



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:49 AM GMT

PDB ID : 2UWW
Title : X-RAY HIGH RESOLUTION STRUCTURE OF THE PHOTOSYNTHETIC REACTION CENTER FROM RB. SPHAEROIDES AT PH 6.5 IN THE NEUTRAL STATE
Authors : Koepke, J.; Diehm, R.; Fritzsche, G.
Deposited on : 2007-03-23
Resolution : 2.05 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

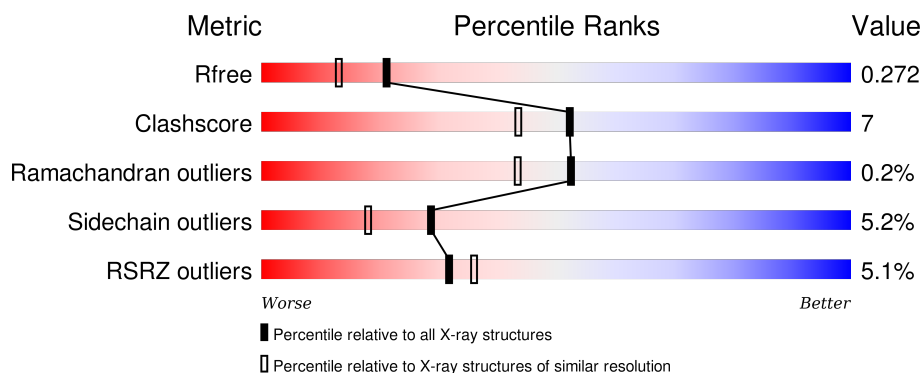
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

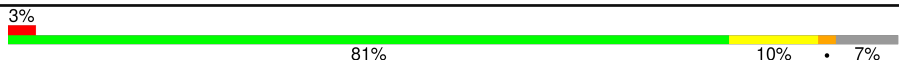


The reported resolution of this entry is 2.05 Å.

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	1192 (2.04-2.04)
Clashscore	102246	1269 (2.04-2.04)
Ramachandran outliers	100387	1258 (2.04-2.04)
Sidechain outliers	100360	1258 (2.04-2.04)
RSRZ outliers	91569	1194 (2.04-2.04)

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	1292	-	-	-	X
13	SPO	M	1313	-	-	-	X
14	CDL	M	1314	-	-	-	X
4	GOL	H	1252	-	-	X	X
5	BCL	L	1282	X	-	-	-
5	BCL	L	1290	X	-	-	-
5	BCL	M	1304	X	-	-	-
5	BCL	M	1305	X	-	-	-
6	LDA	L	1283	-	-	-	X
6	LDA	L	1284	-	-	-	X
6	LDA	L	1285	-	-	-	X
6	LDA	L	1286	-	-	-	X
6	LDA	L	1287	-	-	-	X
6	LDA	M	1306	-	-	-	X
6	LDA	M	1307	-	-	-	X
6	LDA	M	1308	-	-	-	X
8	UQ2	L	1289[A]	-	-	-	X
8	UQ2	L	1289[B]	-	-	-	X

2 Entry composition [i](#)

There are 15 unique types of molecules in this entry. The entry contains 7772 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	0	1
			1830	1169	315	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.

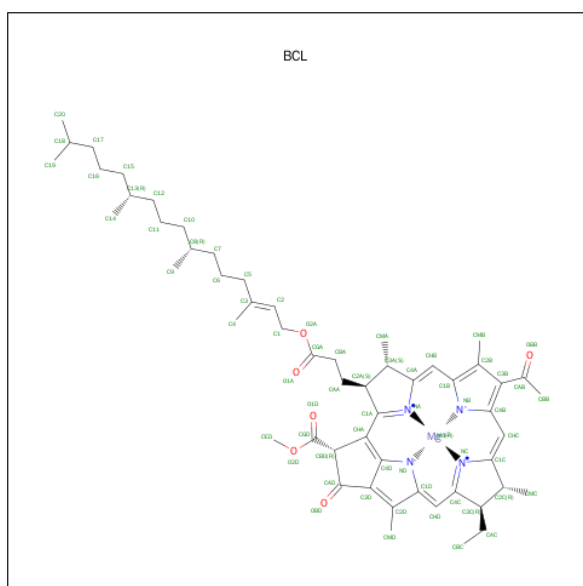
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	M	303	Total	C	N	O	S	0	0	1
			2409	1607	395	397	10			

- 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		

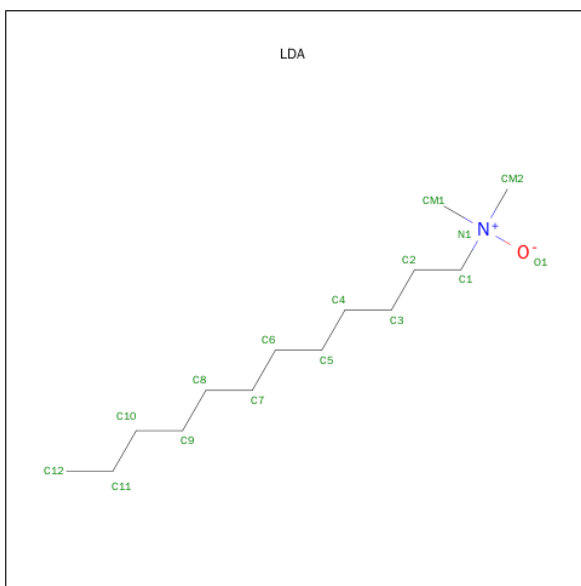
- Molecule 5 is BACTERIOCHLOROPHYLL A (three-letter code: BCL) (formula: $C_{55}H_{74}MgN_4O_6$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	L	1	Total 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

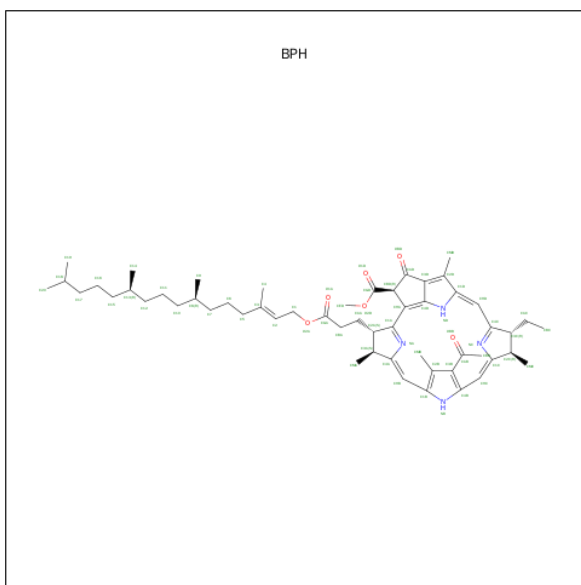
- Molecule 6 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula:

C₁₄H₃₁NO).



