



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 10:18 PM GMT

PDB ID : 3V3Y
Title : Photosynthetic Reaction Center From Rhodobacter Sphaeroides strain RV
Authors : Gabdulkhakov, A.G.; Fufina, T.Y.; Vasilieva, L.G.; Shuvalov, V.A.
Deposited on : 2011-12-14
Resolution : 2.80 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

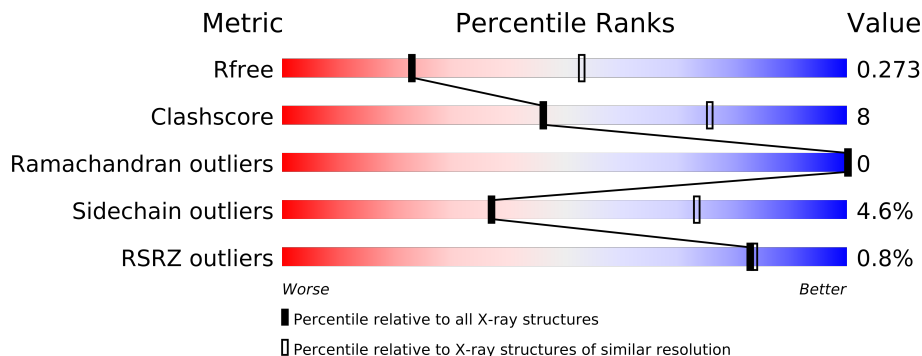
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.80 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}	66092	1799 (2.80-2.80)
Clashscore	79885	2295 (2.80-2.80)
Ramachandran outliers	78287	2252 (2.80-2.80)
Sidechain outliers	78261	2254 (2.80-2.80)
RSRZ outliers	66119	1802 (2.80-2.80)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	H	241	
2	L	281	
3	M	302	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
11	PO4	M	801	-	X
4	LDA	H	702	-	X
4	LDA	H	704	-	X
4	LDA	M	701	-	X
4	LDA	M	703	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
4	LDA	M	705	-	X
4	LDA	M	707	-	X
4	LDA	M	708	-	X
7	U10	L	502	-	X
8	DIO	L	900	-	X
8	DIO	L	901	-	X
8	DIO	M	902	-	X

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 7270 atoms, of which 0 are hydrogen and 0 are deuterium.

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	0
			1840	1178	315	338	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
			2233	1508	355	362	8			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	178	THR	SER	SEE REMARK 999	UNP P0C0Y8

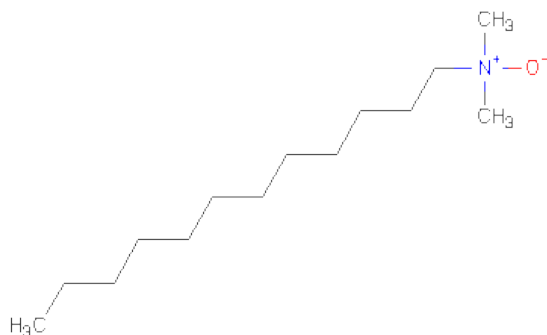
- Molecule 3 is a protein called Reaction center protein M chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	M	302	Total	C	N	O	S	0	0	0
			2409	1608	394	397	10			

There is a discrepancy between the modelled and reference sequences:

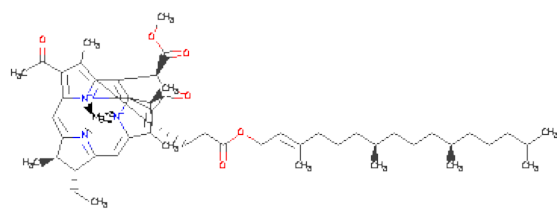
Chain	Residue	Modelled	Actual	Comment	Reference
M	8	THR	SER	SEE REMARK 999	UNP P0C0Y9

- Molecule 4 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula: C₁₄H₃₁NO).



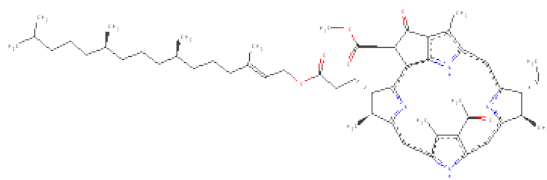
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	H	1	Total	C	N	O	0	0
			16	14	1	1		
4	H	1	Total	C	N	O	0	0
			16	14	1	1		
4	H	1	Total	C	N	O	0	0
			16	14	1	1		
4	M	1	Total	C	N	O	0	0
			16	14	1	1		
4	M	1	Total	C	N	O	0	0
			16	14	1	1		
4	M	1	Total	C	N	O	0	0
			16	14	1	1		
4	M	1	Total	C	N	O	0	0
			16	14	1	1		

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



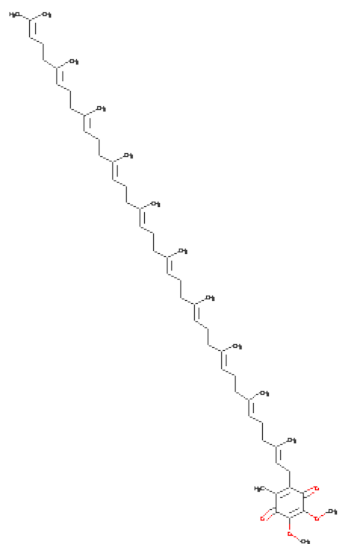
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
5	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
5	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
5	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

- Molecule 6 is BACTERIOPHEOPHYTIN A (three-letter code: BPH) (formula: C₅₅H₇₆N₄O₆).



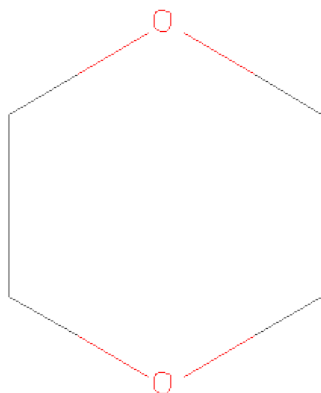
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	L	1	Total	C	N	O	0	0
			65	55	4	6		
6	M	1	Total	C	N	O	0	0
			65	55	4	6		

- Molecule 7 is UBIQUINONE-10 (three-letter code: U10) (formula: $C_{59}H_{90}O_4$).



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

- Molecule 8 is 1,4-DIETHYLENE DIOXIDE (three-letter code: DIO) (formula: $C_4H_8O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	L	1	Total	C	O	0	0
			6	4	2		
8	L	1	Total	C	O	0	0
			6	4	2		
8	M	1	Total	C	O	0	0
			6	4	2		

- Molecule 9 is FE (III) ION (three-letter code: FE) (formula: Fe).

