Full wwPDB X-ray Structure Validation Report (i)

Mar 3, 2024 – 09:49 PM EST

PDB ID	:	6MEZ
Title	:	X-ray structure of the Fenna-Matthews-Olsen antenna complex from Prosthecochloris aestuarii
Authors	:	Selvaraj, B.; Lu, X.; Cuneo, M.J.; Myles, D.A.A.
Deposited on	:	2018-09-07
Resolution	:	1.74 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 (i) 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 (i)) were used in the production of this report:

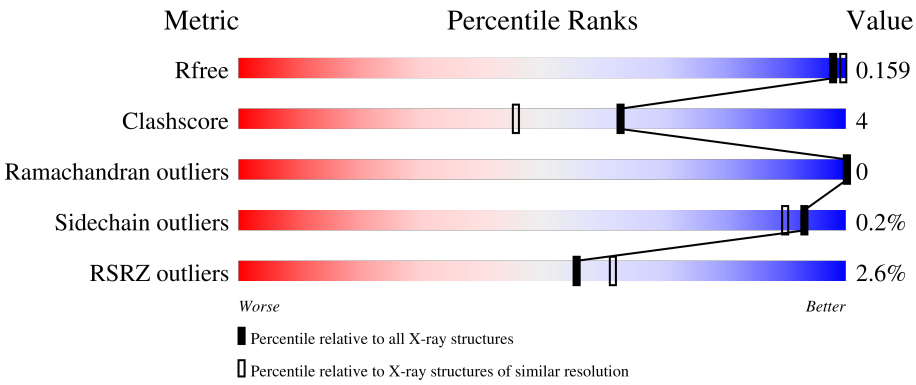
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.74 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	3764 (1.76-1.72)
Clashscore	141614	3923 (1.76-1.72)
Ramachandran outliers	138981	3878 (1.76-1.72)
Sidechain outliers	138945	3878 (1.76-1.72)
RSRZ outliers	127900	3705 (1.76-1.72)

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 <=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	360	3% 92% 7% •
1	B	360	2% 89% 11%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 7812 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.

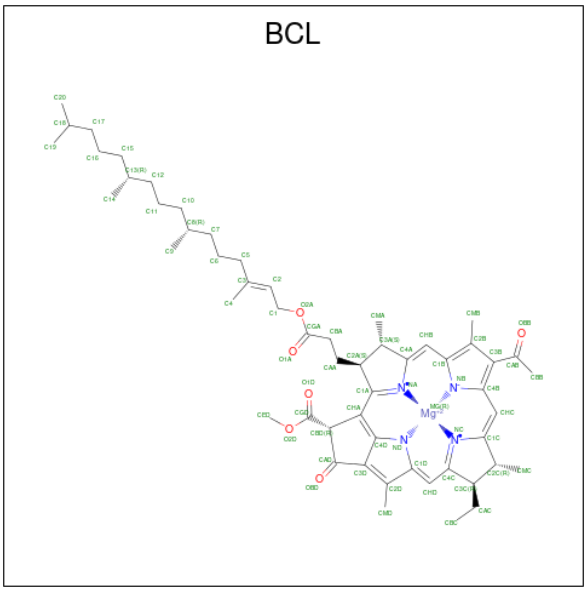
- Molecule 1 is a protein called Bacteriochlorophyll a protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	358	3135	1983	546	598	8	0	60	0
1	B	360	3185	2022	559	596	8	0	60	1

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	117	SER	GLN	conflict	UNP P11741
B	117	SER	GLN	conflict	UNP P11741

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



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

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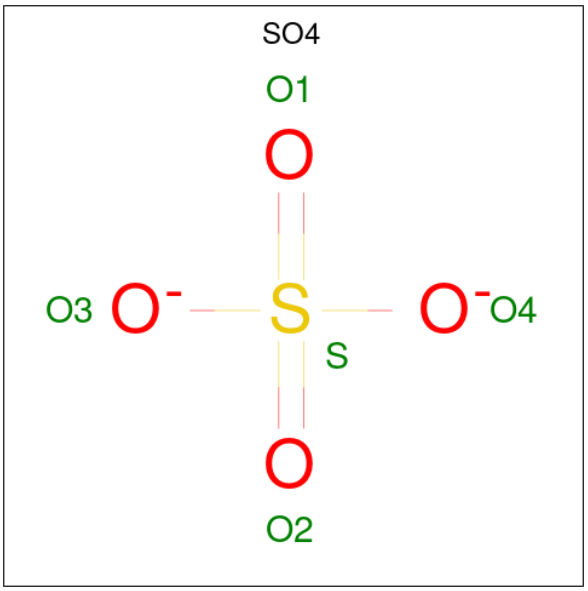
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Mg	N	O		
2	A	1	66	55	1	4	6	0	0
			Total	C	Mg	N	O		
2	A	1	79	68	1	4	6	0	1
			Total	C	Mg	N	O		
2	A	1	66	55	1	4	6	0	0
			Total	C	Mg	N	O		
2	A	1	66	55	1	4	6	0	0
			Total	C	Mg	N	O		
2	A	1	76	62	1	4	9	0	1
			Total	C	Mg	N	O		
2	A	1	70	58	1	4	7	0	1
			Total	C	Mg	N	O		
2	B	1	66	55	1	4	6	0	0
			Total	C	Mg	N	O		
2	B	1	66	55	1	4	6	0	0
			Total	C	Mg	N	O		
2	B	1	79	68	1	4	6	0	1
			Total	C	Mg	N	O		
2	B	1	66	55	1	4	6	0	0
			Total	C	Mg	N	O		
2	B	1	66	55	1	4	6	0	0
			Total	C	Mg	N	O		
2	B	1	84	69	1	5	9	0	1
			Total	C	Mg	N	O		
2	B	1	72	61	1	4	6	0	1

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0

- Molecule 4 is water.

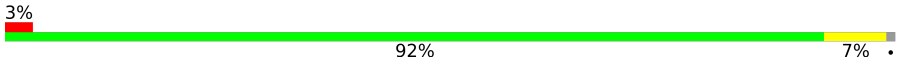
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	228	Total O 228 228	0	0
4	B	246	Total O 246 246	0	0

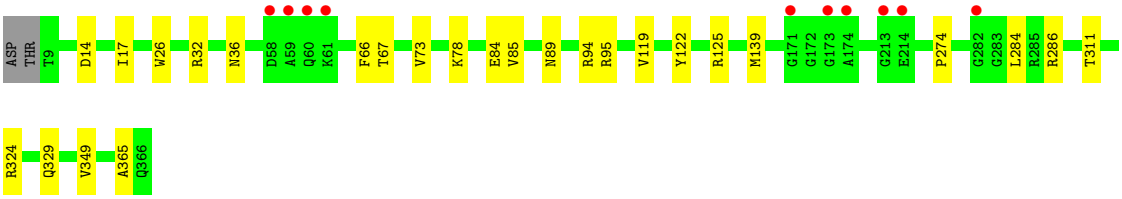
3 Residue-property plots (i)

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

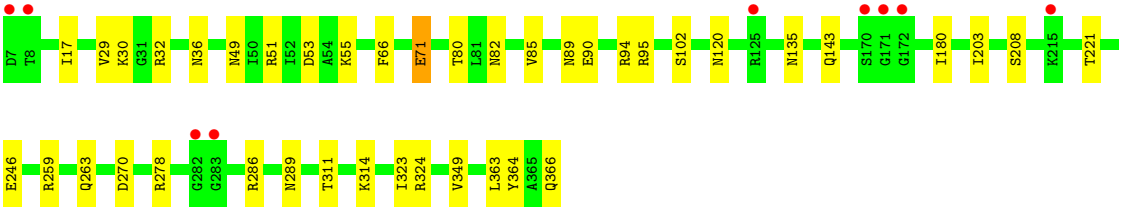
Chain A:





• Molecule 1: Bacteriochlorophyll a protein

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α, β, γ	83.64Å 83.64Å 294.78Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.65 – 1.74 19.65 – 1.74	Depositor EDS
% Data completeness (in resolution range)	93.4 (19.65-1.74) 93.4 (19.65-1.74)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.03 (at 1.74Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.132 , 0.159 0.134 , 0.159	Depositor DCC
R_{free} test set	3693 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	18.2	Xtriage
Anisotropy	0.005	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 51.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	0.025 for -h-k,k,-l	Xtriage
F_o,F_c correlation	0.98	EDS
Total number of atoms	7812	wwPDB-VP
Average B, all atoms (Å^2)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.12% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: BCL, SO4

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	0.60	0/3272	0.62	0/4436
1	B	0.60	0/3332	0.61	0/4511
All	All	0.60	0/6604	0.62	0/8947

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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	3135	0	3019	17	0
1	B	3185	0	3134	29	0
2	A	489	0	368	5	0
2	B	499	0	414	6	0
3	A	15	0	0	1	0
3	B	15	0	0	1	0
4	A	228	0	0	2	0
4	B	246	0	0	8	0
All	All	7812	0	6935	56	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 4.

All (56) 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:B:135:ASN:HD21	1:B:289:ASN:HD21	1.22	0.86
1:A:286[A]:ARG:NH2	4:A:502:HOH:O	2.28	0.67
1:B:89:ASN:ND2	1:B:95:ARG:HE	1.94	0.65
1:A:89:ASN:ND2	1:A:95:ARG:HE	1.94	0.64
1:B:120:ASN:HD22	1:B:143:GLN:HE21	1.46	0.64
1:B:89:ASN:HD21	1:B:95:ARG:HE	1.44	0.63
1:A:89:ASN:HD21	1:A:95:ARG:HE	1.47	0.63
1:B:311[B]:THR:HG21	1:B:349:VAL:HG21	1.81	0.62
1:B:49[B]:ASN:HD21	1:B:259[B]:ARG:HH22	1.48	0.62
1:B:30[A]:LYS:NZ	1:B:270[A]:ASP:OD2	2.30	0.60
1:B:82[B]:ASN:OD1	1:B:102:SER:OG	2.16	0.58
1:B:246[A]:GLU:OE2	4:B:501:HOH:O	2.15	0.58
1:B:180[B]:ILE:HD11	2:B:401:BCL:H162	1.87	0.56
1:A:67[B]:THR:HG23	1:A:84[B]:GLU:HG2	1.87	0.56
1:B:30[B]:LYS:NZ	4:B:507:HOH:O	2.34	0.56
3:B:410:SO4:O2	4:B:502:HOH:O	2.17	0.56
2:B:402:BCL:HMB1	2:B:402:BCL:HBB3	1.88	0.55
2:B:401:BCL:HMB1	2:B:401:BCL:HBB2	1.88	0.54
1:B:55:LYS:NZ	4:B:508:HOH:O	2.34	0.53
1:A:36[A]:ASN:ND2	4:A:504:HOH:O	2.41	0.53
1:A:73[B]:VAL:HG12	1:A:78:LYS:HG2	1.89	0.52
1:A:311[B]:THR:HG21	1:A:349:VAL:HG21	1.91	0.52
1:B:286[A]:ARG:HB3	1:B:363:LEU:HD23	1.91	0.52
1:B:90[A]:GLU:OE1	1:B:94:ARG:HD2	2.10	0.51
2:A:401:BCL:HMB1	2:A:401:BCL:HBB2	1.93	0.51
1:B:36[A]:ASN:ND2	4:B:512:HOH:O	2.43	0.51
1:B:246[A]:GLU:H	1:B:246[A]:GLU:CD	2.16	0.49
1:B:32[A]:ARG:NE	4:B:513:HOH:O	2.45	0.49
1:B:120:ASN:ND2	1:B:143:GLN:HE21	2.07	0.49
1:A:284:LEU:HD23	1:A:365:ALA:HB2	1.96	0.47
1:B:208[B]:SER:OG	1:B:221[B]:THR:HG22	2.15	0.47
2:B:402:BCL:HBB2	2:B:407[E]:BCL:H193	1.97	0.46
2:A:402:BCL:HMB1	2:A:402:BCL:HBB3	1.97	0.46
3:A:410:SO4:O3	1:B:314:LYS:NZ	2.48	0.46
1:A:66:PHE:HB3	1:A:85[A]:VAL:HG13	1.98	0.45
1:B:263:GLN:NE2	4:B:517:HOH:O	2.48	0.45
1:B:17[B]:ILE:HD12	1:B:29[B]:VAL:HG12	1.98	0.45
1:B:180[B]:ILE:HD13	1:B:203:ILE:HD12	1.98	0.45
1:A:324[A]:ARG:HH11	1:A:324[A]:ARG:HB3	1.81	0.45
1:B:66:PHE:HB3	1:B:85[A]:VAL:HG13	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:71[B]:GLU:HG2	1:B:80:THR:HG22	1.98	0.44
1:A:17:ILE:HD11	2:A:404:BCL:HAA1	2.00	0.44
1:A:26:TRP:HA	1:A:274:PRO:HA	2.01	0.42
1:B:323[B]:ILE:HD13	1:B:364:TYR:HB3	2.01	0.42
1:A:139[B]:MET:HB2	1:A:139[B]:MET:HE2	1.97	0.41
1:B:51[C]:ARG:NH2	1:B:53:ASP:OD2	2.54	0.41
2:B:404:BCL:CBB	2:B:404:BCL:HMB1	2.50	0.41
1:A:329[B]:GLN:HE21	1:A:329[B]:GLN:HA	1.84	0.41
1:A:14[B]:ASP:OD1	1:A:32[B]:ARG:HG2	2.21	0.41
1:A:122:TYR:CD2	1:A:125:ARG:HD2	2.55	0.41
2:A:403[B]:BCL:H141	2:A:403[B]:BCL:H162	1.89	0.41
1:B:324[B]:ARG:NH1	1:B:366:GLN:O	2.54	0.41
1:A:94[B]:ARG:HG3	1:A:119:VAL:HG22	2.03	0.41
1:B:278:ARG:NE	4:B:520:HOH:O	2.50	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	411/360 (114%)	405 (98%)	6 (2%)	0	100	100
1	B	416/360 (116%)	412 (99%)	4 (1%)	0	100	100
All	All	827/720 (115%)	817 (99%)	10 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	338/299 (113%)	338 (100%)	0	100	100
1	B	348/299 (116%)	346 (99%)	2 (1%)	86	79
All	All	686/598 (115%)	684 (100%)	2 (0%)	93	89

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

Mol	Chain	Res	Type
1	B	71[A]	GLU
1	B	71[B]	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	79	ASN
1	A	89	ASN
1	A	166	GLN
1	A	206	ASN
1	B	79	ASN
1	B	89	ASN
1	B	120	ASN
1	B	135	ASN
1	B	209	ASN
1	B	263	GLN
1	B	359	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

28 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	404	-	64,74,74	1.21	6 (9%)	78,115,115	1.55	10 (12%)
2	BCL	A	401	-	64,74,74	1.32	6 (9%)	78,115,115	1.60	11 (14%)
3	SO4	B	409	-	4,4,4	0.14	0	6,6,6	0.06	0
3	SO4	B	410	-	4,4,4	0.14	0	6,6,6	0.06	0
2	BCL	B	404	-	64,74,74	1.28	6 (9%)	78,115,115	1.50	10 (12%)
2	BCL	A	405	1	64,74,74	1.36	7 (10%)	78,115,115	1.43	10 (12%)
3	SO4	B	408	-	4,4,4	0.13	0	6,6,6	0.08	0
3	SO4	A	409	-	4,4,4	0.15	0	6,6,6	0.07	0
2	BCL	B	403[A]	-	64,74,74	1.34	6 (9%)	78,115,115	1.47	10 (12%)
3	SO4	A	410	-	4,4,4	0.15	0	6,6,6	0.07	0
2	BCL	A	407[A]	-	64,74,74	1.41	6 (9%)	78,115,115	1.63	12 (15%)
2	BCL	B	407[F]	-	64,74,74	1.49	9 (14%)	78,115,115	1.59	16 (20%)
2	BCL	A	406[D]	-	64,74,74	1.34	7 (10%)	78,115,115	1.59	11 (14%)
2	BCL	B	401	-	64,74,74	1.33	6 (9%)	78,115,115	1.58	12 (15%)
2	BCL	A	403[A]	-	64,74,74	1.27	5 (7%)	78,115,115	1.45	8 (10%)
2	BCL	B	405	1	64,74,74	1.40	7 (10%)	78,115,115	1.50	10 (12%)
2	BCL	B	403[B]	-	64,74,74	1.34	6 (9%)	78,115,115	1.47	10 (12%)
2	BCL	A	402	4	64,74,74	1.43	6 (9%)	78,115,115	1.59	9 (11%)
2	BCL	A	407[B]	-	64,74,74	1.40	6 (9%)	78,115,115	1.65	13 (16%)
2	BCL	B	407[E]	-	64,74,74	1.48	9 (14%)	78,115,115	1.59	16 (20%)
3	SO4	A	408	-	4,4,4	0.14	0	6,6,6	0.05	0
2	BCL	A	406[C]	-	64,74,74	1.34	7 (10%)	78,115,115	1.60	11 (14%)
2	BCL	A	403[B]	-	64,74,74	1.27	5 (7%)	78,115,115	1.50	10 (12%)
2	BCL	B	402	4	64,74,74	1.37	5 (7%)	78,115,115	1.55	11 (14%)

