311	LDA	O1-N1	-14.24	1.26	1.39
6	M	1306	LDA	O1-N1	-14.09	1.26	1.39
6	M	1305	LDA	O1-N1	-14.06	1.26	1.39
14	M	1316	CDL	C11-CA5	-7.79	1.27	1.50
14	M	1316	CDL	C12-C11	-6.71	1.26	1.52
14	M	1316	CDL	C32-C31	-6.67	1.26	1.52
14	M	1316	CDL	C33-C32	-5.53	1.19	1.51
14	M	1316	CDL	C34-C33	-5.25	1.21	1.51
8	L	1285[A]	UQ2	O2-C2	-5.04	1.23	1.37
8	L	1285[B]	UQ2	O2-C2	-4.74	1.24	1.37
8	L	1285[B]	UQ2	O3-C3	-4.56	1.25	1.37
8	L	1285[A]	UQ2	O3-C3	-4.48	1.25	1.37
12	M	1314	U10	O4-C4	-4.43	1.25	1.37
14	M	1316	CDL	C16-C15	-4.34	1.26	1.51
7	M	1313	BPH	C3D-C4D	-4.30	1.35	1.41
14	M	1316	CDL	C17-C16	-4.27	1.26	1.51
14	M	1316	CDL	C20-C19	-4.25	1.27	1.51
14	M	1316	CDL	C19-C18	-4.18	1.27	1.51
12	M	1314	U10	O3-C3	-4.09	1.26	1.37
7	L	1284	BPH	C3D-CAD	-3.73	1.39	1.46
14	M	1316	CDL	C13-C12	-3.45	1.31	1.51
7	L	1284	BPH	C3D-C4D	-3.32	1.37	1.41
8	L	1285[A]	UQ2	C3-C4	-3.17	1.39	1.48
12	M	1314	U10	C4-C5	-3.13	1.39	1.48
8	L	1285[B]	UQ2	C3-C4	-3.09	1.40	1.48
7	M	1313	BPH	C3D-CAD	-3.09	1.40	1.46
7	M	1313	BPH	C1B-C2B	-3.04	1.39	1.45
14	M	1316	CDL	C37-C36	-3.04	1.34	1.51
6	M	1307	LDA	C1-N1	-3.02	1.45	1.51

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	M	1316	CDL	C79-C78	-2.94	1.34	1.51
14	M	1316	CDL	C22-C21	-2.91	1.34	1.51
14	M	1316	CDL	C80-C79	-2.86	1.35	1.51
7	L	1284	BPH	O2D-CGD	-2.71	1.26	1.33
7	M	1313	BPH	O2A-CGA	-2.71	1.25	1.33
12	M	1314	U10	C3-C2	-2.70	1.41	1.48
7	M	1313	BPH	O2D-CGD	-2.66	1.26	1.33
8	L	1285[B]	UQ2	C2-C1	-2.65	1.41	1.48
7	L	1284	BPH	C1B-C2B	-2.59	1.40	1.45
5	M	1303	BCL	O2D-CGD	-2.56	1.26	1.33
5	L	1282	BCL	O2A-CGA	-2.54	1.25	1.33
8	L	1285[A]	UQ2	C6-C1	-2.49	1.39	1.46
5	L	1282	BCL	C3D-CAD	-2.47	1.38	1.45
5	M	1304	BCL	C3C-C4C	-2.44	1.48	1.51
6	M	1310	LDA	C1-N1	-2.42	1.47	1.51
6	M	1309	LDA	C1-N1	-2.39	1.47	1.51
6	M	1306	LDA	C1-N1	-2.35	1.47	1.51
5	L	1282	BCL	O2D-CGD	-2.33	1.27	1.33
6	L	1711	LDA	C1-N1	-2.33	1.47	1.51
5	M	1304	BCL	O2D-CGD	-2.29	1.27	1.33
5	L	1286	BCL	C3D-CAD	-2.27	1.39	1.45
6	M	1308	LDA	C1-N1	-2.21	1.47	1.51
5	L	1286	BCL	O2D-CGD	-2.16	1.27	1.33
5	M	1303	BCL	C3D-CAD	-2.14	1.39	1.45
6	M	1311	LDA	C1-N1	-2.14	1.47	1.51
5	M	1304	BCL	C3D-CAD	-2.09	1.39	1.45
5	M	1303	BCL	O2A-CGA	-2.07	1.27	1.33
7	L	1284	BPH	O2A-CGA	-2.06	1.27	1.33
8	L	1285[A]	UQ2	C2-C1	-2.01	1.43	1.48
8	L	1285[A]	UQ2	C6-C5	2.01	1.40	1.35
7	L	1284	BPH	C1D-CHD	2.43	1.49	1.40
12	M	1314	U10	C6-C1	2.69	1.41	1.35
8	L	1285[B]	UQ2	C6-C5	2.81	1.41	1.35
7	M	1313	BPH	C1D-CHD	2.99	1.51	1.40
7	L	1284	BPH	CHD-C4C	3.43	1.46	1.38
7	M	1313	BPH	CHB-C4A	3.48	1.46	1.40
7	L	1284	BPH	C3D-C2D	3.62	1.48	1.40
5	M	1304	BCL	C2-C3	3.64	1.40	1.33
5	L	1282	BCL	C2-C3	3.76	1.40	1.33
7	L	1284	BPH	CHC-C4B	3.77	1.49	1.40
7	M	1313	BPH	CHD-C4C	3.83	1.47	1.38
13	M	1315	SPO	C21-C20	3.85	1.46	1.35

