



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 19, 2020 – 08:28 pm BST

PDB ID : 3EOJ
Title : Fmo protein from Prosthecochloris Aestuarii 2K AT 1.3A Resolution
Authors : Tronrud, D.E.; Wen, J.; Gay, L.; Blankenship, R.E.
Deposited on : 2008-09-27
Resolution : 1.30 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

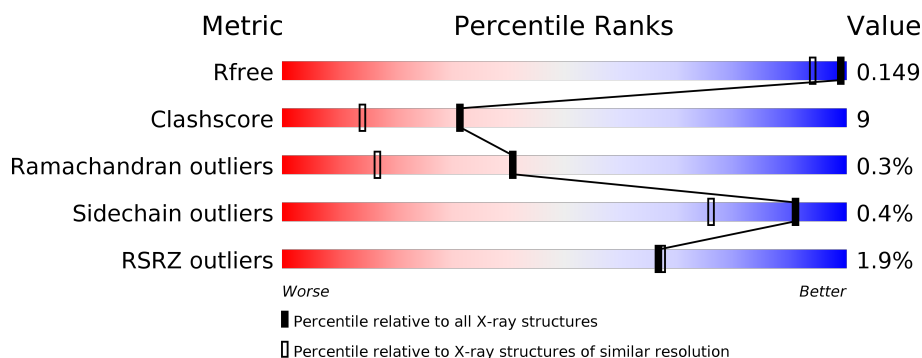
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.30 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))
R_{free}	130704	1058 (1.30-1.30)
Clashscore	141614	1101 (1.30-1.30)
Ramachandran outliers	138981	1058 (1.30-1.30)
Sidechain outliers	138945	1058 (1.30-1.30)
RSRZ outliers	127900	1029 (1.30-1.30)

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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	366	<div> <div>2%</div> <div> <div></div> <div>82%</div> <div>15%</div> <div>..</div> </div> </div>

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 4115 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.

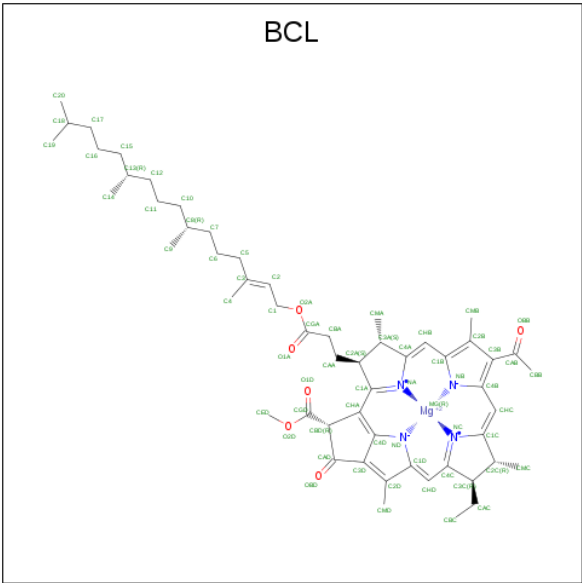
- Molecule 1 is a protein called Bacteriochlorophyll a protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	359	Total	C	N	O	S	0	60	1
			3082	1974	527	573	8			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	117	SER	GLN	SEE REMARK 999	UNP P11741

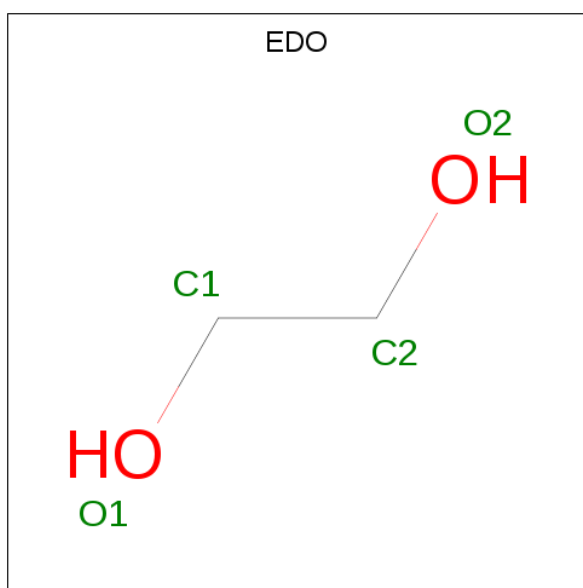
- Molecule 2 is BACTERIOCHLOROPHYLL A (three-letter code: BCL) (formula: C₅₅H₇₄MgN₄O₆).



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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
2	A	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
2	A	1	Total	C	Mg	N	O	0	1
			84	69	1	5	9		
2	A	1	Total	C	Mg	N	O	0	1
			83	71	1	4	7		
2	A	1	Total	C	Mg	N	O	0	1
			47	36	1	4	6		

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	1
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		

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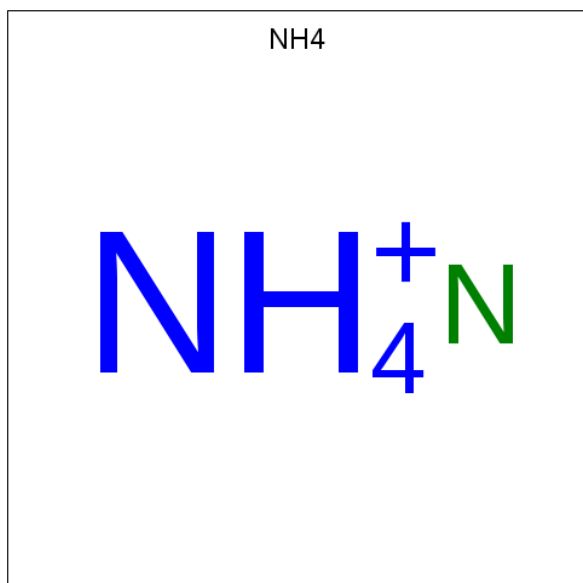
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	1
3	A	1	Total C O 4 2 2	0	1
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	1

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Na 1 1	0	0

- Molecule 5 is AMMONIUM ION (three-letter code: NH4) (formula: H₄N).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total N 2 2	0	1

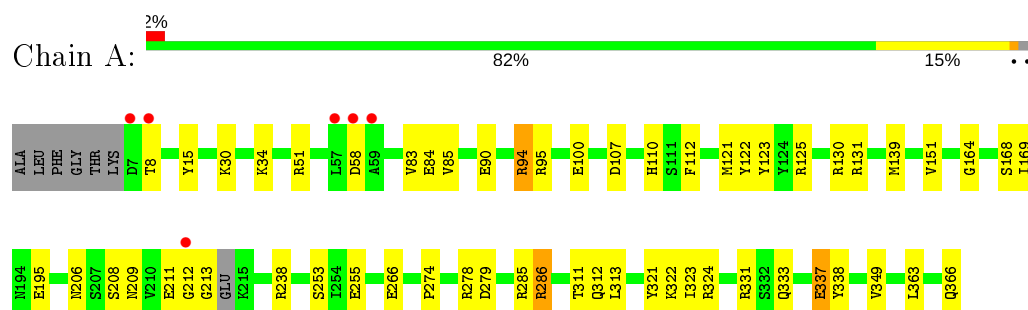
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	406	Total O 408 408	0	50

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

- Molecule 1: Bacteriochlorophyll a protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α , β , γ	111.24 Å 111.24 Å 98.20 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 1.30 48.40 – 1.30	Depositor EDS
% Data completeness (in resolution range)	94.9 (50.00-1.30) 92.4 (48.40-1.30)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.36 (at 1.30 Å)	Xtriage
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.135 , 0.161 0.134 , 0.149	Depositor DCC
R_{free} test set	8438 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	11.1	Xtriage
Anisotropy	0.173	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 56.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.033 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	4115	wwPDB-VP
Average B, all atoms (Å ²)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.48% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BCL, NH4, EDO, NA

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	6.77	4/3302 (0.1%)	1.65	38/4466 (0.9%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	213[A]	GLY	CA-C	271.60	5.86	1.51
1	A	213[B]	GLY	CA-C	271.60	5.86	1.51
1	A	139[A]	MET	SD-CE	33.99	3.68	1.77
1	A	139[B]	MET	SD-CE	33.99	3.68	1.77

