wwPDB EM Validation Summary Report (i)

Nov 16, 2022 – 12:44 AM JST

PDB ID	:	6M32
EMDB ID	:	EMD-30069
Title	:	Cryo-EM structure of FMO-RC complex from green sulfur bacteria
Authors	:	Chen, J.H.; Zhang, X.
Deposited on	:	2020-03-02
Resolution	:	2.70 Å(reported)

This is a wwPDB EM Validation Summary 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/EMValidationReportHelp
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 (1)) were used in the production of this report:

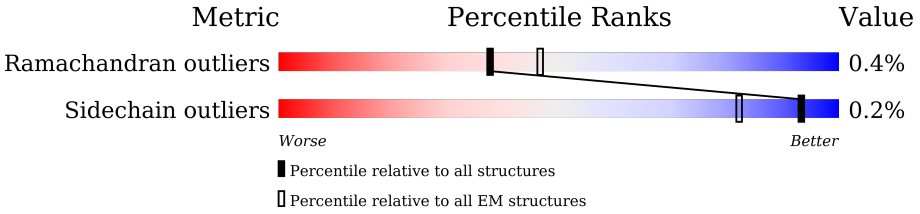
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.70 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)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	E	366	14% 99%
1	F	366	12% 98%
1	G	366	9% 97%
2	D	143	41% 64% 34%
3	B	231	10% 41% 59%
4	A	731	13% 85% 14%
4	a	731	17% 84% 14%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
9	F39	A	817	-	X	-	-
9	F39	a	817	-	X	-	-

2 Entry composition (i)

There are 13 unique types of molecules in this entry. The entry contains 23566 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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					AltConf	Trace
			Total	C	N	O	S		
1	E	362	2815	1783	501	524	7	0	0
1	F	358	2789	1770	496	516	7	0	0
1	G	358	2789	1770	496	516	7	0	0

- Molecule 2 is a protein called P840 reaction center 17 kDa protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	D	94	766	484	137	141	4	0	0

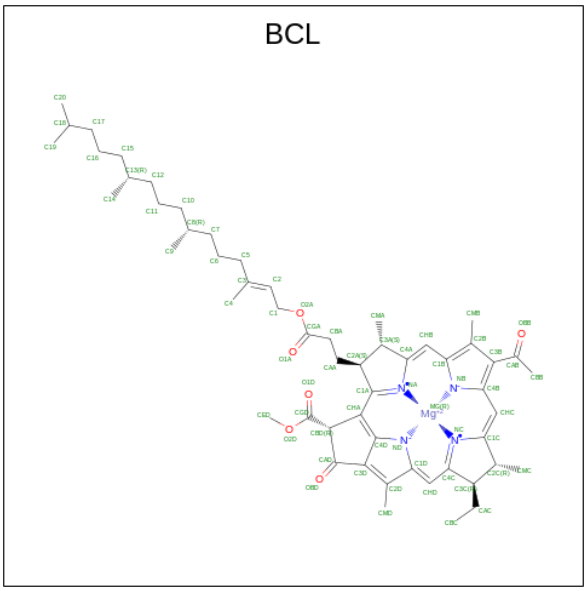
- Molecule 3 is a protein called Photosystem P840 reaction center iron-sulfur protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	B	95	731	469	115	138	9	0	0

- Molecule 4 is a protein called Photosystem P840 reaction center, large subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	A	628	5030	3360	798	846	26	0	0
4	a	628	5030	3360	798	846	26	0	0

- Molecule 5 is BACTERIOCHLOROPHYLL A (three-letter code: BCL) (formula: $C_{55}H_{74}MgN_4O_6$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
5	E	1	508	420	8	32	48	0
5	E	1	508	420	8	32	48	0
5	E	1	508	420	8	32	48	0
5	E	1	508	420	8	32	48	0
5	E	1	508	420	8	32	48	0
5	E	1	508	420	8	32	48	0
5	E	1	508	420	8	32	48	1
5	E	1	508	420	8	32	48	0
5	F	1	508	420	8	32	48	0
5	F	1	508	420	8	32	48	0
5	F	1	508	420	8	32	48	0
5	F	1	508	420	8	32	48	0
5	F	1	508	420	8	32	48	0
5	F	1	508	420	8	32	48	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
5	F	1	508	420	8	32	48	0
			Total	C	Mg	N	O	
5	F	1	508	420	8	32	48	1
			Total	C	Mg	N	O	
5	G	1	508	420	8	32	48	1
			Total	C	Mg	N	O	
5	G	1	508	420	8	32	48	0
			Total	C	Mg	N	O	
5	G	1	508	420	8	32	48	0
			Total	C	Mg	N	O	
5	G	1	508	420	8	32	48	0
			Total	C	Mg	N	O	
5	G	1	508	420	8	32	48	0
			Total	C	Mg	N	O	
5	G	1	508	420	8	32	48	0
			Total	C	Mg	N	O	
5	G	1	508	420	8	32	48	0
			Total	C	Mg	N	O	
5	G	1	508	420	8	32	48	0
			Total	C	Mg	N	O	
5	A	1	642	510	12	48	72	0
			Total	C	Mg	N	O	
5	A	1	642	510	12	48	72	0
			Total	C	Mg	N	O	
5	A	1	642	510	12	48	72	0
			Total	C	Mg	N	O	
5	A	1	642	510	12	48	72	0
			Total	C	Mg	N	O	
5	A	1	642	510	12	48	72	0
			Total	C	Mg	N	O	
5	A	1	642	510	12	48	72	0
			Total	C	Mg	N	O	
5	A	1	642	510	12	48	72	0
			Total	C	Mg	N	O	
5	A	1	642	510	12	48	72	0
			Total	C	Mg	N	O	
5	A	1	642	510	12	48	72	0
			Total	C	Mg	N	O	
5	A	1	642	510	12	48	72	0
			Total	C	Mg	N	O	
5	A	1	642	510	12	48	72	0

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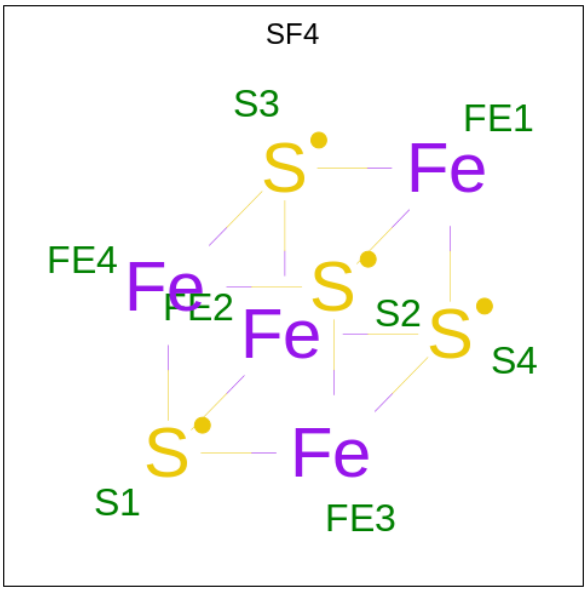
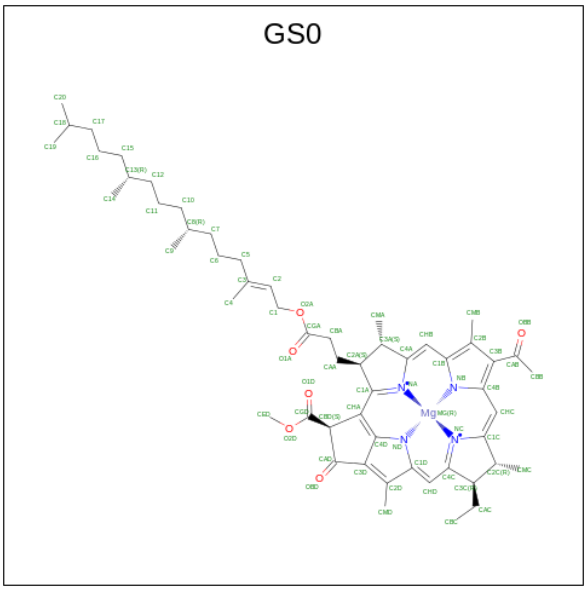
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
5	A	1	642	510	12	48	72	0
5	a	1	642	510	12	48	72	0
5	a	1	642	510	12	48	72	0
5	a	1	642	510	12	48	72	0
5	a	1	642	510	12	48	72	0
5	a	1	642	510	12	48	72	0
5	a	1	642	510	12	48	72	0
5	a	1	642	510	12	48	72	0
5	a	1	642	510	12	48	72	0
5	a	1	642	510	12	48	72	0
5	a	1	642	510	12	48	72	0
5	a	1	642	510	12	48	72	0
5	a	1	642	510	12	48	72	0

- Molecule 6 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
6	B	1	16	8	8	0
			Total	Fe	S	
6	B	1	16	8	8	0
			Total	Fe	S	
6	A	1	8	4	4	0

- Molecule 7 is Bacteriochlorophyll A isomer (three-letter code: GS0) (formula: $C_{55}H_{74}MgN_4O_6$).



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

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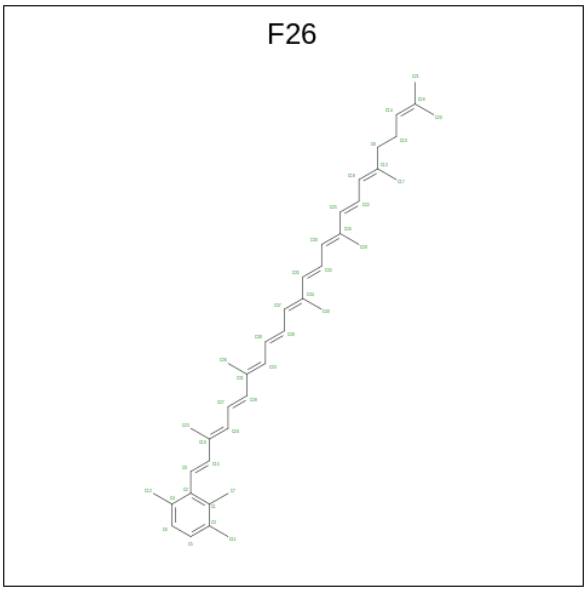
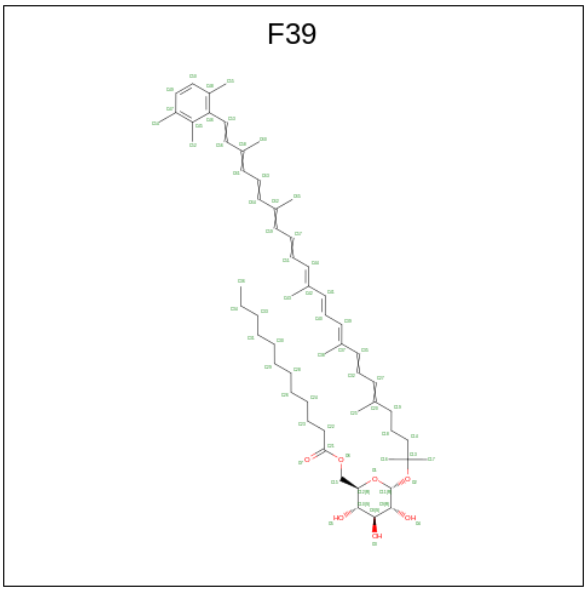
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
7	a	1	66	55	1	4	6	0

- Molecule 8 is 2-[(1E,3E,5E,7E,9E,11E,13E,15E,17E,19E)-3,7,12,16,20,24-hexamethylpentacosa-1,3,5,7,9,11,13,15,17,19,23-undecaenyl]-1,3,4-trimethyl-benzene (three-letter code: F26) (formula: $C_{40}H_{52}$).



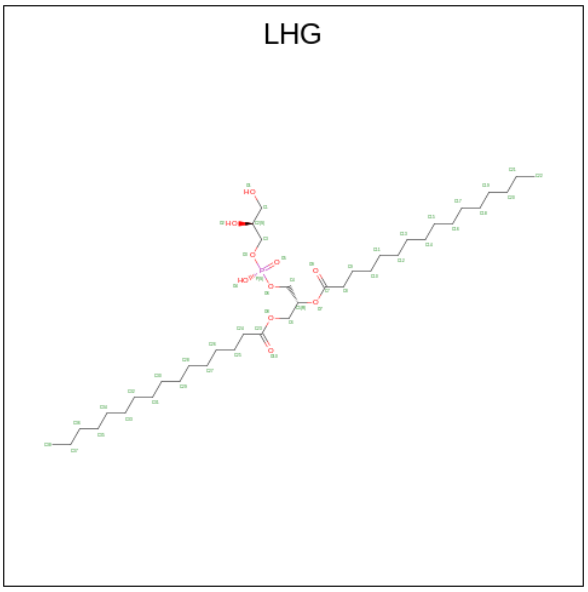
Mol	Chain	Residues	Atoms		AltConf
			Total	C	
8	A	1	40	40	0
8	a	1	40	40	0

- Molecule 9 is [(2R,3S,4S,5R,6R)-6-[(10E,12E,14E)-2,6,10,14,19,23-hexamethyl-25-(2,3,6-trimethylphenyl)pentacosa-6,8,10,12,14,16,18,20,22,24-decaen-2-yl]oxy-3,4,5-tris(oxidanyl)oxan-2-yl]methyl dodecanoate (three-letter code: F39) (formula: $C_{58}H_{86}O_7$).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
9	A	1	65	58	7	0
9	a	1	65	58	7	0

- Molecule 10 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: $C_{38}H_{75}O_{10}P$).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
10	A	1	46	35	10	1	0

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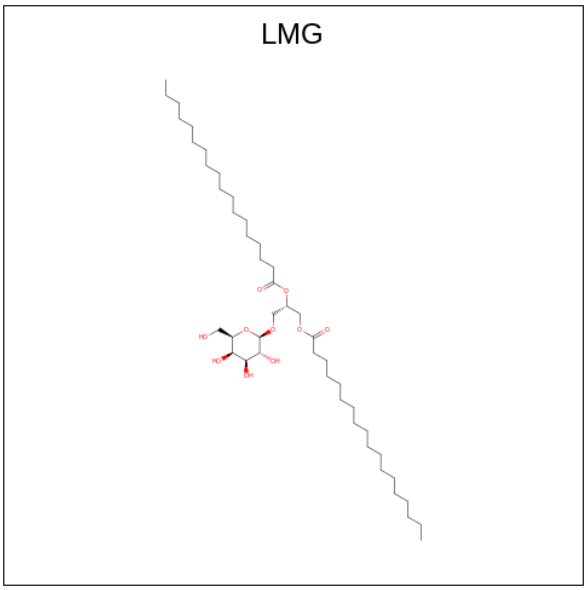
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
10	a	1	46	35	10	1	0

- Molecule 11 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: $C_{45}H_{86}O_{10}$).

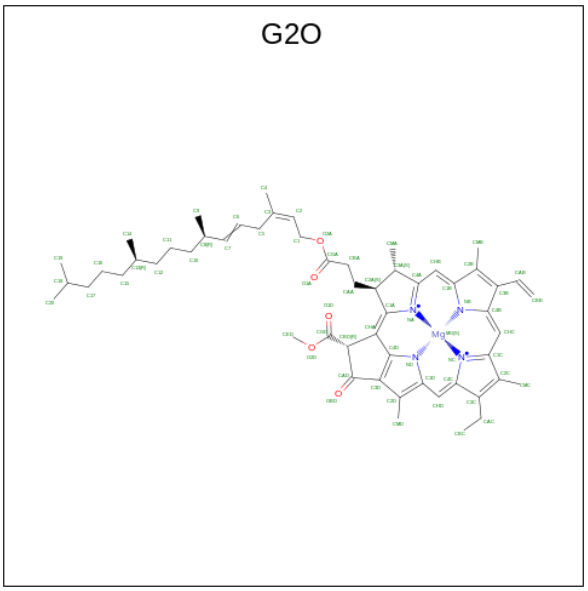


Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
11	A	1	44	34	10	0
11	a	1	44	34	10	0

- Molecule 12 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
			Total	Ca	
12	A	1	1	1	0
12	a	1	1	1	0

- Molecule 13 is Chlorophyll A ester (three-letter code: G2O) (formula: $C_{55}H_{70}MgN_4O_5$).



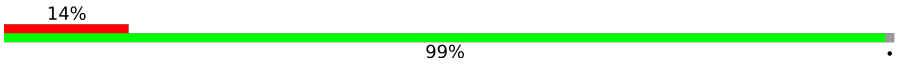
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
13	A	1	130	110	2	8	10	0
			Total	C	Mg	N	O	
13	A	1	130	110	2	8	10	0
			Total	C	Mg	N	O	
13	a	1	130	110	2	8	10	0
			Total	C	Mg	N	O	
13	a	1	130	110	2	8	10	0

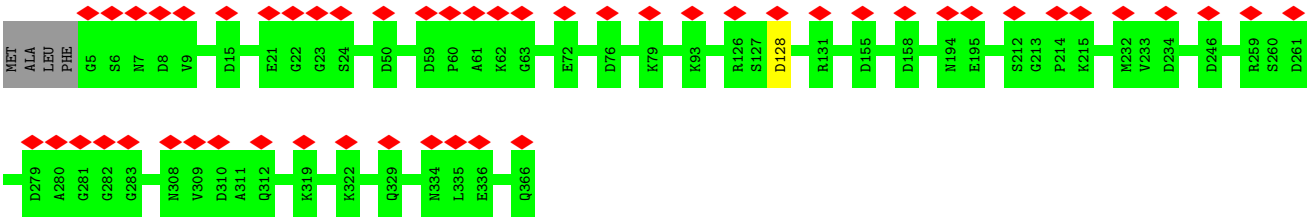
3 Residue-property plots (i)

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 atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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

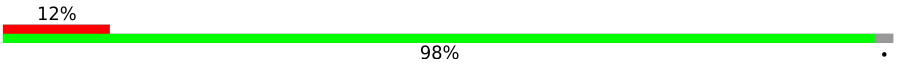
Chain E:

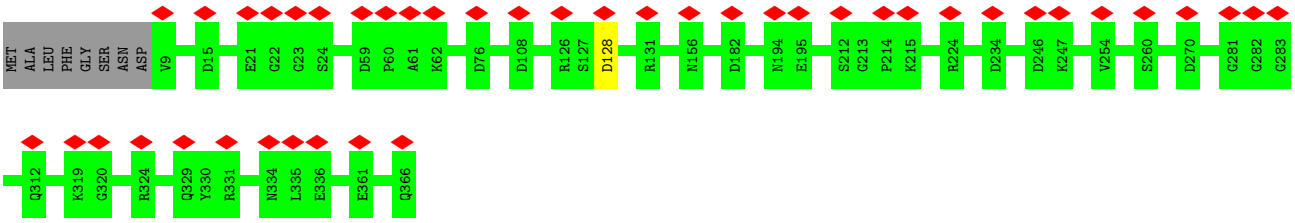




• Molecule 1: Bacteriochlorophyll a protein

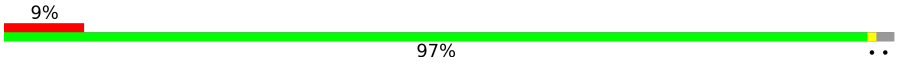
Chain F:

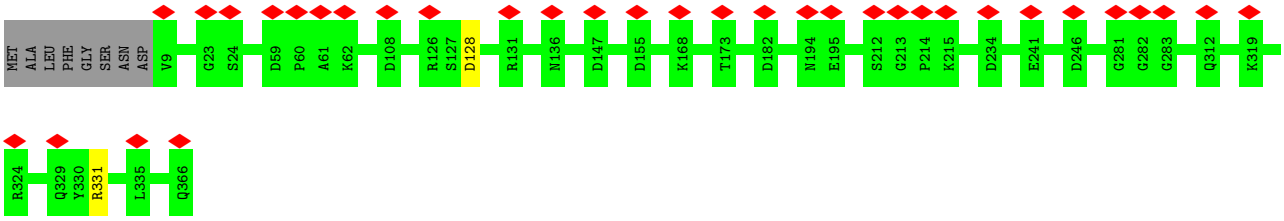




• Molecule 1: Bacteriochlorophyll a protein

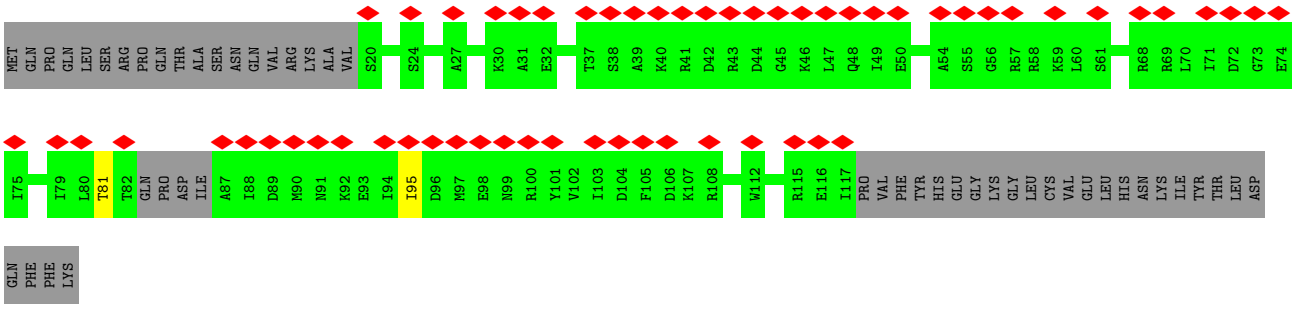
Chain G:





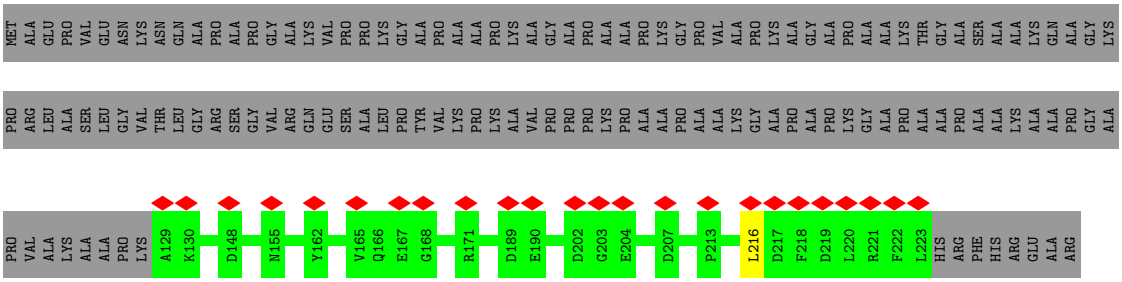
• Molecule 2: P840 reaction center 17 kDa protein

Chain D:



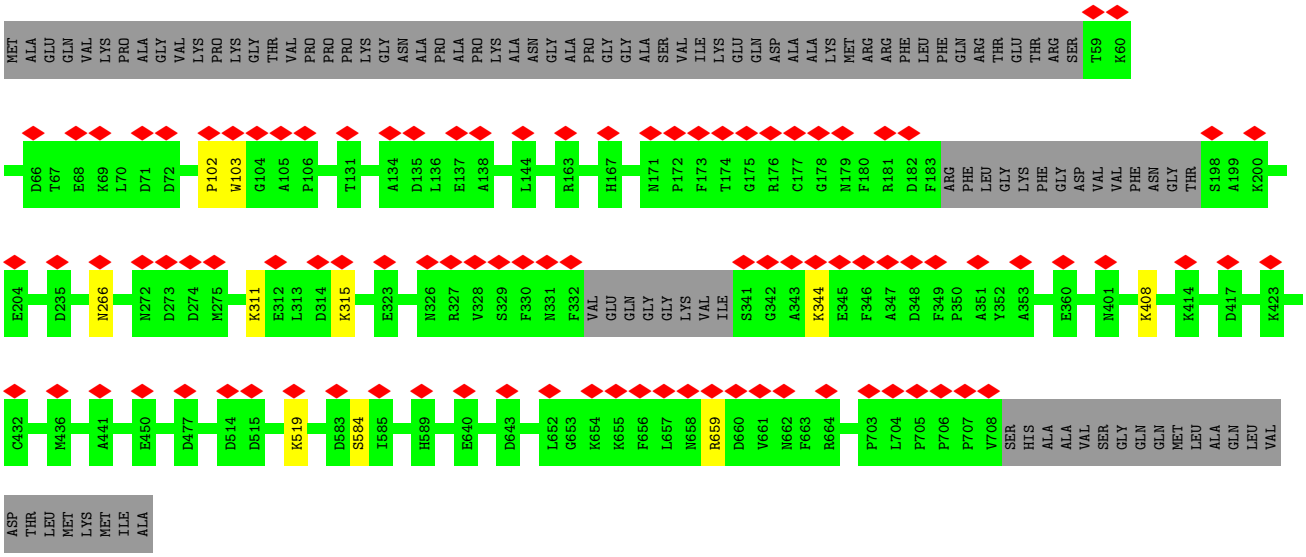
• Molecule 3: Photosystem P840 reaction center iron-sulfur protein

Chain B:



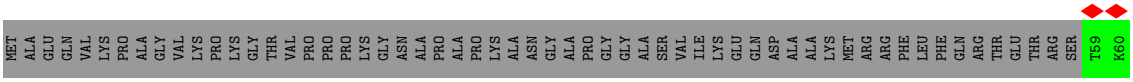
• Molecule 4: Photosystem P840 reaction center, large subunit

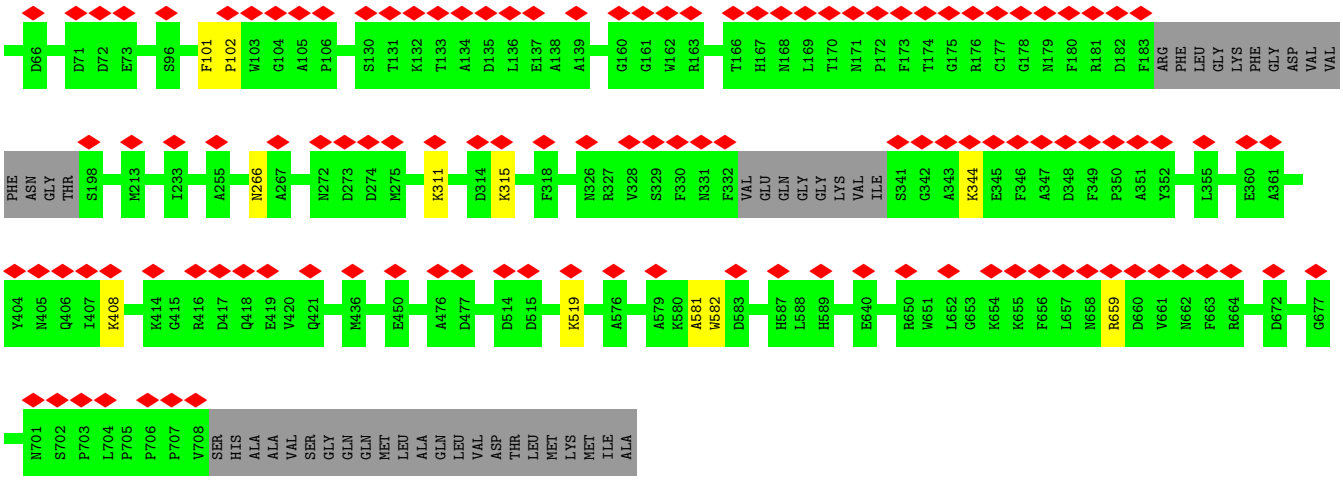
Chain A:



• Molecule 4: Photosystem P840 reaction center, large subunit

Chain a:




D66
D71 D72 E73
S96
F101 P102 W103 G104 A105 P106
S130 T131 K132 T133 A134 D135 L136 E137 A138 A139
G160 G161 W162 R163
T166 H167 N168 L169 T170 N171 P172 F173 T174 G175 R176 C177 G178 N179 F180 R181 D182 F183
ARG PHE LEU GLY LYS PHE GLY ASP VAL VAL
PHE ASN GLY THR S198 M213 T233 A255 N266 A267 N272 D273 D274 M275 K311 D314 K315 F318 N326 R327 V328 S329 F330 N331 F332
VAL GLU GLN GLY GLY LYS VAL ILE
S341 G342 A343 K344 E345 F346 A347 D348 F349 P350 A351 Y352 L355 E360 A361
Y404 N405 Q406 I407 K408 K414 G415 R416 D417 Q418 E419 V420 Q421 M436 E450 A476 D477 D514 D515 K519 A576 A579 K580 A581 W582 D583 H587 L588 H589 E640 R650 W651 L652 G653 K654 K655 F656 L657 N658 R659 D660 V661 N662 F663 R664 D672 G677
N701 S702 P703 L704 P705 P706 P707 V708
SER HIS ALA ALA VAL SER GLY GLN GLN MET LEU ALA GLN LEU VAL ASP THR LEU MET LYS MET ILE ALA

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	268430	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	47	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	38244	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.163	Depositor
Minimum map value	-0.048	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.0341	Depositor
Map size (Å)	209.12001, 209.12001, 209.12001	wwPDB
Map dimensions	160, 160, 160	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.307, 1.307, 1.307	Depositor

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: SF4, LHG, CA, F39, LMG, F26, G2O, GS0, 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	E	0.31	0/2885	0.53	1/3910 (0.0%)
1	F	0.31	0/2859	0.53	1/3875 (0.0%)
1	G	0.31	0/2859	0.53	1/3875 (0.0%)
2	D	0.28	0/778	0.56	0/1043
3	B	0.32	0/749	0.56	0/1013
4	A	0.32	0/5207	0.51	2/7097 (0.0%)
4	a	0.31	0/5207	0.50	2/7097 (0.0%)
All	All	0.31	0/20544	0.52	7/27910 (0.0%)

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
3	B	0	1
4	A	0	3
4	a	0	3
All	All	0	7

There are no bond length outliers.

