



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 12:45 PM GMT

PDB ID : 3BSD
Title : Light harvesting protein from RC of Chlorobium tepidum
Authors : Nelson, N.; Frolow, F.; Brn-Shem, A.
Deposited on : 2007-12-23
Resolution : 2.30 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>

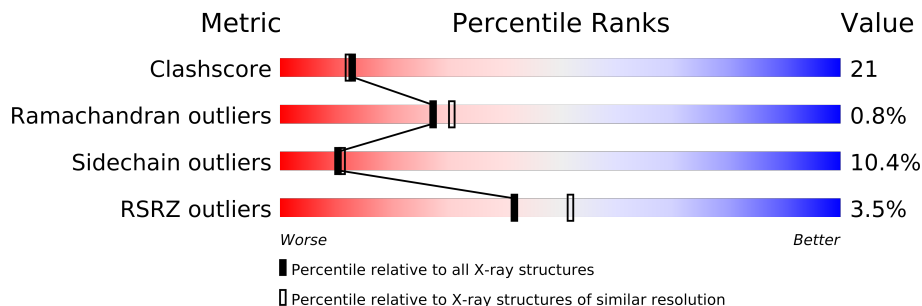
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.30 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))
Clashscore	79885	3679 (2.30-2.30)
Ramachandran outliers	78287	3642 (2.30-2.30)
Sidechain outliers	78261	3641 (2.30-2.30)
RSRZ outliers	66119	2930 (2.30-2.30)

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	A	366	

2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 3481 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.

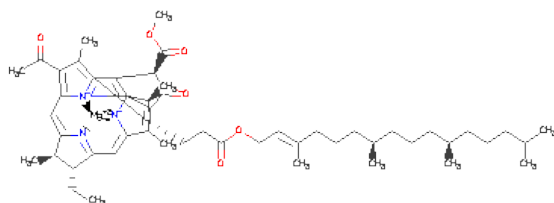
- Molecule 1 is a protein called Bacteriochlorophyll a protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	359	Total	C	N	O	S	0	0	0
			2798	1774	497	520	7			

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		

- Molecule 3 is BACTERIOCHLOROPHYLL A (three-letter code: BCL) (formula: C₅₅H₇₄MgN₄O₆).



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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
3	A	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
3	A	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
3	A	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
3	A	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
3	A	1	Total	C	Mg	N	O	0	0
			42	33	1	4	4		

- Molecule 4 is water.

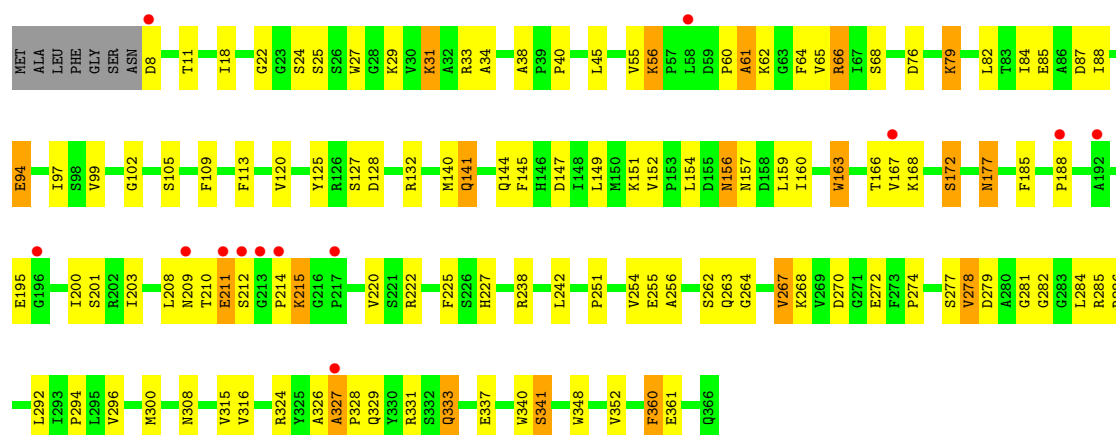
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	178	Total	O	0	0
			178	178		

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: Bacteriochlorophyll a protein

Chain A: 



4 Data and refinement statistics

Property	Value	Source
Space group	I 41 3 2	Depositor
Cell constants a, b, c, α , β , γ	167.69Å 167.69Å 167.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.82 – 2.30 44.82 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.7 (44.82-2.30) 99.1 (44.82-2.30)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.00 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.2.0013	Depositor
R, R_{free}	0.174 , 0.273 0.182 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	48.5	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 65.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 18046 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	3481	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.42% 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, MG

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	A	0.76	0/2868	0.80	2/3886 (0.1%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	238	ARG	NE-CZ-NH2	-5.61	117.50	120.30
1	A	76	ASP	N-CA-C	-5.38	96.47	111.00

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	A	2798	0	2736	102	0
2	A	1	0	0	0	0
3	A	504	0	549	51	0
4	A	178	0	0	23	0
All	All	3481	0	3285	137	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 21.