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	213[A]	GLY	CA-C-O	-36.76	54.43	120.60
1	A	213[B]	GLY	CA-C-O	-36.76	54.43	120.60
1	A	139[A]	MET	CG-SD-CE	-29.38	53.19	100.20
1	A	139[B]	MET	CG-SD-CE	-29.38	53.19	100.20
1	A	94[A]	ARG	NE-CZ-NH2	15.73	128.16	120.30
1	A	94[B]	ARG	NE-CZ-NH2	15.73	128.16	120.30
1	A	107	ASP	CB-CG-OD1	14.56	131.41	118.30
1	A	131	ARG	NE-CZ-NH1	13.63	127.11	120.30
1	A	130[A]	ARG	CD-NE-CZ	9.47	136.86	123.60
1	A	130[B]	ARG	CD-NE-CZ	9.47	136.86	123.60
1	A	107	ASP	CB-CG-OD2	-8.61	110.55	118.30
1	A	94[A]	ARG	NE-CZ-NH1	-7.99	116.30	120.30
1	A	94[B]	ARG	NE-CZ-NH1	-7.99	116.30	120.30
1	A	123[A]	TYR	CB-CG-CD1	7.92	125.75	121.00
1	A	123[B]	TYR	CB-CG-CD1	7.92	125.75	121.00
1	A	58	ASP	C-N-CA	-6.91	104.42	121.70
1	A	123[A]	TYR	CB-CG-CD2	-6.85	116.89	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	123[B]	TYR	CB-CG-CD2	-6.85	116.89	121.00
1	A	83	VAL	CA-CB-CG2	6.82	121.12	110.90
1	A	279	ASP	CB-CG-OD1	6.82	124.44	118.30
1	A	238	ARG	NE-CZ-NH1	-6.67	116.96	120.30
1	A	286[A]	ARG	NE-CZ-NH1	6.59	123.60	120.30
1	A	286[B]	ARG	NE-CZ-NH1	6.59	123.60	120.30
1	A	366	GLN	CA-CB-CG	6.55	127.82	113.40
1	A	110	HIS	CA-CB-CG	6.17	124.09	113.60
1	A	331[A]	ARG	NE-CZ-NH2	-5.87	117.36	120.30
1	A	331[B]	ARG	NE-CZ-NH2	-5.87	117.36	120.30
1	A	337[A]	GLU	OE1-CD-OE2	5.58	130.00	123.30
1	A	337[B]	GLU	OE1-CD-OE2	5.58	130.00	123.30
1	A	130[A]	ARG	NE-CZ-NH2	-5.50	117.55	120.30
1	A	130[B]	ARG	NE-CZ-NH2	-5.50	117.55	120.30
1	A	321	TYR	CB-CG-CD2	5.45	124.27	121.00
1	A	95	ARG	NE-CZ-NH2	-5.23	117.69	120.30
1	A	130[A]	ARG	NE-CZ-NH1	5.20	122.90	120.30
1	A	130[B]	ARG	NE-CZ-NH1	5.20	122.90	120.30
1	A	212[A]	GLY	C-N-CA	5.15	133.11	122.30
1	A	212[B]	GLY	C-N-CA	5.15	133.11	122.30
1	A	95	ARG	NE-CZ-NH1	5.11	122.86	120.30

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	3082	0	3033	39	0
2	A	562	0	431	20	0
3	A	60	0	89	12	0
4	A	1	0	0	0	0
5	A	2	0	0	1	0
6	A	408	0	0	10	0
All	All	4115	0	3553	59	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 9.

All (59) 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:208[A]:SER:O	1:A:209[A]:ASN:ND2	1.93	1.01
2:A:375:BCL:H191	2:A:377[E]:BCL:H203	1.53	0.91
1:A:195[B]:GLU:OE2	5:A:2378[B]:NH4:N	2.06	0.88
1:A:337[B]:GLU:HG2	6:A:1100:HOH:O	1.72	0.86
2:A:377[E]:BCL:H151	2:A:377[E]:BCL:H192	1.57	0.85
1:A:208[A]:SER:C	1:A:209[A]:ASN:ND2	2.31	0.84
1:A:285:ARG:HH22	3:A:387:EDO:H11	1.52	0.74
1:A:122:TYR:HB3	1:A:125[C]:ARG:HH11	1.53	0.73
1:A:30[B]:LYS:HG3	6:A:1254:HOH:O	1.92	0.70
1:A:209[B]:ASN:ND2	1:A:211[B]:GLU:HG2	2.06	0.69
1:A:209[B]:ASN:HD22	1:A:211[B]:GLU:HG2	1.56	0.69
1:A:164[B]:GLY:O	1:A:168[B]:SER:N	2.26	0.68
2:A:377[E]:BCL:C15	2:A:377[E]:BCL:H192	2.23	0.68
1:A:285:ARG:HH22	3:A:387:EDO:C1	2.06	0.68
1:A:206[B]:ASN:ND2	6:A:1149:HOH:O	2.22	0.67
2:A:375:BCL:H191	2:A:377[E]:BCL:C20	2.24	0.67
1:A:51[A]:ARG:HG2	1:A:255[A]:GLU:HG2	1.79	0.65
1:A:121[B]:MET:SD	2:A:378[B]:BCL:HED2	2.37	0.64
2:A:375:BCL:HMB1	2:A:375:BCL:HBB2	1.79	0.64
2:A:374:BCL:CBB	2:A:374:BCL:HMB1	2.28	0.63
1:A:169[B]:ILE:HD12	1:A:176:PHE:CD2	2.33	0.63
2:A:372:BCL:HMB1	2:A:372:BCL:HBB3	1.82	0.61
1:A:322[A]:LYS:HD2	6:A:1174:HOH:O	2.03	0.59
1:A:90:GLU:OE1	1:A:94[A]:ARG:HD3	2.02	0.58
1:A:208[A]:SER:C	1:A:209[A]:ASN:HD22	2.02	0.57
1:A:8:THR:O	6:A:1230:HOH:O	2.18	0.56
1:A:169[B]:ILE:HG13	6:A:1191:HOH:O	2.04	0.56
1:A:209[B]:ASN:HD22	1:A:211[B]:GLU:CG	2.18	0.56
2:A:378[B]:BCL:HBB3	2:A:378[B]:BCL:HMB1	1.88	0.56
2:A:372:BCL:HMB1	2:A:372:BCL:CBB	2.37	0.55
1:A:253:SER:OG	3:A:382:EDO:C1	2.55	0.55
1:A:100[B]:GLU:OE2	3:A:385:EDO:O1	2.24	0.54
1:A:286[A]:ARG:HB3	1:A:363:LEU:HD23	1.90	0.54
2:A:378[B]:BCL:HBD	2:A:378[B]:BCL:HAA1	1.90	0.53
3:A:391[A]:EDO:H22	6:A:1121:HOH:O	2.09	0.51
1:A:312[A]:GLN:HG2	1:A:313:LEU:N	2.26	0.49
1:A:34:LYS:HG2	1:A:266[B]:GLU:HG3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:391[A]:EDO:H22	6:A:1136:HOH:O	2.12	0.49
1:A:112:PHE:O	3:A:383[A]:EDO:H21	2.14	0.48
1:A:169[B]:ILE:CG1	6:A:1191:HOH:O	2.61	0.48
1:A:285:ARG:NH2	3:A:387:EDO:H11	2.27	0.46
2:A:374:BCL:HBB2	2:A:374:BCL:HMB1	1.98	0.46
2:A:374:BCL:HBB3	2:A:374:BCL:HMB1	1.97	0.46
1:A:15:TYR:CE1	2:A:374:BCL:H43	2.52	0.44
1:A:311[B]:THR:HG21	1:A:349:VAL:HG21	1.99	0.44
2:A:373[A]:BCL:H203	2:A:373[A]:BCL:H161	1.63	0.44
1:A:278:ARG:CG	3:A:391[A]:EDO:H12	2.49	0.43
1:A:323[A]:ILE:HD12	1:A:338:TYR:CD1	2.54	0.43
1:A:333[B]:GLN:HB3	1:A:338:TYR:CD1	2.54	0.42
3:A:392:EDO:H21	6:A:1141:HOH:O	2.19	0.42
1:A:253:SER:OG	3:A:382:EDO:H12	2.20	0.42
1:A:274:PRO:HG2	2:A:375:BCL:HMB3	2.01	0.41
2:A:374:BCL:C1B	2:A:375:BCL:H42	2.50	0.41
1:A:84:GLU:OE1	3:A:385:EDO:O1	2.38	0.41

