



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 07:19 AM UTC

PDB ID : 3ENI / pdb_00003eni
Title : Crystal structure of the Fenna-Matthews-Olson Protein from Chlorobaculum Tepidum
Authors : Tronrud, D.; Camara-Artigas, A.; Blankenship, R.; Allen, J.P.
Deposited on : 2008-09-25
Resolution : 2.20 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

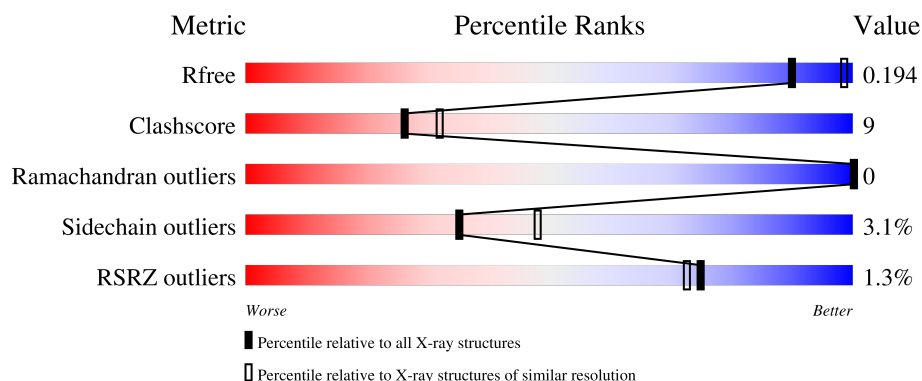
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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 of 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	365	% 84% 13% ..
1	C	365	2% 83% 13% ..

2 Entry composition [i](#)

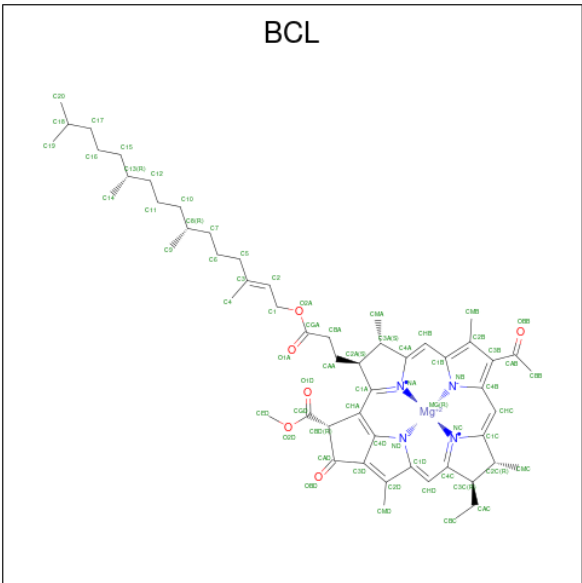
There are 3 unique types of molecules in this entry. The entry contains 6773 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	358	Total	C	N	O	S	0	0	1
			2719	1734	468	510	7			
1	C	357	Total	C	N	O	S	0	0	2
			2726	1734	476	509	7			

- Molecule 2 is BACTERIOCHLOROPHYLL A (CCD ID: BCL) (formula: $C_{55}H_{74}MgN_4O_6$).



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
			71	60	1	4	6		
2	A	1	Total	C	Mg	N	O	0	1
			84	69	1	5	9		

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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	1
			83	71	1	4	7		
2	A	1	Total	C	Mg	N	O	0	1
			79	68	1	4	6		
2	A	1	Total	C	Mg	N	O	0	1
			46	35	1	4	6		
2	C	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
2	C	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
2	C	1	Total	C	Mg	N	O	0	1
			71	60	1	4	6		
2	C	1	Total	C	Mg	N	O	0	1
			84	69	1	5	9		
2	C	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
2	C	1	Total	C	Mg	N	O	0	1
			83	71	1	4	7		
2	C	1	Total	C	Mg	N	O	0	1
			79	68	1	4	6		
2	C	1	Total	C	Mg	N	O	0	1
			46	35	1	4	6		

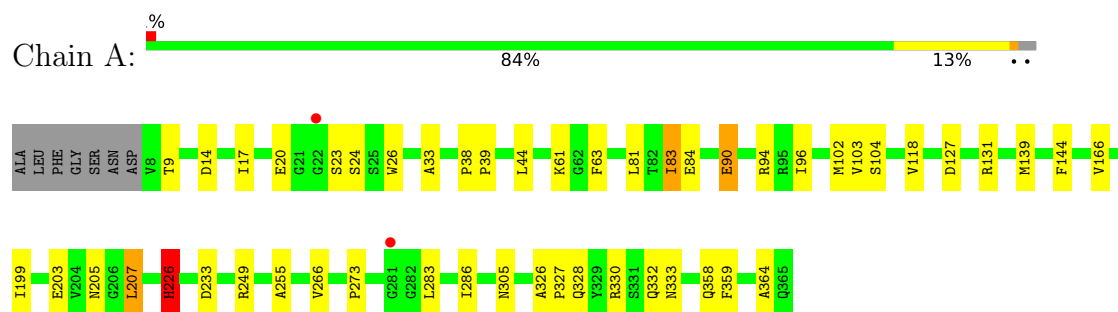
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	104	Total	O	0	1
			104	104		
3	C	102	Total	O	0	1
			102	102		

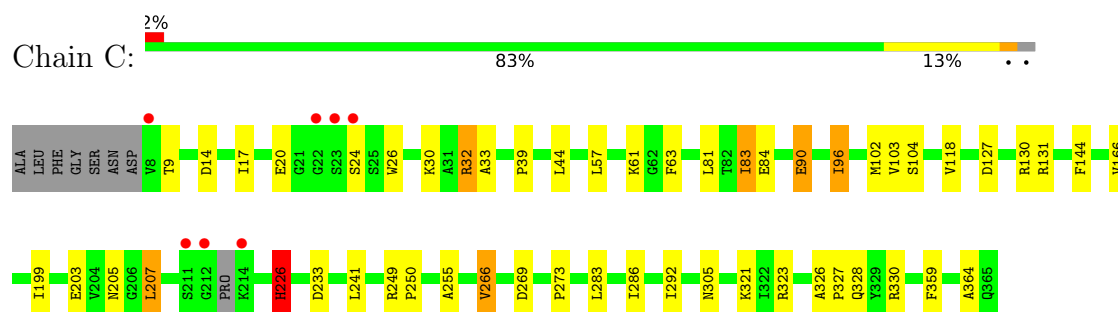
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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



- Molecule 1: Bacteriochlorophyll a protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 3 2	Depositor
Cell constants a, b, c, α , β , γ	169.10Å 169.10Å 169.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.20 20.00 – 2.20	Depositor EDS
% Data completeness (in resolution range)	86.5 (20.00-2.20) 86.5 (20.00-2.20)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.38 (at 2.14Å)	Xtriage
Refinement program	BUSTER-TNT 2.1.1	Depositor
R, R_{free}	0.163 , 0.207 0.154 , 0.194	Depositor DCC
R_{free} test set	2102 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	25.2	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 55.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	6773	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.18% 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

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	0.84	1/2788 (0.0%)	0.95	4/3791 (0.1%)
1	C	0.83	1/2793 (0.0%)	0.95	4/3793 (0.1%)
All	All	0.83	2/5581 (0.0%)	0.95	8/7584 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	292	ILE	CA-CB	5.88	1.57	1.54
1	A	38	PRO	CA-C	5.19	1.55	1.52

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	286	ILE	N-CA-C	-7.67	99.69	109.58
1	A	286	ILE	N-CA-C	-6.34	101.40	109.58
1	C	226	HIS	CB-CA-C	5.32	118.33	110.14
1	A	226	HIS	CB-CA-C	5.23	118.19	110.14
1	A	358	GLN	N-CA-C	5.20	117.85	110.10
1	C	90	GLU	N-CA-C	-5.20	105.76	112.68
1	C	130	ARG	N-CA-C	5.20	117.34	111.11
1	A	90	GLU	N-CA-C	-5.03	106.00	112.68

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	2719	0	2566	29	0
1	C	2726	0	2593	33	0
2	A	561	0	431	23	0
2	C	561	0	431	28	0
3	A	104	0	0	3	0
3	C	102	0	0	2	0
All	All	6773	0	6021	109	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 (109) 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)
2:A:375:BCL:C19	2:A:377[E]:BCL:H203	2.13	0.77
1:C:20:GLU:OE2	1:C:249:ARG:NH2	2.20	0.74
2:C:375:BCL:C19	2:C:377[E]:BCL:H203	2.17	0.74
1:A:20:GLU:OE2	1:A:249:ARG:NH2	2.22	0.72
2:A:375:BCL:H193	2:A:377[E]:BCL:H203	1.70	0.72
1:C:327:PRO:HD2	1:C:359:PHE:CD1	2.24	0.72
2:C:372:BCL:H92	2:C:372:BCL:H52	1.75	0.69
2:A:372:BCL:H52	2:A:372:BCL:H92	1.76	0.68
2:A:372:BCL:H151	2:A:373[A]:BCL:C20	2.24	0.67
2:C:375:BCL:H193	2:C:377[E]:BCL:H203	1.74	0.67
1:C:81:LEU:HD12	1:C:103:VAL:HG22	1.77	0.66
2:C:372:BCL:H151	2:C:373[A]:BCL:C20	2.26	0.65
1:A:81:LEU:HD12	1:A:103:VAL:HG22	1.78	0.65
2:C:372:BCL:H92	2:C:372:BCL:C5	2.26	0.65
2:A:372:BCL:H92	2:A:372:BCL:C5	2.27	0.64
1:A:327:PRO:HD2	1:A:359:PHE:CD1	2.34	0.63
2:A:375:BCL:H193	2:A:377[E]:BCL:C20	2.30	0.62
1:C:39:PRO:HG2	1:C:44:LEU:HD21	1.81	0.62
2:A:375:BCL:H191	2:A:377[E]:BCL:H203	1.82	0.60
1:C:321:LYS:CG	1:C:323:ARG:HH21	2.15	0.59
2:C:375:BCL:H193	2:C:377[E]:BCL:C20	2.32	0.59
1:A:90:GLU:OE1	1:A:94:ARG:NH1	2.36	0.58
1:C:30:LYS:HG2	1:C:269:ASP:OD1	2.05	0.57
1:C:61:LYS:CG	1:C:63:PHE:HD2	2.18	0.57
2:C:375:BCL:H191	2:C:377[E]:BCL:H203	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:372:BCL:H151	2:A:373[A]:BCL:H203	1.86	0.56
1:A:39:PRO:HG2	1:A:44:LEU:HD21	1.88	0.55
1:A:61:LYS:CG	1:A:63:PHE:HD2	2.20	0.55
1:C:127:ASP:O	1:C:131:ARG:HG2	2.07	0.55
1:C:203:GLU:CD	1:C:205:ASN:HD21	2.15	0.55
2:A:378[B]:BCL:HBB3	2:A:378[B]:BCL:HMB1	1.89	0.54
1:A:23:SER:N	1:A:24:SER:N	2.56	0.54
1:A:139:MET:HE1	3:A:1141:HOH:O	2.08	0.54
1:C:17:ILE:HD11	2:C:374:BCL:HAA1	1.90	0.53
1:C:203:GLU:CG	1:C:205:ASN:HD21	2.21	0.53
1:A:127:ASP:O	1:A:131:ARG:HG2	2.09	0.53
2:C:374:BCL:HMB1	2:C:374:BCL:HBB3	1.91	0.52
1:A:283:LEU:HD23	1:A:364:ALA:HB2	1.92	0.52
1:A:24:SER:HA	3:A:1075:HOH:O	2.10	0.52
2:C:372:BCL:H151	2:C:373[A]:BCL:H203	1.90	0.52
1:A:9:THR:HB	1:A:305:ASN:O	2.09	0.51
1:A:328:GLN:HA	1:A:328:GLN:OE1	2.09	0.51
1:C:90:GLU:HG3	1:C:96:ILE:HD13	1.92	0.51
1:C:24:SER:HA	3:C:1091:HOH:O	2.11	0.51
1:A:203:GLU:CD	1:A:205:ASN:HD21	2.18	0.50
2:C:378[B]:BCL:HMB1	2:C:378[B]:BCL:HBB3	1.92	0.50
1:A:326:ALA:HA	1:A:327:PRO:C	2.36	0.50
2:A:372:BCL:H91	2:A:373[A]:BCL:H101	1.92	0.50
1:C:326:ALA:HA	1:C:327:PRO:C	2.37	0.50
1:A:17:ILE:HD11	2:A:374:BCL:HAA1	1.93	0.49
1:C:26:TRP:HA	1:C:273:PRO:HA	1.95	0.48
2:A:372:BCL:HMB3	2:A:372:BCL:CBB	2.43	0.48
1:C:9:THR:HB	1:C:305:ASN:O	2.14	0.48
1:C:33:ALA:HB3	1:C:266:VAL:HG13	1.95	0.48
2:A:378[B]:BCL:HBD	2:A:378[B]:BCL:HAA1	1.95	0.48
2:C:372:BCL:HMB3	2:C:372:BCL:CBB	2.43	0.48
2:C:372:BCL:H91	2:C:373[A]:BCL:H101	1.96	0.48
1:A:203:GLU:CG	1:A:205:ASN:HD21	2.26	0.47
1:A:26:TRP:HA	1:A:273:PRO:HA	1.97	0.47
1:C:328:GLN:HA	1:C:328:GLN:OE1	2.15	0.47
1:C:199:ILE:HD13	1:C:226:HIS:HB2	1.95	0.47
1:A:102:MET:HE2	1:A:102:MET:HB3	1.84	0.47
1:C:283:LEU:HD23	1:C:364:ALA:HB2	1.95	0.47
1:A:199:ILE:HD13	1:A:226:HIS:HB2	1.96	0.47
2:A:374:BCL:HBB3	2:A:374:BCL:HMB1	1.96	0.47
2:A:377[E]:BCL:H162	2:A:377[E]:BCL:H192	1.55	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:166:VAL:HG22	1:A:207:LEU:HD12	1.98	0.46
1:C:249:ARG:NE	3:C:1139:HOH:O	2.30	0.46
2:A:378[B]:BCL:HAA1	2:A:378[B]:BCL:CBD	2.46	0.46
2:C:377[E]:BCL:H162	2:C:377[E]:BCL:H192	1.57	0.46
2:C:378[B]:BCL:HAA1	2:C:378[B]:BCL:HBD	1.97	0.45
1:C:81:LEU:CD1	1:C:103:VAL:HG22	2.46	0.45
2:C:378[B]:BCL:HAA1	2:C:378[B]:BCL:CBD	2.46	0.44
2:C:374:BCL:HHC	2:C:374:BCL:OBB	2.17	0.44
1:A:83:ILE:HG13	1:A:84:GLU:N	2.32	0.44
2:C:378[B]:BCL:H2C	2:C:378[B]:BCL:HBC3	1.51	0.44
1:A:81:LEU:CD1	1:A:103:VAL:HG22	2.47	0.43
2:A:372:BCL:H162	2:A:372:BCL:H203	1.43	0.43
1:A:90:GLU:HG3	1:A:96:ILE:HD13	1.99	0.43
1:A:33:ALA:HB3	1:A:266:VAL:HG13	2.01	0.43
1:C:32:ARG:HH22	1:C:269:ASP:CG	2.26	0.43
1:C:203:GLU:CG	1:C:205:ASN:ND2	2.82	0.43
2:C:372:BCL:H203	2:C:372:BCL:H162	1.36	0.43
2:C:378[B]:BCL:HAA1	2:C:378[B]:BCL:CGD	2.49	0.43
1:C:166:VAL:HG22	1:C:207:LEU:HD12	2.01	0.42
1:C:255:ALA:HB3	2:C:375:BCL:H92	2.00	0.42
2:C:372:BCL:HMB3	2:C:372:BCL:HBB3	2.00	0.42
1:A:255:ALA:HB3	2:A:375:BCL:H92	2.00	0.42
1:C:83:ILE:HG13	1:C:84:GLU:N	2.35	0.42
1:A:118:VAL:HA	1:A:144:PHE:O	2.20	0.42
2:C:376[B]:BCL:HAC2	2:C:377[B]:BCL:OBB	2.20	0.41
1:C:118:VAL:HA	1:C:144:PHE:O	2.20	0.41
1:C:203:GLU:HG2	1:C:205:ASN:ND2	2.36	0.41
2:C:378[B]:BCL:HBA1	2:C:378[B]:BCL:H3A	1.81	0.41
1:A:144:PHE:HB3	3:A:1146:HOH:O	2.19	0.41
2:A:378[B]:BCL:HAA1	2:A:378[B]:BCL:CGD	2.51	0.41
1:C:57:LEU:HD12	1:C:57:LEU:HA	1.87	0.41
1:C:249:ARG:HB2	1:C:250:PRO:CD	2.51	0.41
1:A:332:GLN:HG2	1:A:333:ASN:N	2.35	0.41
2:A:372:BCL:HMB3	2:A:372:BCL:HBB3	2.03	0.40
1:C:241:LEU:HD12	1:C:241:LEU:C	2.46	0.40
1:C:102:MET:HE2	1:C:102:MET:HB3	1.86	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	354/365 (97%)	346 (98%)	8 (2%)	0	100	100
1	C	351/365 (96%)	345 (98%)	6 (2%)	0	100	100
All	All	705/730 (97%)	691 (98%)	14 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	273/301 (91%)	266 (97%)	7 (3%)	40	55
1	C	278/301 (92%)	268 (96%)	10 (4%)	31	42
All	All	551/602 (92%)	534 (97%)	17 (3%)	35	48