All (137) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:327:ALA:HB3	1:A:328:PRO:CD	1.82	1.09
3:A:373:BCL:C2	4:A:568:HOH:O	2.04	1.04
1:A:327:ALA:CB	1:A:328:PRO:CD	2.37	1.02
1:A:327:ALA:HB3	1:A:328:PRO:HD2	1.40	1.01
3:A:373:BCL:C3	4:A:568:HOH:O	2.12	0.97
1:A:152:VAL:HG21	3:A:367:BCL:HHC	1.51	0.92
1:A:327:ALA:CB	1:A:328:PRO:HD3	2.04	0.88
3:A:373:BCL:C5	4:A:568:HOH:O	2.25	0.85
1:A:327:ALA:HB2	1:A:361:GLU:H	1.40	0.84
1:A:195:GLU:HG3	1:A:300:MET:SD	2.19	0.83
1:A:151:LYS:HG2	1:A:220:VAL:HG22	1.60	0.83
1:A:56:LYS:HG3	1:A:251:PRO:HB3	1.62	0.81
1:A:84:ILE:HG21	3:A:372:BCL:H42	1.61	0.81
1:A:327:ALA:HB1	1:A:328:PRO:HD3	1.60	0.80
1:A:66:ARG:HD3	1:A:87:ASP:OD1	1.82	0.80
1:A:141:GLN:HE21	1:A:141:GLN:H	1.26	0.79
1:A:147:ASP:OD1	1:A:222:ARG:NH1	2.17	0.78
1:A:125:TYR:HB2	3:A:400:BCL:HHC	1.64	0.77
1:A:188:PRO:HG3	3:A:373:BCL:H42	1.69	0.75
1:A:315:VAL:HG23	1:A:340:TRP:CZ3	2.22	0.74
1:A:113:PHE:HZ	4:A:458:HOH:O	1.72	0.73
1:A:212:SER:HB3	1:A:220:VAL:HG21	1.70	0.73
1:A:29:LYS:HG3	1:A:272:GLU:HG3	1.70	0.73
1:A:328:PRO:HD2	1:A:360:PHE:CD2	2.25	0.71
1:A:34:ALA:HB3	1:A:267:VAL:HG13	1.72	0.71
1:A:168:LYS:O	1:A:172:SER:HB3	1.91	0.70
1:A:177:ASN:ND2	4:A:470:HOH:O	2.24	0.70
3:A:400:BCL:HBB3	3:A:400:BCL:HMB1	1.73	0.69
3:A:373:BCL:H2	4:A:568:HOH:O	1.79	0.68
3:A:372:BCL:HBC1	3:A:373:BCL:HMC2	1.78	0.65
1:A:315:VAL:HG23	1:A:340:TRP:HZ3	1.62	0.65
3:A:400:BCL:HBC2	3:A:400:BCL:HHD	1.79	0.64
3:A:372:BCL:HBB3	3:A:372:BCL:HMB1	1.81	0.63
1:A:31:LYS:HE2	1:A:33:ARG:HG3	1.80	0.62
1:A:55:VAL:CG2	1:A:65:VAL:CG1	2.78	0.61
1:A:141:GLN:NE2	1:A:141:GLN:H	1.97	0.61
1:A:18:ILE:HD11	3:A:370:BCL:HAA1	1.82	0.61
3:A:370:BCL:HBB2	3:A:371:BCL:H51	1.81	0.61
1:A:145:PHE:N	4:A:564:HOH:O	2.29	0.61
1:A:94:GLU:HG2	4:A:411:HOH:O	2.00	0.61

