



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 16, 2018 – 04:09 PM EST

PDB ID : 2GMR
Title : Photosynthetic reaction center mutant from Rhodobacter sphaeroides with Asp L210 replaced with Asn
Authors : Stachnik, J.M.; Hermes, S.; Gerwert, K.; Hofmann, E.
Deposited on : 2006-04-07
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

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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030736
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : rb-20030736

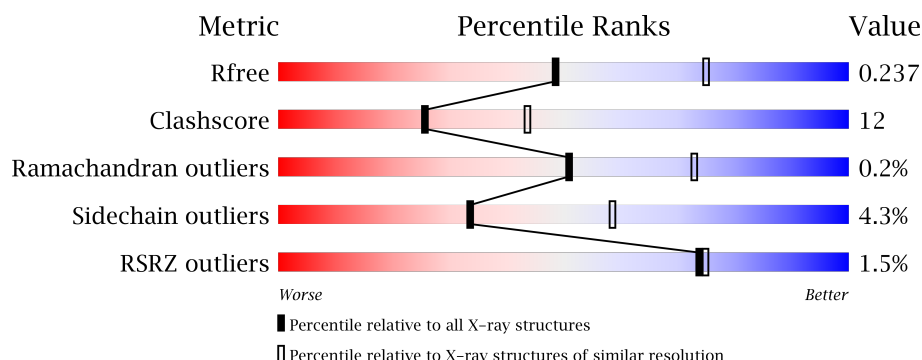
1 Overall quality at a glance

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}	100719	3846 (2.50-2.50)
Clashscore	112137	4554 (2.50-2.50)
Ramachandran outliers	110173	4463 (2.50-2.50)
Sidechain outliers	110143	4465 (2.50-2.50)
RSRZ outliers	101464	3876 (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	L	281	
2	M	307	
3	H	260	

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
4	BCL	L	301	X	-	-	X
5	BPH	L	305	X	-	-	-
5	BPH	M	310	X	-	-	-
7	LDA	L	307	-	-	-	X
9	SPN	M	312	-	-	-	X

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 7286 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 Photosynthetic Reaction center protein L chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	280	Total	C	N	O	S	0	0	0
			2227	1505	355	359	8			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	210	ASN	ASP	ENGINEERED	UNP Q3J1A5

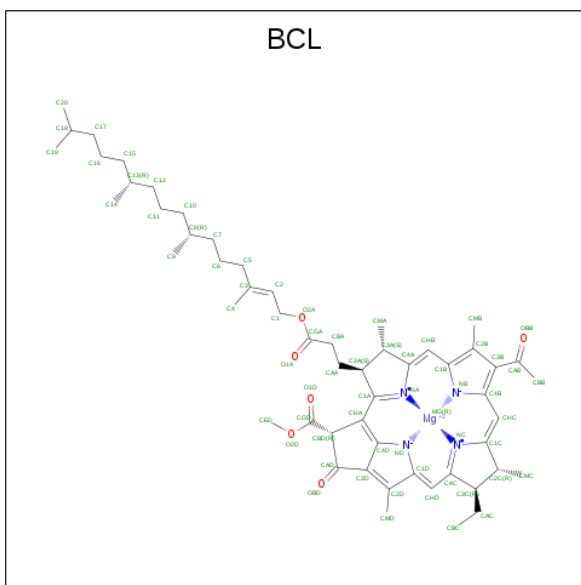
- Molecule 2 is a protein called Photosynthetic Reaction center protein M chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	M	297	Total	C	N	O	S	0	0	0
			2368	1582	387	389	10			

- Molecule 3 is a protein called Photosynthetic reaction center protein H chain.

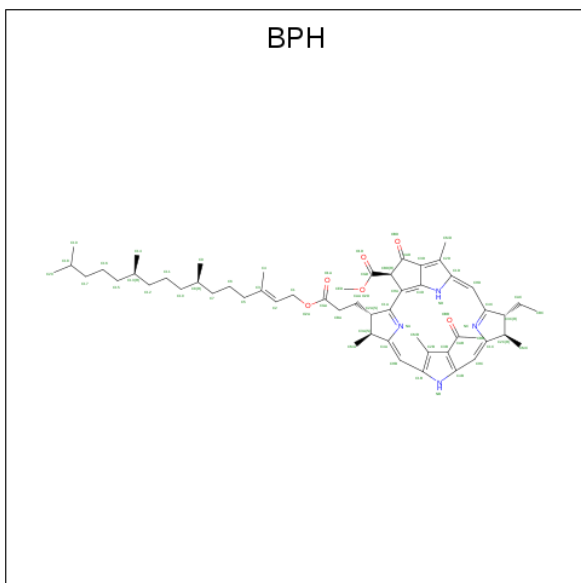
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	248	Total	C	N	O	S	0	0	0
			1883	1204	322	347	10			

- Molecule 4 is BACTERIOCHLOROPHYLL A (three-letter code: BCL) (formula: C₅₅H₇₄MgN₄O₆).



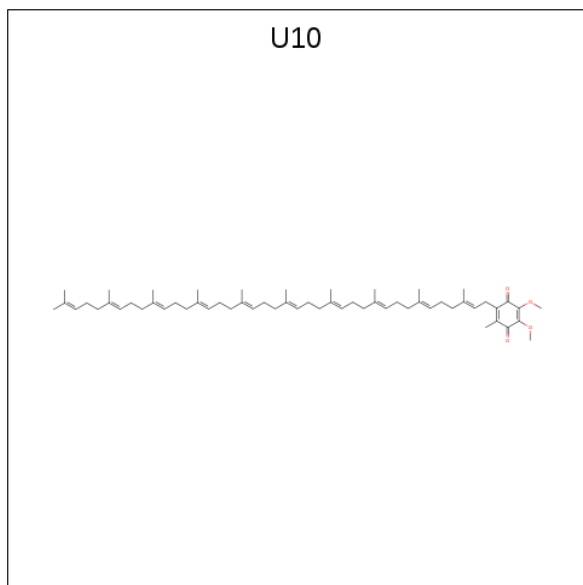
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
4	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
4	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
4	M	1	Total 66	C 55	Mg 1	N 4	O 6	0	0

- Molecule 5 is BACTERIOPHEOPHYTIN A (three-letter code: BPH) (formula: $C_{55}H_{76}N_4O_6$).



