Full wwPDB X-ray Structure Validation Report ⓘ

Mar 24, 2022 – 12:15 pm GMT

PDB ID	:	5H8Z
Title	:	Crystal structure of the C49A C353A mutant Fenna-Matthews-Olson Protein from Chlorobaculum Tepidum
Authors	:	Lu, X.; Cuneo, M.J.; Myles, D.A.A.
Deposited on	:	2015-12-25
Resolution	:	1.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

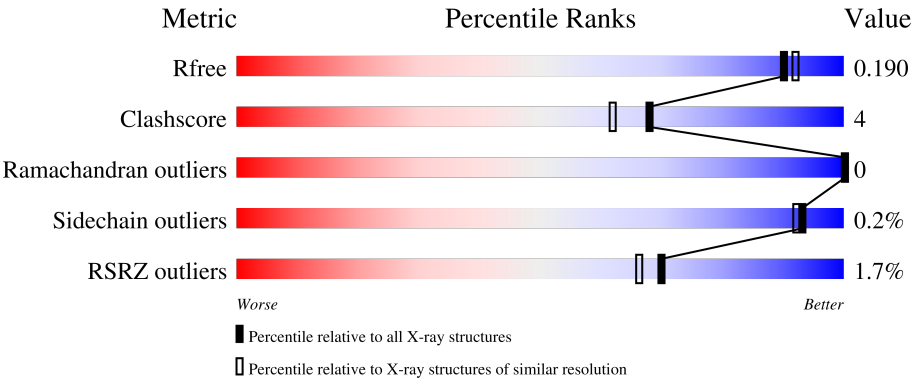
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.27
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.27

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 1.80 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	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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	365	2% 96%
1	C	365	2% 94%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 7201 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.

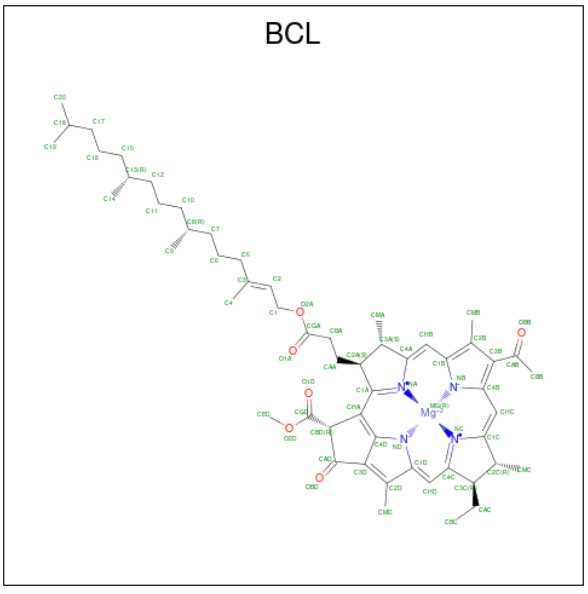
- Molecule 1 is a protein called Bacteriochlorophyll a protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	358	Total	C	N	O	S	0	9	0
			2818	1791	488	534	5			
1	C	358	Total	C	N	O	S	0	8	0
			2802	1780	487	529	6			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	49	ALA	CYS	engineered mutation	UNP Q46393
A	353	ALA	CYS	engineered mutation	UNP Q46393
C	49	ALA	CYS	engineered mutation	UNP Q46393
C	353	ALA	CYS	engineered mutation	UNP Q46393

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 71	C 60	Mg 1	N 4	O 6	0	1
2	A	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
2	A	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
2	A	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
2	A	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
2	A	1	Total 76	C 62	Mg 1	N 4	O 9	0	1
2	A	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
2	A	1	Total 46	C 35	Mg 1	N 4	O 6	0	1
2	C	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
2	C	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
2	C	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
2	C	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
2	C	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
2	C	1	Total 76	C 62	Mg 1	N 4	O 9	0	1
2	C	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
2	C	1	Total 46	C 35	Mg 1	N 4	O 6	0	1

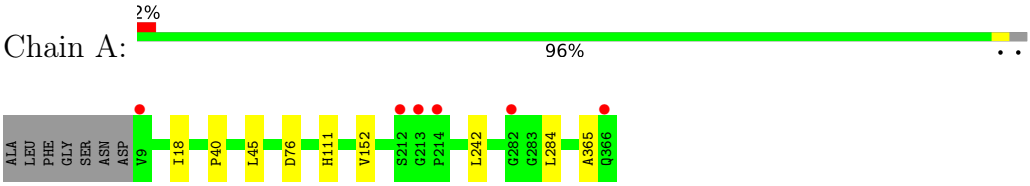
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	279	Total 279	O 279	0	0
3	C	261	Total 261	O 261	0	0

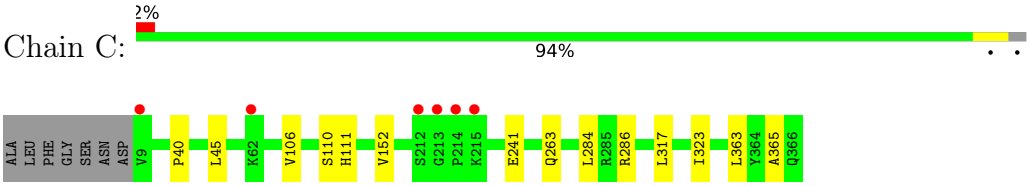
3 Residue-property plots (i)

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



• Molecule 1: Bacteriochlorophyll a protein



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 3 2	Depositor
Cell constants a, b, c, α, β, γ	168.36Å 168.36Å 168.36Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.84 – 1.80 19.84 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.9 (19.84-1.80) 95.1 (19.84-1.80)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.30 (at 1.80Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.159 , 0.189 0.162 , 0.190	Depositor DCC
R_{free} test set	1998 reflections (2.65%)	wwPDB-VP
Wilson B-factor (Å^2)	21.2	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	7201	wwPDB-VP
Average B, all atoms (Å^2)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.09% 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

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	0.69	0/2888	0.67	0/3925
1	C	0.69	2/2872 (0.1%)	0.68	0/3904
All	All	0.69	2/5760 (0.0%)	0.68	0/7829

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	110	SER	C-N	8.86	1.54	1.34
1	C	241	GLU	CD-OE2	-5.24	1.19	1.25

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	111	HIS	Mainchain

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	2818	0	2683	6	0
1	C	2802	0	2663	7	0
2	A	523	0	439	17	0
2	C	518	0	487	15	0
3	A	279	0	0	1	0
3	C	261	0	0	1	0
All	All	7201	0	6272	42	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 (42) 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:C:407:BCL:HBB2	2:C:407:BCL:HMB1	1.83	0.60
2:A:402:BCL:HMB1	2:A:402:BCL:HBB3	1.84	0.59
2:A:407:BCL:HMB1	2:A:407:BCL:HBB2	1.85	0.58
1:C:284:LEU:HD23	1:C:365:ALA:HB2	1.90	0.54
1:C:263:GLN:NE2	3:C:501:HOH:O	2.19	0.52
1:C:106:VAL:HB	2:C:401:BCL:HED2	1.94	0.50
2:A:403:BCL:HHC	2:A:403:BCL:CBB	2.42	0.49
2:C:404:BCL:CBB	2:C:404:BCL:HMB1	2.43	0.49
1:A:18:ILE:HD11	2:A:404:BCL:HAA1	1.94	0.49
2:A:405:BCL:H62	2:A:405:BCL:H102	1.55	0.49
2:C:405:BCL:HMB1	2:C:405:BCL:HBB2	1.96	0.48
1:A:76:ASP:OD2	3:A:501:HOH:O	2.20	0.48
2:A:408[B]:BCL:HMB1	2:A:408[B]:BCL:HBB3	1.95	0.48
2:C:403:BCL:HHC	2:C:403:BCL:CBB	2.46	0.46
1:A:40:PRO:HG2	1:A:45:LEU:HD21	1.96	0.46
2:C:408[B]:BCL:HMB1	2:C:408[B]:BCL:HBB3	1.98	0.46
2:A:404:BCL:HMB1	2:A:404:BCL:HBB3	1.97	0.46
2:C:405:BCL:H193	2:C:407:BCL:H18	1.98	0.46
1:A:242:LEU:C	1:A:242:LEU:HD12	2.36	0.45
2:C:401:BCL:HMB1	2:C:401:BCL:HBB2	1.98	0.45
1:C:286:ARG:HB3	1:C:363:LEU:HD23	1.99	0.45
2:C:403:BCL:H42	2:C:405:BCL:H151	1.97	0.45
1:C:40:PRO:HG2	1:C:45:LEU:HD21	1.99	0.44
2:A:405:BCL:HBB2	2:A:405:BCL:HMB1	1.98	0.44
2:C:402:BCL:HMB1	2:C:402:BCL:HBB3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:404:BCL:HMB1	2:C:404:BCL:HBB3	2.00	0.44
2:A:402:BCL:HMB1	2:A:402:BCL:CBB	2.49	0.43
2:C:402:BCL:H203	2:C:402:BCL:H162	1.73	0.43
2:A:403:BCL:H61	2:A:403:BCL:H102	1.83	0.42
2:A:402:BCL:HAC2	2:A:407:BCL:H71	2.00	0.42
1:C:152:VAL:HB	2:C:401:BCL:HBB3	2.00	0.42
1:C:317:LEU:HD11	1:C:323:ILE:HG13	2.02	0.42
2:A:405:BCL:OBB	2:A:405:BCL:HHC	2.21	0.41
2:C:403:BCL:HHC	2:C:403:BCL:HBB2	2.02	0.41
2:A:402:BCL:H162	2:A:402:BCL:H122	1.94	0.41
2:A:407:BCL:HMB1	2:A:407:BCL:CBB	2.51	0.40
1:A:284:LEU:HD23	1:A:365:ALA:HB2	2.04	0.40
2:A:402:BCL:H91	2:A:403:BCL:H101	2.02	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	365/365 (100%)	357 (98%)	8 (2%)	0	100	100
1	C	364/365 (100%)	358 (98%)	6 (2%)	0	100	100
All	All	729/730 (100%)	715 (98%)	14 (2%)	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	290/299 (97%)	289 (100%)	1 (0%)	92 91
1	C	287/299 (96%)	287 (100%)	0	100 100
All	All	577/598 (96%)	576 (100%)	1 (0%)	93 92

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	111	HIS

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

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

19 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	C	403	-	58,74,74	1.57	7 (12%)	69,115,115	1.56	11 (15%)
2	BCL	A	403	-	58,74,74	1.59	10 (17%)	69,115,115	1.71	12 (17%)
2	BCL	A	402	3	58,74,74	1.49	6 (10%)	69,115,115	1.51	11 (15%)
2	BCL	C	406[C]	-	58,74,74	1.39	7 (12%)	69,115,115	1.56	11 (15%)
2	BCL	C	408[B]	1	35,54,74	1.71	5 (14%)	41,91,115	1.78	12 (29%)
2	BCL	A	401[B]	-	58,74,74	1.45	6 (10%)	69,115,115	1.52	13 (18%)
2	BCL	A	408[B]	1	35,54,74	1.52	4 (11%)	41,91,115	1.69	11 (26%)
2	BCL	A	407	-	58,74,74	1.45	6 (10%)	69,115,115	1.68	17 (24%)
2	BCL	A	406[D]	-	58,74,74	1.45	4 (6%)	69,115,115	1.59	12 (17%)
2	BCL	A	404	-	58,74,74	1.35	5 (8%)	69,115,115	1.46	12 (17%)
2	BCL	C	405	1	58,74,74	1.39	5 (8%)	69,115,115	1.69	17 (24%)
2	BCL	C	407	-	58,74,74	1.43	4 (6%)	69,115,115	1.42	9 (13%)
2	BCL	C	401	-	58,74,74	1.39	6 (10%)	69,115,115	1.51	11 (15%)
2	BCL	A	401[A]	-	58,74,74	1.43	6 (10%)	69,115,115	1.53	13 (18%)
2	BCL	A	406[C]	-	58,74,74	1.44	5 (8%)	69,115,115	1.55	13 (18%)
2	BCL	A	405	1	58,74,74	1.35	4 (6%)	69,115,115	1.44	13 (18%)
2	BCL	C	402	3	58,74,74	1.39	5 (8%)	69,115,115	1.52	13 (18%)
2	BCL	C	406[D]	-	58,74,74	1.43	8 (13%)	69,115,115	1.62	11 (15%)
2	BCL	C	404	-	58,74,74	1.48	5 (8%)	69,115,115	1.60	11 (15%)

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	C	403	-	-	9/37/137/137	-
2	BCL	A	403	-	-	6/37/137/137	-
2	BCL	A	402	3	-	3/37/137/137	-
2	BCL	C	406[C]	-	-	3/37/137/137	-
2	BCL	C	408[B]	1	-	2/11/113/137	-
2	BCL	A	401[B]	-	-	2/37/137/137	-
2	BCL	A	408[B]	1	-	2/11/113/137	-
2	BCL	A	407	-	-	9/37/137/137	-
2	BCL	A	406[D]	-	-	4/37/137/137	-
2	BCL	A	404	-	-	0/37/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BCL	C	405	1	-	7/37/137/137	-
2	BCL	C	407	-	-	4/37/137/137	-
2	BCL	C	401	-	-	2/37/137/137	-
2	BCL	A	401[A]	-	-	2/37/137/137	-
2	BCL	A	406[C]	-	-	5/37/137/137	-
2	BCL	A	405	1	-	7/37/137/137	-
2	BCL	C	402	3	-	5/37/137/137	-
2	BCL	C	406[D]	-	-	2/37/137/137	-
2	BCL	C	404	-	-	0/37/137/137	-

