Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 07:41 AM 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 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

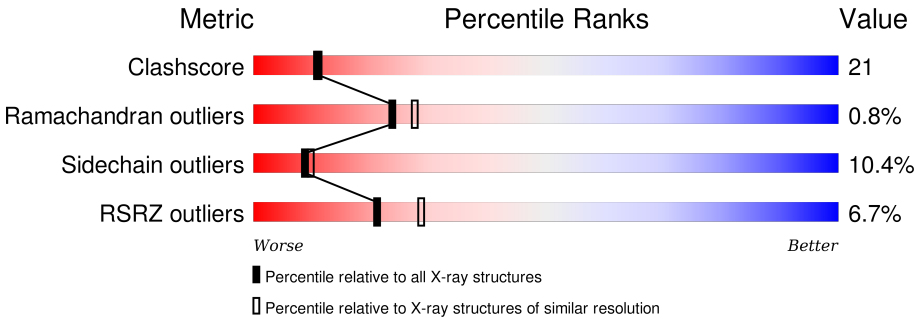
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (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. 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 <=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	A	366	7%, 65%, 28%, 5%

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
3	BCL	A	367	X	-	-	-
3	BCL	A	368	X	-	-	-
3	BCL	A	369	X	-	-	-
3	BCL	A	370	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	BCL	A	371	X	-	-	-
3	BCL	A	372	X	-	-	-
3	BCL	A	373	X	-	-	-

2 Entry composition

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

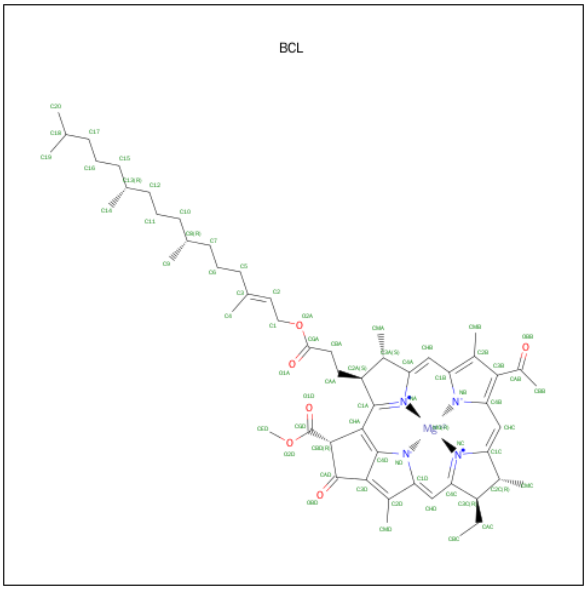
- Molecule 1 is a protein called Bacteriochlorophyll a protein.

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: $C_{55}H_{74}MgN_4O_6$).



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
			Total	C	Mg	N	O		
3	A	1	66	55	1	4	6	0	0
3	A	1	66	55	1	4	6	0	0
3	A	1	66	55	1	4	6	0	0
3	A	1	66	55	1	4	6	0	0
3	A	1	66	55	1	4	6	0	0
3	A	1	42	33	1	4	4	0	0

- Molecule 4 is water.

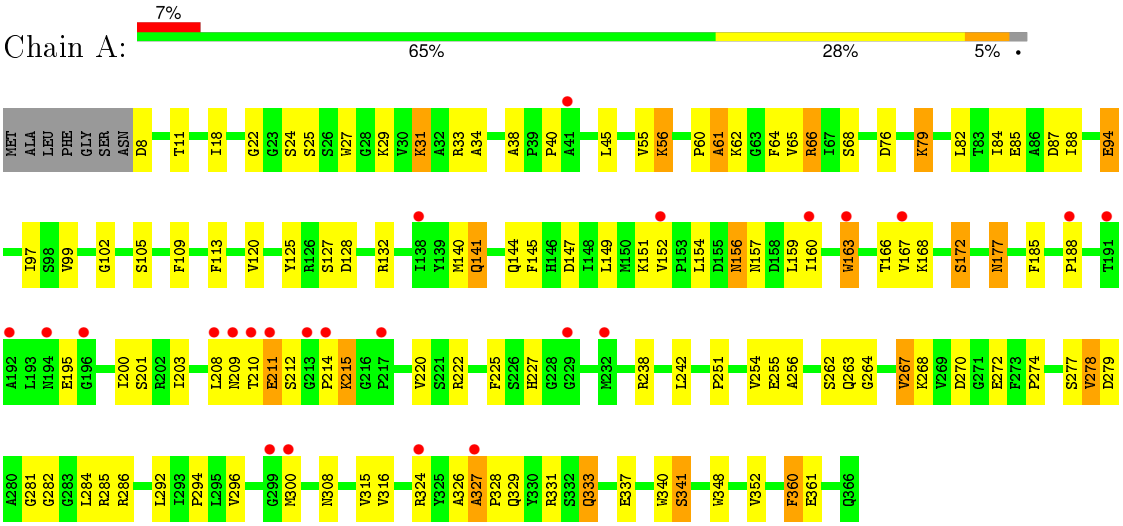
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	178	178	178	0	0