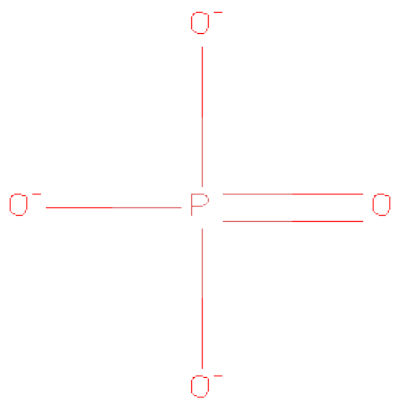
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	M	1	Total	Fe	0	0
			1	1		

- Molecule 10 is SPEROIDENONE (three-letter code: SPN) (formula: C₄₁H₇₀O₂).



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

- Molecule 11 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	M	1	Total	O	P	0	0
			5	4	1		
11	M	1	Total	O	P	0	0
			5	4	1		
11	M	1	Total	O	P	0	0
			5	4	1		

- Molecule 12 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	M	1	Total 1	Cl 1	0	0

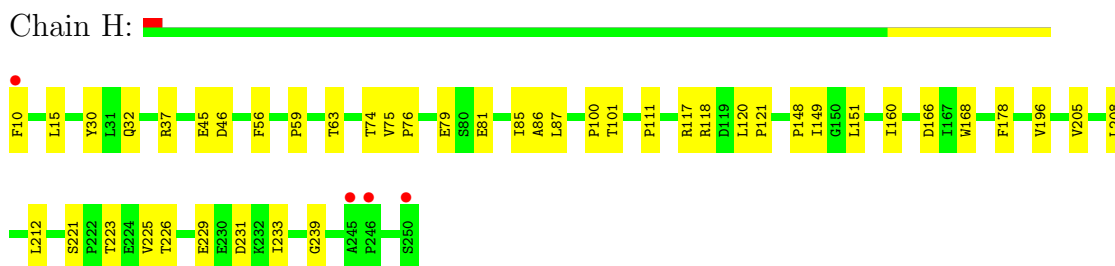
- Molecule 13 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	H	40	Total 40	O 40	0	0
13	L	21	Total 21	O 21	0	0
13	M	31	Total 31	O 31	0	0

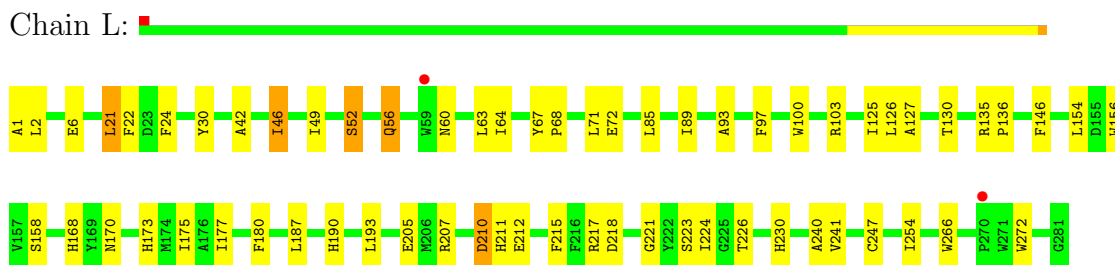
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

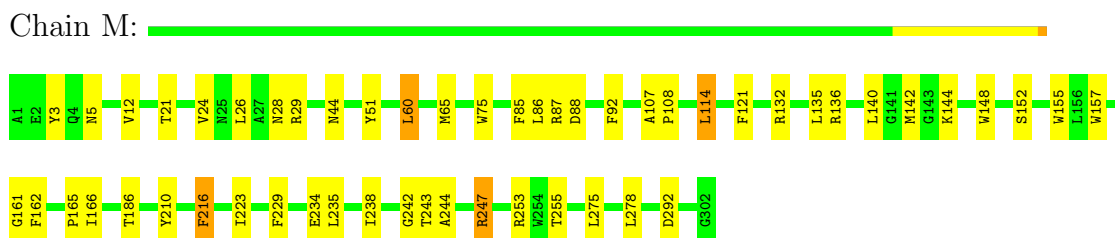
- Molecule 1: Reaction center protein H chain



- Molecule 2: Reaction center protein L chain



- Molecule 3: Reaction center protein M chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	139.75Å 139.75Å 185.60Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.94 – 2.80 26.60 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.4 (19.94-2.80) 99.2 (26.60-2.80)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.73 (at 2.80Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.2_869)	Depositor
R, R_{free}	0.244 , 0.284 0.237 , 0.273	Depositor DCC
R_{free} test set	2638 reflections (5.11%)	DCC
Wilson B-factor (Å ²)	40.8	Xtriage
Anisotropy	0.152	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 16.0	EDS
Estimated twinning fraction	0.000 for -h,-k,l	Xtriage
L-test for twinning	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Outliers	0 of 51770 reflections	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	7270	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.13% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BCL, LDA, DIO, CL, BPH, PO4, FE, 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	H	0.48	0/1889	0.67	0/2569
2	L	0.47	0/2321	0.61	0/3177
3	M	0.48	0/2501	0.60	0/3415
All	All	0.48	0/6711	0.62	0/9161

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	H	1840	0	1845	24	0
2	L	2233	0	2189	40	0
3	M	2409	0	2323	40	0
4	H	48	0	93	5	0
4	M	80	0	155	3	0
5	L	66	0	74	4	0
5	M	198	0	222	13	0
6	L	65	0	76	6	0
6	M	65	0	76	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	L	48	0	63	5	0
7	M	48	0	63	1	0
8	L	12	0	16	2	0
8	M	6	0	8	0	0
9	M	1	0	0	0	0
10	M	43	0	70	6	0
11	M	15	0	0	0	0
12	M	1	0	0	0	0
13	H	40	0	0	0	0
13	L	21	0	0	0	0
13	M	31	0	0	1	0
All	All	7270	0	7273	119	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 8.