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	413/366 (113%)	408 (99%)	3 (1%)	2 (0%)	29 6

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	170[A]	SER
1	A	170[B]	SER

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	335/303 (111%)	333 (99%)	2 (1%)	86	65

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	324[A]	ARG
1	A	324[B]	ARG

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

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 36 ligands modelled in this entry, 2 are modelled with single atom and 1 is monoatomic - leaving 33 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	EDO	A	384	-	3,3,3	0.55	0	2,2,2	0.32	0
2	BCL	A	374	1	58,74,74	1.19	4 (6%)	69,115,115	1.44	9 (13%)
3	EDO	A	392	-	3,3,3	0.69	0	2,2,2	0.37	0
3	EDO	A	382	-	3,3,3	0.59	0	2,2,2	0.46	0
3	EDO	A	390	-	3,3,3	0.58	0	2,2,2	0.35	0
3	EDO	A	379	-	3,3,3	0.36	0	2,2,2	0.22	0
2	BCL	A	375	1	58,74,74	1.29	5 (8%)	69,115,115	1.25	10 (14%)
3	EDO	A	388[A]	-	3,3,3	0.73	0	2,2,2	0.47	0
2	BCL	A	371[A]	-	58,74,74	1.27	4 (6%)	69,115,115	1.25	10 (14%)
3	EDO	A	380	-	3,3,3	0.43	0	2,2,2	0.19	0
3	EDO	A	381	-	3,3,3	0.24	0	2,2,2	1.90	1 (50%)
3	EDO	A	393[B]	-	3,3,3	0.58	0	2,2,2	0.56	0
3	EDO	A	383[A]	-	3,3,3	0.26	0	2,2,2	0.53	0
2	BCL	A	373[A]	-	58,74,74	1.25	4 (6%)	69,115,115	1.30	7 (10%)
3	EDO	A	391[A]	-	3,3,3	0.28	0	2,2,2	0.78	0
3	EDO	A	387	-	3,3,3	0.72	0	2,2,2	0.72	0
2	BCL	A	373[B]	-	58,74,74	1.25	4 (6%)	69,115,115	1.35	7 (10%)
3	EDO	A	385	-	3,3,3	0.74	0	2,2,2	0.26	0
3	EDO	A	386	-	3,3,3	0.36	0	2,2,2	0.53	0
3	EDO	A	389	-	3,3,3	0.78	0	2,2,2	1.41	0
2	BCL	A	372	6	58,74,74	1.18	4 (6%)	69,115,115	1.25	8 (11%)
2	BCL	A	378[B]	1	39,55,74	1.37	3 (7%)	46,92,115	2.16	12 (26%)
2	BCL	A	371[B]	-	58,74,74	1.25	4 (6%)	69,115,115	1.20	9 (13%)

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	EDO	A	384	-	-	0/1/1/1	-
2	BCL	A	374	1	-	0/37/137/137	-
3	EDO	A	392	-	-	0/1/1/1	-
3	EDO	A	382	-	-	1/1/1/1	-
3	EDO	A	390	-	-	0/1/1/1	-
3	EDO	A	379	-	-	0/1/1/1	-
2	BCL	A	375	1	-	4/37/137/137	-
3	EDO	A	388[A]	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BCL	A	371[A]	-	-	4/37/137/137	-
3	EDO	A	380	-	-	1/1/1/1	-
3	EDO	A	381	-	-	1/1/1/1	-
3	EDO	A	393[B]	-	-	0/1/1/1	-
3	EDO	A	383[A]	-	-	1/1/1/1	-
2	BCL	A	373[A]	-	-	9/37/137/137	-
3	EDO	A	391[A]	-	-	0/1/1/1	-
3	EDO	A	387	-	-	0/1/1/1	-
2	BCL	A	373[B]	-	-	7/37/137/137	-
3	EDO	A	385	-	-	0/1/1/1	-
3	EDO	A	386	-	-	1/1/1/1	-
3	EDO	A	389	-	-	0/1/1/1	-
2	BCL	A	372	6	-	1/37/137/137	-
2	BCL	A	378[B]	1	-	0/15/115/137	-
2	BCL	A	371[B]	-	-	5/37/137/137	-

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	374	BCL	C4B-NB	5.59	1.40	1.35
2	A	371[A]	BCL	C1B-NB	5.33	1.40	1.35
2	A	371[B]	BCL	C1B-NB	5.33	1.40	1.35
2	A	378[B]	BCL	C1B-NB	4.78	1.39	1.35
2	A	373[A]	BCL	C4B-NB	4.78	1.39	1.35
2	A	373[B]	BCL	C4B-NB	4.78	1.39	1.35
2	A	373[A]	BCL	MG-NA	4.72	2.17	2.06
2	A	373[B]	BCL	MG-NA	4.72	2.17	2.06
2	A	371[A]	BCL	MG-NA	4.47	2.16	2.06
2	A	371[B]	BCL	MG-NA	4.47	2.16	2.06
2	A	375	BCL	C4B-NB	4.32	1.39	1.35
2	A	375	BCL	MG-NA	4.28	2.16	2.06
2	A	374	BCL	MG-NA	4.05	2.15	2.06
2	A	372	BCL	C1B-NB	3.80	1.38	1.35
2	A	372	BCL	MG-NA	3.72	2.15	2.06
2	A	375	BCL	C1B-NB	3.70	1.38	1.35
2	A	378[B]	BCL	MG-NA	3.52	2.14	2.06
2	A	375	BCL	MG-NC	3.33	2.14	2.06
2	A	374	BCL	C1B-NB	3.05	1.37	1.35
2	A	372	BCL	C4B-NB	2.88	1.37	1.35
2	A	378[B]	BCL	MG-NC	2.73	2.12	2.06
2	A	373[A]	BCL	C1B-NB	2.48	1.37	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	373[B]	BCL	C1B-NB	2.48	1.37	1.35
2	A	373[A]	BCL	MG-NC	2.47	2.12	2.06
2	A	373[B]	BCL	MG-NC	2.47	2.12	2.06
2	A	372	BCL	MG-NC	2.45	2.12	2.06
2	A	371[A]	BCL	C3C-C4C	2.36	1.54	1.51
2	A	371[B]	BCL	C3C-C4C	2.36	1.54	1.51
2	A	374	BCL	MG-NC	2.26	2.11	2.06
2	A	371[A]	BCL	MG-NC	2.08	2.11	2.06
2	A	371[B]	BCL	MG-NC	2.08	2.11	2.06
2	A	375	BCL	C5-C3	2.04	1.55	1.51