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:327:ALA:CB	1:A:361:GLU:H	2.13	0.60
1:A:113:PHE:HB3	1:A:152:VAL:HG22	1.84	0.60
1:A:177:ASN:HB3	1:A:203:ILE:HG13	1.83	0.59
3:A:373:BCL:HED2	3:A:373:BCL:H2	1.85	0.59
1:A:8:ASP:HA	4:A:512:HOH:O	2.03	0.58
1:A:55:VAL:CG2	1:A:65:VAL:HG13	2.34	0.58
1:A:40:PRO:HG2	1:A:45:LEU:HD21	1.86	0.58
3:A:371:BCL:C14	3:A:373:BCL:HHD	2.34	0.57
1:A:209:ASN:HB3	1:A:220:VAL:HB	1.87	0.57
3:A:373:BCL:HMB1	3:A:373:BCL:HBB2	1.88	0.56
1:A:254:VAL:CG2	3:A:372:BCL:H171	2.36	0.56
1:A:331:ARG:NH1	1:A:341:SER:O	2.39	0.56
1:A:278:VAL:HG23	1:A:279:ASP:O	2.06	0.55
1:A:128:ASP:O	1:A:132:ARG:HG2	2.06	0.55
1:A:163:TRP:CH2	1:A:210:THR:OG1	2.60	0.55
3:A:367:BCL:H41	3:A:367:BCL:H203	1.89	0.54
1:A:22:GLY:O	1:A:25:SER:HB3	2.06	0.54
3:A:372:BCL:HMB1	3:A:372:BCL:CBB	2.37	0.54
1:A:326:ALA:HA	1:A:361:GLU:O	2.08	0.54
1:A:144:GLN:HG3	4:A:564:HOH:O	2.07	0.54
1:A:24:SER:N	4:A:433:HOH:O	2.41	0.53
1:A:84:ILE:CG2	3:A:372:BCL:H42	2.34	0.53
1:A:167:VAL:HG22	1:A:208:LEU:HD13	1.91	0.53
1:A:156:ASN:HD22	1:A:156:ASN:N	2.07	0.53
1:A:27:TRP:HA	1:A:274:PRO:HA	1.90	0.53
1:A:156:ASN:H	1:A:159:LEU:HD12	1.74	0.52
1:A:254:VAL:HG23	3:A:372:BCL:H171	1.92	0.51
1:A:56:LYS:HD2	4:A:516:HOH:O	2.10	0.51
1:A:55:VAL:O	1:A:251:PRO:HA	2.12	0.50
3:A:373:BCL:HED2	3:A:373:BCL:C2	2.41	0.50
1:A:38:ALA:O	1:A:264:GLY:HA2	2.12	0.49
1:A:82:LEU:HD21	4:A:458:HOH:O	2.12	0.49
1:A:157:ASN:HA	1:A:160:ILE:HG12	1.94	0.49
3:A:372:BCL:HHD	3:A:372:BCL:HBC2	1.94	0.49
3:A:370:BCL:HBB3	3:A:370:BCL:HMB1	1.95	0.48
3:A:368:BCL:HMB1	3:A:368:BCL:HBB3	1.95	0.48
1:A:315:VAL:CG2	1:A:340:TRP:CZ3	2.93	0.48
1:A:125:TYR:CB	3:A:400:BCL:HHC	2.40	0.48
3:A:367:BCL:H41	3:A:367:BCL:C20	2.44	0.48
1:A:263:GLN:NE2	4:A:528:HOH:O	2.46	0.48
1:A:88:ILE:HD11	3:A:372:BCL:O1A	2.14	0.48
1:A:84:ILE:HB	4:A:458:HOH:O	2.13	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:11:THR:HG23	1:A:308:ASN:HB2	1.96	0.48
1:A:156:ASN:HD22	1:A:156:ASN:H	1.60	0.47
1:A:327:ALA:CB	4:A:418:HOH:O	2.62	0.47
1:A:60:PRO:O	1:A:61:ALA:CB	2.62	0.47
1:A:109:PHE:CZ	3:A:367:BCL:HMA3	2.51	0.46
1:A:141:GLN:HE21	1:A:141:GLN:N	2.04	0.46
1:A:185:PHE:CE1	1:A:200:ILE:HG13	2.50	0.46
1:A:125:TYR:HD1	1:A:127:SER:H	1.64	0.46
3:A:368:BCL:HBA2	3:A:368:BCL:H3A	1.79	0.45
1:A:188:PRO:CG	3:A:373:BCL:H42	2.43	0.45
1:A:120:VAL:N	4:A:564:HOH:O	2.48	0.45
1:A:214:PRO:HA	4:A:541:HOH:O	2.16	0.45
1:A:62:LYS:HE2	1:A:64:PHE:CE1	2.52	0.45
1:A:256:ALA:HB3	3:A:371:BCL:H93	1.99	0.45
1:A:166:THR:HG21	3:A:367:BCL:H101	1.99	0.44
1:A:286:ARG:NH1	1:A:361:GLU:OE2	2.44	0.44
1:A:281:GLY:C	4:A:419:HOH:O	2.55	0.44
1:A:348:TRP:CZ2	1:A:352:VAL:HG11	2.53	0.44
1:A:294:PRO:HB3	3:A:370:BCL:HHC	1.99	0.44
3:A:371:BCL:H172	3:A:372:BCL:H72	2.01	0.43
1:A:316:VAL:HG22	1:A:337:GLU:HG3	1.99	0.43
1:A:327:ALA:HB3	1:A:360:PHE:HD2	1.83	0.43
3:A:369:BCL:H62	3:A:369:BCL:H101	1.58	0.43
1:A:333:GLN:HA	1:A:337:GLU:O	2.18	0.43
1:A:154:LEU:HB3	1:A:160:ILE:HG23	2.00	0.43
1:A:282:GLY:CA	4:A:419:HOH:O	2.65	0.43
1:A:292:LEU:O	1:A:296:VAL:HG23	2.18	0.43
3:A:368:BCL:CBB	3:A:368:BCL:HMB1	2.49	0.42
3:A:370:BCL:C1A	3:A:370:BCL:CGA	2.97	0.42
3:A:371:BCL:H92	3:A:371:BCL:H111	1.57	0.42
3:A:371:BCL:H42	3:A:371:BCL:H11	1.90	0.42
1:A:94:GLU:O	1:A:120:VAL:HA	2.20	0.42
1:A:79:LYS:HB2	1:A:79:LYS:HE3	1.71	0.42
3:A:372:BCL:CHD	3:A:372:BCL:HBC2	2.49	0.42
1:A:55:VAL:HG22	1:A:65:VAL:HG13	2.01	0.42
1:A:284:LEU:CD2	1:A:324:ARG:HG3	2.50	0.42
1:A:277:SER:HG	1:A:285:ARG:HH21	1.64	0.41
1:A:327:ALA:HB1	4:A:418:HOH:O	2.18	0.41
1:A:152:VAL:CG2	3:A:367:BCL:HHC	2.35	0.41
3:A:367:BCL:HBB2	3:A:367:BCL:HMB1	2.02	0.41
3:A:370:BCL:H62	3:A:370:BCL:H93	1.96	0.41
1:A:203:ILE:HG22	1:A:225:PHE:HB3	2.02	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:60:PRO:O	1:A:61:ALA:HB2	2.20	0.41
1:A:102:GLY:HA2	4:A:504:HOH:O	2.20	0.41
3:A:368:BCL:H121	3:A:368:BCL:H162	1.66	0.41
1:A:62:LYS:HE2	1:A:64:PHE:HE1	1.86	0.41
3:A:367:BCL:HMB1	3:A:367:BCL:CBB	2.51	0.41
3:A:368:BCL:C19	3:A:372:BCL:HHB	2.50	0.41
1:A:360:PHE:C	1:A:360:PHE:CD2	2.94	0.41
3:A:400:BCL:HBC2	3:A:400:BCL:CHD	2.49	0.41
1:A:242:LEU:C	1:A:242:LEU:HD12	2.41	0.40
3:A:373:BCL:H2	3:A:373:BCL:CED	2.51	0.40
1:A:210:THR:HA	1:A:211:GLU:HA	1.64	0.40
3:A:373:BCL:HMB1	3:A:373:BCL:CBB	2.51	0.40
1:A:282:GLY:N	4:A:419:HOH:O	2.53	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	A	357/366 (98%)	335 (94%)	19 (5%)	3 (1%)	27	30

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	327	ALA
1	A	61	ALA
1	A	215	LYS