All (119) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
5:M:303:BCL:H62	5:M:304:BCL:H202	1.62	0.82
1:H:81:GLU:HG3	1:H:85:ILE:HD11	1.66	0.78
1:H:63:THR:HG1	1:H:74:THR:HG1	1.33	0.77
3:M:229:PHE:HB2	3:M:244:ALA:HB2	1.72	0.72
2:L:30:TYR:O	2:L:103:ARG:NH2	2.26	0.69
6:L:402:BPH:HHC	6:L:402:BPH:HBB3	1.76	0.68
6:L:402:BPH:HBB2	3:M:210:TYR:HB3	1.78	0.65
2:L:190:HIS:HD1	7:L:502:U10:H4M1	1.61	0.65
4:H:702:LDA:HM22	3:M:253:ARG:HH22	1.62	0.64
1:H:111:PRO:O	3:M:247:ARG:NH2	2.31	0.64
3:M:234:GLU:O	3:M:238:ILE:HG13	1.99	0.63
1:H:30:TYR:CZ	4:H:704:LDA:H12	2.34	0.62
1:H:111:PRO:HB2	1:H:239:GLY:HA2	1.82	0.61
3:M:136:ARG:NH2	13:M:336:HOH:O	2.33	0.61
2:L:49:ILE:HG12	2:L:89:ILE:HD13	1.83	0.60
5:M:304:BCL:H192	6:M:401:BPH:H7C2	1.84	0.60
2:L:71:LEU:H	2:L:71:LEU:HD12	1.69	0.58
1:H:120:LEU:N	1:H:226:THR:HB	2.19	0.57
3:M:161:GLY:HA3	10:M:600:SPN:H201	1.86	0.57
2:L:266:TRP:CG	8:L:900:DIO:H21	2.42	0.55
1:H:120:LEU:H	1:H:226:THR:HB	1.72	0.55
5:L:302:BCL:HBB2	5:M:304:BCL:NA	2.20	0.55
6:M:401:BPH:HHC	6:M:401:BPH:HBB3	1.88	0.55
2:L:60:ASN:O	2:L:64:ILE:HG13	2.07	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
5:L:302:BCL:NA	5:M:304:BCL:HBB2	2.23	0.53
3:M:157:TRP:CD1	10:M:600:SPN:H202	2.43	0.53
6:L:402:BPH:HHC	6:L:402:BPH:CBB	2.39	0.53
2:L:97:PHE:HB3	2:L:125:ILE:HG12	1.90	0.53
3:M:243:THR:O	3:M:247:ARG:HG2	2.09	0.53
1:H:196:VAL:HG12	1:H:205:VAL:HG22	1.91	0.52
2:L:210:ASP:OD1	2:L:210:ASP:N	2.43	0.52
1:H:117:ARG:HD2	3:M:242:GLY:HA2	1.92	0.52
3:M:275:LEU:HD23	3:M:278:LEU:HD23	1.93	0.51
2:L:266:TRP:CD2	8:L:900:DIO:H21	2.47	0.50
2:L:180:PHE:CE2	2:L:240:ALA:HB1	2.47	0.49
5:M:305:BCL:HMB1	5:M:305:BCL:HBB2	1.95	0.48
2:L:127:ALA:O	2:L:130:THR:HB	2.12	0.48
7:L:502:U10:H122	7:L:502:U10:H101	1.52	0.48
3:M:28:ASN:HB2	3:M:51:TYR:CE2	2.49	0.48
5:M:303:BCL:H111	5:M:303:BCL:H142	1.69	0.48
1:H:149:ILE:HD13	1:H:166:ASP:HA	1.95	0.48
2:L:187:LEU:HD13	3:M:216:PHE:CG	2.49	0.48
2:L:193:LEU:HG	2:L:212:GLU:HG2	1.96	0.48
3:M:21:THR:HG23	3:M:26:LEU:HD21	1.95	0.47
1:H:86:ALA:HB1	1:H:101:THR:OG1	2.13	0.47
1:H:148:PRO:HA	1:H:151:LEU:HD12	1.97	0.47
2:L:224:ILE:HG22	7:L:502:U10:C2	2.44	0.47
5:M:303:BCL:C4B	10:M:600:SPN:H152	2.45	0.47
1:H:87:LEU:HD23	1:H:100:PRO:HA	1.96	0.47
1:H:37:ARG:HB3	1:H:75:VAL:HB	1.97	0.46
5:M:303:BCL:CAB	10:M:600:SPN:H162	2.46	0.46
2:L:103:ARG:NH1	3:M:255:THR:O	2.42	0.46
2:L:175:ILE:HG12	7:L:502:U10:H261	1.97	0.46
4:M:703:LDA:H11	4:M:703:LDA:H41	1.60	0.46
2:L:170:ASN:O	2:L:173:HIS:HB3	2.15	0.46
2:L:1:ALA:C	2:L:2:LEU:HD23	2.37	0.45
5:M:303:BCL:H2	6:M:401:BPH:CMB	2.46	0.45
3:M:60:LEU:HA	6:M:401:BPH:H4C2	1.98	0.45
2:L:135:ARG:HB3	2:L:136:PRO:HD3	1.98	0.45
3:M:85:PHE:HD2	3:M:86:LEU:HD12	1.81	0.45
1:H:121:PRO:HB3	1:H:225:VAL:O	2.17	0.45
2:L:180:PHE:CD2	2:L:240:ALA:HB1	2.52	0.44
5:L:302:BCL:CGA	5:M:305:BCL:HBC1	2.48	0.44
1:H:81:GLU:HG3	1:H:85:ILE:CD1	2.44	0.44
3:M:107:ALA:HA	3:M:108:PRO:HD3	1.86	0.44
3:M:75:TRP:HE1	10:M:600:SPN:HMA2	1.82	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:L:215:PHE:HB2	3:M:142:MET:HE1	2.00	0.43
3:M:162:PHE:O	3:M:166:ILE:HG12	2.18	0.43
2:L:205:GLU:O	2:L:207:ARG:NH1	2.51	0.43
2:L:217:ARG:O	2:L:221:GLY:HA2	2.18	0.43
3:M:114:LEU:HD13	3:M:114:LEU:HA	1.80	0.43
2:L:223:SER:O	3:M:44:ASN:ND2	2.48	0.43
3:M:223:ILE:HD13	3:M:223:ILE:HA	1.87	0.43
7:L:502:U10:H72	7:L:502:U10:H1M1	1.81	0.43
1:H:32:GLN:HG2	1:H:56:PHE:CE2	2.53	0.43
3:M:65:MET:HB3	3:M:121:PHE:CD2	2.54	0.43
3:M:235:LEU:HD23	3:M:235:LEU:HA	1.75	0.43
2:L:93:ALA:HB2	6:L:402:BPH:H122	2.01	0.43
4:H:704:LDA:HM11	4:H:704:LDA:H22	1.79	0.43
1:H:59:PRO:HG2	1:H:76:PRO:HD3	2.00	0.43
2:L:218:ASP:OD1	3:M:29:ARG:HD3	2.19	0.43
3:M:3:TYR:CZ	3:M:5:ASN:HA	2.53	0.43
5:M:304:BCL:HHC	5:M:304:BCL:OBB	2.19	0.43
2:L:146:PHE:HB3	2:L:156:TRP:CD2	2.54	0.42
2:L:230:HIS:CD2	3:M:223:ILE:HG13	2.55	0.42
1:H:229:GLU:O	1:H:233:ILE:HG13	2.20	0.42
1:H:168:TRP:HB2	1:H:178:PHE:HB2	2.01	0.42
1:H:118:ARG:HD3	1:H:120:LEU:HD12	2.02	0.42
2:L:22:PHE:HA	2:L:24:PHE:CE2	2.55	0.42
2:L:42:ALA:O	2:L:46:ILE:HB	2.19	0.42
5:M:303:BCL:HHC	5:M:303:BCL:OBB	2.19	0.42
4:M:705:LDA:HM13	4:M:705:LDA:H21	1.73	0.42
2:L:100:TRP:CH2	7:M:501:U10:H261	2.54	0.42
3:M:135:LEU:HD23	3:M:135:LEU:HA	1.92	0.42
1:H:212:LEU:HD23	1:H:212:LEU:HA	1.87	0.42
2:L:52:SER:O	2:L:56:GLN:HB2	2.20	0.42
5:M:303:BCL:H61	5:M:303:BCL:H102	1.93	0.41
3:M:24:VAL:HG11	3:M:29:ARG:NH1	2.36	0.41
3:M:157:TRP:CE2	10:M:600:SPN:HM73	2.55	0.41
4:H:702:LDA:H121	4:M:701:LDA:H91	2.02	0.41
6:M:401:BPH:H3A	6:M:401:BPH:HBA2	1.82	0.41
2:L:67:TYR:HA	2:L:68:PRO:HD3	1.93	0.41
3:M:140:LEU:HA	3:M:140:LEU:HD23	1.95	0.41
4:H:702:LDA:HM22	3:M:253:ARG:NH2	2.31	0.41
2:L:2:LEU:HB3	2:L:6:GLU:HB3	2.02	0.41
2:L:272:TRP:CG	3:M:87:ARG:HB2	2.56	0.41
1:H:208:LEU:HA	1:H:208:LEU:HD23	1.88	0.41
5:L:302:BCL:HBB3	5:L:302:BCL:HMB1	2.03	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:M:152:SER:O	3:M:155:TRP:HB3	2.21	0.41
2:L:207:ARG:HG3	2:L:211:HIS:CD2	2.57	0.40
2:L:173:HIS:O	2:L:177:ILE:HG13	2.21	0.40
3:M:162:PHE:C	3:M:165:PRO:HD2	2.42	0.40
3:M:88:ASP:HB2	3:M:92:PHE:CZ	2.56	0.40
2:L:168:HIS:HE1	3:M:186:THR:HB	1.87	0.40
2:L:21:LEU:HA	2:L:21:LEU:HD13	1.86	0.40
2:L:241:VAL:HG21	6:L:402:BPH:H2C	2.04	0.40
6:L:402:BPH:H112	6:L:402:BPH:H7C2	1.65	0.40
3:M:132:ARG:O	3:M:136:ARG:HG2	2.20	0.40
1:H:160:ILE:HD13	1:H:160:ILE:HA	1.88	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	239/241 (99%)	232 (97%)	7 (3%)	0	100	100
2	L	279/281 (99%)	271 (97%)	8 (3%)	0	100	100
3	M	300/302 (99%)	282 (94%)	18 (6%)	0	100	100
All	All	818/824 (99%)	785 (96%)	33 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	196/196 (100%)	188 (96%)	8 (4%)	41	77
2	L	220/220 (100%)	206 (94%)	14 (6%)	25	58
3	M	236/236 (100%)	228 (97%)	8 (3%)	49	84
All	All	652/652 (100%)	622 (95%)	30 (5%)	37	73