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	ASP
1	A	83	ILE
1	A	104	SER
1	A	207	LEU
1	A	226	HIS
1	A	233	ASP
1	A	330	ARG
1	C	14	ASP

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Mol	Chain	Res	Type
1	C	32	ARG
1	C	83	ILE
1	C	96	ILE
1	C	104	SER
1	C	207	LEU
1	C	226	HIS
1	C	233	ASP
1	C	266	VAL
1	C	330	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	197	GLN
1	A	205	ASN
1	A	311	GLN
1	C	205	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

36 ligands are modelled in this entry.

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$
2	BCL	A	371[B]	-	69,74,74	1.31	10 (14%)	79,115,115	1.53	10 (12%)
2	BCL	C	373[A]	-	69,74,74	1.24	7 (10%)	79,115,115	1.51	13 (16%)
2	BCL	C	374	1	69,74,74	1.38	10 (14%)	79,115,115	1.42	10 (12%)
2	BCL	A	372	3	69,74,74	1.44	10 (14%)	79,115,115	1.58	9 (11%)
2	BCL	A	371[A]	-	69,74,74	1.31	10 (14%)	79,115,115	1.52	10 (12%)
2	BCL	A	373[B]	-	69,74,74	1.27	7 (10%)	79,115,115	1.57	13 (16%)
2	BCL	A	373[A]	-	69,74,74	1.28	7 (10%)	79,115,115	1.54	13 (16%)
2	BCL	C	378[B]	1	49,54,74	1.40	6 (12%)	55,91,115	1.63	7 (12%)
2	BCL	A	375	1	69,74,74	1.43	8 (11%)	79,115,115	1.45	10 (12%)
2	BCL	C	371[A]	-	69,74,74	1.44	9 (13%)	79,115,115	1.48	10 (12%)
2	BCL	C	371[B]	-	69,74,74	1.44	9 (13%)	79,115,115	1.49	10 (12%)
2	BCL	C	372	3	69,74,74	1.38	9 (13%)	79,115,115	1.57	10 (12%)
2	BCL	C	373[B]	-	69,74,74	1.23	7 (10%)	79,115,115	1.55	13 (16%)
2	BCL	C	375	1	69,74,74	1.22	5 (7%)	79,115,115	1.49	13 (16%)
2	BCL	A	378[B]	1	49,54,74	1.41	6 (12%)	55,91,115	1.63	9 (16%)
2	BCL	A	374	1	69,74,74	1.34	7 (10%)	79,115,115	1.43	10 (12%)

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
2	BCL	A	371[B]	-	-	6/41/137/137	-
2	BCL	C	373[A]	-	-	9/41/137/137	-
2	BCL	C	374	1	-	0/41/137/137	-
2	BCL	A	372	3	-	10/41/137/137	-
2	BCL	A	371[A]	-	-	4/41/137/137	-
2	BCL	A	373[B]	-	-	13/41/137/137	-
2	BCL	A	373[A]	-	-	11/41/137/137	-
2	BCL	C	378[B]	1	-	6/17/113/137	-
2	BCL	A	375	1	-	7/41/137/137	-
2	BCL	C	371[A]	-	-	5/41/137/137	-
2	BCL	C	371[B]	-	-	7/41/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BCL	C	372	3	-	10/41/137/137	-
2	BCL	C	373[B]	-	-	11/41/137/137	-
2	BCL	C	375	1	-	11/41/137/137	-
2	BCL	A	378[B]	1	-	6/17/113/137	-
2	BCL	A	374	1	-	0/41/137/137	-

All (127) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	371[A]	BCL	MG-NA	5.85	2.20	2.06
2	C	371[B]	BCL	MG-NA	5.85	2.20	2.06
2	C	373[A]	BCL	MG-NA	5.54	2.19	2.06
2	C	373[B]	BCL	MG-NA	5.54	2.19	2.06
2	C	372	BCL	MG-NA	5.51	2.19	2.06
2	A	375	BCL	MG-NA	5.47	2.19	2.06
2	A	374	BCL	MG-NA	5.36	2.19	2.06
2	A	378[B]	BCL	MG-NA	5.19	2.18	2.06
2	C	378[B]	BCL	MG-NA	5.13	2.18	2.06
2	A	371[A]	BCL	MG-NA	4.96	2.18	2.06
2	A	371[B]	BCL	MG-NA	4.96	2.18	2.06
2	A	373[A]	BCL	MG-NA	4.82	2.17	2.06
2	A	373[B]	BCL	MG-NA	4.82	2.17	2.06
2	C	374	BCL	MG-NC	4.77	2.17	2.06
2	C	375	BCL	MG-NA	4.70	2.17	2.06
2	A	372	BCL	MG-NA	4.56	2.17	2.06
2	A	372	BCL	MG-NC	4.44	2.16	2.06
2	A	375	BCL	MG-NC	4.43	2.16	2.06
2	C	374	BCL	MG-NA	4.05	2.15	2.06
2	A	378[B]	BCL	MG-NC	3.92	2.15	2.06
2	C	378[B]	BCL	MG-NC	3.66	2.15	2.06
2	A	375	BCL	C1D-ND	3.60	1.42	1.37
2	A	371[A]	BCL	MG-NC	3.46	2.14	2.06
2	A	371[B]	BCL	MG-NC	3.46	2.14	2.06
2	A	372	BCL	C3B-C4B	3.42	1.47	1.41
2	A	374	BCL	C1D-ND	3.41	1.42	1.37
2	C	374	BCL	CHD-C1D	3.38	1.45	1.38
2	C	371[A]	BCL	MG-NC	3.36	2.14	2.06
2	C	371[B]	BCL	MG-NC	3.36	2.14	2.06
2	A	374	BCL	CMB-C2B	3.27	1.57	1.50
2	C	373[A]	BCL	C5-C3	3.26	1.58	1.51
2	C	373[B]	BCL	C5-C3	3.26	1.58	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	375	BCL	C3B-C4B	3.24	1.47	1.41
2	C	372	BCL	O2A-CGA	-3.22	1.24	1.33
2	A	374	BCL	MG-NC	3.19	2.13	2.06
2	C	371[A]	BCL	C3B-C4B	3.16	1.47	1.41
2	C	371[B]	BCL	C3B-C4B	3.16	1.47	1.41
2	A	374	BCL	CHD-C1D	3.10	1.44	1.38
2	C	372	BCL	C3B-C4B	3.09	1.47	1.41
2	A	375	BCL	O1A-CGA	-3.08	1.13	1.22
2	C	375	BCL	MG-NC	3.07	2.13	2.06
2	C	372	BCL	CAC-C3C	3.06	1.59	1.54
2	A	372	BCL	C3C-C4C	3.04	1.55	1.51
2	A	373[A]	BCL	C5-C3	3.03	1.57	1.51
2	A	373[B]	BCL	C5-C3	3.03	1.57	1.51
2	A	375	BCL	CHD-C1D	3.00	1.44	1.38
2	C	372	BCL	MG-NC	2.98	2.13	2.06
2	A	378[B]	BCL	CHD-C1D	2.97	1.44	1.38
2	C	371[A]	BCL	CMB-C2B	2.97	1.56	1.50
2	C	371[B]	BCL	CMB-C2B	2.97	1.56	1.50
2	C	371[A]	BCL	CAC-C3C	2.95	1.59	1.54
2	C	371[B]	BCL	CAC-C3C	2.95	1.59	1.54
2	A	373[A]	BCL	CHD-C1D	2.93	1.44	1.38
2	A	373[B]	BCL	CHD-C1D	2.93	1.44	1.38
2	C	378[B]	BCL	CHD-C1D	2.93	1.44	1.38
2	A	373[A]	BCL	C3B-C4B	2.91	1.46	1.41
2	A	373[B]	BCL	C3B-C4B	2.91	1.46	1.41
2	A	378[B]	BCL	C3B-C4B	2.90	1.46	1.41
2	A	372	BCL	CHD-C1D	2.89	1.44	1.38
2	A	373[A]	BCL	MG-NC	2.81	2.12	2.06
2	A	373[B]	BCL	MG-NC	2.81	2.12	2.06
2	A	372	BCL	O2A-CGA	-2.80	1.25	1.33
2	C	378[B]	BCL	C3B-C4B	2.74	1.46	1.41
2	A	372	BCL	O1A-CGA	-2.74	1.14	1.22
2	C	374	BCL	OBD-CAD	2.69	1.27	1.22
2	C	375	BCL	CHD-C1D	2.68	1.43	1.38
2	C	375	BCL	C3B-C4B	2.66	1.46	1.41
2	C	373[A]	BCL	MG-NC	2.66	2.12	2.06
2	C	373[B]	BCL	MG-NC	2.66	2.12	2.06
2	A	373[A]	BCL	O1A-CGA	-2.62	1.14	1.22
2	A	373[B]	BCL	O1A-CGA	-2.62	1.14	1.22
2	A	371[A]	BCL	C1D-C2D	-2.57	1.40	1.45
2	A	371[B]	BCL	C1D-C2D	-2.57	1.40	1.45
2	A	373[A]	BCL	OBD-CAD	2.57	1.26	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	373[B]	BCL	OBD-CAD	2.57	1.26	1.22
2	A	371[A]	BCL	CHD-C1D	2.54	1.43	1.38
2	A	371[B]	BCL	CHD-C1D	2.54	1.43	1.38
2	C	371[A]	BCL	CHD-C1D	2.50	1.43	1.38
2	C	371[B]	BCL	CHD-C1D	2.50	1.43	1.38
2	C	374	BCL	C1-C2	2.48	1.56	1.49
2	C	374	BCL	C1D-ND	2.48	1.41	1.37
2	A	371[A]	BCL	CAA-C2A	2.47	1.58	1.54
2	A	371[B]	BCL	CAA-C2A	2.47	1.58	1.54
2	A	371[A]	BCL	C3D-C4D	-2.44	1.38	1.44
2	A	371[B]	BCL	C3D-C4D	-2.44	1.38	1.44
2	A	372	BCL	CAC-C3C	2.43	1.58	1.54
2	A	374	BCL	C3B-C4B	2.40	1.45	1.41
2	C	373[A]	BCL	C3B-C4B	2.40	1.45	1.41
2	C	373[B]	BCL	C3B-C4B	2.40	1.45	1.41
2	C	372	BCL	C1D-ND	2.38	1.41	1.37
2	C	372	BCL	CHD-C1D	2.36	1.43	1.38
2	C	373[A]	BCL	CHD-C1D	2.36	1.43	1.38
2	C	373[B]	BCL	CHD-C1D	2.36	1.43	1.38
2	A	371[A]	BCL	C5-C3	2.34	1.56	1.51
2	A	371[B]	BCL	C5-C3	2.34	1.56	1.51
2	C	374	BCL	C9-C8	2.32	1.60	1.52
2	A	374	BCL	C5-C3	2.27	1.56	1.51
2	A	371[A]	BCL	C9-C8	2.27	1.59	1.52
2	A	371[B]	BCL	C9-C8	2.27	1.59	1.52
2	C	374	BCL	C3B-C4B	2.22	1.45	1.41
2	C	373[A]	BCL	C3D-C4D	-2.20	1.39	1.44
2	C	373[B]	BCL	C3D-C4D	-2.20	1.39	1.44
2	A	372	BCL	CMB-C2B	2.17	1.55	1.50
2	C	372	BCL	C2-C3	-2.15	1.28	1.33
2	A	378[B]	BCL	C1D-ND	2.12	1.40	1.37
2	C	375	BCL	C5-C3	2.11	1.55	1.51
2	C	371[A]	BCL	C3D-C4D	-2.11	1.39	1.44
2	C	371[B]	BCL	C3D-C4D	-2.11	1.39	1.44
2	A	378[B]	BCL	C3D-C4D	-2.10	1.39	1.44
2	C	374	BCL	CMB-C2B	2.09	1.55	1.50
2	A	375	BCL	CHC-C1C	2.08	1.42	1.37
2	C	371[A]	BCL	O1A-CGA	-2.07	1.16	1.22
2	C	371[B]	BCL	O1A-CGA	-2.07	1.16	1.22
2	C	378[B]	BCL	C3D-C4D	-2.06	1.39	1.44
2	A	371[A]	BCL	C3B-C4B	2.05	1.45	1.41
2	A	371[B]	BCL	C3B-C4B	2.05	1.45	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	371[A]	BCL	CAC-C3C	2.04	1.57	1.54
2	A	371[B]	BCL	CAC-C3C	2.04	1.57	1.54
2	C	378[B]	BCL	CHB-C1B	2.04	1.44	1.39
2	C	374	BCL	C3D-C4D	-2.03	1.39	1.44
2	C	371[A]	BCL	OBD-CAD	2.01	1.26	1.22
2	C	371[B]	BCL	OBD-CAD	2.01	1.26	1.22
2	A	372	BCL	C2-C3	-2.01	1.28	1.33
2	C	372	BCL	C3D-C4D	-2.01	1.39	1.44
2	A	375	BCL	CBD-CGD	-2.01	1.46	1.52
2	C	373[A]	BCL	CMD-C2D	2.01	1.54	1.50
2	C	373[B]	BCL	CMD-C2D	2.01	1.54	1.50