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	M	1313	BPH	CHC-C4B	3.95	1.50	1.40
5	M	1303	BCL	C2-C3	4.07	1.40	1.33
7	M	1313	BPH	C3D-C2D	4.12	1.50	1.40
7	L	1284	BPH	CHB-C4A	4.15	1.48	1.40
13	M	1315	SPO	C26-C25	4.23	1.45	1.34
14	M	1316	CDL	OA6-CA5	4.29	1.47	1.34
14	M	1316	CDL	OB8-CB7	4.46	1.46	1.33
5	L	1286	BCL	C2-C3	4.51	1.41	1.33
14	M	1316	CDL	OB6-CB5	4.61	1.48	1.34
13	M	1315	SPO	C15-C16	4.61	1.46	1.34
14	M	1316	CDL	OA8-CA7	4.66	1.47	1.33
13	M	1315	SPO	C10-C11	4.70	1.46	1.34
7	L	1284	BPH	CHC-C1C	4.90	1.46	1.36
12	M	1314	U10	C38-C39	5.09	1.47	1.32
13	M	1315	SPO	C6-C5	5.11	1.46	1.31
8	L	1285[A]	UQ2	C13-C14	5.14	1.48	1.32
8	L	1285[B]	UQ2	C13-C14	5.17	1.48	1.32
13	M	1315	SPO	C37-C38	5.49	1.49	1.32
5	L	1286	BCL	O1A-CGA	5.51	1.39	1.22
7	M	1313	BPH	O1A-CGA	5.78	1.39	1.22
7	M	1313	BPH	CHC-C1C	5.80	1.47	1.36
5	L	1282	BCL	O1A-CGA	5.83	1.40	1.22
5	M	1304	BCL	O1A-CGA	5.87	1.40	1.22
5	M	1303	BCL	O1A-CGA	6.15	1.41	1.22
7	L	1284	BPH	CHB-C1B	6.20	1.50	1.38
7	L	1284	BPH	O1A-CGA	6.24	1.41	1.22
7	M	1313	BPH	CHB-C1B	6.36	1.51	1.38
12	M	1314	U10	C18-C19	6.96	1.46	1.33
7	M	1313	BPH	O1D-CGD	7.10	1.39	1.21
12	M	1314	U10	C28-C29	7.10	1.46	1.33
7	L	1284	BPH	C2-C3	7.26	1.47	1.33
12	M	1314	U10	C23-C24	7.28	1.47	1.33
7	M	1313	BPH	C2-C3	7.70	1.48	1.33
7	L	1284	BPH	O1D-CGD	7.73	1.40	1.21
12	M	1314	U10	C8-C9	7.74	1.48	1.33
8	L	1285[A]	UQ2	C8-C9	7.79	1.48	1.33
13	M	1315	SPO	C32-C33	8.02	1.48	1.33
8	L	1285[B]	UQ2	C8-C9	8.19	1.49	1.33
7	M	1313	BPH	OBB-CAB	8.21	1.41	1.23
12	M	1314	U10	C13-C14	8.27	1.49	1.33
12	M	1314	U10	C33-C34	8.33	1.49	1.33
13	M	1315	SPO	C14-C12	8.36	1.46	1.35