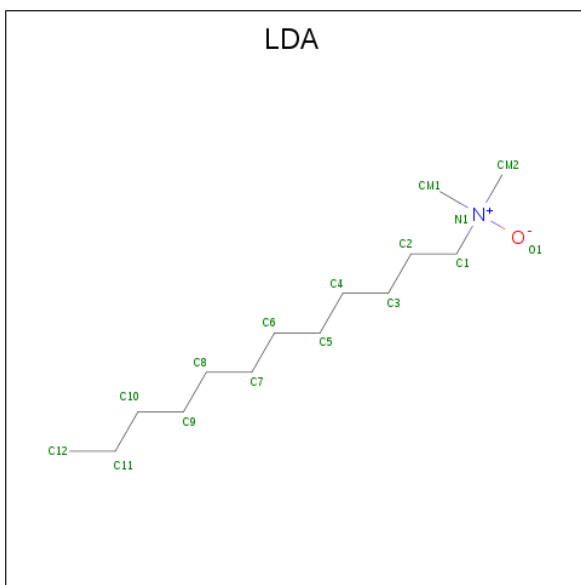
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	L	1	Total	C	N	O	0	0
			65	55	4	6		
5	M	1	Total	C	N	O	0	0
			65	55	4	6		

- Molecule 6 is UBIQUINONE-10 (three-letter code: U10) (formula: $C_{59}H_{90}O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	L	1	Total	C	O	33	0
			63	59	4		
6	M	1	Total	C	O	16	0
			63	59	4		

- Molecule 7 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula: $C_{14}H_{31}NO$).

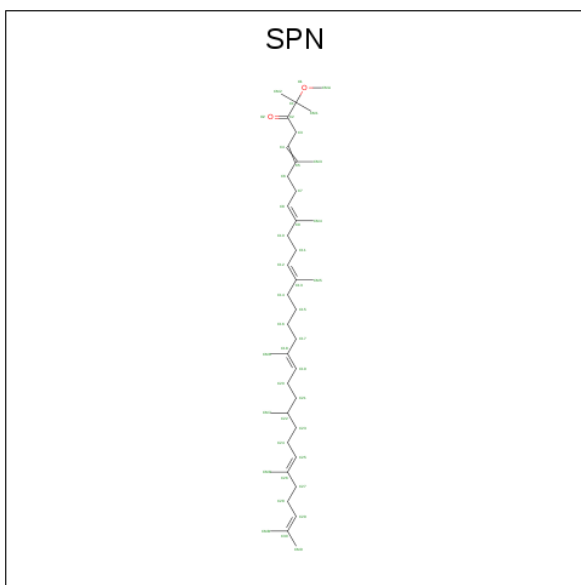


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	L	1	Total	C	N	O	0	0
			16	14	1	1		
7	M	1	Total	C	N	O	0	0
			16	14	1	1		
7	M	1	Total	C	N	O	0	0
			16	14	1	1		
7	H	1	Total	C	N	O	0	0
			16	14	1	1		

- Molecule 8 is FE (II) ION (three-letter code: FE2) (formula: Fe).

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

- Molecule 9 is SPEROIDENONE (three-letter code: SPN) (formula: C₄₁H₇₀O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	M	1	Total	C	O	0	0
			43	41	2		

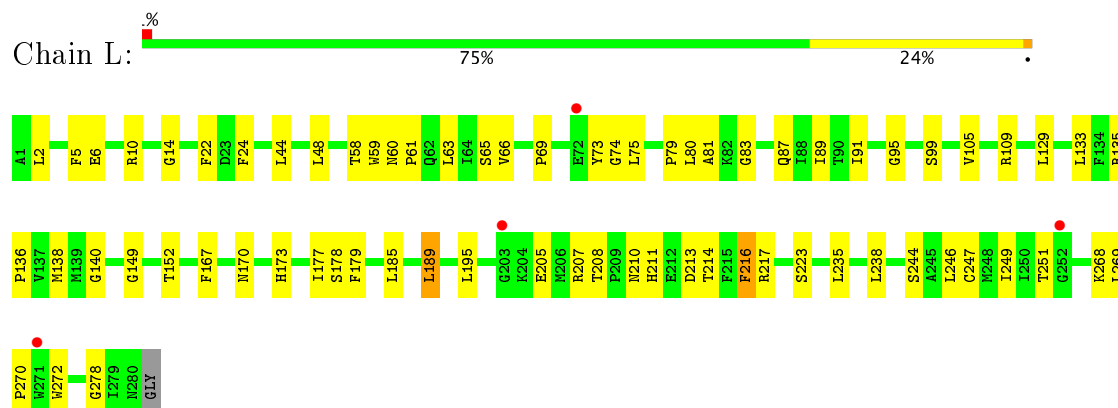
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	L	45	Total	O	0	0
			45	45		
10	M	65	Total	O	0	0
			65	65		
10	H	70	Total	O	0	0
			70	70		

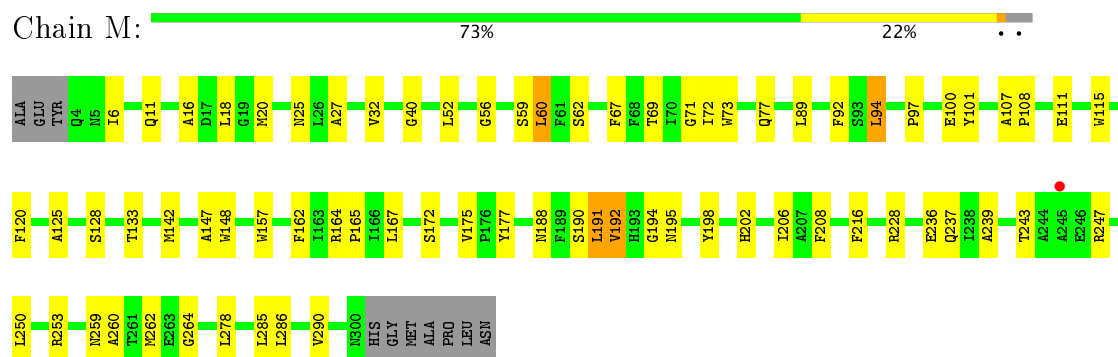
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

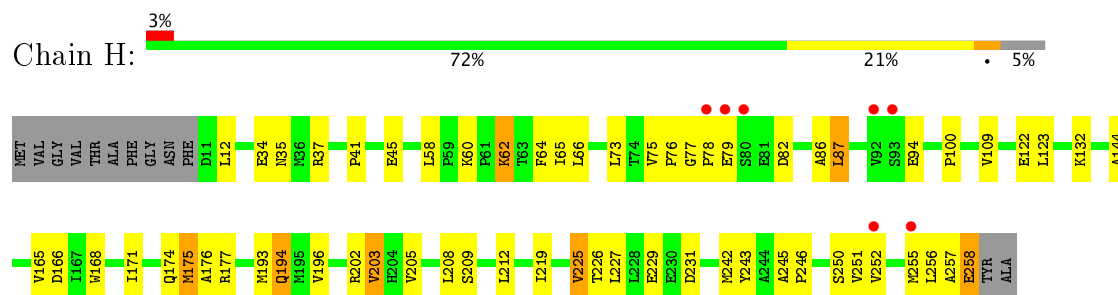
- Molecule 1: Photosynthetic Reaction center protein L chain