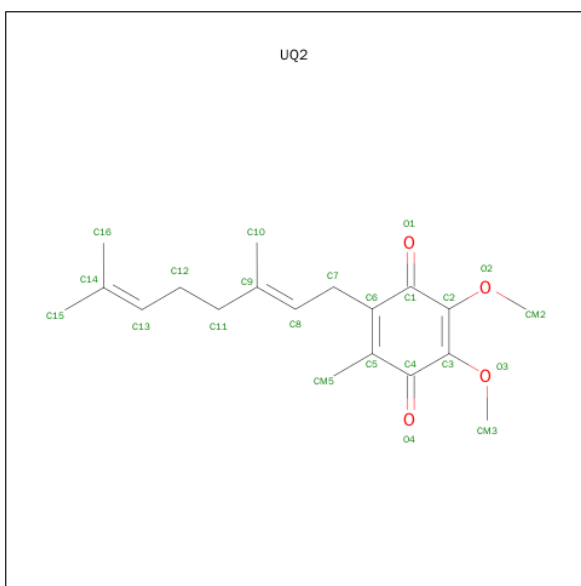
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	L	1	Total	C	N	O	0	0
			16	14	1	1		
6	L	1	Total	C	N	O	0	0
			16	14	1	1		
6	L	1	Total	C	N	O	0	0
			16	14	1	1		
6	L	1	Total	C	N	O	0	0
			16	14	1	1		
6	L	1	Total	C	N	O	0	0
			16	14	1	1		
6	M	1	Total	C	N	O	0	0
			16	14	1	1		
6	M	1	Total	C	N	O	0	0
			16	14	1	1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

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



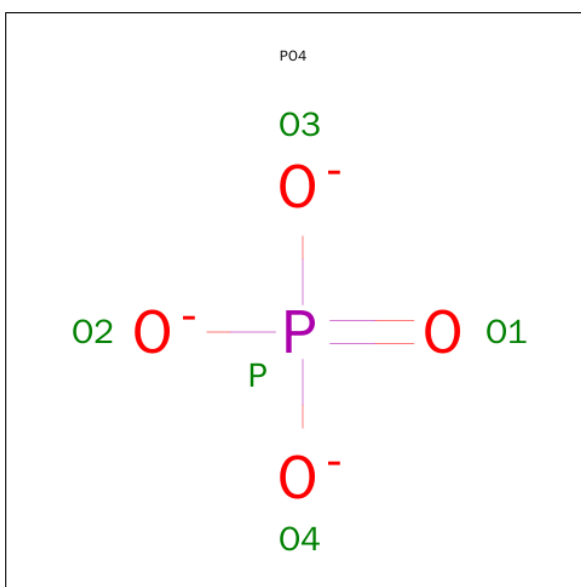
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	L	1	Total	C	N	O	0	0
			65	55	4	6		
7	M	1	Total	C	N	O	0	0
			65	55	4	6		

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



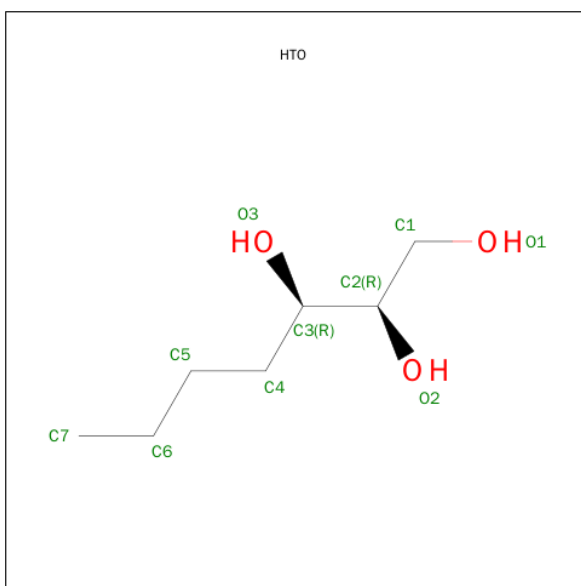
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	L	1	Total	C	O	0	1
			46	38	8		

- 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: $C_7H_{16}O_3$).

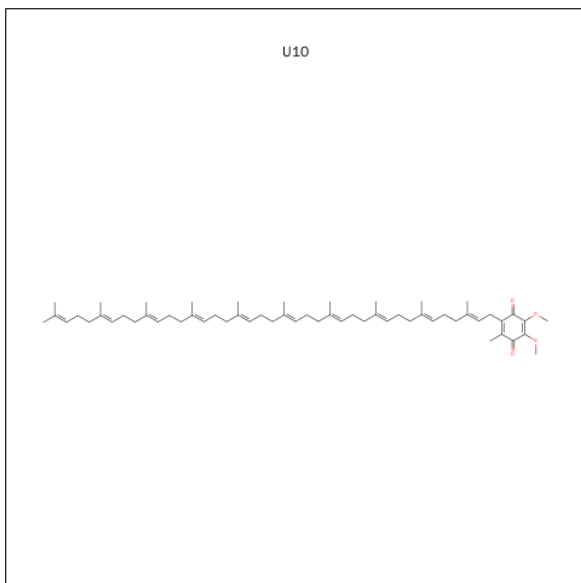


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	L	1	Total	C	O	0	0
			10	7	3		

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

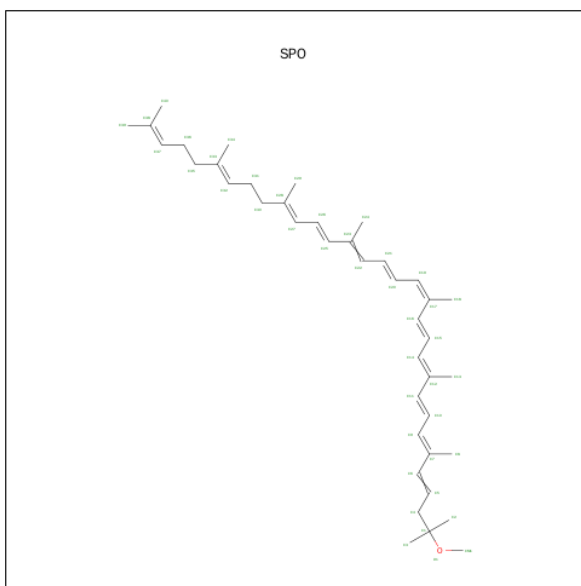
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	M	1	Total	Fe	0	0
			1	1		

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



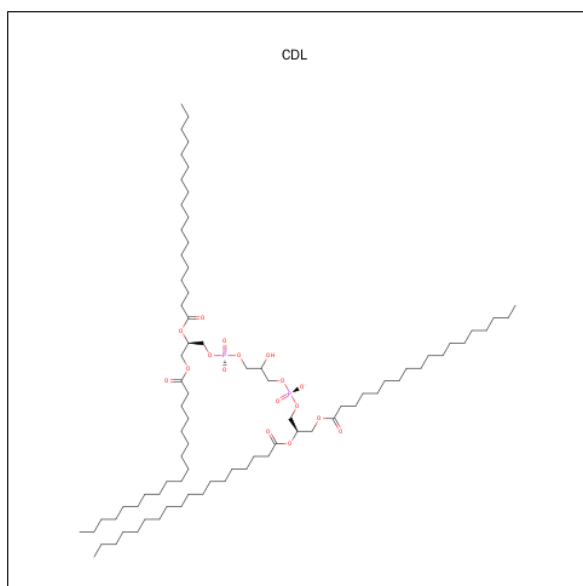
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	M	1	Total	C	O	0	0
			48	44	4		

- 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		

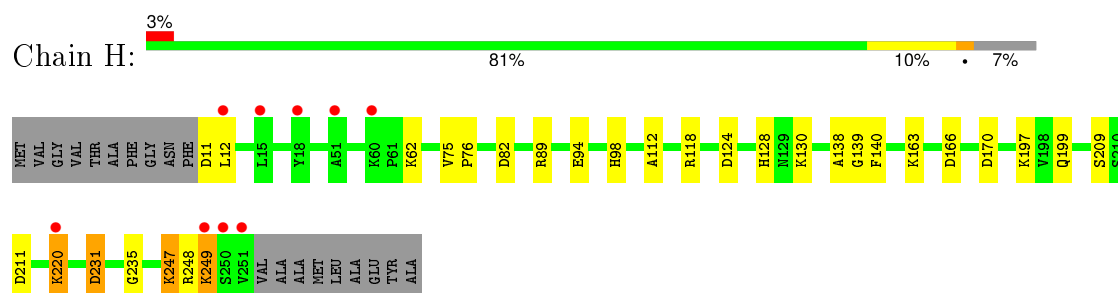
- Molecule 15 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	H	198	Total	O	0	0
			198	198		
15	L	132	Total	O	0	0
			132	132		
15	M	158	Total	O	0	0
			158	158		