3 Residue-property plots (i)

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

- Molecule 1: Bacteriochlorophyll a protein

Chain A:



4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [1]	2.00 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.2.0013	Depositor
R, R_{free}	0.174 , 0.273 0.181 , (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)	0.30 , 51.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BCL, 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(^{o})	Ideal(^{o})
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 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	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

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 21.

All (137) 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: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	Interatomic distance (Å)	Clash overlap (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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:84:ILE:HB	4:A:458:HOH:O	2.13	0.48
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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 (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	357/366 (98%)	335 (94%)	19 (5%)	3 (1%)	24 27

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 (i)

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%)	9 10

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

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Mol	Chain	Res	Type
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 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 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	-	53,74,74	1.95	6 (11%)	57,115,115	2.40	19 (33%)
3	BCL	A	368	4	53,74,74	2.04	6 (11%)	57,115,115	2.15	16 (28%)
3	BCL	A	369	1	53,74,74	2.21	4 (7%)	57,115,115	2.09	14 (24%)
3	BCL	A	370	1	53,74,74	2.08	5 (9%)	57,115,115	1.96	9 (15%)
3	BCL	A	371	1	53,74,74	1.86	6 (11%)	57,115,115	2.24	17 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	BCL	A	372	1	53,74,74	2.14	6 (11%)	57,115,115	2.29	14 (24%)
3	BCL	A	373	1	53,74,74	2.22	5 (9%)	57,115,115	2.24	15 (26%)
3	BCL	A	400	1	28,50,74	2.52	3 (10%)	30,86,115	2.94	12 (40%)

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	0/37/137/137	0/0/9/9
3	BCL	A	368	4	2/2/21/25	1/37/137/137	0/0/9/9
3	BCL	A	369	1	2/2/21/25	0/37/137/137	0/0/9/9
3	BCL	A	370	1	2/2/21/25	0/37/137/137	0/0/9/9
3	BCL	A	371	1	2/2/21/25	0/37/137/137	0/0/9/9
3	BCL	A	372	1	2/2/21/25	1/37/137/137	0/0/9/9
3	BCL	A	373	1	2/2/21/25	0/37/137/137	0/0/9/9
3	BCL	A	400	1	-	0/8/108/137	0/0/9/9

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	368	BCL	O2A-CGA	-2.86	1.24	1.33
3	A	370	BCL	O2D-CGD	-2.77	1.26	1.33
3	A	367	BCL	C3D-CAD	-2.73	1.38	1.45
3	A	373	BCL	O2D-CGD	-2.59	1.26	1.33
3	A	400	BCL	O2D-CGD	-2.58	1.26	1.33
3	A	400	BCL	C3D-CAD	-2.54	1.38	1.45
3	A	371	BCL	C3D-CAD	-2.54	1.38	1.45
3	A	371	BCL	O2D-CGD	-2.52	1.26	1.33
3	A	369	BCL	O2A-CGA	-2.50	1.25	1.33
3	A	373	BCL	O2A-CGA	-2.49	1.25	1.33
3	A	372	BCL	O2D-CGD	-2.42	1.27	1.33
3	A	367	BCL	O2A-CGA	-2.40	1.26	1.33
3	A	367	BCL	O2D-CGD	-2.30	1.27	1.33
3	A	370	BCL	C3D-CAD	-2.28	1.39	1.45
3	A	368	BCL	O2D-CGD	-2.25	1.27	1.33
3	A	372	BCL	O2A-CGA	-2.19	1.26	1.33
3	A	371	BCL	CHD-C4C	2.13	1.47	1.41
3	A	372	BCL	CHD-C4C	2.21	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	373	BCL	CHD-C4C	2.35	1.48	1.41
3	A	368	BCL	CHD-C4C	2.41	1.48	1.41
3	A	367	BCL	C2-C3	3.18	1.39	1.33
3	A	372	BCL	C2-C3	3.23	1.39	1.33
3	A	370	BCL	C2-C3	3.32	1.39	1.33
3	A	371	BCL	C2-C3	3.55	1.39	1.33
3	A	368	BCL	C2-C3	3.84	1.40	1.33
3	A	369	BCL	C2-C3	4.02	1.40	1.33
3	A	369	BCL	O1A-CGA	4.87	1.37	1.22
3	A	373	BCL	O1A-CGA	5.35	1.38	1.22
3	A	367	BCL	O1A-CGA	5.86	1.40	1.22
3	A	371	BCL	O1A-CGA	6.09	1.40	1.22
3	A	370	BCL	O1A-CGA	6.21	1.41	1.22
3	A	372	BCL	O1A-CGA	6.40	1.41	1.22
3	A	368	BCL	O1A-CGA	6.47	1.42	1.22
3	A	371	BCL	OBD-CAD	9.73	1.37	1.22
3	A	367	BCL	OBD-CAD	10.83	1.38	1.22
3	A	368	BCL	OBD-CAD	11.09	1.39	1.22
3	A	370	BCL	OBD-CAD	11.98	1.40	1.22
3	A	400	BCL	OBD-CAD	12.29	1.41	1.22
3	A	372	BCL	OBD-CAD	12.46	1.41	1.22
3	A	369	BCL	OBD-CAD	13.53	1.43	1.22
3	A	373	BCL	OBD-CAD	13.67	1.43	1.22