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	10	PHE
1	H	15	LEU
1	H	45	GLU
1	H	46	ASP
1	H	79	GLU
1	H	221	SER
1	H	223	THR
1	H	231	ASP
2	L	21	LEU
2	L	46	ILE
2	L	52	SER
2	L	56	GLN
2	L	63	LEU
2	L	72	GLU
2	L	85	LEU
2	L	126	LEU
2	L	154	LEU
2	L	158	SER
2	L	210	ASP
2	L	226	THR
2	L	247	CYS
2	L	254	ILE
3	M	12	VAL
3	M	60	LEU
3	M	114	LEU
3	M	144	LYS
3	M	148	TRP
3	M	216	PHE
3	M	247	ARG
3	M	292	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA chains 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 25 ligands modelled in this entry, 2 are monoatomic - leaving 23 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	LDA	H	702	-	15,15,15	3.63	2 (13%)	17,17,17	0.73	0
4	LDA	H	704	-	15,15,15	3.61	2 (13%)	17,17,17	0.93	1 (5%)
4	LDA	H	709	-	15,15,15	3.65	2 (13%)	17,17,17	0.52	0
5	BCL	L	302	-	74,74,74	1.32	5 (6%)	97,115,115	1.88	27 (27%)
6	BPH	L	402	-	70,70,70	0.99	4 (5%)	94,101,101	1.28	12 (12%)
7	U10	L	502	-	48,48,63	3.18	12 (25%)	59,61,79	1.77	18 (30%)
8	DIO	L	900	-	6,6,6	0.78	0	6,6,6	0.80	0
8	DIO	L	901	-	6,6,6	0.73	0	6,6,6	0.97	0
5	BCL	M	303	-	74,74,74	1.38	7 (9%)	97,115,115	2.05	30 (30%)
5	BCL	M	304	-	74,74,74	1.34	6 (8%)	97,115,115	1.93	25 (25%)
5	BCL	M	305	-	74,74,74	1.30	6 (8%)	97,115,115	2.06	25 (25%)
6	BPH	M	401	-	70,70,70	1.10	6 (8%)	94,101,101	1.17	7 (7%)
7	U10	M	501	-	48,48,63	3.06	14 (29%)	59,61,79	1.82	15 (25%)
10	SPN	M	600	-	42,42,42	1.26	6 (14%)	52,52,52	1.81	17 (32%)
4	LDA	M	701	-	15,15,15	3.71	1 (6%)	17,17,17	0.83	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	LDA	M	703	-	15,15,15	3.57	2 (13%)	17,17,17	0.55	0
4	LDA	M	705	-	15,15,15	3.79	2 (13%)	17,17,17	1.08	1 (5%)
4	LDA	M	707	-	15,15,15	3.63	2 (13%)	17,17,17	0.74	1 (5%)
4	LDA	M	708	-	15,15,15	3.82	2 (13%)	17,17,17	0.82	1 (5%)
11	PO4	M	800	-	4,4,4	0.44	0	6,6,6	0.31	0
11	PO4	M	801	-	4,4,4	0.08	0	6,6,6	0.33	0
11	PO4	M	803	-	4,4,4	0.16	0	6,6,6	0.32	0
8	DIO	M	902	-	6,6,6	0.72	0	6,6,6	0.92	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	LDA	H	702	-	-	0/13/13/13	0/0/0/0
4	LDA	H	704	-	-	0/13/13/13	0/0/0/0
4	LDA	H	709	-	-	0/13/13/13	0/0/0/0
5	BCL	L	302	-	-	0/41/137/137	0/0/9/9
6	BPH	L	402	-	-	0/49/105/105	0/0/6/6
7	U10	L	502	-	-	0/45/69/87	0/1/1/1
8	DIO	L	900	-	-	0/0/6/6	0/1/1/1
8	DIO	L	901	-	-	0/0/6/6	0/1/1/1
5	BCL	M	303	-	-	0/41/137/137	0/0/9/9
5	BCL	M	304	-	-	0/41/137/137	0/0/9/9
5	BCL	M	305	-	-	0/41/137/137	0/0/9/9
6	BPH	M	401	-	-	0/49/105/105	0/0/6/6
7	U10	M	501	-	-	0/45/69/87	0/1/1/1
10	SPN	M	600	-	-	0/51/51/51	0/0/0/0
4	LDA	M	701	-	-	0/13/13/13	0/0/0/0
4	LDA	M	703	-	-	0/13/13/13	0/0/0/0
4	LDA	M	705	-	-	0/13/13/13	0/0/0/0
4	LDA	M	707	-	-	0/13/13/13	0/0/0/0
4	LDA	M	708	-	-	0/13/13/13	0/0/0/0
11	PO4	M	800	-	-	0/0/0/0	0/0/0/0
11	PO4	M	801	-	-	0/0/0/0	0/0/0/0
11	PO4	M	803	-	-	0/0/0/0	0/0/0/0
8	DIO	M	902	-	-	0/0/6/6	0/1/1/1