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	128	ASP	CB-CG-OD2	6.18	123.86	118.30
1	F	128	ASP	CB-CG-OD2	6.16	123.84	118.30
1	G	128	ASP	CB-CG-OD2	6.13	123.82	118.30
4	a	266	ASN	N-CA-C	5.76	126.56	111.00
4	A	266	ASN	N-CA-C	5.76	126.55	111.00

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	A	311	LYS	Peptide
4	A	344	LYS	Peptide
4	A	519	LYS	Peptide
3	B	216	LEU	Peptide
4	a	311	LYS	Peptide

5.2 Too-close contacts (i)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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 PDB entries followed by that with respect to all EM entries.

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	E	360/366 (98%)	339 (94%)	21 (6%)	0	100	100
1	F	356/366 (97%)	338 (95%)	18 (5%)	0	100	100
1	G	356/366 (97%)	338 (95%)	18 (5%)	0	100	100
2	D	90/143 (63%)	71 (79%)	17 (19%)	2 (2%)	6	17
3	B	93/231 (40%)	76 (82%)	17 (18%)	0	100	100
4	A	622/731 (85%)	568 (91%)	51 (8%)	3 (0%)	29	54
4	a	622/731 (85%)	571 (92%)	46 (7%)	5 (1%)	19	43
All	All	2499/2934 (85%)	2301 (92%)	188 (8%)	10 (0%)	38	60

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	95	ILE
4	A	102	PRO
4	a	102	PRO

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Mol	Chain	Res	Type
4	A	659	ARG
4	a	659	ARG

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 PDB entries followed by that with respect to all EM entries.

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	E	299/302 (99%)	299 (100%)	0	100	100
1	F	296/302 (98%)	296 (100%)	0	100	100
1	G	296/302 (98%)	295 (100%)	1 (0%)	92	98
2	D	83/128 (65%)	83 (100%)	0	100	100
3	B	80/162 (49%)	80 (100%)	0	100	100
4	A	521/599 (87%)	519 (100%)	2 (0%)	91	97
4	a	521/599 (87%)	520 (100%)	1 (0%)	93	98
All	All	2096/2394 (88%)	2092 (100%)	4 (0%)	93	98

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	331	ARG
4	A	103	TRP
4	A	408	LYS
4	a	408	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	F	37	ASN
1	G	312	GLN
1	G	329	GLN
4	A	237	GLN
4	a	237	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)

Of 67 ligands modelled in this entry, 2 are monoatomic - leaving 65 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
8	F26	a	816	-	40,40,40	2.01	15 (37%)	46,50,50	2.00	10 (21%)
5	BCL	F	378[B]	1	38,54,74	1.88	7 (18%)	45,91,115	2.36	18 (40%)
5	BCL	E	376	-	58,74,74	1.59	8 (13%)	69,115,115	2.17	23 (33%)
5	BCL	E	375	1	58,74,74	1.60	8 (13%)	69,115,115	2.13	24 (34%)
5	BCL	A	804	-	38,54,74	1.89	8 (21%)	45,91,115	2.31	19 (42%)
5	BCL	a	809	4	38,54,74	1.86	6 (15%)	45,91,115	2.45	19 (42%)
11	LMG	a	819	4	44,44,55	0.78	1 (2%)	52,52,63	1.33	4 (7%)
10	LHG	A	818	-	45,45,48	0.64	1 (2%)	48,51,54	1.27	6 (12%)
5	BCL	G	371	1	58,74,74	1.60	7 (12%)	69,115,115	2.31	25 (36%)
5	BCL	E	373	-	58,74,74	1.61	9 (15%)	69,115,115	2.20	24 (34%)
7	GS0	a	801	-	64,74,74	1.73	12 (18%)	78,115,115	2.17	24 (30%)
10	LHG	a	818	-	45,45,48	0.63	1 (2%)	48,51,54	1.27	6 (12%)
5	BCL	a	806	-	58,74,74	1.61	9 (15%)	69,115,115	2.10	24 (34%)
5	BCL	G	372	-	58,74,74	1.58	7 (12%)	69,115,115	2.14	24 (34%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
13	G2O	A	803	-	67,73,73	2.73	24 (35%)	75,113,113	1.56	10 (13%)
5	BCL	A	807	4	38,54,74	1.92	9 (23%)	45,91,115	2.32	17 (37%)
5	BCL	A	814	-	38,54,74	1.87	6 (15%)	45,91,115	2.41	19 (42%)
5	BCL	G	375	1	58,74,74	1.60	8 (13%)	69,115,115	2.13	24 (34%)
5	BCL	A	808	-	58,74,74	1.59	8 (13%)	69,115,115	2.05	21 (30%)
5	BCL	G	374	-	58,74,74	1.59	7 (12%)	69,115,115	2.14	24 (34%)
5	BCL	F	373	-	58,74,74	1.61	9 (15%)	69,115,115	2.20	24 (34%)
5	BCL	a	808	-	58,74,74	1.60	8 (13%)	69,115,115	2.05	21 (30%)
5	BCL	F	372	-	58,74,74	1.59	7 (12%)	69,115,115	2.14	24 (34%)
6	SF4	A	821	4	0,12,12	-	-	-		
9	F39	A	817	-	66,66,66	8.01	53 (80%)	79,85,85	4.33	29 (36%)
5	BCL	A	812	4	58,74,74	1.61	9 (15%)	69,115,115	2.08	23 (33%)
5	BCL	a	812	4	58,74,74	1.60	9 (15%)	69,115,115	2.08	23 (33%)
5	BCL	a	811	4	58,74,74	1.60	8 (13%)	69,115,115	2.18	23 (33%)
9	F39	a	817	-	66,66,66	8.01	53 (80%)	79,85,85	4.33	29 (36%)
5	BCL	G	373	-	58,74,74	1.61	9 (15%)	69,115,115	2.20	23 (33%)
5	BCL	F	371	1	58,74,74	1.60	7 (12%)	69,115,115	2.31	24 (34%)
13	G2O	A	802	4	67,73,73	2.70	24 (35%)	75,113,113	1.50	7 (9%)
5	BCL	a	810	4	38,54,74	1.82	8 (21%)	45,91,115	2.47	19 (42%)
6	SF4	B	302	3	0,12,12	-	-	-		
5	BCL	A	815	-	38,54,74	1.86	7 (18%)	45,91,115	2.44	19 (42%)
5	BCL	F	375	1	58,74,74	1.59	8 (13%)	69,115,115	2.13	25 (36%)
7	GS0	A	801	-	64,74,74	1.72	12 (18%)	78,115,115	2.17	24 (30%)
5	BCL	E	371	1	58,74,74	1.60	8 (13%)	69,115,115	2.30	25 (36%)
5	BCL	a	804	-	38,54,74	1.89	8 (21%)	45,91,115	2.32	19 (42%)
8	F26	A	816	-	40,40,40	2.00	15 (37%)	46,50,50	2.00	12 (26%)
5	BCL	a	805	-	48,64,74	1.76	8 (16%)	57,103,115	2.24	22 (38%)
6	SF4	B	301	3	0,12,12	-	-	-		
11	LMG	A	819	4	44,44,55	0.78	1 (2%)	52,52,63	1.33	4 (7%)
5	BCL	F	376	-	58,74,74	1.60	7 (12%)	69,115,115	2.17	23 (33%)
5	BCL	A	810	4	38,54,74	1.82	8 (21%)	45,91,115	2.47	19 (42%)
5	BCL	E	377	-	58,74,74	1.59	8 (13%)	69,115,115	2.17	23 (33%)
13	G2O	a	803	-	67,73,73	2.73	24 (35%)	75,113,113	1.55	10 (13%)
5	BCL	E	374	-	58,74,74	1.59	7 (12%)	69,115,115	2.14	25 (36%)
5	BCL	A	805	-	48,64,74	1.76	9 (18%)	57,103,115	2.24	22 (38%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
13	G2O	a	802	4	67,73,73	2.70	24 (35%)	75,113,113	1.49	7 (9%)
5	BCL	E	378[B]	1	38,54,74	1.87	7 (18%)	45,91,115	2.36	17 (37%)
5	BCL	a	807	4	38,54,74	1.92	9 (23%)	45,91,115	2.32	17 (37%)
5	BCL	F	377	-	58,74,74	1.59	7 (12%)	69,115,115	2.16	23 (33%)
5	BCL	F	374	-	58,74,74	1.58	7 (12%)	69,115,115	2.14	24 (34%)
5	BCL	A	809	4	38,54,74	1.86	7 (18%)	45,91,115	2.46	19 (42%)
5	BCL	G	376	-	58,74,74	1.60	8 (13%)	69,115,115	2.17	23 (33%)
5	BCL	G	377	-	58,74,74	1.59	7 (12%)	69,115,115	2.17	23 (33%)
5	BCL	A	813	-	38,54,74	1.87	9 (23%)	45,91,115	2.33	18 (40%)
5	BCL	a	814	-	38,54,74	1.86	6 (15%)	45,91,115	2.40	18 (40%)
5	BCL	a	815	-	38,54,74	1.86	8 (21%)	45,91,115	2.44	19 (42%)
5	BCL	a	813	-	38,54,74	1.87	9 (23%)	45,91,115	2.33	17 (37%)
5	BCL	G	378[B]	1	38,54,74	1.87	8 (21%)	45,91,115	2.36	18 (40%)
5	BCL	E	372	-	58,74,74	1.59	8 (13%)	69,115,115	2.14	23 (33%)
5	BCL	A	806	-	58,74,74	1.62	9 (15%)	69,115,115	2.09	24 (34%)
5	BCL	A	811	4	58,74,74	1.60	8 (13%)	69,115,115	2.18	23 (33%)

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
8	F26	a	816	-	-	15/36/36/36	0/1/1/1
5	BCL	F	378[B]	1	-	3/13/113/137	-
5	BCL	E	376	-	-	11/37/137/137	-
5	BCL	E	375	1	-	11/37/137/137	-
5	BCL	A	804	-	-	11/13/113/137	-
5	BCL	a	809	4	-	4/13/113/137	-
11	LMG	a	819	4	-	19/39/59/70	0/1/1/1
10	LHG	A	818	-	-	21/50/50/53	-
5	BCL	G	371	1	-	12/37/137/137	-
5	BCL	E	373	-	-	13/37/137/137	-
7	GS0	a	801	-	-	12/37/137/137	-
10	LHG	a	818	-	-	21/50/50/53	-
5	BCL	a	806	-	-	10/37/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	BCL	G	372	-	-	17/37/137/137	-
13	G2O	A	803	-	-	18/39/115/115	-
5	BCL	A	807	4	-	5/13/113/137	-
5	BCL	A	814	-	-	5/13/113/137	-
5	BCL	G	375	1	-	11/37/137/137	-
5	BCL	A	808	-	-	18/37/137/137	-
5	BCL	G	374	-	-	14/37/137/137	-
5	BCL	F	373	-	-	13/37/137/137	-
5	BCL	a	808	-	-	18/37/137/137	-
5	BCL	F	372	-	-	17/37/137/137	-
6	SF4	A	821	4	-	-	0/6/5/5
9	F39	A	817	-	-	40/58/78/78	0/2/2/2
5	BCL	A	812	4	-	14/37/137/137	-
5	BCL	a	812	4	-	14/37/137/137	-
5	BCL	a	811	4	-	17/37/137/137	-
9	F39	a	817	-	-	40/58/78/78	0/2/2/2
5	BCL	G	373	-	-	13/37/137/137	-
5	BCL	F	371	1	-	12/37/137/137	-
13	G2O	A	802	4	-	12/39/115/115	-
5	BCL	a	810	4	-	8/13/113/137	-
6	SF4	B	302	3	-	-	0/6/5/5
5	BCL	A	815	-	-	7/13/113/137	-
5	BCL	F	375	1	-	11/37/137/137	-
7	GS0	A	801	-	-	12/37/137/137	-
5	BCL	E	371	1	-	12/37/137/137	-
5	BCL	a	804	-	-	11/13/113/137	-
8	F26	A	816	-	-	15/36/36/36	0/1/1/1
5	BCL	a	805	-	-	12/25/125/137	-
6	SF4	B	301	3	-	-	0/6/5/5
11	LMG	A	819	4	-	19/39/59/70	0/1/1/1
5	BCL	F	376	-	-	11/37/137/137	-
5	BCL	A	810	4	-	8/13/113/137	-
5	BCL	E	377	-	-	12/37/137/137	-
13	G2O	a	803	-	-	18/39/115/115	-
5	BCL	E	374	-	-	14/37/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	BCL	A	805	-	-	12/25/125/137	-
13	G2O	a	802	4	-	12/39/115/115	-
5	BCL	E	378[B]	1	-	3/13/113/137	-
5	BCL	a	807	4	-	5/13/113/137	-
5	BCL	F	377	-	-	12/37/137/137	-
5	BCL	F	374	-	-	14/37/137/137	-
5	BCL	A	809	4	-	4/13/113/137	-
5	BCL	G	376	-	-	11/37/137/137	-
5	BCL	G	377	-	-	12/37/137/137	-
5	BCL	A	813	-	-	5/13/113/137	-
5	BCL	a	814	-	-	5/13/113/137	-
5	BCL	a	815	-	-	7/13/113/137	-
5	BCL	a	813	-	-	5/13/113/137	-
5	BCL	G	378[B]	1	-	3/13/113/137	-
5	BCL	E	372	-	-	17/37/137/137	-
5	BCL	A	806	-	-	10/37/137/137	-
5	BCL	A	811	4	-	17/37/137/137	-

The worst 5 of 636 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	817	F39	C27-C20	26.99	1.62	1.34
9	a	817	F39	C27-C20	26.91	1.62	1.34
9	a	817	F39	C39-C37	22.04	1.65	1.35
9	A	817	F39	C39-C37	22.01	1.65	1.35
9	A	817	F39	C44-C42	20.11	1.62	1.35

The worst 5 of 1219 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	a	817	F39	C57-C59-C62	-11.74	110.55	127.31
9	A	817	F39	C57-C59-C62	-11.73	110.56	127.31
9	A	817	F39	C51-C44-C42	-11.21	111.31	127.31
9	a	817	F39	C51-C44-C42	-11.20	111.33	127.31
9	A	817	F39	C40-C39-C37	-11.17	111.37	127.31

There are no chirality outliers.

5 of 785 torsion outliers are listed below:

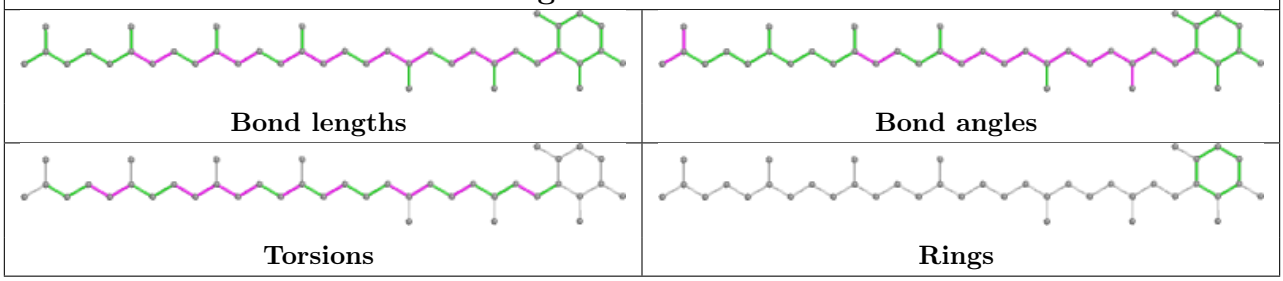
Mol	Chain	Res	Type	Atoms
5	E	371	BCL	C1A-C2A-CAA-CBA
5	E	371	BCL	C3A-C2A-CAA-CBA
5	E	371	BCL	CBD-CGD-O2D-CED
5	E	371	BCL	O1D-CGD-O2D-CED
5	E	373	BCL	C2C-C3C-CAC-CBC

There are no ring outliers.

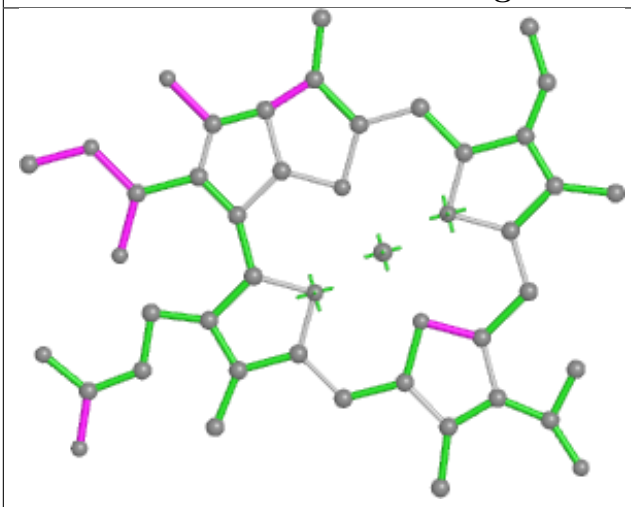
No monomer is involved in short contacts.

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.

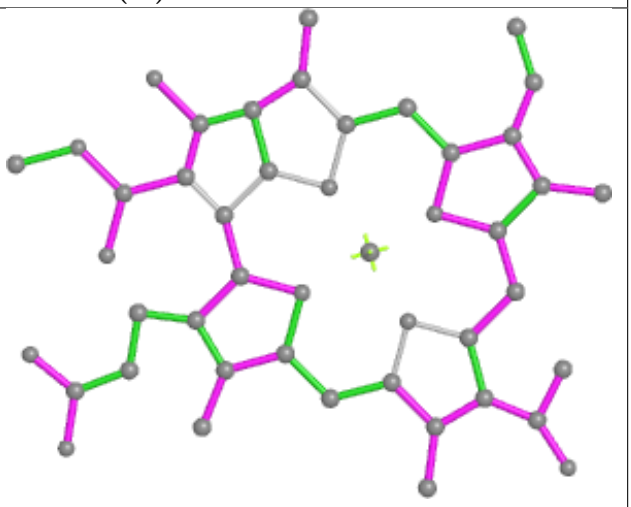
Ligand F26 a 816



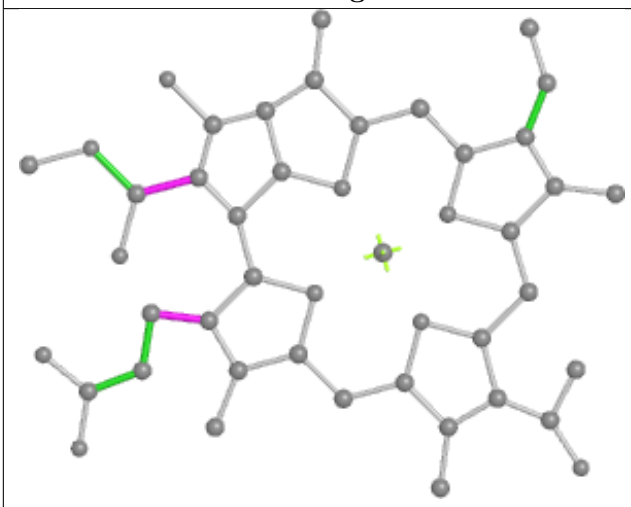
Ligand BCL F 378 (B)