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	L	1284	BPH	OBB-CAB	8.98	1.42	1.23
13	M	1315	SPO	C19-C17	9.07	1.47	1.35
13	M	1315	SPO	C22-C23	9.13	1.47	1.35
13	M	1315	SPO	C9-C7	9.40	1.48	1.35
7	L	1284	BPH	OBD-CAD	11.56	1.40	1.22
5	M	1303	BCL	OBD-CAD	11.80	1.40	1.22
5	M	1304	BCL	OBD-CAD	12.00	1.40	1.22
7	M	1313	BPH	OBD-CAD	12.08	1.40	1.22
5	L	1286	BCL	OBD-CAD	12.10	1.40	1.22
13	M	1315	SPO	C27-C28	12.51	1.47	1.34
5	L	1282	BCL	OBD-CAD	12.54	1.41	1.22

All (133) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	M	1304	BCL	CMB-C2B-C1B	-7.26	116.35	128.36
5	L	1286	BCL	CMB-C2B-C1B	-7.23	116.39	128.36
5	L	1282	BCL	CMB-C2B-C1B	-6.84	117.05	128.36
5	M	1303	BCL	CMB-C2B-C1B	-6.35	117.87	128.36
5	L	1282	BCL	O1D-CGD-CBD	-5.20	117.17	124.62
13	M	1315	SPO	C20-C19-C17	-5.00	119.97	127.20
7	M	1313	BPH	OBD-CAD-CBD	-4.54	119.09	125.94
7	L	1284	BPH	O1D-CGD-CBD	-4.53	118.13	124.62
7	L	1284	BPH	OBD-CAD-CBD	-4.52	119.12	125.94
13	M	1315	SPO	C21-C22-C23	-4.49	120.72	127.20
13	M	1315	SPO	C10-C9-C7	-4.44	120.79	127.20
7	M	1313	BPH	CHC-C4B-NB	-4.28	116.75	124.91
7	L	1284	BPH	OBD-CAD-C3D	-4.15	119.88	128.35
13	M	1315	SPO	C15-C14-C12	-3.77	121.75	127.20
8	L	1285[A]	UQ2	O1-C1-C6	-3.66	114.80	121.68
7	M	1313	BPH	O1D-CGD-CBD	-3.61	119.44	124.62
5	M	1303	BCL	C1D-CHD-C4C	-3.57	120.61	126.07
12	M	1314	U10	C27-C28-C29	-3.50	120.14	127.76
5	M	1303	BCL	O1D-CGD-CBD	-3.31	119.89	124.62
7	L	1284	BPH	C1C-NC-C4C	-3.27	107.09	110.44
12	M	1314	U10	C22-C23-C24	-3.26	120.68	127.76
8	L	1285[A]	UQ2	CM5-C5-C6	-3.05	117.57	124.10
5	L	1282	BCL	C1D-CHD-C4C	-2.99	121.50	126.07
7	M	1313	BPH	O2D-CGD-O1D	-2.98	117.64	123.79
13	M	1315	SPO	C4-C5-C6	-2.97	120.44	124.67
5	L	1282	BCL	CMD-C2D-C3D	-2.94	119.34	125.09
7	L	1284	BPH	CHC-C4B-NB	-2.88	119.43	124.91