All (108) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	402	BCL	C1B-NB	6.44	1.40	1.35
2	C	404	BCL	C1B-NB	6.20	1.40	1.35
2	A	406[C]	BCL	C1B-NB	6.11	1.40	1.35
2	A	406[D]	BCL	C1B-NB	6.11	1.40	1.35
2	C	403	BCL	C1B-NB	6.06	1.40	1.35
2	A	407	BCL	MG-NA	6.01	2.20	2.06
2	A	401[A]	BCL	C1B-NB	5.44	1.40	1.35
2	A	401[B]	BCL	C1B-NB	5.44	1.40	1.35
2	C	407	BCL	C1B-NB	5.33	1.40	1.35
2	C	408[B]	BCL	C1B-NB	5.29	1.39	1.35
2	C	402	BCL	C1B-NB	5.25	1.39	1.35
2	C	402	BCL	MG-NA	5.23	2.18	2.06
2	A	405	BCL	C1B-NB	5.20	1.39	1.35
2	A	403	BCL	C1B-NB	5.19	1.39	1.35
2	C	405	BCL	MG-NA	5.18	2.18	2.06
2	A	408[B]	BCL	C1B-NB	5.17	1.39	1.35
2	A	403	BCL	MG-NA	5.17	2.18	2.06
2	A	401[A]	BCL	MG-NA	5.11	2.18	2.06
2	A	401[B]	BCL	MG-NA	5.11	2.18	2.06
2	C	404	BCL	MG-NA	5.10	2.18	2.06
2	C	407	BCL	MG-NA	5.09	2.18	2.06
2	C	406[C]	BCL	MG-NA	4.95	2.18	2.06
2	C	406[D]	BCL	MG-NA	4.95	2.18	2.06
2	C	408[B]	BCL	MG-NA	4.91	2.17	2.06
2	A	404	BCL	MG-NA	4.88	2.17	2.06
2	C	405	BCL	C1B-NB	4.83	1.39	1.35
2	C	401	BCL	MG-NA	4.78	2.17	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	402	BCL	MG-NA	4.67	2.17	2.06
2	C	401	BCL	C1B-NB	4.65	1.39	1.35
2	C	403	BCL	MG-NA	4.64	2.17	2.06
2	A	405	BCL	MG-NA	4.63	2.17	2.06
2	A	406[C]	BCL	MG-NA	4.55	2.17	2.06
2	A	406[D]	BCL	MG-NA	4.55	2.17	2.06
2	C	406[C]	BCL	C1B-NB	4.48	1.39	1.35
2	C	406[D]	BCL	C1B-NB	4.48	1.39	1.35
2	A	408[B]	BCL	MG-NA	4.46	2.16	2.06
2	A	404	BCL	C1B-NB	4.40	1.39	1.35
2	A	406[C]	BCL	MG-NC	4.18	2.16	2.06
2	A	406[D]	BCL	MG-NC	4.18	2.16	2.06
2	C	403	BCL	C2-C3	-4.05	1.23	1.33
2	A	405	BCL	MG-NC	3.97	2.15	2.06
2	C	406[C]	BCL	MG-NC	3.96	2.15	2.06
2	C	406[D]	BCL	MG-NC	3.96	2.15	2.06
2	A	407	BCL	C1B-NB	3.85	1.38	1.35
2	C	401	BCL	MG-NC	3.82	2.15	2.06
2	C	405	BCL	MG-NC	3.82	2.15	2.06
2	A	403	BCL	C4B-NB	3.65	1.38	1.35
2	C	407	BCL	MG-NC	3.63	2.14	2.06
2	A	403	BCL	OBD-CAD	3.55	1.27	1.22
2	C	404	BCL	MG-NC	3.48	2.14	2.06
2	C	402	BCL	OBD-CAD	3.31	1.26	1.22
2	C	408[B]	BCL	MG-NC	3.29	2.14	2.06
2	A	404	BCL	MG-NC	3.18	2.13	2.06
2	A	407	BCL	MG-NC	3.15	2.13	2.06
2	A	408[B]	BCL	MG-NC	3.10	2.13	2.06
2	C	402	BCL	MG-NC	3.07	2.13	2.06
2	A	403	BCL	C5-C3	3.07	1.57	1.51
2	A	404	BCL	C4B-NB	3.00	1.37	1.35
2	A	402	BCL	MG-NC	3.00	2.13	2.06
2	C	405	BCL	O2A-CGA	-2.93	1.24	1.33
2	A	407	BCL	C4B-NB	2.91	1.37	1.35
2	C	406[C]	BCL	C4B-NB	2.87	1.37	1.35
2	C	406[D]	BCL	C4B-NB	2.87	1.37	1.35
2	A	402	BCL	O2A-CGA	-2.86	1.24	1.33
2	C	404	BCL	C5-C3	2.78	1.57	1.51
2	A	401[A]	BCL	MG-NC	2.75	2.12	2.06
2	A	401[B]	BCL	MG-NC	2.75	2.12	2.06
2	C	406[C]	BCL	CAC-C3C	2.73	1.59	1.54
2	C	406[D]	BCL	CAC-C3C	2.73	1.59	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	404	BCL	C1-C2	2.73	1.57	1.49
2	C	408[B]	BCL	C4B-NB	2.71	1.37	1.35
2	C	402	BCL	C4B-NB	2.69	1.37	1.35
2	A	402	BCL	OBD-CAD	2.64	1.26	1.22
2	A	403	BCL	MG-NC	2.56	2.12	2.06
2	C	401	BCL	C4B-NB	2.53	1.37	1.35
2	C	403	BCL	MG-NC	2.51	2.12	2.06
2	C	405	BCL	C4B-NB	2.48	1.37	1.35
2	C	403	BCL	C4B-NB	2.44	1.37	1.35
2	C	406[C]	BCL	O2A-CGA	-2.40	1.26	1.33
2	C	406[D]	BCL	O2A-CGA	-2.40	1.26	1.33
2	A	403	BCL	C2-C3	-2.38	1.27	1.33
2	A	402	BCL	C5-C3	2.29	1.56	1.51
2	C	401	BCL	CAA-C2A	2.29	1.58	1.54
2	A	403	BCL	CAC-C3C	2.28	1.58	1.54
2	A	401[A]	BCL	C9-C8	2.26	1.60	1.52
2	A	401[B]	BCL	C9-C8	2.26	1.60	1.52
2	A	407	BCL	C1-C2	2.26	1.55	1.49
2	A	403	BCL	C6-C5	-2.26	1.43	1.52
2	C	406[C]	BCL	C3C-C4C	2.25	1.54	1.51
2	C	406[D]	BCL	C3C-C4C	2.25	1.54	1.51
2	C	408[B]	BCL	OBB-CAB	2.25	1.29	1.22
2	C	404	BCL	C1-C2	2.20	1.55	1.49
2	A	403	BCL	C3B-CAB	-2.19	1.43	1.49
2	A	406[C]	BCL	C4B-NB	2.19	1.37	1.35
2	A	406[D]	BCL	C4B-NB	2.19	1.37	1.35
2	A	401[A]	BCL	OBD-CAD	2.18	1.25	1.22
2	A	401[B]	BCL	OBD-CAD	2.18	1.25	1.22
2	A	401[A]	BCL	CAA-C2A	2.17	1.58	1.54
2	A	401[B]	BCL	CAA-C2A	2.17	1.58	1.54
2	C	407	BCL	O2A-CGA	-2.17	1.27	1.33
2	A	408[B]	BCL	C3D-CAD	-2.15	1.40	1.46
2	C	403	BCL	C3D-CAD	-2.12	1.40	1.46
2	C	401	BCL	CBD-CGD	-2.10	1.45	1.52
2	A	407	BCL	O1A-CGA	-2.08	1.16	1.22
2	A	406[C]	BCL	OBD-CAD	2.06	1.25	1.22
2	C	406[D]	BCL	OBD-CAD	2.03	1.25	1.22
2	A	405	BCL	C1-C2	2.01	1.55	1.49
2	C	403	BCL	OBD-CAD	2.00	1.25	1.22

All (233) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	403	BCL	C6-C7-C8	-6.06	96.32	115.92
2	C	406[C]	BCL	C4A-NA-C1A	5.37	109.12	106.71
2	C	406[D]	BCL	C4A-NA-C1A	5.37	109.12	106.71
2	C	404	BCL	CAD-C3D-C4D	-4.99	105.69	108.47
2	A	407	BCL	C4A-NA-C1A	4.75	108.84	106.71
2	C	406[D]	BCL	CAD-C3D-C4D	-4.71	105.84	108.47
2	A	406[C]	BCL	C4A-NA-C1A	4.66	108.80	106.71
2	A	406[D]	BCL	C4A-NA-C1A	4.66	108.80	106.71
2	A	403	BCL	C4A-NA-C1A	4.61	108.78	106.71
2	C	407	BCL	C4A-NA-C1A	4.50	108.73	106.71
2	A	406[C]	BCL	C16-C15-C13	-4.48	101.42	115.92
2	A	406[D]	BCL	C16-C15-C13	-4.48	101.42	115.92
2	C	405	BCL	C4-C3-C5	-4.48	107.74	115.27
2	C	401	BCL	C4A-NA-C1A	4.47	108.71	106.71
2	C	403	BCL	C4A-NA-C1A	4.40	108.69	106.71
2	A	404	BCL	C4A-NA-C1A	4.37	108.67	106.71
2	A	401[A]	BCL	CMB-C2B-C1B	-4.35	121.78	128.46
2	A	401[B]	BCL	CMB-C2B-C1B	-4.35	121.78	128.46
2	A	402	BCL	C1-C2-C3	-4.30	118.61	126.04
2	A	402	BCL	CMB-C2B-C1B	-4.30	121.86	128.46
2	C	402	BCL	CMB-C2B-C1B	-4.27	121.91	128.46
2	A	406[D]	BCL	CAD-C3D-C4D	-4.26	106.09	108.47
2	A	407	BCL	C6-C5-C3	4.26	124.64	113.45
2	C	406[C]	BCL	CMB-C2B-C1B	-4.20	122.00	128.46
2	C	406[D]	BCL	CMB-C2B-C1B	-4.20	122.00	128.46
2	A	403	BCL	CMB-C2B-C1B	-4.19	122.03	128.46
2	C	403	BCL	CMB-C2B-C1B	-4.16	122.08	128.46
2	A	401[A]	BCL	OBD-CAD-CBD	-4.07	120.08	125.89
2	A	401[B]	BCL	OBD-CAD-CBD	-4.07	120.08	125.89
2	C	404	BCL	C4A-NA-C1A	3.98	108.50	106.71
2	C	403	BCL	OBD-CAD-CBD	-3.97	120.23	125.89
2	C	401	BCL	OBD-CAD-CBD	-3.95	120.26	125.89
2	C	404	BCL	C1C-NC-C4C	3.87	108.44	106.71
2	A	407	BCL	O2A-CGA-O1A	-3.85	113.87	123.59
2	C	401	BCL	C1-C2-C3	-3.85	119.38	126.04
2	C	408[B]	BCL	C4A-NA-C1A	3.83	108.43	106.71
2	A	404	BCL	CMB-C2B-C1B	-3.82	122.60	128.46
2	A	405	BCL	CMB-C2B-C1B	-3.76	122.68	128.46
2	C	408[B]	BCL	CMB-C2B-C1B	-3.75	122.71	128.46
2	A	407	BCL	CMB-C2B-C1B	-3.65	122.85	128.46
2	A	408[B]	BCL	CMB-C2B-C1B	-3.65	122.86	128.46
2	C	402	BCL	C4A-NA-C1A	3.63	108.34	106.71
2	C	404	BCL	OBD-CAD-CBD	-3.62	120.73	125.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	405	BCL	OBD-CAD-CBD	-3.59	120.77	125.89
2	C	402	BCL	C1-C2-C3	-3.59	119.84	126.04
2	A	402	BCL	CAD-C3D-C4D	-3.58	106.47	108.47
2	A	406[C]	BCL	C1C-NC-C4C	3.57	108.31	106.71
2	A	406[D]	BCL	C1C-NC-C4C	3.57	108.31	106.71
2	A	406[C]	BCL	CMB-C2B-C1B	-3.54	123.02	128.46
2	A	406[D]	BCL	CMB-C2B-C1B	-3.54	123.02	128.46
2	C	408[B]	BCL	CAD-C3D-C4D	-3.51	106.51	108.47
2	A	403	BCL	OBD-CAD-CBD	-3.50	120.89	125.89
2	A	401[A]	BCL	C4A-NA-C1A	3.50	108.28	106.71
2	A	401[B]	BCL	C4A-NA-C1A	3.50	108.28	106.71
2	C	401	BCL	CMB-C2B-C1B	-3.47	123.13	128.46
2	C	405	BCL	CAD-C3D-C4D	-3.43	106.56	108.47
2	A	403	BCL	CHA-C1A-NA	-3.38	118.66	126.40
2	A	402	BCL	OBD-CAD-CBD	-3.36	121.09	125.89
2	C	402	BCL	OBD-CAD-CBD	-3.35	121.10	125.89
2	A	407	BCL	CAD-C3D-C4D	-3.27	106.64	108.47
2	C	404	BCL	CMD-C2D-C3D	3.27	130.80	124.68
2	A	405	BCL	OBD-CAD-CBD	-3.26	121.23	125.89
2	C	405	BCL	CHA-C1A-NA	-3.26	118.94	126.40
2	A	401[A]	BCL	CMB-C2B-C3B	3.25	130.77	124.68
2	A	401[B]	BCL	CMB-C2B-C3B	3.25	130.77	124.68
2	C	407	BCL	CMB-C2B-C1B	-3.25	123.46	128.46
2	A	402	BCL	CMB-C2B-C3B	3.25	130.76	124.68
2	A	408[B]	BCL	OBD-CAD-CBD	-3.25	121.26	125.89
2	A	405	BCL	CAD-C3D-C4D	-3.25	106.66	108.47
2	C	403	BCL	CAD-C3D-C4D	-3.24	106.67	108.47
2	A	406[C]	BCL	OBD-CAD-CBD	-3.21	121.30	125.89
2	A	402	BCL	C4A-NA-C1A	3.20	108.14	106.71
2	C	405	BCL	CMD-C2D-C3D	3.19	130.65	124.68
2	A	401[A]	BCL	CHA-C1A-NA	-3.19	119.09	126.40
2	A	401[B]	BCL	CHA-C1A-NA	-3.19	119.09	126.40
2	C	402	BCL	CAD-C3D-C4D	-3.17	106.70	108.47
2	C	405	BCL	C7-C6-C5	-3.16	104.77	113.36
2	C	404	BCL	CMB-C2B-C1B	-3.15	123.62	128.46
2	C	405	BCL	CMB-C2B-C1B	-3.14	123.64	128.46
2	C	405	BCL	C6-C5-C3	3.13	121.67	113.45
2	C	406[C]	BCL	OBD-CAD-CBD	-3.11	121.45	125.89
2	A	401[A]	BCL	C1-C2-C3	-3.11	120.67	126.04
2	A	401[B]	BCL	C1-C2-C3	-3.11	120.67	126.04
2	A	405	BCL	CHA-C1A-NA	-3.10	119.30	126.40
2	C	406[C]	BCL	CAD-C3D-C4D	-3.09	106.75	108.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	403	BCL	CHA-C1A-NA	-3.08	119.35	126.40
2	C	401	BCL	CHA-C1A-NA	-3.07	119.36	126.40
2	C	407	BCL	OBD-CAD-CBD	-3.06	121.52	125.89
2	A	404	BCL	CAD-C3D-C4D	-3.06	106.77	108.47
2	C	404	BCL	CHA-C1A-NA	-3.05	119.41	126.40
2	A	401[A]	BCL	C2A-C1A-CHA	3.05	129.19	123.86
2	A	401[B]	BCL	C2A-C1A-CHA	3.05	129.19	123.86
2	A	403	BCL	CAD-C3D-C4D	-3.03	106.78	108.47
2	A	404	BCL	CHA-C1A-NA	-3.02	119.47	126.40
2	C	408[B]	BCL	CHA-C1A-NA	-3.02	119.49	126.40
2	A	403	BCL	CMB-C2B-C3B	3.01	130.32	124.68
2	C	407	BCL	C1C-NC-C4C	3.01	108.06	106.71
2	C	405	BCL	C4A-NA-C1A	3.01	108.06	106.71
2	A	405	BCL	CMB-C2B-C3B	3.00	130.30	124.68
2	A	404	BCL	OBD-CAD-CBD	-3.00	121.61	125.89
2	A	408[B]	BCL	CHA-C1A-NA	-2.97	119.59	126.40
2	C	402	BCL	CHA-C1A-NA	-2.96	119.62	126.40
2	C	403	BCL	CMB-C2B-C3B	2.96	130.22	124.68
2	A	406[D]	BCL	C2A-C1A-CHA	2.95	129.02	123.86
2	C	406[C]	BCL	C6-C7-C8	-2.94	106.43	115.92
2	C	406[D]	BCL	C6-C7-C8	-2.94	106.43	115.92
2	A	403	BCL	C4-C3-C5	2.93	120.19	115.27
2	C	406[D]	BCL	CHA-C1A-NA	-2.92	119.70	126.40
2	A	404	BCL	CMD-C2D-C3D	2.92	130.14	124.68
2	A	402	BCL	CHA-C1A-NA	-2.91	119.72	126.40
2	C	406[D]	BCL	OBD-CAD-CBD	-2.91	121.74	125.89
2	C	404	BCL	C2A-C1A-CHA	2.89	128.91	123.86
2	A	402	BCL	CMD-C2D-C3D	2.89	130.08	124.68
2	C	401	BCL	CAD-C3D-C4D	-2.86	106.88	108.47
2	A	407	BCL	C1C-NC-C4C	2.86	107.99	106.71
2	C	402	BCL	CMB-C2B-C3B	2.86	130.02	124.68
2	C	406[D]	BCL	C2A-C1A-CHA	2.85	128.84	123.86
2	C	408[B]	BCL	OBD-CAD-CBD	-2.85	121.83	125.89
2	C	408[B]	BCL	O2D-CGD-O1D	-2.85	118.27	123.84
2	A	403	BCL	C2A-C1A-CHA	2.84	128.83	123.86
2	A	401[A]	BCL	CAD-C3D-C4D	-2.84	106.89	108.47
2	A	401[B]	BCL	CAD-C3D-C4D	-2.84	106.89	108.47
2	C	401	BCL	C2A-C1A-CHA	2.83	128.81	123.86
2	C	407	BCL	CHA-C1A-NA	-2.83	119.93	126.40
2	A	402	BCL	C1-O2A-CGA	-2.82	109.03	116.44
2	A	407	BCL	CHA-C1A-NA	-2.82	119.93	126.40
2	A	407	BCL	OBD-CAD-CBD	-2.82	121.86	125.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	407	BCL	C1-C2-C3	-2.82	121.16	126.04
2	C	408[B]	BCL	CMB-C2B-C3B	2.82	129.95	124.68
2	A	405	BCL	C4A-NA-C1A	2.81	107.97	106.71
2	A	408[B]	BCL	CMB-C2B-C3B	2.81	129.94	124.68
2	C	408[B]	BCL	C2A-C1A-CHA	2.81	128.78	123.86
2	A	406[D]	BCL	OBD-CAD-CBD	-2.81	121.88	125.89
2	C	403	BCL	C6-C7-C8	-2.79	106.91	115.92
2	A	404	BCL	C2A-C1A-CHA	2.79	128.73	123.86
2	A	408[B]	BCL	O2D-CGD-O1D	-2.77	118.43	123.84
2	C	404	BCL	CMB-C2B-C3B	2.76	129.84	124.68
2	A	406[D]	BCL	CHA-C1A-NA	-2.75	120.10	126.40
2	C	406[C]	BCL	CMB-C2B-C3B	2.74	129.81	124.68
2	C	406[D]	BCL	CMB-C2B-C3B	2.74	129.81	124.68
2	A	403	BCL	CMD-C2D-C3D	2.74	129.81	124.68
2	C	406[C]	BCL	CHA-C1A-NA	-2.74	120.13	126.40
2	C	405	BCL	C1-C2-C3	-2.74	121.31	126.04
2	C	405	BCL	C2A-C1A-CHA	2.71	128.60	123.86
2	A	406[C]	BCL	C2A-C1A-CHA	2.71	128.59	123.86
2	A	404	BCL	CMB-C2B-C3B	2.70	129.74	124.68
2	C	403	BCL	CMD-C2D-C3D	2.70	129.73	124.68
2	C	408[B]	BCL	OBB-CAB-C3B	2.68	124.74	119.99
2	A	405	BCL	C2A-C1A-CHA	2.66	128.51	123.86
2	C	407	BCL	CMB-C2B-C3B	2.64	129.62	124.68
2	A	406[C]	BCL	CAD-C3D-C4D	-2.63	107.00	108.47
2	A	407	BCL	O2A-CGA-CBA	2.58	120.01	111.91
2	A	405	BCL	CMD-C2D-C3D	2.56	129.47	124.68
2	A	406[C]	BCL	CHA-C1A-NA	-2.56	120.53	126.40
2	C	401	BCL	OBB-CAB-CBB	-2.56	114.40	120.17
2	C	406[C]	BCL	C2A-C1A-CHA	2.56	128.34	123.86
2	C	402	BCL	C1C-NC-C4C	2.55	107.85	106.71
2	C	408[B]	BCL	C4B-C3B-CAB	-2.55	122.20	127.13
2	A	407	BCL	CMB-C2B-C3B	2.53	129.41	124.68
2	A	407	BCL	C11-C10-C8	-2.53	107.75	115.92
2	C	403	BCL	C2A-C1A-CHA	2.52	128.26	123.86
2	A	406[C]	BCL	OBB-CAB-CBB	-2.51	114.51	120.17
2	A	406[D]	BCL	OBB-CAB-CBB	-2.51	114.51	120.17
2	A	401[A]	BCL	CED-O2D-CGD	2.50	121.59	115.94
2	A	401[B]	BCL	CED-O2D-CGD	2.50	121.59	115.94
2	C	405	BCL	C4B-C3B-CAB	-2.50	122.31	127.13
2	A	406[C]	BCL	CMB-C2B-C3B	2.49	129.34	124.68
2	A	406[D]	BCL	CMB-C2B-C3B	2.49	129.34	124.68
2	A	405	BCL	C4B-C3B-CAB	-2.49	122.32	127.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	401	BCL	CMB-C2B-C3B	2.49	129.34	124.68
2	C	403	BCL	O2A-C1-C2	-2.47	102.13	108.64
2	C	405	BCL	CMB-C2B-C3B	2.46	129.28	124.68
2	A	404	BCL	C1C-NC-C4C	2.45	107.81	106.71
2	A	405	BCL	C1C-NC-C4C	2.45	107.81	106.71
2	A	408[B]	BCL	C4B-C3B-CAB	-2.45	122.40	127.13
2	A	406[D]	BCL	CMD-C2D-C3D	2.44	129.25	124.68
2	C	406[C]	BCL	C11-C10-C8	2.44	123.79	115.92
2	C	406[D]	BCL	C11-C10-C8	2.44	123.79	115.92
2	C	406[C]	BCL	OBB-CAB-CBB	-2.42	114.72	120.17
2	C	406[D]	BCL	OBB-CAB-CBB	-2.42	114.72	120.17
2	C	407	BCL	CAD-C3D-C4D	-2.42	107.12	108.47
2	C	405	BCL	O2A-C1-C2	-2.39	102.34	108.64
2	C	402	BCL	C2A-C1A-CHA	2.37	128.00	123.86
2	A	408[B]	BCL	C2A-C1A-CHA	2.37	128.00	123.86
2	A	406[C]	BCL	CMD-C2D-C3D	2.36	129.10	124.68
2	C	408[B]	BCL	O2D-CGD-CBD	2.36	115.46	111.27
2	C	402	BCL	CMD-C2D-C3D	2.35	129.07	124.68
2	A	402	BCL	C2A-C1A-CHA	2.34	127.94	123.86
2	A	408[B]	BCL	C1C-NC-C4C	2.32	107.75	106.71
2	A	404	BCL	CAC-C3C-C4C	-2.32	107.43	112.58
2	A	407	BCL	C2A-C1A-CHA	2.32	127.92	123.86
2	A	408[B]	BCL	CAD-C3D-C4D	-2.31	107.18	108.47
2	C	407	BCL	C6-C7-C8	-2.30	108.48	115.92
2	C	403	BCL	O2A-CGA-O1A	-2.29	117.81	123.59
2	C	405	BCL	C5-C3-C2	2.27	125.71	121.12
2	A	401[A]	BCL	OBD-CAD-C3D	2.26	131.74	127.98
2	A	401[B]	BCL	OBD-CAD-C3D	2.26	131.74	127.98
2	A	408[B]	BCL	C4A-NA-C1A	2.26	107.72	106.71
2	A	402	BCL	O2A-C1-C2	-2.23	102.79	108.64
2	A	403	BCL	C11-C12-C13	-2.20	108.79	115.92
2	A	404	BCL	OBB-CAB-CBB	-2.20	115.23	120.17
2	C	404	BCL	C11-C12-C13	-2.19	108.83	115.92
2	C	407	BCL	C2A-C1A-CHA	2.19	127.69	123.86
2	C	406[D]	BCL	CMD-C2D-C3D	2.18	128.76	124.68
2	C	405	BCL	C1C-NC-C4C	2.18	107.69	106.71
2	A	407	BCL	C7-C6-C5	2.18	119.27	113.36
2	C	404	BCL	C6-C7-C8	-2.17	108.89	115.92
2	C	402	BCL	OBB-CAB-CBB	-2.17	115.28	120.17
2	A	408[B]	BCL	OBB-CAB-C3B	2.15	123.81	119.99
2	A	405	BCL	O2D-CGD-O1D	-2.14	119.66	123.84
2	A	406[C]	BCL	O2D-CGD-O1D	-2.14	119.66	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	408[B]	BCL	CMD-C2D-C3D	2.12	128.65	124.68
2	C	406[C]	BCL	CMD-C2D-C3D	2.12	128.65	124.68
2	A	407	BCL	CMD-C2D-C3D	2.11	128.63	124.68
2	A	407	BCL	C4-C3-C5	-2.10	111.73	115.27
2	A	401[A]	BCL	CAA-C2A-C1A	2.10	118.86	111.97
2	A	401[B]	BCL	CAA-C2A-C1A	2.10	118.86	111.97
2	A	407	BCL	C1-O2A-CGA	2.07	121.86	116.44
2	A	405	BCL	C7-C6-C5	-2.06	107.76	113.36
2	A	405	BCL	C4-C3-C5	-2.06	111.81	115.27
2	C	402	BCL	C4B-C3B-CAB	-2.06	123.15	127.13
2	C	401	BCL	C6-C5-C3	2.05	118.84	113.45
2	A	403	BCL	C1-C2-C3	-2.04	122.51	126.04
2	C	401	BCL	CAA-CBA-CGA	-2.04	107.29	113.25
2	C	405	BCL	OBB-CAB-C3B	2.03	123.60	119.99
2	A	404	BCL	O2D-CGD-O1D	-2.02	119.89	123.84
2	A	401[A]	BCL	C4C-CHD-C1D	2.01	128.85	125.88
2	A	401[B]	BCL	C4C-CHD-C1D	2.01	128.85	125.88
2	C	402	BCL	C19-C18-C17	-2.01	99.12	111.54
2	A	401[A]	BCL	OBB-CAB-CBB	-2.01	115.65	120.17
2	A	401[B]	BCL	OBB-CAB-CBB	-2.01	115.65	120.17
2	A	406[C]	BCL	C9-C8-C10	-2.00	104.04	111.29
2	A	406[D]	BCL	C9-C8-C10	-2.00	104.04	111.29