All (170) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	372	BCL	C1-C2-C3	-5.83	116.64	126.20
2	A	371[A]	BCL	C1-C2-C3	-5.82	116.66	126.20
2	A	371[B]	BCL	C1-C2-C3	-5.82	116.66	126.20
2	C	372	BCL	C1-C2-C3	-5.65	116.94	126.20
2	C	372	BCL	C4D-CHA-C1A	5.45	127.75	121.24
2	C	378[B]	BCL	C4D-CHA-C1A	5.41	127.70	121.24
2	A	372	BCL	C4D-CHA-C1A	5.38	127.66	121.24
2	A	378[B]	BCL	C4D-CHA-C1A	5.36	127.64	121.24
2	A	374	BCL	C4D-CHA-C1A	5.26	127.52	121.24
2	A	371[A]	BCL	C4D-CHA-C1A	5.24	127.49	121.24
2	A	371[B]	BCL	C4D-CHA-C1A	5.24	127.49	121.24
2	C	371[A]	BCL	C1-C2-C3	-5.21	117.65	126.20
2	C	371[B]	BCL	C1-C2-C3	-5.21	117.65	126.20
2	C	371[A]	BCL	C4D-CHA-C1A	5.16	127.40	121.24
2	C	371[B]	BCL	C4D-CHA-C1A	5.16	127.40	121.24
2	C	374	BCL	C4D-CHA-C1A	5.06	127.27	121.24
2	A	375	BCL	C4D-CHA-C1A	5.02	127.23	121.24
2	C	375	BCL	C4D-CHA-C1A	5.00	127.21	121.24
2	C	375	BCL	C1-C2-C3	-4.86	118.24	126.20
2	A	373[A]	BCL	C4D-CHA-C1A	4.52	126.63	121.24
2	A	373[B]	BCL	C4D-CHA-C1A	4.52	126.63	121.24
2	C	373[A]	BCL	C4D-CHA-C1A	4.50	126.61	121.24
2	C	373[B]	BCL	C4D-CHA-C1A	4.50	126.61	121.24
2	A	374	BCL	C4A-NA-C1A	4.26	108.62	106.68
2	C	373[B]	BCL	C11-C10-C8	4.23	130.01	115.97
2	C	373[A]	BCL	CHD-C1D-ND	-4.14	118.98	124.80
2	C	373[B]	BCL	CHD-C1D-ND	-4.14	118.98	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	373[A]	BCL	C1D-ND-C4D	-4.12	103.42	106.31
2	A	373[B]	BCL	C1D-ND-C4D	-4.12	103.42	106.31
2	A	373[A]	BCL	CHD-C1D-ND	-4.08	119.06	124.80
2	A	373[B]	BCL	CHD-C1D-ND	-4.08	119.06	124.80
2	A	372	BCL	C4A-NA-C1A	4.06	108.53	106.68
2	A	373[B]	BCL	C11-C10-C8	4.04	129.39	115.97
2	A	372	BCL	CHD-C1D-ND	-4.01	119.16	124.80
2	A	378[B]	BCL	CHD-C1D-ND	-3.98	119.21	124.80
2	C	378[B]	BCL	CHD-C1D-ND	-3.94	119.25	124.80
2	A	371[A]	BCL	C4A-NA-C1A	3.90	108.46	106.68
2	A	371[B]	BCL	C4A-NA-C1A	3.90	108.46	106.68
2	C	373[A]	BCL	C1D-ND-C4D	-3.90	103.57	106.31
2	C	373[B]	BCL	C1D-ND-C4D	-3.90	103.57	106.31
2	C	378[B]	BCL	C1D-ND-C4D	-3.86	103.60	106.31
2	C	372	BCL	CHD-C1D-ND	-3.83	119.41	124.80
2	C	371[A]	BCL	CHD-C1D-ND	-3.83	119.41	124.80
2	C	371[B]	BCL	CHD-C1D-ND	-3.83	119.41	124.80
2	A	378[B]	BCL	C1D-ND-C4D	-3.80	103.64	106.31
2	C	371[A]	BCL	C1D-ND-C4D	-3.78	103.66	106.31
2	C	371[B]	BCL	C1D-ND-C4D	-3.78	103.66	106.31
2	A	374	BCL	C1D-ND-C4D	-3.69	103.72	106.31
2	A	374	BCL	CHD-C1D-ND	-3.68	119.62	124.80
2	C	378[B]	BCL	C4A-NA-C1A	3.65	108.34	106.68
2	A	372	BCL	C1D-ND-C4D	-3.64	103.76	106.31
2	A	371[A]	BCL	CHD-C1D-ND	-3.63	119.69	124.80
2	A	371[B]	BCL	CHD-C1D-ND	-3.63	119.69	124.80
2	C	374	BCL	C4A-NA-C1A	3.54	108.30	106.68
2	C	372	BCL	C4A-NA-C1A	3.51	108.28	106.68
2	A	378[B]	BCL	C4A-NA-C1A	3.50	108.28	106.68
2	C	371[A]	BCL	C4A-NA-C1A	3.50	108.28	106.68
2	C	371[B]	BCL	C4A-NA-C1A	3.50	108.28	106.68
2	C	374	BCL	C1D-ND-C4D	-3.45	103.89	106.31
2	A	371[A]	BCL	C1D-ND-C4D	-3.43	103.90	106.31
2	A	371[B]	BCL	C1D-ND-C4D	-3.43	103.90	106.31
2	A	373[A]	BCL	C4A-NA-C1A	3.41	108.23	106.68
2	A	373[B]	BCL	C4A-NA-C1A	3.41	108.23	106.68
2	C	373[B]	BCL	C6-C7-C8	-3.37	104.77	115.97
2	A	375	BCL	C1-C2-C3	-3.36	120.69	126.20
2	C	373[A]	BCL	CHA-C1A-NA	-3.34	118.82	126.39
2	C	373[B]	BCL	CHA-C1A-NA	-3.34	118.82	126.39
2	A	375	BCL	C1D-ND-C4D	-3.32	103.99	106.31
2	C	374	BCL	O2D-CGD-O1D	-3.29	117.45	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	375	BCL	CHD-C1D-ND	-3.27	120.20	124.80
2	C	374	BCL	CHD-C1D-ND	-3.24	120.24	124.80
2	A	372	BCL	O2D-CGD-CBD	3.19	116.81	111.23
2	A	375	BCL	CHD-C1D-ND	-3.15	120.37	124.80
2	A	373[B]	BCL	C16-C15-C13	-3.12	105.59	115.97
2	C	373[A]	BCL	C4A-NA-C1A	3.10	108.09	106.68
2	C	373[B]	BCL	C4A-NA-C1A	3.10	108.09	106.68
2	C	374	BCL	C1C-NC-C4C	3.09	108.09	106.68
2	C	372	BCL	CHA-C1A-NA	-3.05	119.49	126.39
2	C	373[A]	BCL	C2A-C1A-CHA	3.03	129.13	123.87
2	C	373[B]	BCL	C2A-C1A-CHA	3.03	129.13	123.87
2	C	373[A]	BCL	C6-C7-C8	-3.03	105.89	115.97
2	A	375	BCL	CHA-C1A-NA	-3.03	119.53	126.39
2	C	371[A]	BCL	CHA-C1A-NA	-3.03	119.54	126.39
2	C	371[B]	BCL	CHA-C1A-NA	-3.03	119.54	126.39
2	A	378[B]	BCL	CHA-C1A-NA	-3.02	119.56	126.39
2	A	373[A]	BCL	O2D-CGD-O1D	-3.01	117.99	123.85
2	A	373[B]	BCL	O2D-CGD-O1D	-3.01	117.99	123.85
2	C	378[B]	BCL	CHA-C1A-NA	-2.99	119.61	126.39
2	C	375	BCL	C1D-ND-C4D	-2.97	104.23	106.31
2	A	371[A]	BCL	C2A-C1A-CHA	2.95	128.99	123.87
2	A	371[B]	BCL	C2A-C1A-CHA	2.95	128.99	123.87
2	A	373[A]	BCL	CHA-C1A-NA	-2.95	119.71	126.39
2	A	373[B]	BCL	CHA-C1A-NA	-2.95	119.71	126.39
2	C	374	BCL	CHA-C1A-NA	-2.92	119.77	126.39
2	A	371[A]	BCL	CHA-C1A-NA	-2.91	119.81	126.39
2	A	371[B]	BCL	CHA-C1A-NA	-2.91	119.81	126.39
2	A	373[A]	BCL	CAC-C3C-C4C	2.90	119.03	112.58
2	A	373[B]	BCL	CAC-C3C-C4C	2.90	119.03	112.58
2	C	374	BCL	O2D-CGD-CBD	2.89	116.29	111.23
2	C	372	BCL	O2D-CGD-CBD	2.87	116.25	111.23
2	A	375	BCL	C2A-C1A-CHA	2.86	128.84	123.87
2	A	372	BCL	CHA-C1A-NA	-2.86	119.91	126.39
2	C	375	BCL	CHA-C1A-NA	-2.85	119.95	126.39
2	A	374	BCL	CHA-C1A-NA	-2.83	119.97	126.39
2	A	373[A]	BCL	C6-C7-C8	-2.83	106.55	115.97
2	A	375	BCL	C4A-NA-C1A	2.82	107.97	106.68
2	A	373[A]	BCL	C11-C10-C8	-2.82	106.60	115.97
2	C	371[A]	BCL	O2A-CGA-O1A	-2.79	116.64	123.63
2	C	371[B]	BCL	O2A-CGA-O1A	-2.79	116.64	123.63
2	C	372	BCL	C1D-ND-C4D	-2.77	104.37	106.31
2	A	373[B]	BCL	C6-C7-C8	-2.75	106.82	115.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	373[A]	BCL	C11-C10-C8	-2.74	106.87	115.97
2	C	374	BCL	C2A-C1A-CHA	2.74	128.62	123.87
2	C	375	BCL	C2A-C1A-CHA	2.73	128.61	123.87
2	C	378[B]	BCL	C2A-C1A-CHA	2.72	128.59	123.87
2	A	374	BCL	C2A-C1A-CHA	2.72	128.58	123.87
2	A	378[B]	BCL	C2A-C1A-CHA	2.70	128.56	123.87
2	A	374	BCL	O2D-CGD-CBD	2.69	115.94	111.23
2	A	373[A]	BCL	C2A-C1A-CHA	2.67	128.50	123.87
2	A	373[B]	BCL	C2A-C1A-CHA	2.67	128.50	123.87
2	A	372	BCL	C2A-C1A-CHA	2.66	128.49	123.87
2	C	378[B]	BCL	OBB-CAB-C3B	2.65	125.12	120.43
2	A	375	BCL	O2D-CGD-O1D	-2.64	118.71	123.85
2	A	378[B]	BCL	OBB-CAB-C3B	2.63	125.09	120.43
2	C	375	BCL	O2D-CGD-O1D	-2.63	118.72	123.85
2	C	371[A]	BCL	C2A-C1A-CHA	2.63	128.43	123.87
2	C	371[B]	BCL	C2A-C1A-CHA	2.63	128.43	123.87
2	A	374	BCL	O2A-CGA-O1A	-2.60	117.11	123.63
2	C	372	BCL	O2D-CGD-O1D	-2.59	118.81	123.85
2	A	374	BCL	O2D-CGD-O1D	-2.59	118.81	123.85
2	C	372	BCL	C2A-C1A-CHA	2.58	128.35	123.87
2	A	375	BCL	C16-C15-C13	-2.58	107.39	115.97
2	A	373[A]	BCL	O2A-CGA-O1A	-2.54	117.27	123.63
2	A	373[B]	BCL	O2A-CGA-O1A	-2.54	117.27	123.63
2	C	375	BCL	C16-C15-C13	-2.52	107.58	115.97
2	C	373[B]	BCL	C16-C15-C13	-2.42	107.92	115.97
2	C	373[A]	BCL	O2D-CGD-CBD	2.42	115.45	111.23
2	C	373[B]	BCL	O2D-CGD-CBD	2.42	115.45	111.23
2	C	375	BCL	C1C-NC-C4C	2.41	107.78	106.68
2	A	378[B]	BCL	C1C-NC-C4C	2.37	107.76	106.68
2	A	371[A]	BCL	O2D-CGD-O1D	-2.37	119.24	123.85
2	A	371[B]	BCL	O2D-CGD-O1D	-2.37	119.24	123.85
2	A	375	BCL	C15-C13-C12	-2.30	100.42	112.07
2	C	374	BCL	C1-C2-C3	-2.29	122.45	126.20
2	C	373[A]	BCL	CBC-CAC-C3C	-2.28	108.57	113.41
2	C	373[B]	BCL	CBC-CAC-C3C	-2.28	108.57	113.41
2	A	371[A]	BCL	OBB-CAB-CBB	-2.27	114.68	119.77
2	A	371[B]	BCL	OBB-CAB-CBB	-2.27	114.68	119.77
2	A	372	BCL	C15-C13-C12	-2.25	100.66	112.07
2	C	375	BCL	O2A-CGA-O1A	-2.25	118.00	123.63
2	C	373[A]	BCL	C16-C15-C13	2.16	123.13	115.97
2	C	375	BCL	C15-C13-C12	-2.15	101.19	112.07
2	C	371[A]	BCL	O2A-CGA-CBA	2.13	118.34	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	371[B]	BCL	O2A-CGA-CBA	2.13	118.34	111.83
2	C	371[A]	BCL	O2D-CGD-CBD	2.13	114.96	111.23
2	C	371[B]	BCL	O2D-CGD-CBD	2.13	114.96	111.23
2	A	373[A]	BCL	O2D-CGD-CBD	2.12	114.94	111.23
2	A	373[B]	BCL	O2D-CGD-CBD	2.12	114.94	111.23
2	C	375	BCL	C9-C8-C10	-2.09	103.82	111.27
2	A	371[A]	BCL	O2D-CGD-CBD	2.09	114.89	111.23
2	A	371[B]	BCL	O2D-CGD-CBD	2.09	114.89	111.23
2	A	374	BCL	C1C-NC-C4C	2.08	107.63	106.68
2	C	373[A]	BCL	O2D-CGD-O1D	-2.07	119.82	123.85
2	C	373[B]	BCL	O2D-CGD-O1D	-2.07	119.82	123.85
2	A	373[A]	BCL	C16-C15-C13	2.06	122.80	115.97
2	C	375	BCL	C6-C5-C3	2.03	118.42	113.47
2	C	373[A]	BCL	CHD-C1D-C2D	2.02	129.70	125.49
2	C	373[B]	BCL	CHD-C1D-C2D	2.02	129.70	125.49
2	C	372	BCL	C11-C10-C8	-2.01	109.30	115.97
2	A	378[B]	BCL	C4D-C3D-CAD	-2.00	105.93	108.11

There are no chirality outliers.