All (81) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	M	708	LDA	O1-N1	-14.51	1.25	1.39
4	M	705	LDA	O1-N1	-14.36	1.25	1.39
4	M	701	LDA	O1-N1	-14.14	1.26	1.39
4	H	709	LDA	O1-N1	-13.86	1.26	1.39
4	H	702	LDA	O1-N1	-13.82	1.26	1.39
4	M	707	LDA	O1-N1	-13.78	1.26	1.39
4	H	704	LDA	O1-N1	-13.72	1.26	1.39
4	M	703	LDA	O1-N1	-13.53	1.26	1.39
7	L	502	U10	C13-C14	8.15	1.49	1.32
7	L	502	U10	C8-C9	8.04	1.49	1.32
7	M	501	U10	C13-C14	7.95	1.49	1.32
7	L	502	U10	C18-C19	7.65	1.48	1.32
7	M	501	U10	C33-C34	7.62	1.48	1.32
7	L	502	U10	C28-C29	7.60	1.48	1.32
7	L	502	U10	C23-C24	7.49	1.48	1.32
7	L	502	U10	C33-C34	7.47	1.48	1.32
7	M	501	U10	C18-C19	7.38	1.47	1.32
7	L	502	U10	C38-C39	7.02	1.48	1.34
7	M	501	U10	C8-C9	6.98	1.47	1.32
7	M	501	U10	C28-C29	6.96	1.47	1.32
7	M	501	U10	C38-C39	6.95	1.48	1.34
7	M	501	U10	C23-C24	6.59	1.46	1.32
5	M	305	BCL	C4B-NB	5.53	1.41	1.34
5	L	302	BCL	C4B-NB	5.50	1.41	1.34
5	M	303	BCL	C1B-NB	5.40	1.41	1.34
5	M	304	BCL	C4B-NB	5.25	1.41	1.34
5	M	303	BCL	C4B-NB	5.09	1.40	1.34
5	M	304	BCL	C1B-NB	5.08	1.40	1.34
5	L	302	BCL	C1B-NB	4.79	1.40	1.34
7	M	501	U10	O3-C3	-4.75	1.24	1.36
7	L	502	U10	O3-C3	-4.56	1.25	1.36
5	L	302	BCL	MG-ND	-4.54	1.95	2.05
5	M	303	BCL	MG-ND	-4.41	1.95	2.05
5	M	305	BCL	C1B-NB	4.40	1.40	1.34
7	M	501	U10	O4-C4	-4.28	1.25	1.36
5	M	304	BCL	MG-ND	-4.24	1.95	2.05
7	L	502	U10	O4-C4	-3.96	1.26	1.36
5	M	305	BCL	MG-ND	-3.94	1.96	2.05
5	M	303	BCL	MG-NB	-3.91	1.96	2.05
5	M	305	BCL	MG-NB	-3.91	1.96	2.05
5	M	304	BCL	MG-NB	-3.62	1.97	2.05
10	M	600	SPN	C25-C26	3.56	1.40	1.32
6	L	402	BPH	CHD-C4C	3.51	1.49	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	L	302	BCL	MG-NB	-3.47	1.97	2.05
6	M	401	BPH	CHD-C4C	3.33	1.48	1.41
10	M	600	SPN	C8-C9	3.32	1.39	1.32
10	M	600	SPN	C19-C18	3.14	1.39	1.32
6	M	401	BPH	C1B-NB	3.01	1.39	1.36
7	L	502	U10	C3-C2	-2.81	1.40	1.48
7	M	501	U10	C4-C5	-2.74	1.40	1.48
7	M	501	U10	C3-C2	-2.65	1.41	1.48
6	L	402	BPH	C4B-NB	2.65	1.39	1.36
10	M	600	SPN	C12-C13	2.63	1.38	1.32
5	M	303	BCL	C1C-NC	-2.62	1.33	1.39
4	M	705	LDA	C1-N1	-2.61	1.46	1.51
7	L	502	U10	C4-C5	-2.60	1.41	1.48
6	M	401	BPH	C4C-NC	-2.58	1.28	1.34
6	M	401	BPH	C4D-ND	-2.51	1.34	1.38
10	M	600	SPN	C4-C5	2.42	1.37	1.32
5	M	305	BCL	MG-NA	-2.41	2.00	2.07
5	M	304	BCL	C1B-C2B	-2.37	1.37	1.40
5	M	303	BCL	MG-NA	-2.32	2.00	2.07
5	M	305	BCL	C1C-NC	-2.27	1.34	1.39
4	M	708	LDA	C1-N1	-2.26	1.47	1.51
6	M	401	BPH	C4B-NB	2.25	1.39	1.36
4	H	704	LDA	C1-N1	-2.24	1.47	1.51
4	M	707	LDA	C1-N1	-2.20	1.47	1.51
6	M	401	BPH	C4D-C3D	2.18	1.44	1.41
6	L	402	BPH	C4D-ND	-2.18	1.35	1.38
7	M	501	U10	C6-C5	-2.15	1.40	1.46
6	L	402	BPH	C1B-NB	2.14	1.38	1.36
7	M	501	U10	C1-C2	-2.12	1.38	1.46
5	M	303	BCL	C1B-C2B	-2.11	1.37	1.40
4	H	709	LDA	C1-N1	-2.11	1.47	1.51
5	M	304	BCL	C1C-NC	-2.11	1.34	1.39
5	L	302	BCL	C1C-NC	-2.10	1.34	1.39
7	L	502	U10	C41-C39	2.08	1.51	1.40
7	M	501	U10	C41-C39	2.08	1.51	1.40
4	M	703	LDA	C1-N1	-2.07	1.47	1.51
4	H	702	LDA	C1-N1	-2.05	1.47	1.51
10	M	600	SPN	C1-C2	-2.01	1.50	1.54