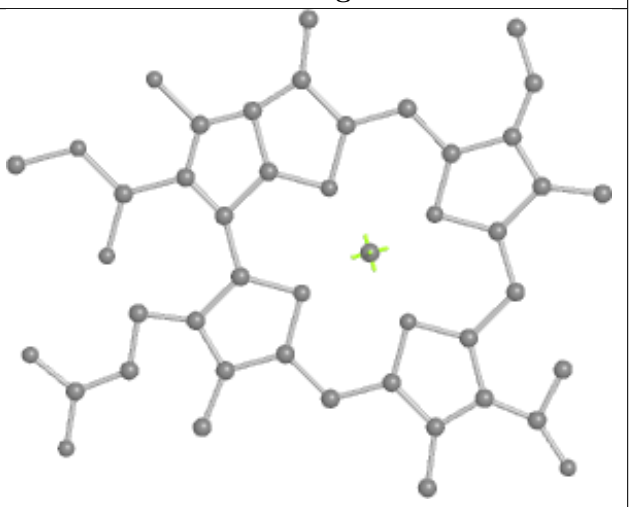
Bond lengths



Bond angles

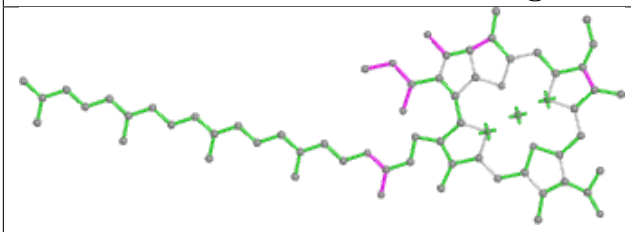


Torsions

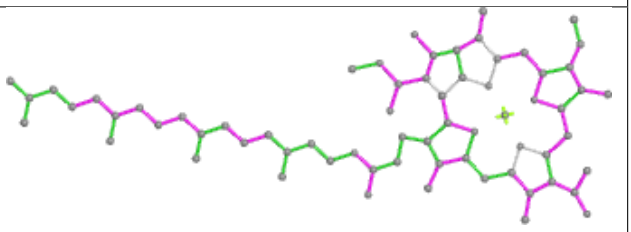


Rings

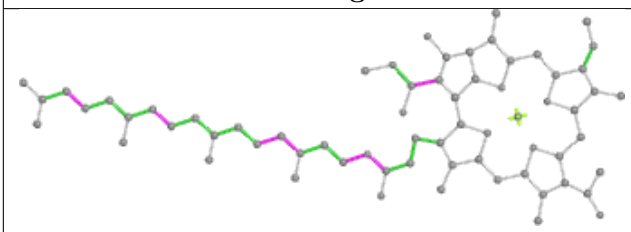
Ligand BCL E 376



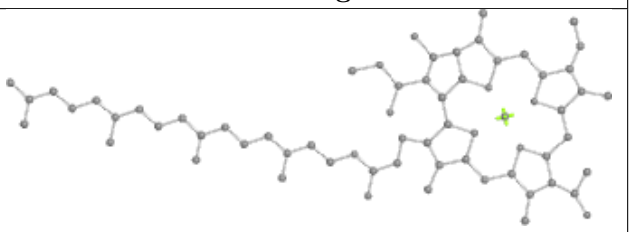
Bond lengths



Bond angles

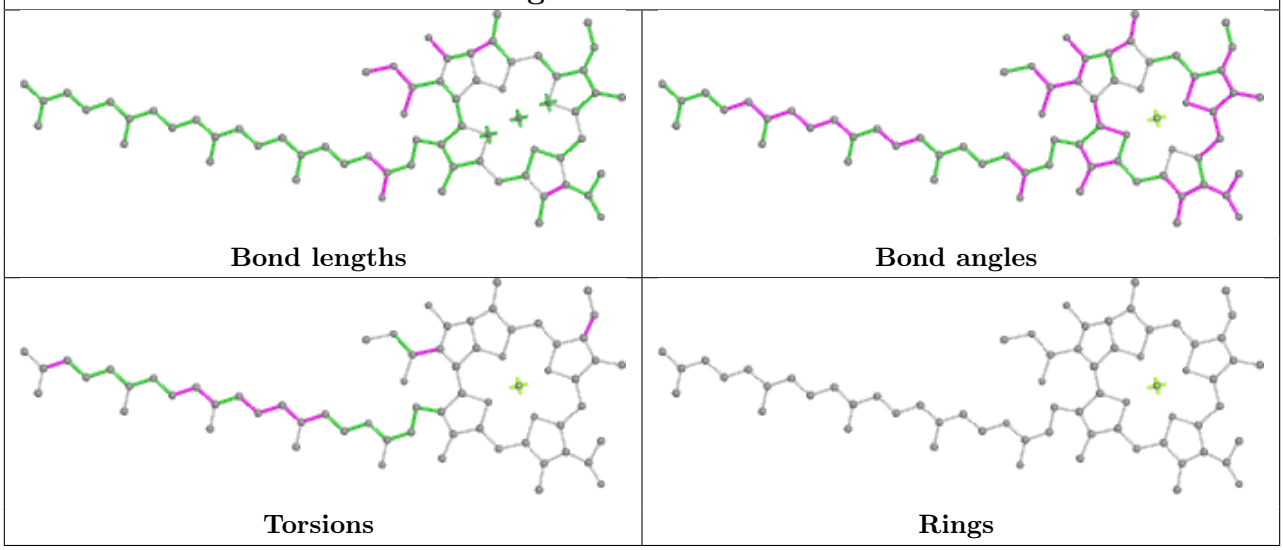


Torsions

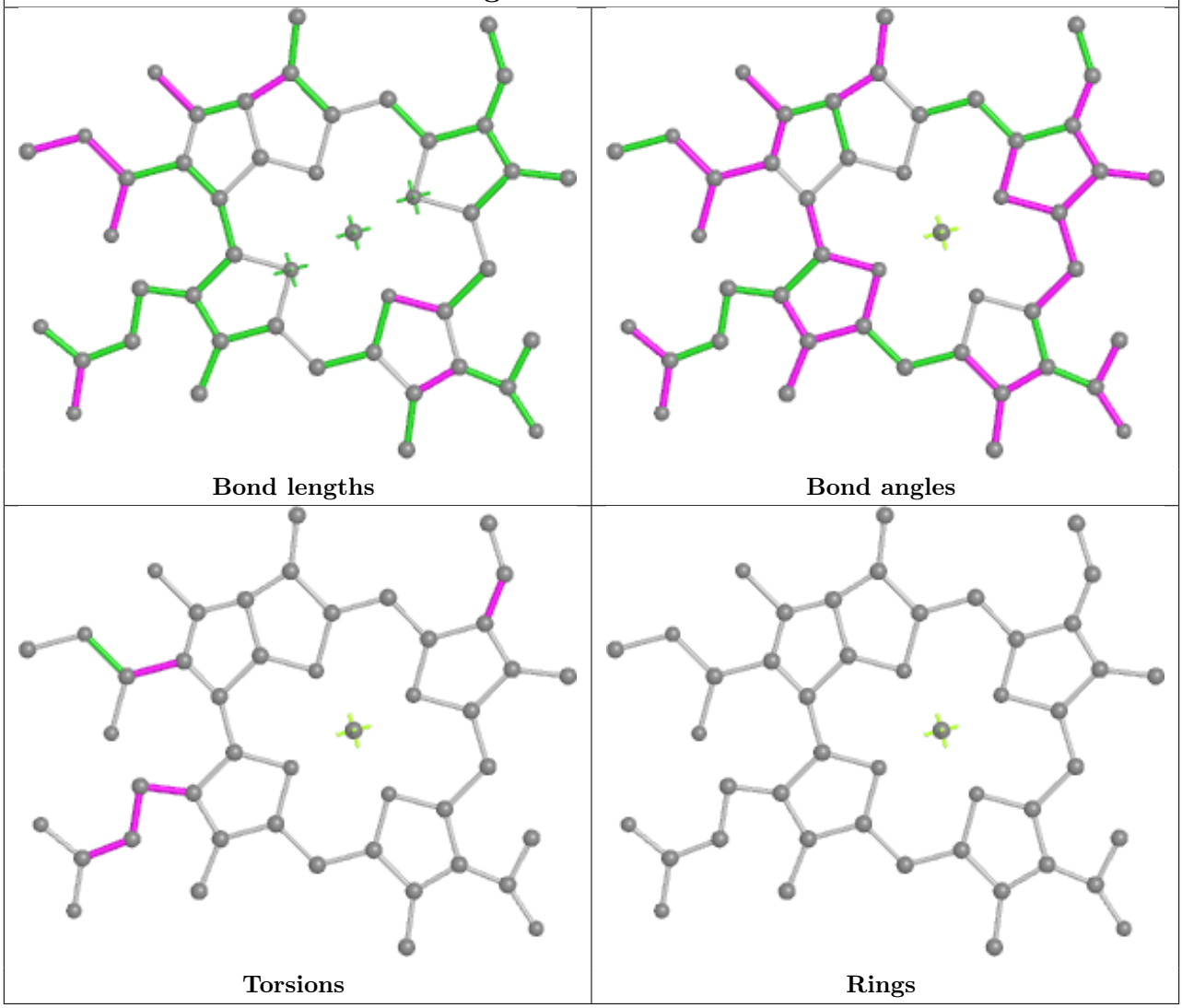


Rings

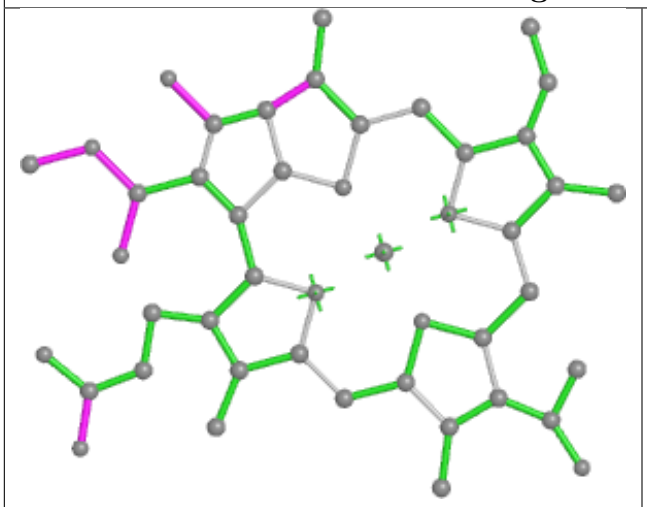
Ligand BCL E 375



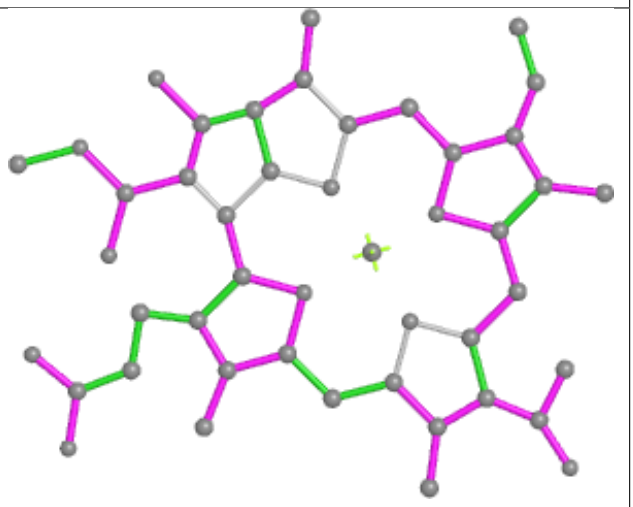
Ligand BCL A 804



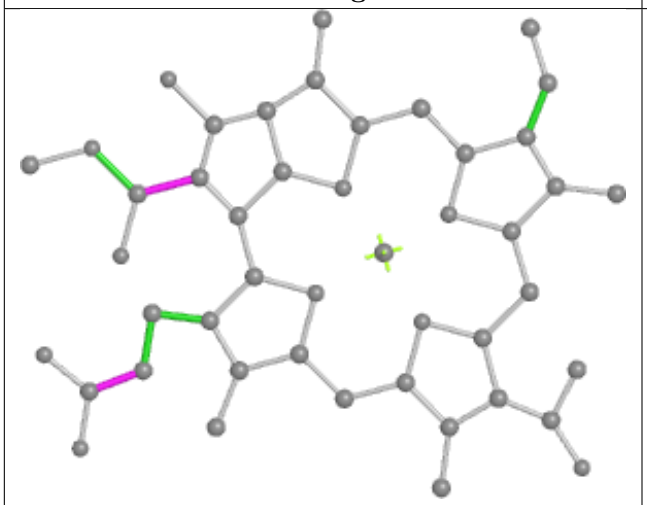
Ligand BCL a 809



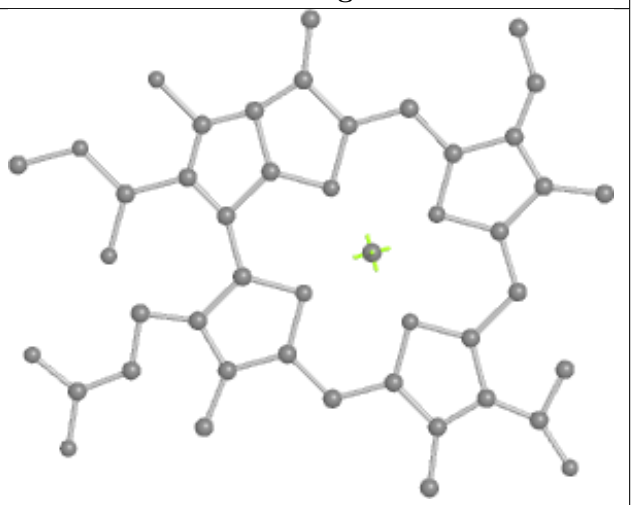
Bond lengths



Bond angles

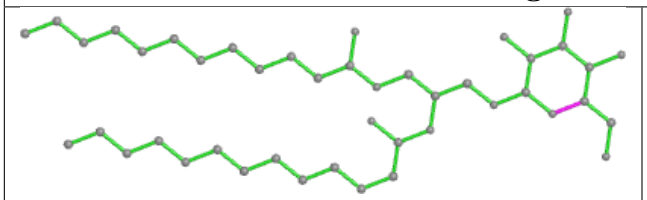


Torsions

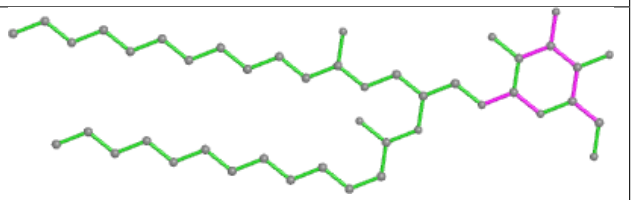


Rings

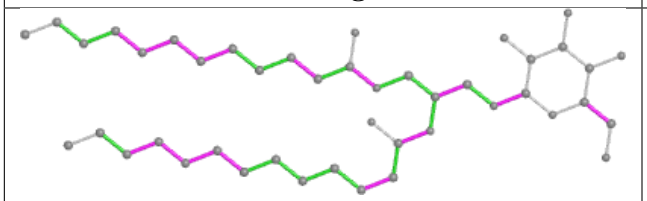
Ligand LMG a 819



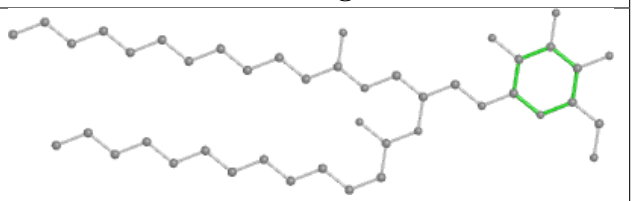
Bond lengths



Bond angles

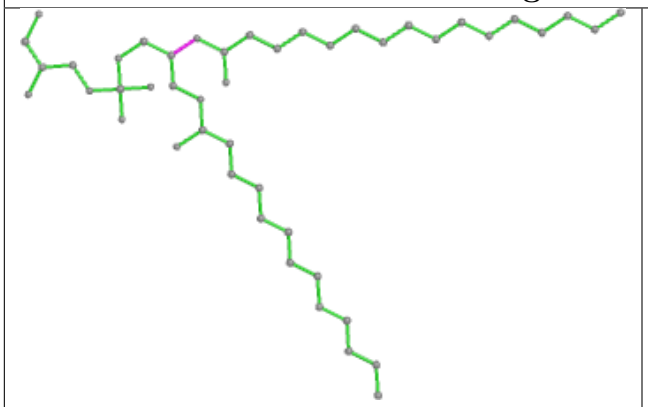


Torsions



Rings

Ligand LHG A 818



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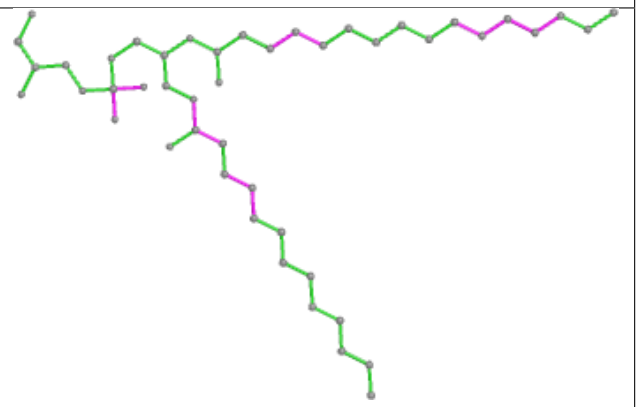
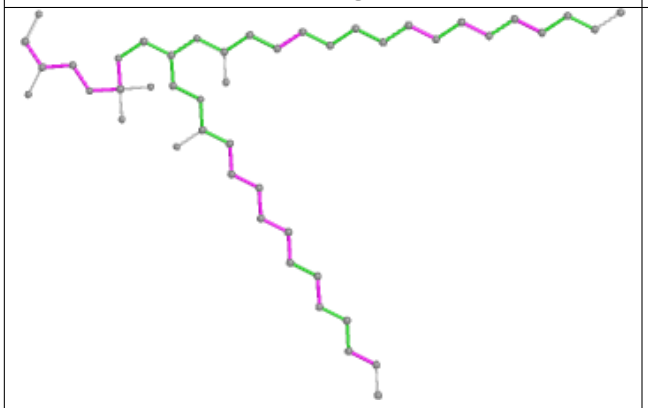
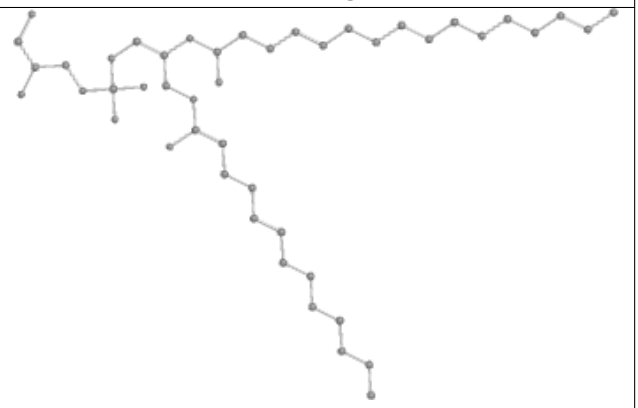


Bond angles

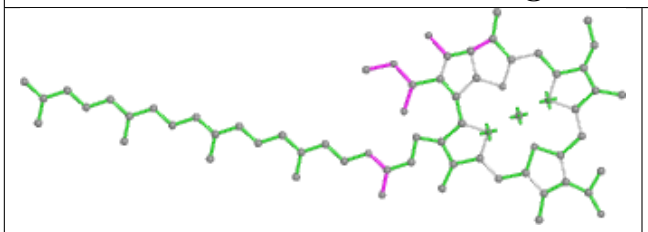


Torsions

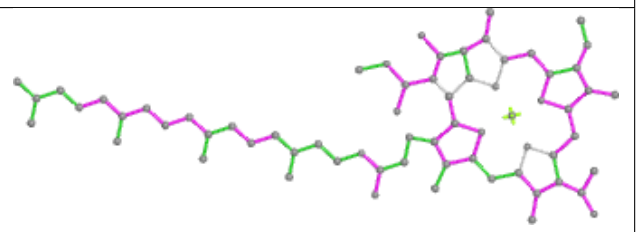


Rings

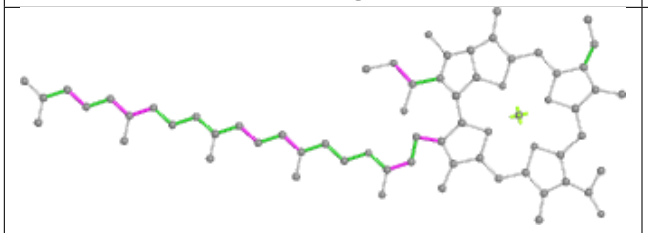
Ligand BCL G 371



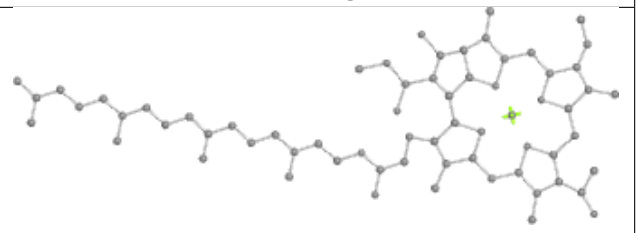
Bond lengths



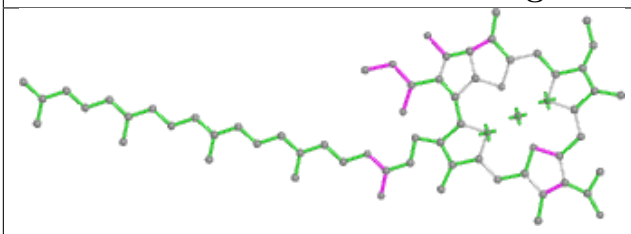
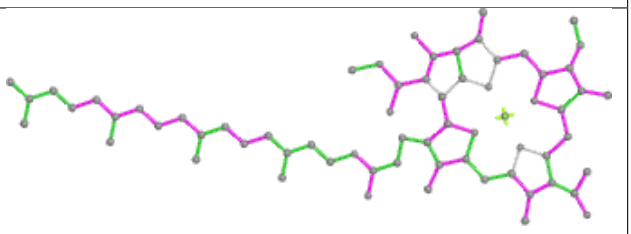
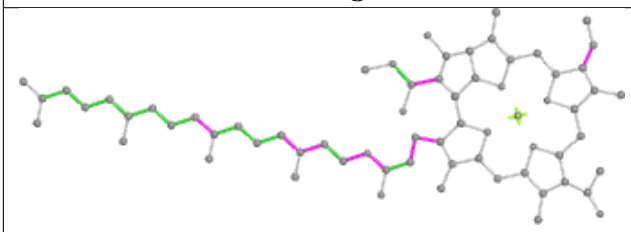
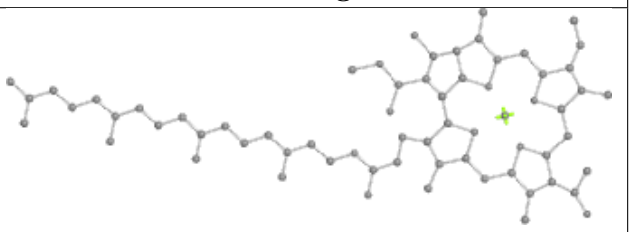
Bond angles

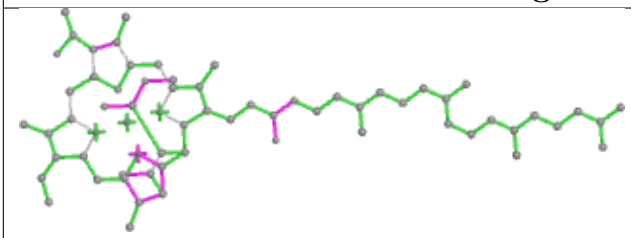
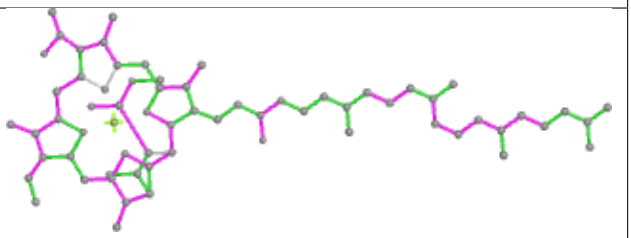
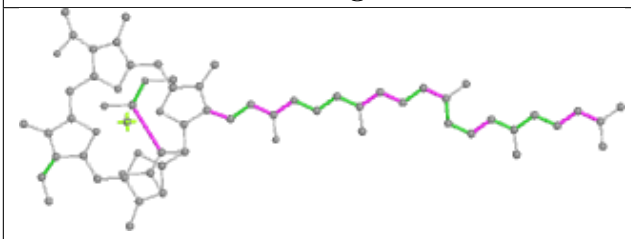
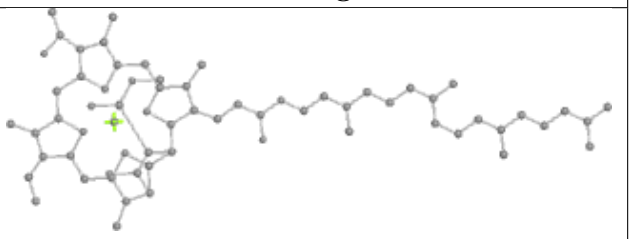


Torsions

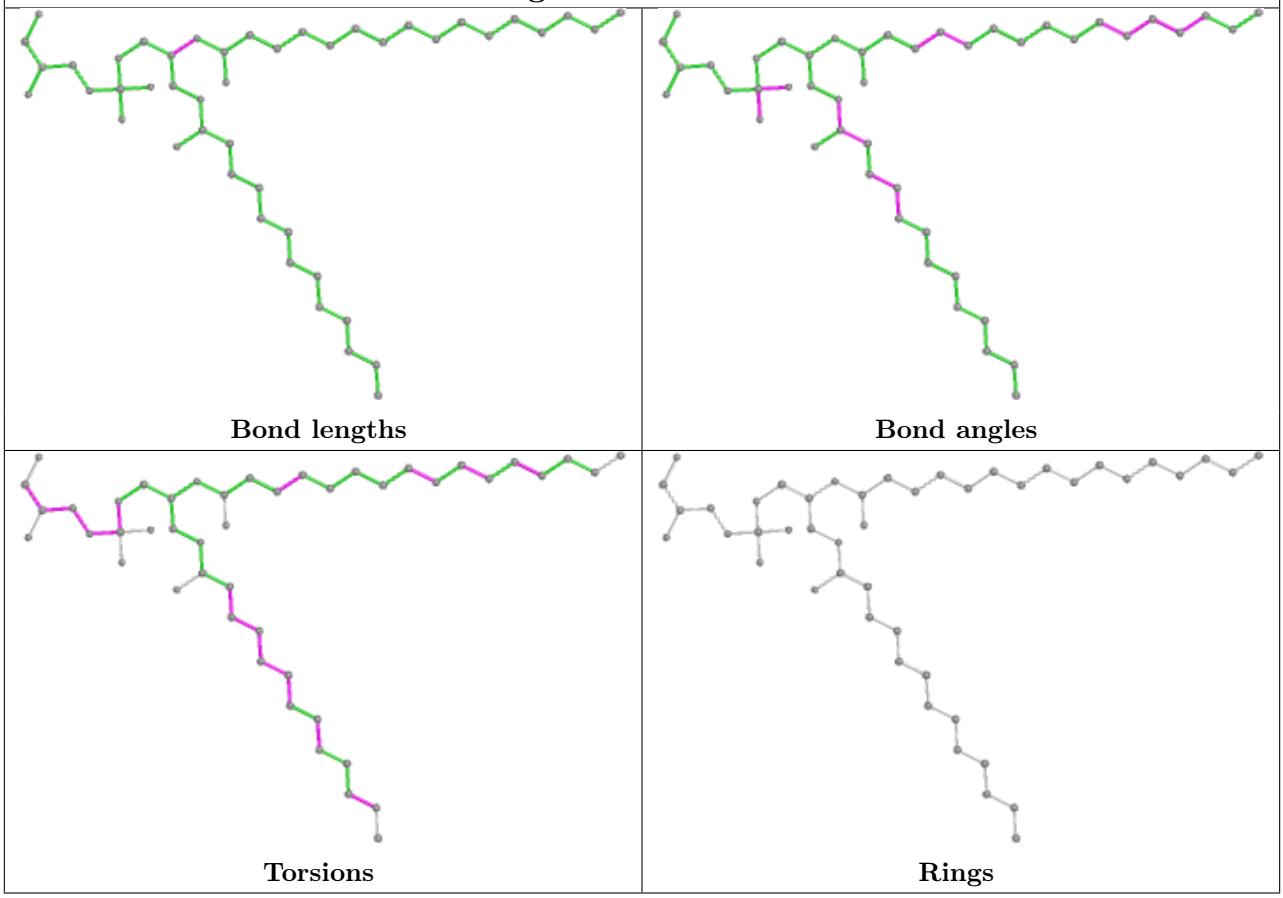


Rings

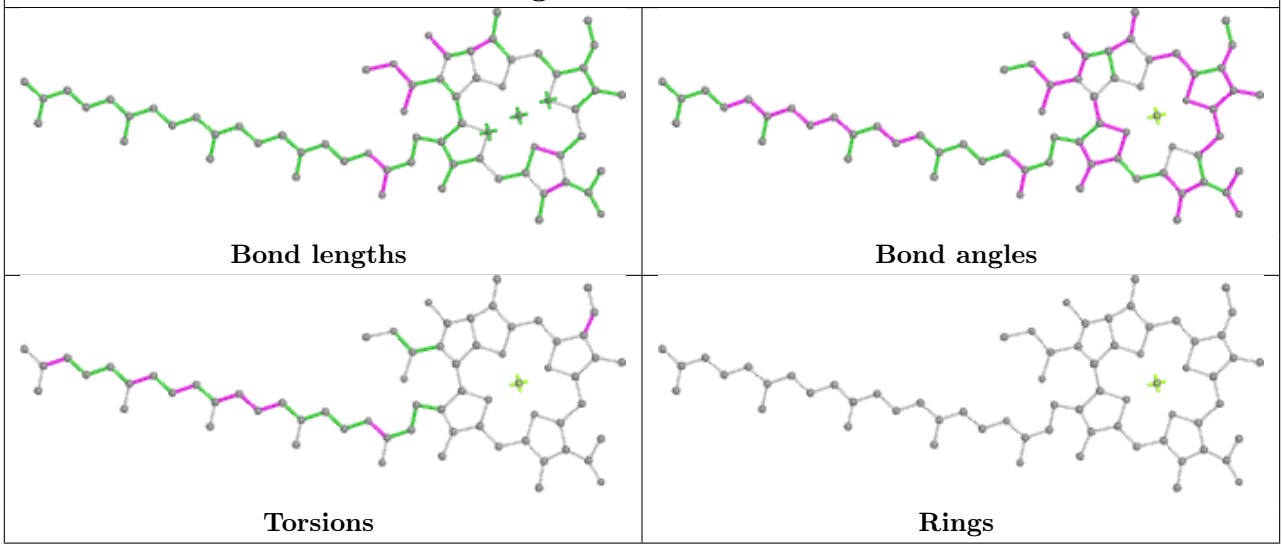
Ligand BCL E 373	
 Bond lengths	 Bond angles
 Torsions	 Rings