There are no chirality outliers.

All (74) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	403	BCL	C2C-C3C-CAC-CBC
2	A	403	BCL	C4C-C3C-CAC-CBC
2	A	406[C]	BCL	CHA-CBD-CGD-O1D
2	A	406[C]	BCL	CHA-CBD-CGD-O2D
2	C	403	BCL	C2C-C3C-CAC-CBC
2	C	403	BCL	C4C-C3C-CAC-CBC
2	C	403	BCL	C4-C3-C5-C6
2	C	403	BCL	C2-C3-C5-C6
2	A	403	BCL	C4-C3-C5-C6
2	A	403	BCL	C2-C3-C5-C6
2	C	402	BCL	C13-C15-C16-C17
2	A	405	BCL	C5-C6-C7-C8
2	C	405	BCL	C8-C10-C11-C12
2	A	407	BCL	C4-C3-C5-C6
2	C	405	BCL	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
2	A	407	BCL	C2-C3-C5-C6
2	C	405	BCL	C2-C3-C5-C6
2	A	405	BCL	C4-C3-C5-C6
2	A	405	BCL	C2-C3-C5-C6
2	A	405	BCL	CAA-CBA-CGA-O2A
2	A	408[B]	BCL	C4C-C3C-CAC-CBC
2	A	407	BCL	C11-C10-C8-C7
2	A	406[D]	BCL	CAD-CBD-CGD-O2D
2	C	403	BCL	CAD-CBD-CGD-O2D
2	C	405	BCL	CAD-CBD-CGD-O2D
2	C	408[B]	BCL	CAD-CBD-CGD-O2D
2	C	406[C]	BCL	CHA-CBD-CGD-O1D
2	C	406[C]	BCL	CHA-CBD-CGD-O2D
2	C	407	BCL	C4-C3-C5-C6
2	C	405	BCL	CAA-CBA-CGA-O2A
2	C	407	BCL	C16-C17-C18-C19
2	C	407	BCL	C2-C3-C5-C6
2	C	402	BCL	C11-C12-C13-C15
2	A	407	BCL	C11-C10-C8-C9
2	A	407	BCL	C16-C17-C18-C19
2	C	406[C]	BCL	C10-C11-C12-C13
2	C	406[D]	BCL	C10-C11-C12-C13
2	C	403	BCL	C10-C11-C12-C13
2	A	406[C]	BCL	C4-C3-C5-C6
2	A	406[D]	BCL	C4-C3-C5-C6
2	A	405	BCL	CAA-CBA-CGA-O1A
2	C	402	BCL	C11-C12-C13-C14
2	A	408[B]	BCL	CAD-CBD-CGD-O2D
2	C	406[D]	BCL	CAD-CBD-CGD-O2D
2	C	401	BCL	CAA-CBA-CGA-O2A
2	A	401[A]	BCL	CAA-CBA-CGA-O2A
2	A	401[B]	BCL	CAA-CBA-CGA-O2A
2	A	402	BCL	CHA-CBD-CGD-O1D
2	A	402	BCL	CHA-CBD-CGD-O2D
2	A	405	BCL	CHA-CBD-CGD-O2D
2	A	407	BCL	CHA-CBD-CGD-O1D
2	A	407	BCL	CHA-CBD-CGD-O2D
2	C	402	BCL	CHA-CBD-CGD-O1D
2	C	402	BCL	CHA-CBD-CGD-O2D
2	C	403	BCL	CHA-CBD-CGD-O2D
2	C	405	BCL	CHA-CBD-CGD-O2D
2	C	407	BCL	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
2	A	406[C]	BCL	C11-C10-C8-C9
2	A	406[D]	BCL	C11-C10-C8-C9
2	C	408[B]	BCL	C1A-C2A-CAA-CBA
2	C	405	BCL	CAA-CBA-CGA-O1A
2	A	401[A]	BCL	CAA-CBA-CGA-O1A
2	A	401[B]	BCL	CAA-CBA-CGA-O1A
2	C	401	BCL	CAA-CBA-CGA-O1A
2	C	403	BCL	CAA-CBA-CGA-O2A
2	A	402	BCL	CAD-CBD-CGD-O1D
2	C	403	BCL	CAA-CBA-CGA-O1A
2	A	403	BCL	CAA-CBA-CGA-O2A
2	A	403	BCL	CAA-CBA-CGA-O1A
2	A	405	BCL	C6-C7-C8-C10
2	A	406[C]	BCL	C2-C3-C5-C6
2	A	406[D]	BCL	C2-C3-C5-C6
2	A	407	BCL	C15-C16-C17-C18
2	A	407	BCL	CAA-CBA-CGA-O2A

There are no ring outliers.

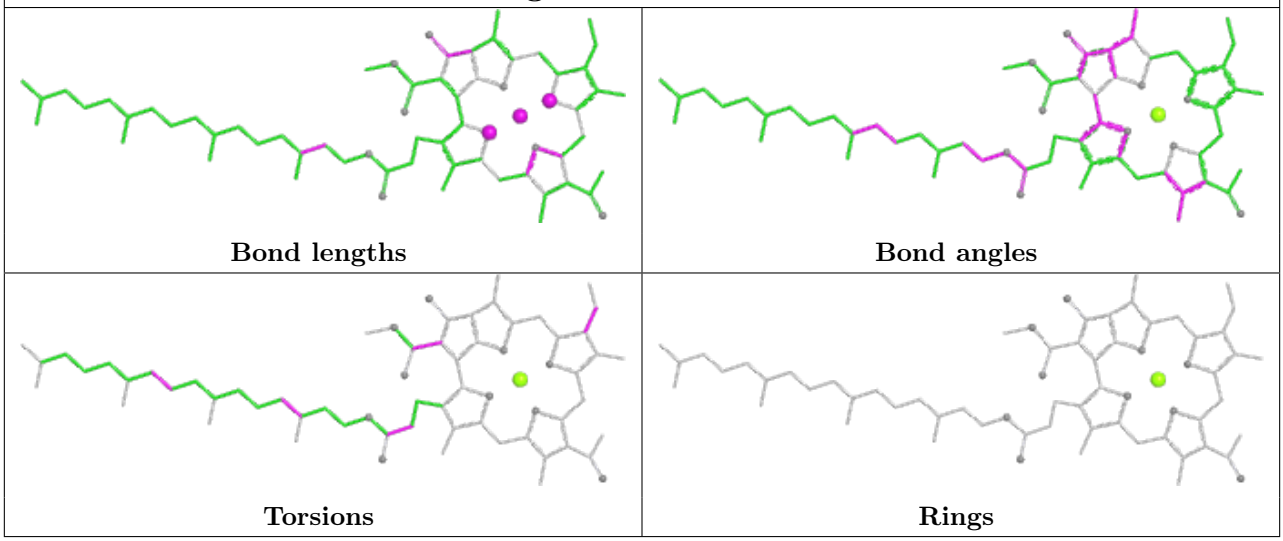
13 monomers are involved in 32 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	403	BCL	3	0
2	A	403	BCL	3	0
2	A	402	BCL	6	0
2	C	408[B]	BCL	1	0
2	A	408[B]	BCL	1	0
2	A	407	BCL	3	0
2	A	404	BCL	2	0
2	C	405	BCL	3	0
2	C	407	BCL	2	0
2	C	401	BCL	3	0
2	A	405	BCL	4	0
2	C	402	BCL	3	0
2	C	404	BCL	2	0