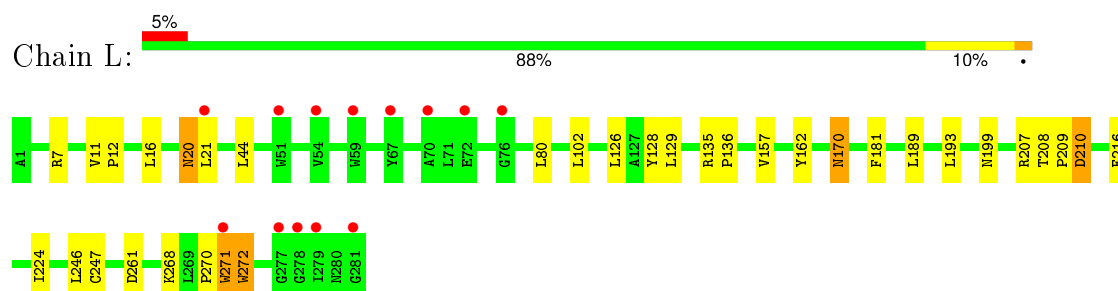
3 Residue-property plots [i](#)

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.

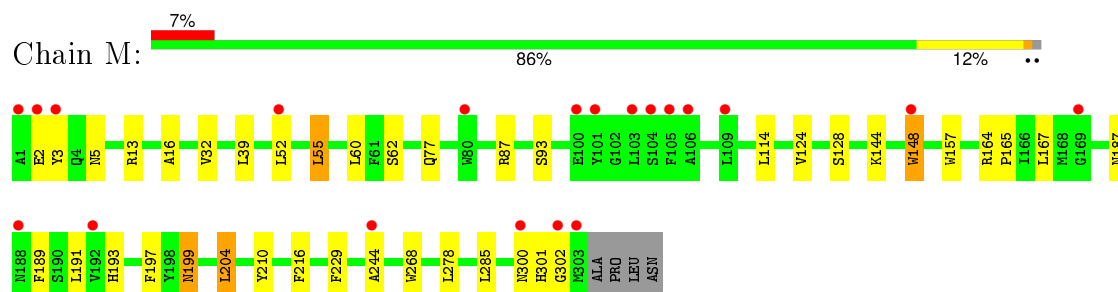
• Molecule 1: REACTION CENTER PROTEIN H CHAIN



• 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	138.69Å 138.69Å 184.61Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	119.52 – 2.05 29.81 – 2.03	Depositor EDS
% Data completeness (in resolution range)	99.2 (119.52-2.05) 89.3 (29.81-2.03)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.06 (at 2.03Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.205 , 0.233 0.272 , 0.272	Depositor DCC
R_{free} test set	2589 reflections (2.29%)	DCC
Wilson B-factor (Å ²)	33.1	Xtriage
Anisotropy	0.117	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 43.2	EDS
Estimated twinning fraction	0.019 for -h,-k,l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	1 of 131143 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	7772	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.53% 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