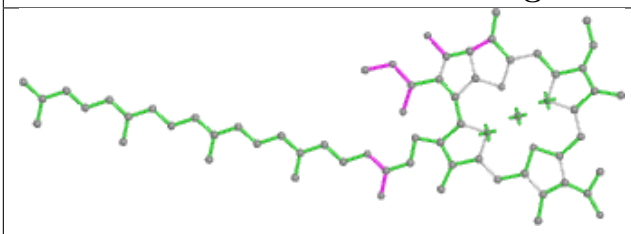
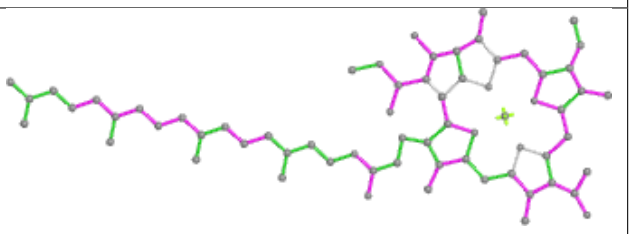
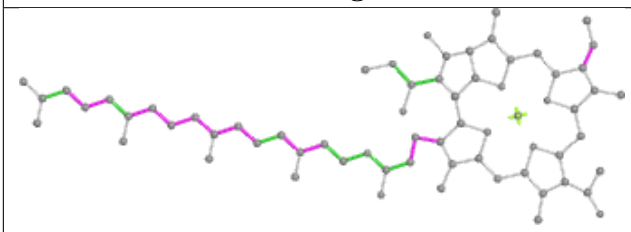
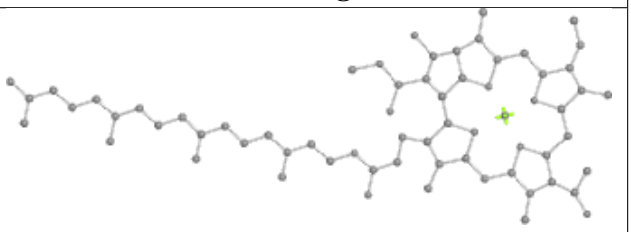
Ligand GS0 a 801	
 Bond lengths	 Bond angles
 Torsions	 Rings

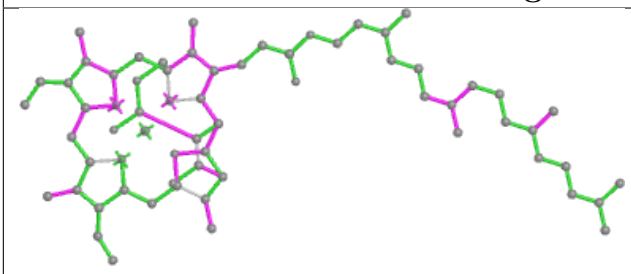
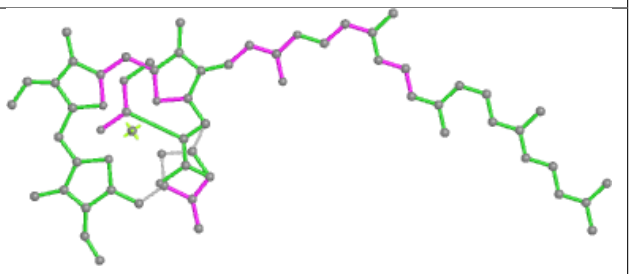
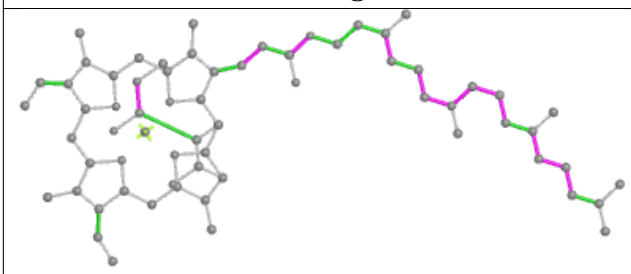
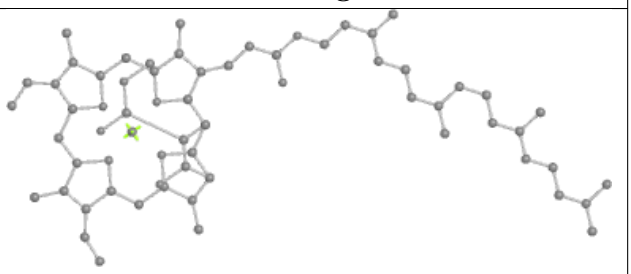
Ligand LHG a 818



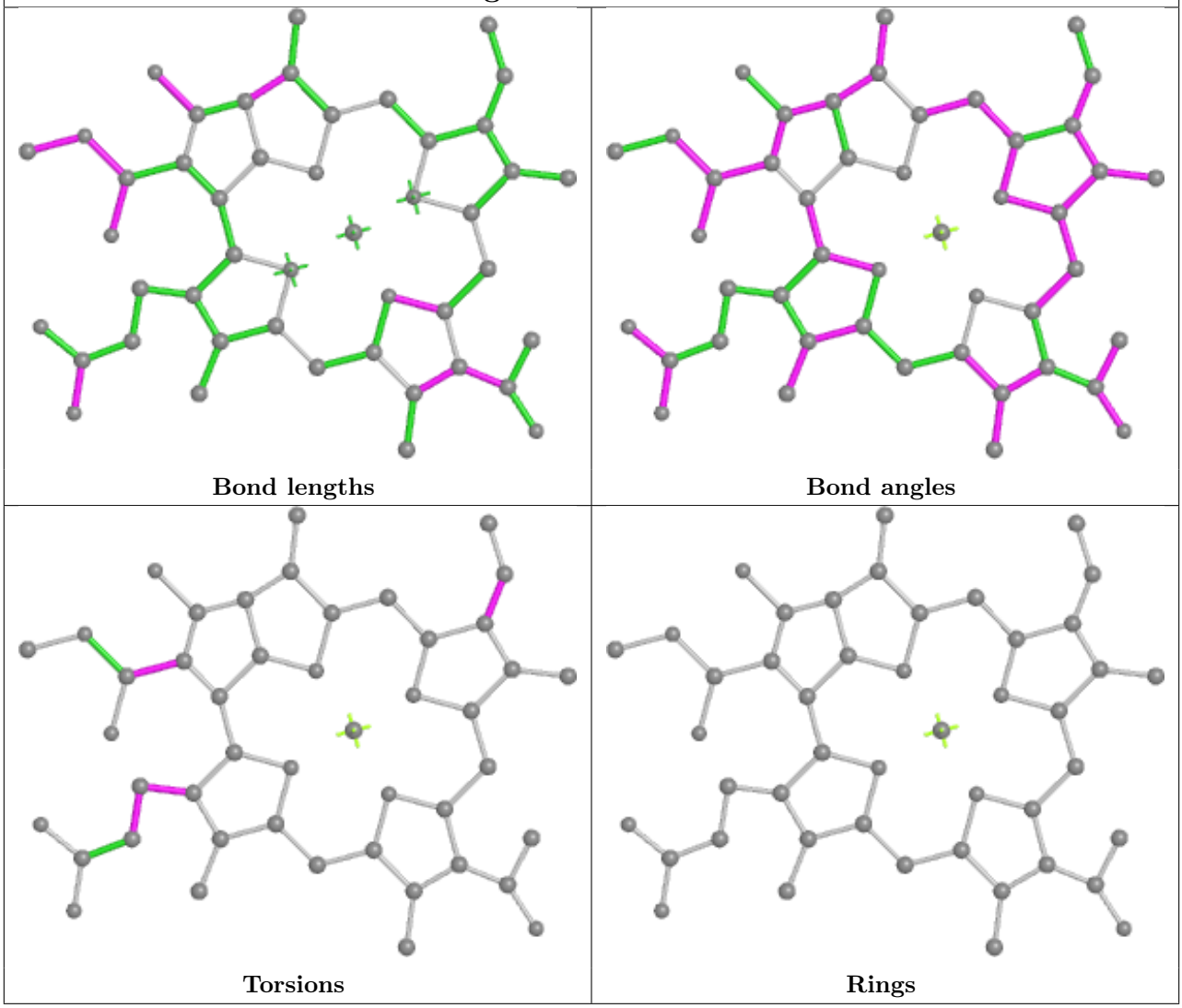
Ligand BCL a 806



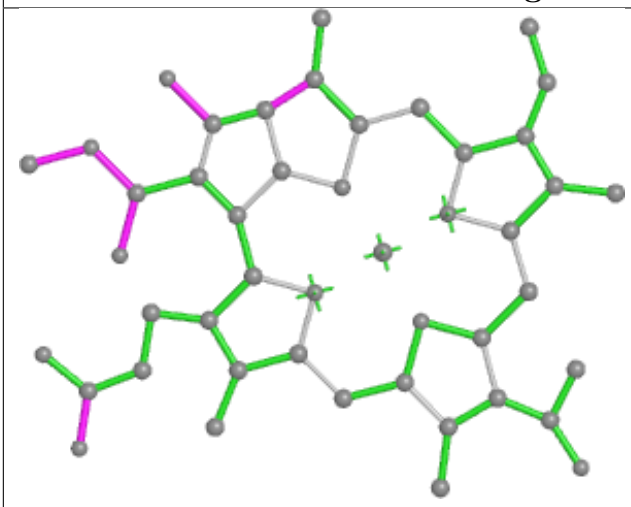
Ligand BCL G 372	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand G2O A 803	
 Bond lengths	 Bond angles
 Torsions	 Rings