- Molecule 2: Photosynthetic Reaction center protein M chain



- Molecule 3: Photosynthetic reaction center protein H chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	76.85Å 134.72Å 141.64Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.43 – 2.50 38.43 – 2.50	Depositor EDS
% Data completeness (in resolution range)	97.3 (38.43-2.50) 97.4 (38.43-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.02 (at 2.51Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.215 , 0.250 0.203 , 0.237	Depositor DCC
R_{free} test set	2514 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	42.9	Xtriage
Anisotropy	0.740	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 51.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.022 for -h,l,k	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7286	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.11% 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, 0.333 respectively for untwinned datasets, and 0.375, 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, LDA, BPH, FE2, SPN, U10

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	L	0.38	0/2315	0.58	0/3170
2	M	0.41	0/2458	0.57	0/3356
3	H	0.36	0/1931	0.64	1/2627 (0.0%)
All	All	0.38	0/6704	0.59	1/9153 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
3	H	203	VAL	N-CA-C	-5.58	95.94	111.00

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	L	2227	0	2186	48	0
2	M	2368	0	2288	59	0
3	H	1883	0	1895	49	0
4	L	198	0	222	17	0
4	M	66	0	74	5	0
5	L	65	0	76	0	0
5	M	65	0	76	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	L	63	0	90	6	0
6	M	63	0	90	1	0
7	H	16	0	31	2	0
7	L	16	0	31	0	0
7	M	32	0	62	5	0
8	M	1	0	0	0	0
9	M	43	0	69	8	0
10	H	70	0	0	6	0
10	L	45	0	0	1	0
10	M	65	0	0	3	0
All	All	7286	0	7190	168	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 12.