All (116) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	369	BCL	CMB-C2B-C1B	-7.38	116.15	128.36
3	A	372	BCL	CMB-C2B-C1B	-7.34	116.23	128.36
3	A	367	BCL	CMB-C2B-C1B	-7.33	116.23	128.36
3	A	373	BCL	CMB-C2B-C1B	-7.14	116.55	128.36
3	A	370	BCL	CMB-C2B-C1B	-7.11	116.60	128.36
3	A	367	BCL	C1D-CHD-C4C	-7.09	115.24	126.07
3	A	400	BCL	CMB-C2B-C1B	-6.80	117.11	128.36
3	A	400	BCL	CHD-C4C-NC	-6.28	117.78	125.06
3	A	368	BCL	CMB-C2B-C1B	-6.05	118.36	128.36
3	A	371	BCL	CHB-C4A-NA	-6.01	116.20	124.51
3	A	367	BCL	CHD-C4C-NC	-5.92	118.19	125.06
3	A	369	BCL	O1D-CGD-CBD	-5.91	116.15	124.62
3	A	371	BCL	CMB-C2B-C1B	-5.64	119.03	128.36
3	A	372	BCL	C1D-CHD-C4C	-5.57	117.57	126.07
3	A	400	BCL	C1D-CHD-C4C	-5.32	117.94	126.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	367	BCL	CHC-C1C-NC	-5.30	117.18	124.51
3	A	373	BCL	C4-C3-C2	-4.99	113.71	123.50
3	A	373	BCL	OBD-CAD-CBD	-4.97	118.44	125.94
3	A	368	BCL	CHD-C4C-NC	-4.35	120.01	125.06
3	A	371	BCL	O1D-CGD-CBD	-4.35	118.39	124.62
3	A	372	BCL	O1D-CGD-CBD	-4.18	118.64	124.62
3	A	368	BCL	C1D-CHD-C4C	-4.12	119.78	126.07
3	A	368	BCL	O1D-CGD-CBD	-4.08	118.78	124.62
3	A	367	BCL	O1D-CGD-CBD	-3.86	119.09	124.62
3	A	400	BCL	CAA-C2A-C3A	-3.84	107.00	116.20
3	A	372	BCL	CHB-C4A-NA	-3.79	119.27	124.51
3	A	368	BCL	O2A-CGA-O1A	-3.79	113.72	123.49
3	A	368	BCL	CHC-C1C-NC	-3.74	119.34	124.51
3	A	400	BCL	CMD-C2D-C3D	-3.64	117.96	125.09
3	A	371	BCL	C3C-C4C-CHD	-3.61	115.27	123.33
3	A	370	BCL	O2D-CGD-O1D	-3.43	116.71	123.79
3	A	400	BCL	O1D-CGD-CBD	-3.37	119.80	124.62
3	A	371	BCL	C1D-CHD-C4C	-3.34	120.97	126.07
3	A	400	BCL	CHB-C4A-NA	-3.16	120.14	124.51
3	A	368	BCL	CMD-C2D-C3D	-3.13	118.97	125.09
3	A	373	BCL	C1D-CHD-C4C	-3.07	121.39	126.07
3	A	368	BCL	OBD-CAD-CBD	-2.99	121.42	125.94
3	A	372	BCL	O2D-CGD-O1D	-2.90	117.81	123.79
3	A	373	BCL	O2A-CGA-O1A	-2.89	116.03	123.49
3	A	373	BCL	C6-C7-C8	-2.87	105.97	115.49
3	A	372	BCL	C6-C5-C3	-2.85	106.22	112.48
3	A	369	BCL	CHC-C1C-NC	-2.79	120.65	124.51
3	A	373	BCL	O2D-CGD-O1D	-2.73	118.16	123.79
3	A	371	BCL	C7-C6-C5	-2.72	105.04	113.06
3	A	367	BCL	C4-C3-C2	-2.71	118.19	123.50
3	A	368	BCL	CHB-C4A-NA	-2.67	120.82	124.51
3	A	367	BCL	CAA-CBA-CGA	-2.64	105.58	113.32
3	A	371	BCL	CHD-C4C-NC	-2.59	122.05	125.06
3	A	367	BCL	CMD-C2D-C3D	-2.57	120.05	125.09
3	A	372	BCL	CMD-C2D-C3D	-2.55	120.09	125.09
3	A	371	BCL	OBD-CAD-C3D	-2.52	123.22	128.35
3	A	370	BCL	O1D-CGD-CBD	-2.50	121.04	124.62
3	A	369	BCL	CHD-C4C-NC	-2.49	122.17	125.06
3	A	369	BCL	OBD-CAD-CBD	-2.47	122.21	125.94
3	A	368	BCL	CHA-C1A-NA	-2.46	120.02	126.06
3	A	371	BCL	CBC-CAC-C3C	-2.45	107.57	113.57