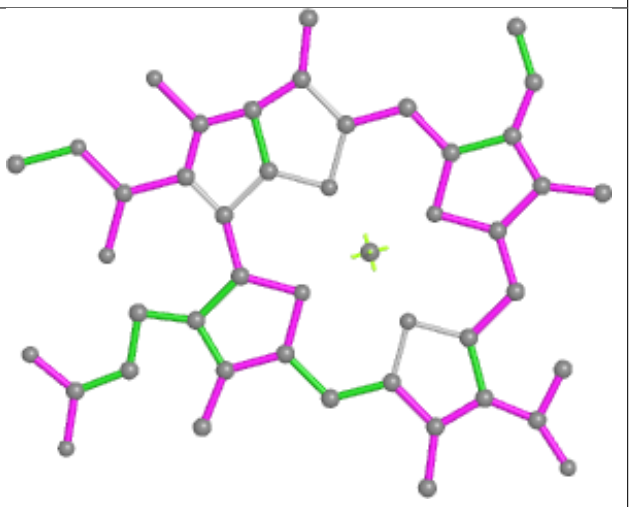
Ligand BCL A 807



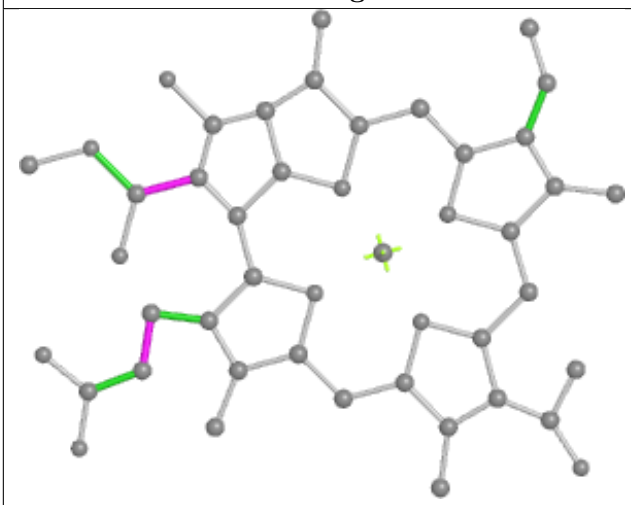
Ligand BCL A 814



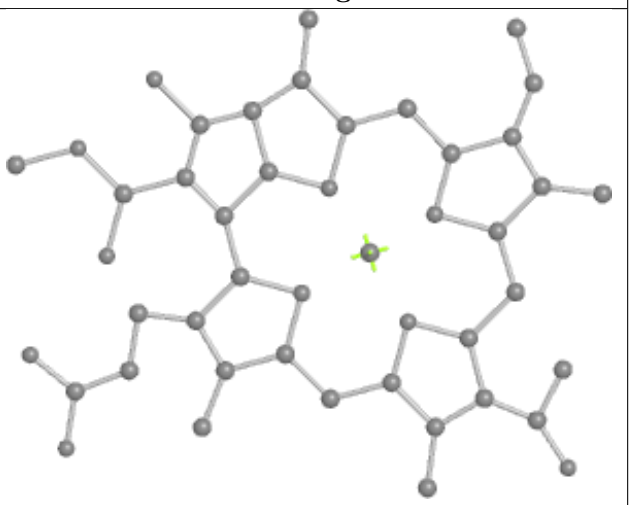
Bond lengths



Bond angles

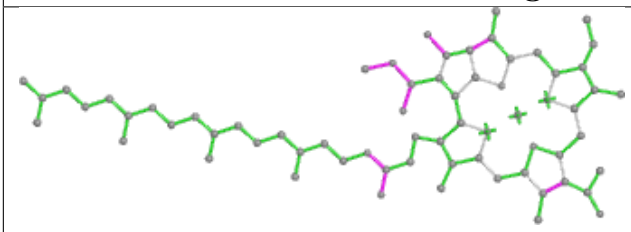


Torsions

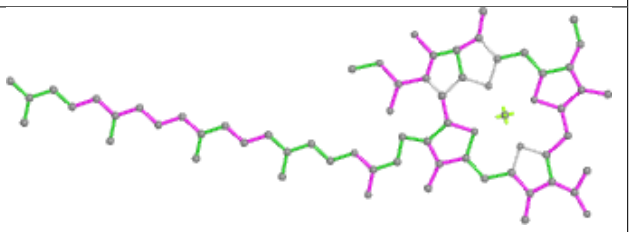


Rings

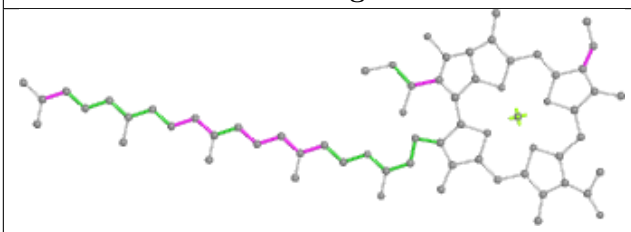
Ligand BCL G 375



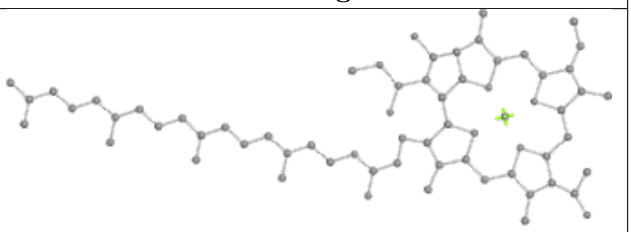
Bond lengths



Bond angles

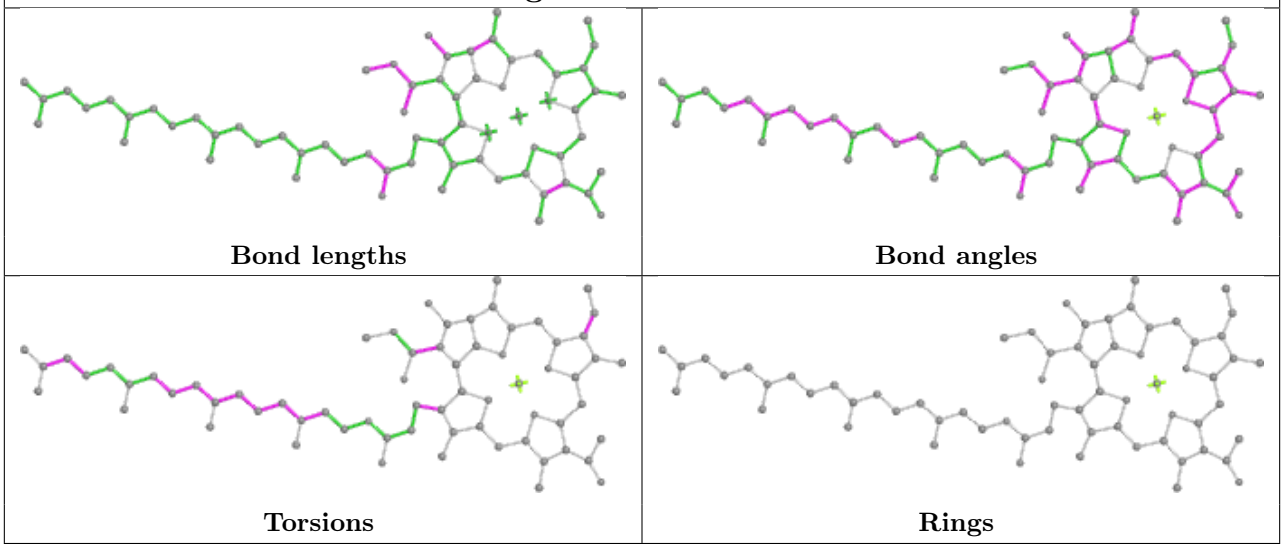


Torsions

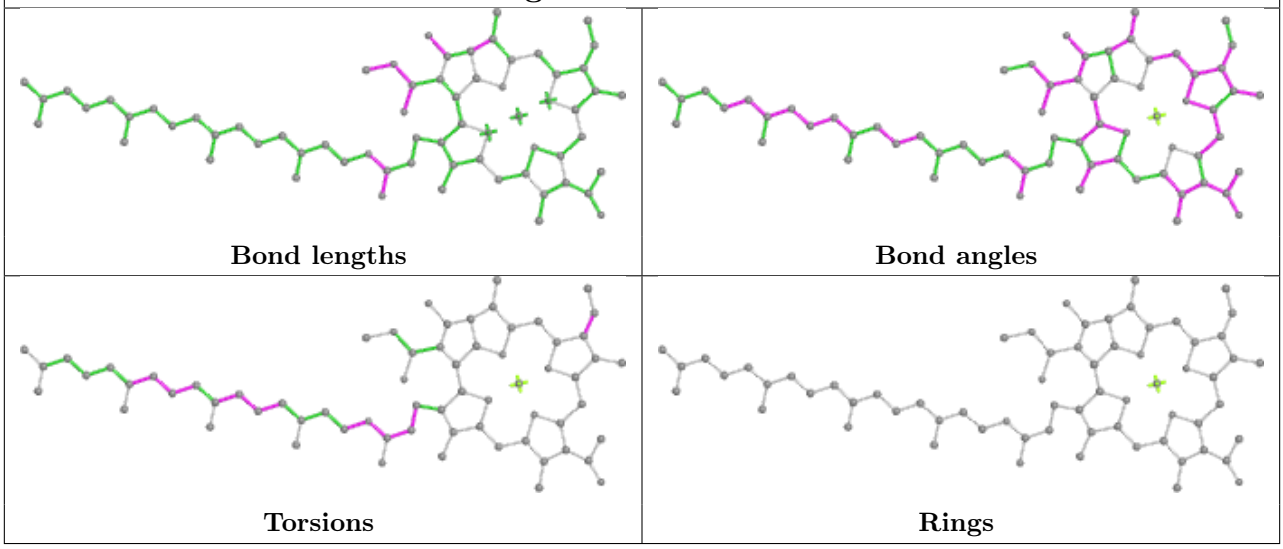


Rings

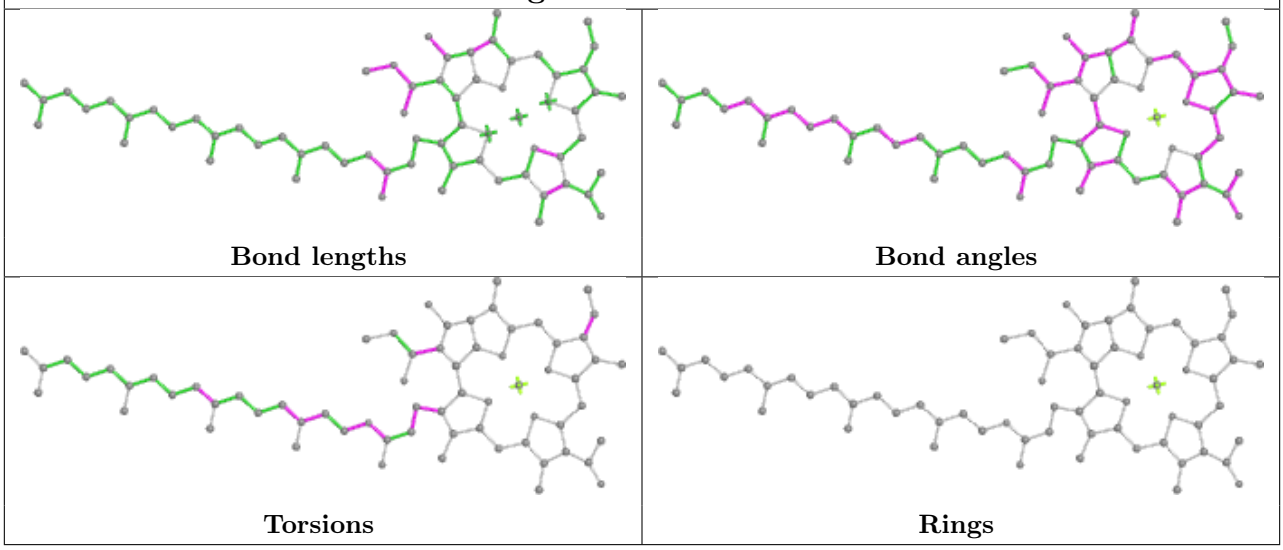
Ligand BCL A 808



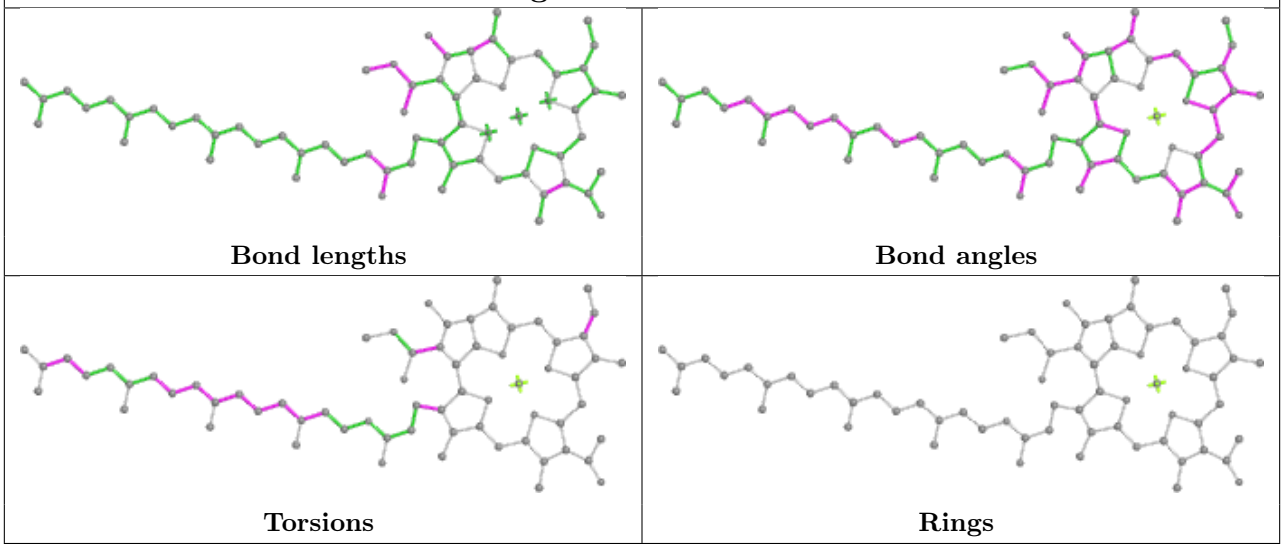
Ligand BCL G 374



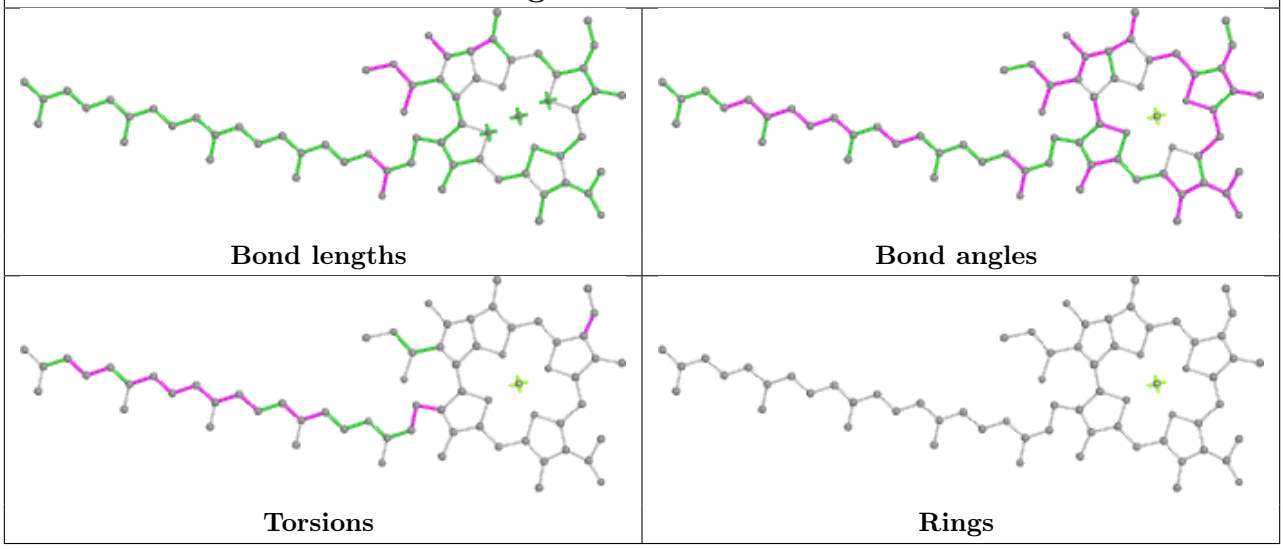
Ligand BCL F 373



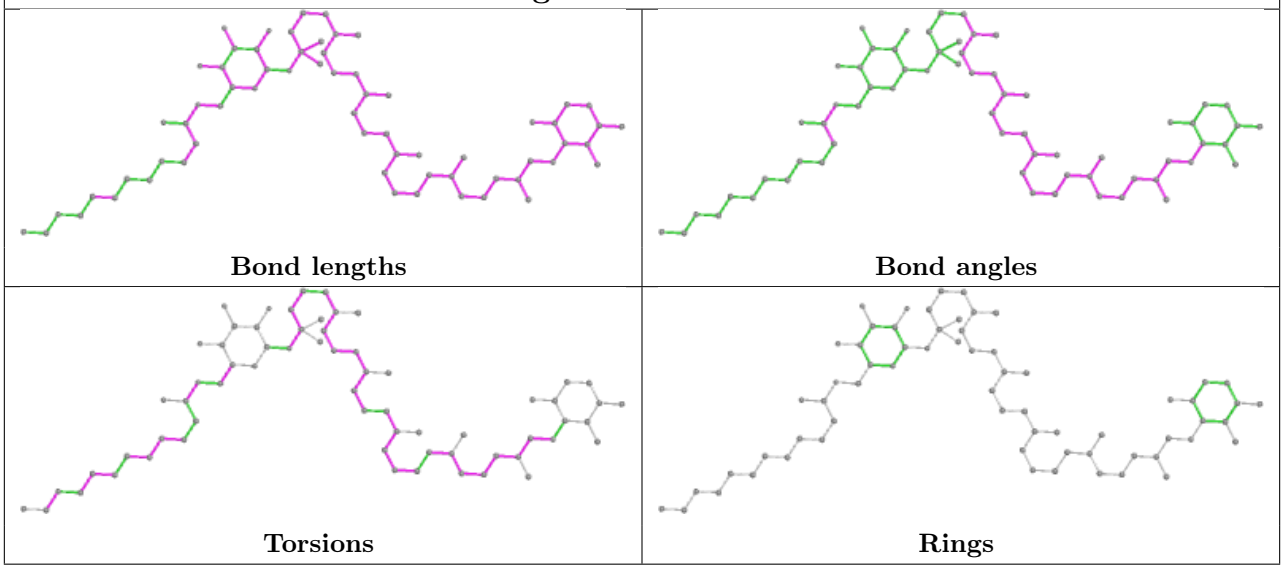
Ligand BCL a 808



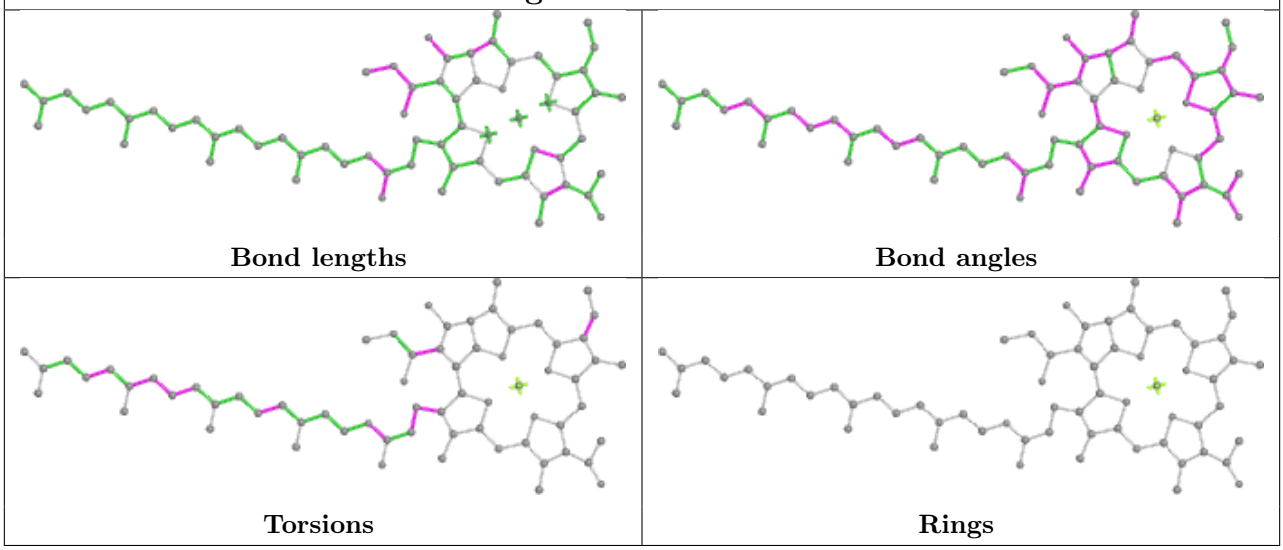
Ligand BCL F 372



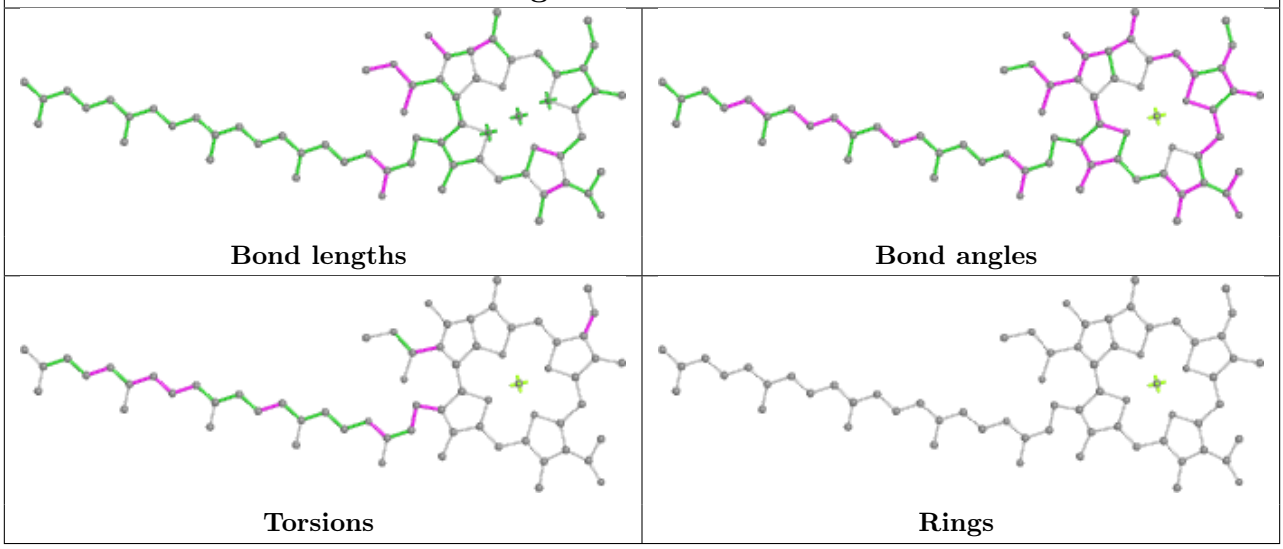
Ligand F39 A 817



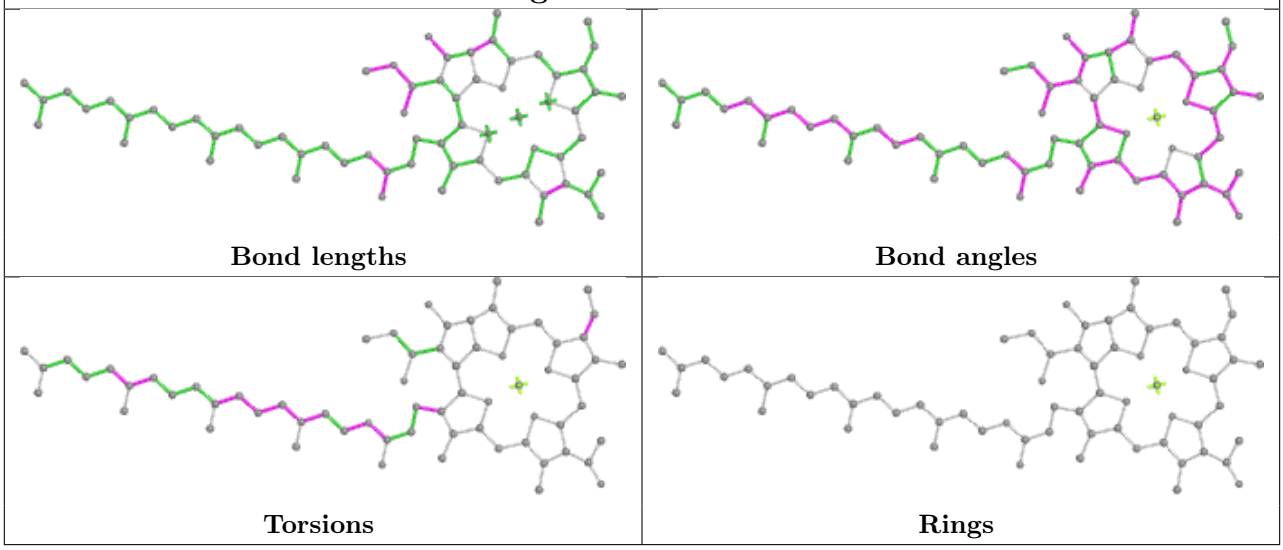
Ligand BCL A 812



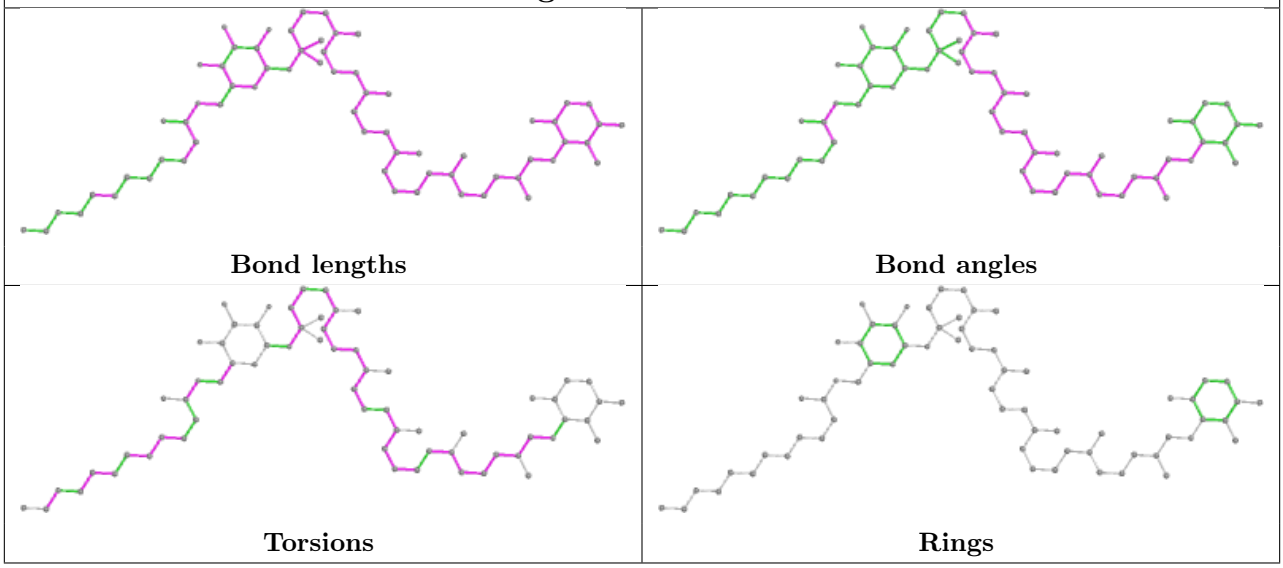
Ligand BCL a 812



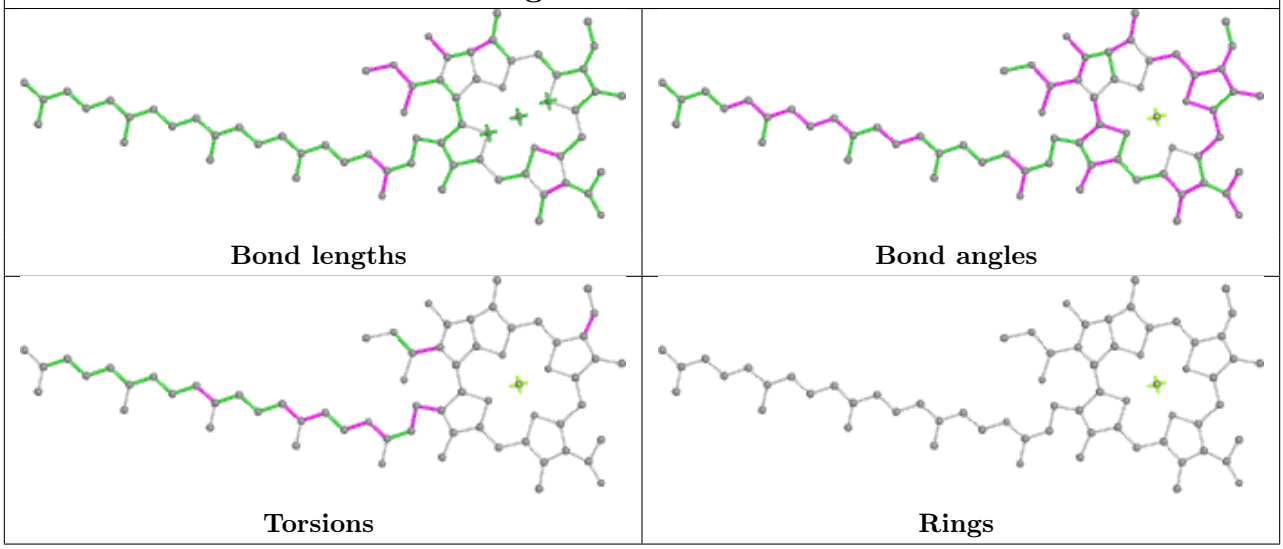
Ligand BCL a 811



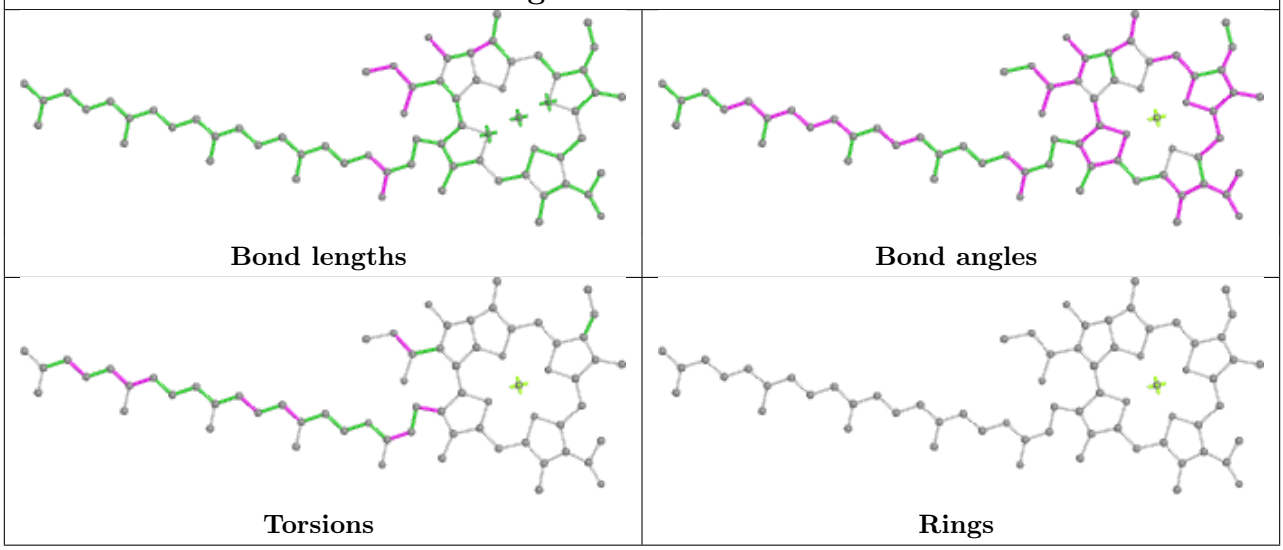
Ligand F39 a 817



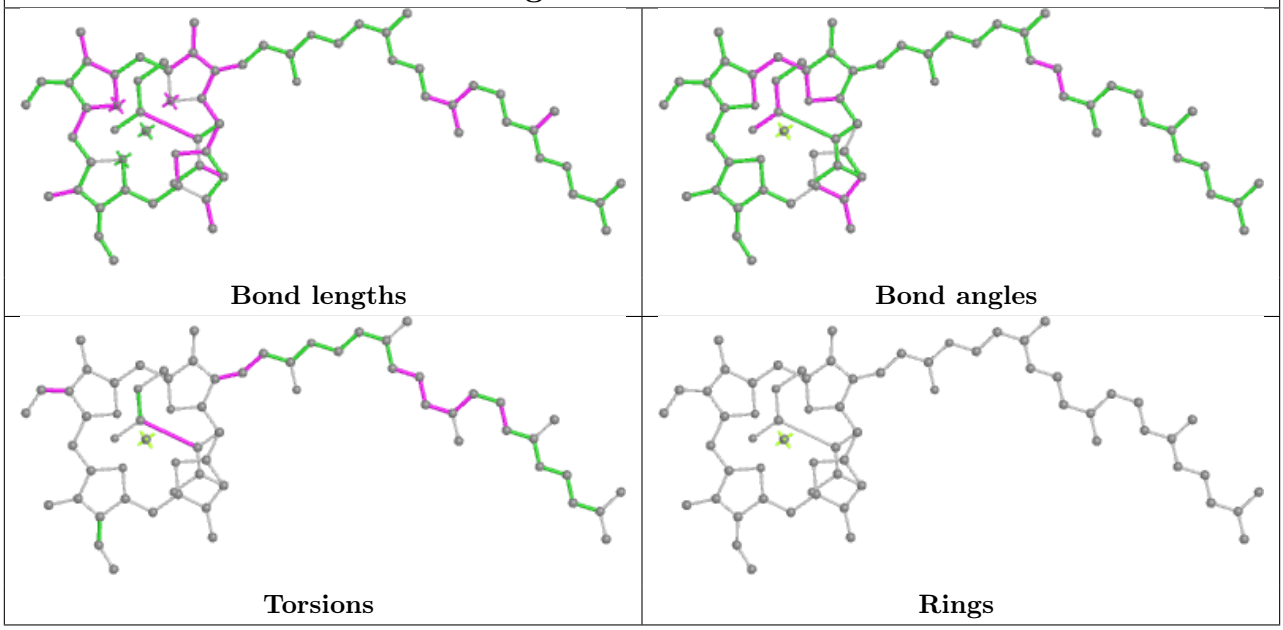
Ligand BCL G 373



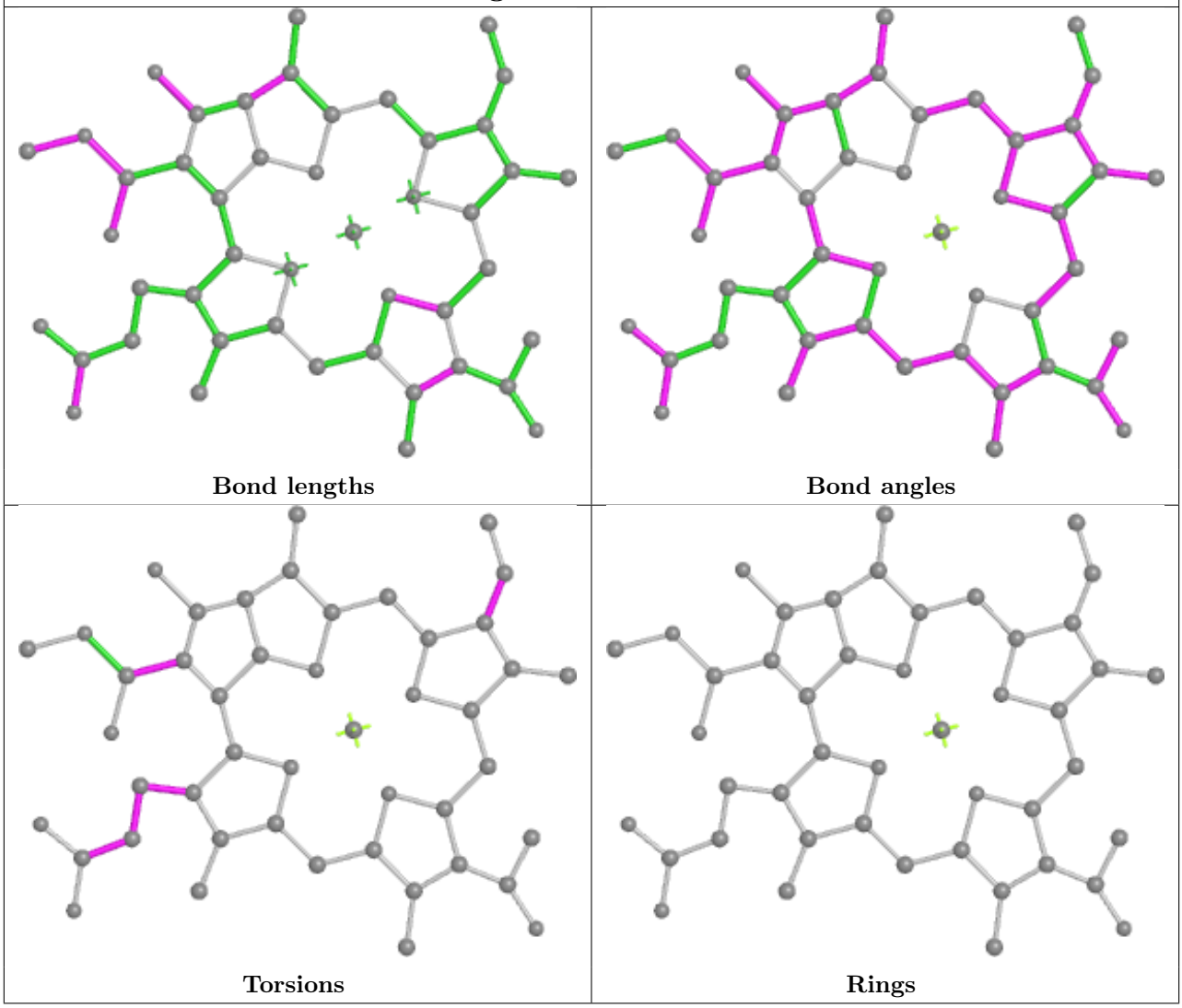
Ligand BCL F 371



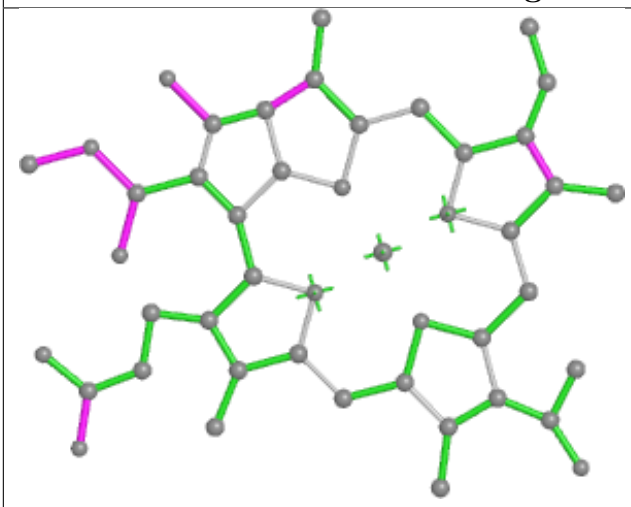
Ligand G2O A 802



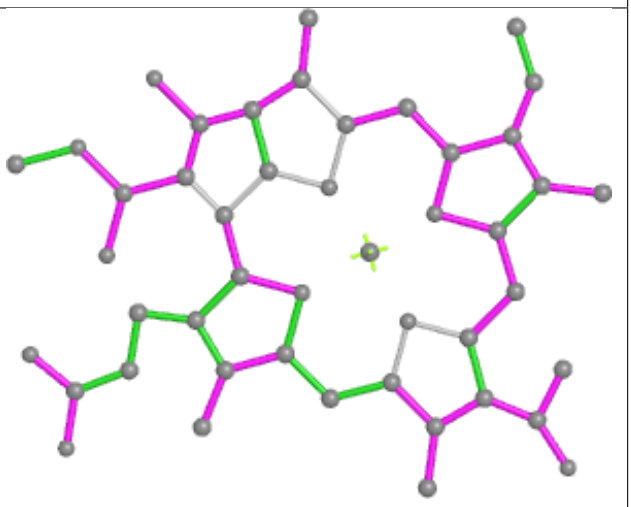