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	405	1	-	5/37/137/137	-
2	BCL	A	404	-	-	0/37/137/137	-
2	BCL	B	403[A]	-	-	7/37/137/137	-
2	BCL	B	405	1	-	4/37/137/137	-
2	BCL	A	401	-	-	3/37/137/137	-
2	BCL	A	407[A]	-	-	2/37/137/137	-
2	BCL	B	404	-	-	2/37/137/137	-
2	BCL	B	403[B]	-	-	5/37/137/137	-
2	BCL	A	402	4	-	2/37/137/137	-
2	BCL	A	406[D]	-	-	5/37/137/137	-
2	BCL	A	407[B]	-	-	2/37/137/137	-
2	BCL	B	407[E]	-	-	5/37/137/137	-
2	BCL	B	401	-	-	2/37/137/137	-
2	BCL	A	403[A]	-	-	7/37/137/137	-
2	BCL	B	407[F]	-	-	3/37/137/137	-
2	BCL	A	406[C]	-	-	7/37/137/137	-
2	BCL	A	403[B]	-	-	5/37/137/137	-
2	BCL	B	402	4	-	2/37/137/137	-

All (115) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	405	BCL	C1B-NB	5.87	1.40	1.35
2	B	402	BCL	MG-NA	5.68	2.19	2.06
2	A	407[A]	BCL	C1B-NB	5.62	1.40	1.35
2	A	407[B]	BCL	C1B-NB	5.62	1.40	1.35
2	B	407[E]	BCL	C1B-NB	5.62	1.40	1.35
2	B	407[F]	BCL	C1B-NB	5.62	1.40	1.35
2	A	402	BCL	MG-NA	5.42	2.19	2.06
2	A	406[C]	BCL	C1B-NB	5.28	1.39	1.35
2	A	406[D]	BCL	C1B-NB	5.28	1.39	1.35
2	B	401	BCL	MG-NA	5.27	2.18	2.06
2	B	407[E]	BCL	MG-NA	5.21	2.18	2.06
2	B	407[F]	BCL	MG-NA	5.21	2.18	2.06
2	A	405	BCL	MG-NA	5.17	2.18	2.06
2	A	401	BCL	C1B-NB	5.09	1.39	1.35
2	A	405	BCL	C1B-NB	5.09	1.39	1.35
2	B	403[A]	BCL	C1B-NB	5.00	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	403[B]	BCL	C1B-NB	5.00	1.39	1.35
2	B	402	BCL	C1B-NB	4.99	1.39	1.35
2	A	406[C]	BCL	MG-NA	4.88	2.17	2.06
2	A	406[D]	BCL	MG-NA	4.88	2.17	2.06
2	A	403[A]	BCL	MG-NA	4.83	2.17	2.06
2	A	403[B]	BCL	MG-NA	4.83	2.17	2.06
2	A	403[A]	BCL	C1B-NB	4.82	1.39	1.35
2	A	403[B]	BCL	C1B-NB	4.82	1.39	1.35
2	A	407[A]	BCL	MG-NA	4.81	2.17	2.06
2	A	407[B]	BCL	MG-NA	4.81	2.17	2.06
2	A	401	BCL	MG-NA	4.78	2.17	2.06
2	B	403[A]	BCL	MG-NA	4.76	2.17	2.06
2	B	403[B]	BCL	MG-NA	4.76	2.17	2.06
2	B	401	BCL	C1B-NB	4.73	1.39	1.35
2	A	404	BCL	MG-NA	4.70	2.17	2.06
2	A	402	BCL	C1B-NB	4.67	1.39	1.35
2	B	404	BCL	MG-NA	4.55	2.17	2.06
2	B	404	BCL	C1B-NB	4.49	1.39	1.35
2	B	405	BCL	MG-NA	4.31	2.16	2.06
2	A	404	BCL	C1B-NB	4.23	1.39	1.35
2	A	402	BCL	C1D-ND	3.64	1.42	1.37
2	A	402	BCL	C4B-NB	3.56	1.38	1.35
2	A	402	BCL	MG-NC	3.48	2.14	2.06
2	B	401	BCL	MG-NC	3.39	2.14	2.06
2	B	407[E]	BCL	MG-NC	3.29	2.14	2.06
2	B	407[F]	BCL	MG-NC	3.29	2.14	2.06
2	B	403[A]	BCL	MG-NC	3.24	2.14	2.06
2	B	403[B]	BCL	MG-NC	3.24	2.14	2.06
2	B	405	BCL	MG-NC	3.22	2.13	2.06
2	A	401	BCL	MG-NC	3.18	2.13	2.06
2	B	404	BCL	MG-NC	3.10	2.13	2.06
2	A	407[A]	BCL	MG-NC	3.10	2.13	2.06
2	A	407[B]	BCL	MG-NC	3.10	2.13	2.06
2	A	406[C]	BCL	MG-NC	3.08	2.13	2.06
2	A	406[D]	BCL	MG-NC	3.08	2.13	2.06
2	B	405	BCL	CHD-C1D	3.06	1.44	1.38
2	B	402	BCL	MG-NC	3.02	2.13	2.06
2	A	403[A]	BCL	MG-NC	3.02	2.13	2.06
2	A	403[B]	BCL	MG-NC	3.02	2.13	2.06
2	B	404	BCL	CHD-C1D	3.01	1.44	1.38
2	A	402	BCL	CHD-C1D	3.00	1.44	1.38
2	A	405	BCL	MG-NC	2.99	2.13	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	402	BCL	C4B-NB	2.93	1.37	1.35
2	B	407[E]	BCL	C4B-NB	2.89	1.37	1.35
2	B	407[F]	BCL	C4B-NB	2.89	1.37	1.35
2	A	401	BCL	C1D-ND	2.88	1.41	1.37
2	B	402	BCL	CHD-C1D	2.85	1.43	1.38
2	A	404	BCL	MG-NC	2.81	2.12	2.06
2	B	407[E]	BCL	C1D-ND	2.80	1.41	1.37
2	B	407[F]	BCL	C1D-ND	2.80	1.41	1.37
2	B	403[A]	BCL	C4B-NB	2.78	1.37	1.35
2	B	403[B]	BCL	C4B-NB	2.78	1.37	1.35
2	A	405	BCL	CHD-C1D	2.73	1.43	1.38
2	B	407[E]	BCL	CHD-C1D	2.71	1.43	1.38
2	B	407[F]	BCL	CHD-C1D	2.71	1.43	1.38
2	B	404	BCL	C4B-NB	2.71	1.37	1.35
2	A	405	BCL	O1A-CGA	-2.63	1.14	1.22
2	A	404	BCL	C4B-NB	2.62	1.37	1.35
2	A	406[C]	BCL	CHD-C1D	2.61	1.43	1.38
2	A	406[D]	BCL	CHD-C1D	2.61	1.43	1.38
2	B	405	BCL	C1D-ND	2.55	1.40	1.37
2	A	407[A]	BCL	C1D-ND	2.54	1.40	1.37
2	A	407[B]	BCL	C1D-ND	2.54	1.40	1.37
2	B	403[A]	BCL	O1A-CGA	-2.54	1.15	1.22
2	B	403[B]	BCL	O1A-CGA	-2.54	1.15	1.22
2	B	407[E]	BCL	CAC-C3C	2.54	1.59	1.54
2	B	407[F]	BCL	CAC-C3C	2.54	1.59	1.54
2	B	405	BCL	C4B-NB	2.48	1.37	1.35
2	B	403[A]	BCL	CHD-C1D	2.46	1.43	1.38
2	B	403[B]	BCL	CHD-C1D	2.46	1.43	1.38
2	A	405	BCL	C1D-ND	2.43	1.40	1.37
2	B	401	BCL	C1D-ND	2.41	1.40	1.37
2	B	407[E]	BCL	O1A-CGA	-2.40	1.15	1.22
2	B	407[F]	BCL	O1A-CGA	-2.40	1.15	1.22
2	A	406[C]	BCL	O1A-CGA	-2.39	1.15	1.22
2	A	406[D]	BCL	O1A-CGA	-2.39	1.15	1.22
2	A	404	BCL	CHD-C1D	2.28	1.42	1.38
2	A	407[A]	BCL	O2A-CGA	-2.27	1.26	1.33
2	A	407[B]	BCL	O2A-CGA	-2.27	1.26	1.33
2	A	401	BCL	OBD-CAD	2.23	1.26	1.22
2	A	403[A]	BCL	CHD-C1D	2.22	1.42	1.38
2	A	403[B]	BCL	CHD-C1D	2.22	1.42	1.38
2	A	407[A]	BCL	C4B-NB	2.21	1.37	1.35
2	A	407[B]	BCL	C4B-NB	2.21	1.37	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	405	BCL	O1A-CGA	-2.20	1.16	1.22
2	B	401	BCL	CHD-C1D	2.19	1.42	1.38
2	A	403[A]	BCL	C1D-ND	2.17	1.40	1.37
2	A	403[B]	BCL	C1D-ND	2.17	1.40	1.37
2	A	405	BCL	C4B-NB	2.15	1.37	1.35
2	A	401	BCL	CHD-C1D	2.14	1.42	1.38
2	B	401	BCL	C4B-NB	2.10	1.37	1.35
2	B	407[E]	BCL	CMB-C2B	2.06	1.55	1.51
2	B	407[F]	BCL	CMB-C2B	2.06	1.55	1.51
2	A	404	BCL	CBD-CGD	-2.05	1.46	1.52
2	A	406[C]	BCL	C3D-C4D	-2.04	1.39	1.44
2	B	404	BCL	C3D-C4D	-2.04	1.39	1.44
2	A	406[D]	BCL	C3D-C4D	-2.03	1.39	1.44
2	A	406[C]	BCL	C4B-NB	2.03	1.37	1.35
2	A	406[D]	BCL	C4B-NB	2.03	1.37	1.35