All (73) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	378[B]	BCL	C4A-NA-C1A	6.82	109.77	106.71
2	A	378[B]	BCL	C4D-C3D-CAD	-6.41	104.90	108.47
2	A	374	BCL	C4A-NA-C1A	5.81	109.32	106.71
2	A	374	BCL	C1C-NC-C4C	5.45	109.16	106.71
2	A	373[A]	BCL	C1C-NC-C4C	4.75	108.84	106.71
2	A	373[B]	BCL	C1C-NC-C4C	4.75	108.84	106.71
2	A	378[B]	BCL	CMB-C2B-C1B	-4.58	121.42	128.46
2	A	378[B]	BCL	CBA-CAA-C2A	3.90	125.37	113.86
2	A	373[B]	BCL	C17-C16-C15	3.85	130.92	113.24
2	A	371[A]	BCL	CHA-C1A-NA	-3.59	118.17	126.40
2	A	371[B]	BCL	CHA-C1A-NA	-3.59	118.17	126.40
2	A	375	BCL	C4-C3-C5	-3.44	109.49	115.27
2	A	378[B]	BCL	OBD-CAD-CBD	-3.41	121.02	125.89
2	A	373[A]	BCL	C4A-NA-C1A	3.41	108.24	106.71
2	A	373[B]	BCL	C4A-NA-C1A	3.41	108.24	106.71
2	A	374	BCL	CMD-C2D-C3D	3.32	130.90	124.68
2	A	375	BCL	C1C-NC-C4C	3.28	108.18	106.71
2	A	374	BCL	OBD-CAD-CBD	-3.27	121.23	125.89
2	A	373[A]	BCL	CHA-C1A-NA	-3.24	118.97	126.40
2	A	373[B]	BCL	CHA-C1A-NA	-3.24	118.97	126.40
2	A	371[A]	BCL	C1-C2-C3	-3.22	120.47	126.04
2	A	371[B]	BCL	C1-C2-C3	-3.22	120.47	126.04
2	A	372	BCL	CMB-C2B-C3B	3.17	130.62	124.68
2	A	372	BCL	CMB-C2B-C1B	-3.15	123.62	128.46
2	A	374	BCL	CMB-C2B-C1B	-3.09	123.71	128.46
2	A	375	BCL	CMB-C2B-C1B	-3.04	123.79	128.46
2	A	374	BCL	CMB-C2B-C3B	2.91	130.13	124.68
2	A	375	BCL	OBD-CAD-CBD	-2.80	121.89	125.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	373[A]	BCL	OBD-CAD-CBD	-2.72	122.00	125.89
2	A	373[B]	BCL	OBD-CAD-CBD	-2.72	122.00	125.89
2	A	373[A]	BCL	CMD-C2D-C3D	2.72	129.77	124.68
2	A	373[B]	BCL	CMD-C2D-C3D	2.72	129.77	124.68
2	A	371[A]	BCL	OBD-CAD-CBD	-2.70	122.04	125.89
2	A	371[B]	BCL	OBD-CAD-CBD	-2.70	122.04	125.89
2	A	372	BCL	CMD-C2D-C3D	2.68	129.70	124.68
2	A	372	BCL	C4D-C3D-CAD	-2.66	106.99	108.47
2	A	372	BCL	C1-C2-C3	-2.66	121.44	126.04
2	A	371[A]	BCL	C2A-C1A-CHA	2.65	128.49	123.86
2	A	371[B]	BCL	C2A-C1A-CHA	2.65	128.49	123.86
3	A	381	EDO	O1-C1-C2	2.64	130.91	111.91
2	A	375	BCL	CHA-C1A-NA	-2.63	120.38	126.40
2	A	372	BCL	OBD-CAD-CBD	-2.60	122.18	125.89
2	A	378[B]	BCL	CMD-C2D-C3D	2.55	129.45	124.68
2	A	378[B]	BCL	O2A-CGA-O1A	-2.54	115.17	123.14
2	A	378[B]	BCL	C4B-C3B-CAB	-2.54	122.22	127.13
2	A	371[A]	BCL	CMB-C2B-C1B	-2.54	124.56	128.46
2	A	371[B]	BCL	CMB-C2B-C1B	-2.54	124.56	128.46
2	A	372	BCL	CHA-C1A-NA	-2.51	120.66	126.40
2	A	375	BCL	O2A-CGA-O1A	-2.48	117.32	123.59
2	A	375	BCL	CMB-C2B-C3B	2.46	129.27	124.68
2	A	375	BCL	C4-C3-C2	2.44	129.94	123.68
2	A	371[A]	BCL	CMB-C2B-C3B	2.43	129.23	124.68
2	A	371[B]	BCL	CMB-C2B-C3B	2.43	129.23	124.68
2	A	373[A]	BCL	C2A-C1A-CHA	2.39	128.04	123.86
2	A	373[B]	BCL	C2A-C1A-CHA	2.39	128.04	123.86
2	A	378[B]	BCL	O2A-CGA-CBA	2.32	121.38	112.23
2	A	371[A]	BCL	C16-C15-C13	-2.26	108.60	115.92
2	A	373[A]	BCL	C11-C10-C8	2.26	123.22	115.92
2	A	374	BCL	C4D-C3D-CAD	-2.26	107.21	108.47
2	A	374	BCL	C2A-C1A-CHA	2.20	127.70	123.86
2	A	378[B]	BCL	CHD-C4C-NC	-2.19	122.64	125.08
2	A	371[A]	BCL	CAA-C2A-C1A	2.18	119.12	111.97
2	A	371[B]	BCL	CAA-C2A-C1A	2.18	119.12	111.97
2	A	372	BCL	OBB-CAB-C3B	2.18	123.86	119.99
2	A	375	BCL	CMD-C2D-C3D	2.16	128.72	124.68
2	A	371[A]	BCL	C4D-C3D-CAD	-2.14	107.28	108.47
2	A	371[B]	BCL	C4D-C3D-CAD	-2.14	107.28	108.47
2	A	378[B]	BCL	OBB-CAB-CBB	-2.11	115.42	120.17
2	A	374	BCL	CHA-C1A-NA	-2.10	121.58	126.40
2	A	378[B]	BCL	C2A-C3A-C4A	2.08	105.22	101.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	375	BCL	C4D-C3D-CAD	-2.06	107.32	108.47
2	A	371[A]	BCL	CBA-CAA-C2A	2.04	119.88	113.86
2	A	371[B]	BCL	CBA-CAA-C2A	2.04	119.88	113.86

There are no chirality outliers.

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	373[A]	BCL	C4C-C3C-CAC-CBC
2	A	373[B]	BCL	C4C-C3C-CAC-CBC
2	A	373[B]	BCL	C13-C15-C16-C17
2	A	373[B]	BCL	C15-C16-C17-C18
2	A	373[A]	BCL	C15-C16-C17-C18
2	A	373[A]	BCL	C13-C15-C16-C17
3	A	381	EDO	O1-C1-C2-O2
3	A	383[A]	EDO	O1-C1-C2-O2
2	A	373[A]	BCL	C2C-C3C-CAC-CBC
2	A	373[B]	BCL	C2C-C3C-CAC-CBC
2	A	373[A]	BCL	C10-C11-C12-C13
2	A	375	BCL	CAA-CBA-CGA-O2A
2	A	371[B]	BCL	C13-C15-C16-C17
2	A	375	BCL	C2-C3-C5-C6
2	A	375	BCL	CAD-CBD-CGD-O2D
2	A	375	BCL	C4-C3-C5-C6
2	A	373[A]	BCL	C5-C6-C7-C8
2	A	372	BCL	C13-C15-C16-C17
3	A	380	EDO	O1-C1-C2-O2
2	A	373[A]	BCL	C16-C17-C18-C20
2	A	373[B]	BCL	C6-C7-C8-C10
3	A	382	EDO	O1-C1-C2-O2
3	A	386	EDO	O1-C1-C2-O2
2	A	371[B]	BCL	C16-C17-C18-C19
2	A	371[A]	BCL	C14-C13-C15-C16
2	A	371[A]	BCL	C16-C17-C18-C19
2	A	371[A]	BCL	CAA-CBA-CGA-O2A
2	A	371[B]	BCL	CAA-CBA-CGA-O2A
3	A	388[A]	EDO	O1-C1-C2-O2
2	A	371[B]	BCL	C16-C17-C18-C20
2	A	371[A]	BCL	CAA-CBA-CGA-O1A
2	A	371[B]	BCL	CAA-CBA-CGA-O1A
2	A	373[A]	BCL	CAA-CBA-CGA-O2A
2	A	373[B]	BCL	CAA-CBA-CGA-O2A