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	A	297/302 (98%)	266 (90%)	31 (10%)	10	11

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	LYS
1	A	56	LYS
1	A	66	ARG
1	A	68	SER
1	A	79	LYS
1	A	85	GLU
1	A	94	GLU
1	A	97	ILE
1	A	99	VAL
1	A	105	SER
1	A	140	MET
1	A	141	GLN
1	A	149	LEU
1	A	156	ASN
1	A	163	TRP
1	A	172	SER
1	A	177	ASN
1	A	201	SER
1	A	211	GLU
1	A	215	LYS
1	A	227	HIS
1	A	255	GLU
1	A	262	SER
1	A	267	VAL
1	A	268	LYS
1	A	270	ASP
1	A	278	VAL
1	A	329	GLN
1	A	333	GLN
1	A	341	SER
1	A	360	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	141	GLN
1	A	156	ASN

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 9 ligands modelled in this entry, 1 is monoatomic - leaving 8 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	$\# Z > 2$
3	BCL	A	367	-	74,74,74	1.98	10 (13%)	97,115,115	2.31	25 (25%)
3	BCL	A	368	4	74,74,74	2.05	12 (16%)	97,115,115	2.36	27 (27%)
3	BCL	A	369	1	74,74,74	2.14	11 (14%)	97,115,115	2.04	26 (26%)
3	BCL	A	370	1	74,74,74	2.07	11 (14%)	97,115,115	1.86	18 (18%)
3	BCL	A	371	1	74,74,74	1.90	10 (13%)	97,115,115	2.55	35 (36%)
3	BCL	A	372	1	74,74,74	2.10	10 (13%)	97,115,115	2.32	26 (26%)
3	BCL	A	373	1	74,74,74	2.17	9 (12%)	97,115,115	2.35	30 (30%)
3	BCL	A	400	1	49,50,74	2.44	9 (18%)	66,86,115	2.78	23 (34%)

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
3	BCL	A	367	-	2/2/21/25	0/41/137/137	0/0/9/9
3	BCL	A	368	4	2/2/21/25	1/41/137/137	0/0/9/9
3	BCL	A	369	1	2/2/21/25	0/41/137/137	0/0/9/9
3	BCL	A	370	1	2/2/21/25	0/41/137/137	0/0/9/9
3	BCL	A	371	1	2/2/21/25	0/41/137/137	0/0/9/9
3	BCL	A	372	1	2/2/21/25	1/41/137/137	0/0/9/9
3	BCL	A	373	1	2/2/21/25	0/41/137/137	0/0/9/9
3	BCL	A	400	1	-	0/12/108/137	0/0/9/9

All (82) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	373	BCL	OBD-CAD	14.36	1.43	1.22
3	A	369	BCL	OBD-CAD	14.22	1.43	1.22
3	A	372	BCL	OBD-CAD	13.09	1.41	1.22
3	A	400	BCL	OBD-CAD	12.91	1.41	1.22
3	A	370	BCL	OBD-CAD	12.59	1.40	1.22
3	A	368	BCL	OBD-CAD	11.65	1.39	1.22
3	A	367	BCL	OBD-CAD	11.38	1.38	1.22
3	A	371	BCL	OBD-CAD	10.23	1.37	1.22
3	A	368	BCL	O1A-CGA	6.47	1.42	1.22
3	A	372	BCL	O1A-CGA	6.41	1.41	1.22
3	A	370	BCL	O1A-CGA	6.21	1.41	1.22
3	A	371	BCL	O1A-CGA	6.10	1.40	1.22
3	A	400	BCL	C4D-C3D	-5.95	1.34	1.41
3	A	367	BCL	O1A-CGA	5.87	1.40	1.22
3	A	368	BCL	C4D-C3D	-5.42	1.34	1.41
3	A	373	BCL	O1A-CGA	5.36	1.38	1.22
3	A	371	BCL	C4D-C3D	-5.26	1.35	1.41
3	A	373	BCL	C4D-C3D	-5.18	1.35	1.41
3	A	372	BCL	C4D-C3D	-5.16	1.35	1.41
3	A	370	BCL	C4D-C3D	-5.10	1.35	1.41
3	A	369	BCL	O1A-CGA	4.88	1.37	1.22
3	A	367	BCL	C4D-C3D	-4.56	1.36	1.41
3	A	367	BCL	C3D-CAD	-4.55	1.38	1.47
3	A	400	BCL	C3D-CAD	-4.30	1.38	1.47
3	A	371	BCL	C3D-CAD	-4.30	1.38	1.47
3	A	367	BCL	C1A-NA	4.05	1.41	1.32
3	A	370	BCL	C3D-CAD	-3.93	1.39	1.47
3	A	369	BCL	C2-C3	3.92	1.40	1.32
3	A	400	BCL	C4B-NB	3.78	1.39	1.34
3	A	368	BCL	C2-C3	3.75	1.40	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	373	BCL	C4B-NB	3.58	1.39	1.34
3	A	369	BCL	C4D-C3D	-3.51	1.37	1.41
3	A	371	BCL	C2-C3	3.46	1.39	1.32
3	A	400	BCL	C1A-NA	3.40	1.39	1.32
3	A	368	BCL	C3D-CAD	-3.40	1.40	1.47
3	A	400	BCL	C1B-NB	3.26	1.38	1.34
3	A	370	BCL	C2-C3	3.24	1.39	1.32
3	A	368	BCL	C1A-NA	3.19	1.39	1.32
3	A	371	BCL	C1A-NA	3.17	1.39	1.32
3	A	372	BCL	C2-C3	3.15	1.39	1.32
3	A	372	BCL	C1A-NA	3.15	1.39	1.32
3	A	367	BCL	C2-C3	3.10	1.39	1.32
3	A	369	BCL	C4B-NB	3.08	1.38	1.34
3	A	368	BCL	C4B-NB	3.08	1.38	1.34
3	A	367	BCL	C1C-NC	-3.06	1.32	1.39
3	A	369	BCL	C1C-NC	-2.99	1.32	1.39
3	A	369	BCL	C1A-NA	2.98	1.38	1.32
3	A	368	BCL	CHD-C4C	2.88	1.48	1.39
3	A	372	BCL	C4B-NB	2.86	1.38	1.34
3	A	373	BCL	CHD-C4C	2.83	1.48	1.39
3	A	370	BCL	C1A-NA	2.79	1.38	1.32
3	A	371	BCL	C1C-NC	-2.72	1.33	1.39
3	A	368	BCL	O2A-CGA	-2.71	1.24	1.33
3	A	369	BCL	C3D-CAD	-2.71	1.41	1.47
3	A	373	BCL	C1B-NB	2.71	1.38	1.34
3	A	372	BCL	CHD-C4C	2.70	1.47	1.39
3	A	370	BCL	O2D-CGD	-2.65	1.26	1.33
3	A	372	BCL	C3D-CAD	-2.63	1.42	1.47
3	A	371	BCL	CHD-C4C	2.62	1.47	1.39
3	A	373	BCL	C3D-CAD	-2.62	1.42	1.47
3	A	370	BCL	C4B-NB	2.54	1.37	1.34
3	A	373	BCL	O2D-CGD	-2.48	1.26	1.33
3	A	369	BCL	C1B-NB	2.48	1.37	1.34
3	A	400	BCL	O2D-CGD	-2.47	1.26	1.33
3	A	371	BCL	O2D-CGD	-2.41	1.26	1.33
3	A	370	BCL	CHD-C4C	2.38	1.46	1.39
3	A	368	BCL	C1C-NC	-2.37	1.34	1.39
3	A	369	BCL	O2A-CGA	-2.36	1.25	1.33
3	A	373	BCL	O2A-CGA	-2.36	1.25	1.33
3	A	372	BCL	O2D-CGD	-2.31	1.27	1.33
3	A	367	BCL	CHD-C4C	2.30	1.46	1.39
3	A	367	BCL	O2A-CGA	-2.27	1.26	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	368	BCL	C1B-NB	2.26	1.37	1.34
3	A	400	BCL	CHD-C4C	2.26	1.46	1.39
3	A	370	BCL	C1B-NB	2.26	1.37	1.34
3	A	371	BCL	C4B-NB	2.21	1.37	1.34
3	A	367	BCL	O2D-CGD	-2.20	1.27	1.33
3	A	400	BCL	C1C-NC	-2.17	1.34	1.39
3	A	368	BCL	O2D-CGD	-2.16	1.27	1.33
3	A	369	BCL	CHD-C4C	2.14	1.46	1.39
3	A	372	BCL	O2A-CGA	-2.07	1.26	1.33
3	A	370	BCL	C1C-NC	-2.01	1.34	1.39