All (200) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	402	BCL	CHD-C1D-ND	-5.74	119.18	124.45
2	B	402	BCL	CHD-C1D-ND	-5.50	119.40	124.45
2	A	402	BCL	C4D-CHA-C1A	5.39	127.81	121.25
2	B	405	BCL	C4D-CHA-C1A	5.30	127.70	121.25
2	A	404	BCL	C4D-CHA-C1A	5.29	127.69	121.25
2	A	401	BCL	C4D-CHA-C1A	5.27	127.66	121.25
2	B	404	BCL	C4D-CHA-C1A	5.20	127.58	121.25
2	A	406[C]	BCL	C4D-CHA-C1A	5.15	127.52	121.25
2	A	404	BCL	CHD-C1D-ND	-5.09	119.78	124.45
2	A	405	BCL	C4D-CHA-C1A	5.07	127.42	121.25
2	B	402	BCL	C4D-CHA-C1A	5.07	127.42	121.25
2	B	401	BCL	C4D-CHA-C1A	5.06	127.40	121.25
2	B	404	BCL	CHD-C1D-ND	-5.04	119.83	124.45
2	B	401	BCL	CHD-C1D-ND	-5.02	119.84	124.45
2	B	405	BCL	CHD-C1D-ND	-5.02	119.84	124.45
2	A	407[A]	BCL	CHD-C1D-ND	-5.00	119.86	124.45
2	A	407[B]	BCL	CHD-C1D-ND	-5.00	119.86	124.45
2	A	401	BCL	CHD-C1D-ND	-4.97	119.88	124.45
2	A	403[A]	BCL	C4D-CHA-C1A	4.88	127.19	121.25
2	A	403[B]	BCL	C4D-CHA-C1A	4.88	127.19	121.25
2	A	406[C]	BCL	CHD-C1D-ND	-4.88	119.97	124.45
2	A	406[D]	BCL	CHD-C1D-ND	-4.88	119.97	124.45
2	B	403[A]	BCL	C4D-CHA-C1A	4.78	127.07	121.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	403[B]	BCL	C4D-CHA-C1A	4.78	127.07	121.25
2	A	406[D]	BCL	C4D-CHA-C1A	4.78	127.06	121.25
2	A	405	BCL	CHD-C1D-ND	-4.74	120.10	124.45
2	A	401	BCL	CMB-C2B-C1B	-4.65	121.32	128.46
2	A	407[A]	BCL	C4D-CHA-C1A	4.59	126.84	121.25
2	A	407[B]	BCL	C4D-CHA-C1A	4.59	126.84	121.25
2	B	407[E]	BCL	CHD-C1D-ND	-4.59	120.23	124.45
2	B	407[F]	BCL	CHD-C1D-ND	-4.59	120.23	124.45
2	B	403[A]	BCL	CHD-C1D-ND	-4.58	120.25	124.45
2	B	403[B]	BCL	CHD-C1D-ND	-4.58	120.25	124.45
2	A	404	BCL	CMB-C2B-C1B	-4.49	121.57	128.46
2	A	403[A]	BCL	CHD-C1D-ND	-4.40	120.41	124.45
2	A	403[B]	BCL	CHD-C1D-ND	-4.40	120.41	124.45
2	A	407[A]	BCL	CMB-C2B-C1B	-4.39	121.72	128.46
2	A	407[B]	BCL	CMB-C2B-C1B	-4.39	121.72	128.46
2	B	404	BCL	CMB-C2B-C1B	-4.35	121.78	128.46
2	B	407[E]	BCL	C4D-CHA-C1A	4.30	126.49	121.25
2	B	407[F]	BCL	C4D-CHA-C1A	4.30	126.49	121.25
2	A	406[C]	BCL	CMB-C2B-C1B	-4.29	121.88	128.46
2	A	406[D]	BCL	CMB-C2B-C1B	-4.29	121.88	128.46
2	B	402	BCL	C1-C2-C3	-4.26	118.67	126.04
2	A	407[A]	BCL	C1D-ND-C4D	-4.24	103.33	106.33
2	A	407[B]	BCL	C1D-ND-C4D	-4.24	103.33	106.33
2	A	406[C]	BCL	C1-C2-C3	-4.22	118.75	126.04
2	A	406[D]	BCL	C1-C2-C3	-4.22	118.75	126.04
2	A	402	BCL	C1D-ND-C4D	-4.20	103.35	106.33
2	B	401	BCL	CMB-C2B-C1B	-4.14	122.10	128.46
2	B	405	BCL	CMB-C2B-C1B	-4.02	122.28	128.46
2	B	407[E]	BCL	C1D-ND-C4D	-3.93	103.54	106.33
2	B	407[F]	BCL	C1D-ND-C4D	-3.93	103.54	106.33
2	B	402	BCL	C1D-ND-C4D	-3.83	103.62	106.33
2	A	402	BCL	CMB-C2B-C1B	-3.80	122.62	128.46
2	A	401	BCL	C4A-NA-C1A	3.76	108.40	106.71
2	B	403[A]	BCL	CMB-C2B-C1B	-3.74	122.72	128.46
2	B	403[B]	BCL	CMB-C2B-C1B	-3.74	122.72	128.46
2	B	407[E]	BCL	CMB-C2B-C1B	-3.71	122.76	128.46
2	B	407[F]	BCL	CMB-C2B-C1B	-3.71	122.76	128.46
2	A	403[A]	BCL	CMB-C2B-C1B	-3.66	122.84	128.46
2	A	403[B]	BCL	CMB-C2B-C1B	-3.66	122.84	128.46
2	A	402	BCL	C4A-NA-C1A	3.62	108.33	106.71
2	B	407[E]	BCL	C4A-NA-C1A	3.61	108.33	106.71
2	B	407[F]	BCL	C4A-NA-C1A	3.61	108.33	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	401	BCL	C1D-ND-C4D	-3.61	103.77	106.33
2	B	401	BCL	C1D-ND-C4D	-3.59	103.78	106.33
2	A	407[A]	BCL	O2A-CGA-O1A	-3.57	114.58	123.59
2	A	407[B]	BCL	O2A-CGA-O1A	-3.57	114.58	123.59
2	B	403[A]	BCL	C1D-ND-C4D	-3.57	103.80	106.33
2	B	403[B]	BCL	C1D-ND-C4D	-3.57	103.80	106.33
2	A	403[A]	BCL	C4A-NA-C1A	3.55	108.30	106.71
2	A	403[B]	BCL	C4A-NA-C1A	3.55	108.30	106.71
2	B	407[E]	BCL	O2A-CGA-O1A	-3.53	114.68	123.59
2	B	407[F]	BCL	O2A-CGA-O1A	-3.53	114.68	123.59
2	A	406[C]	BCL	C4A-NA-C1A	3.51	108.28	106.71
2	A	406[D]	BCL	C4A-NA-C1A	3.51	108.28	106.71
2	A	405	BCL	CMB-C2B-C1B	-3.47	123.13	128.46
2	B	402	BCL	CMB-C2B-C1B	-3.47	123.14	128.46
2	A	401	BCL	C1-C2-C3	-3.37	120.22	126.04
2	A	407[A]	BCL	C4A-NA-C1A	3.35	108.21	106.71
2	A	407[B]	BCL	C4A-NA-C1A	3.35	108.21	106.71
2	A	403[A]	BCL	C1D-ND-C4D	-3.35	103.96	106.33
2	A	403[B]	BCL	C1D-ND-C4D	-3.35	103.96	106.33
2	B	401	BCL	C4A-NA-C1A	3.35	108.21	106.71
2	A	405	BCL	CHA-C1A-NA	-3.33	118.77	126.40
2	A	405	BCL	C1D-ND-C4D	-3.24	104.03	106.33
2	A	406[D]	BCL	C1D-ND-C4D	-3.24	104.03	106.33
2	A	402	BCL	C1-C2-C3	-3.24	120.44	126.04
2	A	401	BCL	CHA-C1A-NA	-3.23	119.01	126.40
2	B	403[A]	BCL	CHA-C1A-NA	-3.22	119.02	126.40
2	B	403[B]	BCL	CHA-C1A-NA	-3.22	119.02	126.40
2	B	401	BCL	CHA-C1A-NA	-3.22	119.03	126.40
2	A	401	BCL	CMB-C2B-C3B	3.20	130.67	124.68
2	A	403[A]	BCL	CHA-C1A-NA	-3.20	119.08	126.40
2	A	403[B]	BCL	CHA-C1A-NA	-3.20	119.08	126.40
2	A	407[A]	BCL	CMB-C2B-C3B	3.19	130.65	124.68
2	A	406[C]	BCL	C1D-ND-C4D	-3.18	104.08	106.33
2	B	402	BCL	C4A-NA-C1A	3.16	108.13	106.71
2	A	404	BCL	CMB-C2B-C3B	3.15	130.57	124.68
2	B	404	BCL	CHA-C1A-NA	-3.13	119.23	126.40
2	B	403[A]	BCL	C4A-NA-C1A	3.12	108.11	106.71
2	B	403[B]	BCL	C4A-NA-C1A	3.12	108.11	106.71
2	A	404	BCL	CHA-C1A-NA	-3.11	119.27	126.40
2	B	405	BCL	C1D-ND-C4D	-3.07	104.15	106.33
2	A	402	BCL	CHA-C1A-NA	-3.07	119.37	126.40
2	B	404	BCL	CMB-C2B-C3B	3.07	130.42	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	405	BCL	CHA-C1A-NA	-3.06	119.39	126.40
2	A	403[A]	BCL	C2A-C1A-CHA	3.03	129.16	123.86
2	A	403[B]	BCL	C2A-C1A-CHA	3.03	129.16	123.86
2	B	402	BCL	CHA-C1A-NA	-3.01	119.51	126.40
2	A	406[C]	BCL	CMB-C2B-C3B	3.00	130.30	124.68
2	A	406[D]	BCL	CMB-C2B-C3B	3.00	130.30	124.68
2	A	404	BCL	C1D-ND-C4D	-3.00	104.20	106.33
2	A	406[C]	BCL	C2A-C1A-CHA	2.99	129.09	123.86
2	A	406[C]	BCL	CHA-C1A-NA	-2.98	119.58	126.40
2	A	407[B]	BCL	CMB-C2B-C3B	2.97	130.23	124.68
2	A	404	BCL	C2A-C1A-CHA	2.95	129.02	123.86
2	B	401	BCL	C2A-C1A-CHA	2.94	128.99	123.86
2	A	404	BCL	C4A-NA-C1A	2.91	108.02	106.71
2	B	405	BCL	C2A-C1A-CHA	2.90	128.93	123.86
2	A	405	BCL	C2A-C1A-CHA	2.90	128.92	123.86
2	B	407[E]	BCL	CHA-C1A-NA	-2.89	119.77	126.40
2	B	407[F]	BCL	CHA-C1A-NA	-2.89	119.77	126.40
2	B	404	BCL	C2A-C1A-CHA	2.87	128.88	123.86
2	A	406[D]	BCL	CHA-C1A-NA	-2.85	119.87	126.40
2	B	405	BCL	CMB-C2B-C3B	2.84	129.99	124.68
2	A	406[D]	BCL	C2A-C1A-CHA	2.83	128.80	123.86
2	B	401	BCL	CMB-C2B-C3B	2.81	129.94	124.68
2	B	407[E]	BCL	CMB-C2B-C3B	2.81	129.93	124.68
2	B	407[F]	BCL	CMB-C2B-C3B	2.81	129.93	124.68
2	A	401	BCL	C2A-C1A-CHA	2.78	128.72	123.86
2	A	404	BCL	C1-C2-C3	-2.76	121.27	126.04
2	B	407[E]	BCL	C17-C16-C15	2.75	125.89	113.24
2	A	402	BCL	C2A-C1A-CHA	2.75	128.67	123.86
2	B	402	BCL	C2A-C1A-CHA	2.75	128.67	123.86
2	B	404	BCL	C1D-ND-C4D	-2.75	104.38	106.33
2	A	407[A]	BCL	CHA-C1A-NA	-2.75	120.11	126.40
2	A	407[B]	BCL	CHA-C1A-NA	-2.75	120.11	126.40
2	B	403[A]	BCL	C2A-C1A-CHA	2.72	128.61	123.86
2	B	403[B]	BCL	C2A-C1A-CHA	2.72	128.61	123.86
2	B	403[A]	BCL	C1-C2-C3	-2.61	121.52	126.04
2	B	403[B]	BCL	C1-C2-C3	-2.61	121.52	126.04
2	A	407[B]	BCL	OBB-CAB-CBB	-2.60	114.31	120.17
2	A	406[C]	BCL	C1C-NC-C4C	2.59	107.87	106.71
2	A	406[D]	BCL	C1C-NC-C4C	2.59	107.87	106.71
2	B	403[A]	BCL	CMB-C2B-C3B	2.58	129.51	124.68
2	B	403[B]	BCL	CMB-C2B-C3B	2.58	129.51	124.68
2	A	403[A]	BCL	CMB-C2B-C3B	2.53	129.42	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	403[B]	BCL	CMB-C2B-C3B	2.53	129.42	124.68
2	A	402	BCL	CMB-C2B-C3B	2.51	129.38	124.68
2	B	404	BCL	C4A-NA-C1A	2.51	107.83	106.71
2	A	405	BCL	CMB-C2B-C3B	2.49	129.33	124.68
2	B	403[A]	BCL	C16-C15-C13	-2.49	107.88	115.92
2	A	407[A]	BCL	C15-C13-C12	-2.48	99.10	112.13
2	A	407[B]	BCL	C15-C13-C12	-2.48	99.10	112.13
2	B	405	BCL	C4A-NA-C1A	2.42	107.79	106.71
2	B	407[E]	BCL	C11-C10-C8	-2.35	108.33	115.92
2	B	407[F]	BCL	C11-C10-C8	-2.35	108.33	115.92
2	B	401	BCL	C1-C2-C3	-2.34	122.00	126.04
2	B	404	BCL	C1C-NC-C4C	2.33	107.75	106.71
2	A	406[C]	BCL	OBB-CAB-CBB	-2.31	114.97	120.17
2	A	406[D]	BCL	OBB-CAB-CBB	-2.31	114.97	120.17
2	B	401	BCL	OBB-CAB-CBB	-2.31	114.97	120.17
2	B	407[E]	BCL	C1C-NC-C4C	2.31	107.74	106.71
2	B	407[F]	BCL	C1C-NC-C4C	2.31	107.74	106.71
2	A	401	BCL	OBB-CAB-CBB	-2.29	115.01	120.17
2	B	403[B]	BCL	C11-C10-C8	2.29	123.32	115.92
2	B	407[E]	BCL	C2A-C1A-CHA	2.29	127.86	123.86
2	B	407[F]	BCL	C2A-C1A-CHA	2.29	127.86	123.86
2	A	404	BCL	OBB-CAB-CBB	-2.29	115.02	120.17
2	B	402	BCL	CMB-C2B-C3B	2.28	128.95	124.68
2	A	407[A]	BCL	C2A-C1A-CHA	2.28	127.84	123.86
2	A	407[B]	BCL	C2A-C1A-CHA	2.28	127.84	123.86
2	A	403[B]	BCL	C11-C10-C8	2.27	123.25	115.92
2	B	405	BCL	C4B-C3B-CAB	-2.23	122.83	127.13
2	A	407[A]	BCL	C1-C2-C3	-2.23	122.19	126.04
2	A	407[B]	BCL	C1-C2-C3	-2.23	122.19	126.04
2	B	407[E]	BCL	OBB-CAB-CBB	-2.20	115.21	120.17
2	B	407[F]	BCL	OBB-CAB-CBB	-2.20	115.21	120.17
2	B	407[E]	BCL	O2D-CGD-O1D	-2.17	119.59	123.84
2	B	407[F]	BCL	O2D-CGD-O1D	-2.17	119.59	123.84
2	B	407[E]	BCL	O2A-CGA-CBA	2.17	118.72	111.91
2	B	407[F]	BCL	O2A-CGA-CBA	2.17	118.72	111.91
2	A	407[A]	BCL	O2A-CGA-CBA	2.15	118.66	111.91
2	A	407[B]	BCL	O2A-CGA-CBA	2.15	118.66	111.91
2	B	407[E]	BCL	C1-C2-C3	-2.14	122.33	126.04
2	B	407[F]	BCL	C1-C2-C3	-2.14	122.33	126.04
2	A	401	BCL	C4-C3-C5	-2.13	111.68	115.27
2	A	405	BCL	C4A-NA-C1A	2.13	107.66	106.71
2	A	403[B]	BCL	C17-C16-C15	2.13	123.02	113.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	407[F]	BCL	C17-C16-C15	-2.13	103.47	113.24
2	B	405	BCL	C1C-NC-C4C	2.11	107.65	106.71
2	A	405	BCL	C4B-C3B-CAB	-2.10	123.06	127.13
2	A	405	BCL	O2A-CGA-O1A	-2.09	118.32	123.59
2	B	401	BCL	OBB-CAB-C3B	2.08	123.69	119.99
2	B	401	BCL	C16-C15-C13	-2.04	109.33	115.92
2	B	404	BCL	OBB-CAB-CBB	-2.03	115.60	120.17
2	B	402	BCL	CED-O2D-CGD	2.03	120.52	115.94
2	B	402	BCL	C2D-C1D-ND	2.02	111.59	110.10

There are no chirality outliers.

All (68) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	403[A]	BCL	C2C-C3C-CAC-CBC
2	A	403[A]	BCL	C4C-C3C-CAC-CBC
2	A	403[B]	BCL	C2C-C3C-CAC-CBC
2	A	403[B]	BCL	C4C-C3C-CAC-CBC
2	B	403[A]	BCL	C2C-C3C-CAC-CBC
2	B	403[A]	BCL	C4C-C3C-CAC-CBC
2	B	403[B]	BCL	C2C-C3C-CAC-CBC
2	B	403[B]	BCL	C4C-C3C-CAC-CBC
2	A	406[C]	BCL	C4-C3-C5-C6
2	A	406[D]	BCL	C4-C3-C5-C6
2	A	405	BCL	C4-C3-C5-C6
2	A	405	BCL	C2-C3-C5-C6
2	B	403[A]	BCL	C13-C15-C16-C17
2	A	406[C]	BCL	C2-C3-C5-C6
2	A	406[D]	BCL	C2-C3-C5-C6
2	B	407[E]	BCL	C12-C13-C15-C16
2	B	407[E]	BCL	C14-C13-C15-C16
2	A	403[A]	BCL	C13-C15-C16-C17
2	A	406[C]	BCL	C10-C11-C12-C13
2	A	406[D]	BCL	C10-C11-C12-C13
2	B	403[A]	BCL	C5-C6-C7-C8
2	B	403[A]	BCL	C10-C11-C12-C13
2	A	403[A]	BCL	C5-C6-C7-C8
2	A	403[A]	BCL	C10-C11-C12-C13
2	A	405	BCL	CAD-CBD-CGD-O2D
2	B	405	BCL	CAD-CBD-CGD-O2D
2	A	405	BCL	CHA-CBD-CGD-O1D
2	A	406[C]	BCL	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
2	A	406[C]	BCL	CHA-CBD-CGD-O2D
2	A	401	BCL	C13-C15-C16-C17
2	A	405	BCL	CAA-CBA-CGA-O2A
2	A	406[C]	BCL	C2-C1-O2A-CGA
2	A	406[D]	BCL	C2-C1-O2A-CGA
2	A	407[A]	BCL	CAA-CBA-CGA-O2A
2	A	407[B]	BCL	CAA-CBA-CGA-O2A
2	B	407[E]	BCL	CAA-CBA-CGA-O2A
2	B	407[F]	BCL	CAA-CBA-CGA-O2A
2	B	403[B]	BCL	C6-C7-C8-C10
2	B	405	BCL	CAA-CBA-CGA-O2A
2	B	405	BCL	C2-C3-C5-C6
2	A	403[B]	BCL	C6-C7-C8-C10
2	B	402	BCL	C13-C15-C16-C17
2	B	405	BCL	C4-C3-C5-C6
2	A	401	BCL	CAA-CBA-CGA-O2A
2	A	402	BCL	CHA-CBD-CGD-O1D
2	A	402	BCL	CHA-CBD-CGD-O2D
2	A	407[A]	BCL	CHA-CBD-CGD-O2D
2	A	407[B]	BCL	CHA-CBD-CGD-O2D
2	B	402	BCL	CHA-CBD-CGD-O2D
2	B	407[E]	BCL	CHA-CBD-CGD-O1D
2	B	407[E]	BCL	CHA-CBD-CGD-O2D
2	B	407[F]	BCL	CHA-CBD-CGD-O1D
2	B	407[F]	BCL	CHA-CBD-CGD-O2D
2	B	401	BCL	CAA-CBA-CGA-O2A
2	B	403[A]	BCL	CAA-CBA-CGA-O2A
2	B	403[B]	BCL	CAA-CBA-CGA-O2A
2	A	406[C]	BCL	C16-C17-C18-C20
2	A	406[D]	BCL	C16-C17-C18-C20
2	A	401	BCL	CAA-CBA-CGA-O1A
2	B	404	BCL	CAD-CBD-CGD-O1D
2	B	401	BCL	CAA-CBA-CGA-O1A
2	A	403[A]	BCL	CAA-CBA-CGA-O2A
2	A	403[B]	BCL	CAA-CBA-CGA-O2A
2	B	404	BCL	C2A-CAA-CBA-CGA
2	A	403[A]	BCL	CAA-CBA-CGA-O1A
2	A	403[B]	BCL	CAA-CBA-CGA-O1A
2	B	403[A]	BCL	CAA-CBA-CGA-O1A
2	B	403[B]	BCL	CAA-CBA-CGA-O1A

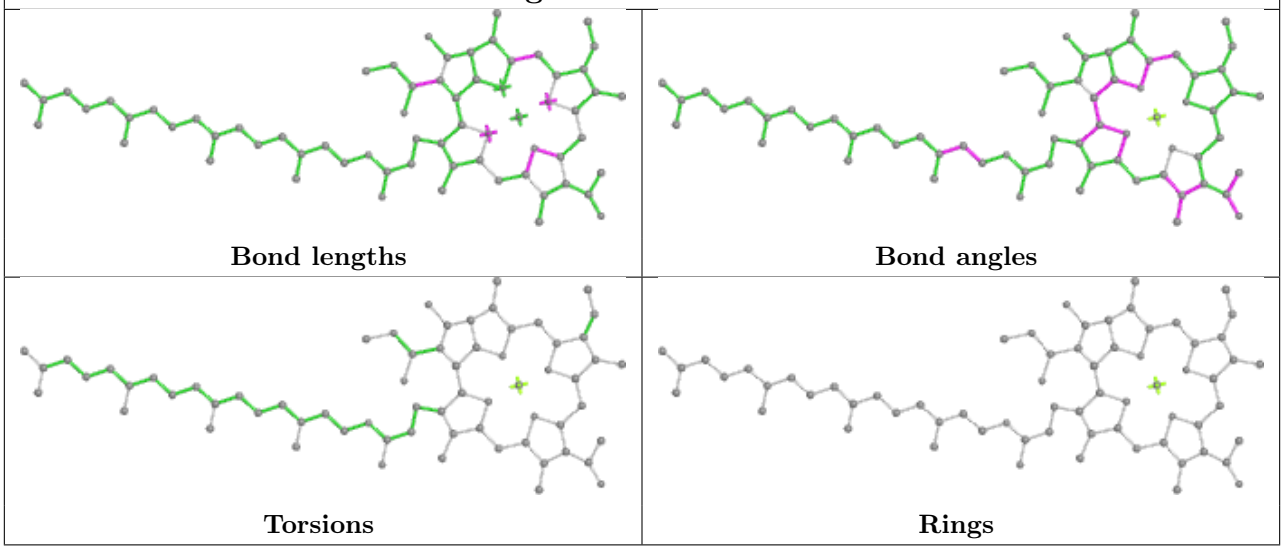
There are no ring outliers.