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	0.68	0/1878	0.77	5/2555 (0.2%)
2	L	0.69	0/2320	0.69	0/3175
3	M	0.68	0/2501	0.70	1/3415 (0.0%)
All	All	0.69	0/6699	0.72	6/9145 (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
1	H	0	1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	M	204	LEU	CB-CG-CD1	5.70	120.68	111.00
1	H	82	ASP	CB-CG-OD2	5.69	123.42	118.30
1	H	211	ASP	CB-CG-OD2	5.47	123.23	118.30
1	H	231	ASP	CB-CG-OD2	5.34	123.10	118.30
1	H	139	GLY	N-CA-C	-5.27	99.92	113.10
1	H	166	ASP	CB-CG-OD2	5.03	122.83	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	H	138	ALA	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	1830	0	1836	18	0
2	L	2232	0	2187	23	0
3	M	2409	0	2321	26	0
4	H	24	0	32	5	0
4	L	12	0	16	1	0
4	M	6	0	8	0	0
5	L	132	0	148	6	0
5	M	132	0	148	20	0
6	L	80	0	155	1	0
6	M	64	0	124	3	0
7	L	65	0	76	6	0
7	M	65	0	76	9	0
8	L	46	0	52	7	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	84	3	0
15	H	198	0	0	5	1
15	L	132	0	0	1	1
15	M	158	0	0	0	0
All	All	7772	0	7402	98	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 (98) 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)
7:L:1288:BPH:HHC	7:L:1288:BPH:HBB3	1.37	1.02
1:H:220:LYS:HD3	15:H:2181:HOH:O	1.75	0.86
5:L:1282:BCL:HHC	5:L:1282:BCL:HBB2	1.59	0.85
1:H:62:LYS:HE3	4:H:1252:GOL:H11	1.60	0.84
3:M:197:PHE:HZ	5:M:1305:BCL:HBB2	1.44	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:197:PHE:CZ	5:M:1305:BCL:HBB2	2.16	0.80
1:H:248:ARG:HA	1:H:249:LYS:CB	2.11	0.79
7:L:1288:BPH:CBB	7:L:1288:BPH:HHC	2.14	0.77
1:H:248:ARG:HA	1:H:249:LYS:HB2	1.67	0.75
7:M:1311:BPH:HBB3	7:M:1311:BPH:HHC	1.69	0.74
4:H:1252:GOL:C3	15:H:2003:HOH:O	2.38	0.71
6:M:1306:LDA:H81	6:M:1308:LDA:H121	1.73	0.70
2:L:181:PHE:CD2	7:M:1311:BPH:HBB1	2.28	0.68
3:M:189:PHE:O	3:M:193:HIS:HD2	1.77	0.67
2:L:181:PHE:HB3	7:M:1311:BPH:HBB2	1.77	0.66
5:L:1282:BCL:HHC	5:L:1282:BCL:CBB	2.27	0.63
7:M:1311:BPH:CBB	7:M:1311:BPH:HHC	2.28	0.63
5:M:1305:BCL:HHC	5:M:1305:BCL:CBB	2.28	0.63
2:L:261:ASP:OD1	15:L:2120:HOH:O	2.16	0.62
4:H:1252:GOL:H31	15:H:2003:HOH:O	1.96	0.62
3:M:144:LYS:N	14:M:1314:CDL:OB3	2.27	0.61
7:L:1288:BPH:CHC	7:L:1288:BPH:HBB3	2.22	0.61
4:H:1252:GOL:H32	15:H:2003:HOH:O	1.99	0.60
2:L:199:ASN:O	14:M:1314:CDL:HB22	2.02	0.59
5:M:1304:BCL:HBB3	5:M:1305:BCL:H41	1.83	0.59
5:M:1304:BCL:CBB	5:M:1304:BCL:HHC	2.34	0.58
2:L:135:ARG:HB3	2:L:136:PRO:HD3	1.85	0.57
1:H:98:HIS:CD2	2:L:7:ARG:HH21	2.22	0.56
2:L:170:ASN:C	2:L:170:ASN:HD22	2.09	0.56
3:M:157:TRP:HB2	5:M:1305:BCL:H71	1.88	0.56
7:L:1288:BPH:CHC	7:L:1288:BPH:CBB	2.81	0.55
1:H:128:HIS:HE1	15:H:2125:HOH:O	1.88	0.55
7:L:1288:BPH:HBB2	3:M:210:TYR:HB3	1.90	0.55
1:H:98:HIS:HD2	2:L:7:ARG:HH21	1.56	0.54
7:M:1311:BPH:HBB3	7:M:1311:BPH:CHC	2.35	0.54
1:H:248:ARG:HA	1:H:249:LYS:HB3	1.91	0.53
3:M:189:PHE:O	3:M:193:HIS:CD2	2.61	0.53
3:M:77:GLN:HE22	3:M:93:SER:H	1.54	0.53
2:L:181:PHE:HB3	7:M:1311:BPH:CBB	2.39	0.53
5:M:1305:BCL:HHC	5:M:1305:BCL:HBB2	1.91	0.53
1:H:197:LYS:HE3	1:H:199:GLN:NE2	2.24	0.52
1:H:209:SER:OG	1:H:247:LYS:HD3	2.10	0.52
5:M:1304:BCL:HBB2	13:M:1313:SPO:H243	1.92	0.52
2:L:128:TYR:HD1	5:L:1282:BCL:HBB1	1.74	0.52
3:M:229:PHE:HB2	3:M:244:ALA:HB2	1.92	0.51
3:M:55:LEU:HD22	3:M:128:SER:HB2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:189:LEU:CD1	8:L:1289[A]:UQ2:H121	2.40	0.51
1:H:75:VAL:HA	1:H:76:PRO:C	2.31	0.51
5:L:1290:BCL:CBB	5:L:1290:BCL:HMB1	2.41	0.50
5:M:1304:BCL:HBB2	5:M:1304:BCL:HHC	1.94	0.50
6:M:1308:LDA:H52	6:M:1309:LDA:H42	1.93	0.50
3:M:16:ALA:HB1	3:M:32:VAL:HG11	1.94	0.50
5:M:1304:BCL:CBB	13:M:1313:SPO:H243	2.42	0.50
2:L:157:VAL:HG11	5:M:1305:BCL:HBB1	1.94	0.49
5:M:1305:BCL:HBD	5:M:1305:BCL:HAA2	1.95	0.49
3:M:167:LEU:HD12	3:M:285:LEU:HD11	1.94	0.48
3:M:199:ASN:HD22	3:M:199:ASN:C	2.16	0.48
1:H:62:LYS:CE	4:H:1252:GOL:H11	2.39	0.48
3:M:197:PHE:HZ	5:M:1305:BCL:CBB	2.19	0.48
2:L:271:TRP:N	2:L:271:TRP:CD1	2.79	0.48
8:L:1289[A]:UQ2:H5M1	8:L:1289[A]:UQ2:H71	1.67	0.47
2:L:162:TYR:OH	3:M:187:ASN:ND2	2.47	0.47
3:M:300:ASN:C	3:M:302:GLY:H	2.17	0.47
1:H:248:ARG:CA	1:H:249:LYS:HB2	2.43	0.47
5:M:1305:BCL:HBB3	5:M:1305:BCL:HHC	1.97	0.46
2:L:199:ASN:HA	4:L:1293:GOL:H31	1.98	0.46
6:L:1287:LDA:H121	8:L:1289[A]:UQ2:H161	1.97	0.46
5:L:1282:BCL:H192	7:L:1288:BPH:H7C2	1.98	0.46
2:L:208:THR:HB	2:L:209:PRO:HD2	1.98	0.46
2:L:193:LEU:HD23	8:L:1289[A]:UQ2:C4	2.46	0.45
1:H:112:ALA:HA	1:H:235:GLY:O	2.17	0.45
5:L:1290:BCL:HMB1	5:L:1290:BCL:HBB3	1.99	0.45
3:M:60:LEU:HD11	7:M:1311:BPH:H161	1.98	0.44
3:M:164:ARG:HB3	3:M:165:PRO:HD3	1.99	0.44
2:L:11:VAL:HB	2:L:12:PRO:HD2	1.99	0.44
5:M:1305:BCL:CHC	5:M:1305:BCL:CBB	2.94	0.44
1:H:89:ARG:NH2	1:H:94:GLU:HG2	2.33	0.43
2:L:224:ILE:HG22	8:L:1289[A]:UQ2:H8	2.00	0.43
1:H:140:PHE:HA	3:M:13:ARG:O	2.19	0.43
3:M:62:SER:OG	3:M:124:VAL:HG22	2.18	0.43
1:H:130:LYS:HE3	1:H:170:ASP:OD2	2.19	0.43
2:L:272:TRP:CD1	3:M:87:ARG:HG3	2.54	0.43
5:M:1304:BCL:H13	5:M:1304:BCL:H102	1.39	0.42
5:M:1304:BCL:HMB2	7:M:1311:BPH:HMB3	2.01	0.42
2:L:20:ASN:N	2:L:20:ASN:HD22	2.17	0.42
5:M:1304:BCL:H71	5:M:1305:BCL:H202	2.02	0.42
5:M:1304:BCL:H101	5:M:1305:BCL:H171	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:M:1311:BPH:H112	7:M:1311:BPH:H7C2	1.81	0.41
8:L:1289[A]:UQ2:H122	8:L:1289[A]:UQ2:H101	1.88	0.41
3:M:278:LEU:HD21	14:M:1314:CDL:H782	2.01	0.41
3:M:148:TRP:HA	3:M:148:TRP:CE3	2.56	0.41
1:H:124:ASP:HB2	2:L:210:ASP:OD2	2.20	0.41
3:M:268:TRP:CD1	12:M:1312:U10:H111	2.56	0.41
6:M:1308:LDA:C5	6:M:1309:LDA:H42	2.52	0.40
3:M:197:PHE:CE1	5:M:1305:BCL:HBB2	2.56	0.40
3:M:3:TYR:CZ	3:M:5:ASN:HA	2.57	0.40
2:L:270:PRO:HG2	2:L:271:TRP:CD1	2.57	0.40
8:L:1289[B]:UQ2:H121	8:L:1289[B]:UQ2:H101	1.50	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:2050:HOH:O	15:L:2077:HOH:O[6_655]	2.18	0.02

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	239/260 (92%)	235 (98%)	3 (1%)	1 (0%)	39	28
2	L	279/281 (99%)	274 (98%)	5 (2%)	0	100	100
3	M	301/307 (98%)	290 (96%)	10 (3%)	1 (0%)	46	36
All	All	819/848 (97%)	799 (98%)	18 (2%)	2 (0%)	52	43

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	249	LYS

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Mol	Chain	Res	Type
3	M	301	HIS

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	195/208 (94%)	188 (96%)	7 (4%)	42	34
2	L	220/220 (100%)	203 (92%)	17 (8%)	16	7
3	M	236/240 (98%)	226 (96%)	10 (4%)	36	28
All	All	651/668 (98%)	617 (95%)	34 (5%)	29	18

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

Mol	Chain	Res	Type
1	H	11	ASP
1	H	12	LEU
1	H	118	ARG
1	H	163	LYS
1	H	220	LYS
1	H	231	ASP
1	H	247	LYS
2	L	16	LEU
2	L	20	ASN
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	207	ARG
2	L	210	ASP
2	L	216	PHE
2	L	246	LEU
2	L	247	CYS