All (210) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	371	BCL	CHC-C4B-NB	-10.14	107.64	124.58
3	A	373	BCL	C2D-C1D-ND	-9.15	102.50	109.41
3	A	400	BCL	C2D-C1D-ND	-9.01	102.61	109.41
3	A	372	BCL	C2D-C1D-ND	-8.89	102.70	109.41
3	A	369	BCL	CMB-C2B-C1B	-8.11	116.15	128.62
3	A	372	BCL	CMB-C2B-C1B	-8.05	116.23	128.62
3	A	367	BCL	CMB-C2B-C1B	-8.05	116.23	128.62
3	A	373	BCL	CMB-C2B-C1B	-7.84	116.55	128.62
3	A	370	BCL	CMB-C2B-C1B	-7.81	116.60	128.62
3	A	368	BCL	CHC-C4B-NB	-7.79	111.57	124.58
3	A	368	BCL	C2D-C1D-ND	-7.57	103.70	109.41
3	A	400	BCL	CMB-C2B-C1B	-7.48	117.11	128.62
3	A	371	BCL	CHB-C4A-NA	-7.07	116.20	124.58
3	A	400	BCL	CHC-C4B-NB	-7.06	112.79	124.58
3	A	368	BCL	CMB-C2B-C1B	-6.67	118.36	128.62
3	A	371	BCL	C1-C2-C3	-6.36	114.88	126.19
3	A	367	BCL	CHC-C1C-NC	-6.24	117.18	124.58
3	A	371	BCL	CMB-C2B-C1B	-6.24	119.03	128.62
3	A	372	BCL	CMB-C2B-C3B	6.04	134.49	124.97
3	A	372	BCL	O2D-CGD-CBD	6.00	123.56	111.33
3	A	367	BCL	C1D-CHD-C4C	-5.98	115.24	125.55
3	A	370	BCL	CMB-C2B-C3B	5.83	134.15	124.97
3	A	367	BCL	CMB-C2B-C3B	5.83	134.15	124.97
3	A	400	BCL	CMB-C2B-C3B	5.82	134.14	124.97
3	A	368	BCL	C4B-CHC-C1C	-5.82	117.95	130.06
3	A	400	BCL	CHD-C4C-NC	-5.60	117.78	125.86
3	A	369	BCL	CMB-C2B-C3B	5.51	133.64	124.97
3	A	371	BCL	C4B-CHC-C1C	-5.41	118.80	130.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	370	BCL	O2D-CGD-CBD	5.36	122.24	111.33
3	A	367	BCL	CHD-C4C-NC	-5.31	118.19	125.86
3	A	373	BCL	CMB-C2B-C3B	5.30	133.33	124.97
3	A	373	BCL	C4-C3-C5	5.28	123.41	115.39
3	A	367	BCL	C4B-CHC-C1C	-5.26	119.11	130.06
3	A	372	BCL	CHC-C4B-NB	-5.23	115.85	124.58
3	A	368	BCL	C4D-ND-C1D	5.17	112.82	106.57
3	A	368	BCL	CMB-C2B-C3B	5.16	133.10	124.97
3	A	372	BCL	C1-C2-C3	-5.14	117.05	126.19
3	A	370	BCL	C2D-C1D-ND	-5.08	105.58	109.41
3	A	371	BCL	CMB-C2B-C3B	4.99	132.83	124.97
3	A	367	BCL	C2D-C1D-ND	-4.99	105.65	109.41
3	A	373	BCL	OBD-CAD-CBD	-4.97	118.44	125.94
3	A	373	BCL	C4-C3-C2	-4.95	113.71	123.52
3	A	372	BCL	C4D-ND-C1D	4.91	112.50	106.57
3	A	369	BCL	CHC-C4B-NB	-4.80	116.56	124.58
3	A	400	BCL	C1B-CHB-C4A	-4.73	120.21	130.06
3	A	400	BCL	C4B-CHC-C1C	-4.65	120.38	130.06
3	A	372	BCL	C1D-CHD-C4C	-4.62	117.57	125.55
3	A	371	BCL	O2D-CGD-CBD	4.62	120.75	111.33
3	A	368	BCL	C3A-C4A-CHB	-4.61	114.74	124.33
3	A	367	BCL	CHC-C4B-NB	-4.61	116.87	124.58
3	A	373	BCL	C4D-ND-C1D	4.53	112.03	106.57
3	A	369	BCL	C4B-CHC-C1C	-4.48	120.72	130.06
3	A	371	BCL	C2D-C1D-ND	-4.48	106.03	109.41
3	A	372	BCL	CHB-C4A-NA	-4.48	119.27	124.58
3	A	400	BCL	CMD-C2D-C3D	-4.45	117.96	124.97
3	A	373	BCL	O2D-CGD-CBD	4.44	120.37	111.33
3	A	368	BCL	CHC-C1C-NC	-4.42	119.34	124.58
3	A	400	BCL	C1D-CHD-C4C	-4.41	117.94	125.55
3	A	369	BCL	O2D-CGD-CBD	4.41	120.31	111.33
3	A	369	BCL	C2B-C1B-NB	-4.40	106.09	109.41
3	A	400	BCL	C4D-ND-C1D	4.32	111.78	106.57
3	A	371	BCL	C2B-C1B-NB	-4.27	106.19	109.41
3	A	400	BCL	C3B-C4B-CHC	-4.26	117.92	126.00
3	A	367	BCL	CAA-C2A-C1A	4.18	122.05	111.62
3	A	373	BCL	C1D-C2D-C3D	4.11	110.15	106.78
3	A	367	BCL	CMD-C2D-C1D	4.10	134.26	126.16
3	A	368	BCL	CHD-C4C-NC	-4.05	120.01	125.86
3	A	369	BCL	O1D-CGD-CBD	-4.04	116.15	124.42
3	A	372	BCL	C4B-CHC-C1C	-4.01	121.72	130.06