All (116) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	373[A]	BCL	C2C-C3C-CAC-CBC
2	A	373[A]	BCL	C4C-C3C-CAC-CBC
2	A	373[B]	BCL	C2C-C3C-CAC-CBC
2	A	373[B]	BCL	C4C-C3C-CAC-CBC
2	A	378[B]	BCL	C2C-C3C-CAC-CBC
2	A	378[B]	BCL	C4C-C3C-CAC-CBC
2	C	373[A]	BCL	C2C-C3C-CAC-CBC
2	C	373[A]	BCL	C4C-C3C-CAC-CBC
2	C	373[B]	BCL	C2C-C3C-CAC-CBC
2	C	373[B]	BCL	C4C-C3C-CAC-CBC
2	C	378[B]	BCL	C2C-C3C-CAC-CBC
2	C	378[B]	BCL	C4C-C3C-CAC-CBC
2	A	372	BCL	C3-C5-C6-C7
2	C	372	BCL	C3-C5-C6-C7
2	A	372	BCL	C6-C7-C8-C9
2	A	373[B]	BCL	C11-C12-C13-C14
2	C	372	BCL	C6-C7-C8-C9
2	C	373[B]	BCL	C11-C12-C13-C14
2	A	378[B]	BCL	C2A-CAA-CBA-CGA
2	C	378[B]	BCL	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
2	A	373[A]	BCL	C13-C15-C16-C17
2	A	373[B]	BCL	C13-C15-C16-C17
2	C	373[A]	BCL	C13-C15-C16-C17
2	C	373[B]	BCL	C13-C15-C16-C17
2	C	372	BCL	C15-C16-C17-C18
2	A	372	BCL	C15-C16-C17-C18
2	A	373[B]	BCL	C16-C17-C18-C19
2	C	375	BCL	CBD-CGD-O2D-CED
2	A	372	BCL	C13-C15-C16-C17
2	C	373[B]	BCL	C16-C17-C18-C19
2	C	372	BCL	C13-C15-C16-C17
2	A	372	BCL	C8-C10-C11-C12
2	C	372	BCL	C8-C10-C11-C12
2	A	372	BCL	C11-C12-C13-C15
2	A	373[A]	BCL	C12-C13-C15-C16
2	C	372	BCL	C11-C12-C13-C15
2	A	375	BCL	C11-C10-C8-C9
2	A	373[A]	BCL	C14-C13-C15-C16
2	C	375	BCL	C11-C10-C8-C9
2	C	373[A]	BCL	C14-C13-C15-C16
2	C	372	BCL	C16-C17-C18-C19
2	A	372	BCL	C16-C17-C18-C19
2	C	375	BCL	C13-C15-C16-C17
2	C	375	BCL	CAA-CBA-CGA-O2A
2	A	373[A]	BCL	C16-C17-C18-C19
2	C	373[A]	BCL	C16-C17-C18-C19
2	A	375	BCL	C11-C10-C8-C7
2	A	372	BCL	C6-C7-C8-C10
2	A	373[B]	BCL	C12-C13-C15-C16
2	C	375	BCL	C11-C10-C8-C7
2	C	372	BCL	C6-C7-C8-C10
2	C	373[A]	BCL	C12-C13-C15-C16
2	C	373[B]	BCL	C12-C13-C15-C16
2	A	375	BCL	C13-C15-C16-C17
2	A	375	BCL	CAA-CBA-CGA-O2A
2	C	375	BCL	O1D-CGD-O2D-CED
2	A	373[B]	BCL	C8-C10-C11-C12
2	C	373[B]	BCL	C16-C17-C18-C20
2	A	373[B]	BCL	C14-C13-C15-C16
2	C	373[B]	BCL	C14-C13-C15-C16
2	A	373[B]	BCL	C16-C17-C18-C20
2	C	373[A]	BCL	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
2	A	372	BCL	C16-C17-C18-C20
2	A	373[A]	BCL	C16-C17-C18-C20
2	C	372	BCL	C16-C17-C18-C20
2	C	375	BCL	C8-C10-C11-C12
2	A	373[A]	BCL	C4-C3-C5-C6
2	A	373[B]	BCL	C4-C3-C5-C6
2	A	375	BCL	C8-C10-C11-C12
2	A	373[A]	BCL	C2-C3-C5-C6
2	A	373[B]	BCL	C2-C3-C5-C6
2	C	371[B]	BCL	C16-C17-C18-C20
2	A	371[B]	BCL	C16-C17-C18-C20
2	A	371[B]	BCL	C16-C17-C18-C19
2	C	371[A]	BCL	CBA-CGA-O2A-C1
2	C	371[B]	BCL	CBA-CGA-O2A-C1
2	C	371[B]	BCL	C16-C17-C18-C19
2	C	373[B]	BCL	C8-C10-C11-C12
2	A	371[A]	BCL	C8-C10-C11-C12
2	A	371[B]	BCL	C8-C10-C11-C12
2	C	373[B]	BCL	C11-C12-C13-C15
2	A	375	BCL	CAA-CBA-CGA-O1A
2	A	373[B]	BCL	C11-C12-C13-C15
2	C	371[A]	BCL	C8-C10-C11-C12
2	C	371[B]	BCL	C8-C10-C11-C12
2	C	375	BCL	C4-C3-C5-C6
2	A	371[A]	BCL	CBA-CGA-O2A-C1
2	A	371[B]	BCL	CBA-CGA-O2A-C1
2	C	372	BCL	C11-C12-C13-C14
2	A	375	BCL	C4-C3-C5-C6
2	A	372	BCL	C11-C12-C13-C14
2	A	378[B]	BCL	C3A-C2A-CAA-CBA
2	C	378[B]	BCL	C3A-C2A-CAA-CBA
2	C	375	BCL	CAA-CBA-CGA-O1A
2	A	373[A]	BCL	C10-C11-C12-C13
2	A	378[B]	BCL	C1A-C2A-CAA-CBA
2	C	378[B]	BCL	C1A-C2A-CAA-CBA
2	C	371[A]	BCL	CAA-CBA-CGA-O2A
2	C	371[B]	BCL	CAA-CBA-CGA-O2A
2	A	371[A]	BCL	O1A-CGA-O2A-C1
2	A	371[B]	BCL	O1A-CGA-O2A-C1
2	C	373[A]	BCL	C2-C3-C5-C6
2	C	373[B]	BCL	C2-C3-C5-C6
2	A	371[A]	BCL	CAA-CBA-CGA-O2A

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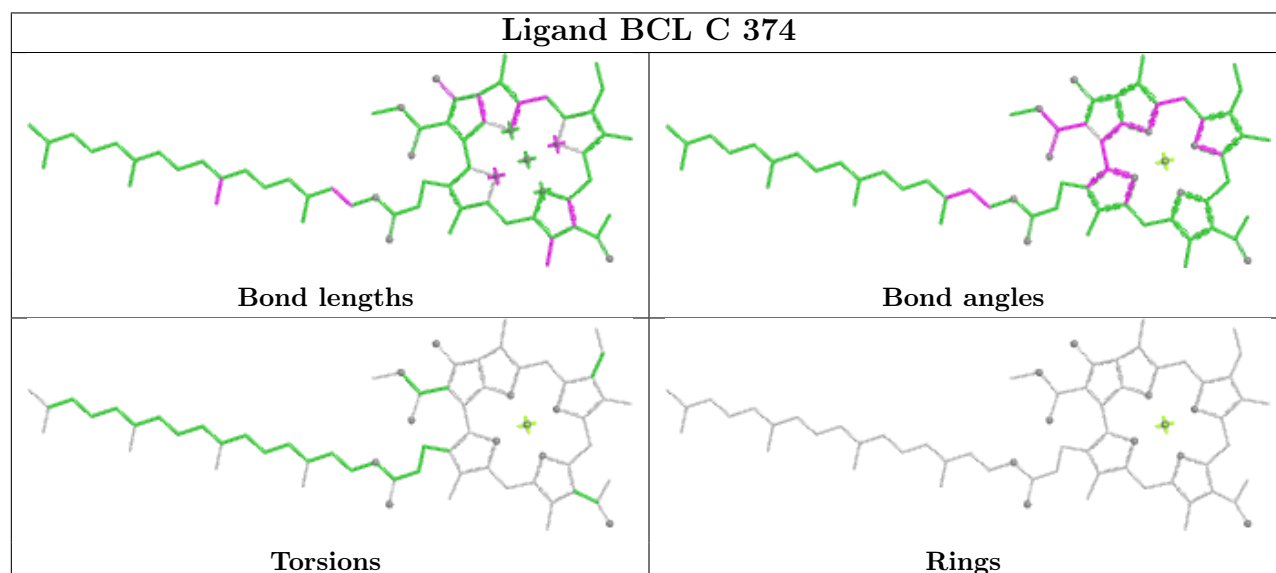
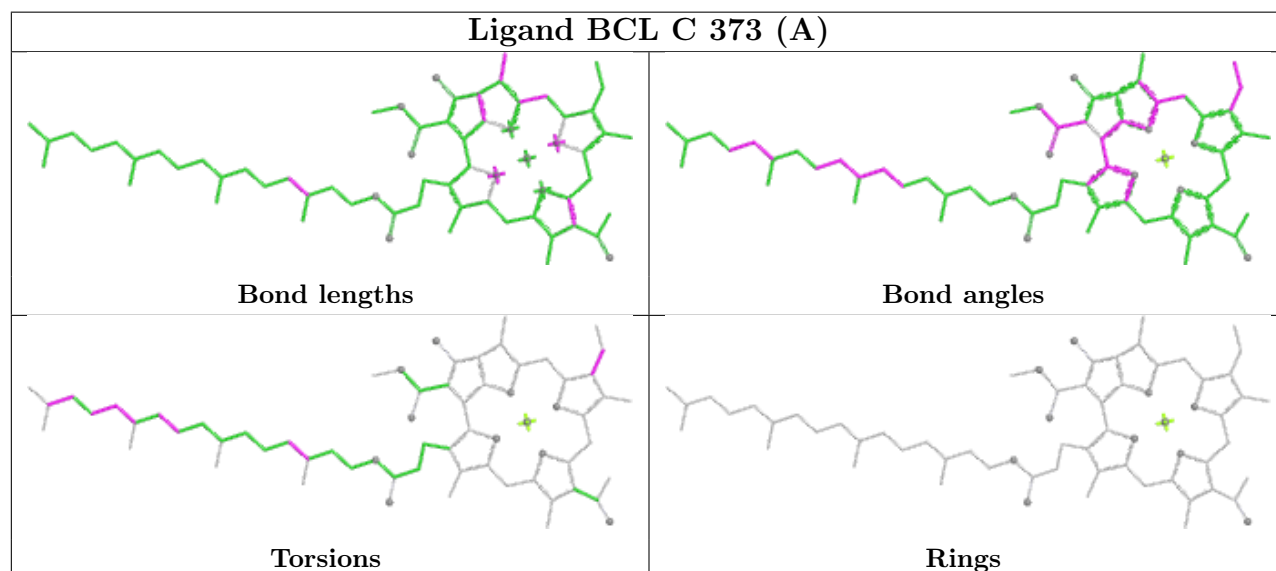
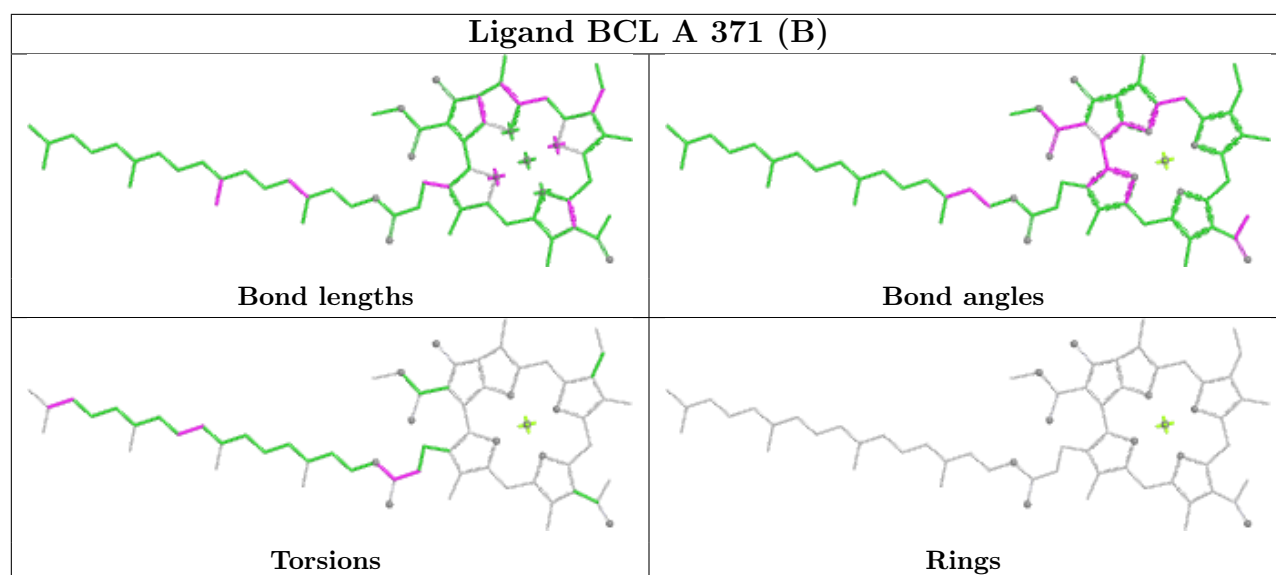
Mol	Chain	Res	Type	Atoms
2	A	371[B]	BCL	CAA-CBA-CGA-O2A
2	C	373[A]	BCL	C10-C11-C12-C13
2	C	375	BCL	C5-C6-C7-C8
2	C	371[A]	BCL	C4-C3-C5-C6
2	C	371[B]	BCL	C4-C3-C5-C6
2	C	375	BCL	C2-C3-C5-C6
2	A	378[B]	BCL	CAD-CBD-CGD-O2D
2	C	378[B]	BCL	CAD-CBD-CGD-O2D
2	C	371[A]	BCL	O1A-CGA-O2A-C1
2	C	371[B]	BCL	O1A-CGA-O2A-C1
2	A	373[A]	BCL	CAA-CBA-CGA-O2A
2	A	373[B]	BCL	CAA-CBA-CGA-O2A