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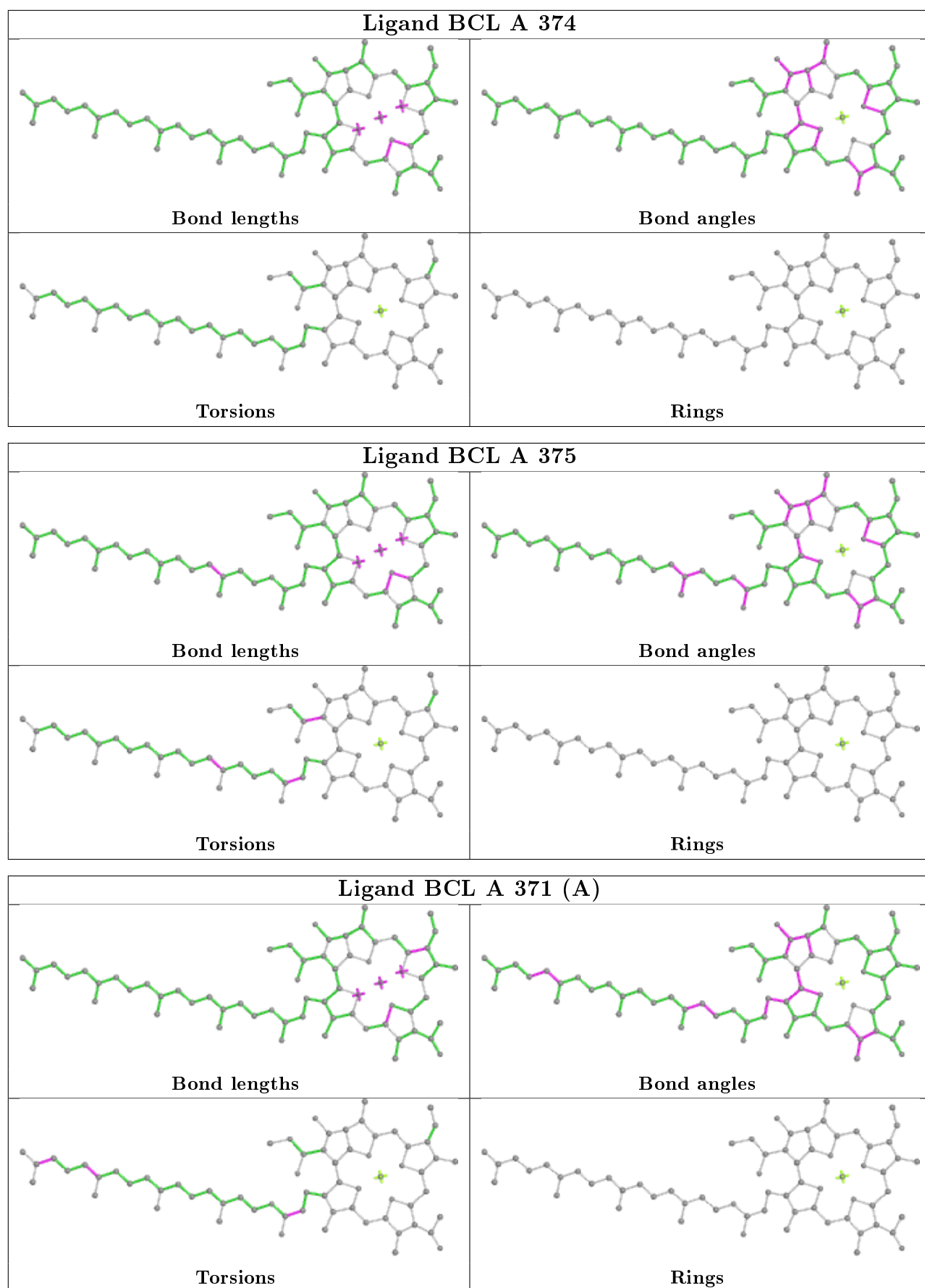
Mol	Chain	Res	Type	Atoms
2	A	373[A]	BCL	CAA-CBA-CGA-O1A
2	A	373[B]	BCL	CAA-CBA-CGA-O1A

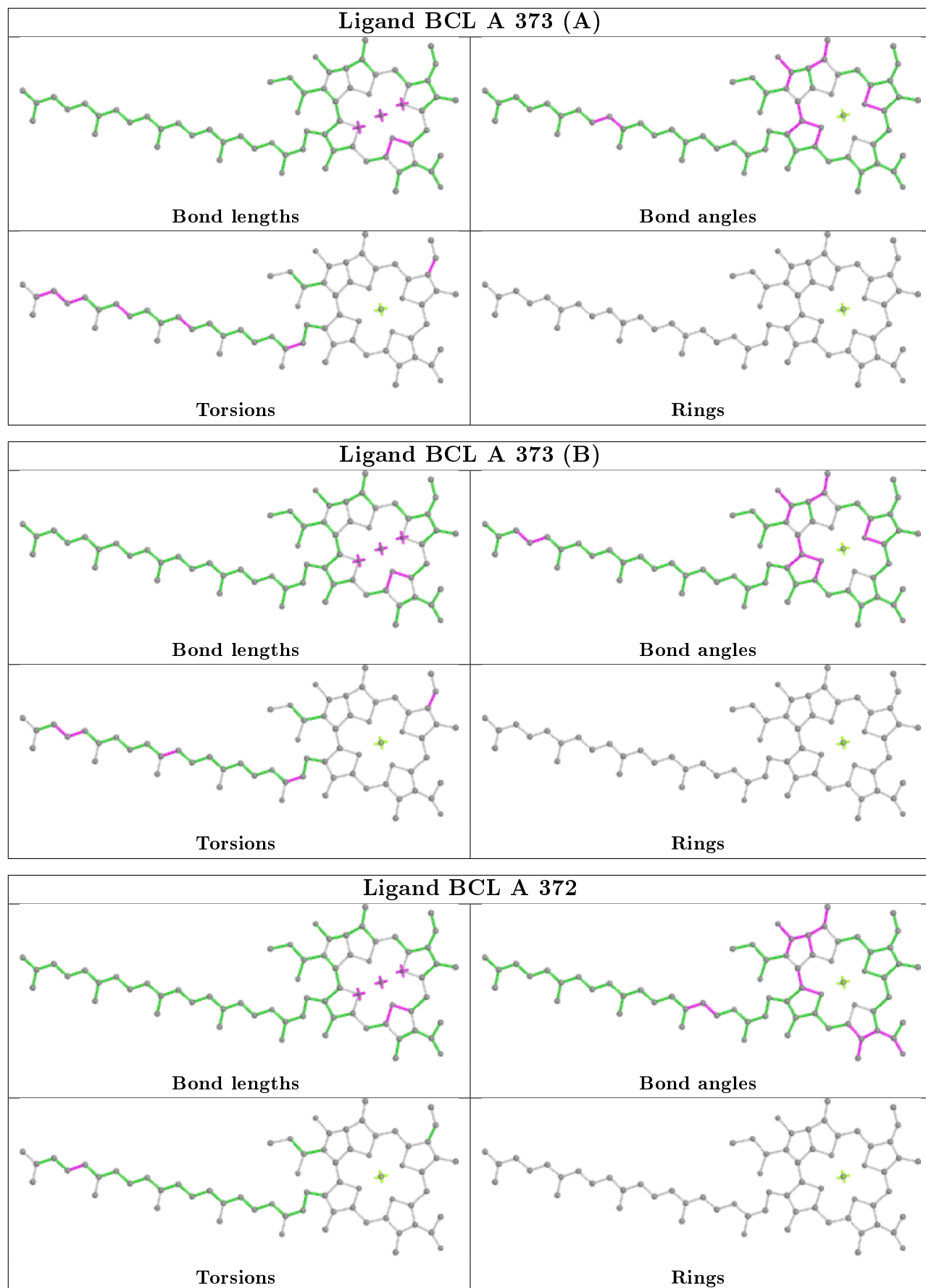
There are no ring outliers.

11 monomers are involved in 27 short contacts:

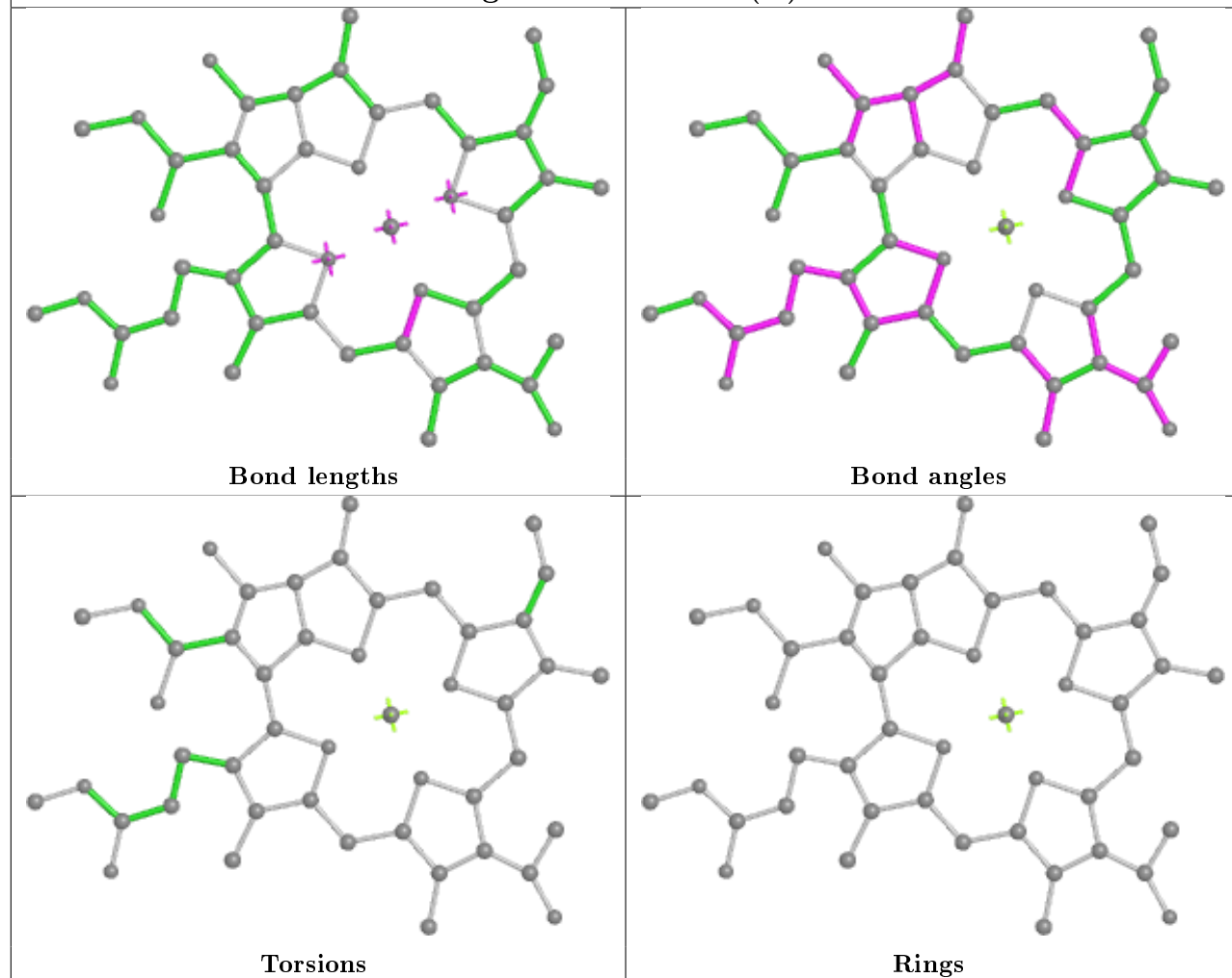
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	374	BCL	5	0
3	A	392	EDO	1	0
3	A	382	EDO	2	0
2	A	375	BCL	5	0
3	A	383[A]	EDO	1	0
2	A	373[A]	BCL	1	0
3	A	391[A]	EDO	3	0
3	A	387	EDO	3	0
3	A	385	EDO	2	0
2	A	372	BCL	2	0
2	A	378[B]	BCL	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

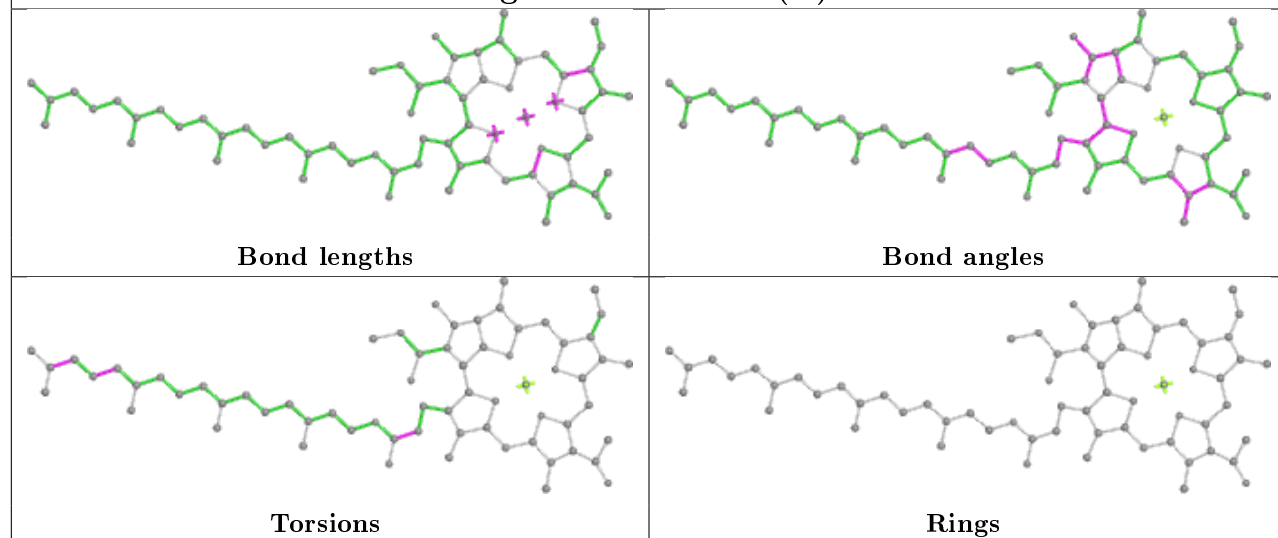




Ligand BCL A 378 (B)



Ligand BCL A 371 (B)



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	359/366 (98%)	-0.21	7 (1%) 66 67	8, 14, 26, 48	14 (3%)

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	8	THR	5.1
1	A	59	ALA	4.5
1	A	212[A]	GLY	3.0
1	A	58	ASP	2.7
1	A	57	LEU	2.4
1	A	7	ASP	2.3
1	A	193	ILE	2.1

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [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. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	EDO	A	382	4/4	0.48	0.22	64,72,72,77	0

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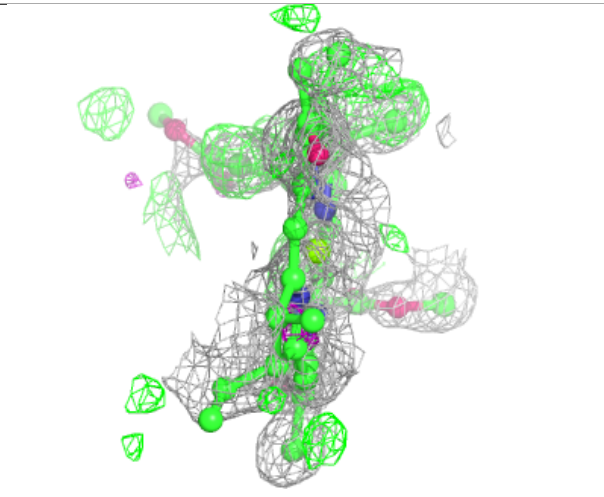
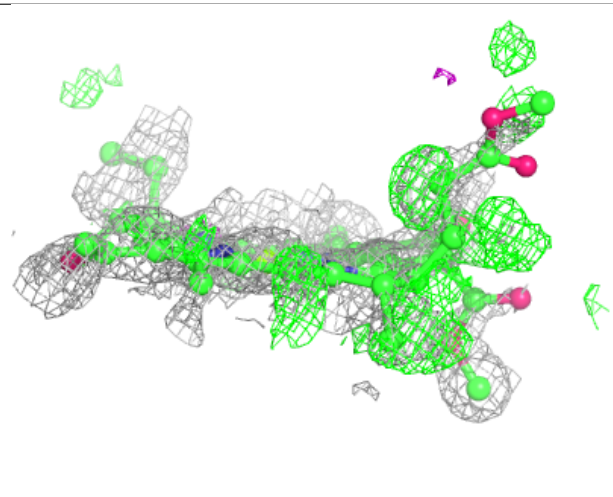
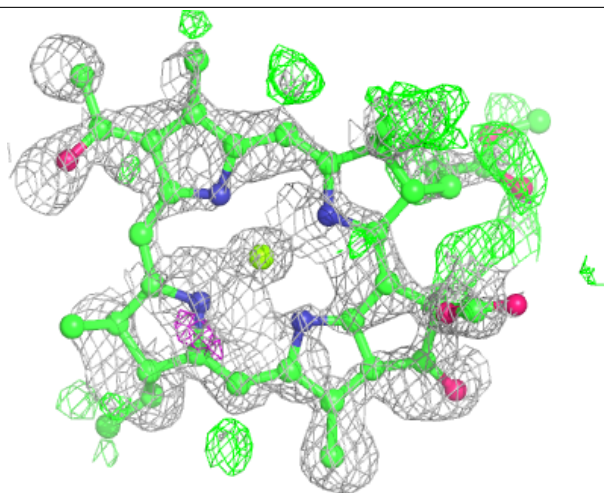
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	EDO	A	391[A]	4/4	0.66	0.31	29,29,39,39	4
3	EDO	A	392	4/4	0.71	0.32	39,41,44,55	0
3	EDO	A	387	4/4	0.81	0.18	23,27,33,45	0
3	EDO	A	384	4/4	0.83	0.21	25,27,38,47	0
3	EDO	A	380	4/4	0.86	0.20	34,35,38,60	0
3	EDO	A	385	4/4	0.86	0.14	34,35,37,42	0
3	EDO	A	383[A]	4/4	0.88	0.12	20,25,28,30	4
5	NH4	A	2378[B]	1/1	0.88	0.91	6,6,6,6	1
5	NH4	A	2378[A]	1/1	0.88	0.91	27,27,27,27	1
3	EDO	A	393[B]	4/4	0.89	0.17	24,27,28,32	4
3	EDO	A	388[A]	4/4	0.90	0.25	17,19,21,22	4
3	EDO	A	379	4/4	0.93	0.11	28,41,43,50	0
2	BCL	A	378[B]	47/66	0.93	0.16	13,19,26,33	47
3	EDO	A	386	4/4	0.94	0.10	25,27,32,39	0
3	EDO	A	390	4/4	0.94	0.15	19,20,30,32	0
3	EDO	A	381	4/4	0.97	0.10	13,19,20,25	0
2	BCL	A	376[A]	56/66	0.97	0.07	8,12,27,29	8
2	BCL	A	376[B]	56/66	0.97	0.07	8,12,27,29	8
2	BCL	A	376[C]	58/66	0.97	0.07	9,12,27,29	10
2	BCL	A	376[D]	58/66	0.97	0.07	9,12,27,29	10
2	BCL	A	377[C]	56/66	0.98	0.10	7,9,14,14	7
2	BCL	A	374	66/66	0.98	0.06	8,11,14,18	0
2	BCL	A	377[B]	53/66	0.98	0.10	7,9,14,14	4
3	EDO	A	389	4/4	0.98	0.12	15,17,28,29	0
2	BCL	A	377[E]	55/66	0.98	0.10	7,9,25,27	6
2	BCL	A	375	66/66	0.98	0.06	9,12,22,30	0
2	BCL	A	377[D]	56/66	0.98	0.10	7,9,14,14	7
2	BCL	A	371[A]	66/66	0.98	0.05	10,12,16,19	5
2	BCL	A	377[F]	55/66	0.98	0.10	7,9,25,31	6
2	BCL	A	371[B]	66/66	0.98	0.05	10,12,15,19	5
2	BCL	A	372	66/66	0.98	0.06	9,11,18,21	0
2	BCL	A	377[A]	53/66	0.98	0.10	7,9,14,14	4
4	NA	A	1232	1/1	0.99	0.29	27,27,27,27	0
2	BCL	A	373[A]	66/66	0.99	0.07	8,10,16,17	13
2	BCL	A	373[B]	66/66	0.99	0.07	8,10,17,19	13