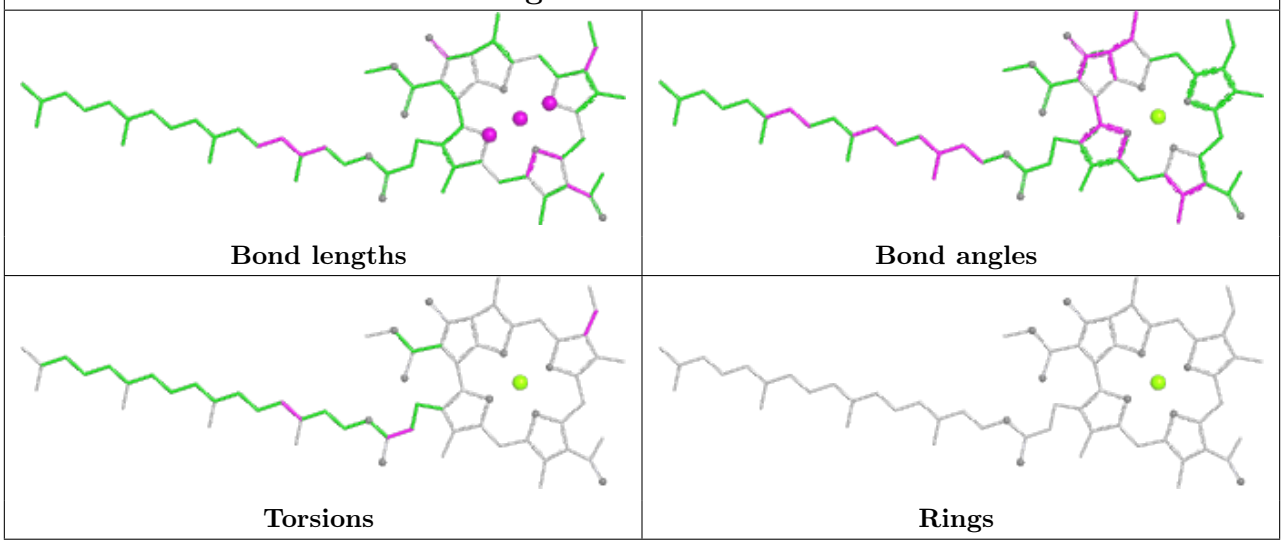
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

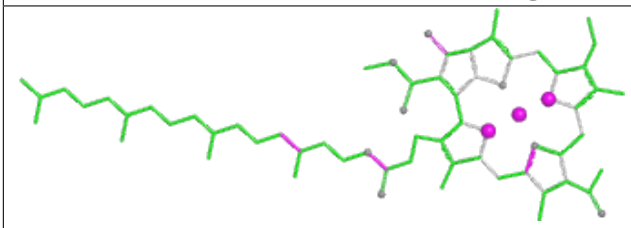
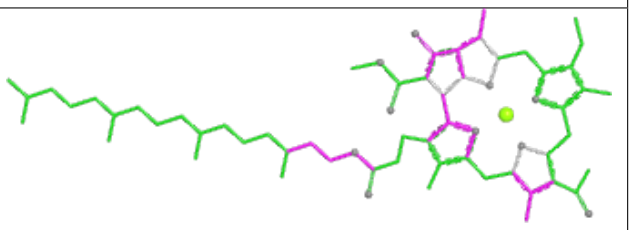
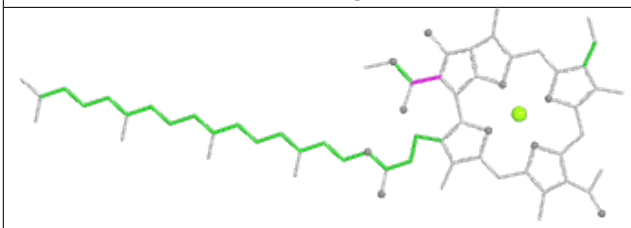
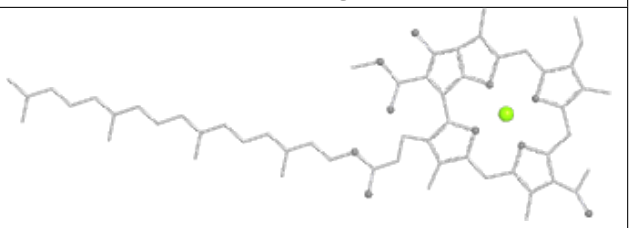
highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified 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 C 403



Ligand BCL A 403



Ligand BCL A 402	
 Bond lengths	 Bond angles
 Torsions	 Rings

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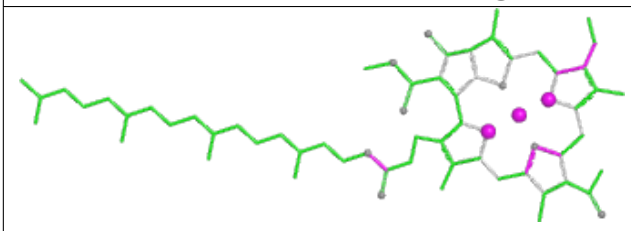
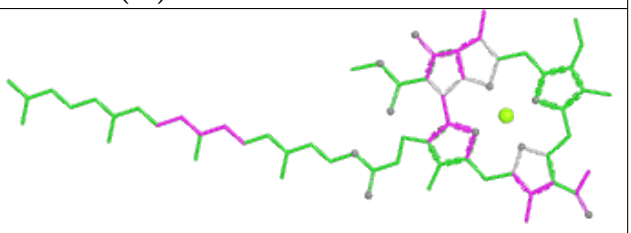
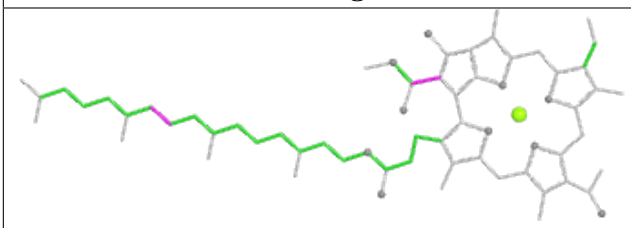
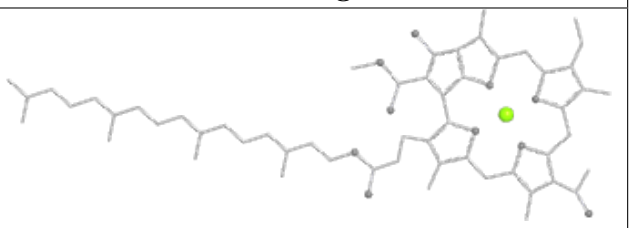
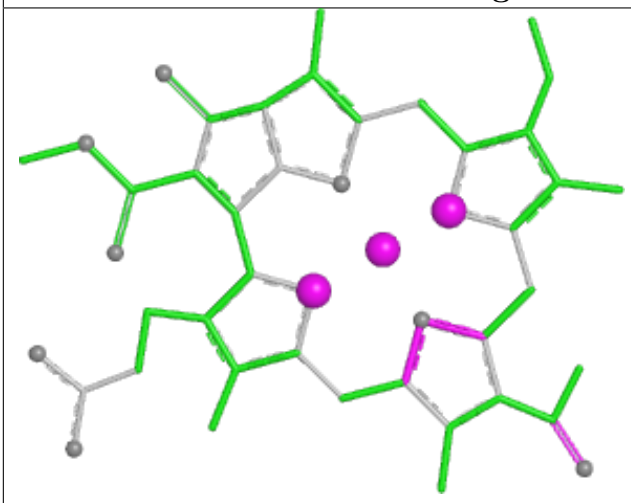
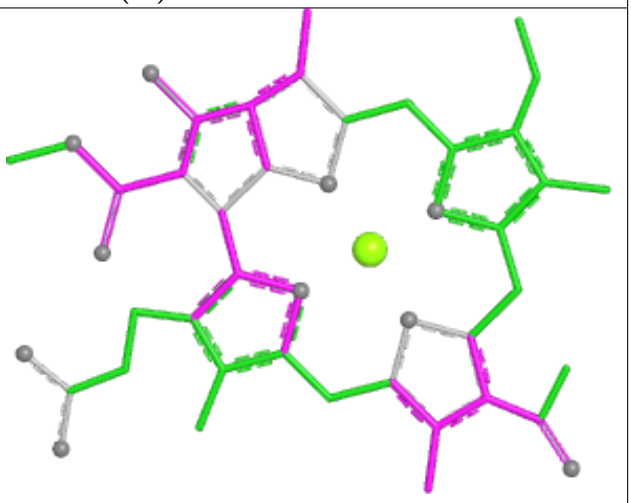
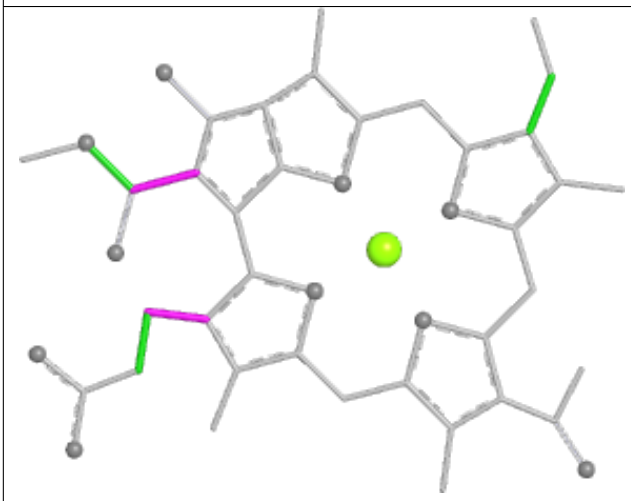
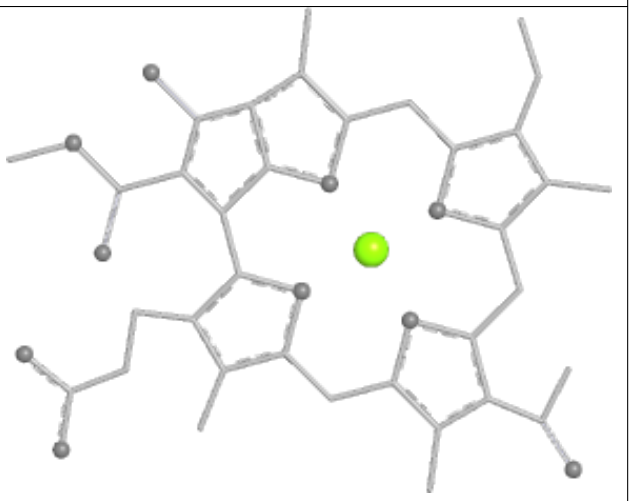
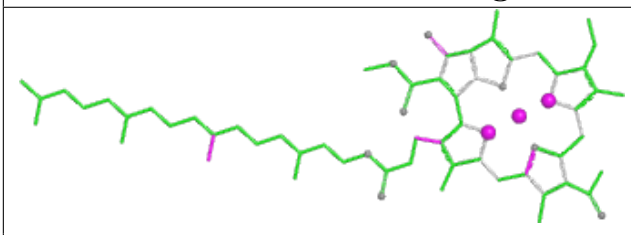
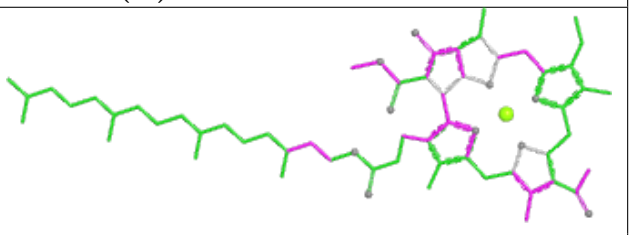
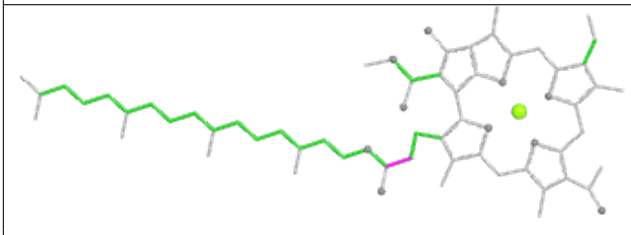
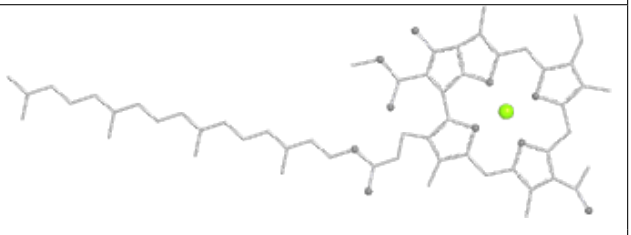
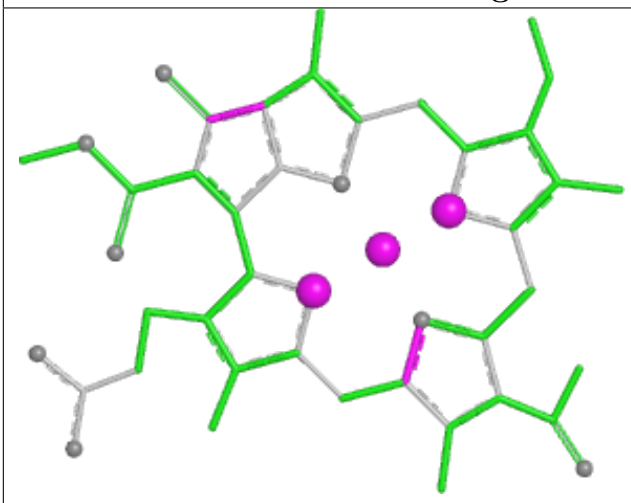
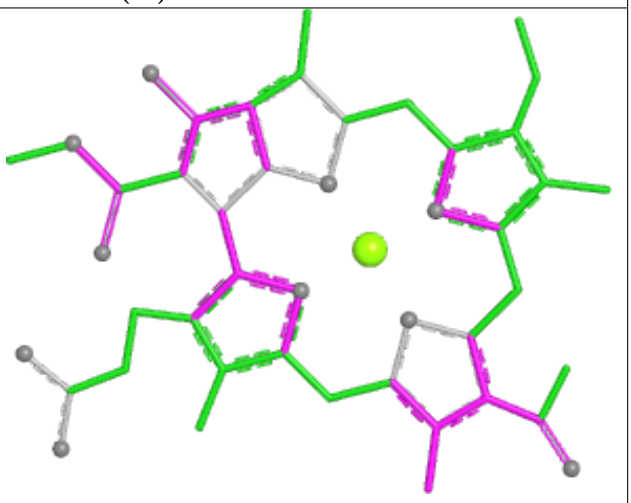
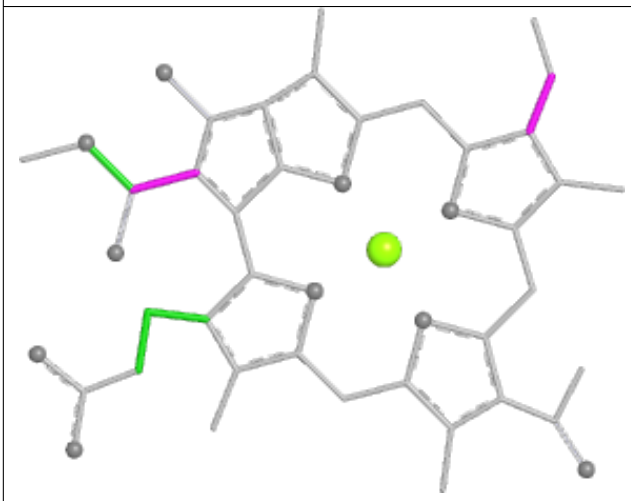
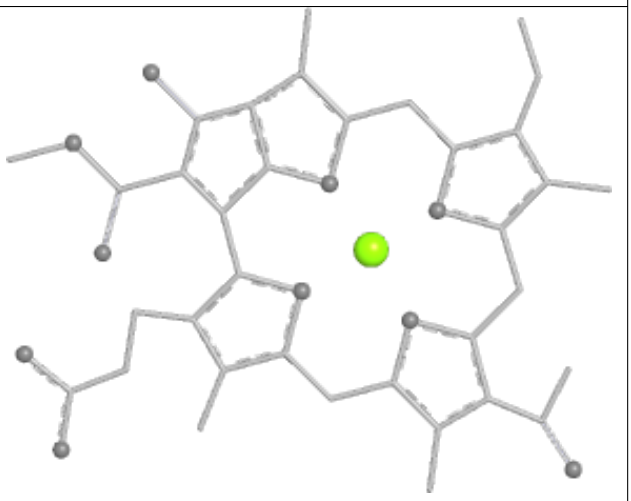
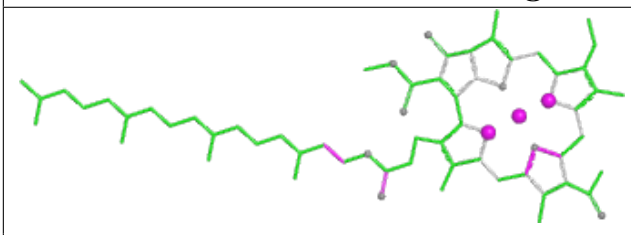
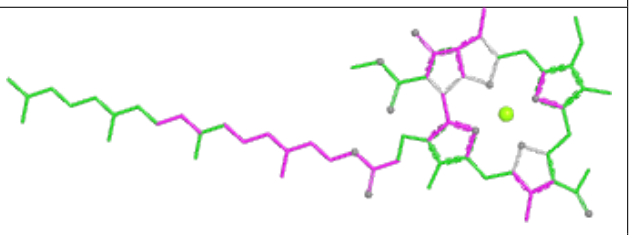
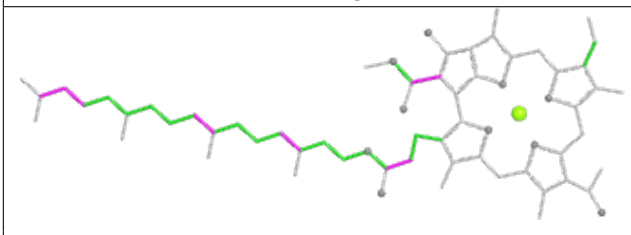
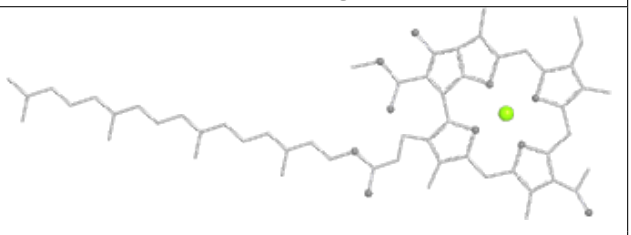
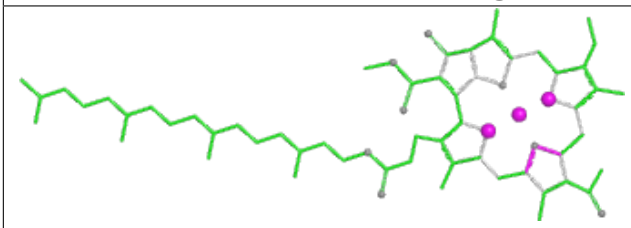
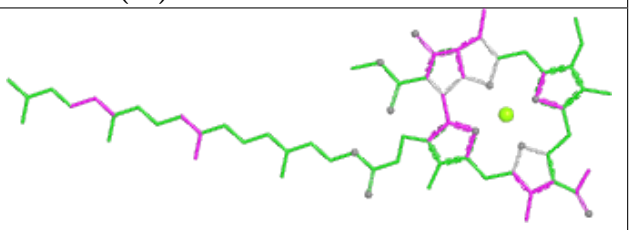
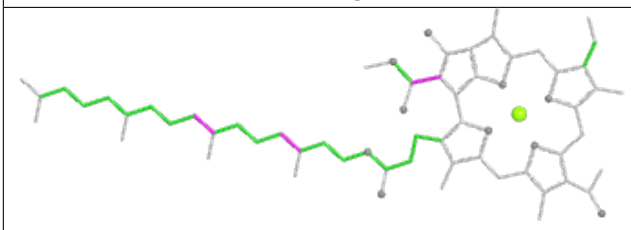
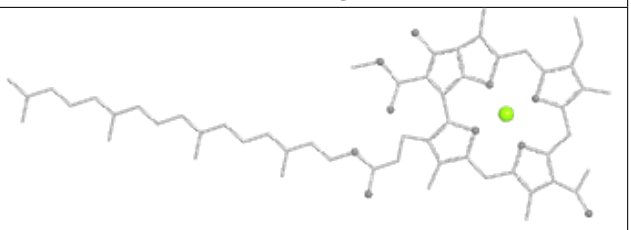
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCL C 408 (B)	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCL A 401 (B)	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCL A 408 (B)	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCL A 407	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCL A 406 (D)	
 Bond lengths	 Bond angles
 Torsions	 Rings