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	M	1315	SPO	C5-C6-C7	-2.85	121.40	125.75
12	M	1314	U10	C30-C29-C28	-2.84	117.93	123.50
12	M	1314	U10	C17-C18-C19	-2.82	121.63	127.76
5	L	1286	BCL	CHC-C1C-NC	-2.71	120.76	124.51
7	M	1313	BPH	CMD-C2D-C3D	-2.67	119.87	125.09
13	M	1315	SPO	C31-C32-C33	-2.66	121.99	127.76
5	M	1303	BCL	OBD-CAD-CBD	-2.64	121.96	125.94
5	M	1304	BCL	O2D-CGD-O1D	-2.59	118.45	123.79
5	L	1282	BCL	CHA-C1A-NA	-2.55	119.77	126.06
5	L	1282	BCL	CHB-C4A-NA	-2.54	121.00	124.51
5	M	1304	BCL	CAC-C3C-C4C	-2.52	106.99	112.58
5	M	1304	BCL	C1D-CHD-C4C	-2.51	122.23	126.07
8	L	1285[B]	UQ2	C5-C6-C1	-2.45	117.33	120.12
6	L	1711	LDA	O1-N1-C1	-2.43	107.54	110.27
12	M	1314	U10	C32-C33-C34	-2.42	122.49	127.76
5	L	1286	BCL	C1D-CHD-C4C	-2.41	122.38	126.07
5	L	1286	BCL	CMD-C2D-C3D	-2.41	120.37	125.09
13	M	1315	SPO	C14-C15-C16	-2.41	115.79	123.13
5	M	1303	BCL	O2D-CGD-O1D	-2.40	118.84	123.79
5	M	1304	BCL	C16-C15-C13	-2.40	107.54	115.49
5	L	1286	BCL	O1D-CGD-CBD	-2.32	121.30	124.62
7	M	1313	BPH	C3B-C2B-C1B	-2.32	102.05	105.77
7	M	1313	BPH	OBD-CAD-C3D	-2.31	123.64	128.35
12	M	1314	U10	C11-C9-C8	-2.29	116.71	121.05
5	L	1282	BCL	O2A-CGA-O1A	-2.28	117.60	123.49
6	M	1305	LDA	CM2-N1-CM1	-2.25	106.29	108.83
7	L	1284	BPH	O2A-CGA-O1A	-2.25	117.70	123.49
5	M	1304	BCL	C7-C6-C5	-2.24	106.44	113.06
7	L	1284	BPH	C4D-C3D-C2D	-2.23	104.20	107.08
5	M	1303	BCL	CHA-C1A-NA	-2.19	120.67	126.06
5	M	1303	BCL	CAA-C2A-C3A	-2.18	106.94	113.22
5	M	1304	BCL	CMD-C2D-C3D	-2.17	120.85	125.09
13	M	1315	SPO	C27-C26-C25	-2.14	116.59	123.13
8	L	1285[A]	UQ2	O4-C4-C3	-2.10	116.25	120.79
14	M	1316	CDL	OB8-CB7-OB9	-2.07	118.15	123.49
5	L	1286	BCL	CHB-C4A-NA	-2.06	121.66	124.51
12	M	1314	U10	C12-C13-C14	-2.06	123.28	127.76
7	L	1284	BPH	CHB-C1B-NB	-2.04	120.84	124.66
8	L	1285[B]	UQ2	C10-C9-C8	-2.04	119.50	123.50
5	L	1286	BCL	O2D-CGD-O1D	-2.04	119.59	123.79
7	M	1313	BPH	C4-C3-C5	2.00	118.47	115.41
5	L	1286	BCL	C4-C3-C5	2.00	118.47	115.41

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	M	1316	CDL	C81-C80-C79	2.04	125.05	114.53
13	M	1315	SPO	C40-C38-C39	2.04	119.66	114.64
12	M	1314	U10	C4M-O4-C4	2.04	123.88	116.61
12	M	1314	U10	C41-C39-C40	2.07	119.72	114.64
5	L	1282	BCL	CAA-CBA-CGA	2.10	119.46	113.32
14	M	1316	CDL	C80-C79-C78	2.10	125.37	114.53
12	M	1314	U10	C3M-O3-C3	2.10	124.10	116.61
13	M	1315	SPO	C8-C7-C6	2.15	121.68	118.10
5	L	1282	BCL	C4A-NA-C1A	2.20	109.20	106.36
8	L	1285[A]	UQ2	C16-C14-C15	2.28	120.23	114.64
5	M	1304	BCL	OB8-CAB-C3B	2.28	123.62	120.00
14	M	1316	CDL	C32-C31-CA7	2.32	122.72	113.59
5	M	1304	BCL	CHD-C4C-NC	2.39	127.83	125.06
12	M	1314	U10	C20-C19-C21	2.39	119.06	115.41
8	L	1285[A]	UQ2	C10-C9-C11	2.40	119.08	115.41
5	L	1282	BCL	O2A-CGA-CBA	2.47	119.43	111.90
14	M	1316	CDL	CA6-OA8-CA7	2.53	123.91	116.85
12	M	1314	U10	C15-C14-C16	2.57	119.33	115.41
13	M	1315	SPO	C34-C33-C35	2.67	119.49	115.41
14	M	1316	CDL	OA8-CA7-C31	2.73	120.22	111.90
5	M	1303	BCL	O2A-CGA-CBA	2.77	120.34	111.90
8	L	1285[B]	UQ2	C10-C9-C11	2.80	119.69	115.41
7	M	1313	BPH	CED-O2D-CGD	2.82	122.61	115.99
7	M	1313	BPH	O2A-CGA-CBA	2.83	120.53	111.90
12	M	1314	U10	C35-C34-C36	2.90	119.84	115.41
5	L	1286	BCL	CED-O2D-CGD	2.93	122.86	115.99
5	M	1304	BCL	C4-C3-C5	2.93	119.88	115.41
7	L	1284	BPH	CED-O2D-CGD	2.93	122.87	115.99
5	M	1304	BCL	CED-O2D-CGD	3.03	123.09	115.99
7	L	1284	BPH	O2A-CGA-CBA	3.05	121.19	111.90
14	M	1316	CDL	OB8-CB7-C71	3.08	121.28	111.90
7	M	1313	BPH	CAC-C3C-C4C	3.14	120.73	112.67
12	M	1314	U10	C25-C24-C26	3.15	120.22	115.41
7	L	1284	BPH	C2B-C1B-NB	3.18	114.50	109.73
7	M	1313	BPH	C2B-C1B-NB	3.18	114.50	109.73
7	M	1313	BPH	C3C-C4C-NC	3.29	111.22	107.93
6	M	1305	LDA	O1-N1-C1	3.37	114.06	110.27
12	M	1314	U10	C10-C9-C11	3.41	120.62	115.41
5	L	1282	BCL	C4-C3-C5	3.55	120.82	115.41
5	M	1304	BCL	O2A-CGA-CBA	3.55	122.71	111.90
5	L	1286	BCL	O2A-CGA-CBA	3.57	122.77	111.90
13	M	1315	SPO	C29-C28-C30	3.65	120.98	115.41