11 monomers are involved in 13 short contacts:

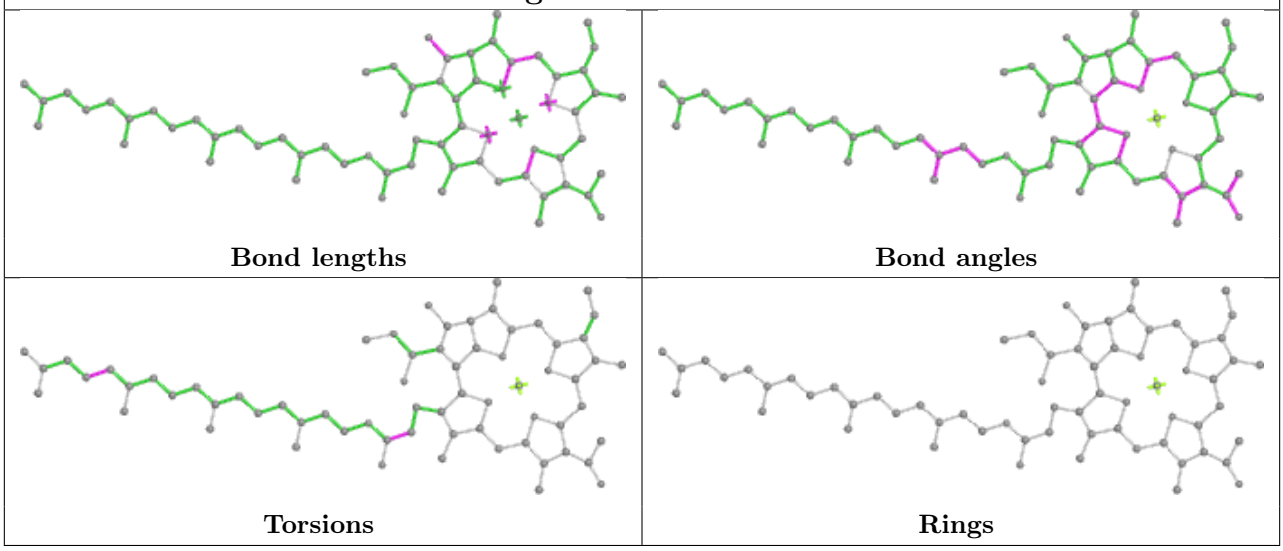
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	404	BCL	1	0
2	A	401	BCL	1	0
3	B	410	SO4	1	0
2	B	404	BCL	1	0
3	A	410	SO4	1	0
2	A	407[A]	BCL	1	0
2	B	401	BCL	2	0
2	A	402	BCL	1	0
2	B	407[E]	BCL	1	0
2	A	403[B]	BCL	1	0
2	B	402	BCL	3	0

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 then 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 404



Ligand BCL A 401



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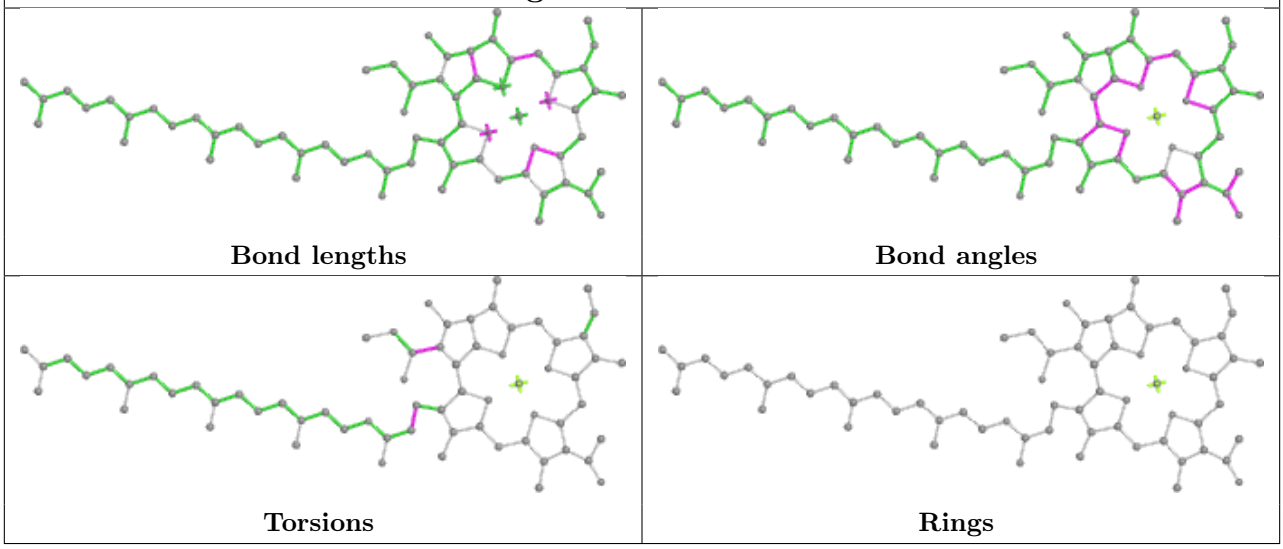

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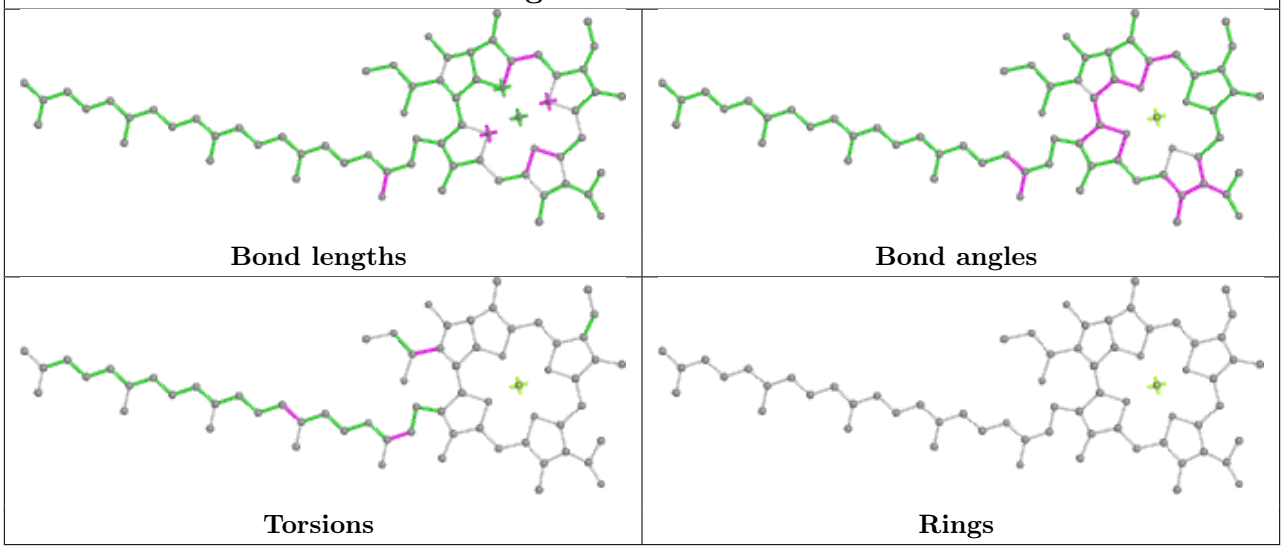

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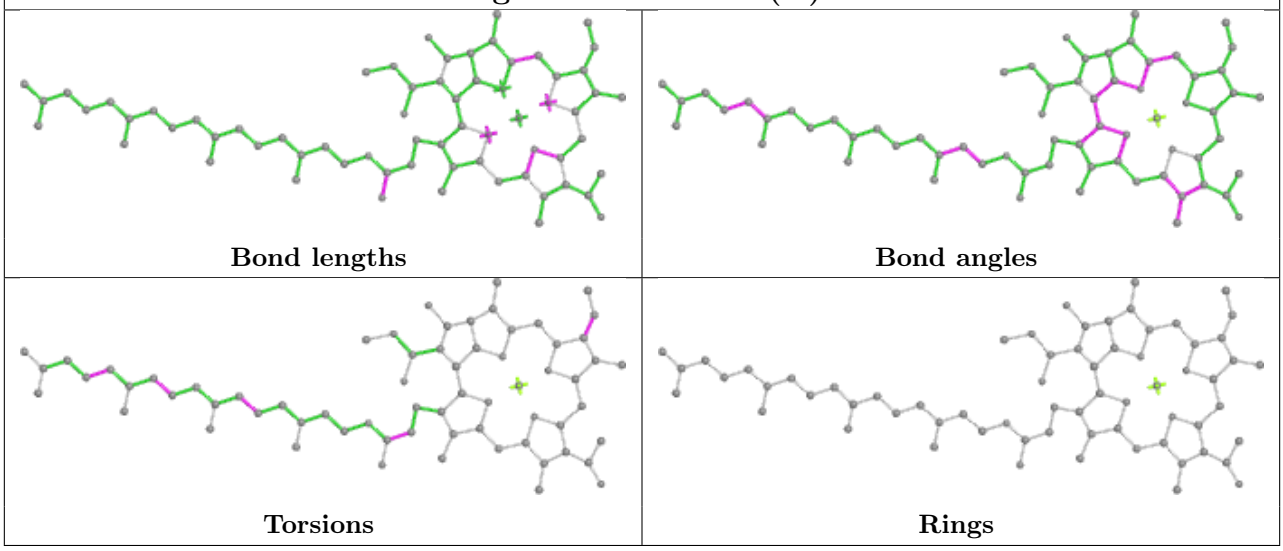

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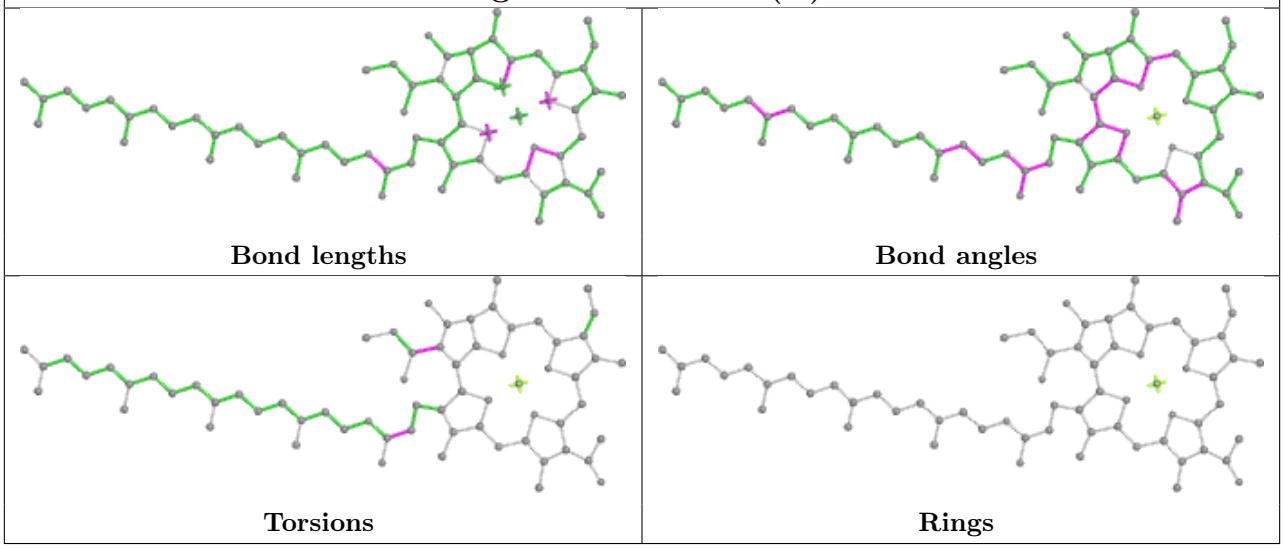

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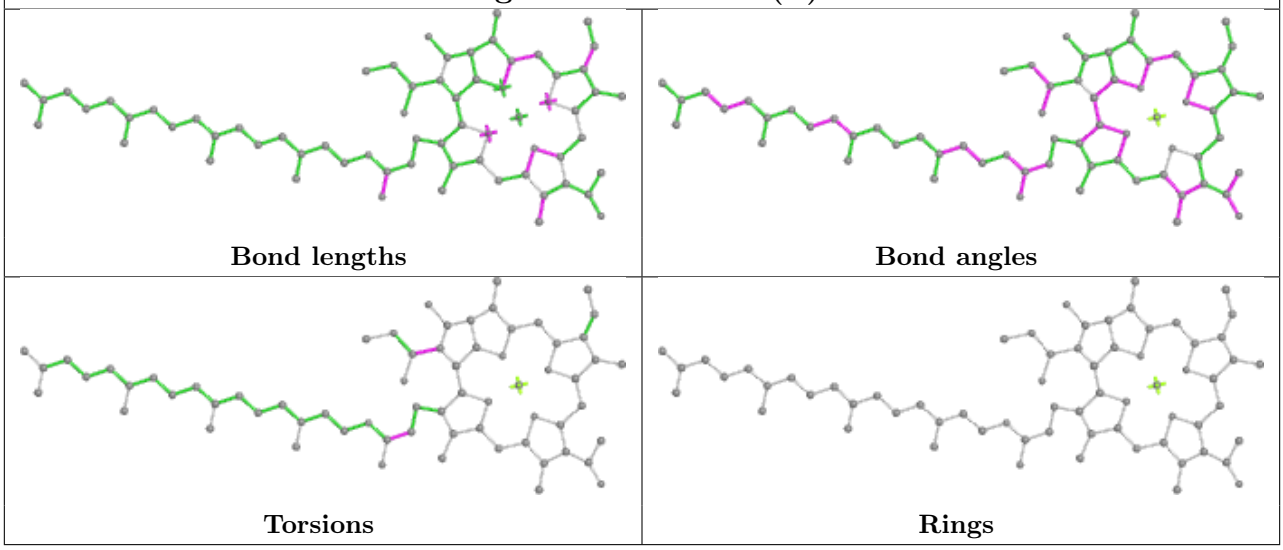

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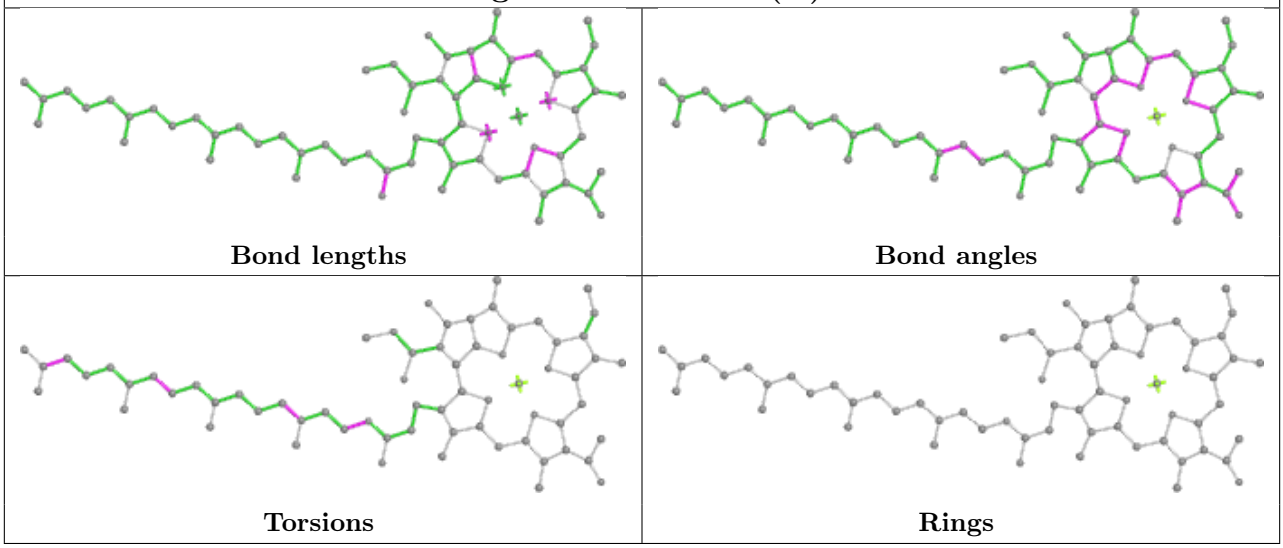

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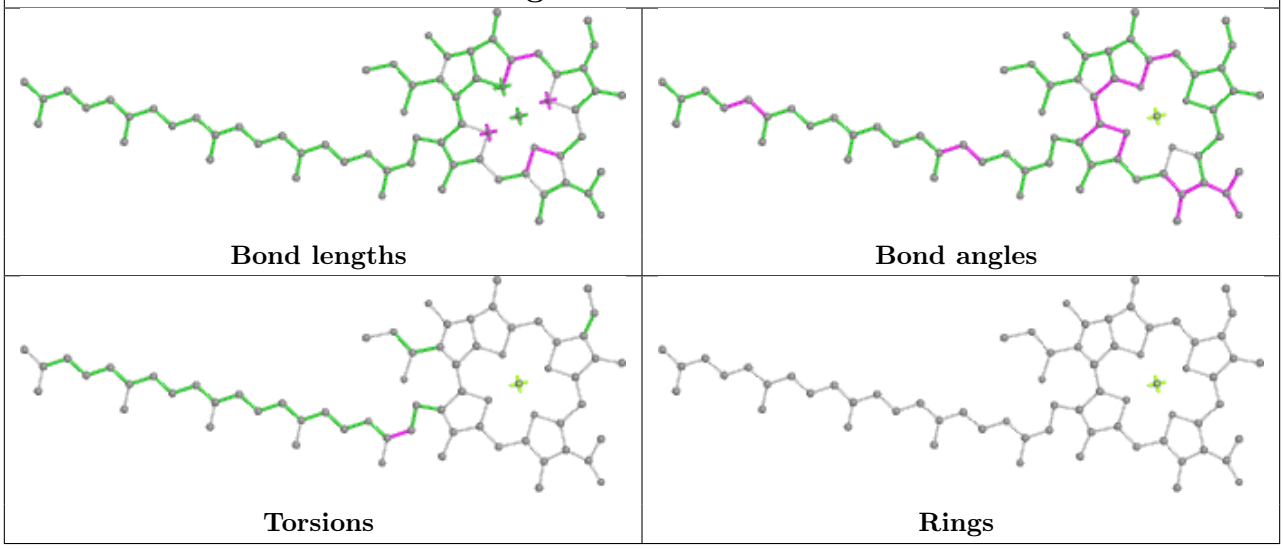