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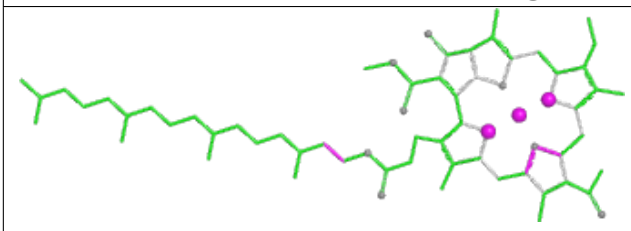
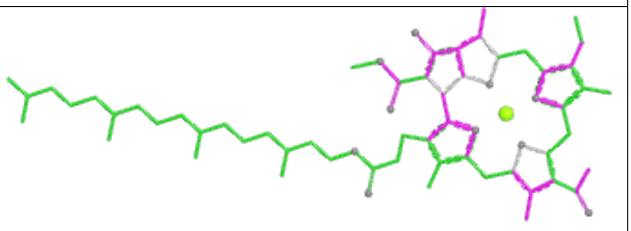
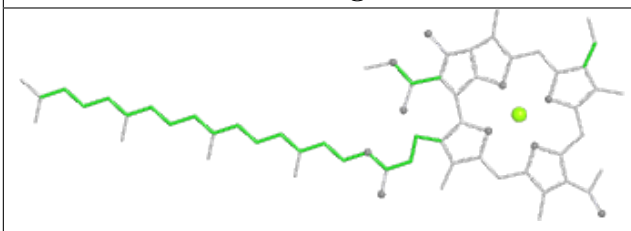
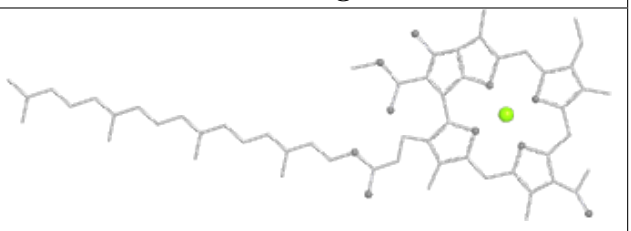
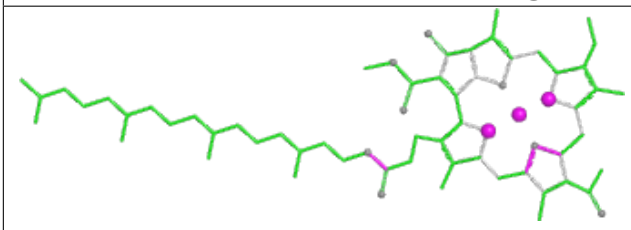
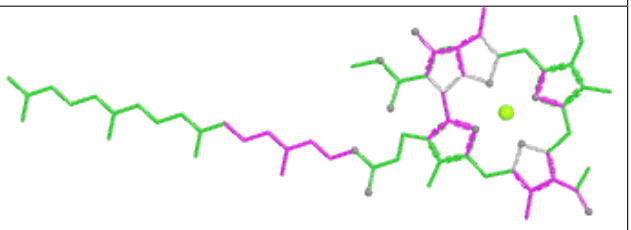
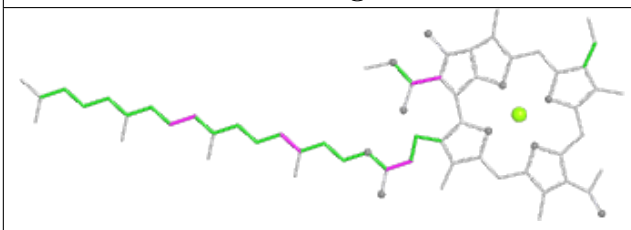
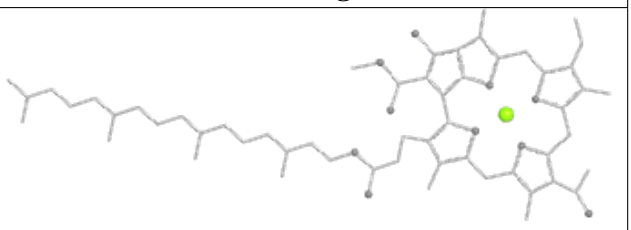
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCL C 405	
 Bond lengths	 Bond angles
 Torsions	 Rings

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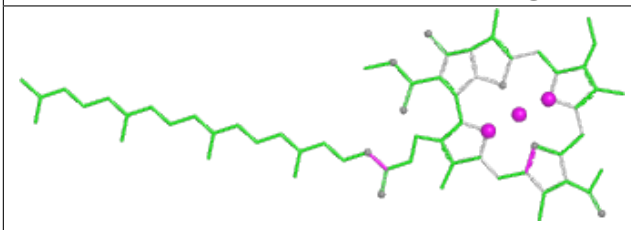
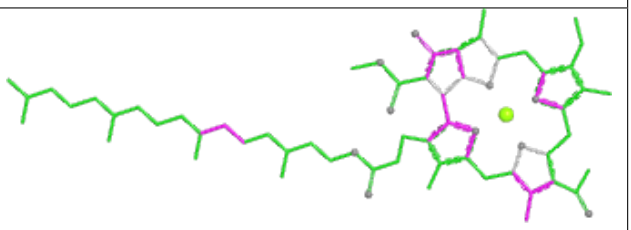
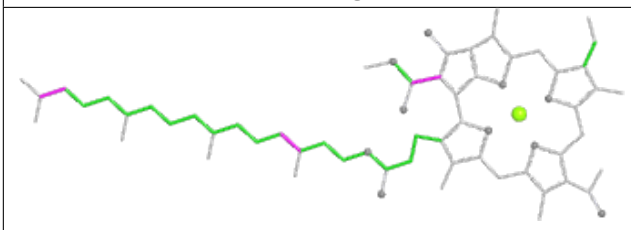
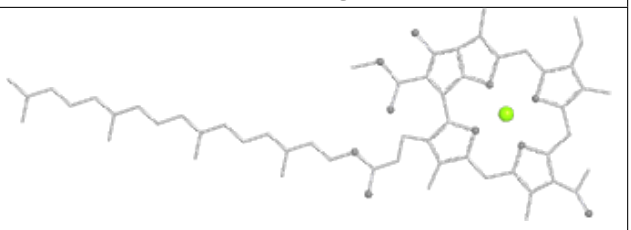
 Bond lengths	 Bond angles
 Torsions	 Rings

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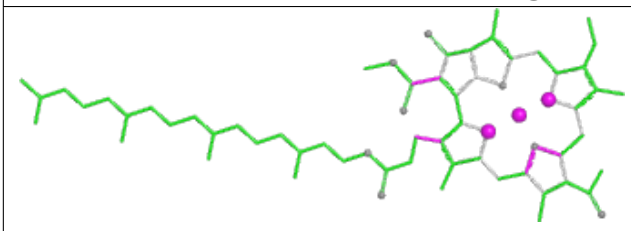
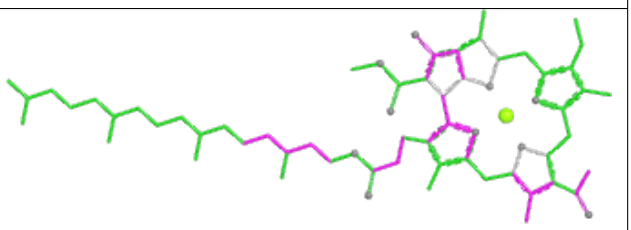
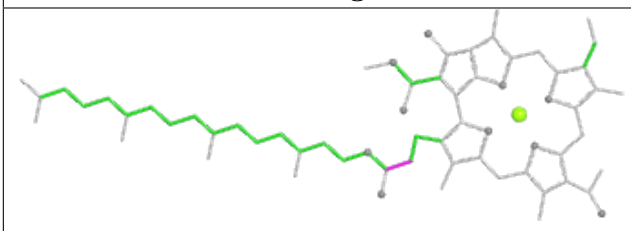
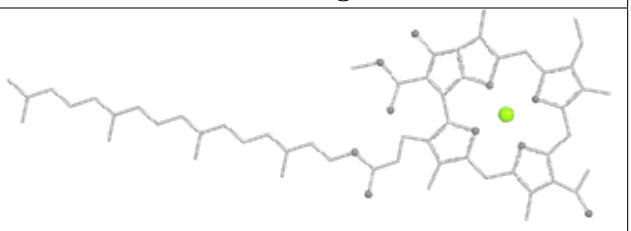
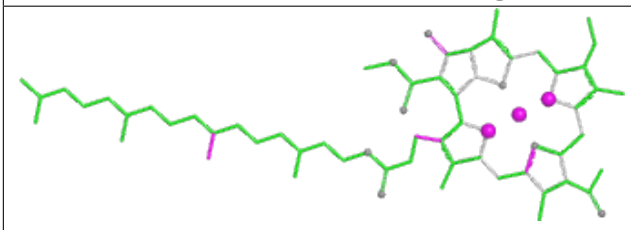
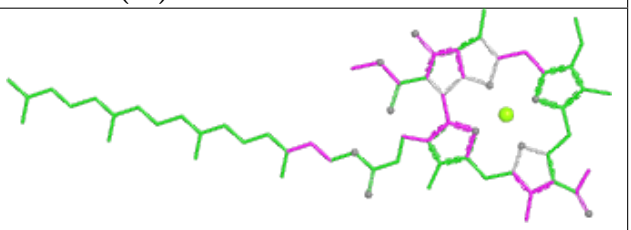
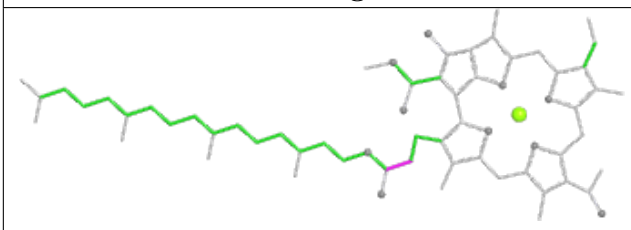
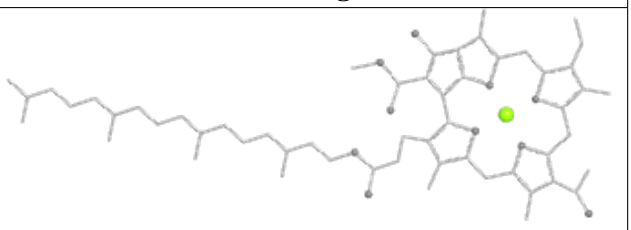
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCL A 401 (A)	
 Bond lengths	 Bond angles
 Torsions	 Rings