All (181) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	M	303	BCL	C2D-C1D-ND	8.64	115.93	109.41
5	M	305	BCL	C2D-C1D-ND	7.81	115.30	109.41
5	M	303	BCL	C4D-ND-C1D	-6.97	98.15	106.57
5	M	305	BCL	C4D-ND-C1D	-6.78	98.38	106.57
5	M	305	BCL	O2D-CGD-CBD	6.56	124.68	111.33
5	M	304	BCL	C2D-C1D-ND	5.86	113.83	109.41
5	L	302	BCL	C2D-C1D-ND	5.74	113.74	109.41
5	M	304	BCL	C4D-ND-C1D	-5.51	99.91	106.57
5	L	302	BCL	C4D-ND-C1D	-5.40	100.05	106.57
10	M	600	SPN	C3-C4-C5	-5.18	118.00	126.76
5	M	305	BCL	CBD-CHA-C1A	5.13	135.47	128.77
5	M	303	BCL	CBD-CHA-C1A	4.71	134.93	128.77
7	M	501	U10	C32-C33-C34	-4.61	117.86	127.80
5	M	304	BCL	O2D-CGD-CBD	4.35	120.18	111.33
7	M	501	U10	C22-C23-C24	-4.32	118.48	127.80
5	M	304	BCL	CBD-CHA-C1A	4.31	134.40	128.77
5	M	303	BCL	C4-C3-C5	4.28	121.90	115.39
5	L	302	BCL	CBD-CHA-C1A	4.24	134.31	128.77
5	M	304	BCL	C2B-C1B-NB	4.18	112.57	109.41
6	L	402	BPH	OBB-CAB-C3B	4.07	126.18	120.07
5	L	302	BCL	CMB-C2B-C1B	-4.06	122.38	128.62
5	M	304	BCL	CHB-C4A-NA	4.00	129.31	124.58
7	M	501	U10	C30-C29-C31	3.87	121.27	115.39
7	M	501	U10	C35-C34-C36	3.83	121.21	115.39
6	M	401	BPH	C6-C5-C3	3.82	121.86	112.78
5	M	304	BCL	CMB-C2B-C1B	-3.74	122.87	128.62
5	M	305	BCL	C2B-C1B-NB	3.73	112.23	109.41
5	L	302	BCL	C2B-C1B-NB	3.70	112.20	109.41
5	M	303	BCL	C3A-C2A-C1A	-3.69	95.87	101.08
4	M	705	LDA	C2-C1-N1	-3.66	107.49	113.80
10	M	600	SPN	C7-C8-C9	-3.64	119.94	127.80
5	M	303	BCL	CMB-C2B-C1B	-3.62	123.05	128.62
6	L	402	BPH	C3B-C2B-C1B	3.59	109.16	107.01
5	M	305	BCL	O2D-CGD-O1D	-3.55	116.58	123.79
7	L	502	U10	O5-C5-C4	-3.54	113.10	120.96
6	M	401	BPH	CMD-C2D-C3D	3.54	130.54	124.97
10	M	600	SPN	CM3-C5-C6	3.49	120.70	115.39
5	L	302	BCL	C4-C3-C5	3.48	120.69	115.39
6	M	401	BPH	OBB-CAB-C3B	3.48	125.29	120.07
7	M	501	U10	C17-C18-C19	-3.46	120.34	127.80
7	L	502	U10	C7-C6-C5	3.40	122.45	118.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	M	304	BCL	CMB-C2B-C3B	3.37	130.27	124.97
5	M	305	BCL	CHB-C4A-NA	3.36	128.56	124.58
5	M	303	BCL	CHB-C4A-NA	3.35	128.55	124.58
5	M	304	BCL	CAA-C2A-C3A	-3.34	105.15	113.04
7	M	501	U10	C25-C24-C26	3.33	120.45	115.39
5	L	302	BCL	C3B-C4B-NB	3.33	111.88	108.64
5	M	305	BCL	C4D-C3D-C2D	-3.31	103.38	107.42
10	M	600	SPN	C24-C25-C26	-3.29	120.70	127.80
5	M	304	BCL	C4D-C3D-C2D	-3.29	103.40	107.42
5	M	303	BCL	O2D-CGD-CBD	3.29	118.03	111.33
5	M	303	BCL	C4D-C3D-C2D	-3.26	103.43	107.42
7	L	502	U10	C22-C23-C24	-3.26	120.77	127.80
6	L	402	BPH	C6-C5-C3	3.26	120.52	112.78
5	M	305	BCL	CHD-C4C-NC	3.25	130.55	125.86
7	L	502	U10	C37-C38-C39	-3.25	120.76	128.63
5	M	304	BCL	C3A-C4A-CHB	-3.19	117.69	124.33
7	M	501	U10	C12-C13-C14	-3.18	120.93	127.80
5	M	303	BCL	C1B-CHB-C4A	-3.18	123.44	130.06
5	M	304	BCL	O2D-CGD-O1D	-3.16	117.37	123.79
5	L	302	BCL	C4D-C3D-C2D	-3.13	103.60	107.42
5	M	305	BCL	CMB-C2B-C1B	-3.12	123.82	128.62
7	L	502	U10	C17-C18-C19	-3.11	121.10	127.80
7	L	502	U10	C32-C33-C34	-3.10	121.11	127.80
6	L	402	BPH	C3A-C2A-C1A	-3.09	97.97	101.91
5	L	302	BCL	CED-O2D-CGD	3.09	123.36	116.02
5	L	302	BCL	C4B-NB-C1B	-3.08	102.70	106.76
5	M	305	BCL	O2A-CGA-CBA	3.07	121.61	111.94
5	L	302	BCL	CHC-C4B-NB	-3.06	119.47	124.58
10	M	600	SPN	C20-C19-C18	-3.03	121.25	127.80
5	M	303	BCL	O1D-CGD-CBD	-3.02	118.24	124.42
5	M	304	BCL	C1-C2-C3	-3.01	120.84	126.19
10	M	600	SPN	CM6-C18-C17	2.98	119.93	115.39
5	L	302	BCL	CMB-C2B-C3B	2.95	129.61	124.97
7	L	502	U10	C20-C19-C21	2.86	119.73	115.39
5	M	305	BCL	CHB-C1B-NB	-2.85	119.82	124.58
5	M	305	BCL	C3B-C4B-NB	2.85	111.41	108.64
5	M	304	BCL	C4-C3-C5	2.81	119.66	115.39
5	M	305	BCL	C4B-NB-C1B	-2.80	103.08	106.76
5	M	305	BCL	O1D-CGD-CBD	-2.78	118.72	124.42
7	L	502	U10	C27-C28-C29	-2.77	121.82	127.80
4	M	701	LDA	O1-N1-CM1	-2.77	105.29	109.01
5	M	304	BCL	CAC-C3C-C2C	-2.77	107.54	113.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	M	304	BCL	C4B-NB-C1B	-2.76	103.12	106.76
7	M	501	U10	C25-C24-C23	-2.75	118.07	123.52
7	M	501	U10	C15-C14-C16	2.74	119.55	115.39
7	L	502	U10	C35-C34-C36	2.73	119.54	115.39
6	L	402	BPH	CMD-C2D-C3D	2.73	129.27	124.97
7	M	501	U10	C27-C28-C29	-2.71	121.95	127.80
7	L	502	U10	C25-C24-C26	2.70	119.49	115.39