All (168) 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:L:214:THR:HG21	2:M:20:MET:H	1.16	1.06
7:M:314:LDA:H82	7:H:261:LDA:H122	1.59	0.85
2:M:16:ALA:HB1	2:M:32:VAL:HG21	1.58	0.83
1:L:210:ASN:O	1:L:214:THR:HG23	1.80	0.82
6:M:311:U10:H202	7:M:314:LDA:H122	1.62	0.80
4:L:304:BCL:HMB1	4:L:304:BCL:HBB2	1.66	0.78
2:M:71:GLY:HA2	9:M:312:SPN:HM32	1.65	0.78
2:M:77:GLN:HE21	2:M:92:PHE:HD2	1.33	0.77
3:H:175:MET:HG2	3:H:176:ALA:N	2.01	0.76
1:L:217:ARG:HD2	10:M:350:HOH:O	1.86	0.76
2:M:243:THR:O	2:M:247:ARG:HG3	1.87	0.75
1:L:105:VAL:O	1:L:109:ARG:HG3	1.89	0.72
2:M:69:THR:O	2:M:72:ILE:HG22	1.92	0.69
1:L:214:THR:HG21	2:M:20:MET:N	2.00	0.67
1:L:207:ARG:HG3	2:M:142:MET:HG2	1.75	0.66
2:M:208:PHE:HE2	7:M:313:LDA:H101	1.58	0.66
3:H:37:ARG:O	3:H:75:VAL:HG22	1.95	0.66
4:L:302:BCL:HBB3	4:L:302:BCL:HMB1	1.76	0.65
3:H:87:LEU:HD13	3:H:109:VAL:HG21	1.78	0.65
4:M:309:BCL:CBB	4:M:309:BCL:HMB1	2.28	0.64
4:L:301:BCL:H8	4:M:309:BCL:H202	1.78	0.64
3:H:209:SER:OG	3:H:212:LEU:HD23	1.98	0.64
2:M:190:SER:O	2:M:194:GLY:O	2.16	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:208:THR:H	1:L:211:HIS:CD2	2.17	0.63
4:L:304:BCL:HMB1	4:L:304:BCL:CBB	2.28	0.62
2:M:260:ALA:HB1	3:H:35:ASN:OD1	2.00	0.61
4:L:302:BCL:HMB1	4:L:302:BCL:CBB	2.30	0.61
3:H:132:LYS:HE2	3:H:171:ILE:HD11	1.84	0.60
3:H:86:ALA:O	3:H:100:PRO:HA	2.01	0.60
2:M:56:GLY:O	2:M:60:LEU:HB2	2.03	0.59
3:H:257:ALA:O	3:H:258:GLU:HG2	2.03	0.58
1:L:14:GLY:O	1:L:109:ARG:HD3	2.03	0.58
2:M:52:LEU:O	2:M:52:LEU:HD12	2.04	0.58
1:L:178:SER:HB3	6:L:306:U10:H212	1.85	0.57
3:H:168:TRP:CZ3	3:H:225:VAL:HG22	2.40	0.57
2:M:16:ALA:CB	2:M:32:VAL:HG21	2.31	0.56
3:H:34:GLU:O	3:H:37:ARG:HG3	2.05	0.56
4:M:309:BCL:HMB1	4:M:309:BCL:HBB3	1.88	0.56
4:L:301:BCL:H112	4:L:301:BCL:H162	1.89	0.55
2:M:162:PHE:CE1	9:M:312:SPN:HMB3	2.42	0.55
3:H:202:ARG:HD3	10:H:280:HOH:O	2.07	0.55
1:L:208:THR:H	1:L:211:HIS:HD2	1.54	0.55
2:M:25:ASN:OD1	2:M:27:ALA:HB3	2.07	0.55
4:L:301:BCL:CBB	4:L:301:BCL:HMB1	2.36	0.55
3:H:122:GLU:HB2	3:H:227:LEU:HD21	1.89	0.54
1:L:278:GLY:HA2	2:M:77:GLN:O	2.07	0.54
3:H:251:VAL:O	3:H:255:MET:HG3	2.08	0.54
2:M:239:ALA:O	3:H:73:LEU:HD22	2.08	0.54
1:L:170:ASN:O	1:L:173:HIS:HB3	2.07	0.54
3:H:257:ALA:C	3:H:258:GLU:HG2	2.28	0.54
3:H:75:VAL:HG22	3:H:76:PRO:HA	1.90	0.54
1:L:75:LEU:HD11	1:L:140:GLY:HA2	1.89	0.53
3:H:87:LEU:CD1	3:H:109:VAL:HG21	2.38	0.53
2:M:18:LEU:HD22	10:M:378:HOH:O	2.07	0.53
3:H:37:ARG:NH2	3:H:62:LYS:HB3	2.24	0.53
3:H:250:SER:OG	3:H:252:VAL:HG22	2.08	0.53
3:H:45:GLU:HG3	3:H:94:GLU:OE1	2.09	0.52
2:M:94:LEU:HD22	2:M:115:TRP:HB2	1.90	0.52
1:L:44:LEU:O	1:L:48:LEU:HD13	2.10	0.52
2:M:202:HIS:CE1	2:M:206:ILE:HD11	2.44	0.52
2:M:188:ASN:O	2:M:192:VAL:HG13	2.10	0.52
2:M:60:LEU:HD22	5:M:310:BPH:H4C3	1.91	0.52
2:M:133:THR:HG22	2:M:147:ALA:HB2	1.92	0.52
2:M:208:PHE:CE2	7:M:313:LDA:H101	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:213:ASP:O	1:L:217:ARG:HB2	2.10	0.51
3:H:62:LYS:HD3	3:H:64:PHE:CZ	2.46	0.50
1:L:2:LEU:HB3	1:L:6:GLU:HB3	1.93	0.50
4:L:301:BCL:HBB3	4:L:301:BCL:HMB1	1.92	0.50
3:H:165:VAL:O	3:H:166:ASP:HB2	2.11	0.50
3:H:242:MET:CE	3:H:243:TYR:CZ	2.94	0.49
1:L:60:ASN:ND2	1:L:63:LEU:HG	2.27	0.49
2:M:164:ARG:HB3	2:M:165:PRO:HD3	1.93	0.49
3:H:252:VAL:O	3:H:256:LEU:HD13	2.13	0.49
1:L:69:PRO:HG3	1:L:83:GLY:HA3	1.93	0.49
1:L:189:LEU:HB3	6:L:306:U10:H4M3	1.93	0.49
1:L:179:PHE:CZ	6:L:306:U10:H203	2.48	0.48
2:M:237:GLN:HB2	2:M:262:MET:HG2	1.95	0.48
2:M:177:TYR:HD1	9:M:312:SPN:H142	1.77	0.48
1:L:22:PHE:HA	1:L:24:PHE:CE2	2.47	0.48
1:L:205:GLU:HG2	3:H:65:ILE:HG22	1.94	0.48
1:L:244:SER:OG	4:L:302:BCL:HMA2	2.13	0.48
2:M:101:TYR:CE2	2:M:107:ALA:HA	2.48	0.48
4:L:301:BCL:H152	4:L:301:BCL:H193	1.95	0.48
4:M:309:BCL:HHC	4:M:309:BCL:OBB	2.14	0.48
3:H:132:LYS:HG2	10:H:305:HOH:O	2.14	0.48
2:M:67:PHE:CE1	9:M:312:SPN:H61	2.49	0.48
2:M:290:VAL:HG21	3:H:12:LEU:HD12	1.95	0.47
3:H:245:ALA:N	3:H:246:PRO:CD	2.77	0.47
3:H:209:SER:HG	3:H:212:LEU:HD23	1.78	0.47
6:L:306:U10:H1M1	6:L:306:U10:C8	2.45	0.47
1:L:79:PRO:O	1:L:81:ALA:N	2.47	0.47
1:L:59:TRP:O	1:L:61:PRO:HD3	2.14	0.47
2:M:120:PHE:HD1	9:M:312:SPN:CM9	2.28	0.47
3:H:242:MET:HE2	3:H:243:TYR:CZ	2.49	0.47
2:M:77:GLN:HG3	2:M:92:PHE:CD2	2.50	0.47
3:H:37:ARG:NH2	3:H:60:LYS:O	2.48	0.46
3:H:168:TRP:HZ3	3:H:225:VAL:HG22	1.79	0.46
1:L:246:LEU:O	1:L:249:ILE:HG22	2.15	0.46
2:M:72:ILE:HG23	2:M:73:TRP:N	2.29	0.46
1:L:216:PHE:CG	6:L:306:U10:H3M3	2.51	0.46
1:L:185:LEU:HD13	5:M:310:BPH:ND	2.30	0.46
1:L:60:ASN:HD22	1:L:63:LEU:CD1	2.28	0.46
1:L:87:GLN:O	1:L:91:ILE:HG12	2.16	0.46
2:M:11:GLN:HB2	3:H:144:ALA:HB3	1.98	0.46
5:M:310:BPH:HHH	5:M:310:BPH:HBC3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:87:LEU:HD12	3:H:100:PRO:HA	1.97	0.46
2:M:148:TRP:HA	2:M:148:TRP:CE3	2.51	0.46
2:M:202:HIS:O	2:M:206:ILE:HG13	2.15	0.46
2:M:236:GLU:HB3	10:H:279:HOH:O	2.14	0.45
7:M:314:LDA:H82	7:H:261:LDA:C12	2.39	0.45
4:L:301:BCL:HHC	4:L:301:BCL:OBB	2.14	0.45
1:L:223:SER:HA	6:L:306:U10:H3M2	1.98	0.45
3:H:132:LYS:HE3	10:H:263:HOH:O	2.15	0.45
2:M:148:TRP:HA	2:M:148:TRP:HE3	1.82	0.45
1:L:149:GLY:HA3	1:L:152:THR:OG1	2.16	0.45
3:H:196:VAL:HG12	3:H:205:VAL:HG22	1.99	0.45
1:L:95:GLY:O	1:L:99:SER:OG	2.22	0.45
2:M:108:PRO:HG2	2:M:111:GLU:HB2	1.99	0.45
1:L:133:LEU:C	1:L:136:PRO:HD2	2.37	0.44
1:L:217:ARG:NH1	10:L:338:HOH:O	2.48	0.44
2:M:97:PRO:O	2:M:172:SER:HB3	2.18	0.44
3:H:37:ARG:O	3:H:75:VAL:CG2	2.63	0.44
4:L:301:BCL:H192	9:M:312:SPN:HM43	2.00	0.44
2:M:167:LEU:HD12	2:M:285:LEU:HD11	1.99	0.43
3:H:41:PRO:HG3	3:H:58:LEU:HD11	1.99	0.43
5:M:310:BPH:H3A	5:M:310:BPH:HBA2	1.79	0.43
2:M:60:LEU:HD22	5:M:310:BPH:C4	2.48	0.43
2:M:60:LEU:HA	5:M:310:BPH:H4C2	2.00	0.43
2:M:228:ARG:HA	3:H:194:GLN:CG	2.48	0.43
2:M:253:ARG:HB2	2:M:259:ASN:HD22	1.83	0.43
2:M:72:ILE:CG2	2:M:73:TRP:N	2.82	0.43
2:M:191:LEU:HD12	2:M:191:LEU:HA	1.89	0.43
3:H:132:LYS:HE2	3:H:171:ILE:CD1	2.48	0.43
3:H:177:ARG:O	3:H:193:MET:HB2	2.19	0.43
1:L:2:LEU:CD2	1:L:10:ARG:CZ	2.96	0.43
4:L:302:BCL:HHC	4:L:302:BCL:OBB	2.19	0.43
3:H:251:VAL:HG23	3:H:252:VAL:N	2.34	0.42
4:L:302:BCL:HBD	4:L:304:BCL:HAC1	2.02	0.42
2:M:278:LEU:HA	2:M:278:LEU:HD12	1.86	0.42
3:H:226:THR:OG1	3:H:229:GLU:HG3	2.20	0.42
2:M:133:THR:HG21	2:M:147:ALA:HA	2.01	0.42
3:H:203:VAL:O	3:H:203:VAL:HG22	2.18	0.42
2:M:175:VAL:N	10:M:356:HOH:O	2.51	0.42
2:M:157:TRP:CE2	9:M:312:SPN:HM73	2.54	0.42
2:M:195:ASN:HB3	2:M:198:TYR:CD1	2.54	0.42
3:H:219:ILE:HG12	10:H:284:HOH:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:78:PRO:O	3:H:79:GLU:C	2.56	0.41
1:L:135:ARG:NH1	1:L:251:THR:O	2.53	0.41
1:L:268:LYS:HD3	1:L:268:LYS:HA	1.86	0.41
1:L:73:TYR:HE2	1:L:79:PRO:HD3	1.86	0.41
4:M:309:BCL:HBD	4:M:309:BCL:HAA2	2.03	0.41
2:M:59:SER:HB2	2:M:128:SER:OG	2.20	0.41
1:L:269:LEU:HA	1:L:270:PRO:HD2	1.86	0.41
1:L:138:MET:SD	1:L:249:ILE:HD11	2.60	0.41
1:L:167:PHE:HB3	4:L:302:BCL:HMC3	2.01	0.41
3:H:77:GLY:HA2	3:H:78:PRO:HD3	1.89	0.41
1:L:65:SER:CB	1:L:152:THR:HG21	2.51	0.41
1:L:66:VAL:HG11	1:L:89:ILE:HD12	2.02	0.41
2:M:264:GLY:HA3	3:H:35:ASN:OD1	2.21	0.41
1:L:73:TYR:O	1:L:74:GLY:C	2.60	0.41
2:M:11:GLN:OE1	2:M:40:GLY:HA3	2.21	0.41
1:L:5:PHE:C	1:L:5:PHE:CD1	2.95	0.40
2:M:100:GLU:CD	2:M:100:GLU:H	2.24	0.40
2:M:62:SER:HB2	2:M:125:ALA:HB2	2.03	0.40
4:L:301:BCL:C14	9:M:312:SPN:H101	2.51	0.40
1:L:6:GLU:HG3	2:M:250:LEU:CD2	2.51	0.40
3:H:202:ARG:CD	10:H:280:HOH:O	2.68	0.40
1:L:177:ILE:HG12	4:L:302:BCL:HMB3	2.03	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	L	278/281 (99%)	262 (94%)	15 (5%)	1 (0%)	38	59
2	M	295/307 (96%)	280 (95%)	15 (5%)	0	100	100
3	H	246/260 (95%)	236 (96%)	9 (4%)	1 (0%)	38	59