Ligand BCL a 810



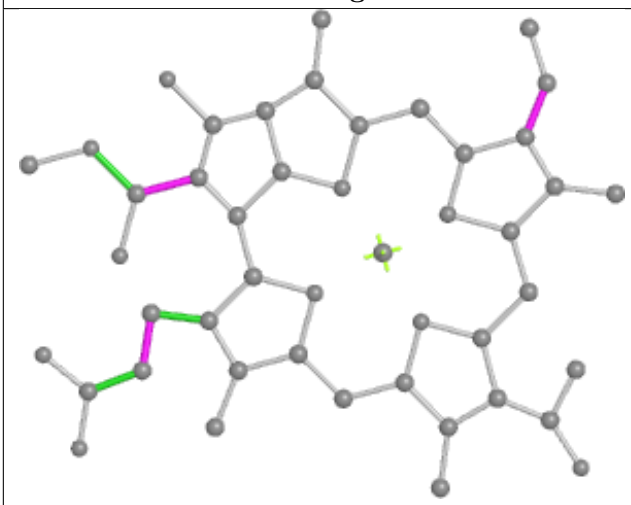
Ligand BCL A 815



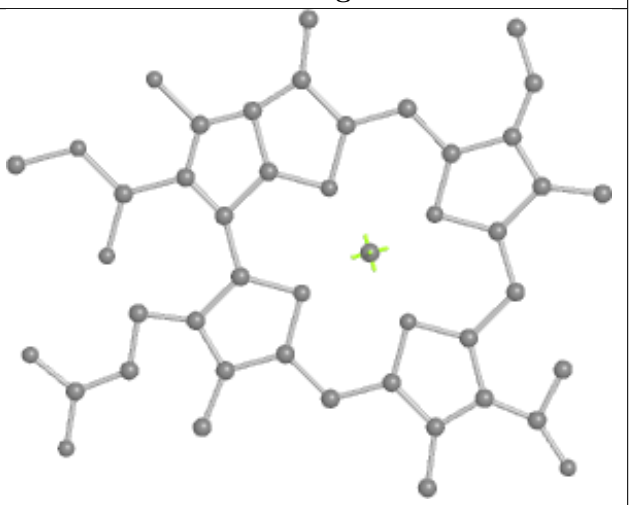
Bond lengths



Bond angles

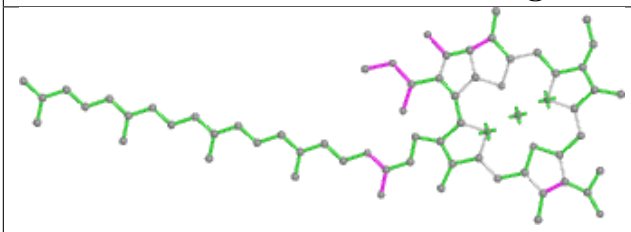


Torsions

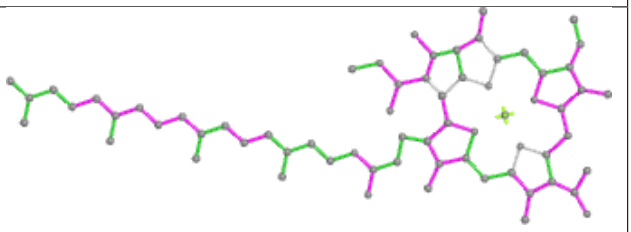


Rings

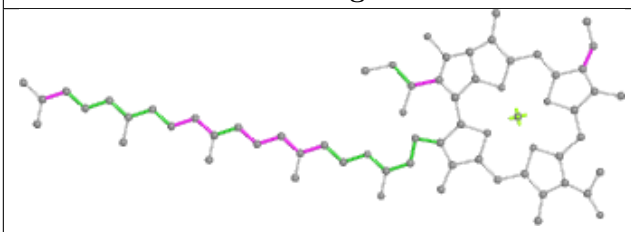
Ligand BCL F 375



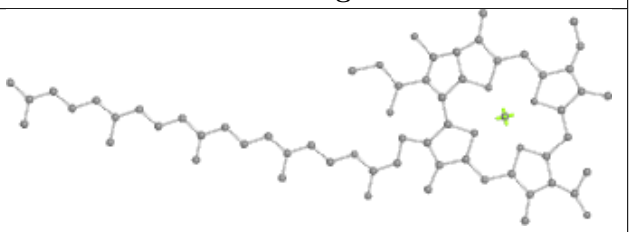
Bond lengths



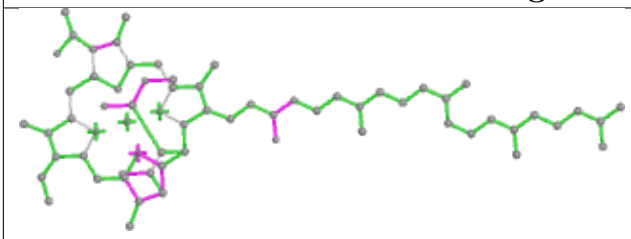
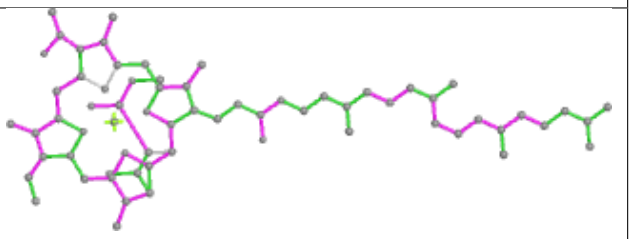
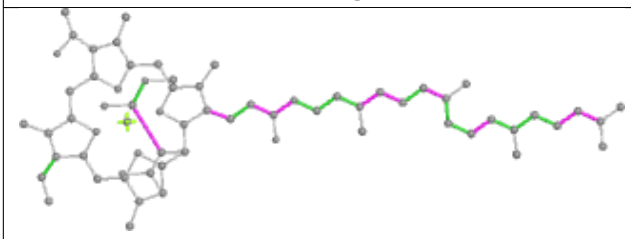
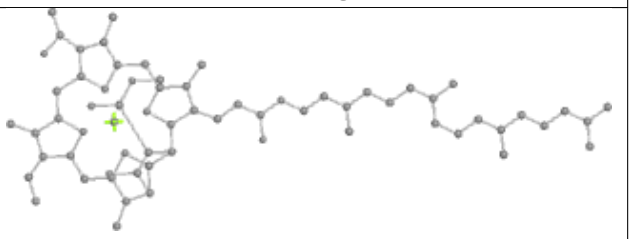
Bond angles

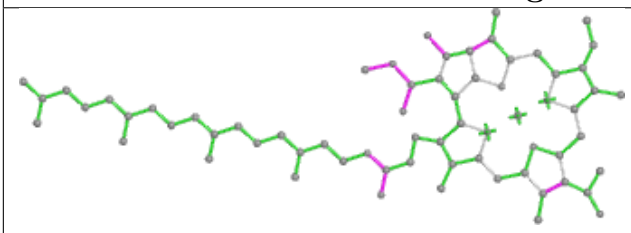
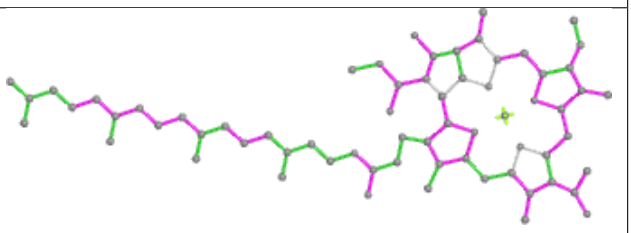
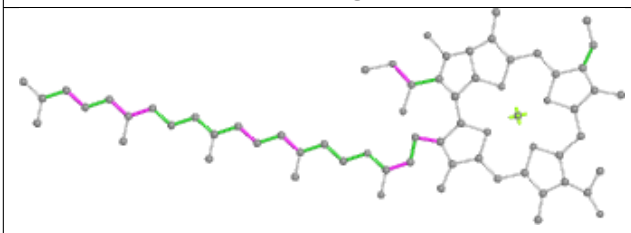
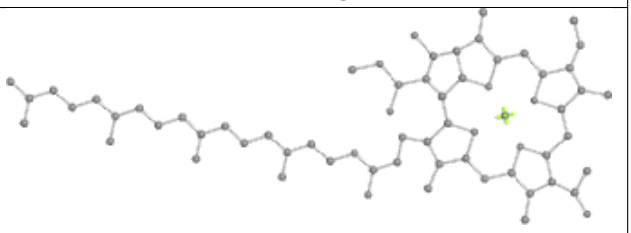


Torsions

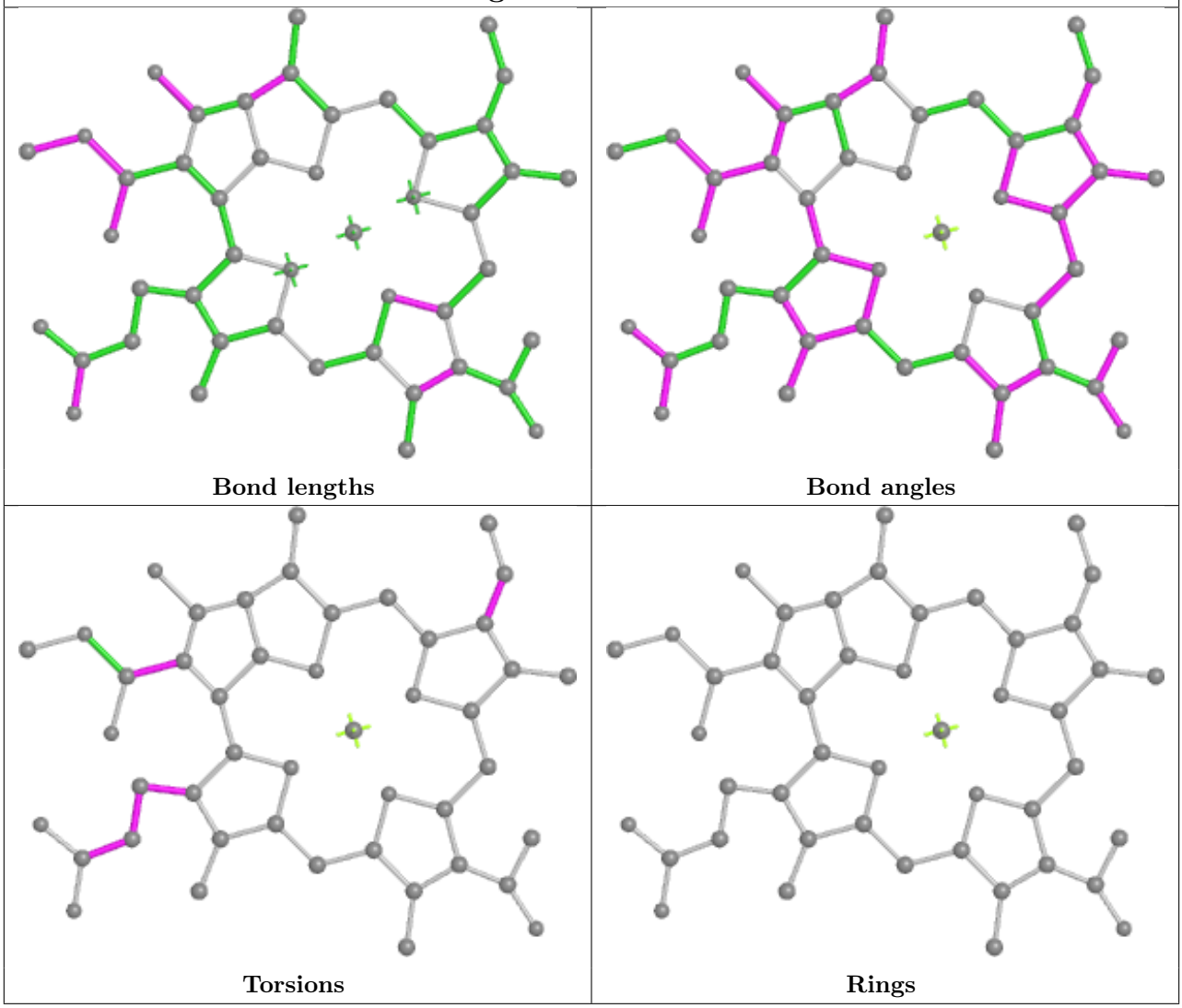


Rings

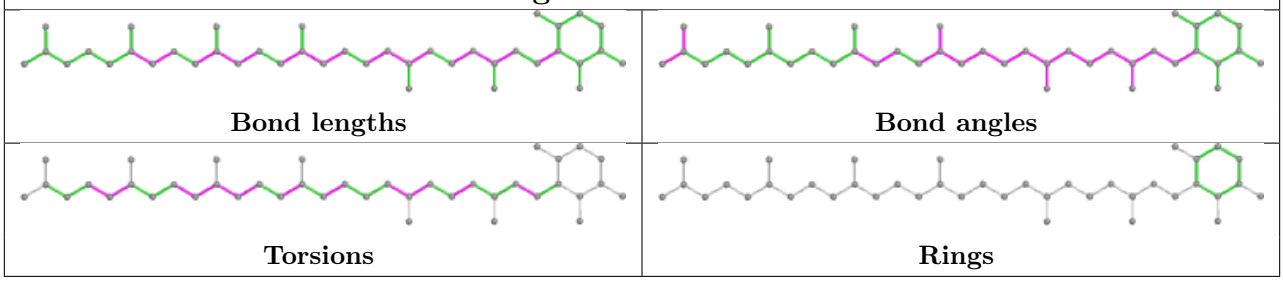
Ligand GS0 A 801	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCL E 371	
 Bond lengths	 Bond angles
 Torsions	 Rings

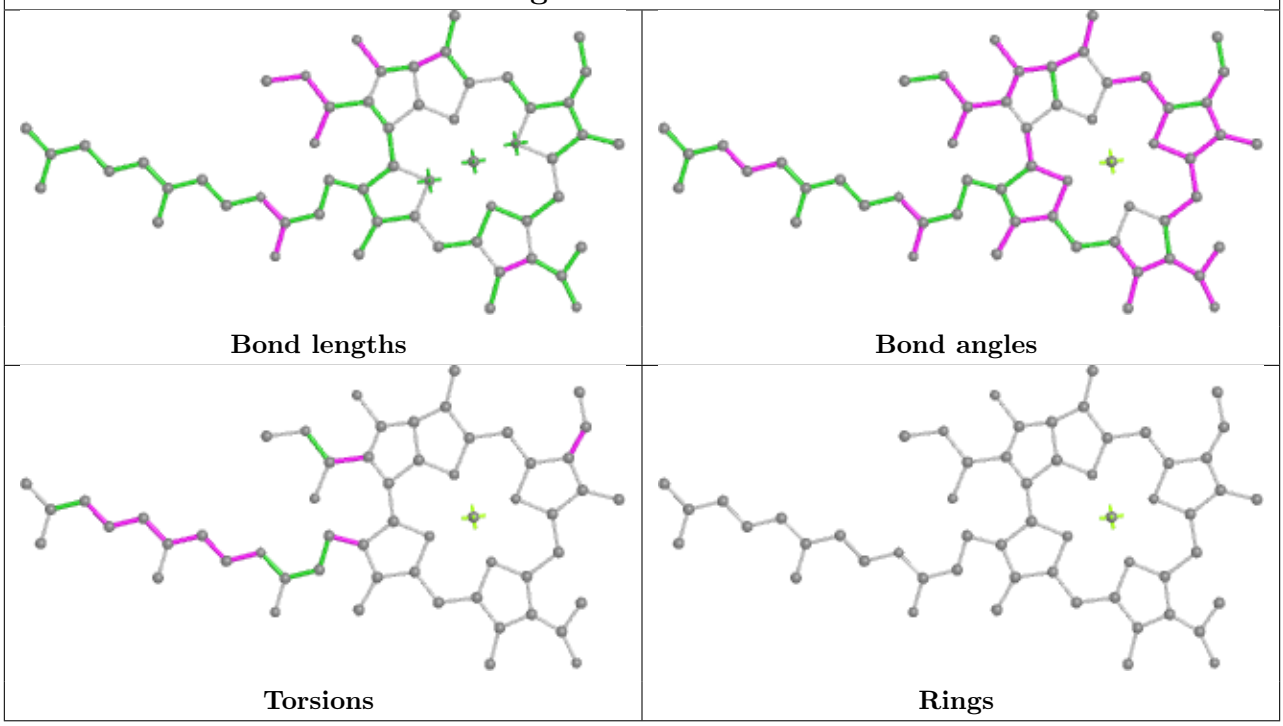
Ligand BCL a 804



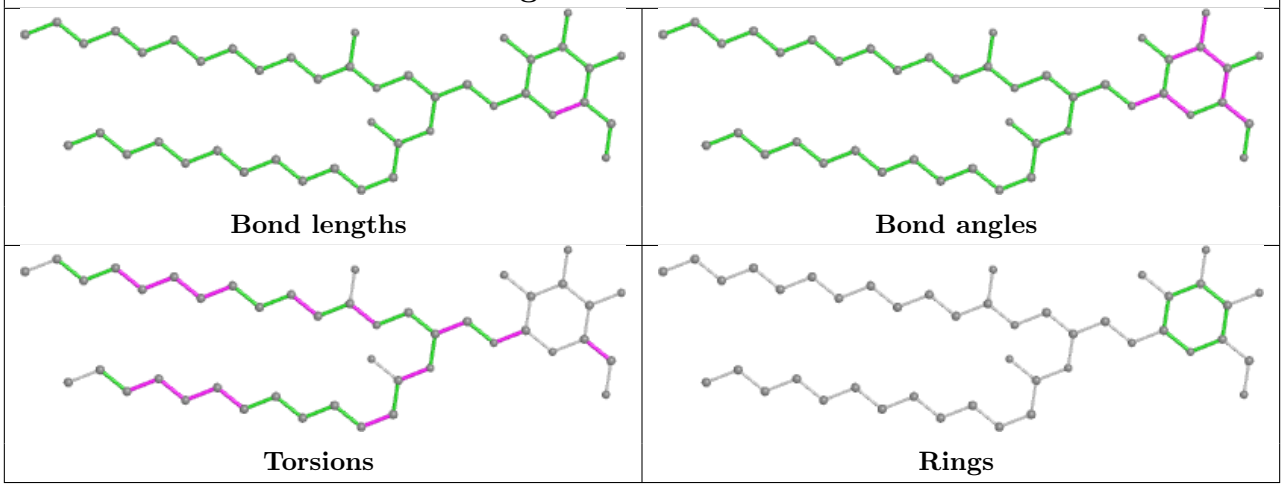
Ligand F26 A 816



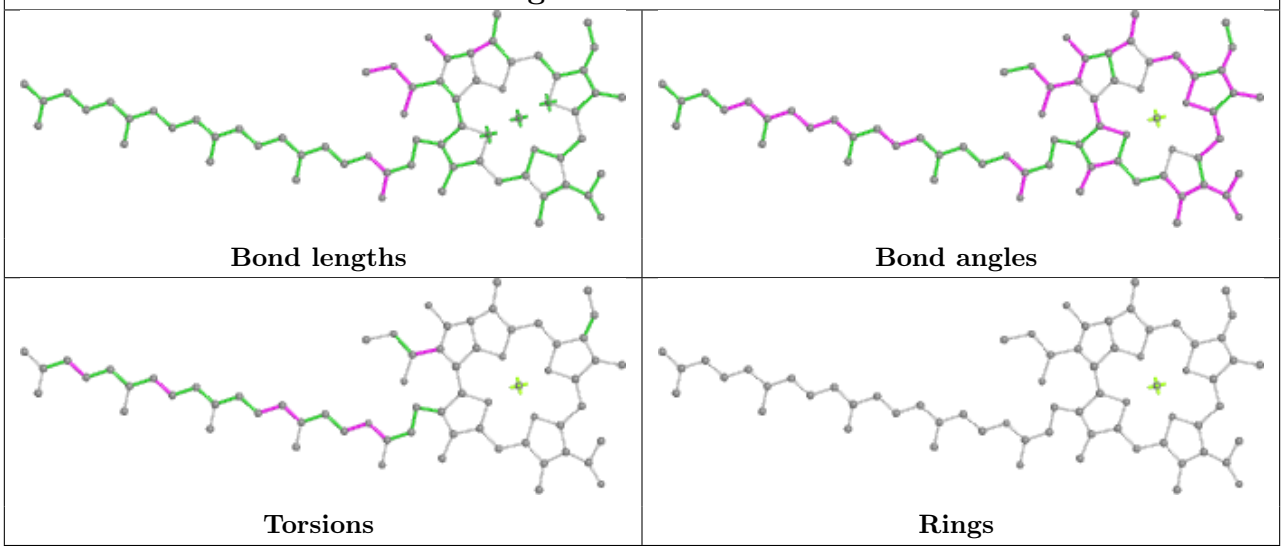
Ligand BCL a 805



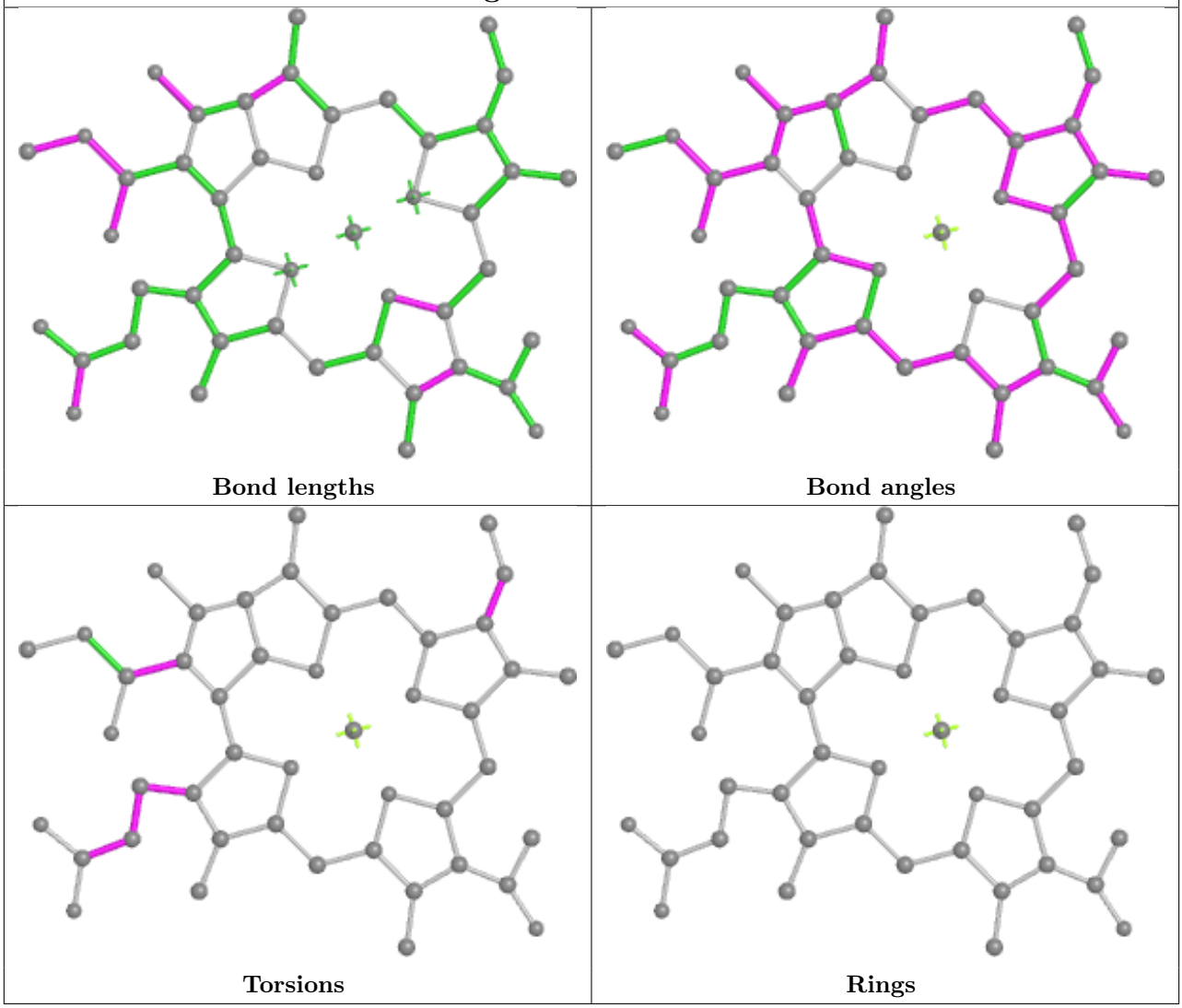
Ligand LMG A 819

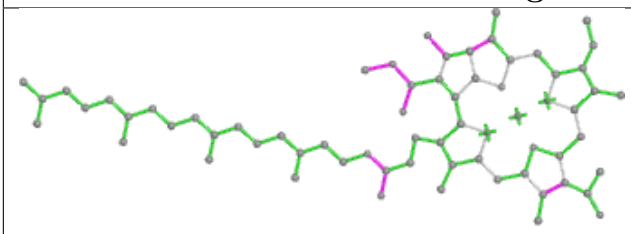
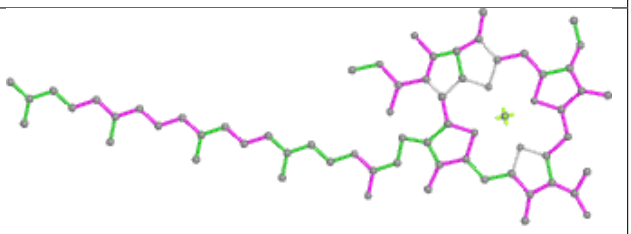
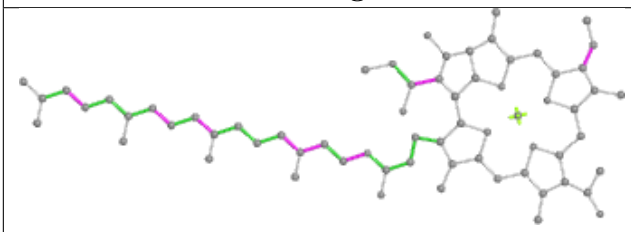
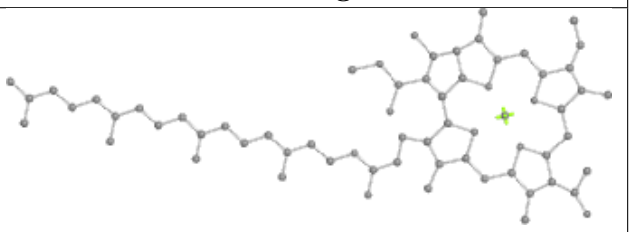