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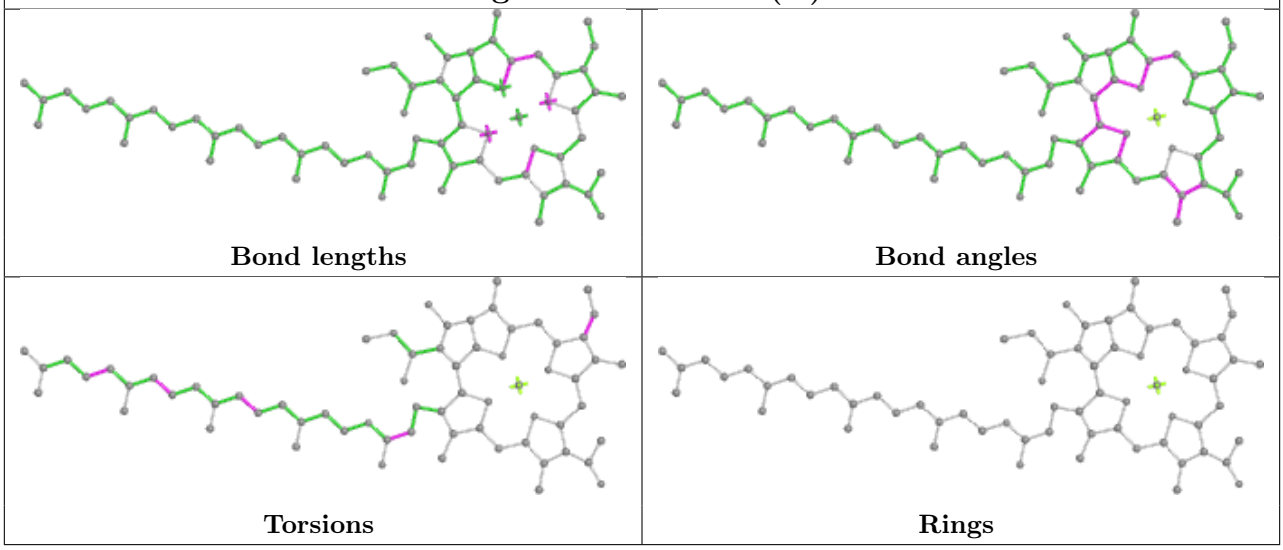

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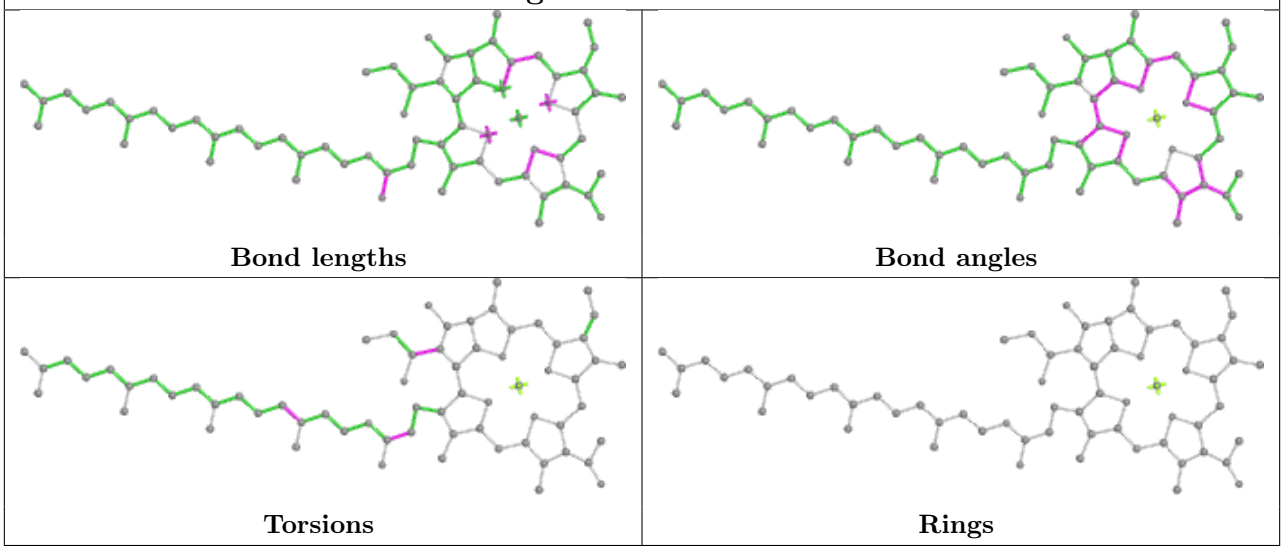

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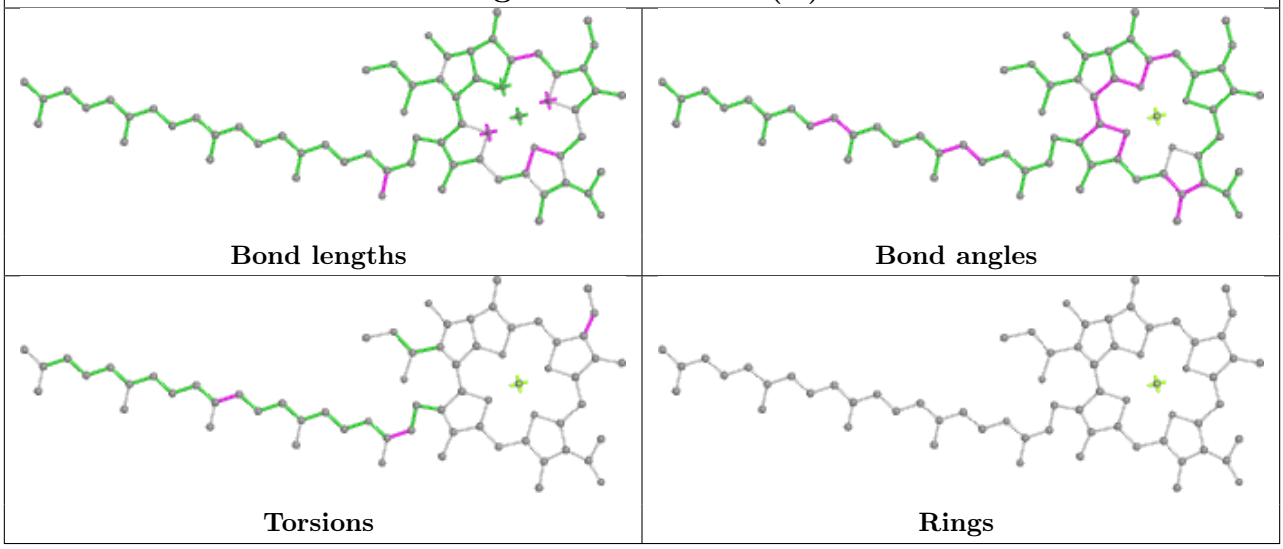
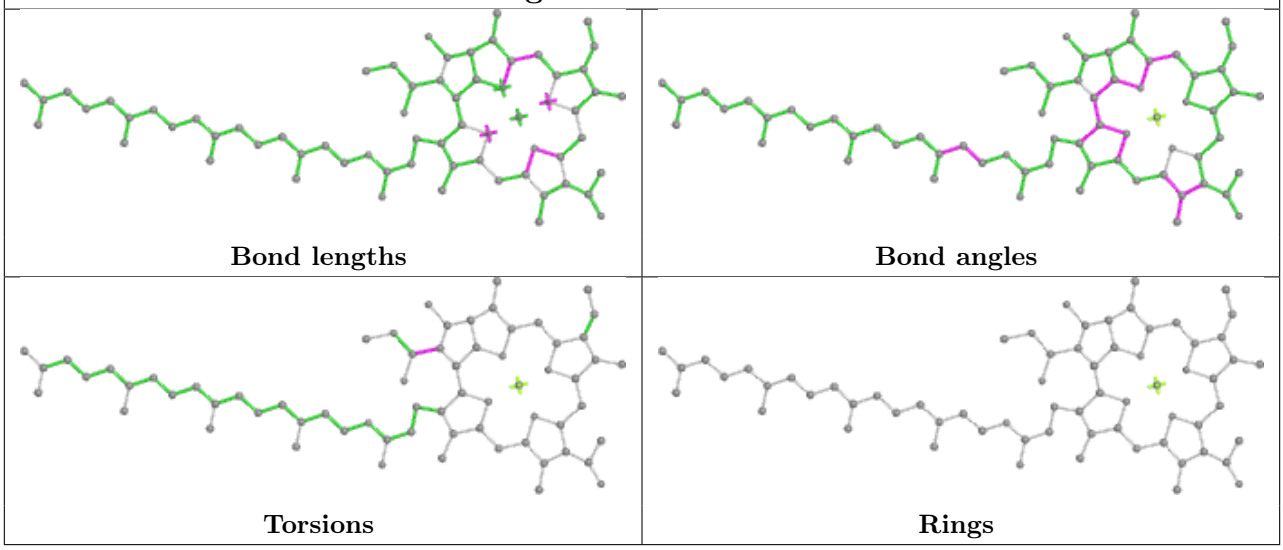


Ligand BCL A 402



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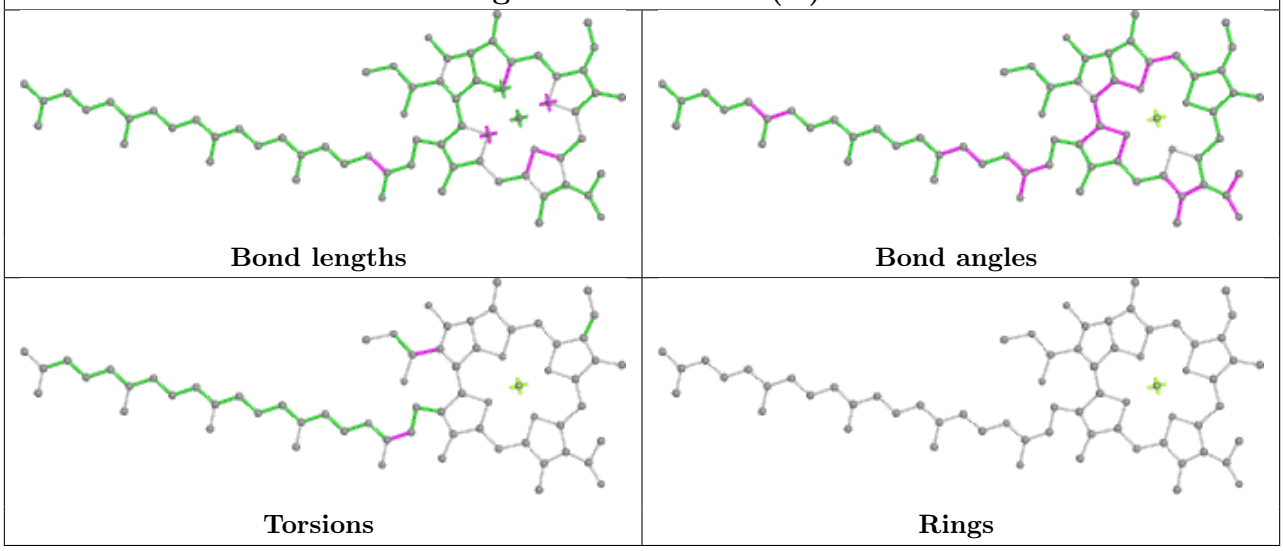

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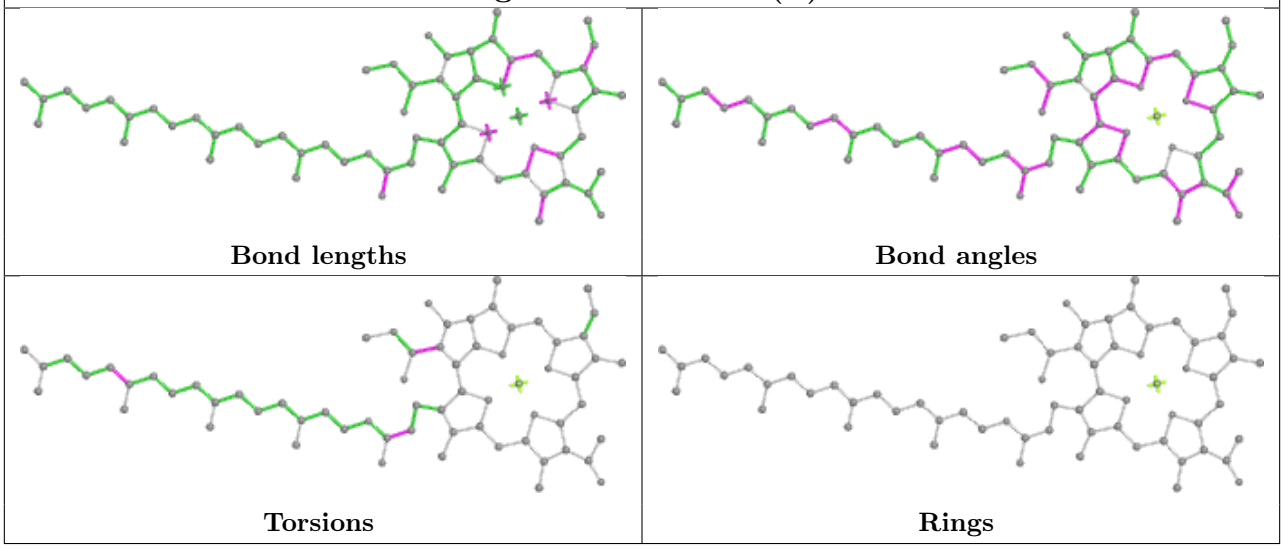
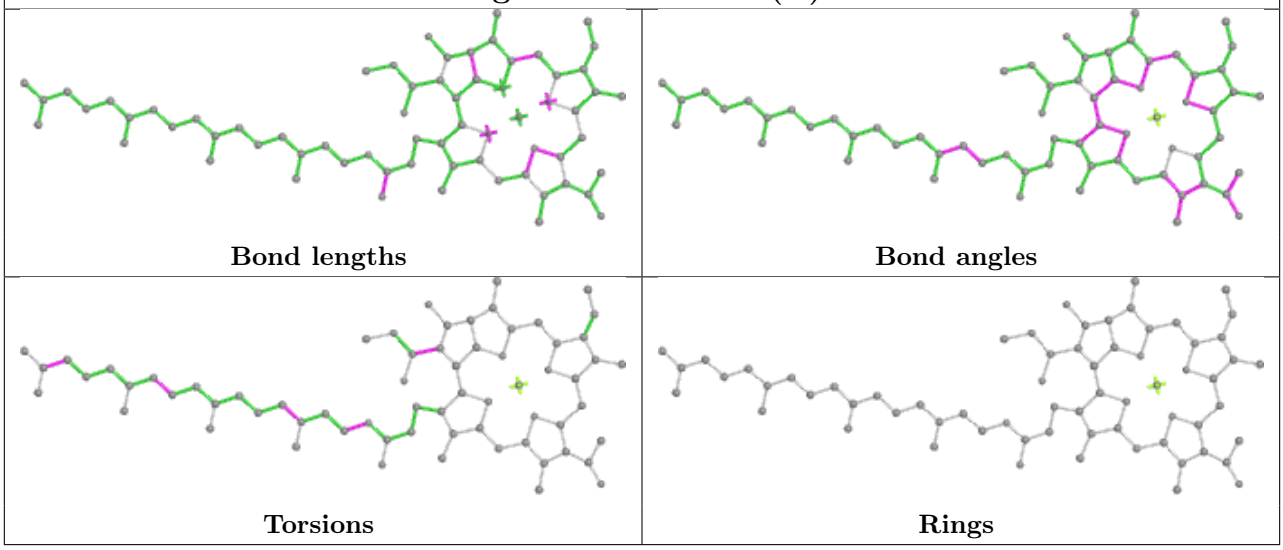
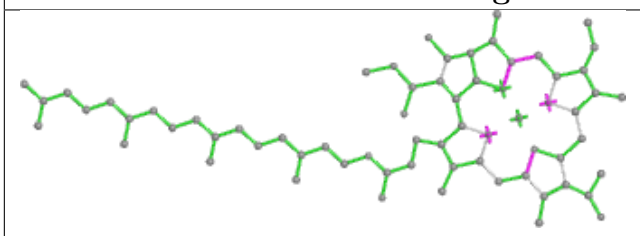
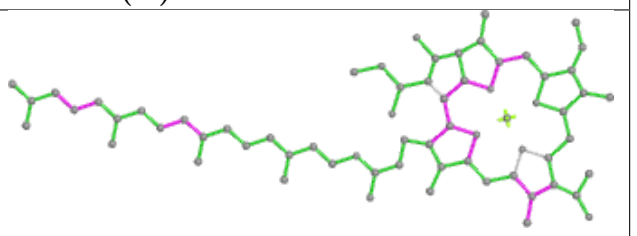
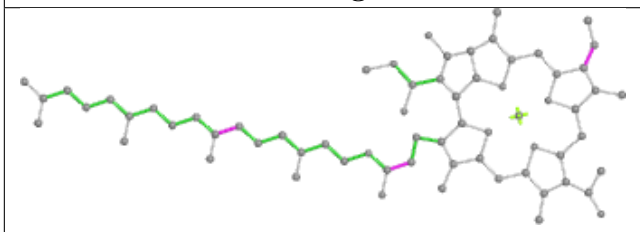
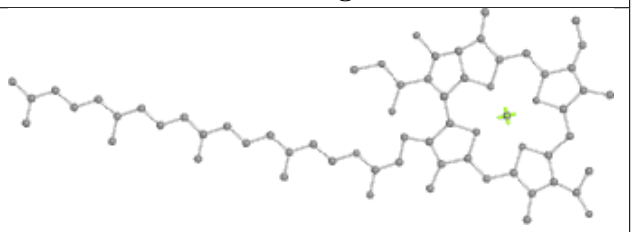
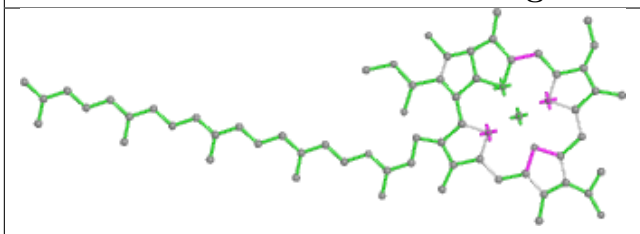
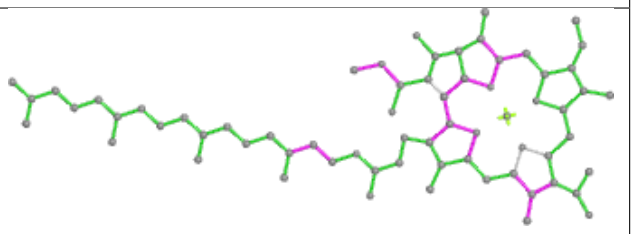
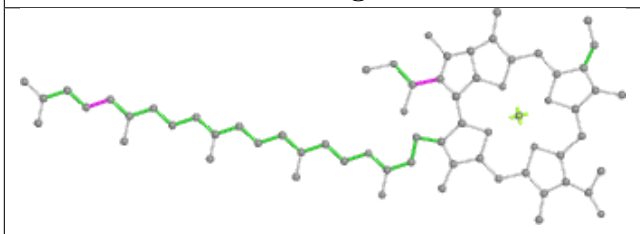
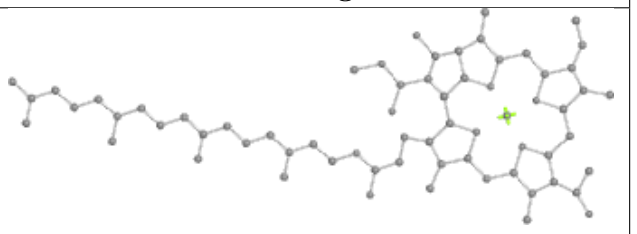