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Mol	Chain	Res	Type
2	L	268	LYS
2	L	271	TRP
2	L	272	TRP
3	M	2	GLU
3	M	39	LEU
3	M	52	LEU
3	M	55	LEU
3	M	114	LEU
3	M	148	TRP
3	M	191	LEU
3	M	199	ASN
3	M	204	LEU
3	M	216	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	98	HIS
1	H	141	HIS
2	L	20	ASN
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	1252	-	5,5,5	0.52	0	5,5,5	1.15	0
4	GOL	H	1253	-	5,5,5	0.36	0	5,5,5	0.24	0
4	GOL	H	1254	-	5,5,5	0.34	0	5,5,5	0.24	0
4	GOL	H	1255	-	5,5,5	0.31	0	5,5,5	0.32	0
5	BCL	L	1282	2	53,74,74	1.98	7 (13%)	57,115,115	1.92	12 (21%)
6	LDA	L	1283	-	15,15,15	3.75	2 (13%)	16,17,17	0.78	1 (6%)
6	LDA	L	1284	-	15,15,15	3.78	2 (13%)	16,17,17	0.59	0
6	LDA	L	1285	-	15,15,15	3.83	2 (13%)	16,17,17	0.63	0
6	LDA	L	1286	-	15,15,15	3.82	2 (13%)	16,17,17	0.69	0
6	LDA	L	1287	-	15,15,15	3.91	2 (13%)	16,17,17	0.95	1 (6%)
7	BPH	L	1288	-	64,70,70	2.84	17 (26%)	73,101,101	1.80	15 (20%)
8	UQ2	L	1289[A]	-	23,23,23	2.61	8 (34%)	28,31,31	1.74	8 (28%)
8	UQ2	L	1289[B]	-	23,23,23	2.71	7 (30%)	28,31,31	1.21	2 (7%)
5	BCL	L	1290	2	53,74,74	2.00	6 (11%)	57,115,115	1.79	15 (26%)
9	PO4	L	1291	-	4,4,4	0.52	0	6,6,6	0.29	0
10	HTO	L	1292	-	9,9,9	0.36	0	8,10,10	0.58	0
4	GOL	L	1293	-	5,5,5	0.35	0	5,5,5	0.78	0
4	GOL	L	1294	-	5,5,5	0.34	0	5,5,5	0.24	0
5	BCL	M	1304	3	53,74,74	1.99	6 (11%)	57,115,115	1.83	10 (17%)
5	BCL	M	1305	3	53,74,74	2.05	5 (9%)	57,115,115	1.90	13 (22%)
6	LDA	M	1306	-	15,15,15	3.57	2 (13%)	16,17,17	0.71	0
6	LDA	M	1307	-	15,15,15	3.79	2 (13%)	16,17,17	0.90	1 (6%)
6	LDA	M	1308	-	15,15,15	3.58	2 (13%)	16,17,17	0.87	1 (6%)
6	LDA	M	1309	-	15,15,15	3.83	2 (13%)	16,17,17	0.66	0
7	BPH	M	1311	-	64,70,70	2.89	18 (28%)	73,101,101	1.77	11 (15%)
12	U10	M	1312	-	48,48,63	3.01	11 (22%)	58,61,79	1.70	12 (20%)
13	SPO	M	1313	-	40,41,41	3.89	12 (30%)	45,50,50	2.21	17 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CDL	M	1314	-	80,80,99	1.95	15 (18%)	82,92,111	2.86	14 (17%)
4	GOL	M	1315	-	5,5,5	0.32	0	5,5,5	0.27	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	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
4	GOL	H	1255	-	-	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
6	LDA	L	1287	-	-	0/13/13/13	0/0/0/0
7	BPH	L	1288	-	-	0/54/105/105	0/1/6/6
8	UQ2	L	1289[A]	-	-	0/15/39/39	0/1/1/1
8	UQ2	L	1289[B]	-	-	0/15/39/39	0/1/1/1
5	BCL	L	1290	2	2/2/21/25	0/37/137/137	0/0/9/9
9	PO4	L	1291	-	-	0/0/0/0	0/0/0/0
10	HTO	L	1292	-	-	0/10/10/10	0/0/0/0
4	GOL	L	1293	-	-	0/4/4/4	0/0/0/0
4	GOL	L	1294	-	-	0/4/4/4	0/0/0/0
5	BCL	M	1304	3	2/2/21/25	1/37/137/137	0/0/9/9
5	BCL	M	1305	3	2/2/21/25	0/37/137/137	0/0/9/9
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 (130) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	L	1287	LDA	O1-N1	-14.85	1.25	1.39
6	L	1285	LDA	O1-N1	-14.56	1.25	1.39
6	L	1286	LDA	O1-N1	-14.55	1.25	1.39
6	M	1309	LDA	O1-N1	-14.53	1.25	1.39
6	M	1307	LDA	O1-N1	-14.45	1.25	1.39
6	L	1284	LDA	O1-N1	-14.33	1.25	1.39
6	L	1283	LDA	O1-N1	-14.28	1.26	1.39
6	M	1308	LDA	O1-N1	-13.59	1.26	1.39
6	M	1306	LDA	O1-N1	-13.42	1.26	1.39
14	M	1314	CDL	C11-CA5	-6.57	1.31	1.50
14	M	1314	CDL	C32-C31	-6.20	1.28	1.52
8	L	1289[A]	UQ2	O2-C2	-4.99	1.23	1.37
8	L	1289[B]	UQ2	O2-C2	-4.68	1.24	1.37
8	L	1289[B]	UQ2	O3-C3	-4.43	1.25	1.37
14	M	1314	CDL	C17-C16	-4.35	1.26	1.51
14	M	1314	CDL	C19-C18	-4.34	1.26	1.51
14	M	1314	CDL	C16-C15	-4.34	1.26	1.51
14	M	1314	CDL	C20-C19	-4.27	1.26	1.51
8	L	1289[A]	UQ2	O3-C3	-4.27	1.25	1.37
7	L	1288	BPH	C3D-CAD	-3.93	1.38	1.46
12	M	1312	U10	O4-C4	-3.84	1.26	1.37
7	M	1311	BPH	C3D-CAD	-3.80	1.39	1.46
12	M	1312	U10	O3-C3	-3.70	1.27	1.37
7	L	1288	BPH	C3D-C4D	-3.40	1.37	1.41
8	L	1289[A]	UQ2	C3-C4	-3.13	1.39	1.48
7	L	1288	BPH	O2D-CGD	-3.08	1.25	1.33
8	L	1289[B]	UQ2	C3-C4	-3.07	1.40	1.48
14	M	1314	CDL	C37-C36	-3.05	1.33	1.51
14	M	1314	CDL	C79-C78	-3.00	1.34	1.51
14	M	1314	CDL	C80-C79	-2.97	1.34	1.51