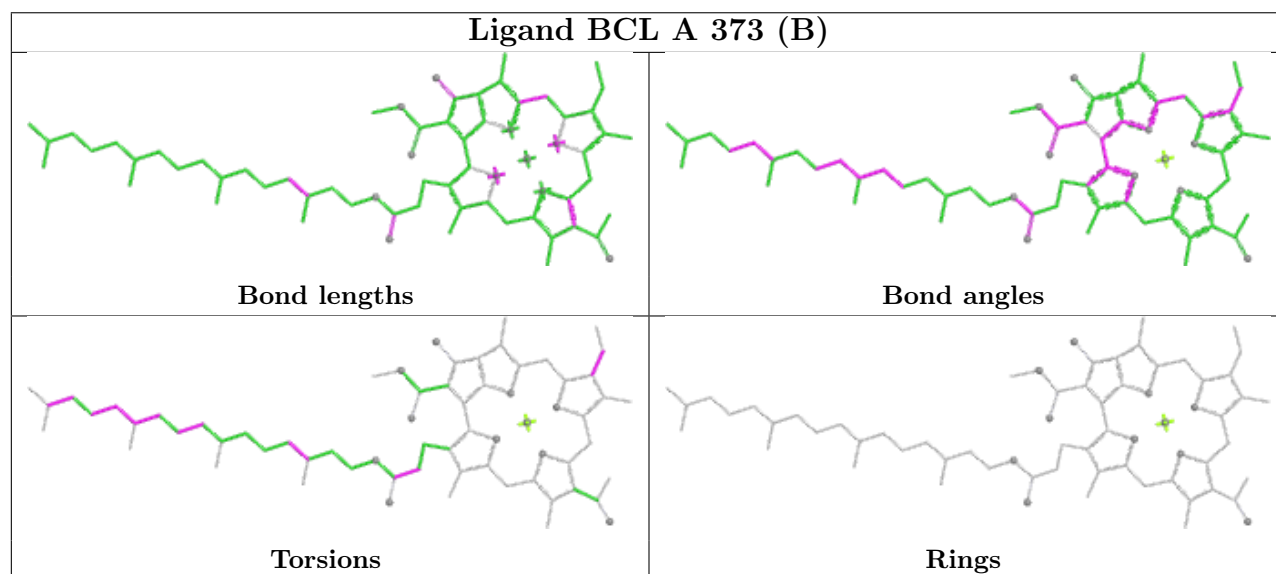
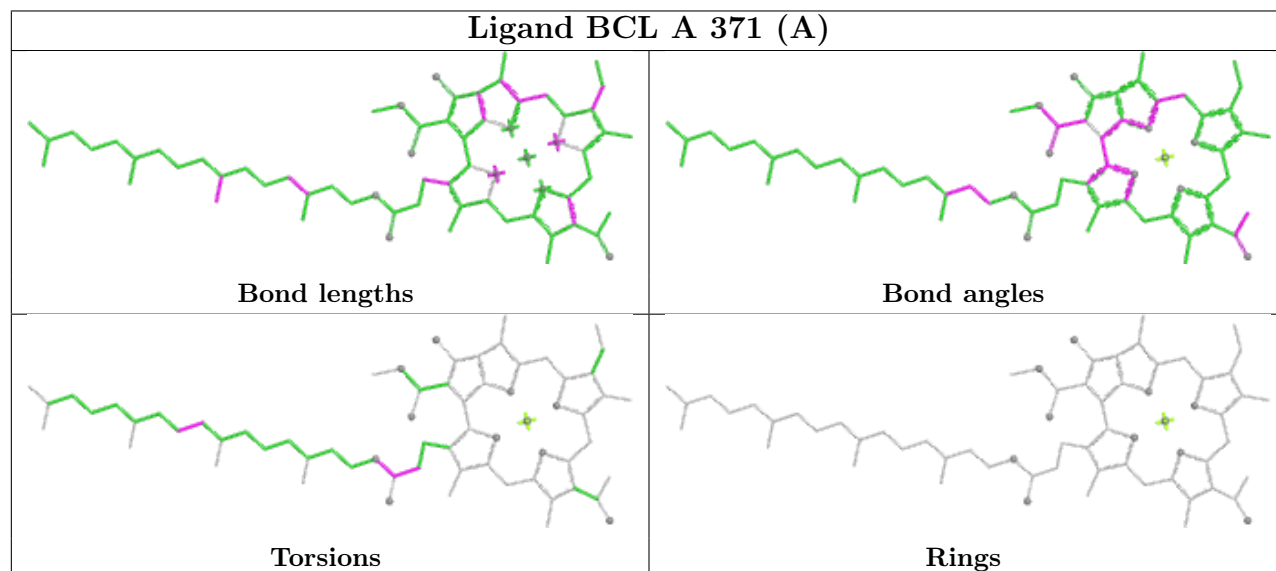
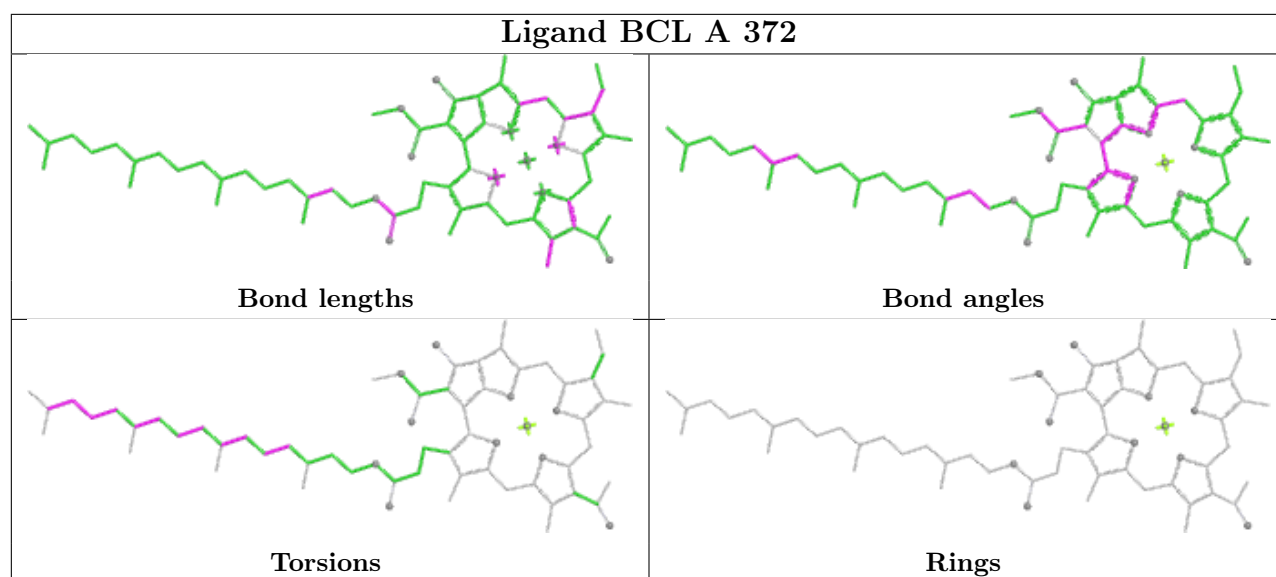
There are no ring outliers.

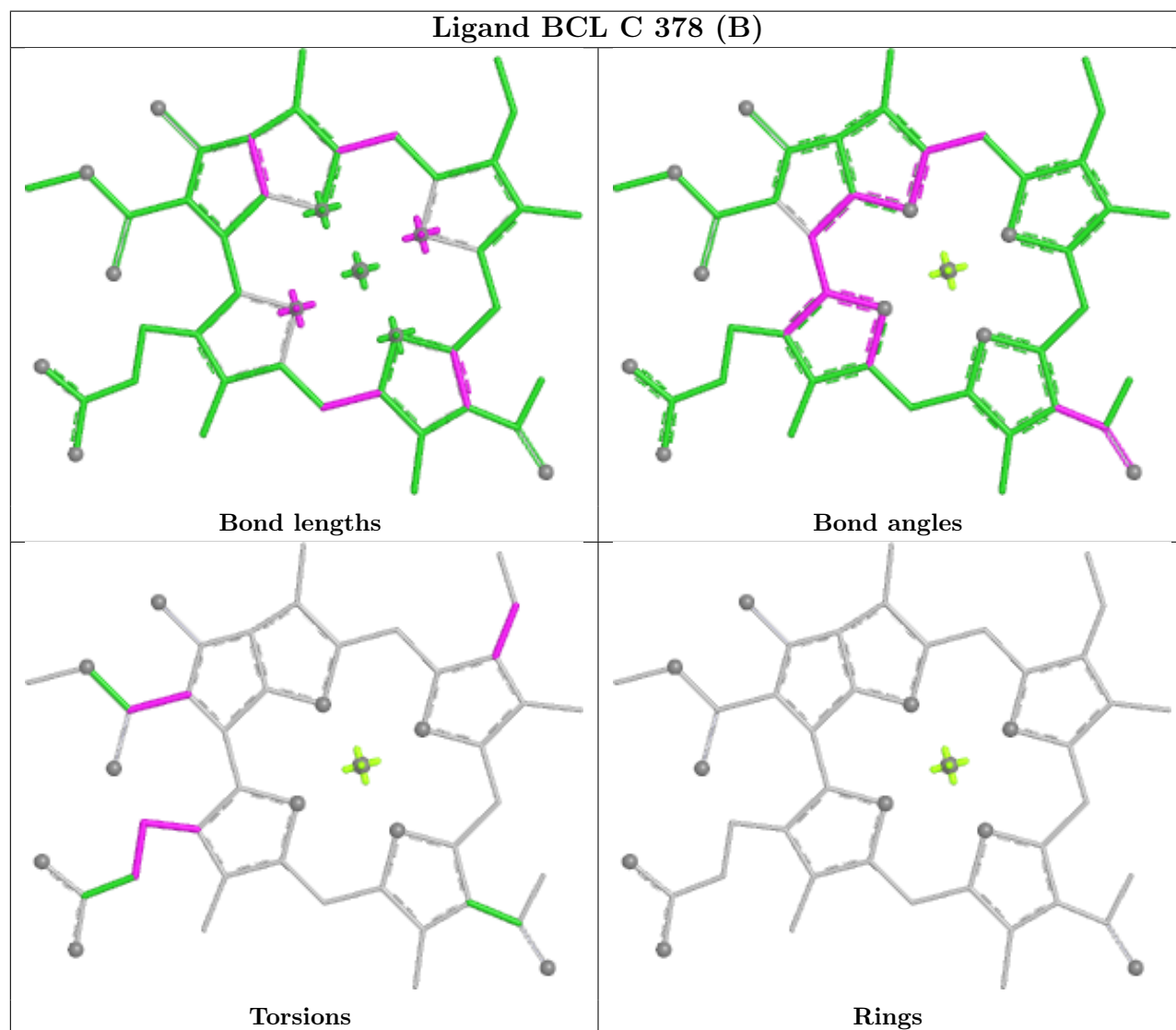
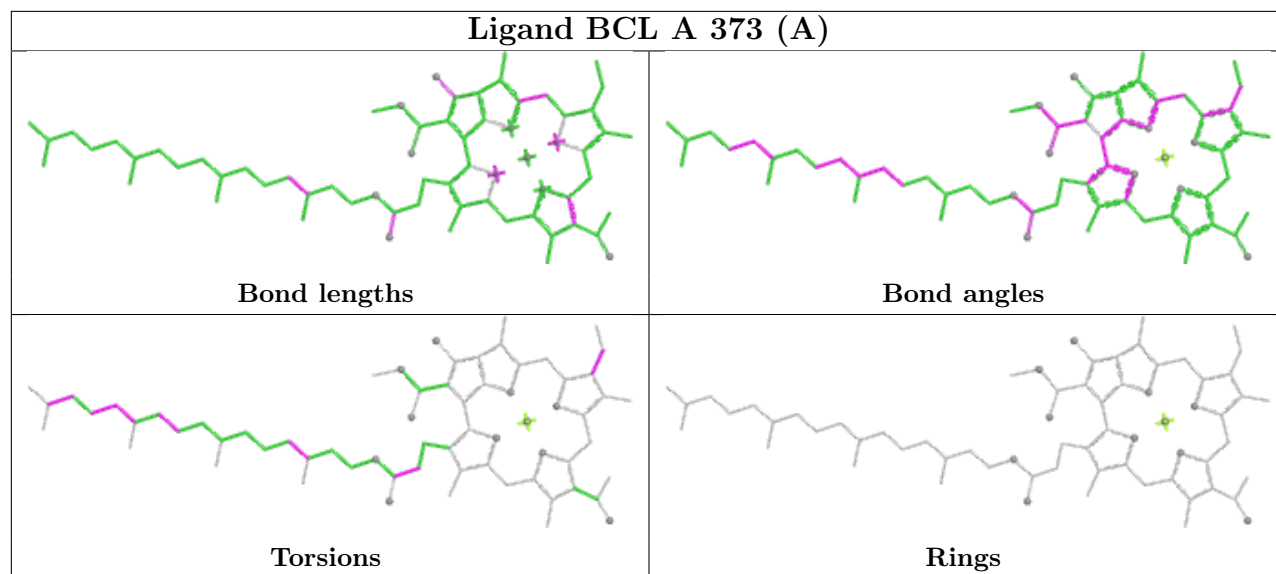
12 monomers are involved in 45 short contacts:

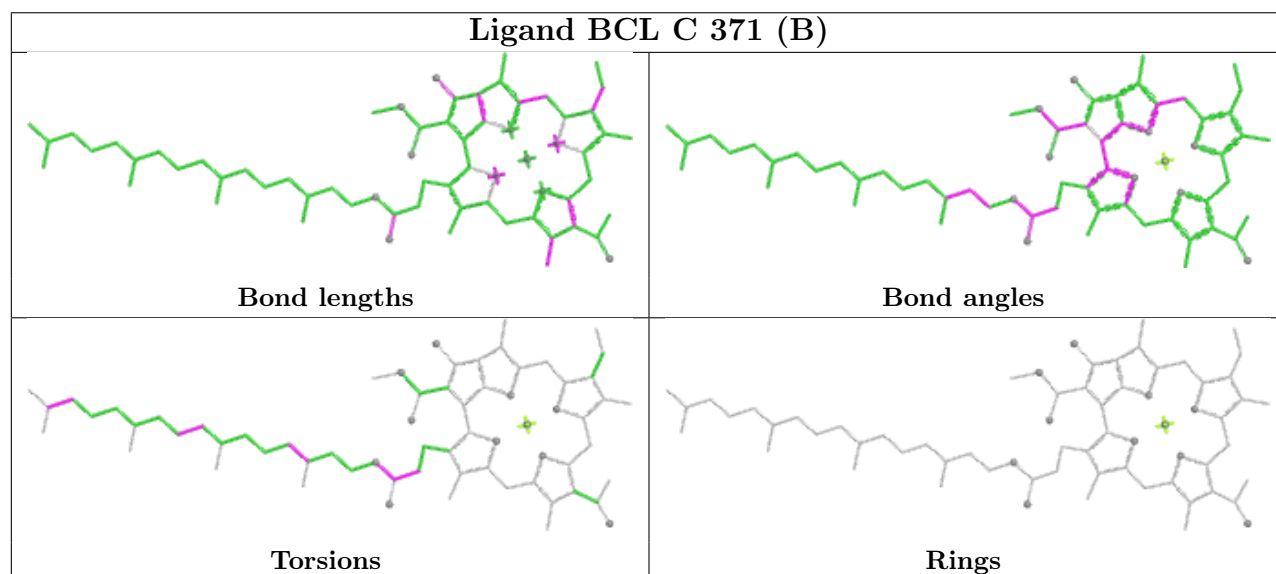
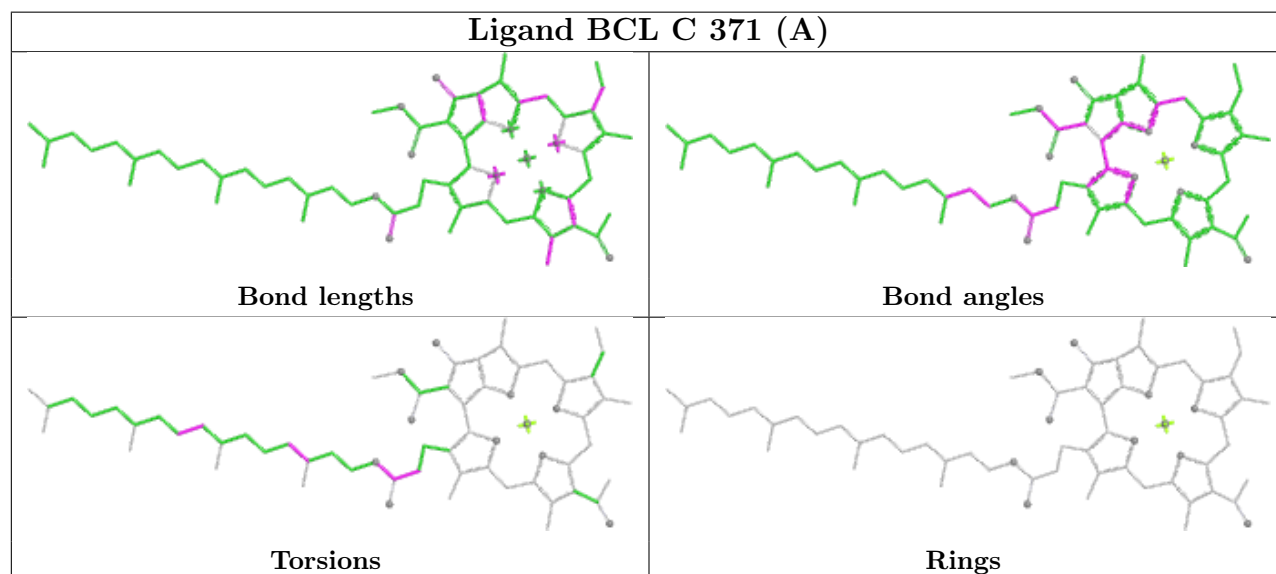
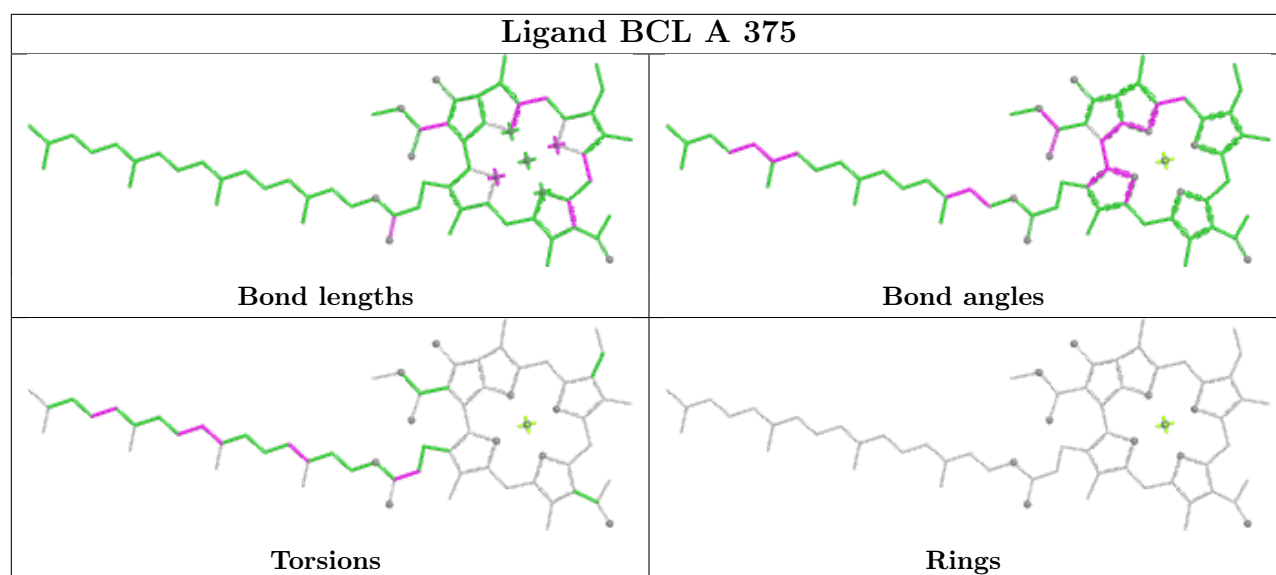
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	373[A]	BCL	3	0
2	C	374	BCL	3	0
2	A	372	BCL	8	0
2	A	373[B]	BCL	1	0
2	A	373[A]	BCL	3	0
2	C	378[B]	BCL	6	0
2	A	375	BCL	5	0
2	C	372	BCL	8	0
2	C	373[B]	BCL	2	0
2	C	375	BCL	5	0
2	A	378[B]	BCL	4	0
2	A	374	BCL	3	0