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	819/848 (97%)	778 (95%)	39 (5%)	2 (0%)	51 73

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	80	LEU
3	H	82	ASP

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	L	220/220 (100%)	211 (96%)	9 (4%)	35 61
2	M	233/240 (97%)	225 (97%)	8 (3%)	42 69
3	H	200/208 (96%)	189 (94%)	11 (6%)	25 46
All	All	653/668 (98%)	625 (96%)	28 (4%)	33 58

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	58	THR
1	L	129	LEU
1	L	189	LEU
1	L	195	LEU
1	L	216	PHE
1	L	235	LEU
1	L	238	LEU
1	L	247	CYS
1	L	272	TRP
2	M	6	ILE
2	M	60	LEU
2	M	89	LEU
2	M	94	LEU
2	M	191	LEU

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Mol	Chain	Res	Type
2	M	192	VAL
2	M	216	PHE
2	M	286	LEU
3	H	62	LYS
3	H	66	LEU
3	H	87	LEU
3	H	123	LEU
3	H	174	GLN
3	H	175	MET
3	H	194	GLN
3	H	208	LEU
3	H	225	VAL
3	H	231	ASP
3	H	258	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	60	ASN
1	L	87	GLN
1	L	183	ASN
1	L	211	HIS
2	M	187	ASN
2	M	259	ASN
3	H	194	GLN

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 14 ligands modelled in this entry, 1 is monoatomic - leaving 13 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
7	LDA	H	261	-	13,15,15	2.59	2 (15%)	14,17,17	0.70	0
4	BCL	L	301	2	55,74,74	1.37	6 (10%)	65,115,115	1.84	14 (21%)
4	BCL	L	302	1	55,74,74	1.50	7 (12%)	65,115,115	1.44	12 (18%)
4	BCL	L	304	1	55,74,74	1.41	6 (10%)	65,115,115	1.68	7 (10%)
5	BPH	L	305	-	65,70,70	1.26	5 (7%)	75,101,101	1.84	15 (20%)
6	U10	L	306	-	63,63,63	1.73	15 (23%)	76,79,79	1.57	20 (26%)
7	LDA	L	307	-	13,15,15	2.80	2 (15%)	14,17,17	0.67	0
4	BCL	M	309	2	55,74,74	1.37	7 (12%)	65,115,115	1.68	12 (18%)
5	BPH	M	310	-	65,70,70	1.28	6 (9%)	75,101,101	1.96	20 (26%)
6	U10	M	311	-	63,63,63	1.63	14 (22%)	76,79,79	1.39	9 (11%)
9	SPN	M	312	-	40,42,42	2.71	19 (47%)	48,52,52	2.45	16 (33%)
7	LDA	M	313	-	13,15,15	2.79	1 (7%)	14,17,17	0.74	1 (7%)
7	LDA	M	314	-	13,15,15	2.88	2 (15%)	14,17,17	0.72	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
7	LDA	H	261	-	-	0/13/13/13	0/0/0/0
4	BCL	L	301	2	1/1/21/25	0/37/137/137	0/0/9/9
4	BCL	L	302	1	-	0/37/137/137	0/0/9/9
4	BCL	L	304	1	-	0/37/137/137	0/0/9/9
5	BPH	L	305	-	1/1/18/22	0/54/105/105	0/1/6/6
6	U10	L	306	-	-	0/63/87/87	0/1/1/1
7	LDA	L	307	-	-	0/13/13/13	0/0/0/0
4	BCL	M	309	2	-	0/37/137/137	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	BPH	M	310	-	1/1/18/22	0/54/105/105	0/1/6/6
6	U10	M	311	-	-	0/63/87/87	0/1/1/1
9	SPN	M	312	-	-	0/50/51/51	0/0/0/0
7	LDA	M	313	-	-	0/13/13/13	0/0/0/0
7	LDA	M	314	-	-	0/13/13/13	0/0/0/0