3	A	400	BCL	O2D-CGD-CBD	3.97	119.42	111.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	368	BCL	O2D-CGD-CBD	3.95	119.39	111.33
3	A	373	BCL	O2A-CGA-CBA	3.93	124.31	111.94
3	A	367	BCL	C2B-C1B-NB	-3.89	106.47	109.41
3	A	373	BCL	CHC-C4B-NB	-3.88	118.09	124.58
3	A	371	BCL	C2B-C1B-CHB	3.84	133.29	126.00
3	A	371	BCL	C3B-C4B-CHC	-3.83	118.73	126.00
3	A	372	BCL	CHB-C1B-NB	-3.82	118.20	124.58
3	A	371	BCL	CMD-C2D-C1D	3.81	133.69	126.16
3	A	368	BCL	CMD-C2D-C3D	-3.81	118.97	124.97
3	A	369	BCL	C2D-C1D-ND	-3.79	106.55	109.41
3	A	373	BCL	C2B-C1B-NB	-3.76	106.57	109.41
3	A	400	BCL	CHB-C4A-NA	-3.75	120.14	124.58
3	A	400	BCL	CMD-C2D-C1D	3.70	133.46	126.16
3	A	371	BCL	C3C-C4C-CHD	-3.69	115.27	123.35
3	A	370	BCL	C4D-ND-C1D	3.66	110.99	106.57
3	A	367	BCL	C1-C2-C3	-3.65	119.70	126.19
3	A	367	BCL	C4D-ND-C1D	3.62	110.94	106.57
3	A	368	BCL	CMD-C2D-C1D	3.62	133.32	126.16
3	A	371	BCL	O2A-CGA-CBA	3.59	123.24	111.94
3	A	368	BCL	O2A-CGA-O1A	-3.55	113.72	123.43
3	A	369	BCL	C1-O2A-CGA	3.53	126.86	116.98
3	A	370	BCL	O2D-CGD-O1D	-3.49	116.71	123.79
3	A	367	BCL	CED-O2D-CGD	3.47	124.29	116.02
3	A	368	BCL	O2A-CGA-CBA	3.46	122.82	111.94
3	A	369	BCL	C1-C2-C3	-3.43	120.09	126.19
3	A	368	BCL	CGD-CBD-CHA	3.35	122.35	110.96
3	A	368	BCL	C1D-CHD-C4C	-3.34	119.78	125.55
3	A	369	BCL	O2A-CGA-CBA	3.33	122.42	111.94
3	A	370	BCL	C2B-C1B-NB	-3.33	106.90	109.41
3	A	373	BCL	C3A-C4A-CHB	-3.33	117.41	124.33
3	A	373	BCL	C4B-CHC-C1C	-3.31	123.16	130.06
3	A	369	BCL	CHC-C1C-NC	-3.31	120.65	124.58
3	A	371	BCL	C1B-CHB-C4A	-3.29	123.21	130.06
3	A	371	BCL	C4D-ND-C1D	3.24	110.48	106.57
3	A	373	BCL	C6-C7-C8	-3.18	105.97	115.14
3	A	368	BCL	CHB-C4A-NA	-3.17	120.82	124.58
3	A	370	BCL	CMA-C3A-C4A	-3.14	102.64	111.76
3	A	400	BCL	CED-O2D-CGD	3.13	123.46	116.02
3	A	367	BCL	CMD-C2D-C3D	-3.12	120.05	124.97
3	A	372	BCL	CMD-C2D-C3D	-3.09	120.09	124.97
3	A	371	BCL	C4B-NB-C1B	3.09	110.84	106.76
3	A	373	BCL	C1-C2-C3	-3.08	120.71	126.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	372	BCL	C1B-CHB-C4A	-3.08	123.66	130.06
3	A	370	BCL	C4-C3-C5	3.07	120.05	115.39
3	A	370	BCL	C3A-C4A-NA	3.05	114.67	110.95
3	A	368	BCL	CHA-C1A-NA	-3.02	120.02	126.22
3	A	370	BCL	O2A-CGA-CBA	3.00	121.37	111.94
3	A	369	BCL	C4D-ND-C1D	3.00	110.19	106.57
3	A	368	BCL	OBD-CAD-CBD	-2.99	121.42	125.94
3	A	373	BCL	C2C-C1C-CHC	-2.98	118.12	124.33
3	A	372	BCL	C3A-C4A-CHB	-2.95	118.20	124.33
3	A	372	BCL	O2D-CGD-O1D	-2.94	117.81	123.79
3	A	371	BCL	O1D-CGD-CBD	-2.94	118.39	124.42
3	A	368	BCL	C1-O2A-CGA	2.87	125.02	116.98
3	A	368	BCL	C2B-C1B-NB	-2.87	107.24	109.41
3	A	371	BCL	C3A-C4A-CHB	-2.86	118.39	124.33
3	A	369	BCL	CED-O2D-CGD	2.85	122.79	116.02
3	A	367	BCL	O2A-CGA-CBA	2.84	120.89	111.94
3	A	372	BCL	O1D-CGD-CBD	-2.82	118.64	124.42
3	A	400	BCL	CHC-C1C-NC	-2.81	121.25	124.58
3	A	400	BCL	CBD-CHA-C1A	2.80	132.43	128.77
3	A	373	BCL	C4D-C3D-C2D	-2.80	104.00	107.42
3	A	373	BCL	O2D-CGD-O1D	-2.77	118.16	123.79
3	A	372	BCL	O2A-CGA-CBA	2.77	120.65	111.94
3	A	372	BCL	C6-C5-C3	-2.76	106.22	112.78
3	A	368	BCL	O1D-CGD-CBD	-2.75	118.78	124.42
3	A	372	BCL	C2B-C1B-NB	-2.74	107.34	109.41
3	A	370	BCL	CMD-C2D-C1D	2.73	131.56	126.16
3	A	368	BCL	C2A-C3A-C4A	2.73	105.60	101.40
3	A	371	BCL	CMD-C2D-C3D	-2.71	120.69	124.97