5	M	303	BCL	C1D-CHD-C4C	-2.69	120.91	125.55
5	M	304	BCL	CHD-C4C-NC	2.69	129.74	125.86
5	M	305	BCL	C11-C12-C13	-2.68	107.42	115.14
5	M	304	BCL	O2A-CGA-CBA	2.68	120.36	111.94
10	M	600	SPN	C11-C12-C13	-2.67	122.03	127.80
5	M	304	BCL	C3B-C4B-NB	2.66	111.23	108.64
5	L	302	BCL	O2A-CGA-CBA	2.65	120.28	111.94
4	M	708	LDA	C2-C1-N1	-2.63	109.27	113.80
5	M	305	BCL	C3C-C4C-CHD	-2.62	117.62	123.35
7	L	502	U10	C30-C29-C31	2.61	119.35	115.39
5	M	304	BCL	CGD-CBD-CAD	-2.60	102.11	110.96
5	M	303	BCL	CHD-C4C-NC	2.60	129.62	125.86
5	M	303	BCL	C6-C5-C3	-2.59	106.62	112.78
5	M	303	BCL	CAA-C2A-C1A	2.57	118.05	111.62
6	L	402	BPH	C4-C3-C5	-2.57	111.48	115.39
7	L	502	U10	C4M-O4-C4	2.56	125.16	116.48
5	M	303	BCL	O2A-C1-C2	-2.56	103.01	108.55
5	M	305	BCL	C4-C3-C5	2.53	119.24	115.39
5	L	302	BCL	CGD-CBD-CHA	2.53	119.55	110.96
5	M	303	BCL	C2B-C1B-NB	2.52	111.32	109.41
5	M	303	BCL	CMB-C2B-C3B	2.50	128.91	124.97
5	M	304	BCL	CHC-C4B-NB	-2.49	120.41	124.58
7	L	502	U10	C3M-O3-C3	2.49	124.94	116.48
5	L	302	BCL	CHB-C4A-NA	2.49	127.52	124.58
5	M	303	BCL	O2A-CGA-CBA	2.49	119.76	111.94
5	L	302	BCL	C1-C2-C3	-2.48	121.78	126.19
7	M	501	U10	C4M-O4-C4	2.45	124.79	116.48
6	L	402	BPH	OBB-CAB-CBB	-2.43	114.09	120.13
6	L	402	BPH	CMB-C2B-C1B	-2.41	124.97	128.65
10	M	600	SPN	C7-C6-C5	2.41	120.71	112.74
6	L	402	BPH	C3A-C4A-NA	-2.41	109.66	112.90
5	L	302	BCL	CHD-C4C-NC	2.41	129.33	125.86
5	L	302	BCL	C2C-C1C-NC	2.40	113.87	110.95
10	M	600	SPN	O1-C1-C2	-2.40	104.54	109.32
6	L	402	BPH	C2C-C3C-C4C	-2.39	98.81	102.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	M	305	BCL	C1D-CHD-C4C	-2.38	121.44	125.55
7	M	501	U10	C37-C38-C39	-2.38	122.86	128.63
7	L	502	U10	O5-C5-C6	-2.36	117.33	121.67
5	M	305	BCL	CMB-C2B-C3B	2.36	128.68	124.97
10	M	600	SPN	CM5-C13-C14	2.36	118.97	115.39
5	L	302	BCL	C11-C10-C8	-2.36	108.35	115.14
5	L	302	BCL	O2D-CGD-CBD	2.35	116.11	111.33
7	M	501	U10	C35-C34-C33	-2.35	118.87	123.52
10	M	600	SPN	CMA-O1-C1	2.33	126.25	112.97
5	M	305	BCL	C16-C15-C13	-2.32	108.46	115.14
6	M	401	BPH	C4D-C3D-C2D	2.32	110.17	107.37
5	L	302	BCL	C11-C12-C13	-2.29	108.55	115.14
5	M	303	BCL	C3C-C4C-CHD	-2.28	118.34	123.35
6	M	401	BPH	CMB-C2B-C1B	-2.26	125.21	128.65
5	M	303	BCL	CHC-C4B-NB	-2.26	120.80	124.58
6	L	402	BPH	C1-O2A-CGA	-2.26	110.65	116.98
10	M	600	SPN	CM3-C5-C4	-2.26	119.05	123.52
10	M	600	SPN	C27-C28-C29	2.25	118.04	111.62
7	M	501	U10	C10-C9-C11	2.25	118.81	115.39
5	M	304	BCL	C1D-CHD-C4C	-2.23	121.70	125.55
5	L	302	BCL	C1B-CHB-C4A	-2.23	125.42	130.06
5	M	303	BCL	CAC-C3C-C2C	-2.22	108.80	113.89
5	M	303	BCL	C3B-C4B-NB	2.22	110.80	108.64
6	M	401	BPH	CAC-C3C-C4C	2.21	118.78	112.68
5	M	303	BCL	C1-C2-C3	-2.21	122.25	126.19
5	M	305	BCL	C6-C5-C3	-2.21	107.53	112.78
5	L	302	BCL	OBB-CAB-CBB	-2.20	114.67	120.13
5	M	305	BCL	OBD-CAD-CBD	2.20	129.25	125.94
5	M	303	BCL	C5-C3-C2	-2.20	116.86	121.08
7	L	502	U10	C7-C6-C1	-2.19	117.98	123.35
7	L	502	U10	O2-C2-C3	-2.18	116.12	120.96
5	L	302	BCL	C7-C6-C5	-2.18	106.58	113.01
7	M	501	U10	C22-C21-C19	-2.18	105.53	112.74
5	M	303	BCL	OBB-CAB-CBB	-2.17	114.73	120.13
6	M	401	BPH	OBB-CAB-CBB	-2.16	114.77	120.13
5	M	303	BCL	C11-C12-C13	-2.16	108.92	115.14
5	M	303	BCL	C4B-NB-C1B	-2.15	103.94	106.76
5	M	303	BCL	CBC-CAC-C3C	-2.13	108.36	113.61
5	M	305	BCL	C3A-C4A-CHB	-2.13	119.90	124.33
5	M	304	BCL	C11-C10-C8	-2.13	109.00	115.14
4	H	704	LDA	C2-C1-N1	-2.12	110.14	113.80
4	M	707	LDA	C2-C1-N1	-2.12	110.15	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	M	305	BCL	O2A-CGA-O1A	-2.12	117.65	123.43
5	L	302	BCL	O2A-C1-C2	-2.12	103.96	108.55
10	M	600	SPN	CM4-C9-C10	2.11	118.59	115.39
7	L	502	U10	C10-C9-C11	2.10	118.59	115.39
10	M	600	SPN	CM8-C26-C27	2.10	118.59	115.39
10	M	600	SPN	C6-C5-C4	-2.10	117.04	121.08
5	L	302	BCL	C1D-CHD-C4C	-2.09	121.94	125.55
5	L	302	BCL	C3C-C4C-CHD	-2.09	118.78	123.35
6	L	402	BPH	C1D-CHD-C4C	-2.08	120.24	128.39
10	M	600	SPN	C17-C18-C19	-2.07	117.09	121.08
5	M	304	BCL	CBC-CAC-C3C	-2.07	108.52	113.61
5	M	304	BCL	C2A-C1A-NA	2.06	113.52	111.24
7	L	502	U10	C7-C8-C9	-2.04	123.30	126.76
5	M	303	BCL	CBB-CAB-C3B	2.04	126.26	120.30