All (92) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	M	313	LDA	O1-N1	-9.87	1.22	1.42
7	L	307	LDA	O1-N1	-9.86	1.22	1.42
7	M	314	LDA	O1-N1	-9.69	1.23	1.42
7	H	261	LDA	O1-N1	-9.08	1.24	1.42
9	M	312	SPN	C10-C9	-5.30	1.39	1.51
9	M	312	SPN	C17-C18	-5.18	1.39	1.51
9	M	312	SPN	C21-C20	-4.22	1.39	1.53
9	M	312	SPN	C10-C11	-4.14	1.39	1.53
6	L	306	U10	O3-C3M	-4.03	1.35	1.45
6	M	311	U10	C7-C8	-3.99	1.44	1.50
4	L	302	BCL	O2D-CED	-3.89	1.36	1.45
7	M	314	LDA	C1-N1	-3.68	1.43	1.51
9	M	312	SPN	C16-C17	-3.45	1.39	1.52
6	L	306	U10	C7-C8	-3.43	1.45	1.50
9	M	312	SPN	C15-C14	-3.39	1.39	1.52
9	M	312	SPN	C20-C19	-3.23	1.39	1.50
9	M	312	SPN	C24-C25	-3.21	1.39	1.50
9	M	312	SPN	C28-C29	-3.21	1.39	1.50
9	M	312	SPN	C7-C8	-3.21	1.39	1.50
9	M	312	SPN	C11-C12	-3.20	1.39	1.50
5	L	305	BPH	O2D-CED	-3.09	1.37	1.45
6	L	306	U10	O4-C4M	-3.04	1.38	1.45
6	M	311	U10	O3-C3M	-3.01	1.38	1.45
4	L	301	BCL	O2D-CED	-2.65	1.38	1.45
5	M	310	BPH	O2D-CED	-2.50	1.39	1.45
6	M	311	U10	C27-C28	-2.46	1.42	1.50
6	M	311	U10	C17-C18	-2.41	1.42	1.50
4	L	302	BCL	C1-C2	-2.39	1.41	1.49
9	M	312	SPN	C21-C22	-2.35	1.39	1.52
4	M	309	BCL	O2D-CED	-2.22	1.40	1.45
7	L	307	LDA	C1-N1	-2.20	1.46	1.51
7	H	261	LDA	C1-N1	-2.12	1.46	1.51
4	L	304	BCL	O2D-CED	-2.12	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	M	312	SPN	C16-C15	-2.09	1.39	1.51
5	M	310	BPH	CHC-C1C	2.02	1.40	1.36
5	L	305	BPH	C4-C3	2.15	1.56	1.50
6	L	306	U10	C6-C1	2.16	1.40	1.35
4	M	309	BCL	C5-C3	2.23	1.56	1.51
6	M	311	U10	C53-C54	2.45	1.39	1.32
4	L	304	BCL	C2-C3	2.46	1.39	1.33
6	L	306	U10	C53-C54	2.47	1.39	1.32
4	L	301	BCL	C2-C3	2.47	1.39	1.33
9	M	312	SPN	C29-C30	2.49	1.39	1.32
6	M	311	U10	C18-C19	2.51	1.39	1.33
6	M	311	U10	C33-C34	2.53	1.39	1.33
4	M	309	BCL	C2-C3	2.59	1.39	1.33
6	M	311	U10	C13-C14	2.60	1.39	1.33
9	M	312	SPN	C8-C9	2.60	1.39	1.33
6	L	306	U10	C43-C44	2.61	1.39	1.33
9	M	312	SPN	C25-C26	2.61	1.39	1.33
6	M	311	U10	C8-C9	2.62	1.39	1.33
9	M	312	SPN	C19-C18	2.62	1.39	1.33
6	M	311	U10	C43-C44	2.62	1.39	1.33
6	M	311	U10	C38-C39	2.62	1.39	1.33
4	L	302	BCL	C2-C3	2.62	1.39	1.33
6	M	311	U10	C23-C24	2.63	1.39	1.33
6	L	306	U10	C23-C24	2.63	1.39	1.33
6	M	311	U10	C48-C49	2.64	1.39	1.33
6	M	311	U10	C28-C29	2.64	1.39	1.33
6	L	306	U10	C33-C34	2.64	1.39	1.33
5	M	310	BPH	C2-C3	2.65	1.39	1.33
6	L	306	U10	C18-C19	2.66	1.39	1.33
6	L	306	U10	C28-C29	2.67	1.39	1.33
9	M	312	SPN	C12-C13	2.67	1.39	1.33
5	L	305	BPH	C2-C3	2.68	1.39	1.33
5	M	310	BPH	C3D-C4D	2.68	1.44	1.41
4	L	302	BCL	O2A-CGA	2.68	1.41	1.33
6	L	306	U10	C38-C39	2.68	1.39	1.33
6	L	306	U10	C13-C14	2.69	1.39	1.33
6	L	306	U10	C48-C49	2.71	1.39	1.33
6	L	306	U10	C8-C9	2.75	1.39	1.33
4	L	301	BCL	O2A-CGA	2.92	1.41	1.33
4	M	309	BCL	O2A-CGA	2.96	1.42	1.33
5	L	305	BPH	O2A-CGA	3.22	1.42	1.33
4	M	309	BCL	O2D-CGD	3.50	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	L	304	BCL	O2A-CGA	3.63	1.44	1.33
4	L	301	BCL	CHB-C4A	3.84	1.38	1.33
6	L	306	U10	C7-C6	3.90	1.58	1.51
4	L	304	BCL	O2D-CGD	3.92	1.43	1.33
4	L	301	BCL	O2D-CGD	3.94	1.43	1.33
4	L	302	BCL	O2D-CGD	4.04	1.43	1.33
5	M	310	BPH	O2A-CGA	4.21	1.45	1.33
4	M	309	BCL	CHC-C1C	4.69	1.39	1.33
4	L	302	BCL	CHB-C4A	4.73	1.39	1.33
4	M	309	BCL	CHB-C4A	4.74	1.39	1.33
4	L	304	BCL	CHB-C4A	4.93	1.39	1.33
4	L	304	BCL	CHC-C1C	5.15	1.40	1.33
4	L	301	BCL	CHC-C1C	5.35	1.40	1.33
5	M	310	BPH	O2D-CGD	5.49	1.47	1.33
4	L	302	BCL	CHC-C1C	5.65	1.40	1.33
5	L	305	BPH	O2D-CGD	5.78	1.47	1.33
9	M	312	SPN	C4-C5	8.22	1.53	1.33