3	A	373	BCL	C11-C10-C8	2.71	122.95	115.14
3	A	373	BCL	O2A-CGA-O1A	-2.71	116.03	123.43
3	A	371	BCL	C7-C6-C5	-2.71	105.04	113.01
3	A	370	BCL	CHC-C4B-NB	-2.70	120.06	124.58
3	A	368	BCL	CED-O2D-CGD	2.70	122.44	116.02
3	A	367	BCL	C4-C3-C2	-2.69	118.19	123.52
3	A	371	BCL	CBD-CHA-C1A	2.69	132.28	128.77
3	A	371	BCL	CED-O2D-CGD	2.68	122.39	116.02
3	A	367	BCL	CHA-C1A-NA	-2.67	120.73	126.22
3	A	370	BCL	C3A-C4A-CHB	-2.67	118.77	124.33
3	A	371	BCL	C1D-CHD-C4C	-2.65	120.97	125.55
3	A	367	BCL	O2D-CGD-CBD	2.65	116.74	111.33
3	A	400	BCL	C2B-C1B-NB	-2.65	107.41	109.41
3	A	373	BCL	CMD-C2D-C3D	-2.65	120.79	124.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	371	BCL	C4A-NA-C1A	2.64	110.17	106.52
3	A	371	BCL	CHD-C4C-NC	-2.64	122.05	125.86
3	A	367	BCL	CGD-CBD-CAD	2.63	119.89	110.96
3	A	367	BCL	O1D-CGD-CBD	-2.60	119.09	124.42
3	A	371	BCL	C2A-C3A-C4A	2.59	105.39	101.40
3	A	369	BCL	C11-C12-C13	-2.58	107.72	115.14
3	A	369	BCL	C3A-C2A-C1A	2.57	104.72	101.08
3	A	370	BCL	C4B-CHC-C1C	-2.56	124.73	130.06
3	A	369	BCL	CHD-C4C-NC	-2.56	122.17	125.86
3	A	369	BCL	CBD-CHA-C1A	2.55	132.10	128.77
3	A	400	BCL	C3A-C4A-NA	2.54	114.04	110.95
3	A	373	BCL	OBD-CAD-C3D	2.54	132.63	127.91
3	A	371	BCL	OBD-CAD-C3D	-2.52	123.22	127.91
3	A	369	BCL	CAC-C3C-C2C	2.51	119.64	113.89
3	A	372	BCL	CMD-C2D-C1D	2.50	131.11	126.16
3	A	369	BCL	OBD-CAD-CBD	-2.47	122.21	125.94
3	A	367	BCL	C4-C3-C5	2.46	119.13	115.39
3	A	371	BCL	CBC-CAC-C3C	-2.45	107.57	113.61
3	A	372	BCL	C1D-C2D-C3D	2.44	108.78	106.78
3	A	371	BCL	CHB-C1B-NB	-2.43	120.52	124.58
3	A	373	BCL	C2C-C1C-NC	2.43	113.90	110.95
3	A	373	BCL	C1D-CHD-C4C	-2.41	121.39	125.55
3	A	371	BCL	C3D-CAD-CBD	2.39	110.97	107.60
3	A	367	BCL	CAA-CBA-CGA	-2.39	105.58	113.27
3	A	369	BCL	C3A-C4A-CHB	-2.32	119.50	124.33
3	A	400	BCL	CHA-C1A-NA	-2.32	121.45	126.22
3	A	373	BCL	C1C-NC-C4C	-2.29	105.01	107.79
3	A	367	BCL	C7-C6-C5	-2.29	106.27	113.01
3	A	400	BCL	CAC-C3C-C4C	2.28	117.65	112.58
3	A	369	BCL	O2A-CGA-O1A	-2.27	117.22	123.43
3	A	372	BCL	C6-C7-C8	-2.27	108.60	115.14
3	A	369	BCL	CMD-C2D-C1D	2.27	130.65	126.16
3	A	367	BCL	C3A-C4A-NA	2.27	113.71	110.95
3	A	369	BCL	C1B-CHB-C4A	-2.26	125.35	130.06
3	A	400	BCL	O1D-CGD-CBD	-2.26	119.80	124.42
3	A	368	BCL	C6-C7-C8	-2.23	108.72	115.14
3	A	368	BCL	C4A-NA-C1A	2.23	109.59	106.52
3	A	369	BCL	C4-C3-C5	2.23	118.77	115.39
3	A	370	BCL	OBD-CAD-C3D	-2.22	123.77	127.91
3	A	370	BCL	C1B-CHB-C4A	-2.21	125.46	130.06
3	A	370	BCL	C11-C10-C8	-2.21	108.78	115.14
3	A	371	BCL	C6-C5-C3	2.19	117.98	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	373	BCL	C3A-C4A-NA	2.17	113.58	110.95
3	A	372	BCL	CAC-C3C-C2C	-2.16	108.94	113.89
3	A	400	BCL	C1D-C2D-C3D	2.14	108.54	106.78
3	A	372	BCL	O2A-C1-C2	2.12	113.15	108.55
3	A	373	BCL	C2A-C1A-NA	2.12	113.59	111.24
3	A	368	BCL	CBD-CHA-C1A	2.11	131.53	128.77
3	A	371	BCL	C2C-C1C-CHC	-2.10	119.96	124.33
3	A	369	BCL	CHA-C1A-NA	-2.08	121.95	126.22
3	A	373	BCL	C9-C8-C10	2.07	118.61	111.02
3	A	371	BCL	C1C-NC-C4C	-2.06	105.28	107.79
3	A	372	BCL	C4A-NA-C1A	2.06	109.36	106.52
3	A	373	BCL	C1B-CHB-C4A	-2.04	125.81	130.06
3	A	371	BCL	C1-O2A-CGA	2.02	122.63	116.98
3	A	372	BCL	CED-O2D-CGD	2.01	120.80	116.02