Ligand BCL A 406 (C)



Ligand BCL A 403 (B)	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCL B 402	
 Bond lengths	 Bond angles
 Torsions	 Rings

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	358/360 (99%)	-0.36	10 (2%)	53	58	11, 20, 40, 83	6 (1%)
1	B	360/360 (100%)	-0.38	9 (2%)	57	63	9, 18, 37, 77	4 (1%)
All	All	718/720 (99%)	-0.37	19 (2%)	56	61	9, 19, 39, 83	10 (1%)

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	7	ASP	5.6
1	A	60	GLN	5.4
1	A	59	ALA	5.2
1	B	8	THR	4.6
1	A	171[A]	GLY	3.7
1	A	282	GLY	3.0
1	B	170[A]	SER	2.8
1	A	214	GLU	2.8
1	A	61	LYS	2.7
1	A	174	ALA	2.6
1	B	171[A]	GLY	2.6
1	B	282	GLY	2.5
1	B	125[A]	ARG	2.3
1	B	215	LYS	2.3
1	B	283	GLY	2.3
1	A	173[A]	GLY	2.2
1	B	172[A]	GLY	2.1
1	A	58	ASP	2.1
1	A	213	GLY	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides 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.

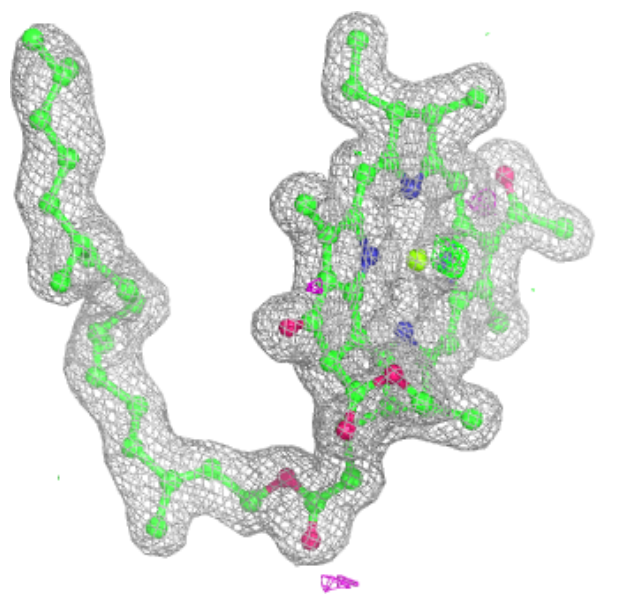
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	SO4	A	409	5/5	0.89	0.21	89,96,98,101	0
3	SO4	A	410	5/5	0.89	0.16	94,95,97,101	0
3	SO4	B	410	5/5	0.89	0.22	96,97,98,102	0
3	SO4	B	408	5/5	0.92	0.23	72,81,87,90	0
3	SO4	A	408	5/5	0.92	0.19	71,83,86,87	0
3	SO4	B	409	5/5	0.94	0.25	90,92,93,95	0
2	BCL	A	405	66/66	0.96	0.07	13,18,36,48	0
2	BCL	A	406[D]	66/66	0.97	0.09	11,16,36,40	10
2	BCL	A	407[A]	66/66	0.97	0.07	9,14,40,54	4
2	BCL	A	407[B]	66/66	0.97	0.07	8,14,40,54	4
2	BCL	B	402	66/66	0.97	0.07	8,13,35,39	0
2	BCL	B	404	66/66	0.97	0.07	8,14,20,26	0
2	BCL	B	405	66/66	0.97	0.07	9,15,36,46	0
2	BCL	B	406[C]	58/66	0.97	0.08	10,15,33,36	10
2	BCL	B	406[D]	58/66	0.97	0.08	9,15,33,36	10
2	BCL	B	406[A]	56/66	0.97	0.08	7,15,33,36	8
2	BCL	B	406[B]	56/66	0.97	0.08	10,15,33,36	8
2	BCL	B	407[E]	66/66	0.97	0.07	7,12,27,37	6
2	BCL	B	407[F]	66/66	0.97	0.07	7,12,28,39	6
2	BCL	A	402	66/66	0.97	0.07	9,15,35,38	0
2	BCL	A	403[A]	66/66	0.97	0.08	10,16,28,33	13
2	BCL	A	403[B]	66/66	0.97	0.08	10,16,27,33	13
2	BCL	A	404	66/66	0.97	0.07	12,16,21,26	0
2	BCL	A	401	66/66	0.97	0.08	11,15,27,34	0
2	BCL	A	406[C]	66/66	0.97	0.09	11,16,36,40	10
2	BCL	B	403[B]	66/66	0.98	0.08	9,14,26,31	13
2	BCL	B	401	66/66	0.98	0.07	11,15,26,36	0
2	BCL	B	403[A]	66/66	0.98	0.08	9,14,28,31	13

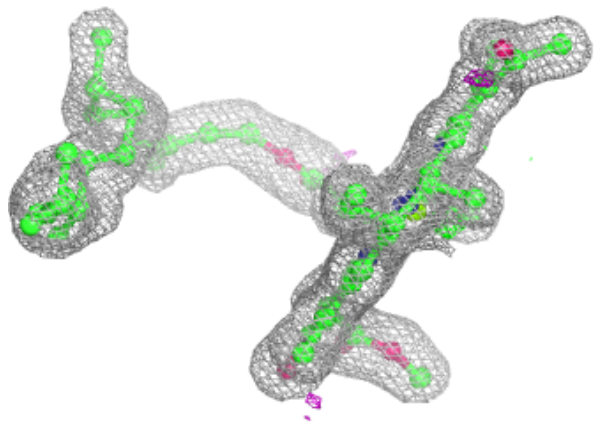
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different

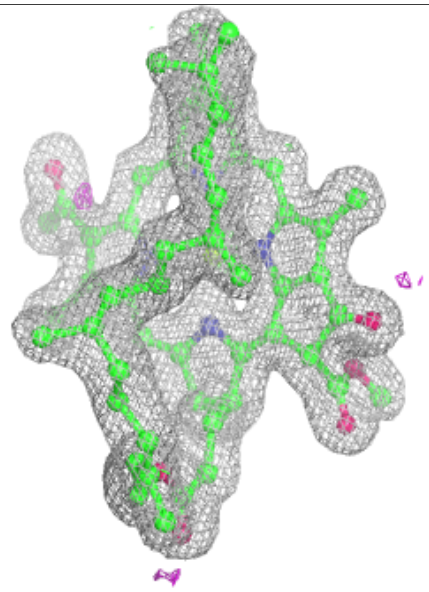
orientation to approximate a three-dimensional view.

Electron density around BCL A 405:

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

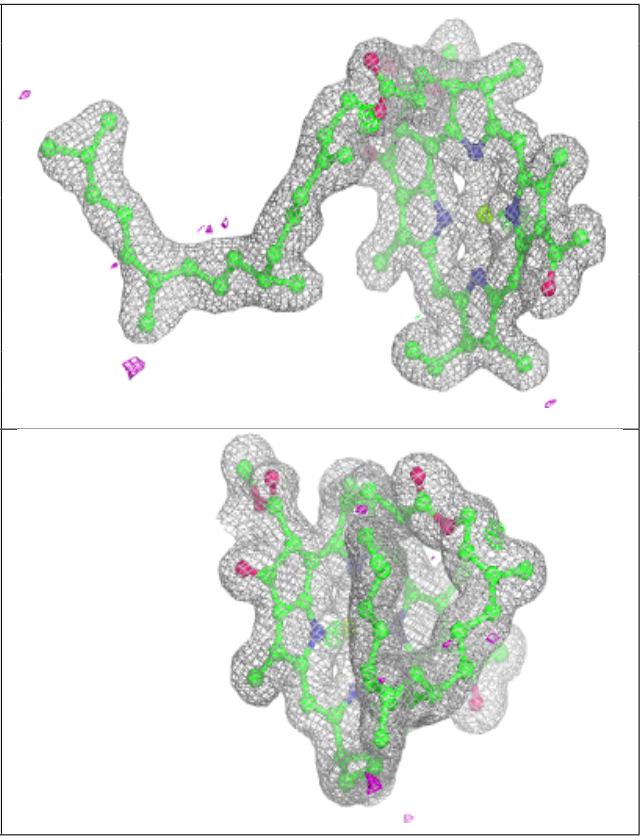






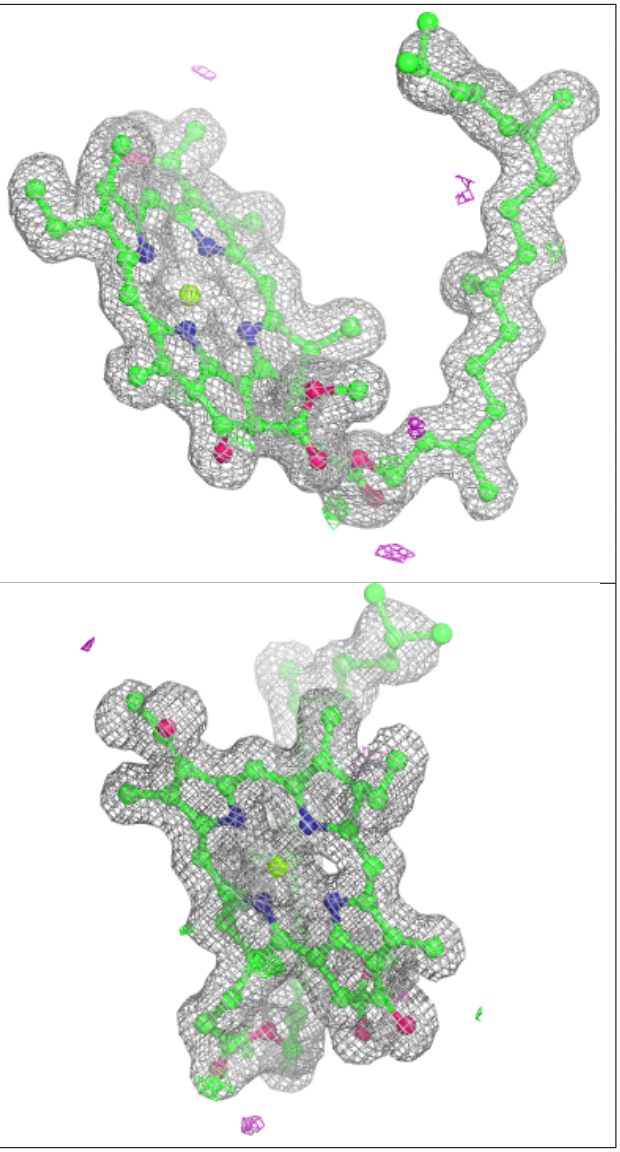
Electron density around BCL A 406 (D):

$2mF_o$-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 407 (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 407 (B):

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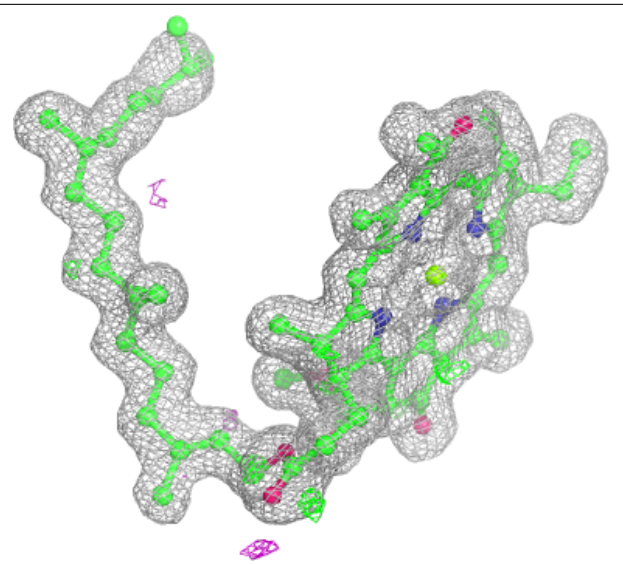
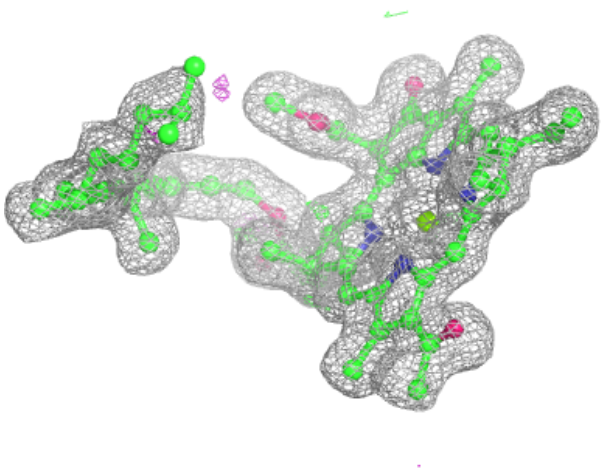
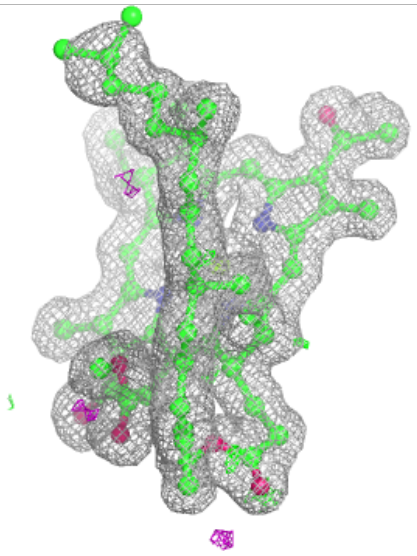
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