7	M	1311	BPH	O2D-CGD	-2.93	1.25	1.33
5	L	1290	BCL	O2D-CGD	-2.92	1.25	1.33
14	M	1314	CDL	C22-C21	-2.90	1.34	1.51
14	M	1314	CDL	C13-C12	-2.90	1.34	1.51
8	L	1289[B]	UQ2	C2-C1	-2.87	1.40	1.48
12	M	1312	U10	C4-C5	-2.77	1.40	1.48
6	M	1306	LDA	C1-N1	-2.76	1.46	1.51
6	M	1308	LDA	C1-N1	-2.73	1.46	1.51
7	M	1311	BPH	O2A-CGA	-2.73	1.25	1.33
5	L	1282	BCL	O2A-CGA	-2.72	1.25	1.33
7	M	1311	BPH	C1B-C2B	-2.55	1.40	1.45
5	L	1290	BCL	C3D-CAD	-2.52	1.38	1.45
5	M	1304	BCL	O2D-CGD	-2.49	1.26	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	L	1284	LDA	C1-N1	-2.48	1.46	1.51
6	L	1287	LDA	C1-N1	-2.45	1.46	1.51
5	L	1282	BCL	O2D-CGD	-2.44	1.26	1.33
7	L	1288	BPH	O2A-CGA	-2.38	1.26	1.33
6	M	1309	LDA	C1-N1	-2.37	1.47	1.51
5	M	1305	BCL	O2D-CGD	-2.32	1.27	1.33
8	L	1289[A]	UQ2	C6-C1	-2.31	1.39	1.46
6	L	1285	LDA	C1-N1	-2.30	1.47	1.51
8	L	1289[A]	UQ2	C2-C1	-2.30	1.42	1.48
7	L	1288	BPH	CBB-CAB	-2.29	1.45	1.50
6	M	1307	LDA	C1-N1	-2.26	1.47	1.51
5	M	1304	BCL	O2A-CGA	-2.25	1.26	1.33
7	M	1311	BPH	C3D-C4D	-2.22	1.38	1.41
5	M	1305	BCL	O2A-CGA	-2.18	1.26	1.33
5	M	1304	BCL	C3D-CAD	-2.16	1.39	1.45
6	L	1286	LDA	C1-N1	-2.14	1.47	1.51
5	L	1290	BCL	O2A-CGA	-2.05	1.27	1.33
5	L	1282	BCL	C3D-CAD	-2.04	1.40	1.45
6	L	1283	LDA	C1-N1	-2.04	1.47	1.51
5	L	1282	BCL	O1D-CGD	2.10	1.26	1.21
8	L	1289[A]	UQ2	C6-C5	2.15	1.40	1.35
7	L	1288	BPH	C1D-CHD	2.18	1.48	1.40
7	M	1311	BPH	CHA-C1A	2.23	1.42	1.37
8	L	1289[B]	UQ2	C6-C5	2.51	1.41	1.35
7	M	1311	BPH	C1D-CHD	2.81	1.51	1.40
12	M	1312	U10	C6-C1	2.93	1.42	1.35
5	L	1282	BCL	C2-C3	3.08	1.39	1.33
7	L	1288	BPH	C3D-C2D	3.21	1.47	1.40
7	M	1311	BPH	C3D-C2D	3.24	1.47	1.40
5	M	1305	BCL	C2-C3	3.42	1.39	1.33
7	L	1288	BPH	CHD-C4C	3.45	1.46	1.38
13	M	1313	SPO	C21-C20	3.47	1.45	1.35
7	L	1288	BPH	CHB-C4A	3.50	1.46	1.40
7	M	1311	BPH	CHD-C4C	3.57	1.47	1.38
7	M	1311	BPH	CHC-C4B	3.77	1.49	1.40
7	L	1288	BPH	CHC-C4B	3.99	1.50	1.40
5	L	1290	BCL	C2-C3	4.02	1.40	1.33
5	M	1304	BCL	C2-C3	4.05	1.40	1.33
13	M	1313	SPO	C15-C16	4.08	1.45	1.34
7	M	1311	BPH	CHB-C4A	4.11	1.48	1.40
13	M	1313	SPO	C26-C25	4.14	1.45	1.34
14	M	1314	CDL	OB8-CB7	4.28	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	M	1314	CDL	OB6-CB5	4.31	1.47	1.34
13	M	1313	SPO	C10-C11	4.47	1.46	1.34
14	M	1314	CDL	OA6-CA5	4.56	1.48	1.34
14	M	1314	CDL	OA8-CA7	4.60	1.47	1.33
8	L	1289[B]	UQ2	C13-C14	4.91	1.47	1.32
13	M	1313	SPO	C6-C5	4.91	1.45	1.31
12	M	1312	U10	C38-C39	5.00	1.47	1.32
8	L	1289[A]	UQ2	C13-C14	5.19	1.48	1.32
7	L	1288	BPH	CHB-C1B	5.28	1.49	1.38
13	M	1313	SPO	C37-C38	5.32	1.48	1.32
7	M	1311	BPH	CHC-C1C	5.34	1.47	1.36
5	L	1282	BCL	O1A-CGA	5.39	1.38	1.22
7	L	1288	BPH	CHC-C1C	5.50	1.47	1.36
5	M	1304	BCL	O1A-CGA	5.57	1.39	1.22
7	M	1311	BPH	CHB-C1B	5.76	1.49	1.38
5	M	1305	BCL	O1A-CGA	5.81	1.40	1.22
7	M	1311	BPH	O1A-CGA	5.90	1.40	1.22
7	L	1288	BPH	O1A-CGA	6.00	1.40	1.22
5	L	1290	BCL	O1A-CGA	6.20	1.41	1.22
7	L	1288	BPH	O1D-CGD	6.67	1.38	1.21
7	M	1311	BPH	O1D-CGD	6.98	1.38	1.21
12	M	1312	U10	C23-C24	6.99	1.46	1.33
12	M	1312	U10	C18-C19	7.12	1.46	1.33
8	L	1289[A]	UQ2	C8-C9	7.42	1.47	1.33
12	M	1312	U10	C28-C29	7.47	1.47	1.33
13	M	1313	SPO	C32-C33	7.55	1.47	1.33
12	M	1312	U10	C13-C14	7.64	1.48	1.33
12	M	1312	U10	C8-C9	7.65	1.48	1.33
7	M	1311	BPH	C2-C3	7.69	1.48	1.33
13	M	1313	SPO	C22-C23	7.69	1.45	1.35
7	L	1288	BPH	C2-C3	7.73	1.48	1.33
13	M	1313	SPO	C14-C12	7.82	1.46	1.35
8	L	1289[B]	UQ2	C8-C9	8.07	1.48	1.33
12	M	1312	U10	C33-C34	8.37	1.49	1.33
13	M	1313	SPO	C19-C17	8.51	1.47	1.35
7	M	1311	BPH	OBB-CAB	8.57	1.42	1.23
13	M	1313	SPO	C9-C7	9.19	1.47	1.35
7	L	1288	BPH	OBD-CAD	9.63	1.37	1.22
7	L	1288	BPH	OBB-CAB	9.99	1.45	1.23
5	M	1304	BCL	OBD-CAD	10.83	1.38	1.22
5	L	1290	BCL	OBD-CAD	10.89	1.39	1.22
5	L	1282	BCL	OBD-CAD	11.07	1.39	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	M	1311	BPH	OBD-CAD	11.23	1.39	1.22
5	M	1305	BCL	OBD-CAD	11.54	1.40	1.22
13	M	1313	SPO	C27-C28	12.00	1.47	1.34