All (14) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	372	BCL	C8
3	A	372	BCL	C13
3	A	371	BCL	C8
3	A	371	BCL	C13
3	A	368	BCL	C8
3	A	368	BCL	C13
3	A	370	BCL	C8
3	A	370	BCL	C13
3	A	369	BCL	C8
3	A	369	BCL	C13
3	A	373	BCL	C8
3	A	373	BCL	C13
3	A	367	BCL	C8
3	A	367	BCL	C13

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	368	BCL	O2A-C1-C2-C3
3	A	372	BCL	C1-C2-C3-C4

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	A	359/366 (98%)	0.00	13 (3%)	41 51	40, 55, 70, 91	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	214	PRO	8.4
1	A	213	GLY	5.3
1	A	209	ASN	3.8
1	A	167	VAL	3.4
1	A	327	ALA	3.2
1	A	196	GLY	2.7
1	A	8	ASP	2.6
1	A	211	GLU	2.6
1	A	212	SER	2.5
1	A	217	PRO	2.4
1	A	58	LEU	2.3
1	A	192	ALA	2.3
1	A	188	PRO	2.1

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(Å ²)	Q<0.9
3	BCL	A	367	66/66	0.18	1.42	46,51,59,65	0
3	BCL	A	372	66/66	0.15	1.39	42,51,58,61	0
3	BCL	A	369	66/66	0.14	0.83	35,44,52,60	0
3	BCL	A	400	42/66	0.16	0.75	71,75,79,80	0
3	BCL	A	370	66/66	0.12	0.28	36,45,47,50	0
3	BCL	A	371	66/66	0.12	0.19	39,49,59,59	0
3	BCL	A	368	66/66	0.12	0.09	39,49,60,62	0
3	BCL	A	373	66/66	0.16	-0.10	36,45,66,67	0
2	MG	A	374	1/1	0.27	-	51,51,51,51	1

6.5 Other polymers

There are no such residues in this entry.