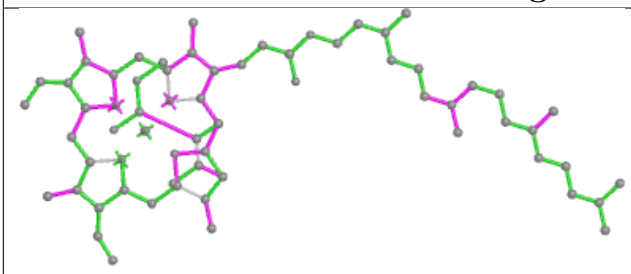
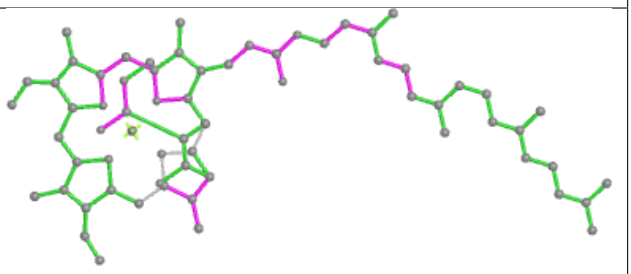
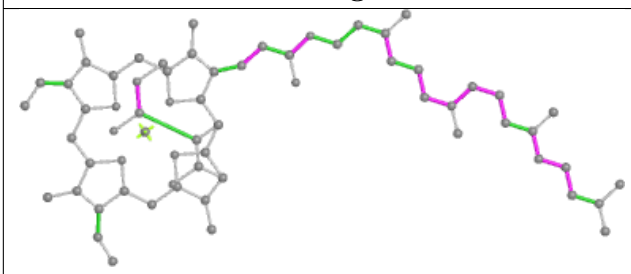
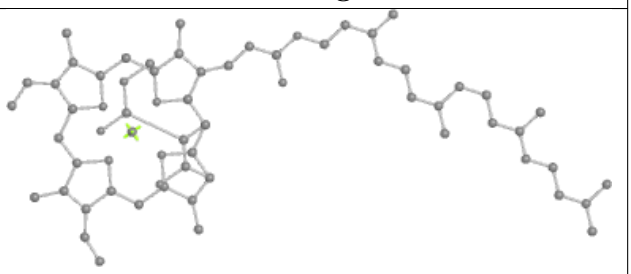
Ligand BCL F 376

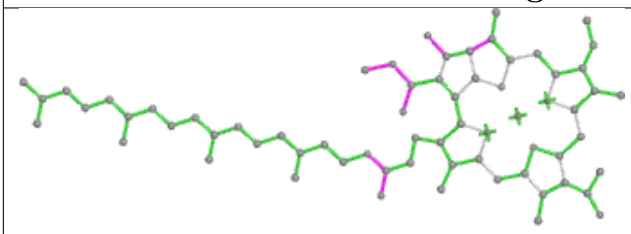
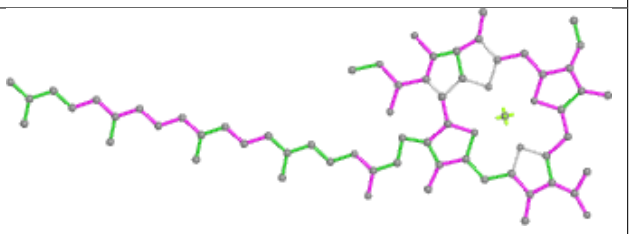
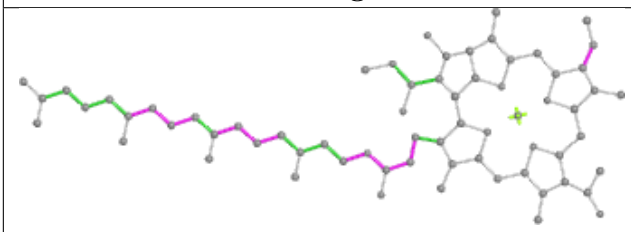
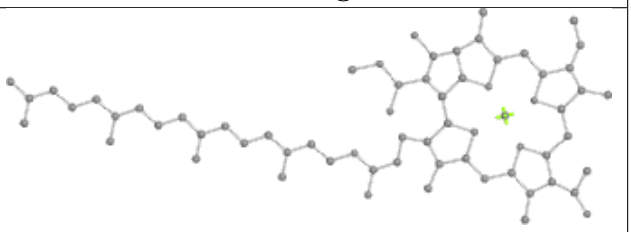


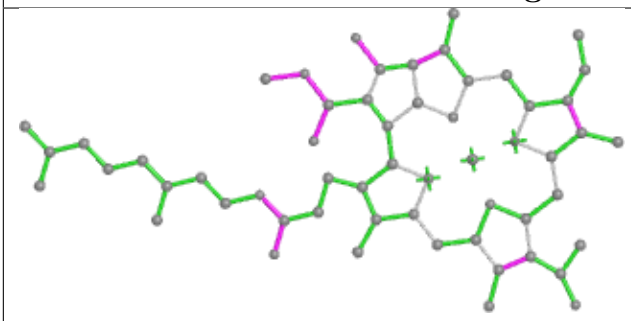
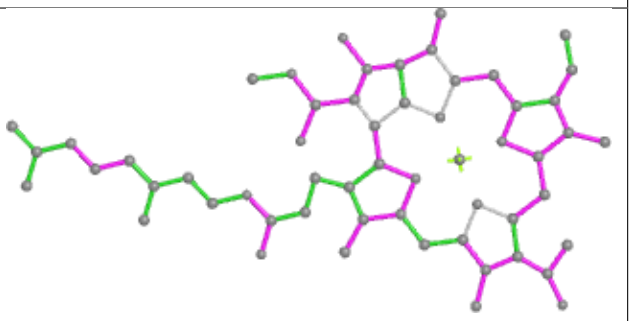
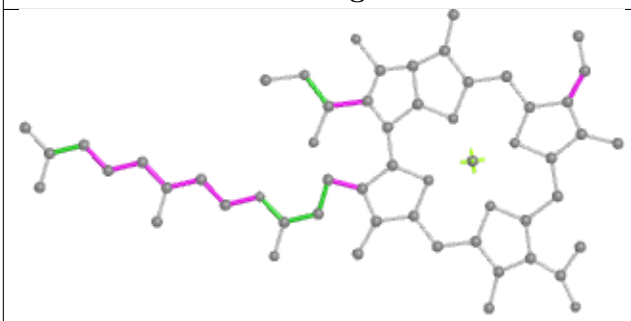
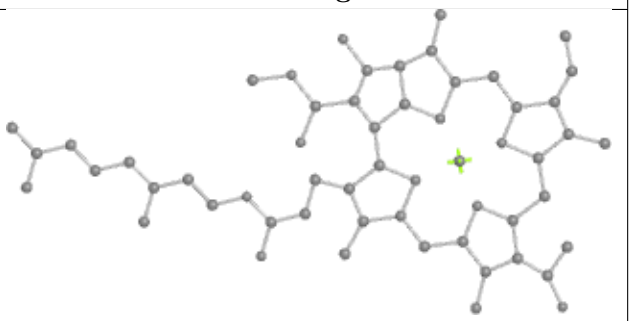
Ligand BCL A 810



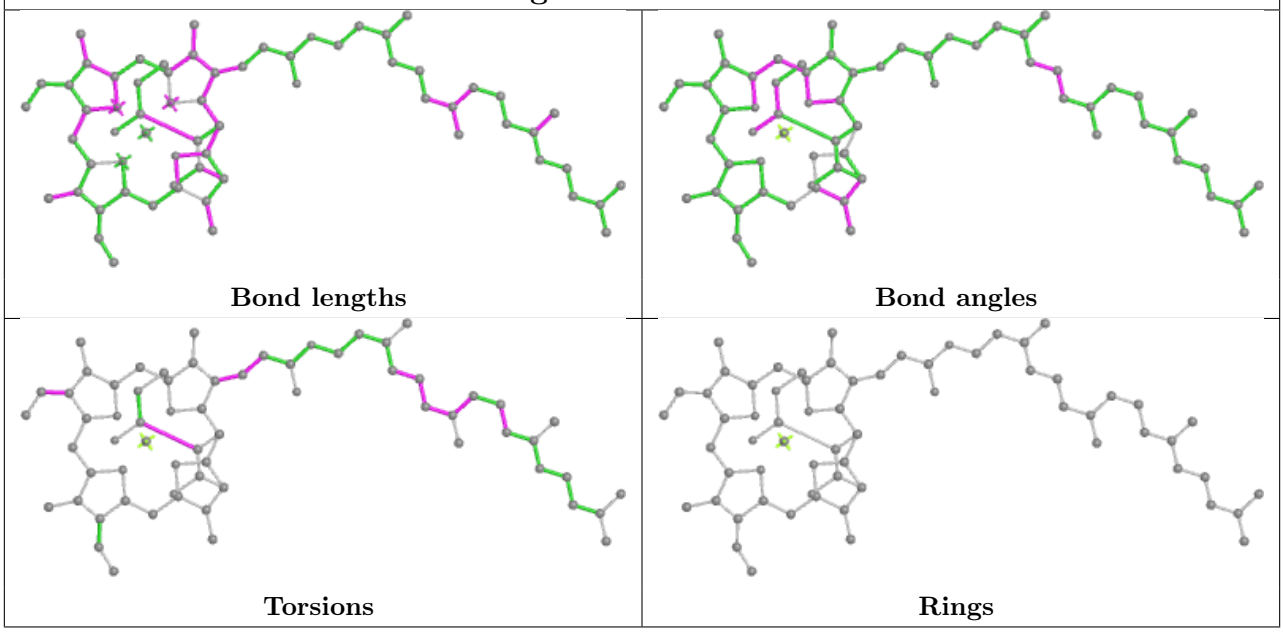
Ligand BCL E 377	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand G2O a 803	
 Bond lengths	 Bond angles
 Torsions	 Rings

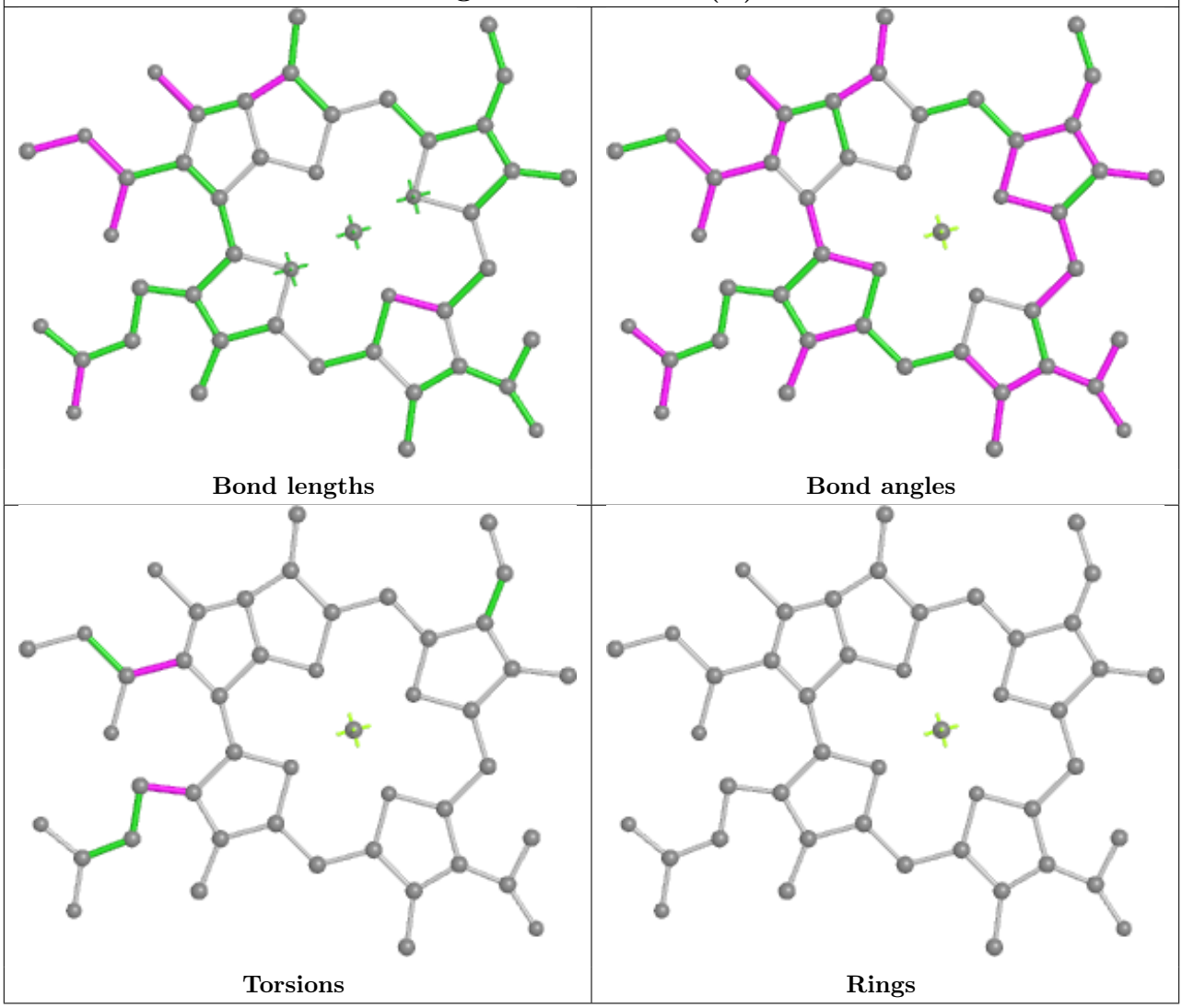
Ligand BCL E 374	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCL A 805	
 Bond lengths	 Bond angles
 Torsions	 Rings

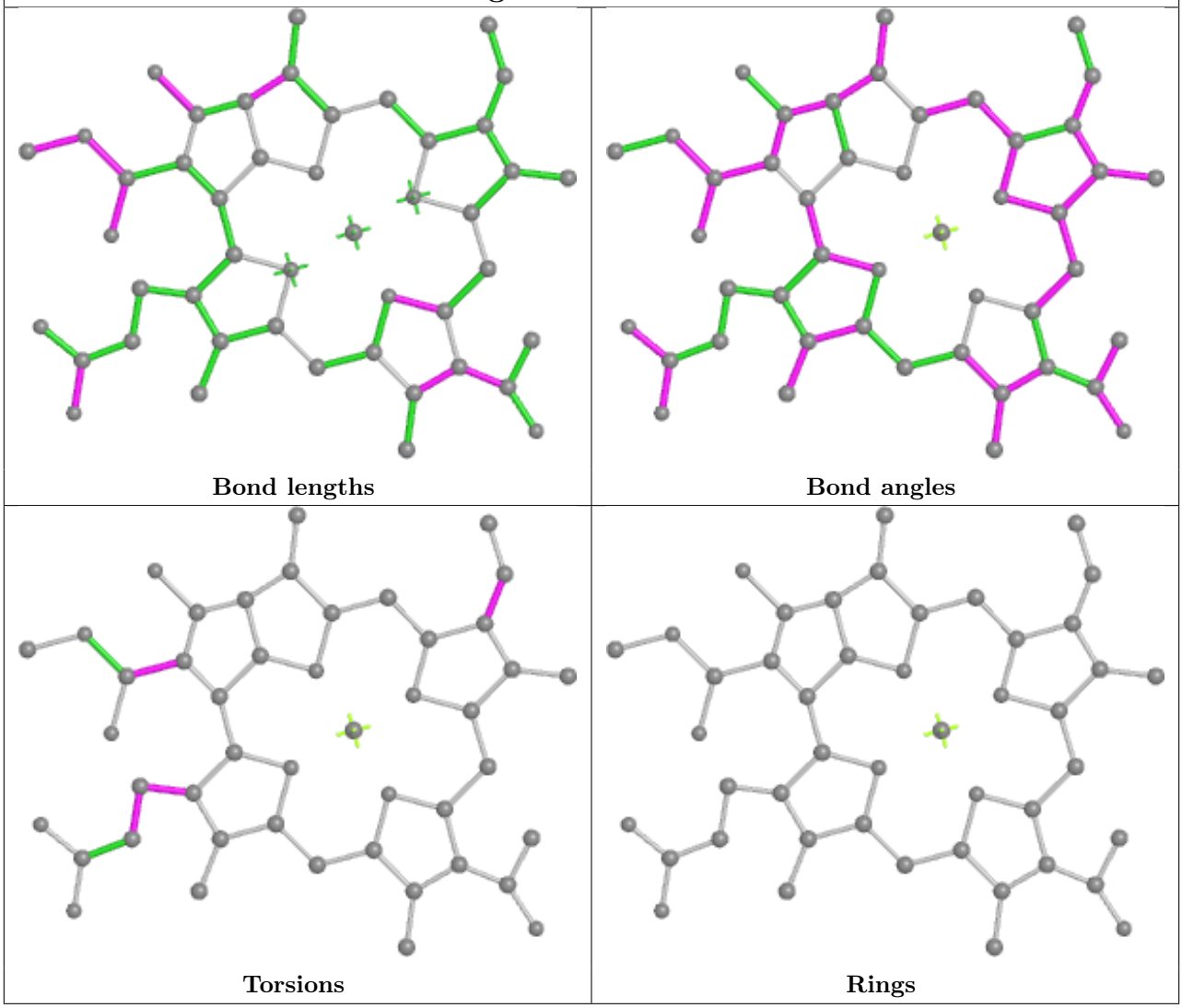
Ligand G2O a 802



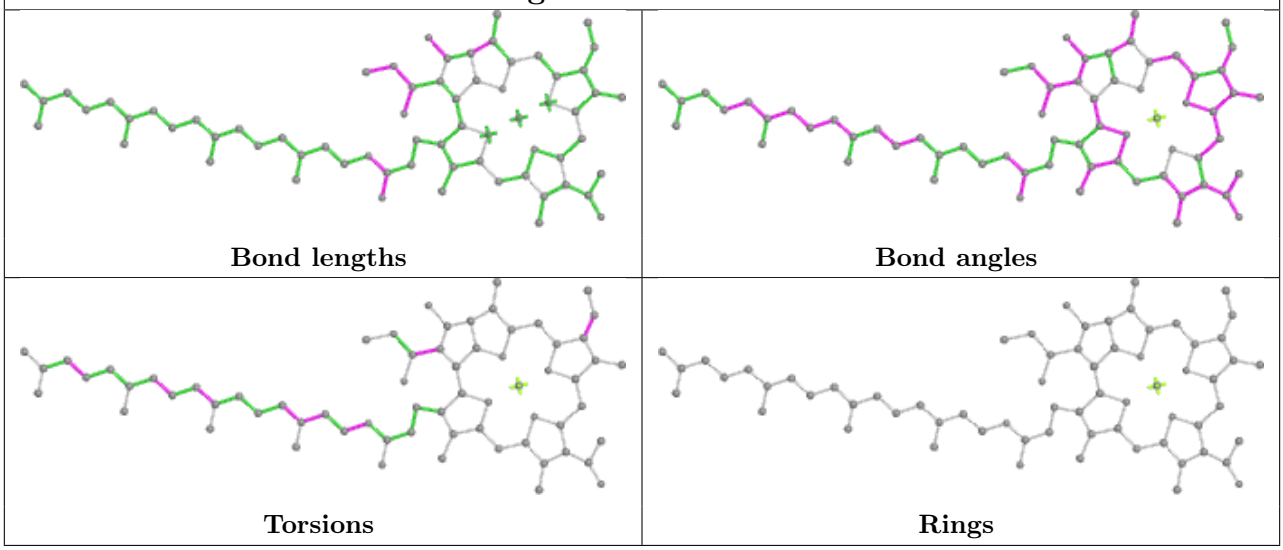
Ligand BCL E 378 (B)



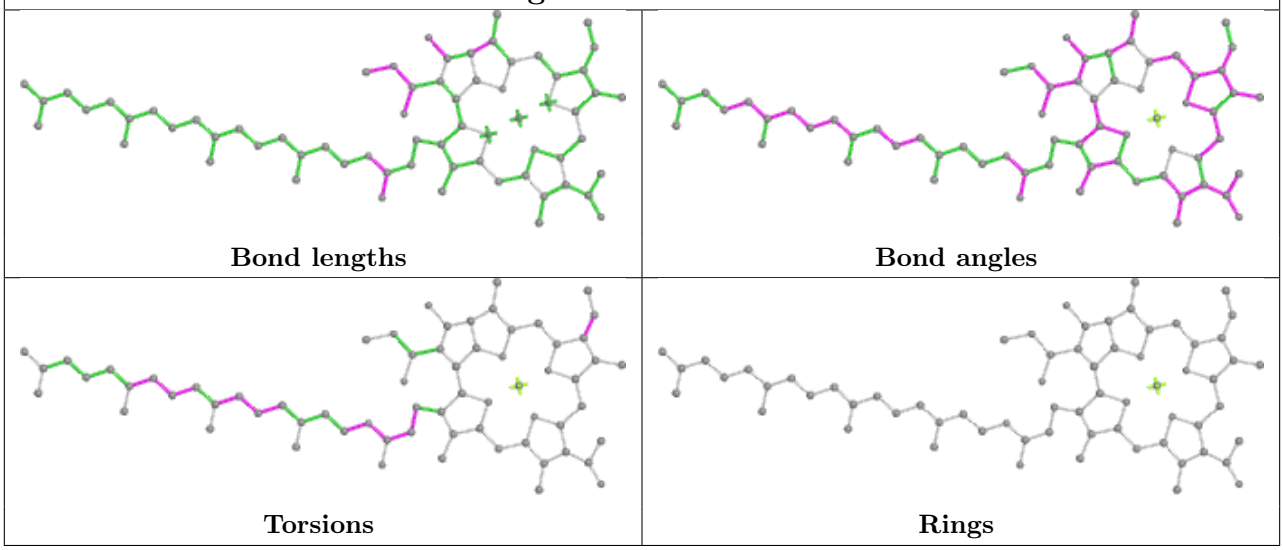
Ligand BCL a 807



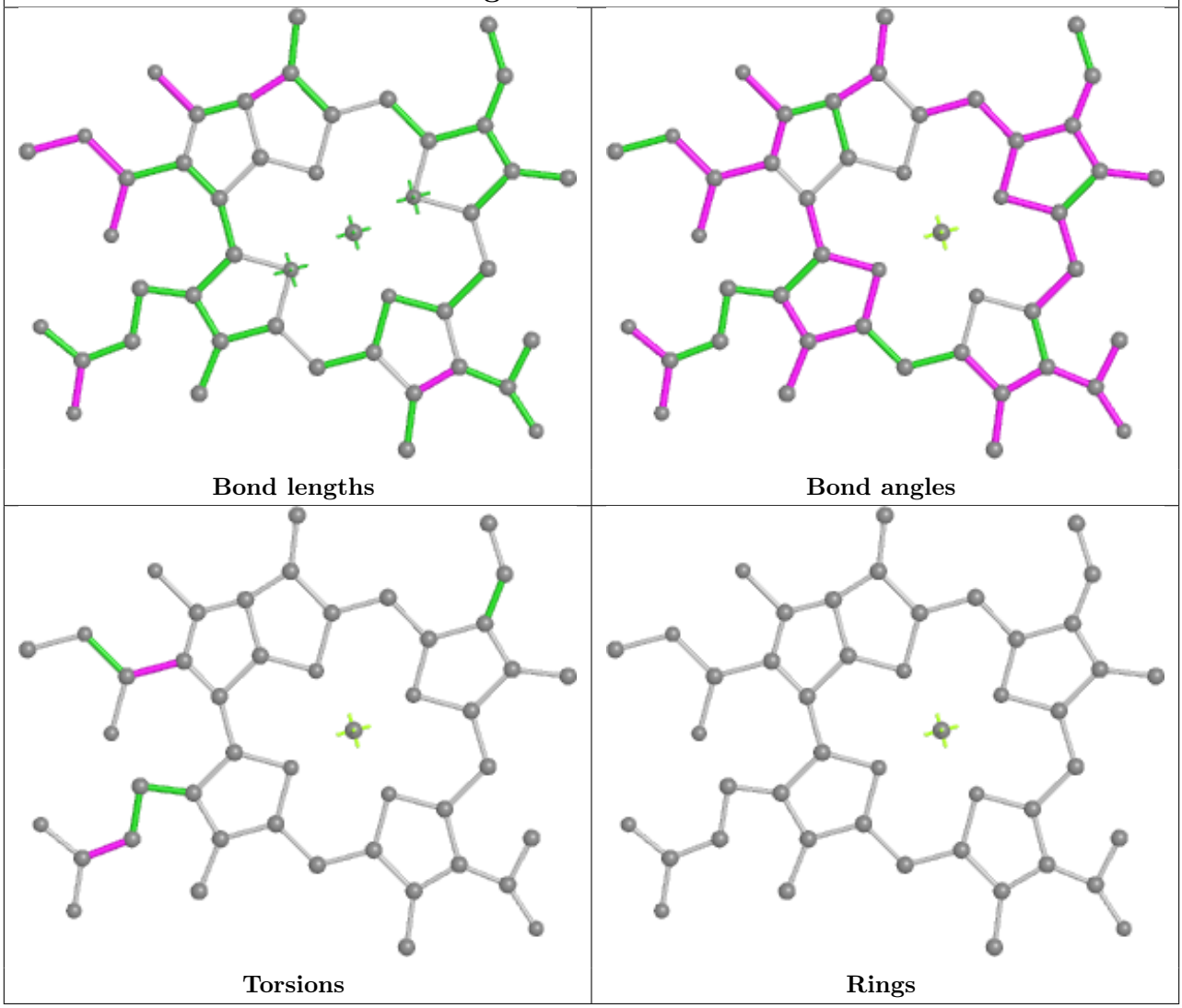
Ligand BCL F 377

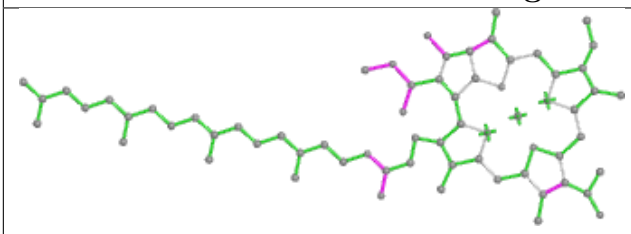
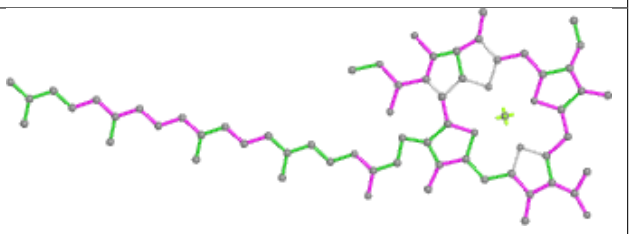
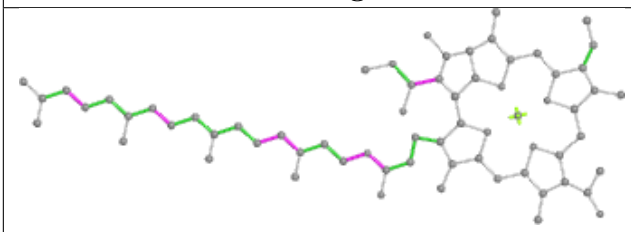
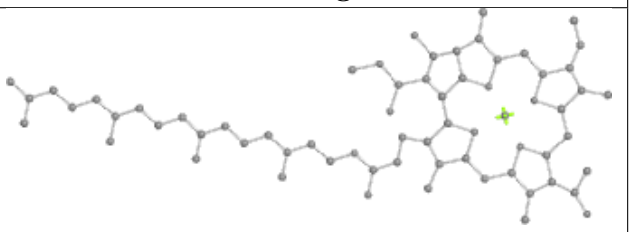