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	L	1285[A]	UQ2	CM3-O3-C3	3.78	130.06	116.61
5	M	1303	BCL	CMB-C2B-C3B	4.12	133.14	125.09
5	L	1282	BCL	CMB-C2B-C3B	4.14	133.18	125.09
14	M	1316	CDL	OB6-CB5-C51	4.42	121.14	111.53
5	L	1286	BCL	CMB-C2B-C3B	4.47	133.84	125.09
5	M	1304	BCL	CMB-C2B-C3B	4.66	134.21	125.09
7	L	1284	BPH	C3C-C4C-NC	4.97	112.91	107.93
14	M	1316	CDL	OA6-CA5-C11	5.02	122.44	111.53
12	M	1314	U10	C30-C29-C31	5.07	123.15	115.41
5	M	1304	BCL	O2D-CGD-CBD	5.67	119.08	111.30
5	L	1286	BCL	O2D-CGD-CBD	5.70	119.12	111.30
7	L	1284	BPH	O2D-CGD-CBD	6.58	120.33	111.30
5	M	1303	BCL	O2D-CGD-CBD	7.26	121.26	111.30
5	L	1282	BCL	O2D-CGD-CBD	7.73	121.90	111.30
7	M	1313	BPH	O2D-CGD-CBD	8.45	122.89	111.30
14	M	1316	CDL	C35-C34-C33	10.39	168.17	114.53
14	M	1316	CDL	C34-C33-C32	10.46	168.54	114.53
14	M	1316	CDL	C13-C12-C11	10.64	152.29	113.29
14	M	1316	CDL	C20-C19-C18	11.33	173.01	114.53
14	M	1316	CDL	C17-C16-C15	11.59	174.41	114.53
14	M	1316	CDL	C12-C11-CA5	12.16	161.41	113.59
14	M	1316	CDL	C33-C32-C31	17.49	177.43	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	M	1304	BCL	C8
5	M	1304	BCL	C13
5	L	1286	BCL	C8
5	L	1286	BCL	C13
5	L	1282	BCL	C8
5	L	1282	BCL	C13

There are no torsion outliers.

There are no ring outliers.