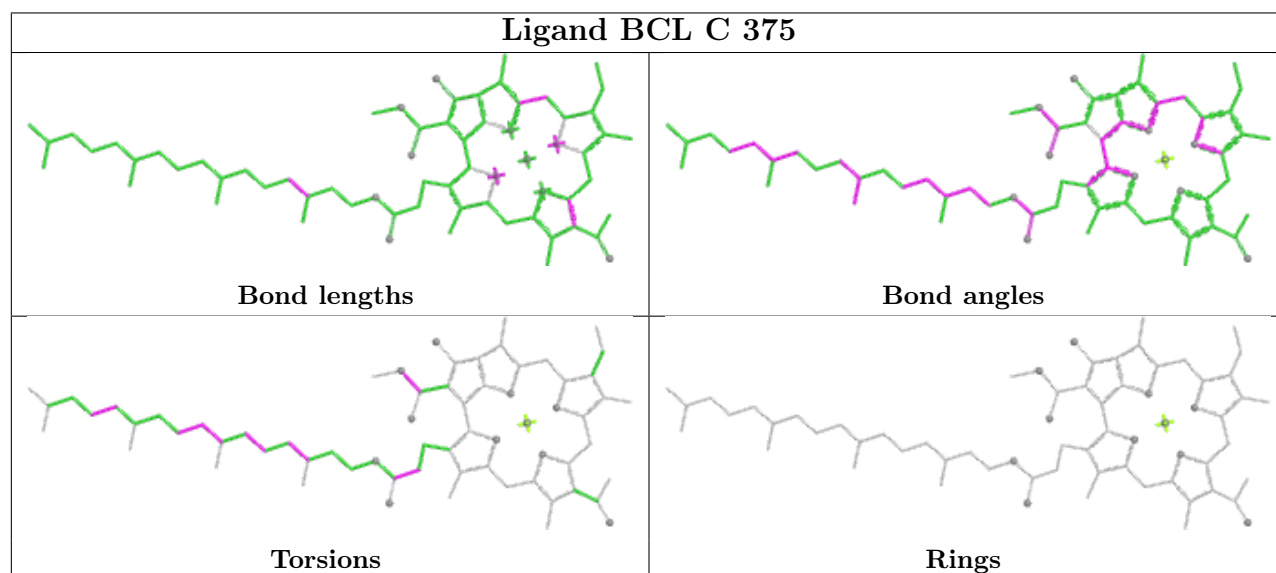
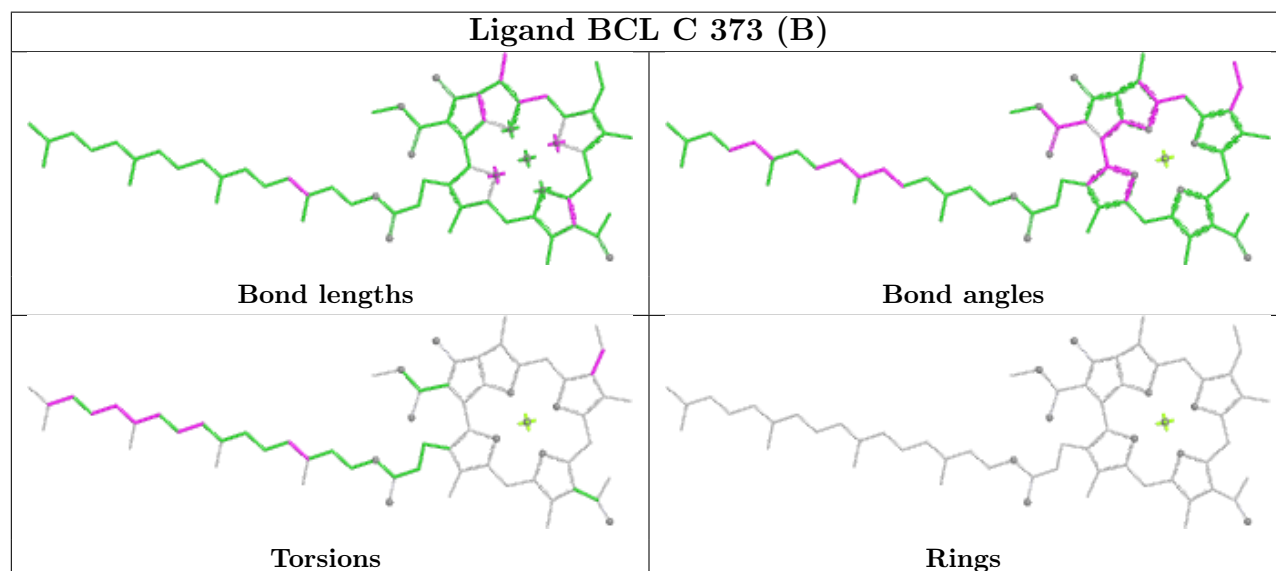
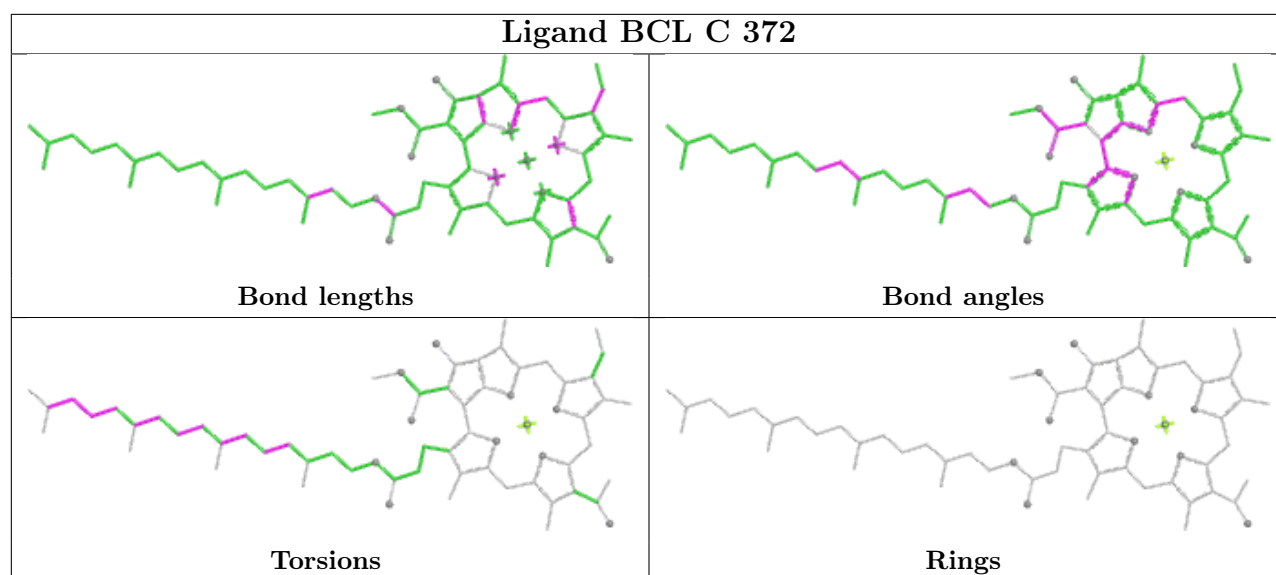
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



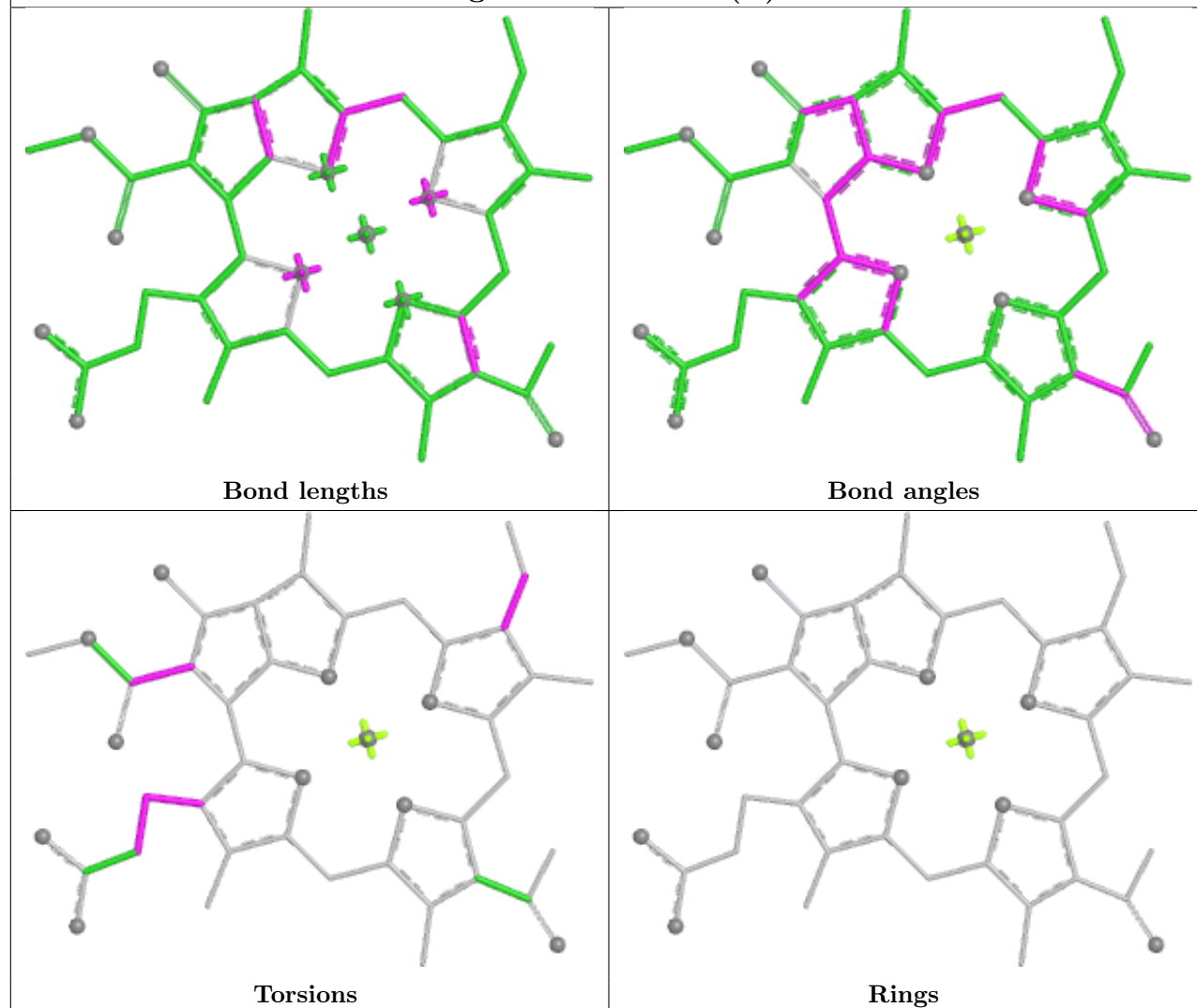




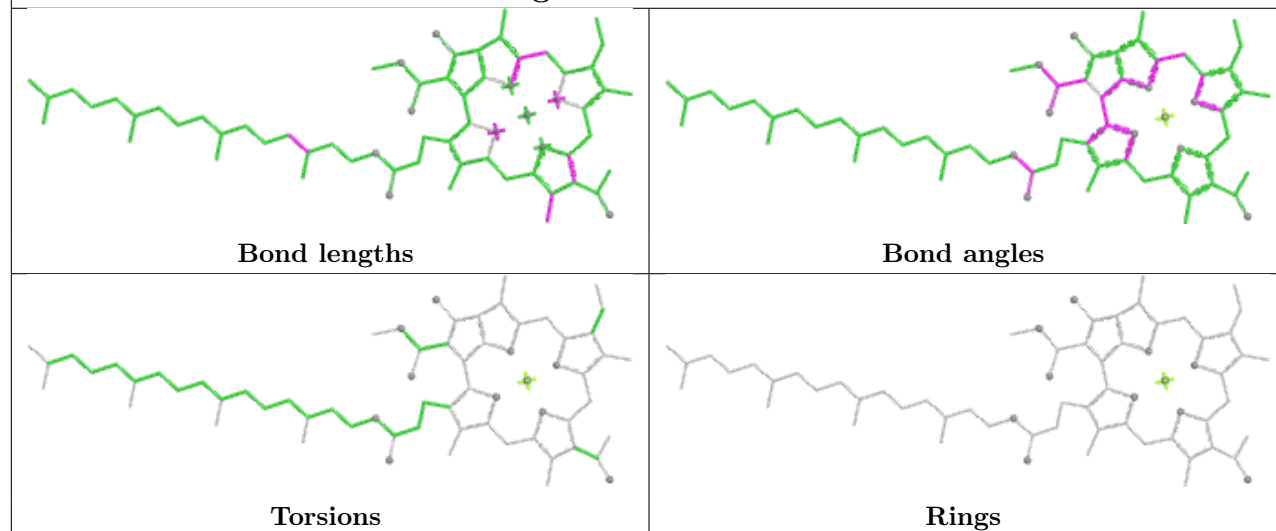




Ligand BCL A 378 (B)