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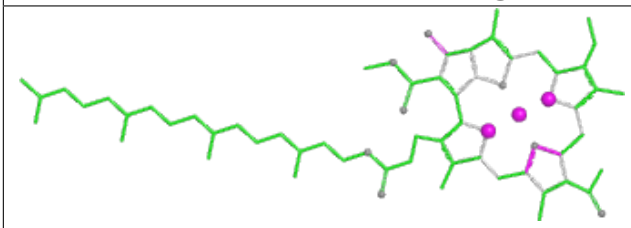
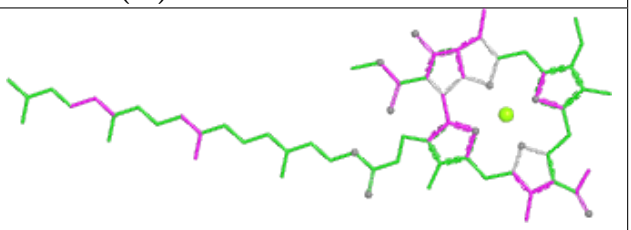
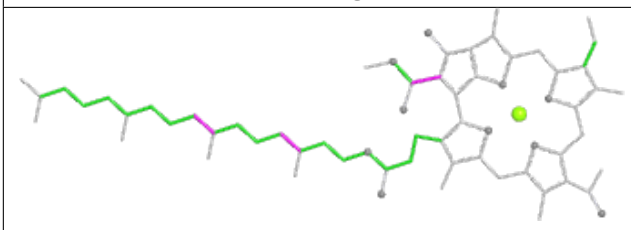
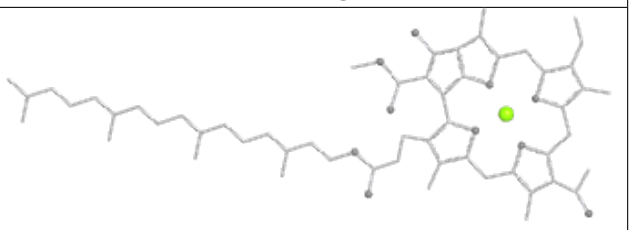
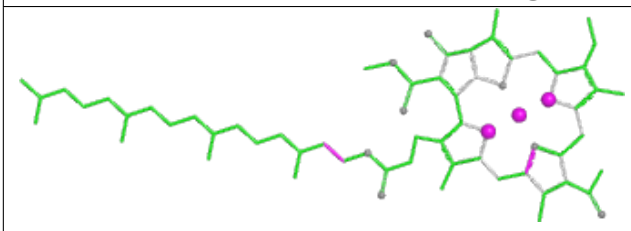
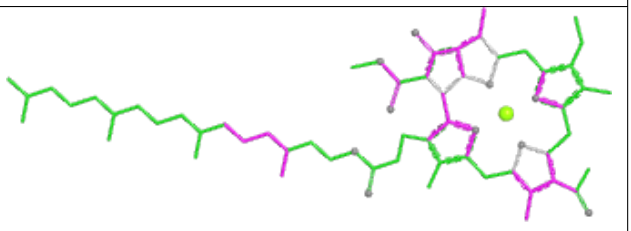
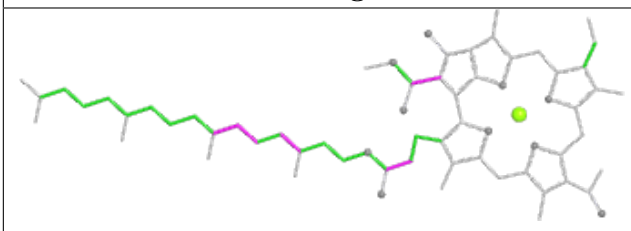
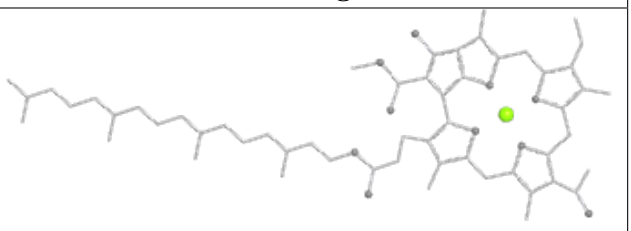
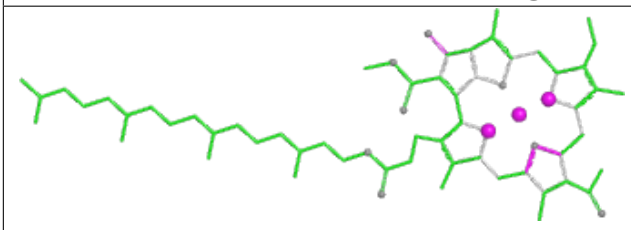
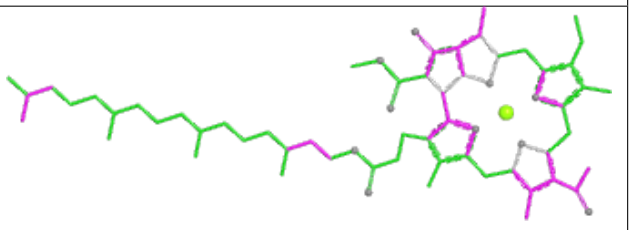
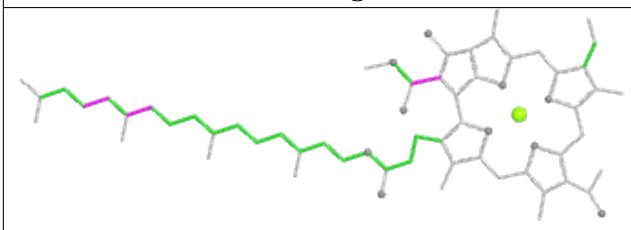
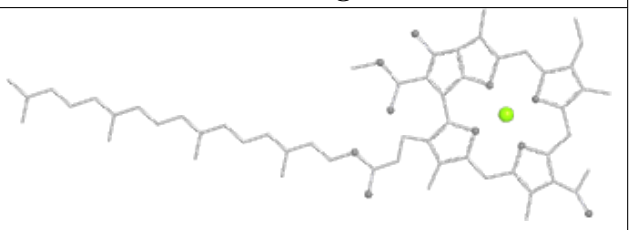
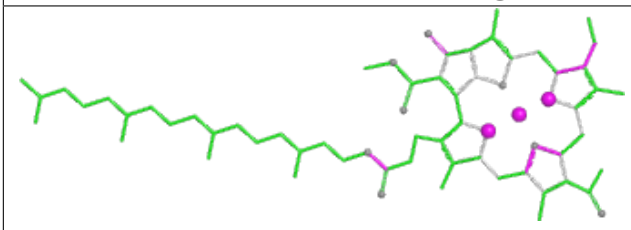
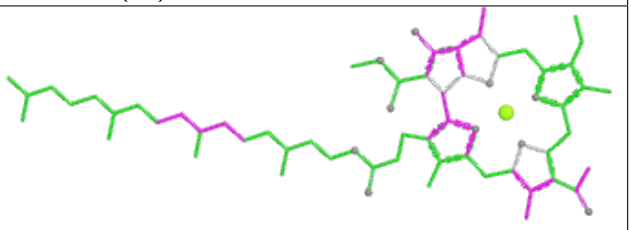
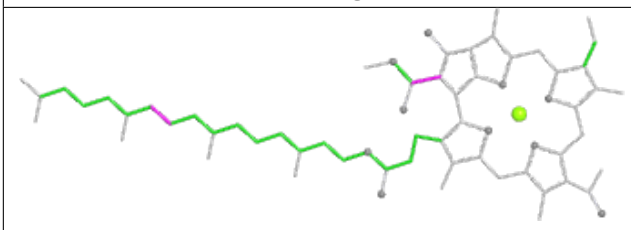
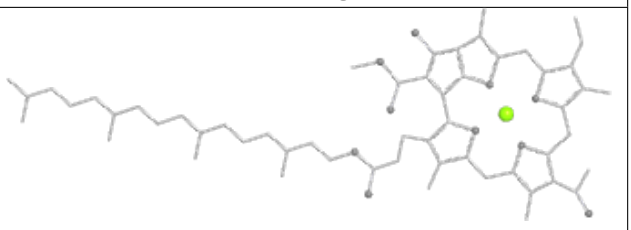
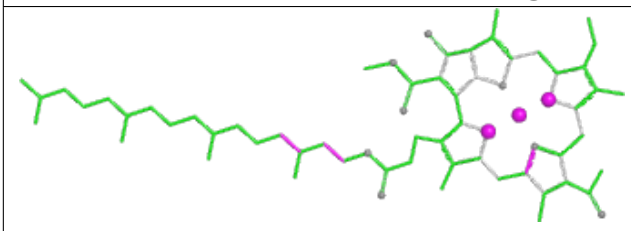
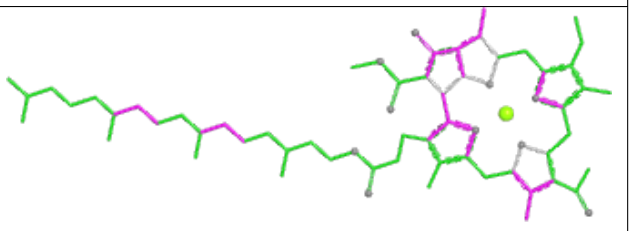
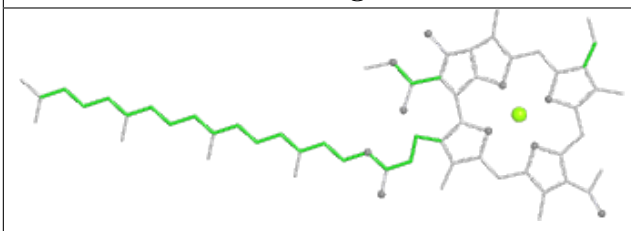
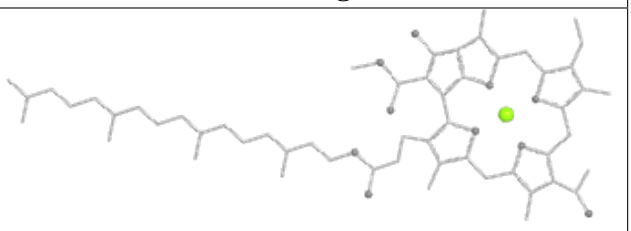
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCL A 405	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCL C 402	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCL C 406 (D)	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCL C 404	
 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

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	358/365 (98%)	-0.39	6 (1%)	70	66	12, 22, 35, 57	0
1	C	358/365 (98%)	-0.35	6 (1%)	70	66	14, 22, 37, 68	0
All	All	716/730 (98%)	-0.37	12 (1%)	70	66	12, 22, 37, 68	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	214	PRO	5.9
1	A	214	PRO	4.3
1	C	212	SER	4.1
1	C	9	VAL	3.1
1	A	282	GLY	2.7
1	C	215	LYS	2.6
1	A	213	GLY	2.5
1	A	9	VAL	2.5
1	C	213	GLY	2.4
1	A	212	SER	2.3
1	C	62	LYS	2.3
1	A	366	GLN	2.2

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands (i)

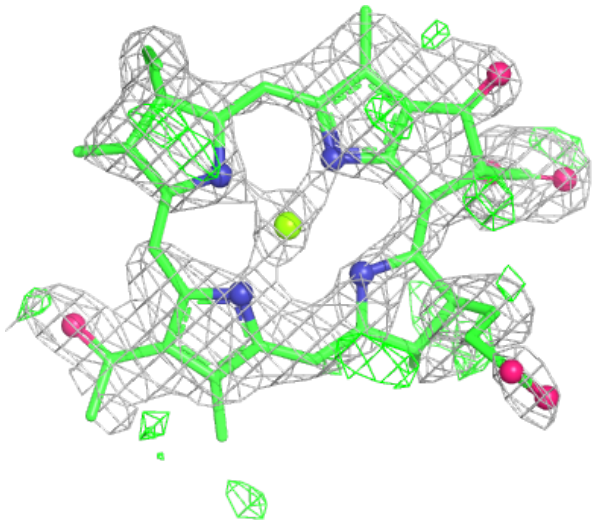
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

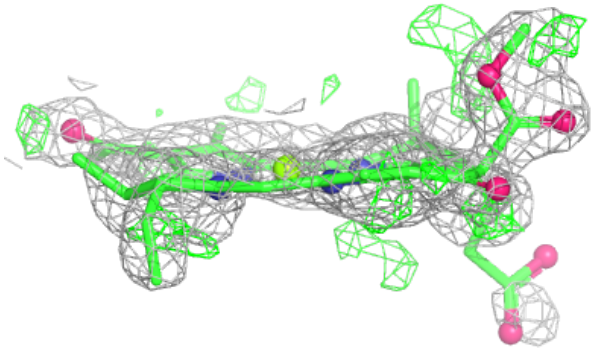
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	BCL	C	408[B]	46/66	0.75	0.24	23,34,49,59	46
2	BCL	A	408[B]	46/66	0.77	0.22	24,32,47,54	46
2	BCL	C	405	66/66	0.95	0.10	15,19,41,51	0
2	BCL	C	402	66/66	0.96	0.10	14,19,31,42	0
2	BCL	A	405	66/66	0.96	0.09	13,18,33,36	0
2	BCL	C	406[C]	66/66	0.96	0.10	16,19,31,37	10
2	BCL	C	406[D]	66/66	0.96	0.10	16,19,31,37	10
2	BCL	A	402	66/66	0.96	0.09	12,18,28,30	0
2	BCL	A	407	66/66	0.97	0.08	11,15,26,38	0
2	BCL	A	401[A]	66/66	0.97	0.13	16,20,22,23	5
2	BCL	C	401	66/66	0.97	0.13	17,21,24,27	0
2	BCL	A	403	66/66	0.97	0.09	11,15,23,28	0
2	BCL	C	403	66/66	0.97	0.10	12,16,24,28	0
2	BCL	C	404	66/66	0.97	0.10	11,17,27,35	0
2	BCL	A	404	66/66	0.97	0.10	10,15,21,23	0
2	BCL	A	401[B]	66/66	0.97	0.13	16,20,22,23	5
2	BCL	A	406[C]	66/66	0.97	0.10	14,18,27,31	10
2	BCL	C	407	66/66	0.97	0.07	13,17,30,39	0
2	BCL	A	406[D]	66/66	0.97	0.10	14,18,27,31	10

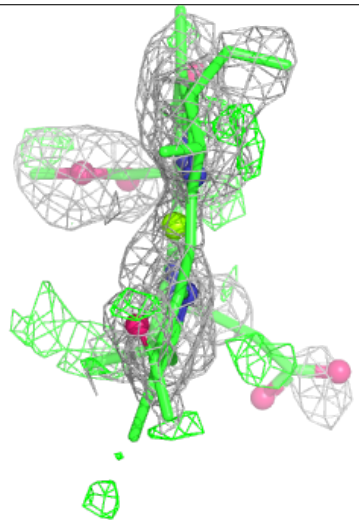
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around BCL C 408 (B):

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

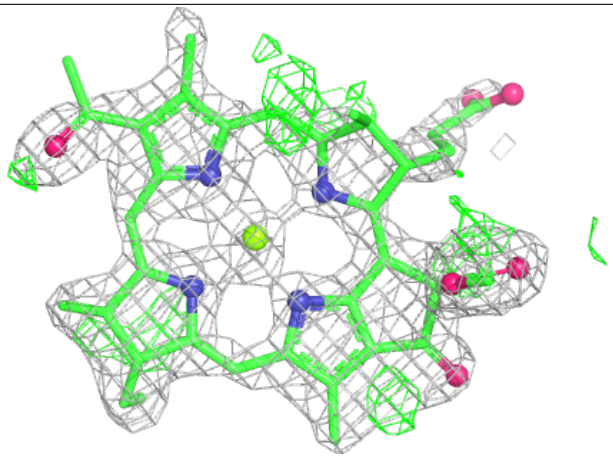


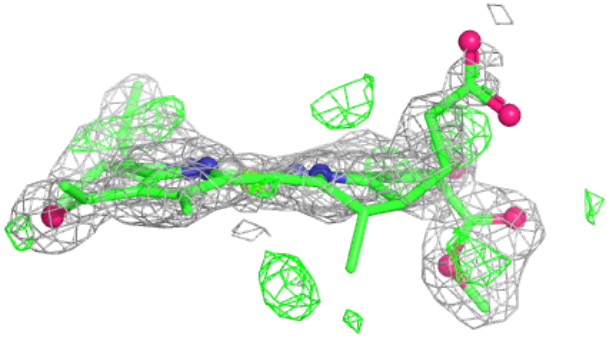


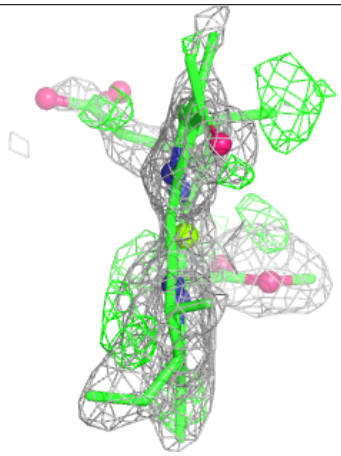


Electron density around BCL A 408 (B):

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

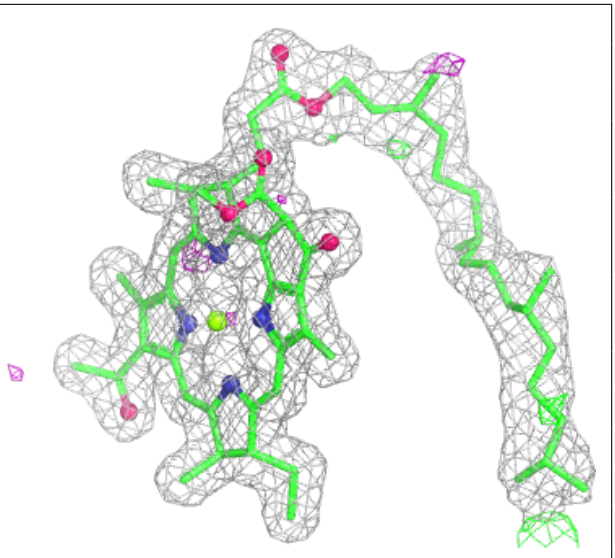


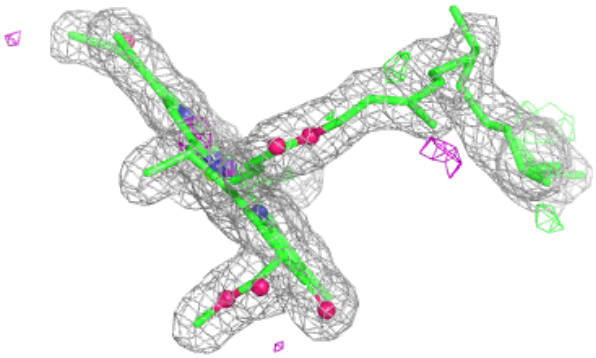


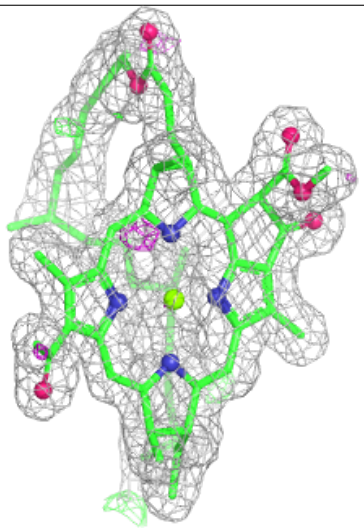


Electron density around BCL C 405:

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

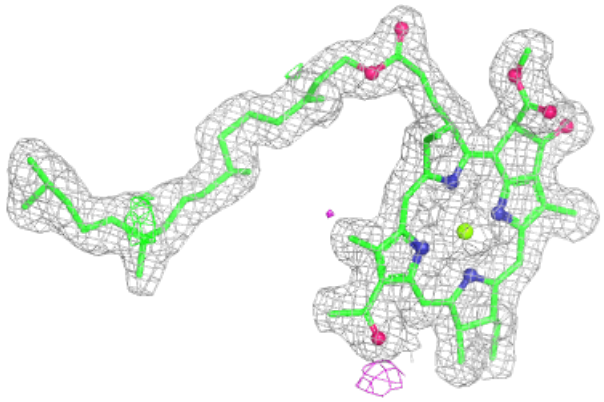


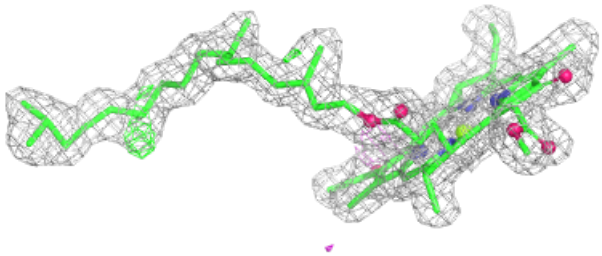


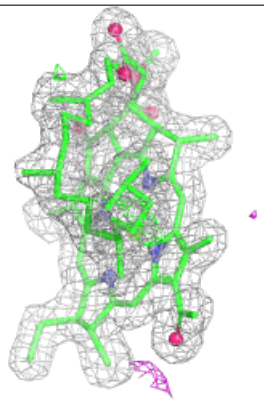


Electron density around BCL C 402:

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

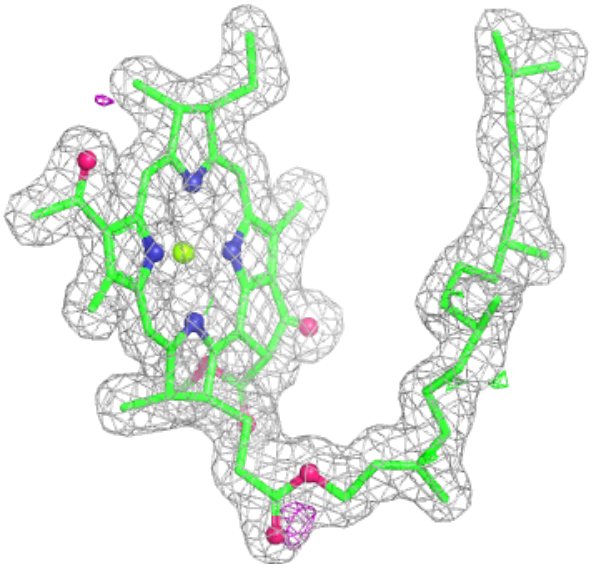


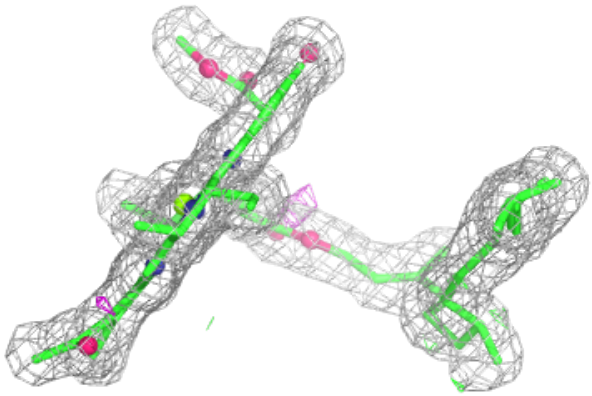


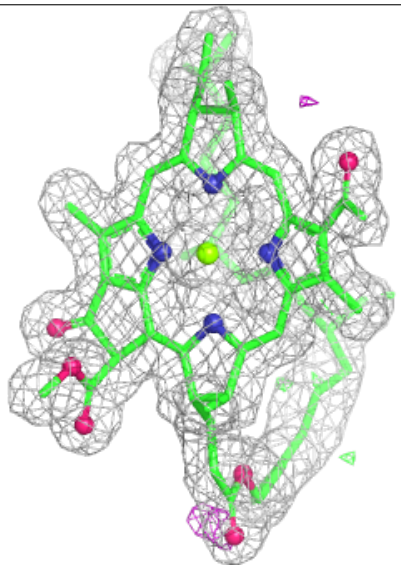


Electron density around BCL A 405:

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

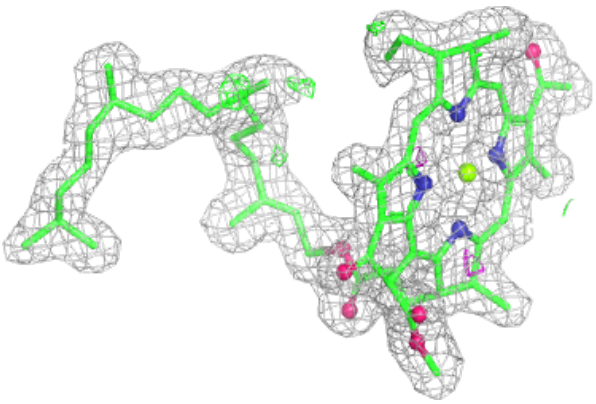


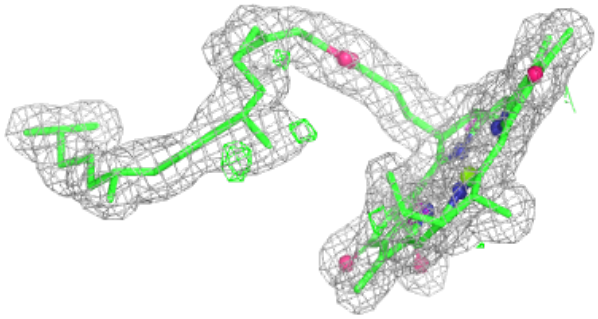


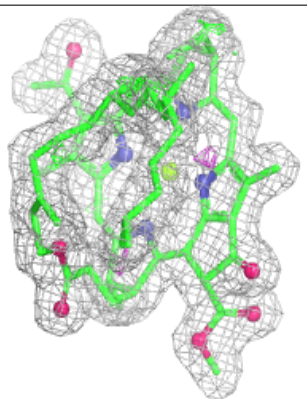


Electron density around BCL C 406 (C):

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

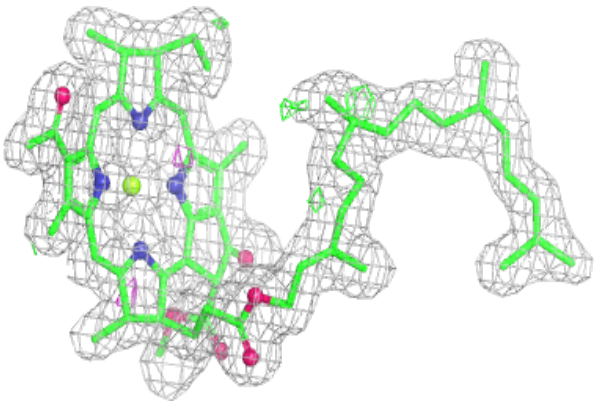


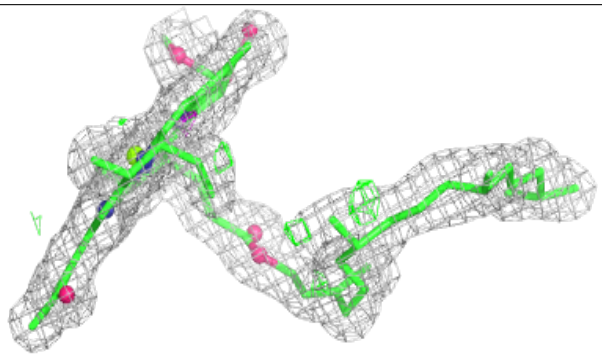


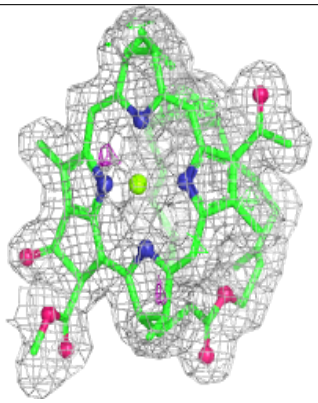


Electron density around BCL C 406 (D):

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

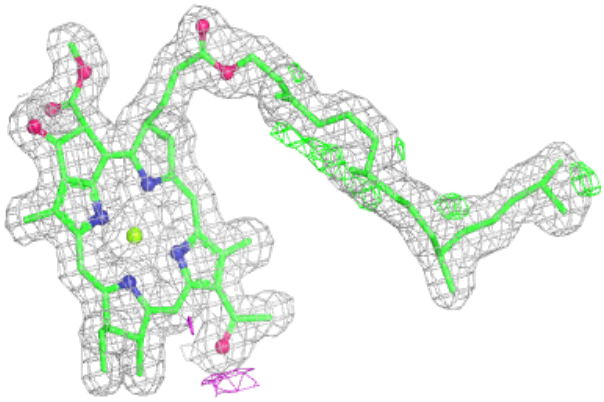


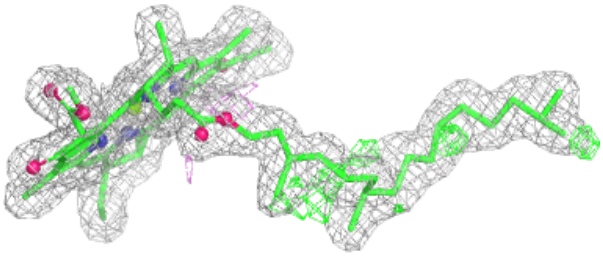


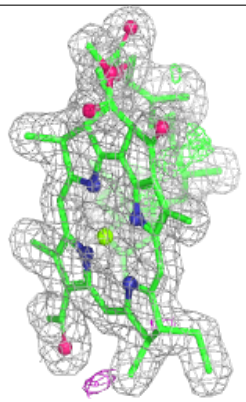


Electron density around BCL A 402:

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

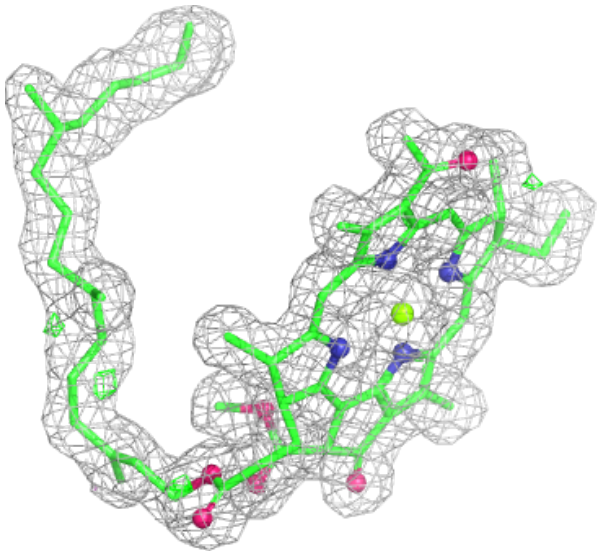


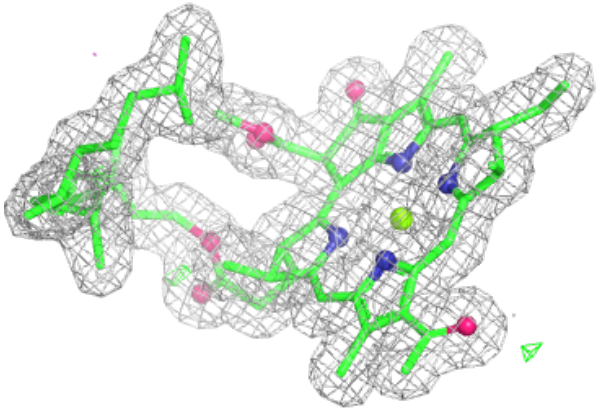


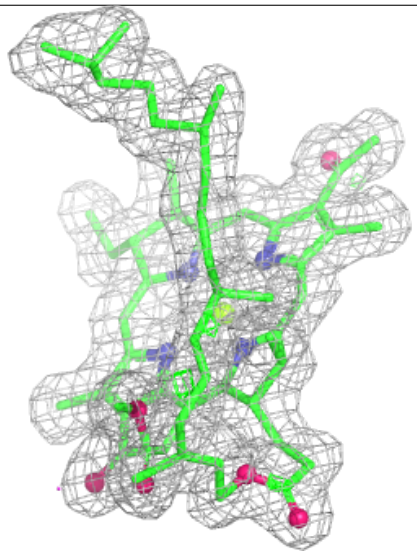


Electron density around BCL A 407:

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

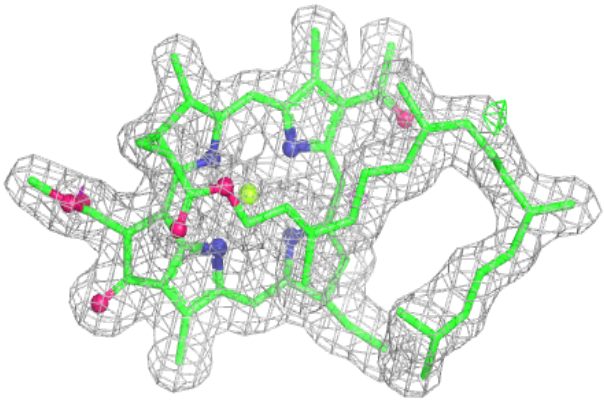


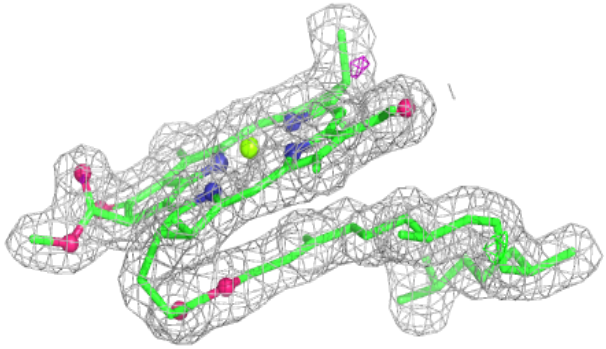




Electron density around BCL A 401 (A):

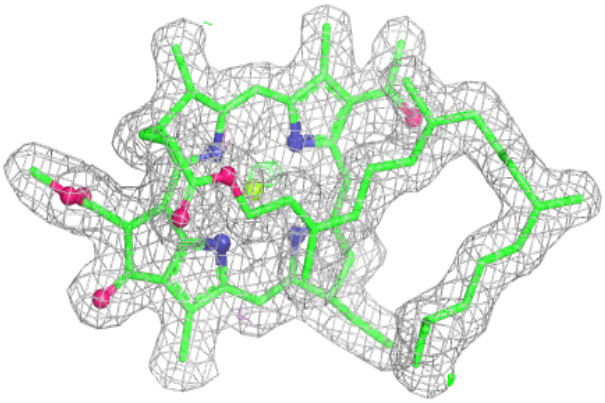
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