17 monomers are involved in 62 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	H	1251	GOL	1	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	L	1282	BCL	5	0
7	L	1284	BPH	9	0
8	L	1285[A]	UQ2	6	0
8	L	1285[B]	UQ2	2	0
5	L	1286	BCL	4	0
10	L	1288	HTO	2	0
4	L	1289	GOL	1	0
6	L	1711	LDA	2	0
5	M	1303	BCL	7	0
5	M	1304	BCL	12	0
6	M	1307	LDA	1	0
6	M	1308	LDA	1	0
7	M	1313	BPH	14	0
12	M	1314	U10	2	0
13	M	1315	SPO	3	0
14	M	1316	CDL	3	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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	H	241/260 (92%)	-0.21	8 (3%)	50	55	38, 48, 61, 105	0
2	L	281/281 (100%)	-0.27	11 (3%)	43	48	35, 44, 69, 77	0
3	M	303/307 (98%)	0.03	16 (5%)	30	34	33, 50, 73, 86	0
All	All	825/848 (97%)	-0.14	35 (4%)	40	45	33, 47, 72, 105	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	M	1	ALA	7.5
1	H	250	SER	6.4
1	H	249	LYS	5.6
3	M	303	MET	5.3
1	H	246	PRO	4.5
2	L	59	TRP	4.0
1	H	251	VAL	3.6
2	L	281	GLY	3.2
3	M	2	GLU	3.1
2	L	277	GLY	3.1
3	M	80	TRP	3.0
1	H	247	LYS	2.9
1	H	220[A]	LYS	2.9
3	M	148[A]	TRP	2.9
3	M	301	HIS	2.8
1	H	60	LYS	2.8
3	M	79	GLY	2.8
2	L	270	PRO	2.8
3	M	223	ILE	2.8
2	L	278	GLY	2.7
2	L	271	TRP	2.6
2	L	202	LYS	2.5
3	M	106	ALA	2.5

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
3	M	82	PRO	2.5
1	H	18	TYR	2.4
3	M	249	ALA	2.4
2	L	272	TRP	2.3
3	M	265	ILE	2.3
3	M	302	GLY	2.2
2	L	188	ALA	2.1
2	L	229	ILE	2.1
2	L	269	LEU	2.0
3	M	3	TYR	2.0
3	M	76	TYR	2.0
3	M	222	THR	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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
6	LDA	M	1311	16/16	0.08	0.62	21.54	115,118,122,122	0
6	LDA	L	1711	16/16	0.51	0.47	11.23	108,112,117,117	0
6	LDA	L	1283	16/16	0.64	0.37	10.43	78,103,114,115	0
10	HTO	L	1288	10/10	0.77	0.46	9.85	83,85,85,86	0
6	LDA	M	1309	16/16	0.56	0.50	9.39	118,120,126,126	0
6	LDA	M	1310	16/16	0.24	0.63	8.47	101,111,118,118	0
4	GOL	H	1251	6/6	0.80	0.31	7.66	70,75,76,76	0
4	GOL	L	1290	6/6	0.79	0.37	7.54	98,99,99,100	0
6	LDA	M	1306	16/16	0.87	0.42	5.10	70,74,86,87	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
6	LDA	M	1305	16/16	0.80	0.31	3.80	70,80,85,85	0
14	CDL	M	1316	81/100	0.67	0.45	3.39	91,107,125,126	0
8	UQ2	L	1285[B]	23/23	0.86	0.32	2.95	42,47,53,54	23
8	UQ2	L	1285[A]	23/23	0.86	0.32	2.84	38,44,54,55	23
13	SPO	M	1315	42/42	0.89	0.21	1.81	44,57,77,80	0
12	U10	M	1314	48/63	0.89	0.26	1.23	36,47,75,78	0
4	GOL	L	1289	6/6	0.88	0.25	1.17	65,69,70,73	0
6	LDA	M	1307	16/16	0.87	0.21	1.13	68,70,76,77	0
7	BPH	M	1313	65/65	0.92	0.21	1.00	38,45,98,99	0
5	BCL	M	1304	66/66	0.98	0.17	0.71	30,36,58,65	0
5	BCL	M	1303	66/66	0.98	0.15	0.70	30,36,89,90	0
7	BPH	L	1284	65/65	0.98	0.14	0.38	29,36,45,48	0
5	BCL	L	1286	66/66	0.97	0.12	0.23	30,38,51,56	0
5	BCL	L	1282	66/66	0.97	0.14	-0.02	29,35,58,61	0
9	PO4	L	1287	5/5	0.97	0.12	-0.42	100,100,101,101	0
11	FE	M	1312	1/1	0.99	0.09	-3.39	34,34,34,34	0
6	LDA	M	1308	16/16	0.67	0.37	-	96,99,107,108	0
4	GOL	H	1252	6/6	0.77	0.32	-	93,94,94,95	0
4	GOL	H	1253	6/6	0.59	0.36	-	103,104,106,106	0
4	GOL	H	1254	6/6	0.85	0.22	-	92,93,93,93	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.