All (126) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	M	312	SPN	C3-C4-C5	-8.79	112.01	126.71
5	M	310	BPH	O1D-CGD-CBD	-6.46	113.00	124.60
5	L	305	BPH	O1D-CGD-CBD	-6.27	113.35	124.60
4	L	304	BCL	O1D-CGD-CBD	-6.06	113.72	124.60
9	M	312	SPN	C6-C5-C4	-5.87	109.09	121.10
4	L	301	BCL	O1D-CGD-CBD	-5.34	115.00	124.60
4	M	309	BCL	O1D-CGD-CBD	-4.94	115.73	124.60
9	M	312	SPN	CM3-C5-C4	-4.70	111.14	123.69
4	L	301	BCL	CMB-C2B-C1B	-4.51	121.53	128.46
4	L	304	BCL	OBD-CAD-CBD	-3.50	120.66	125.94
5	M	310	BPH	OBD-CAD-CBD	-3.48	120.69	125.94
5	L	305	BPH	O2A-CGA-O1A	-3.42	115.06	123.55
5	L	305	BPH	OBD-CAD-CBD	-3.35	120.89	125.94
4	L	302	BCL	OBD-CAD-CBD	-3.14	121.19	125.94
4	L	301	BCL	OBD-CAD-CBD	-3.06	121.32	125.94
4	M	309	BCL	OBD-CAD-CBD	-3.06	121.32	125.94
4	L	302	BCL	O1D-CGD-CBD	-2.95	119.31	124.60
5	M	310	BPH	C4B-C3B-CAB	-2.87	119.48	130.09
5	M	310	BPH	O2A-CGA-O1A	-2.83	116.52	123.55
5	L	305	BPH	C4B-C3B-CAB	-2.77	119.88	130.09
4	M	309	BCL	CMB-C2B-C1B	-2.73	124.26	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L	306	U10	C30-C29-C31	-2.65	110.69	115.29
4	L	302	BCL	O2A-CGA-O1A	-2.52	117.29	123.55
6	L	306	U10	C20-C19-C21	-2.50	110.94	115.29
6	L	306	U10	C35-C34-C36	-2.49	110.96	115.29
6	L	306	U10	C11-C12-C13	-2.46	103.54	111.97
4	L	302	BCL	CMB-C2B-C1B	-2.42	124.74	128.46
5	L	305	BPH	C3A-C4A-NA	-2.42	108.89	113.06
5	M	310	BPH	C3A-C4A-NA	-2.40	108.92	113.06
5	M	310	BPH	C4D-CHA-C1A	-2.39	124.12	130.23
5	M	310	BPH	C2A-C1A-NA	-2.37	109.03	111.91
5	M	310	BPH	CBB-CAB-C3B	-2.35	115.48	120.52
5	M	310	BPH	CAC-C3C-C2C	-2.33	108.38	114.24
6	M	311	U10	C25-C24-C26	-2.28	111.33	115.29
5	L	305	BPH	C4D-CHA-C1A	-2.27	124.44	130.23
4	L	301	BCL	CED-O2D-CGD	-2.27	110.65	115.97
4	L	301	BCL	O2A-CGA-O1A	-2.27	117.92	123.55
9	M	312	SPN	CM3-C5-C6	-2.18	111.51	115.29
4	M	309	BCL	O2A-CGA-O1A	-2.09	118.35	123.55
6	L	306	U10	C50-C49-C51	-2.08	111.68	115.29
4	L	301	BCL	C6-C5-C3	-2.06	107.98	112.66
7	M	313	LDA	CM2-N1-CM1	-2.02	107.13	110.99
6	L	306	U10	C11-C9-C8	-2.02	116.97	121.10
5	L	305	BPH	C4-C3-C5	-2.01	111.80	115.29
6	M	311	U10	C4M-O4-C4	2.01	123.62	116.44
5	M	310	BPH	C5-C3-C2	2.04	125.28	121.10
5	L	305	BPH	C3A-C2A-C1A	2.05	104.10	101.68
6	M	311	U10	C37-C36-C34	2.07	119.94	112.93
9	M	312	SPN	CMB-C30-CM9	2.08	119.46	114.60
4	L	302	BCL	C3C-C2C-C1C	2.09	105.25	101.87
4	L	302	BCL	CMD-C2D-C3D	2.09	128.78	124.89
4	L	302	BCL	CED-O2D-CGD	2.11	120.92	115.97
5	M	310	BPH	C3A-C2A-C1A	2.13	104.19	101.68
6	L	306	U10	C51-C52-C53	2.14	119.31	111.97
5	M	310	BPH	C3C-C2C-C1C	2.16	105.36	101.87
6	M	311	U10	C36-C34-C33	2.16	125.53	121.10
4	M	309	BCL	CMD-C2D-C3D	2.17	128.91	124.89
4	M	309	BCL	C2C-C3C-C4C	2.20	104.63	101.34
4	L	304	BCL	OBB-CAB-C3B	2.22	124.18	119.95
6	L	306	U10	C17-C18-C19	2.22	133.26	127.68
6	L	306	U10	C7-C8-C9	2.23	130.44	126.71
4	M	309	BCL	C3A-C2A-C1A	2.23	104.68	101.34
6	M	311	U10	C41-C39-C38	2.29	125.80	121.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L	304	BCL	C2C-C3C-C4C	2.30	104.79	101.34
5	M	310	BPH	C3A-C4A-CHB	2.32	125.68	121.75
5	M	310	BPH	CMD-C2D-C3D	2.33	129.21	124.89
9	M	312	SPN	CM7-C22-C23	2.36	119.96	111.36
5	M	310	BPH	C2C-C3C-C4C	2.36	104.88	101.34
9	M	312	SPN	CM7-C22-C21	2.36	119.98	111.36
9	M	312	SPN	CM4-C9-C10	2.41	119.46	115.29
6	L	306	U10	C52-C53-C54	2.45	136.54	127.80
6	L	306	U10	C31-C29-C28	2.48	126.17	121.10
5	L	305	BPH	C3A-C4A-CHB	2.49	125.96	121.75
4	L	301	BCL	C2C-C3C-C4C	2.49	105.06	101.34
6	M	311	U10	C47-C48-C49	2.51	133.99	127.68
4	L	301	BCL	C2A-C1A-CHA	2.52	128.38	123.92
5	L	305	BPH	OBB-CAB-C3B	2.52	124.94	120.37
6	L	306	U10	C52-C51-C49	2.53	121.51	112.93
4	L	301	BCL	CMD-C2D-C3D	2.55	129.63	124.89
4	L	302	BCL	C2C-C3C-C4C	2.58	105.21	101.34
4	L	304	BCL	CMD-C2D-C3D	2.59	129.69	124.89
5	L	305	BPH	C1-C2-C3	2.60	130.74	125.96
6	L	306	U10	C42-C43-C44	2.63	134.29	127.68
9	M	312	SPN	CM8-C26-C27	2.70	119.97	115.29
6	L	306	U10	C3M-O3-C3	2.72	126.16	116.44
6	L	306	U10	C36-C34-C33	2.83	126.89	121.10
4	L	302	BCL	OBB-CAB-C3B	2.85	125.37	119.95
5	L	305	BPH	C4A-NA-C1A	2.89	110.50	108.16
5	L	305	BPH	CMD-C2D-C3D	2.93	130.32	124.89
6	L	306	U10	C47-C48-C49	2.93	135.03	127.68
6	L	306	U10	C22-C23-C24	2.98	135.17	127.68
4	L	302	BCL	C4A-NA-C1A	3.00	110.18	106.45
9	M	312	SPN	CM6-C18-C17	3.06	120.60	115.29
5	M	310	BPH	C4A-NA-C1A	3.09	110.66	108.16
9	M	312	SPN	CM5-C13-C14	3.09	120.65	115.29
4	M	309	BCL	OBB-CAB-C3B	3.14	125.94	119.95
5	M	310	BPH	OBB-CAB-C3B	3.20	126.17	120.37
4	L	301	BCL	O2A-CGA-CBA	3.21	121.24	111.90
4	L	301	BCL	CMB-C2B-C3B	3.22	130.88	124.89
6	L	306	U10	C12-C11-C9	3.24	123.90	112.93
4	L	301	BCL	OBB-CAB-C3B	3.27	126.19	119.95
6	M	311	U10	C36-C37-C38	3.28	123.23	111.97
4	M	309	BCL	O2A-CGA-CBA	3.32	121.55	111.90
6	M	311	U10	C27-C28-C29	3.33	136.03	127.68
4	M	309	BCL	C4A-NA-C1A	3.33	110.58	106.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	M	312	SPN	C20-C21-C22	3.38	126.28	116.23
4	L	304	BCL	C4A-NA-C1A	3.38	110.65	106.45
4	L	302	BCL	O2A-CGA-CBA	3.39	121.77	111.90
4	L	301	BCL	C4A-NA-C1A	3.47	110.76	106.45
9	M	312	SPN	CM2-C1-CM1	3.50	120.10	110.85
9	M	312	SPN	C11-C10-C9	3.61	125.14	112.93
4	L	302	BCL	O2D-CGD-CBD	3.76	118.02	111.30
5	M	310	BPH	O2A-CGA-CBA	3.90	123.24	111.90
6	L	306	U10	C12-C13-C14	3.91	137.49	127.68
9	M	312	SPN	C16-C17-C18	4.01	121.75	112.66
4	M	309	BCL	C1-C2-C3	4.02	133.37	125.96
5	L	305	BPH	O2A-CGA-CBA	4.12	123.89	111.90
6	L	306	U10	C32-C33-C34	4.24	138.34	127.68
9	M	312	SPN	CM2-C1-C2	4.50	118.59	109.57
5	M	310	BPH	C1-C2-C3	5.01	135.19	125.96
4	M	309	BCL	O2D-CGD-CBD	5.77	121.61	111.30
6	M	311	U10	C7-C8-C9	5.81	136.43	126.71
4	L	301	BCL	O2D-CGD-CBD	6.51	122.93	111.30
5	L	305	BPH	O2D-CGD-CBD	7.47	124.66	111.30
4	L	304	BCL	O2D-CGD-CBD	7.58	124.84	111.30
5	M	310	BPH	O2D-CGD-CBD	7.75	125.15	111.30