3	A	369	BCL	O2A-CGA-O1A	-2.43	117.22	123.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	400	BCL	CHC-C1C-NC	-2.36	121.25	124.51
3	A	369	BCL	C11-C12-C13	-2.34	107.72	115.49
3	A	369	BCL	C1D-CHD-C4C	-2.31	122.55	126.07
3	A	367	BCL	C7-C6-C5	-2.30	106.27	113.06
3	A	370	BCL	OBD-CAD-C3D	-2.25	123.77	128.35
3	A	371	BCL	CMD-C2D-C3D	-2.25	120.69	125.09
3	A	373	BCL	O1D-CGD-CBD	-2.20	121.46	124.62
3	A	373	BCL	CMD-C2D-C3D	-2.20	120.79	125.09
3	A	367	BCL	CHA-C1A-NA	-2.17	120.73	126.06
3	A	372	BCL	C6-C7-C8	-2.08	108.60	115.49
3	A	372	BCL	CAC-C3C-C2C	-2.06	108.94	114.13
3	A	368	BCL	C6-C7-C8	-2.04	108.72	115.49
3	A	370	BCL	C11-C10-C8	-2.02	108.78	115.49
3	A	372	BCL	CED-O2D-CGD	2.05	120.80	115.99
3	A	373	BCL	OBD-CAD-C3D	2.09	132.63	128.35
3	A	367	BCL	CBA-CAA-C2A	2.14	119.78	113.73
3	A	369	BCL	CAC-C3C-C2C	2.19	119.64	114.13
3	A	369	BCL	C4-C3-C5	2.20	118.77	115.41
3	A	373	BCL	C11-C10-C8	2.25	122.95	115.49
3	A	367	BCL	C6-C5-C3	2.27	117.47	112.48
3	A	400	BCL	CAC-C3C-C4C	2.28	117.65	112.58
3	A	372	BCL	C4A-NA-C1A	2.32	109.36	106.36
3	A	371	BCL	C3D-CAD-CBD	2.39	110.97	107.60
3	A	367	BCL	C4-C3-C5	2.44	119.13	115.41
3	A	368	BCL	C4A-NA-C1A	2.50	109.59	106.36
3	A	371	BCL	C6-C5-C3	2.50	117.98	112.48
3	A	367	BCL	CAA-C2A-C1A	2.72	122.05	112.47
3	A	371	BCL	CED-O2D-CGD	2.73	122.39	115.99
3	A	367	BCL	CGD-CBD-CAD	2.74	119.89	110.62
3	A	368	BCL	CED-O2D-CGD	2.75	122.44	115.99
3	A	372	BCL	O2A-CGA-CBA	2.87	120.65	111.90
3	A	369	BCL	CED-O2D-CGD	2.90	122.79	115.99
3	A	371	BCL	C4A-NA-C1A	2.94	110.17	106.36
3	A	367	BCL	O2A-CGA-CBA	2.95	120.89	111.90
3	A	370	BCL	C4-C3-C5	3.04	120.05	115.41
3	A	370	BCL	O2A-CGA-CBA	3.11	121.37	111.90
3	A	400	BCL	CED-O2D-CGD	3.18	123.46	115.99
3	A	369	BCL	O2A-CGA-CBA	3.45	122.42	111.90
3	A	367	BCL	CED-O2D-CGD	3.54	124.29	115.99
3	A	368	BCL	O2A-CGA-CBA	3.58	122.82	111.90
3	A	371	BCL	O2A-CGA-CBA	3.72	123.24	111.90
3	A	371	BCL	CMB-C2B-C3B	3.96	132.83	125.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	367	BCL	O2D-CGD-CBD	3.96	116.74	111.30
3	A	373	BCL	O2A-CGA-CBA	4.07	124.31	111.90
3	A	368	BCL	CMB-C2B-C3B	4.10	133.10	125.09
3	A	373	BCL	CMB-C2B-C3B	4.21	133.33	125.09
3	A	369	BCL	CMB-C2B-C3B	4.37	133.64	125.09
3	A	400	BCL	CMB-C2B-C3B	4.63	134.14	125.09
3	A	367	BCL	CMB-C2B-C3B	4.63	134.15	125.09
3	A	370	BCL	CMB-C2B-C3B	4.63	134.15	125.09
3	A	372	BCL	CMB-C2B-C3B	4.80	134.49	125.09
3	A	373	BCL	C4-C3-C5	5.24	123.41	115.41
3	A	368	BCL	O2D-CGD-CBD	5.89	119.39	111.30
3	A	400	BCL	O2D-CGD-CBD	5.92	119.42	111.30
3	A	369	BCL	O2D-CGD-CBD	6.57	120.31	111.30
3	A	373	BCL	O2D-CGD-CBD	6.61	120.37	111.30
3	A	371	BCL	O2D-CGD-CBD	6.89	120.75	111.30
3	A	370	BCL	O2D-CGD-CBD	7.97	122.24	111.30
3	A	372	BCL	O2D-CGD-CBD	8.93	123.56	111.30