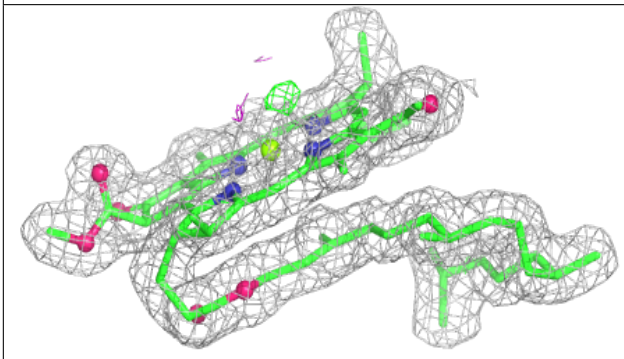


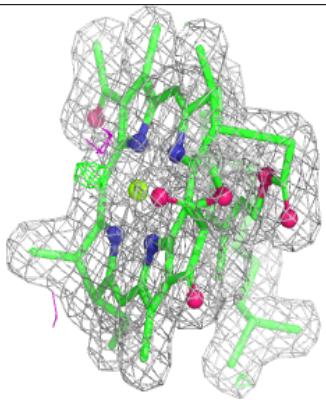


Electron density around BCL C 401:

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

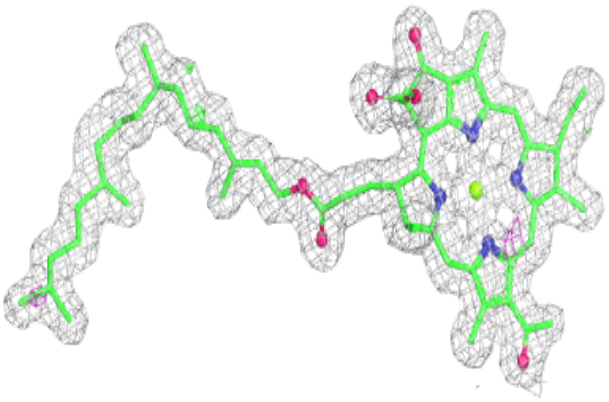


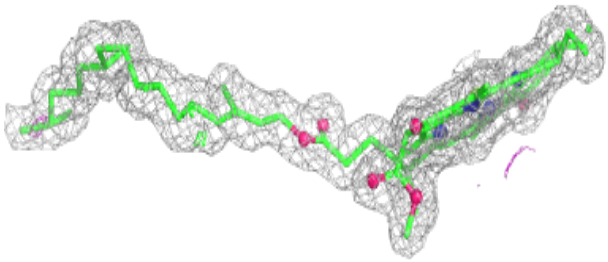


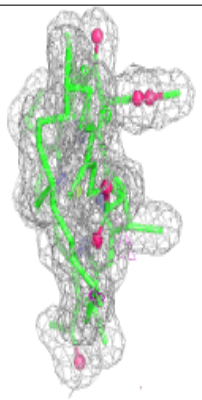


Electron density around BCL A 403:

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

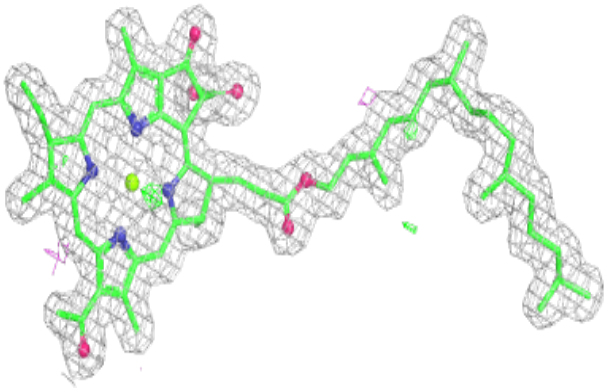


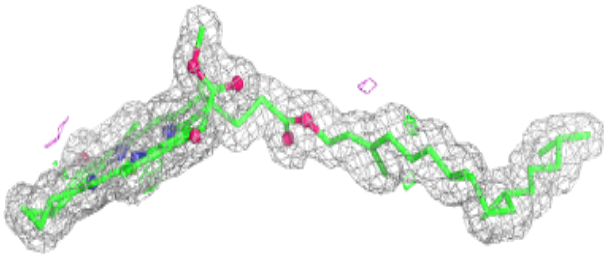


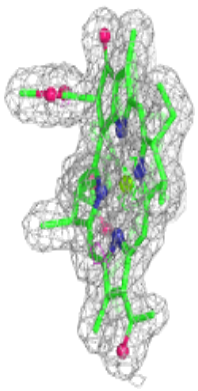


Electron density around BCL C 403:

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

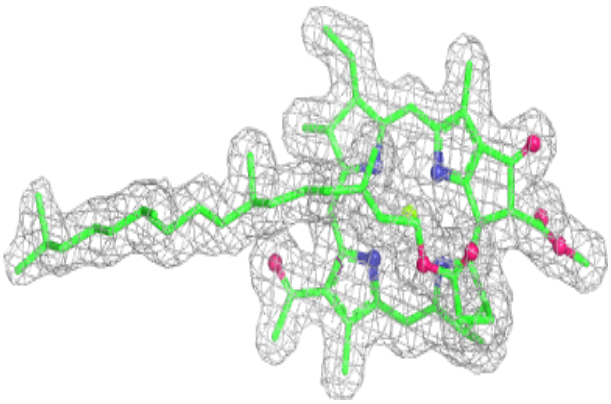


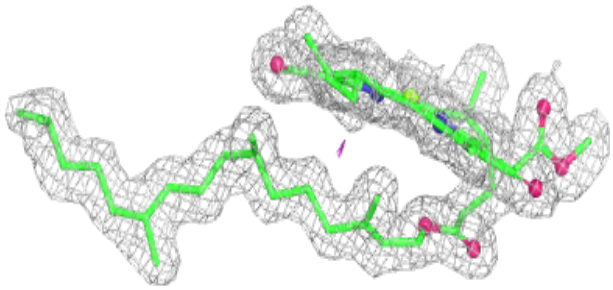


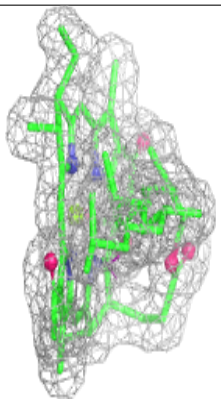


Electron density around BCL C 404:

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

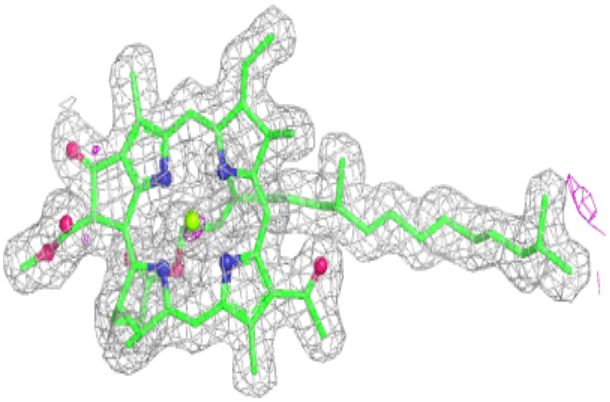


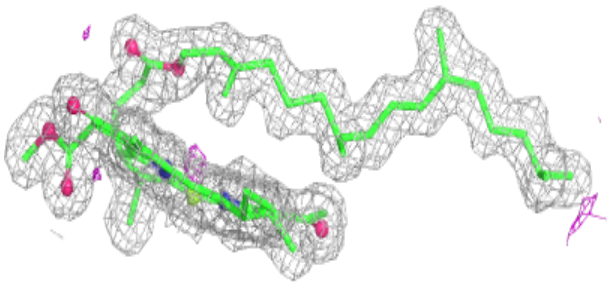


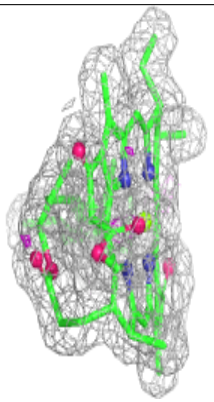


Electron density around BCL A 404:

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

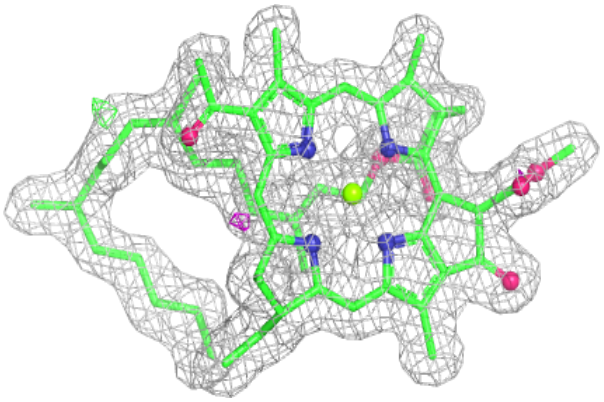


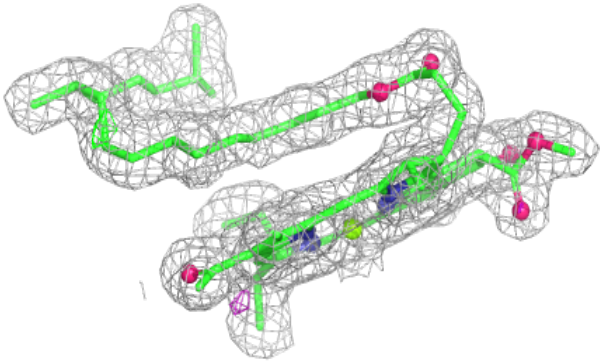


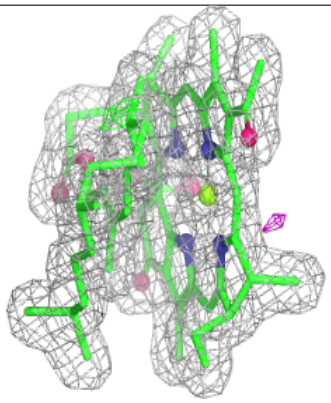


Electron density around BCL A 401 (B):

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

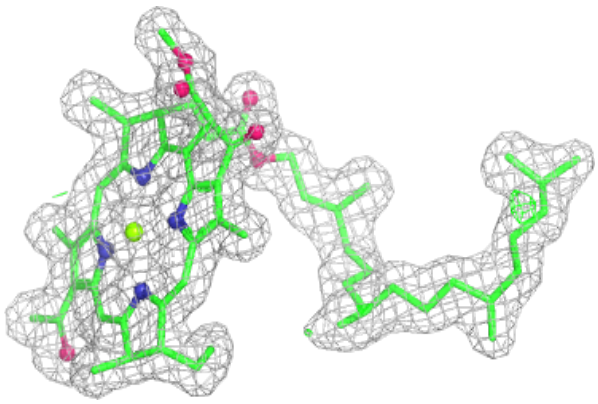


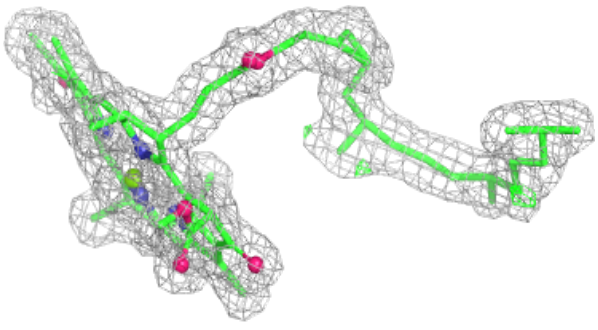


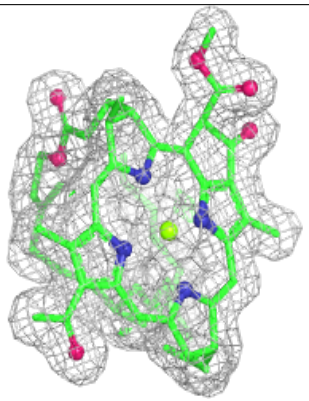


Electron density around BCL A 406 (C):

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

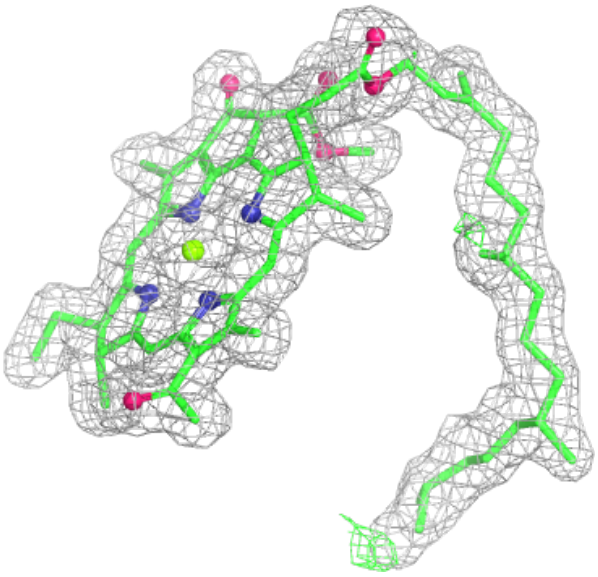


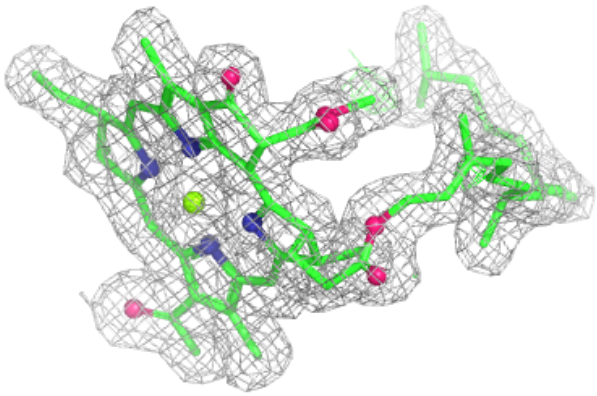


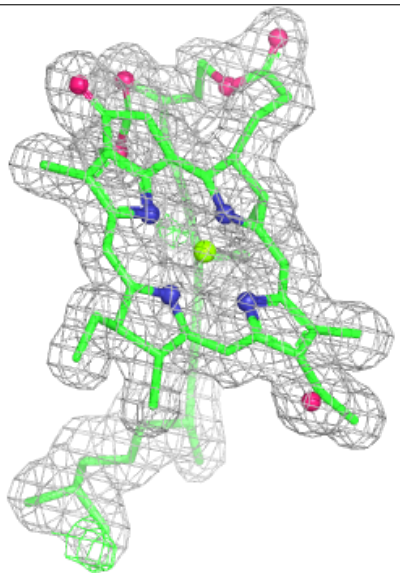


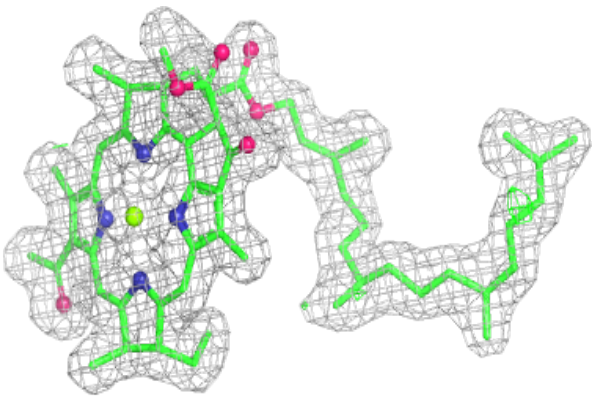
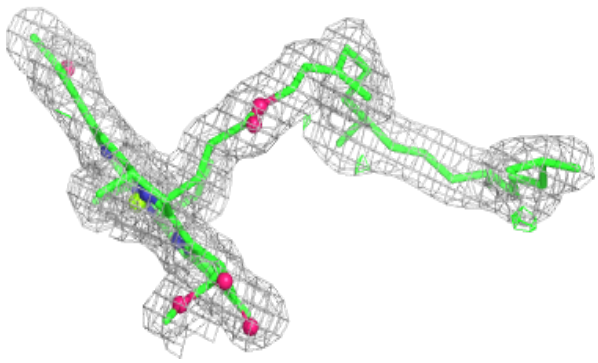
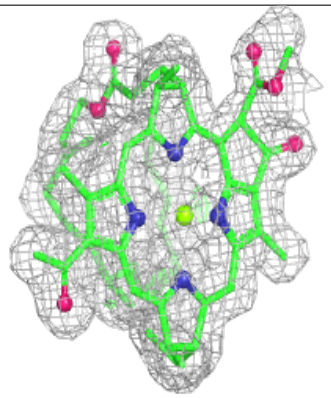
Electron density around BCL C 407:

$2mF_o$-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)	
	

6.5 Other polymers (i)

There are no such residues in this entry.