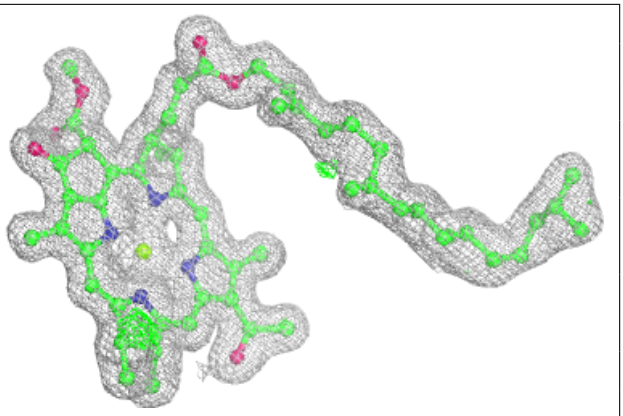


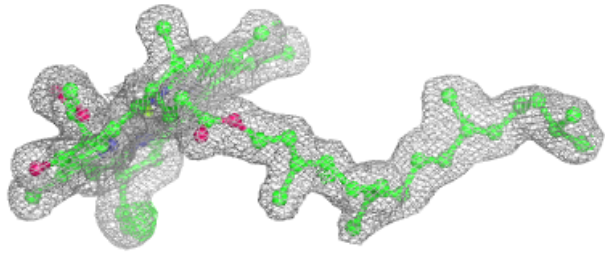


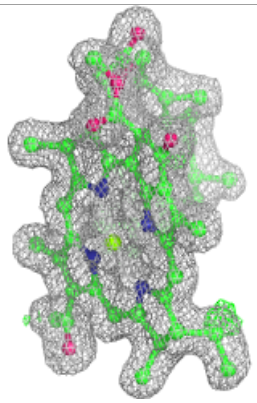


Electron density around BCL B 402:

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

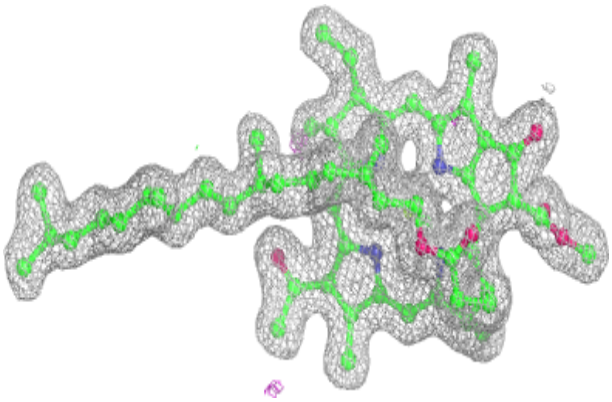


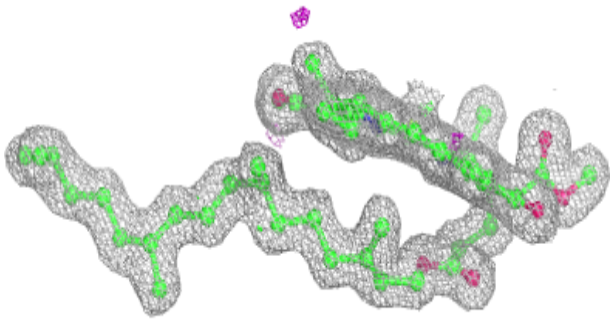


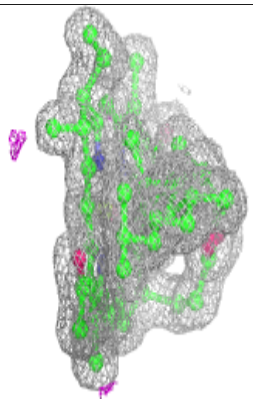


Electron density around BCL B 404:

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

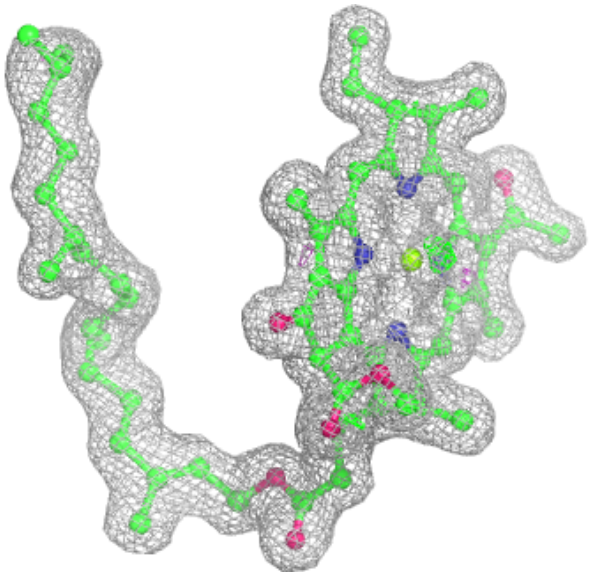


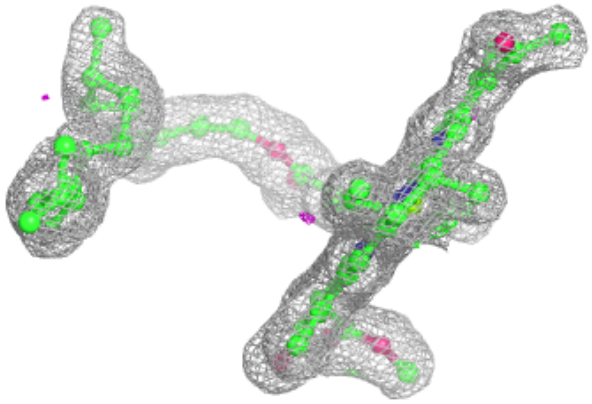




Electron density around BCL B 405:

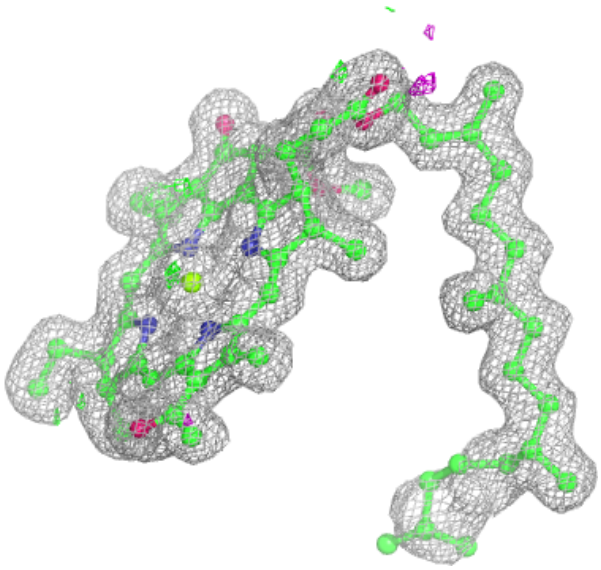
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

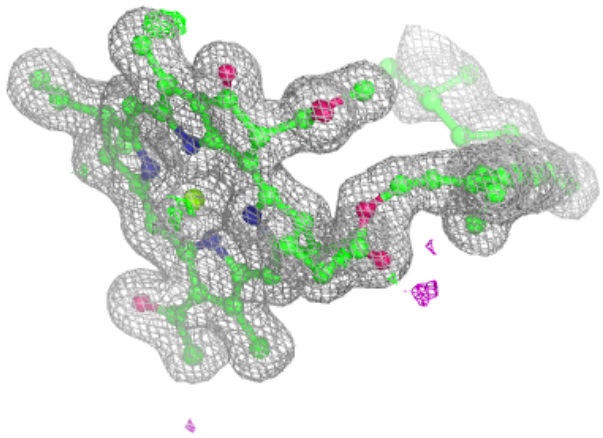


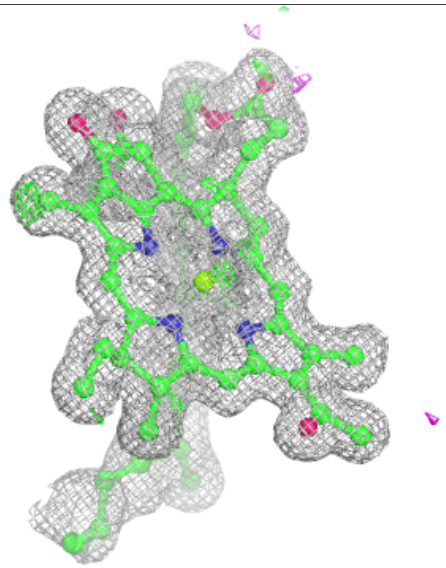


Electron density around BCL B 407 (E):

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

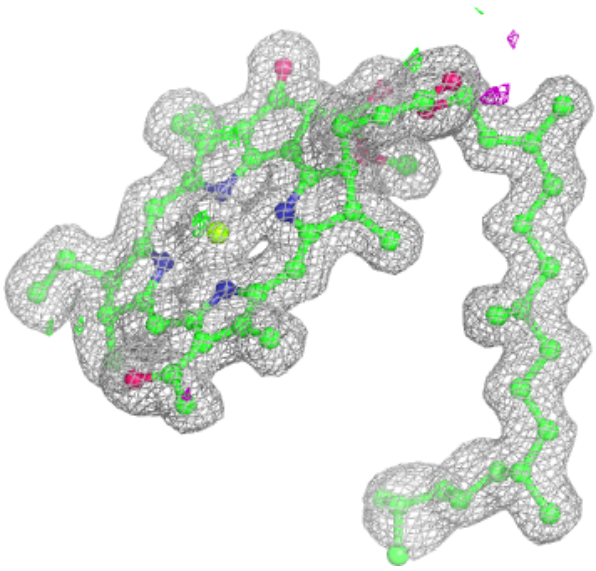


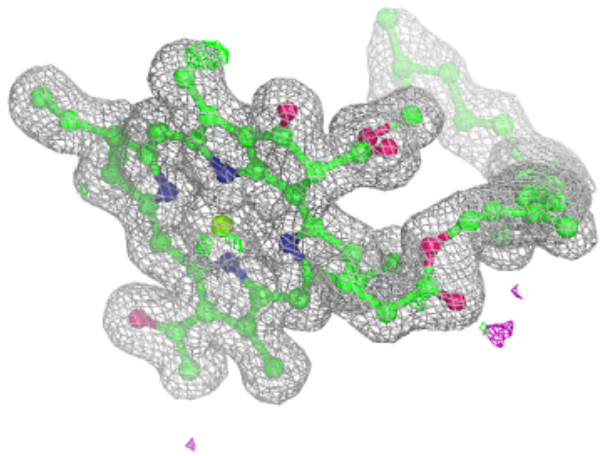


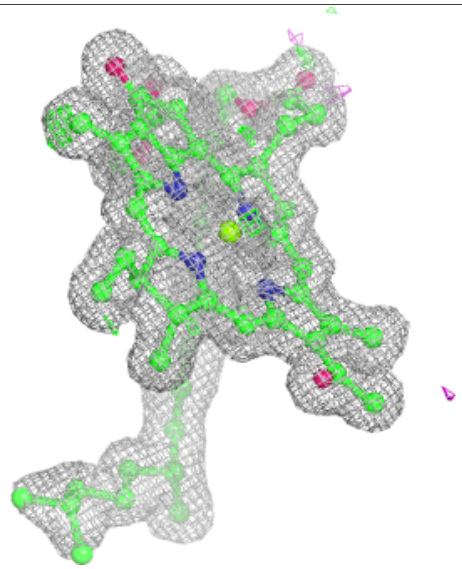


Electron density around BCL B 407 (F):

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

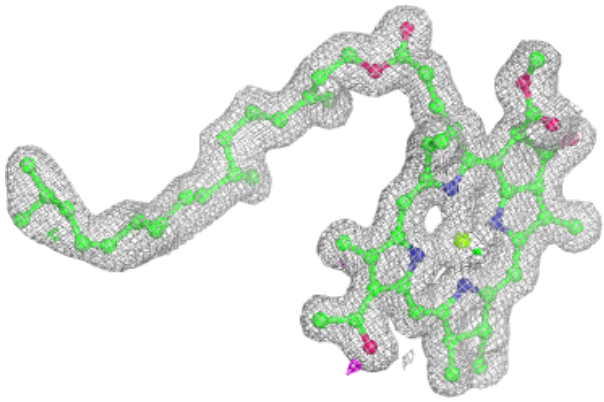


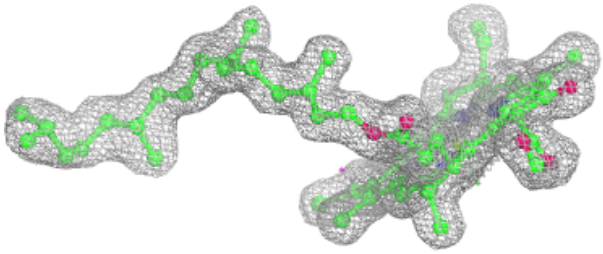


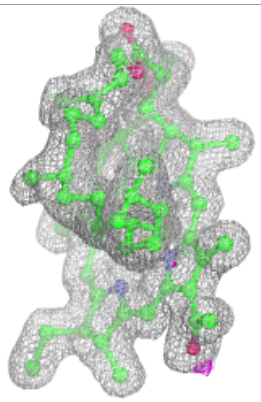


Electron density around BCL A 402:

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

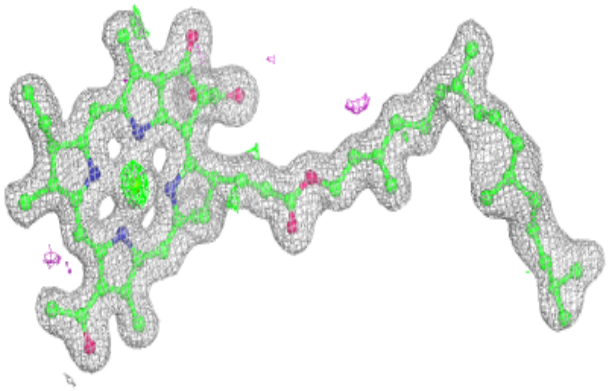


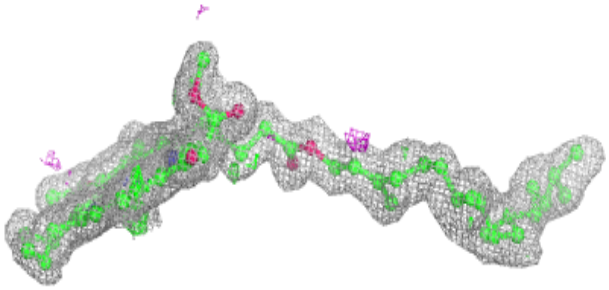


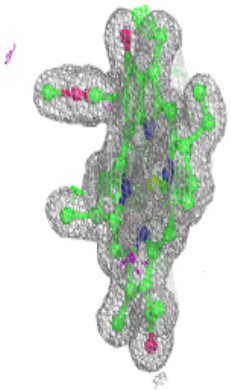


Electron density around BCL A 403 (A):

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

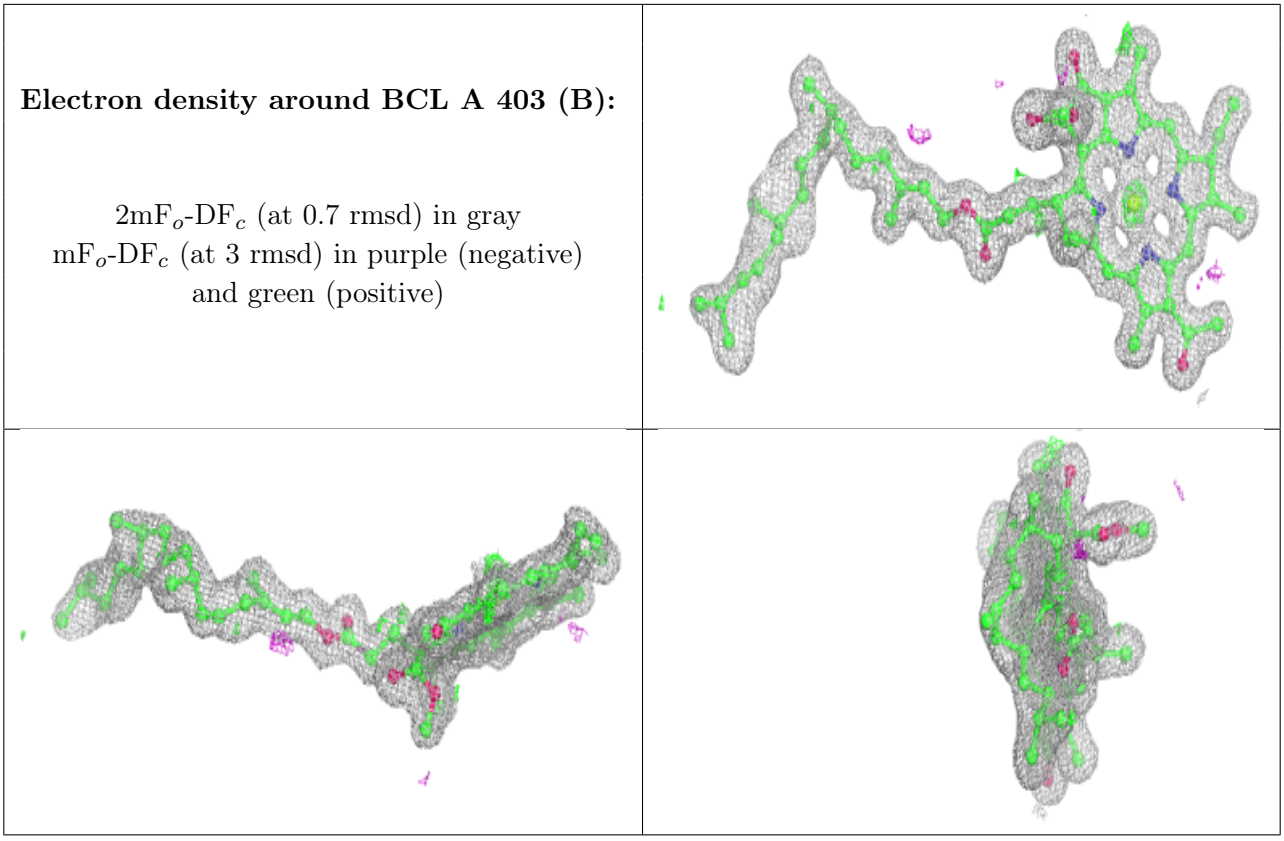






Electron density around BCL A 403 (B):