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	372	BCL	C1-C2-C3-C4
3	A	368	BCL	O2A-C1-C2-C3

There are no ring outliers.

8 monomers are involved in 51 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	367	BCL	8	0
3	A	368	BCL	5	0
3	A	369	BCL	1	0
3	A	370	BCL	6	0
3	A	371	BCL	6	0
3	A	372	BCL	12	0
3	A	373	BCL	13	0
3	A	400	BCL	5	0

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, 95^{th} 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%)	0.32	24 (6%) 21 29	40, 55, 70, 91	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	214	PRO	8.0
1	A	167	VAL	5.0
1	A	160	ILE	5.0
1	A	327	ALA	4.9
1	A	163	TRP	4.0
1	A	213	GLY	4.0
1	A	217	PRO	3.6
1	A	210	THR	3.3
1	A	211	GLU	3.3
1	A	209	ASN	3.1
1	A	152	VAL	2.9
1	A	188	PRO	2.7
1	A	324	ARG	2.6
1	A	192	ALA	2.5
1	A	196	GLY	2.4
1	A	41	ALA	2.3
1	A	194	ASN	2.3
1	A	229	GLY	2.2
1	A	300	MET	2.2
1	A	191	THR	2.1
1	A	208	LEU	2.1
1	A	138	ILE	2.1
1	A	299	GLY	2.0
1	A	232	MET	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} 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
3	BCL	A	400	42/66	0.87	0.19	0.84	71,75,79,80	0
3	BCL	A	372	66/66	0.88	0.15	0.59	42,51,58,61	0
3	BCL	A	369	66/66	0.93	0.16	0.53	35,44,52,60	0
3	BCL	A	368	66/66	0.93	0.14	0.14	39,49,60,62	0
3	BCL	A	367	66/66	0.93	0.16	0.07	46,51,59,65	0
3	BCL	A	371	66/66	0.93	0.13	0.03	39,49,59,59	0
3	BCL	A	370	66/66	0.94	0.12	-0.25	36,45,47,50	0
3	BCL	A	373	66/66	0.96	0.16	-0.74	36,45,66,67	0
2	MG	A	374	1/1	0.99	0.33	-	51,51,51,51	1

6.5 Other polymers (i)

There are no such residues in this entry.