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	116.34	128.36
5	L	1290	BCL	CMB-C2B-C1B	-5.81	118.75	128.36
13	M	1313	SPO	C4-C5-C6	-5.31	117.11	124.67
5	M	1305	BCL	CMB-C2B-C1B	-5.06	120.00	128.36
5	L	1282	BCL	CMB-C2B-C1B	-4.99	120.10	128.36
7	L	1288	BPH	O1D-CGD-CBD	-4.83	117.70	124.62
7	M	1311	BPH	O1D-CGD-CBD	-4.65	117.96	124.62
13	M	1313	SPO	C10-C9-C7	-4.57	120.59	127.20
5	M	1304	BCL	O1D-CGD-CBD	-4.28	118.48	124.62
13	M	1313	SPO	C20-C19-C17	-4.24	121.07	127.20
7	M	1311	BPH	OBD-CAD-CBD	-4.18	119.62	125.94
5	M	1305	BCL	C1D-CHD-C4C	-4.09	119.82	126.07
13	M	1313	SPO	C21-C22-C23	-3.99	121.44	127.20
7	M	1311	BPH	CHC-C4B-NB	-3.85	117.58	124.91
5	L	1282	BCL	O1D-CGD-CBD	-3.74	119.26	124.62
13	M	1313	SPO	C15-C14-C12	-3.51	122.13	127.20
5	L	1282	BCL	C1D-CHD-C4C	-3.49	120.74	126.07
7	L	1288	BPH	OBD-CAD-CBD	-3.39	120.82	125.94
5	M	1304	BCL	OBD-CAD-CBD	-3.23	121.07	125.94
12	M	1312	U10	C30-C29-C28	-3.21	117.20	123.50
8	L	1289[A]	UQ2	O1-C1-C6	-3.19	115.69	121.68
5	M	1305	BCL	C16-C15-C13	-3.17	104.98	115.49
12	M	1312	U10	C22-C23-C24	-3.15	120.90	127.76
5	L	1282	BCL	OBD-CAD-CBD	-3.14	121.20	125.94
5	L	1290	BCL	C1D-CHD-C4C	-3.03	121.45	126.07
12	M	1312	U10	C12-C13-C14	-3.01	121.22	127.76
7	L	1288	BPH	CBB-CAB-C3B	-2.99	113.86	120.52
5	M	1305	BCL	OBD-CAD-CBD	-2.93	121.51	125.94
8	L	1289[A]	UQ2	CM5-C5-C6	-2.82	118.06	124.10
7	L	1288	BPH	C1C-NC-C4C	-2.78	107.59	110.44
5	L	1290	BCL	CHD-C4C-NC	-2.76	121.86	125.06
13	M	1313	SPO	C14-C15-C16	-2.71	114.86	123.13
7	M	1311	BPH	CBA-CAA-C2A	-2.65	106.25	113.73
6	L	1287	LDA	O1-N1-C1	-2.65	107.29	110.27
5	L	1290	BCL	OBD-CAD-CBD	-2.63	121.96	125.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	L	1289[A]	UQ2	C7-C8-C9	-2.58	122.33	126.70
13	M	1313	SPO	C20-C21-C22	-2.55	117.75	123.39
5	L	1282	BCL	CAA-C2A-C3A	-2.55	105.88	113.22
7	L	1288	BPH	C1B-NB-C4B	-2.51	101.55	106.51
12	M	1312	U10	C27-C28-C29	-2.51	122.31	127.76
13	M	1313	SPO	C31-C32-C33	-2.48	122.38	127.76
5	L	1290	BCL	C3C-C4C-CHD	-2.45	117.87	123.33
5	M	1305	BCL	C7-C6-C5	-2.42	105.90	113.06
6	M	1307	LDA	O1-N1-C1	-2.40	107.57	110.27
7	L	1288	BPH	O2A-CGA-O1A	-2.40	117.29	123.49
5	M	1305	BCL	CBB-CAB-C3B	-2.40	113.20	120.33
5	M	1305	BCL	O2D-CGD-O1D	-2.38	118.88	123.79
5	L	1290	BCL	O2A-CGA-O1A	-2.38	117.35	123.49
13	M	1313	SPO	C25-C23-C22	-2.33	115.23	118.98
14	M	1314	CDL	OA6-CA5-OA7	-2.32	117.45	123.67
13	M	1313	SPO	C27-C26-C25	-2.32	116.07	123.13
5	L	1290	BCL	CMD-C2D-C3D	-2.31	120.57	125.09
6	M	1308	LDA	O1-N1-C1	-2.25	107.74	110.27
13	M	1313	SPO	C16-C17-C19	-2.24	115.37	118.98
5	L	1282	BCL	O2D-CGD-O1D	-2.24	119.16	123.79
5	M	1304	BCL	O2A-CGA-O1A	-2.22	117.75	123.49
14	M	1314	CDL	CA4-OA6-CA5	-2.22	112.57	117.89
5	M	1305	BCL	C3C-C4C-CHD	-2.21	118.40	123.33
12	M	1312	U10	O5-C5-C4	-2.18	116.06	120.79
6	L	1283	LDA	O1-N1-C1	-2.15	107.85	110.27
12	M	1312	U10	C17-C18-C19	-2.11	123.18	127.76
5	L	1282	BCL	O2A-CGA-O1A	-2.08	118.11	123.49
7	L	1288	BPH	OBD-CAD-C3D	-2.08	124.12	128.35
7	M	1311	BPH	CAA-C2A-C1A	-2.06	107.45	112.86
8	L	1289[A]	UQ2	C10-C9-C8	-2.04	119.49	123.50
5	M	1304	BCL	C1D-CHD-C4C	-2.03	122.98	126.07
5	L	1282	BCL	C5-C3-C2	-2.02	117.23	121.05
5	L	1290	BCL	O2D-CGD-O1D	-2.01	119.63	123.79
7	L	1288	BPH	OBB-CAB-C3B	2.00	124.17	120.31
5	L	1290	BCL	C4A-NA-C1A	2.00	108.95	106.36
8	L	1289[A]	UQ2	CM2-O2-C2	2.00	123.74	116.61
5	M	1304	BCL	C3D-CAD-CBD	2.01	110.44	107.60
8	L	1289[A]	UQ2	C16-C14-C15	2.06	119.69	114.64
5	L	1290	BCL	C4-C3-C5	2.07	118.56	115.41
8	L	1289[B]	UQ2	C16-C14-C15	2.07	119.73	114.64
7	M	1311	BPH	O2A-CGA-CBA	2.11	118.32	111.90
14	M	1314	CDL	CA6-OA8-CA7	2.15	122.86	116.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	1290	BCL	C14-C13-C12	2.17	119.42	111.08
13	M	1313	SPO	C24-C23-C25	2.19	121.74	118.10
13	M	1313	SPO	C8-C7-C6	2.22	121.78	118.10
12	M	1312	U10	C20-C19-C21	2.30	118.92	115.41
13	M	1313	SPO	C13-C12-C11	2.34	121.99	118.10
7	L	1288	BPH	C2D-C1D-ND	2.36	114.16	110.29
7	L	1288	BPH	CMB-C2B-C1B	2.39	128.95	125.06
13	M	1313	SPO	C40-C38-C39	2.42	120.58	114.64
8	L	1289[B]	UQ2	C10-C9-C11	2.42	119.11	115.41
12	M	1312	U10	C35-C34-C36	2.49	119.21	115.41
5	L	1290	BCL	CED-O2D-CGD	2.62	122.14	115.99
5	M	1304	BCL	CED-O2D-CGD	2.64	122.18	115.99
7	L	1288	BPH	O2A-CGA-CBA	2.75	120.27	111.90
5	L	1282	BCL	CMB-C2B-C3B	2.80	130.56	125.09
13	M	1313	SPO	C34-C33-C35	2.83	119.73	115.41
7	L	1288	BPH	CED-O2D-CGD	2.86	122.70	115.99
5	M	1305	BCL	CMB-C2B-C3B	2.87	130.70	125.09
14	M	1314	CDL	OB8-CB7-C71	2.89	120.70	111.90
5	M	1305	BCL	CED-O2D-CGD	2.91	122.81	115.99
5	L	1290	BCL	O2A-CGA-CBA	3.05	121.20	111.90
14	M	1314	CDL	OA8-CA7-C31	3.10	121.33	111.90
5	L	1282	BCL	O2A-CGA-CBA	3.13	121.44	111.90
7	M	1311	BPH	C2B-C1B-NB	3.14	114.44	109.73
8	L	1289[A]	UQ2	CM3-O3-C3	3.23	128.11	116.61
7	M	1311	BPH	CAC-C3C-C4C	3.24	120.99	112.67
7	M	1311	BPH	CED-O2D-CGD	3.28	123.67	115.99
12	M	1312	U10	C15-C14-C16	3.36	120.53	115.41
5	M	1304	BCL	O2A-CGA-CBA	3.38	122.20	111.90
5	L	1282	BCL	C4-C3-C5	3.49	120.73	115.41
12	M	1312	U10	C10-C9-C11	3.49	120.74	115.41
5	M	1305	BCL	O2A-CGA-CBA	3.59	122.83	111.90
7	L	1288	BPH	C2B-C1B-NB	3.66	115.21	109.73
5	L	1290	BCL	CMB-C2B-C3B	3.80	132.53	125.09
14	M	1314	CDL	C35-C34-C33	3.83	134.30	114.53
12	M	1312	U10	C25-C24-C26	3.86	121.30	115.41
13	M	1313	SPO	C29-C28-C30	4.00	121.52	115.41
5	M	1305	BCL	OB6-CAB-C3B	4.00	126.34	120.00
14	M	1314	CDL	OB6-CB5-C51	4.03	120.30	111.53
8	L	1289[A]	UQ2	C10-C9-C11	4.23	121.87	115.41
5	M	1304	BCL	CMB-C2B-C3B	4.29	133.48	125.09
7	M	1311	BPH	C3C-C4C-NC	4.53	112.47	107.93
7	L	1288	BPH	C3C-C4C-NC	4.79	112.73	107.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	M	1312	U10	C30-C29-C31	4.86	122.84	115.41
5	L	1290	BCL	O2D-CGD-CBD	4.90	118.02	111.30
14	M	1314	CDL	OA6-CA5-C11	5.08	122.57	111.53
14	M	1314	CDL	C12-C11-CA5	5.26	134.27	113.59
5	M	1304	BCL	O2D-CGD-CBD	5.39	118.70	111.30
5	M	1305	BCL	O2D-CGD-CBD	5.53	118.89	111.30
7	M	1311	BPH	O2D-CGD-CBD	6.65	120.43	111.30
14	M	1314	CDL	C33-C32-C31	7.18	139.63	113.29
5	L	1282	BCL	O2D-CGD-CBD	7.48	121.57	111.30
7	L	1288	BPH	O2D-CGD-CBD	7.84	122.05	111.30
14	M	1314	CDL	C34-C33-C32	9.01	161.05	114.53
14	M	1314	CDL	C13-C12-C11	9.46	147.97	113.29
14	M	1314	CDL	C17-C16-C15	11.64	174.65	114.53
14	M	1314	CDL	C20-C19-C18	11.76	175.25	114.53