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	M	310	BPH	C13
4	L	301	BCL	C13
5	L	305	BPH	C13

There are no torsion outliers.

There are no ring outliers.

11 monomers are involved in 44 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	H	261	LDA	2	0
4	L	301	BCL	8	0
4	L	302	BCL	7	0
4	L	304	BCL	3	0
6	L	306	U10	6	0
4	M	309	BCL	5	0
5	M	310	BPH	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	M	311	U10	1	0
9	M	312	SPN	8	0
7	M	313	LDA	2	0
7	M	314	LDA	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	L	280/281 (99%)	-0.28	4 (1%) 75 76	28, 46, 66, 78	0
2	M	297/307 (96%)	-0.27	1 (0%) 93 94	24, 43, 61, 71	0
3	H	248/260 (95%)	-0.32	7 (2%) 53 56	35, 47, 69, 89	0
All	All	825/848 (97%)	-0.29	12 (1%) 74 75	24, 45, 66, 89	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	H	80	SER	3.2
3	H	92	VAL	2.8
3	H	255	MET	2.7
3	H	252	VAL	2.6
1	L	72	GLU	2.6
1	L	203	GLY	2.5
2	M	245	ALA	2.5
1	L	271	TRP	2.4
3	H	93	SER	2.3
3	H	79	GLU	2.1
3	H	78	PRO	2.1
1	L	252	GLY	2.1

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands

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
7	LDA	L	307	16/16	0.84	0.29	9.56	59,63,75,77	0
4	BCL	L	301	66/66	0.96	0.18	2.77	31,38,70,71	0
9	SPN	M	312	43/43	0.88	0.19	2.64	38,46,68,70	0
7	LDA	M	314	16/16	0.92	0.16	1.57	41,46,59,60	0
5	BPH	M	310	65/65	0.94	0.16	1.53	26,35,77,78	0
6	U10	L	306	63/63	0.92	0.16	1.02	51,79,90,90	33
7	LDA	M	313	16/16	0.90	0.16	1.01	39,48,58,60	0
4	BCL	M	309	66/66	0.97	0.15	0.97	27,32,46,53	0
5	BPH	L	305	65/65	0.96	0.14	0.82	27,35,44,46	0
4	BCL	L	304	66/66	0.97	0.15	0.75	26,35,48,50	0
6	U10	M	311	63/63	0.92	0.20	0.65	36,51,92,93	16
4	BCL	L	302	66/66	0.97	0.13	0.56	27,32,39,45	0
8	FE2	M	308	1/1	0.99	0.15	-0.96	37,37,37,37	0
7	LDA	H	261	16/16	0.85	0.31	-	60,63,74,75	0

6.5 Other polymers

There are no such residues in this entry.