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

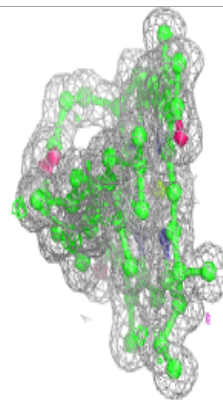
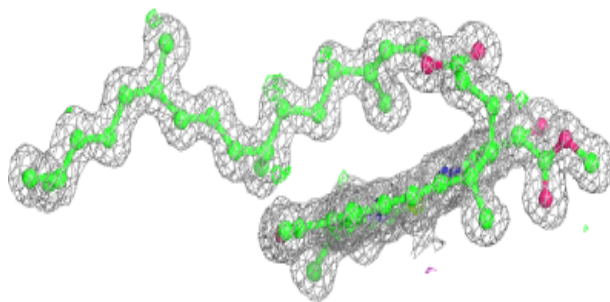
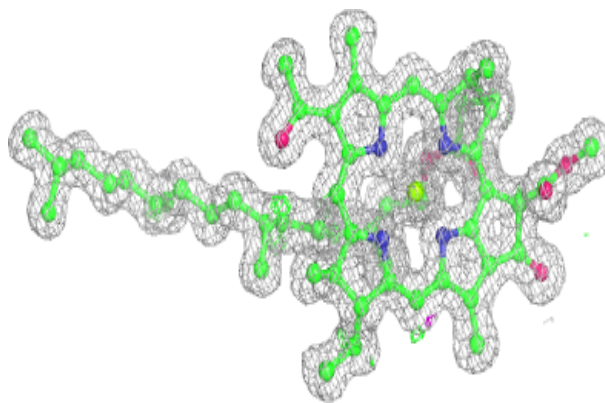
Electron density around BCL A 378 (B):

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



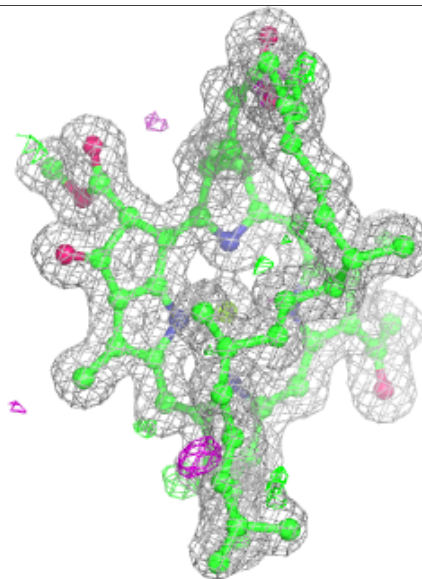
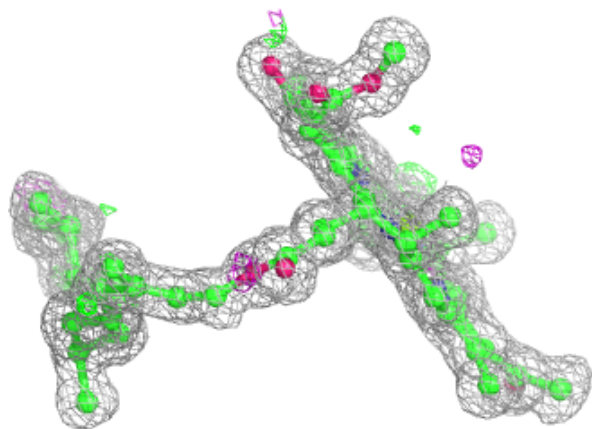
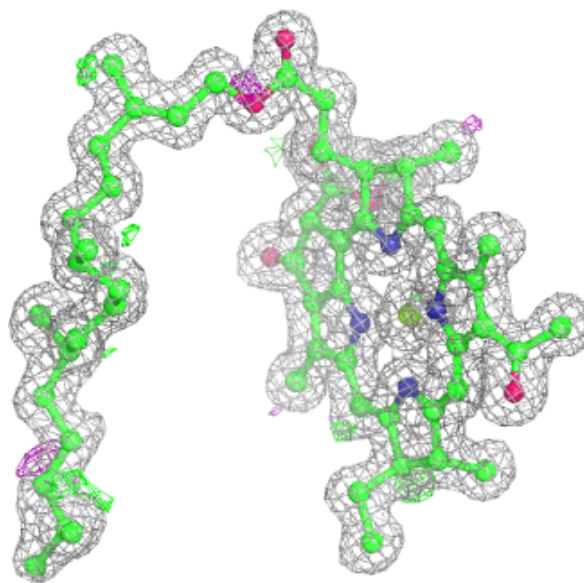
Electron density around BCL A 374:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