$2mF_o$-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 404:

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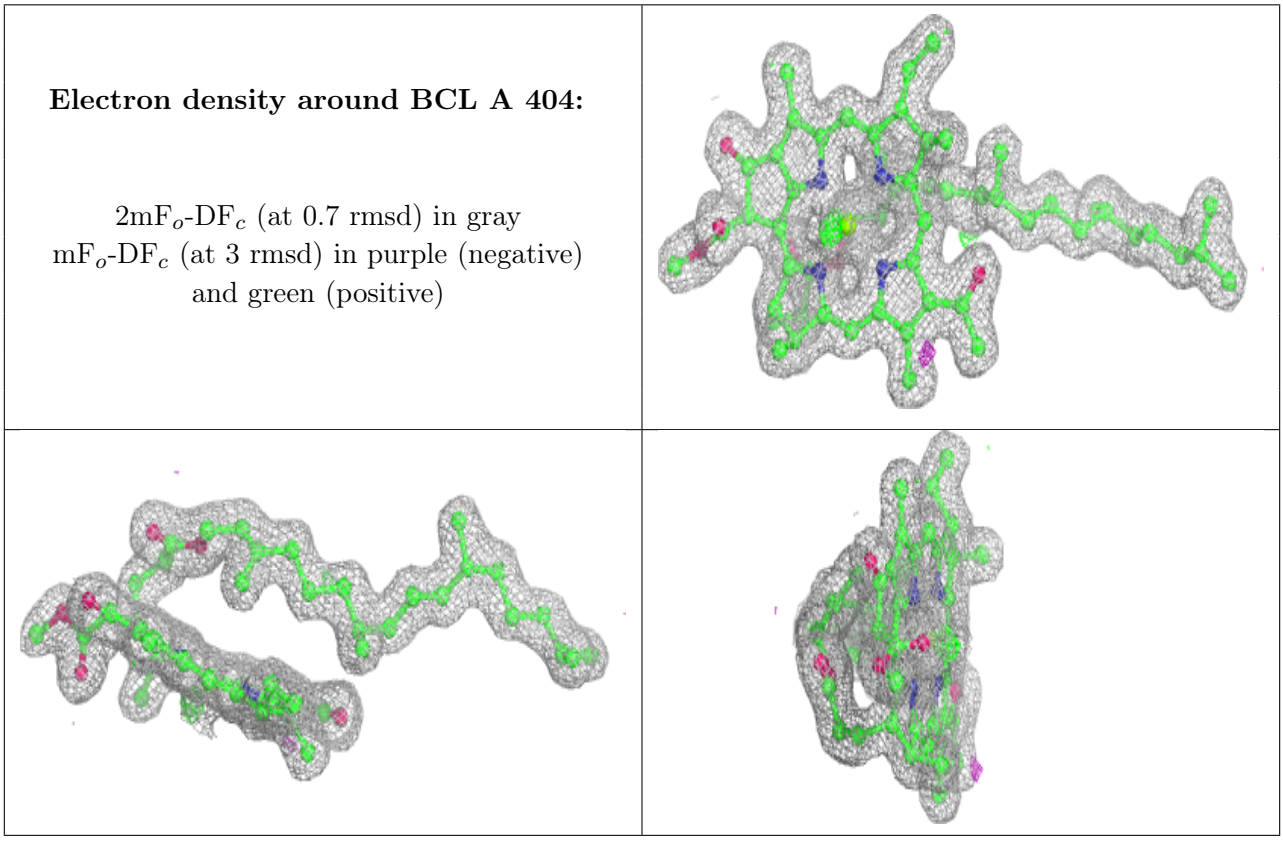
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around BCL A 401:

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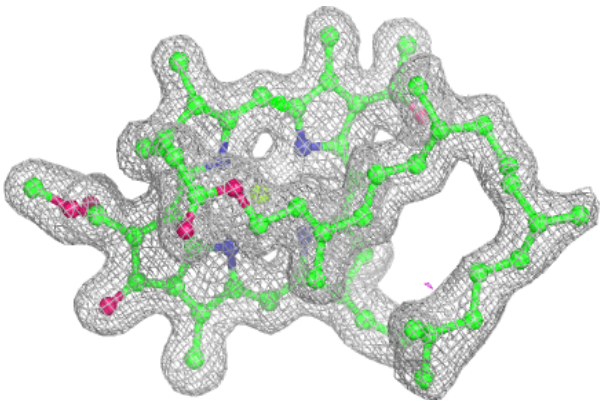
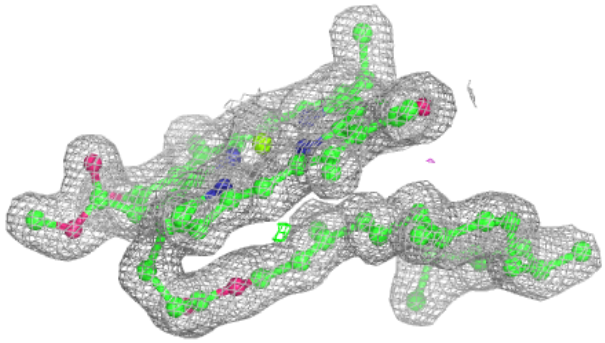
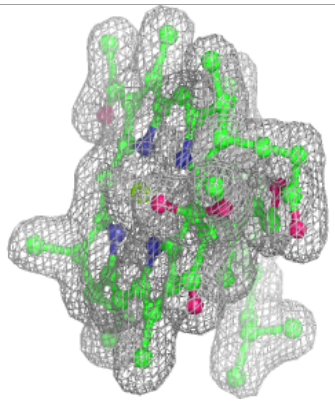
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

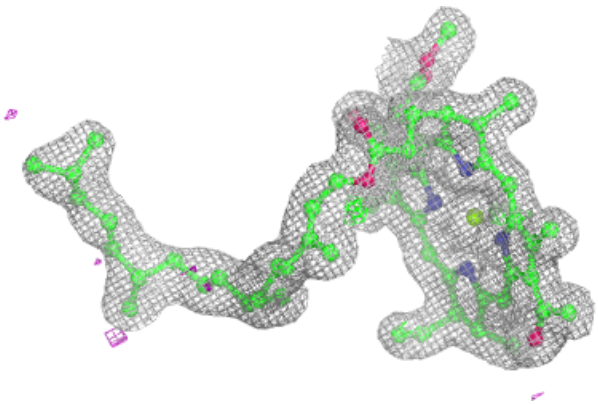


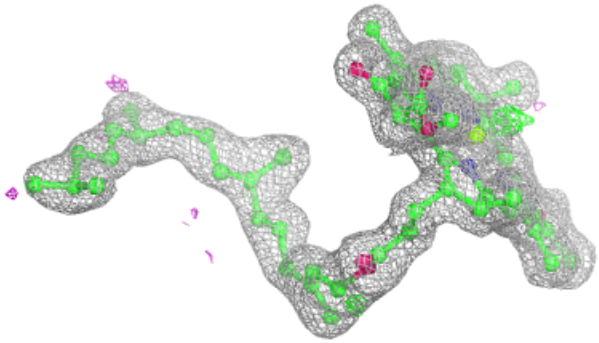


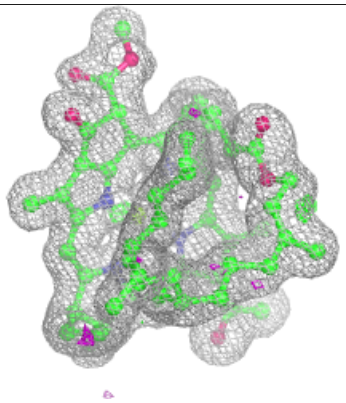


Electron density around BCL A 406 (C):

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

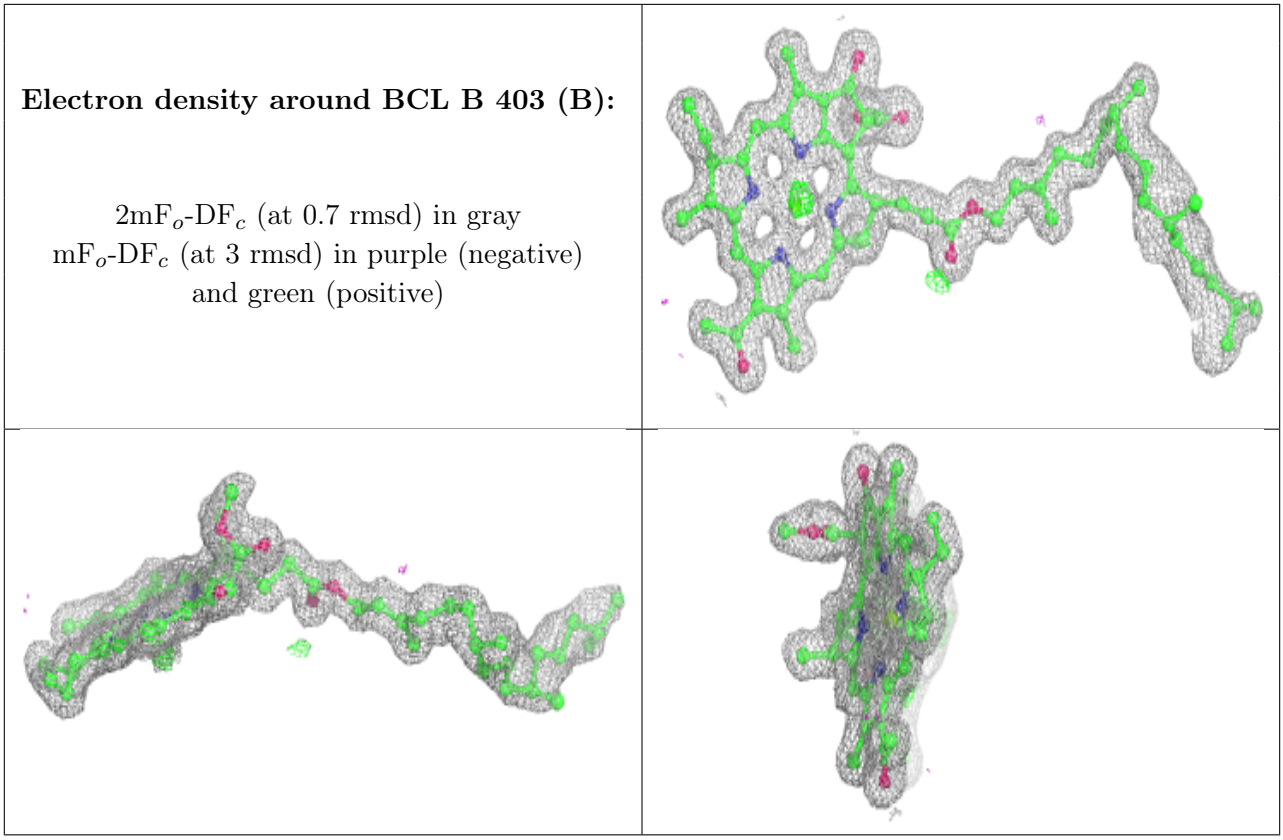






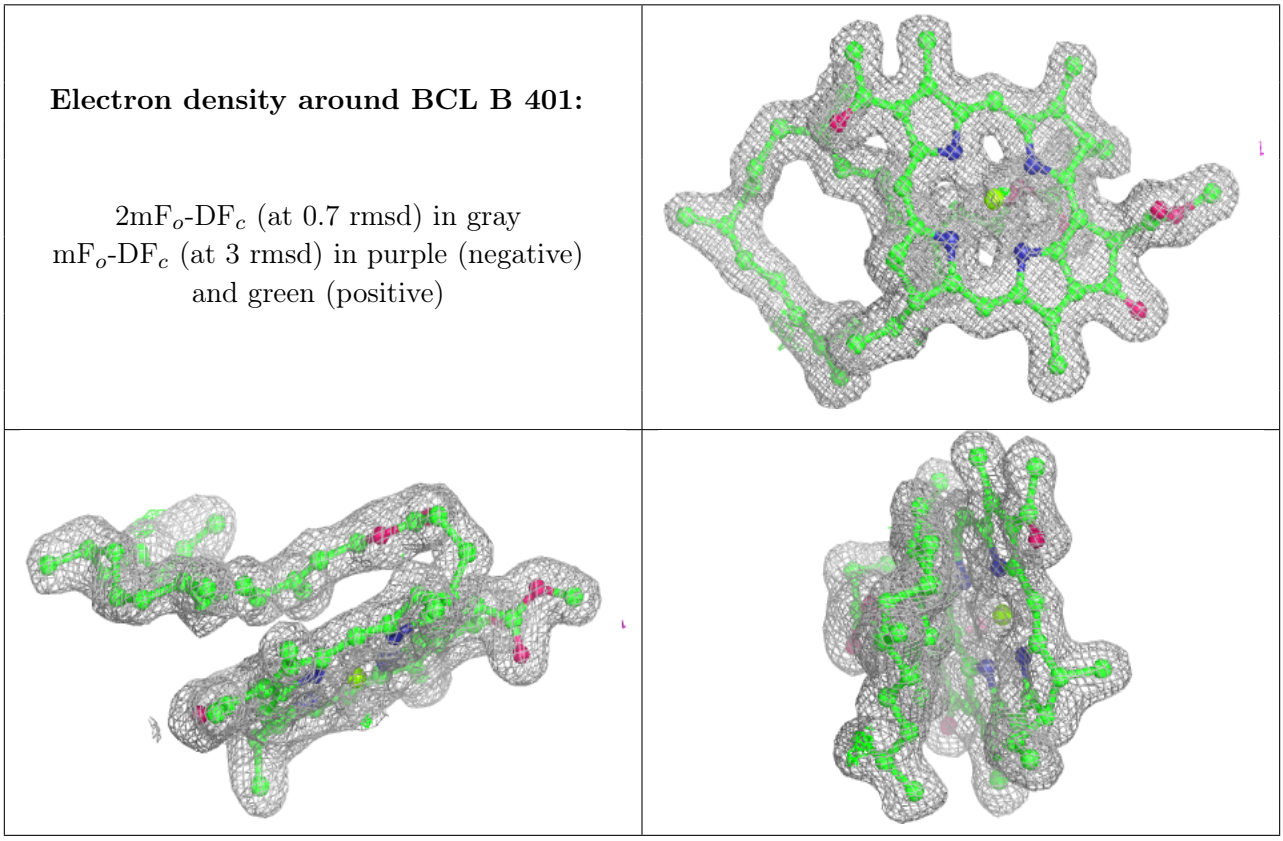
Electron density around BCL B 403 (B):

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



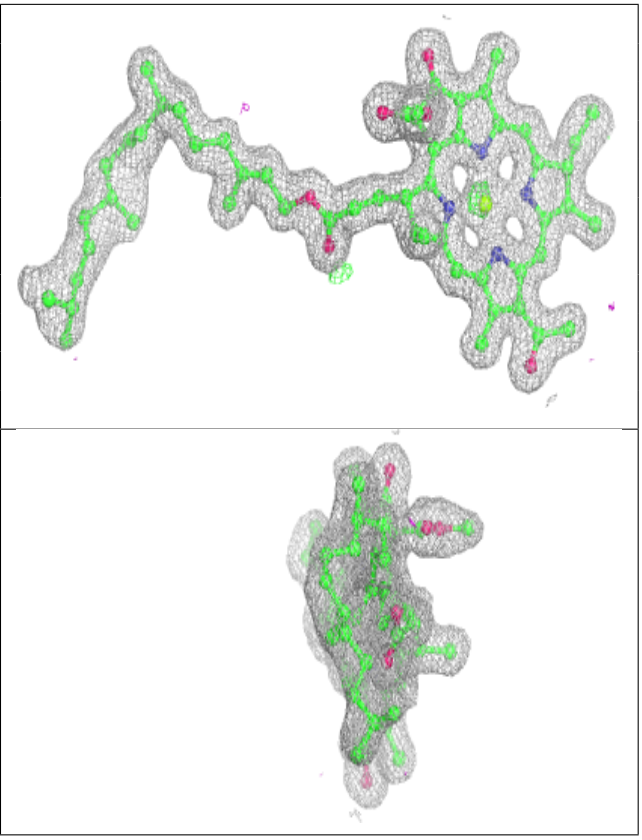
Electron density around BCL B 401:

$2mF_o$-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 B 403 (A):

$2mF_o$-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.