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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	241/241 (100%)	-0.50	4 (1%) 67 68	19, 35, 54, 102	0
2	L	281/281 (100%)	-0.48	2 (0%) 84 85	20, 36, 70, 94	0
3	M	302/302 (100%)	-0.62	0 100 100	21, 39, 65, 82	0
All	All	824/824 (100%)	-0.54	6 (0%) 83 85	19, 36, 65, 102	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	250	SER	4.6
1	H	10	PHE	4.5
2	L	59	TRP	3.7
1	H	245	ALA	2.3
2	L	270	PRO	2.3
1	H	246	PRO	2.2

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

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	RSR	LLDF	B-factors(\AA^2)	Q<0.9
8	DIO	L	901	6/6	0.27	13.89	46,48,53,58	0
8	DIO	M	902	6/6	0.52	12.63	45,53,62,68	0
7	U10	L	502	48/63	0.45	11.99	31,64,107,115	0
4	LDA	H	704	16/16	0.37	6.37	40,50,73,75	0
4	LDA	M	708	16/16	0.32	6.35	35,64,90,93	0
4	LDA	M	707	16/16	0.26	5.85	42,59,91,96	0
11	PO4	M	801	5/5	0.27	4.84	54,68,85,101	0
4	LDA	M	705	16/16	0.46	4.84	36,50,81,81	0
8	DIO	L	900	6/6	0.32	4.24	51,55,63,70	0
4	LDA	M	703	16/16	0.33	4.04	38,49,69,73	0
4	LDA	M	701	16/16	0.21	2.93	21,41,51,55	0
4	LDA	H	702	16/16	0.24	2.54	46,59,70,73	0
7	U10	M	501	48/63	0.17	1.76	19,30,50,61	0
10	SPN	M	600	43/43	0.22	1.49	29,49,77,87	0
5	BCL	M	303	66/66	0.16	1.28	20,29,53,63	0
6	BPH	M	401	65/65	0.17	1.09	23,32,93,104	0
5	BCL	L	302	66/66	0.14	0.33	21,29,38,55	0
6	BPH	L	402	65/65	0.14	0.25	14,28,39,42	0
5	BCL	M	304	66/66	0.14	0.09	22,30,43,60	0
5	BCL	M	305	66/66	0.12	-0.76	21,26,38,52	0
11	PO4	M	803	5/5	0.12	-1.49	66,72,79,87	0
12	CL	M	306	1/1	0.08	-1.71	50,50,50,50	0
9	FE	M	500	1/1	0.09	-1.87	24,24,24,24	0
11	PO4	M	800	5/5	0.06	-3.91	24,33,44,47	0
4	LDA	H	709	16/16	0.39	-	32,57,87,89	0

6.5 Other polymers ⓘ

There are no such residues in this entry.