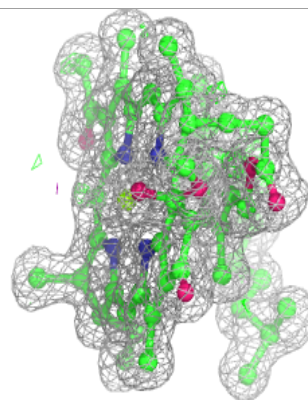
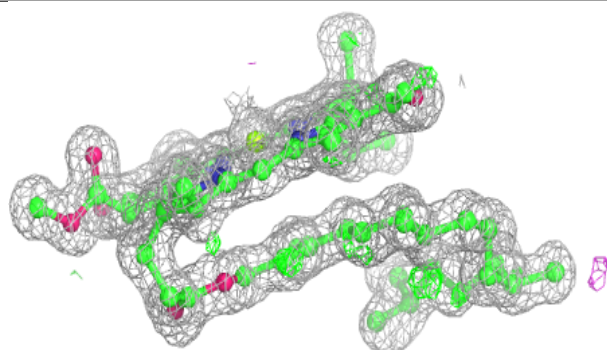
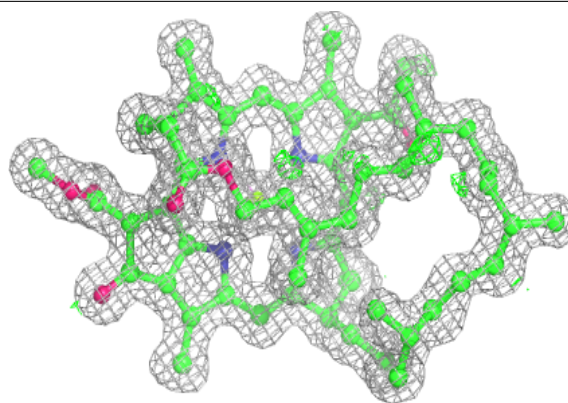
Electron density around BCL A 375:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

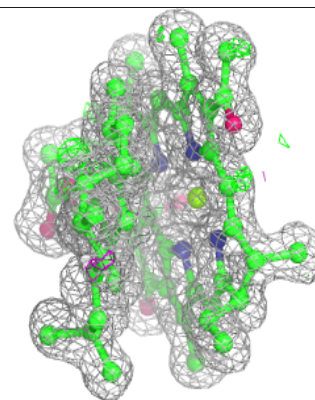
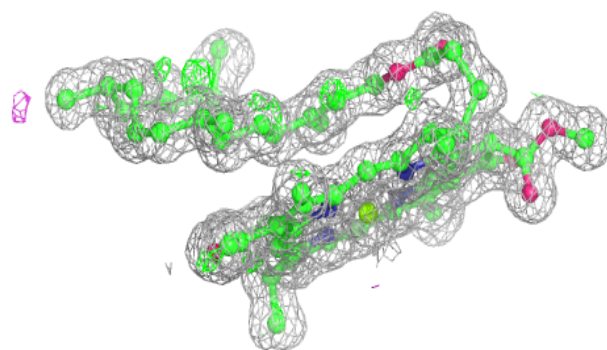
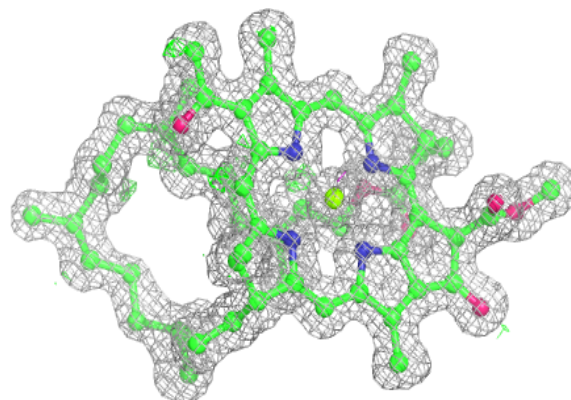


Electron density around BCL A 371 (A):

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

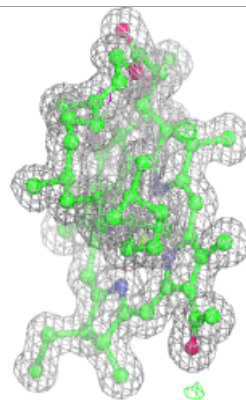
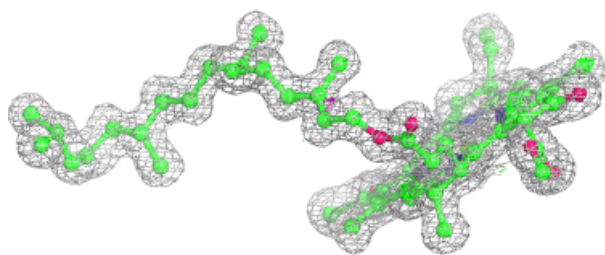
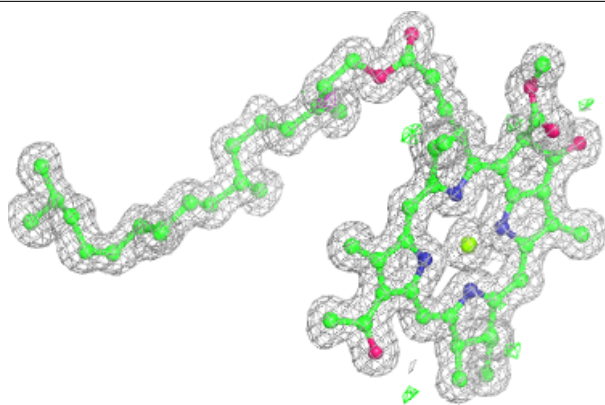
**Electron density around BCL A 371 (B):**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

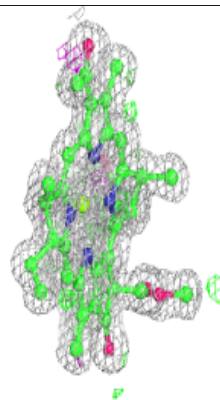
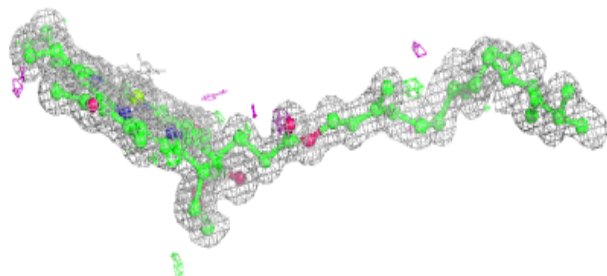
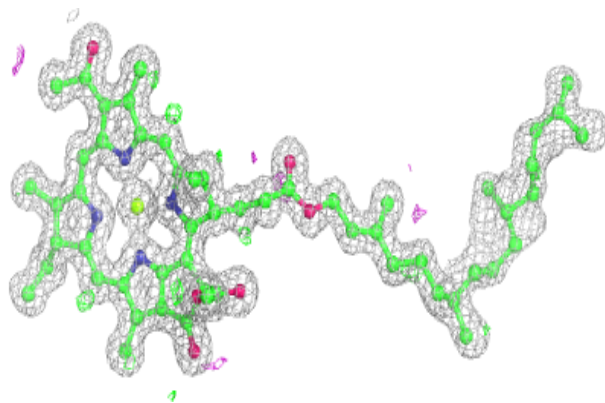


Electron density around BCL A 372:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

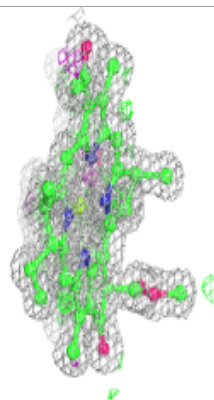
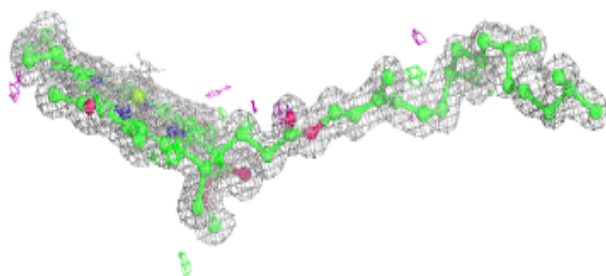
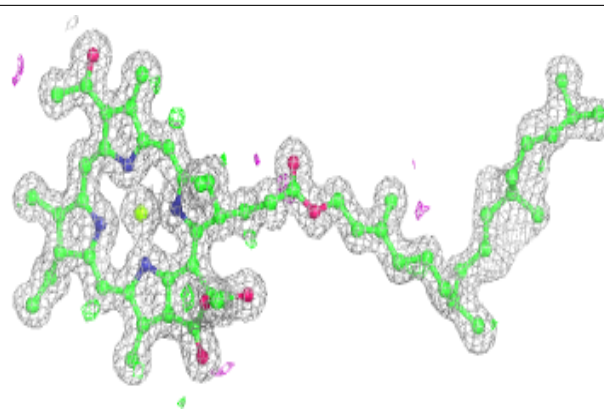
**Electron density around BCL A 373 (A):**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around BCL A 373 (B):

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.