Ligand BCL A 374



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	358/365 (98%)	-0.57	2 (0%) 85 83	16, 27, 50, 67	0
1	C	357/365 (97%)	-0.54	7 (1%) 65 62	16, 27, 50, 65	0
All	All	715/730 (97%)	-0.56	9 (1%) 75 73	16, 27, 50, 67	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	212	GLY	5.7
1	C	214	LYS	4.9
1	C	22	GLY	3.8
1	C	23	SER	2.9
1	C	8	VAL	2.6
1	A	22	GLY	2.4
1	C	24	SER	2.3
1	A	281	GLY	2.3
1	C	211	SER	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 oligosaccharides 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,

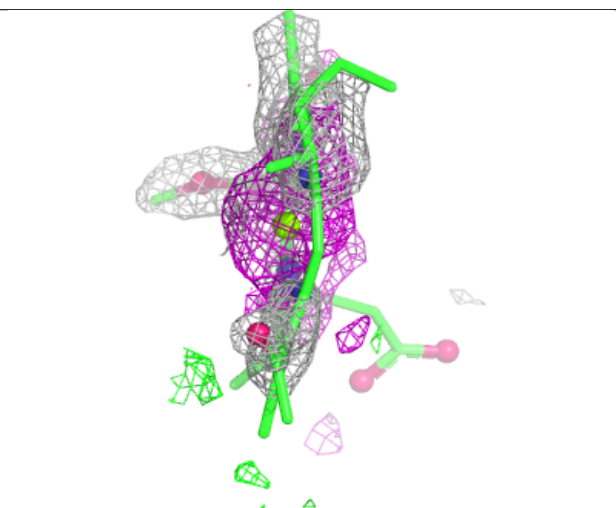
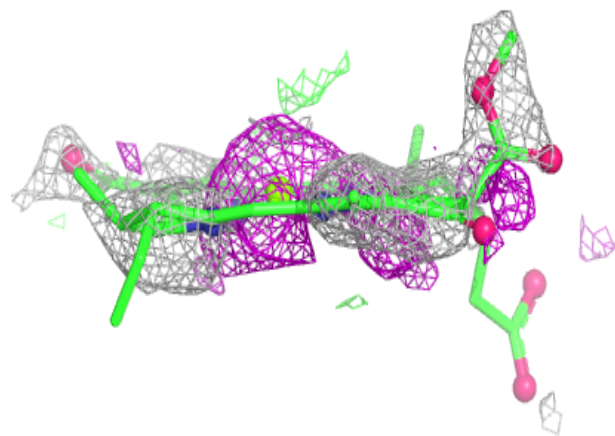
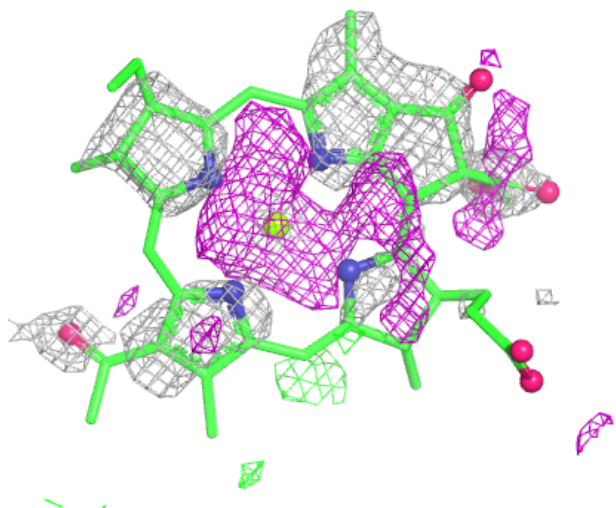
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	BCL	A	378[B]	46/66	0.66	0.18	79,81,88,91	0
2	BCL	C	378[B]	46/66	0.67	0.18	80,82,89,92	0
2	BCL	A	376[C]	58/66	0.95	0.06	12,22,35,36	10
2	BCL	A	376[D]	58/66	0.95	0.06	17,24,35,36	10
2	BCL	A	376[A]	56/66	0.95	0.06	16,22,35,36	8
2	BCL	A	376[B]	56/66	0.95	0.06	17,22,35,36	8
2	BCL	A	372	66/66	0.95	0.07	16,20,47,47	0
2	BCL	A	371[A]	66/66	0.95	0.06	20,23,29,30	5
2	BCL	C	375	66/66	0.95	0.06	20,24,41,44	0
2	BCL	C	376[C]	58/66	0.95	0.06	14,23,36,37	10
2	BCL	C	376[D]	58/66	0.95	0.06	19,25,36,37	10
2	BCL	C	376[A]	56/66	0.95	0.06	17,23,36,37	8
2	BCL	C	376[B]	56/66	0.95	0.06	19,23,36,37	8
2	BCL	C	372	66/66	0.95	0.07	18,21,48,48	0
2	BCL	A	371[B]	66/66	0.95	0.06	20,23,28,29	5
2	BCL	C	371[A]	66/66	0.96	0.05	21,24,30,31	5
2	BCL	C	371[B]	66/66	0.96	0.05	21,24,30,30	5
2	BCL	C	374	66/66	0.96	0.05	16,21,27,30	0
2	BCL	A	375	66/66	0.96	0.05	18,23,39,43	0
2	BCL	A	377[B]	53/66	0.97	0.05	12,17,29,31	4
2	BCL	A	377[C]	56/66	0.97	0.05	12,16,29,31	7
2	BCL	A	377[D]	56/66	0.97	0.05	12,16,29,31	7
2	BCL	A	377[E]	55/66	0.97	0.05	12,18,32,33	6
2	BCL	A	377[F]	55/66	0.97	0.05	12,18,33,35	6
2	BCL	A	373[A]	66/66	0.97	0.05	12,17,21,23	13
2	BCL	A	373[B]	66/66	0.97	0.05	12,17,28,29	13
2	BCL	A	374	66/66	0.97	0.04	15,19,25,28	0
2	BCL	C	377[A]	53/66	0.97	0.05	14,18,30,33	4
2	BCL	C	377[B]	53/66	0.97	0.05	14,18,30,33	4
2	BCL	C	377[C]	56/66	0.97	0.05	14,18,30,33	7
2	BCL	C	377[D]	56/66	0.97	0.05	14,18,30,33	7
2	BCL	C	377[E]	55/66	0.97	0.05	14,20,33,34	6
2	BCL	C	377[F]	55/66	0.97	0.05	14,20,34,36	6
2	BCL	C	373[A]	66/66	0.97	0.05	12,18,22,24	13
2	BCL	C	373[B]	66/66	0.97	0.05	12,18,29,31	13
2	BCL	A	377[A]	53/66	0.97	0.05	12,17,29,31	4

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.

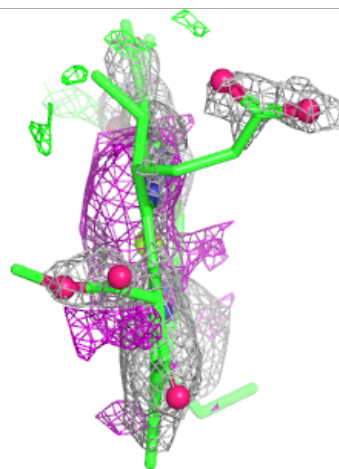
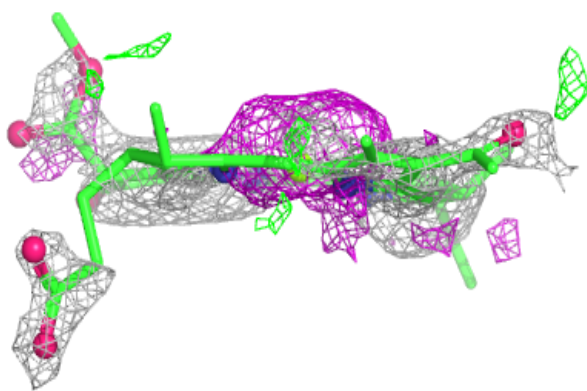
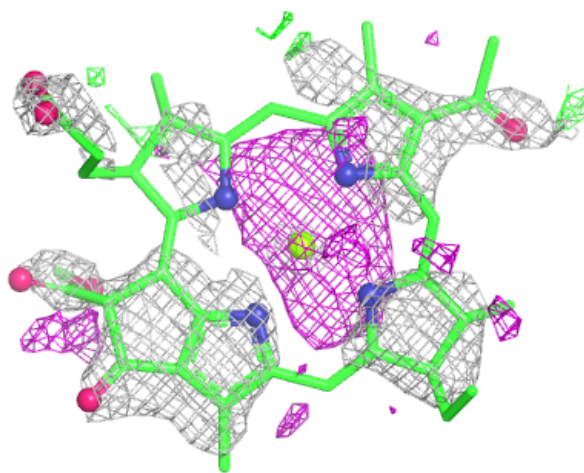
Electron density around BCL A 378 (B):

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



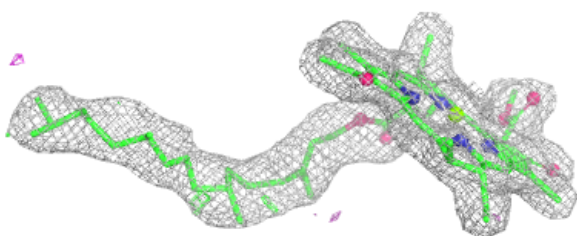
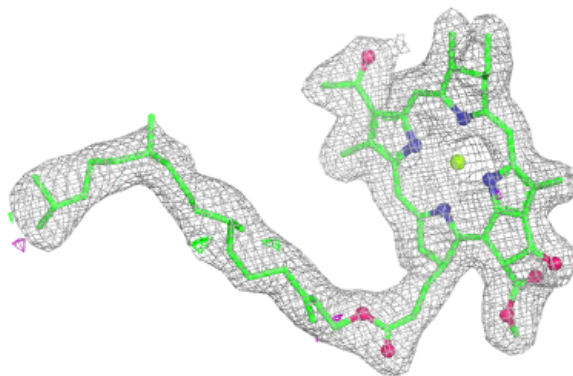
Electron density around BCL C 378 (B):

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

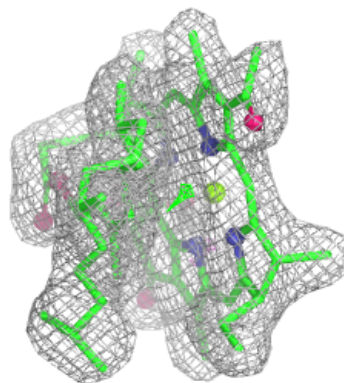
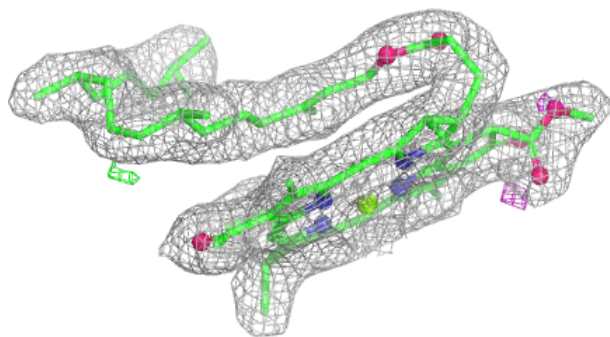
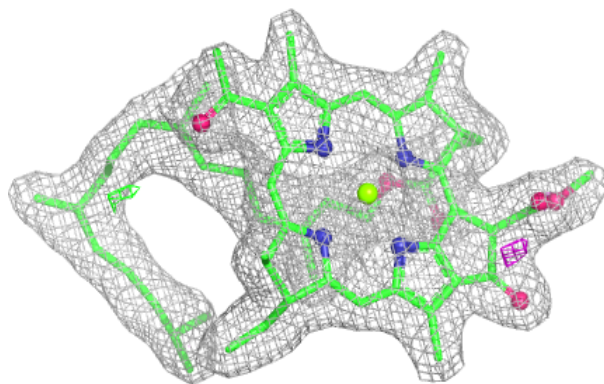


Electron density around BCL A 372:

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

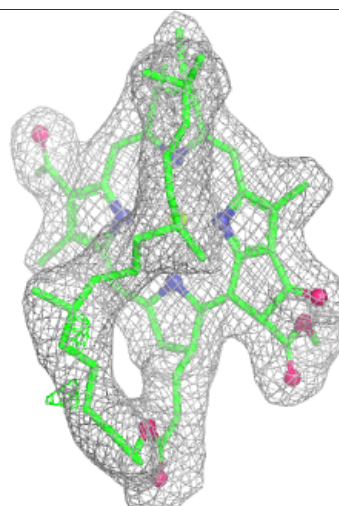
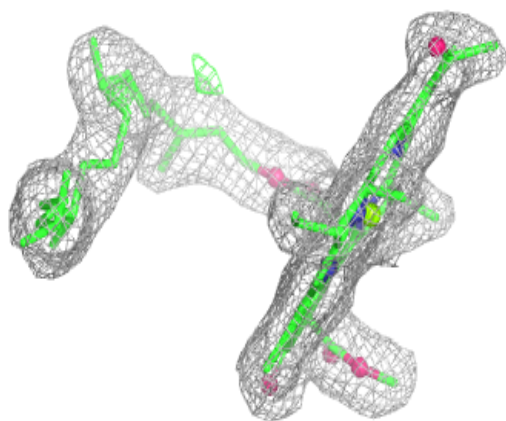
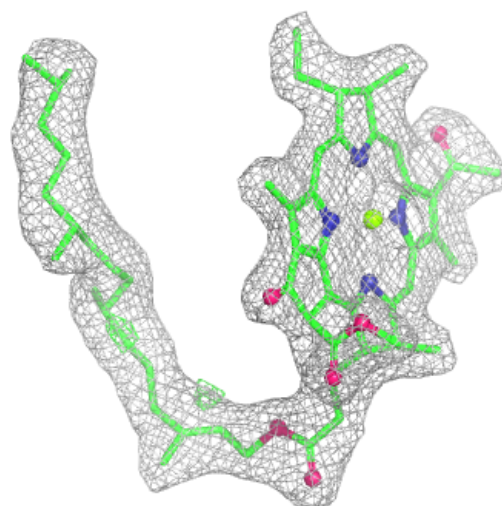
**Electron density around BCL A 371 (A):**

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



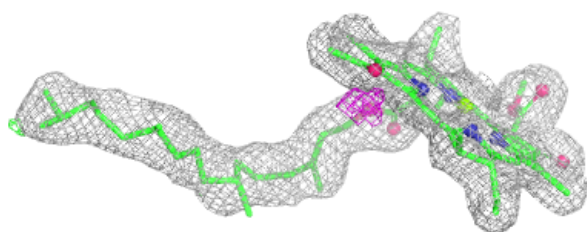
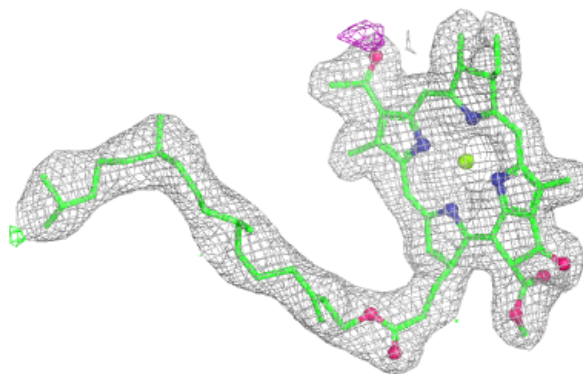
Electron density around BCL C 375:

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

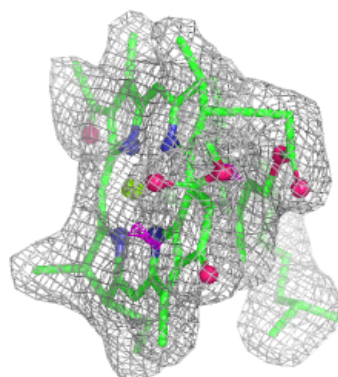
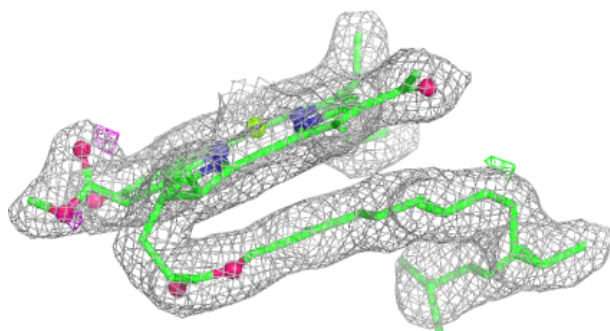
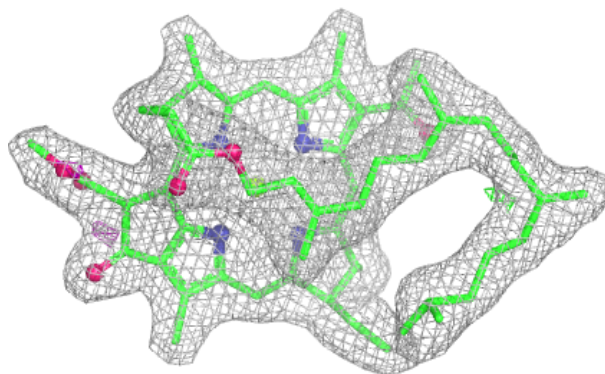


Electron density around BCL C 372:

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

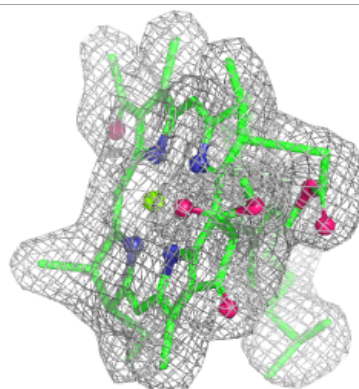
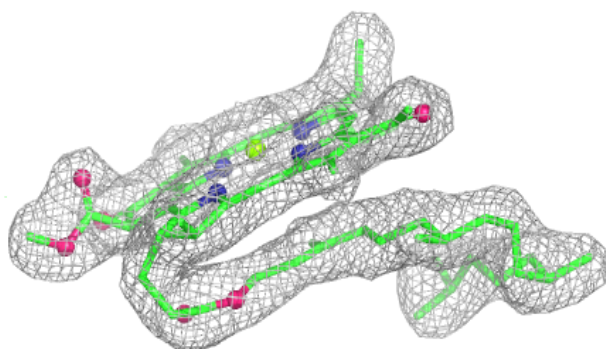
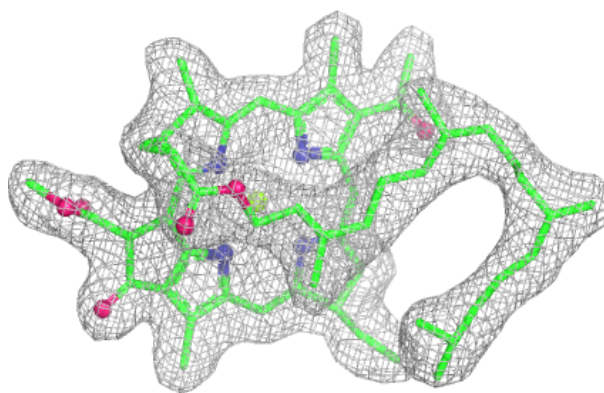
**Electron density around BCL A 371 (B):**

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

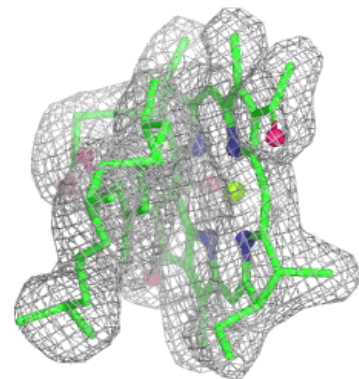
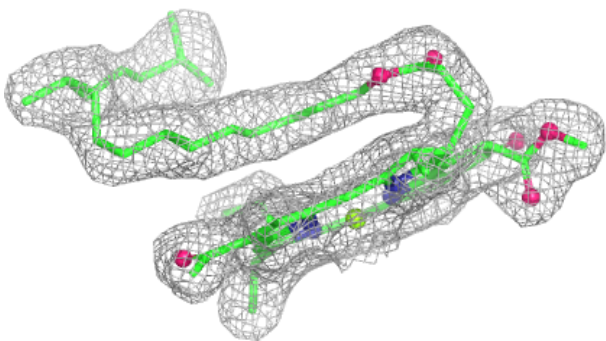
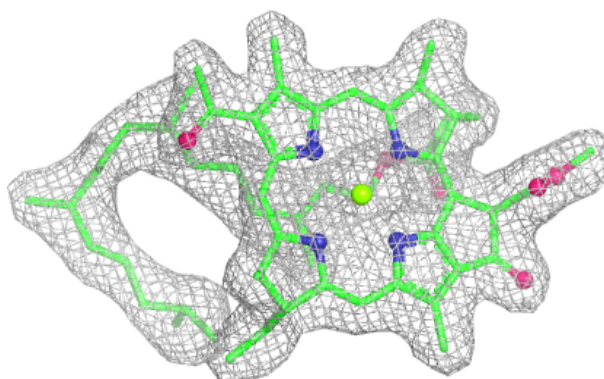


Electron density around BCL C 371 (A):

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

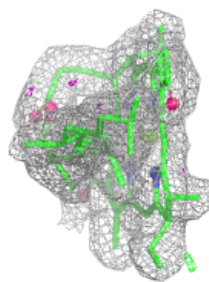
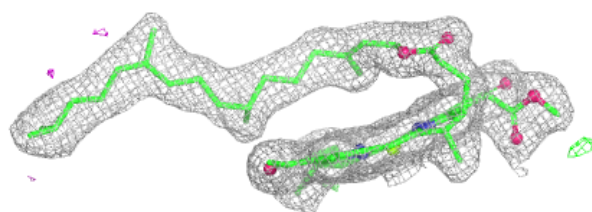
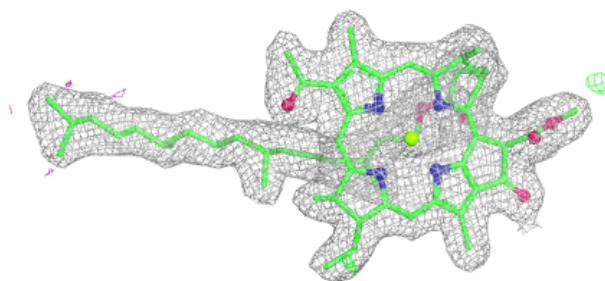
**Electron density around BCL C 371 (B):**

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



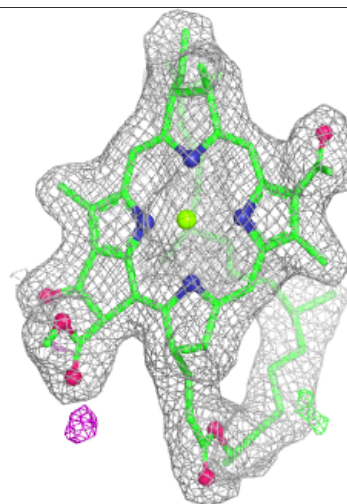
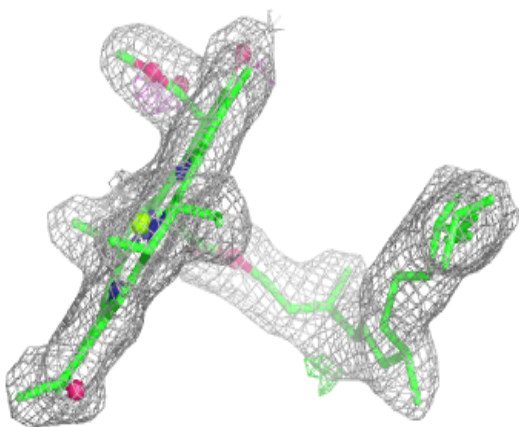
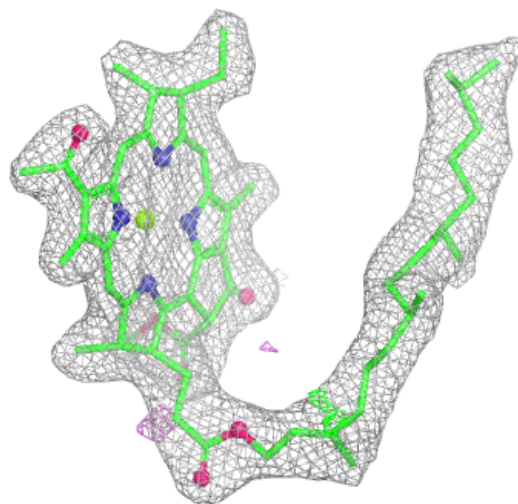
Electron density around BCL C 374:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



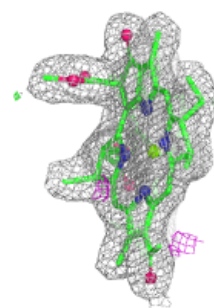
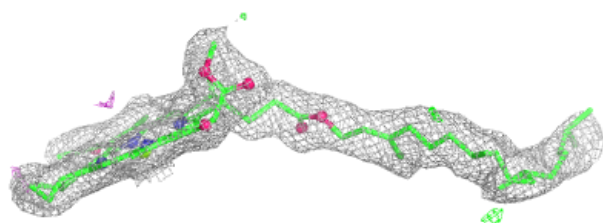
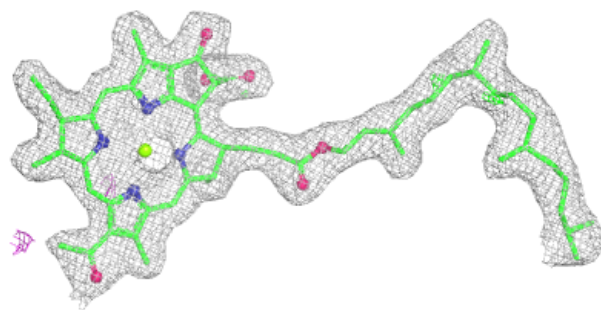
Electron density around BCL A 375:

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

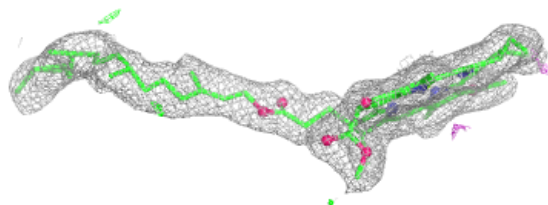
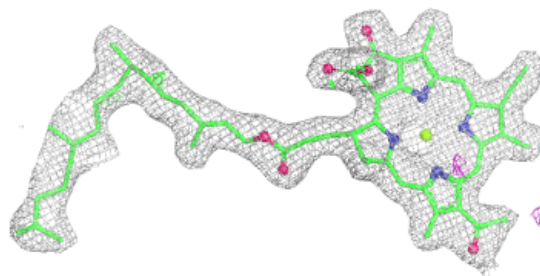


Electron density around BCL A 373 (A):

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

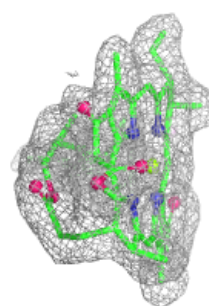
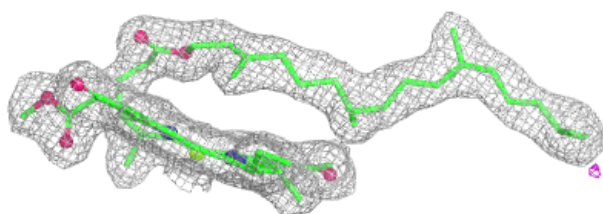
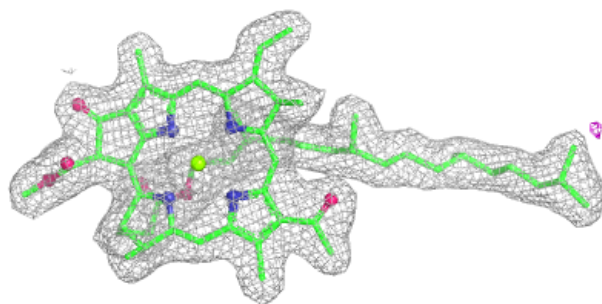
**Electron density around BCL A 373 (B):**

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

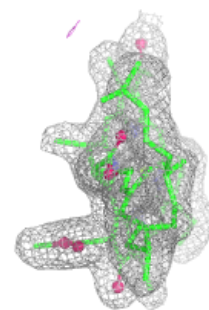
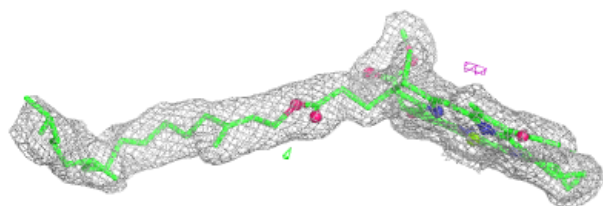
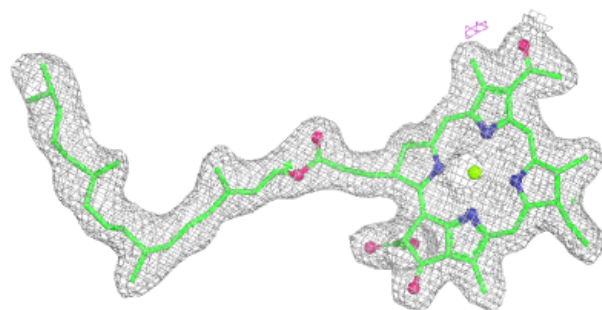


Electron density around BCL A 374:

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

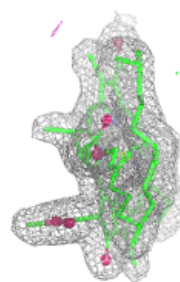
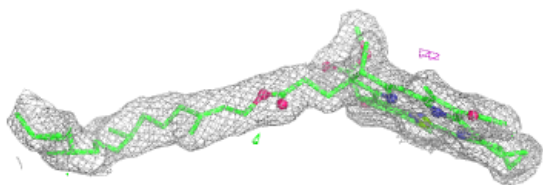
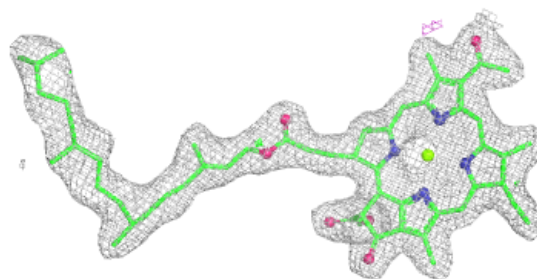
**Electron density around BCL C 373 (A):**

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



Electron density around BCL C 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.