All (8) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	L	1282	BCL	C8
5	L	1282	BCL	C13
5	M	1304	BCL	C8
5	M	1304	BCL	C13
5	M	1305	BCL	C8
5	M	1305	BCL	C13
5	L	1290	BCL	C8
5	L	1290	BCL	C13

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	M	1304	BCL	C1-C2-C3-C4

There are no ring outliers.

17 monomers are involved in 59 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	H	1252	GOL	5	0
5	L	1282	BCL	4	0
6	L	1287	LDA	1	0
7	L	1288	BPH	6	0
8	L	1289[A]	UQ2	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	L	1289[B]	UQ2	1	0
5	L	1290	BCL	2	0
4	L	1293	GOL	1	0
5	M	1304	BCL	9	0
5	M	1305	BCL	14	0
6	M	1306	LDA	1	0
6	M	1308	LDA	3	0
6	M	1309	LDA	2	0
7	M	1311	BPH	9	0
12	M	1312	U10	1	0
13	M	1313	SPO	2	0
14	M	1314	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, 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%)	0.15	9 (3%)	45	51	25, 33, 45, 72	0
2	L	281/281 (100%)	0.42	13 (4%)	36	41	24, 31, 52, 61	0
3	M	303/307 (98%)	0.68	20 (6%)	22	24	22, 35, 56, 67	0
All	All	825/848 (97%)	0.43	42 (5%)	32	36	22, 33, 52, 72	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	M	1	ALA	7.3
1	H	250	SER	6.6
1	H	251	VAL	5.7
3	M	148	TRP	5.0
2	L	281	GLY	4.8
2	L	59	TRP	4.7
1	H	18	TYR	4.3
3	M	106	ALA	3.9
3	M	104	SER	3.6
2	L	277	GLY	3.6
1	H	249	LYS	3.6
3	M	2	GLU	3.4
3	M	101	TYR	3.4
2	L	70	ALA	3.3
3	M	105	PHE	3.2
1	H	15	LEU	3.1
2	L	51	TRP	2.8
2	L	21	LEU	2.8
1	H	12	LEU	2.7
3	M	300	ASN	2.7
2	L	54	VAL	2.7
3	M	80	TRP	2.6
3	M	169	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
3	M	302	GLY	2.6
1	H	51	ALA	2.6
3	M	192	VAL	2.6
2	L	271	TRP	2.5
1	H	60	LYS	2.5
2	L	279	ILE	2.5
3	M	103	LEU	2.4
3	M	3	TYR	2.4
2	L	76	GLY	2.4
2	L	67	TYR	2.4
1	H	220	LYS	2.3
3	M	244	ALA	2.3
3	M	109	LEU	2.3
3	M	52	LEU	2.2
2	L	72	GLU	2.2
3	M	303	MET	2.1
3	M	188	ASN	2.1
2	L	278	GLY	2.0
3	M	100	GLU	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	1286	16/16	0.26	0.51	30.99	81,90,97,97	0
6	LDA	L	1287	16/16	0.65	0.35	20.45	107,108,111,111	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
10	HTO	L	1292	10/10	0.48	0.44	15.51	78,80,80,81	0
6	LDA	L	1283	16/16	0.34	0.42	12.54	73,92,102,102	0
6	LDA	L	1284	16/16	0.28	0.37	8.81	94,97,103,103	0
6	LDA	L	1285	16/16	0.16	0.51	8.25	85,91,98,98	0
4	GOL	H	1252	6/6	0.71	0.21	7.76	41,54,57,59	0
8	UQ2	L	1289[A]	23/23	0.81	0.32	7.03	22,32,49,49	23
8	UQ2	L	1289[B]	23/23	0.81	0.32	6.95	26,33,46,47	23
6	LDA	M	1307	16/16	0.75	0.30	6.16	66,71,80,81	0
14	CDL	M	1314	81/100	0.64	0.42	5.36	62,95,106,107	0
6	LDA	M	1306	16/16	0.78	0.28	4.91	44,66,71,72	0
6	LDA	M	1308	16/16	0.65	0.25	4.48	51,55,57,58	0
13	SPO	M	1313	42/42	0.74	0.26	3.19	34,41,62,66	0
12	U10	M	1312	48/63	0.85	0.18	1.81	24,38,63,64	0
4	GOL	L	1294	6/6	0.78	0.20	1.61	88,89,89,89	0
7	BPH	M	1311	65/65	0.87	0.17	1.36	23,32,86,89	0
4	GOL	L	1293	6/6	0.87	0.19	0.97	45,52,53,56	0
5	BCL	M	1304	66/66	0.90	0.16	0.57	24,29,74,76	0
5	BCL	L	1282	66/66	0.90	0.16	0.48	22,26,53,55	0
5	BCL	L	1290	66/66	0.90	0.15	0.43	23,26,43,50	0
9	PO4	L	1291	5/5	0.89	0.20	0.39	55,56,56,57	0
7	BPH	L	1288	65/65	0.91	0.13	0.22	18,25,36,37	0
5	BCL	M	1305	66/66	0.89	0.16	0.07	20,26,51,58	0
11	FE	M	1310	1/1	0.94	0.06	-5.69	22,22,22,22	0
4	GOL	H	1254	6/6	0.60	0.50	-	111,111,111,111	0
4	GOL	H	1255	6/6	0.43	0.31	-	96,98,98,98	0
4	GOL	M	1315	6/6	0.37	0.33	-	113,114,114,115	0
6	LDA	M	1309	16/16	0.07	0.44	-	94,97,101,102	0
4	GOL	H	1253	6/6	0.71	0.33	-	74,75,75,76	0

6.5 Other polymers ⓘ

There are no such residues in this entry.