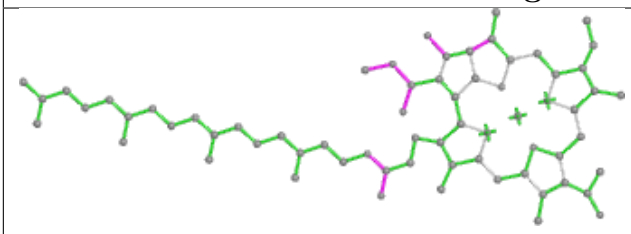
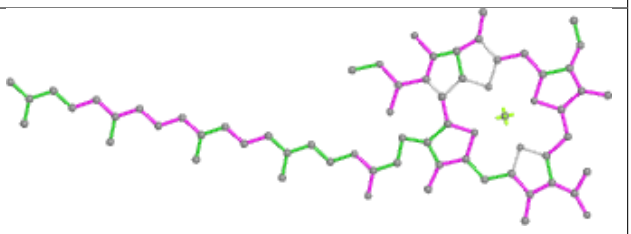
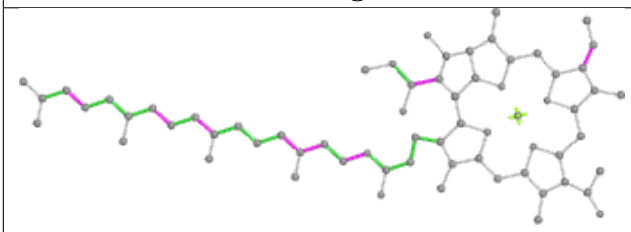
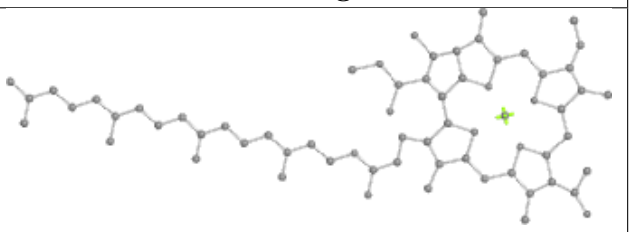
Ligand BCL F 374

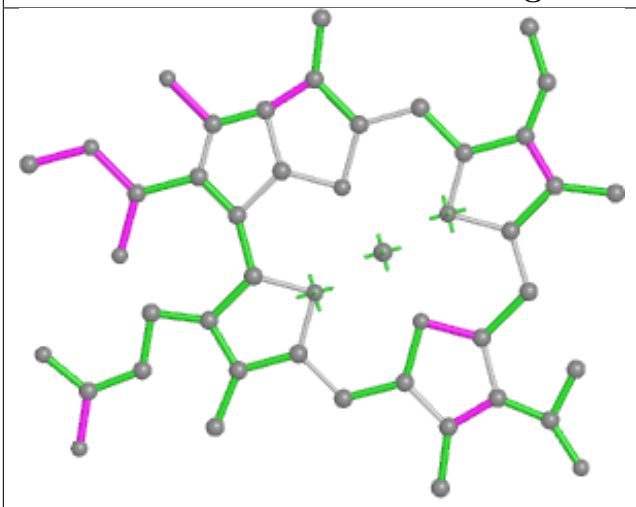
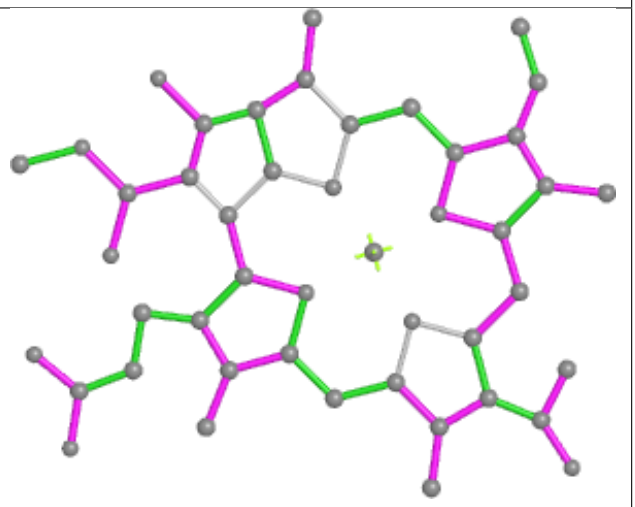
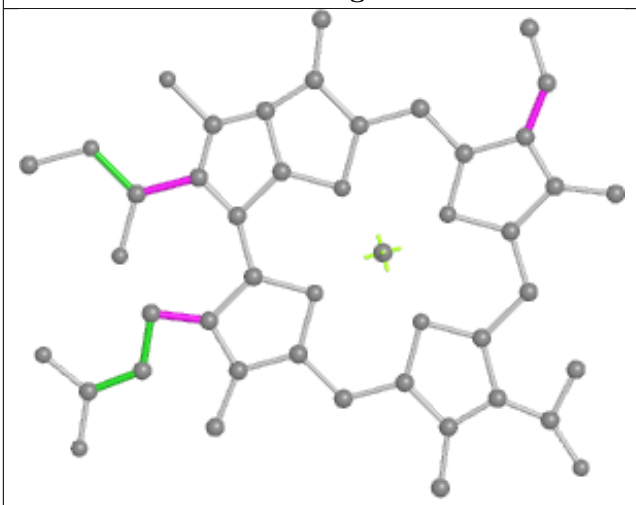
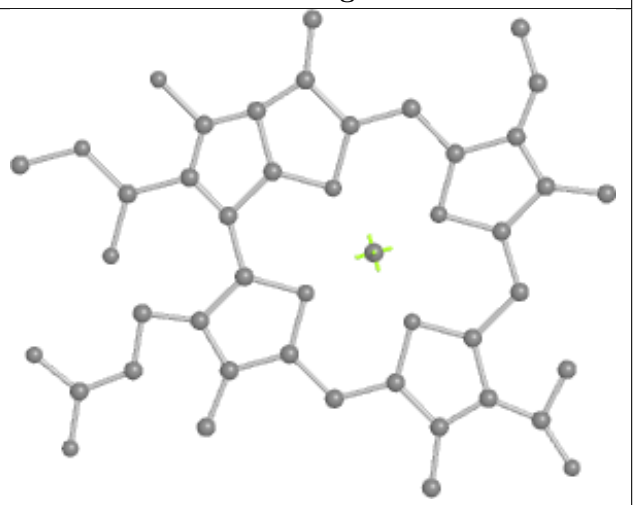


Ligand BCL A 809

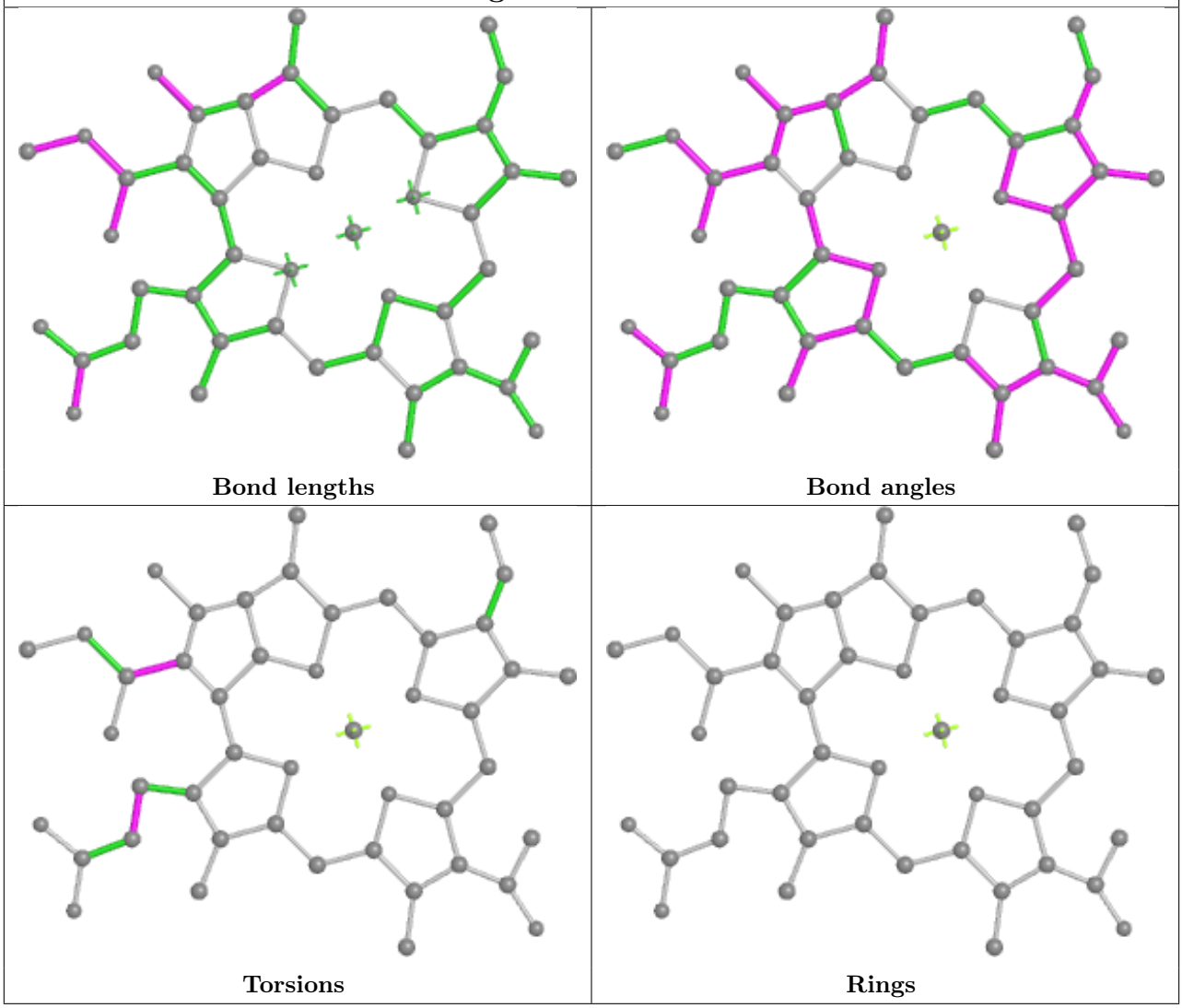


Ligand BCL G 376	
 Bond lengths	 Bond angles
 Torsions	 Rings

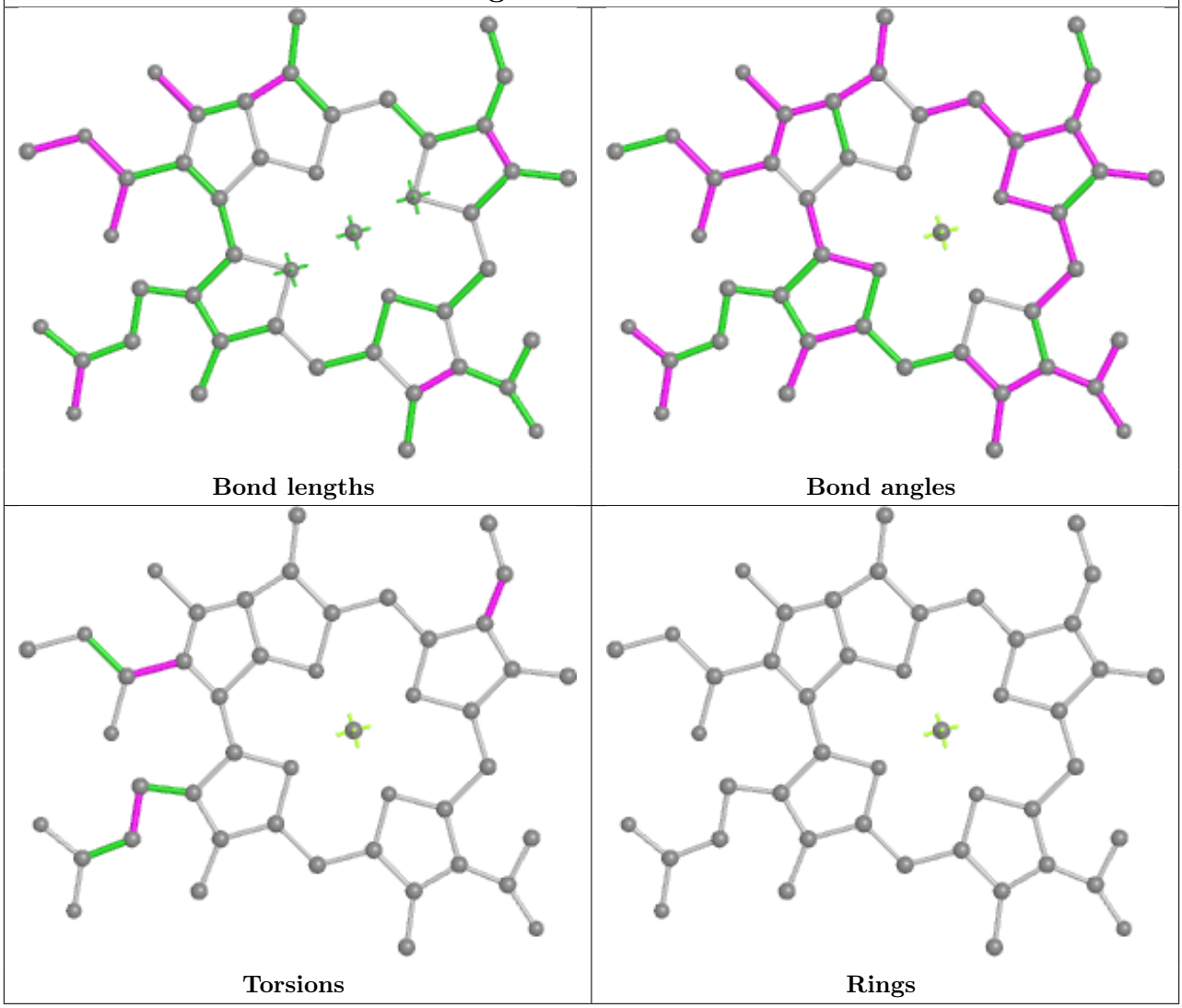
Ligand BCL G 377	
 Bond lengths	 Bond angles
 Torsions	 Rings

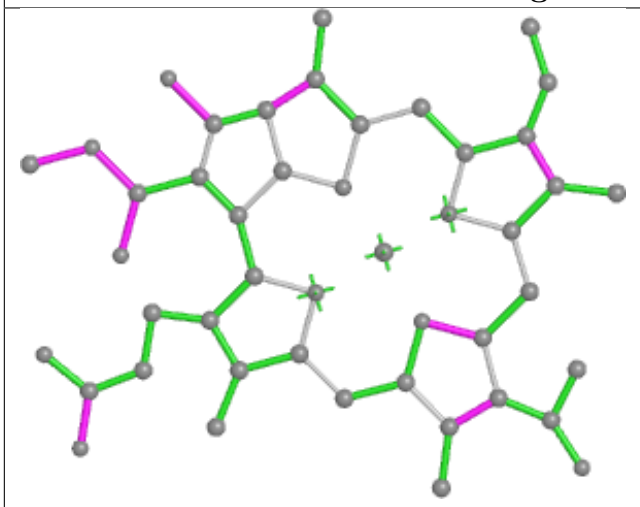
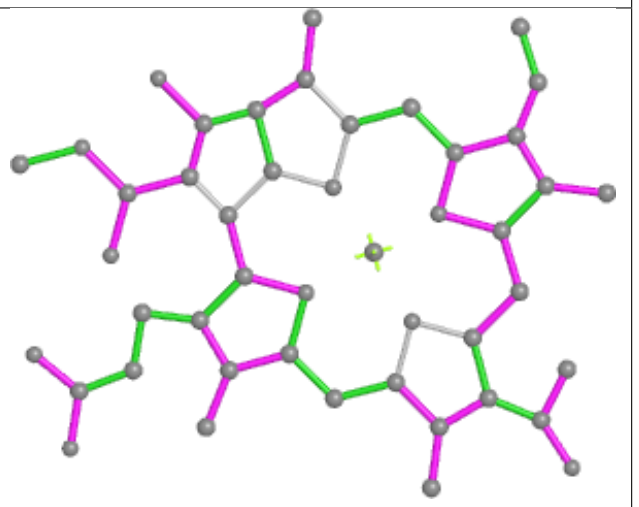
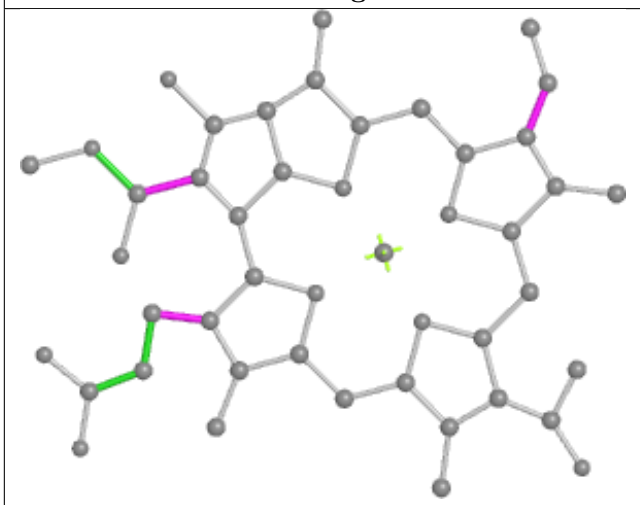
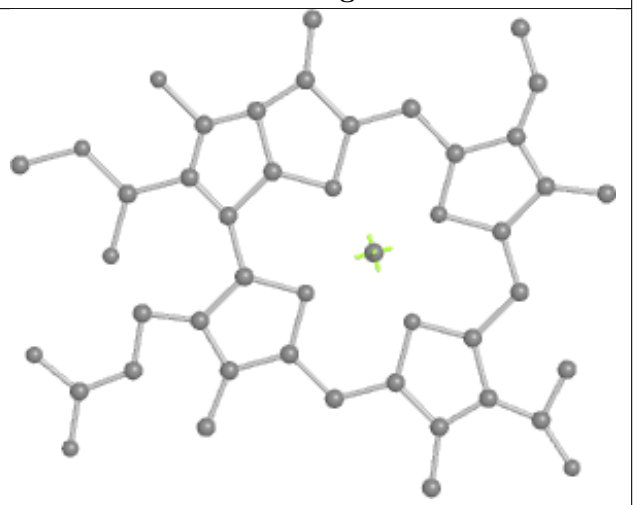
Ligand BCL A 813	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCL a 814

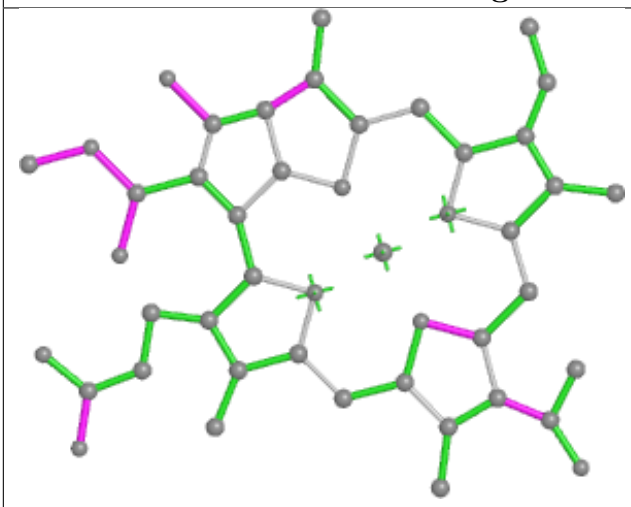


Ligand BCL a 815

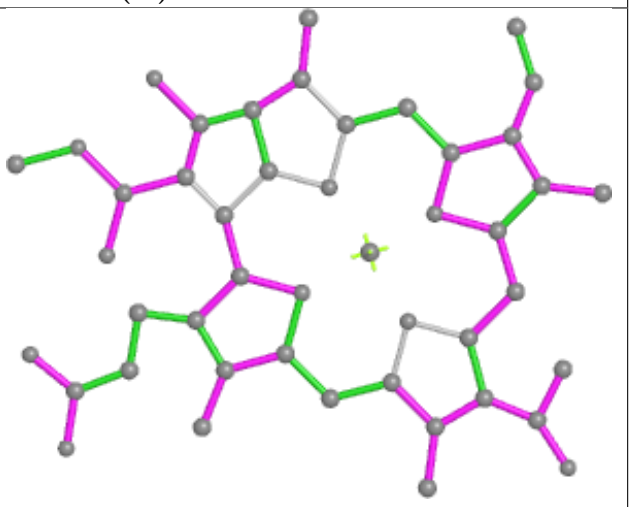


Ligand BCL a 813	
 Bond lengths	 Bond angles
 Torsions	 Rings

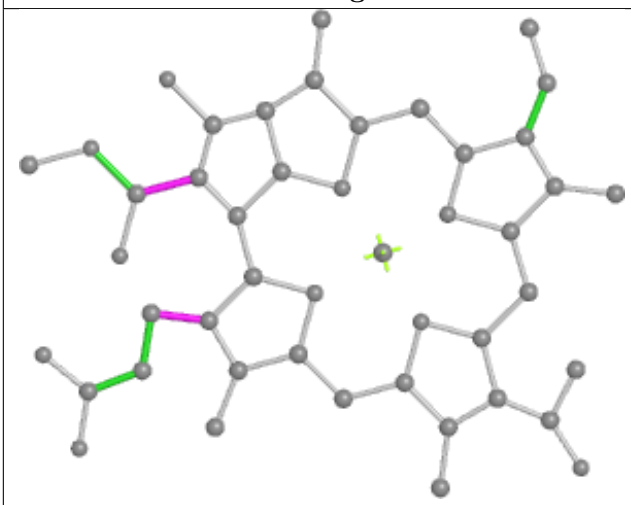
Ligand BCL G 378 (B)



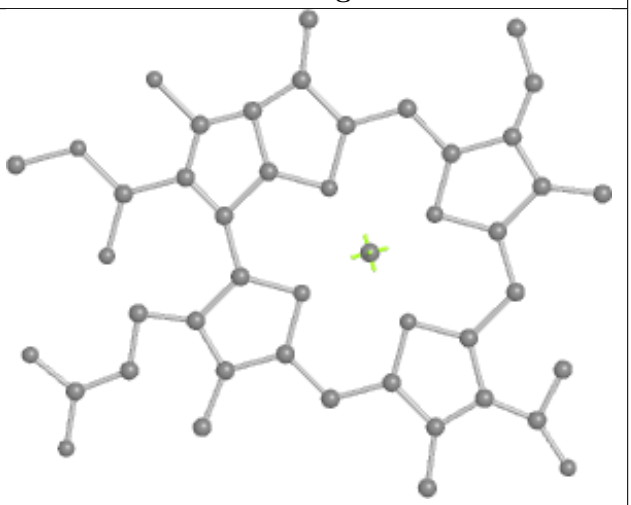
Bond lengths



Bond angles

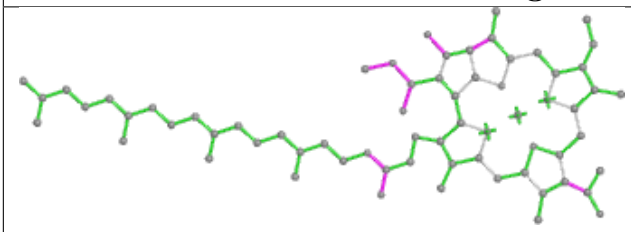


Torsions

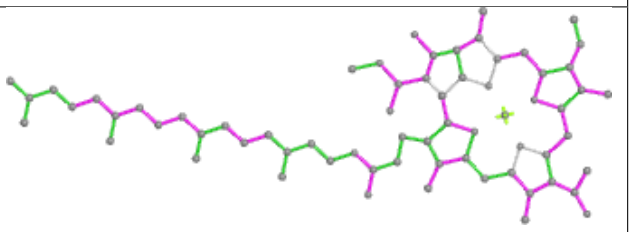


Rings

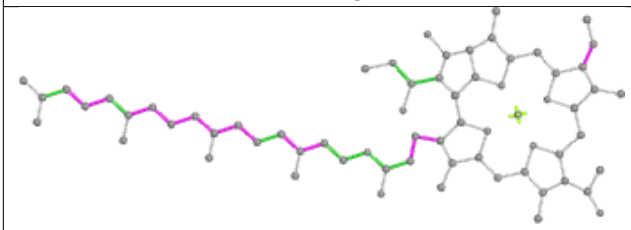
Ligand BCL E 372



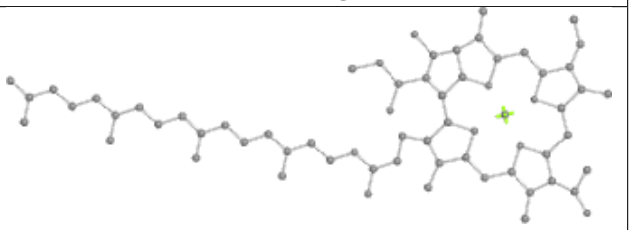
Bond lengths



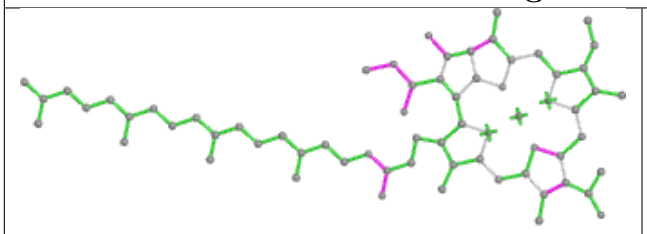
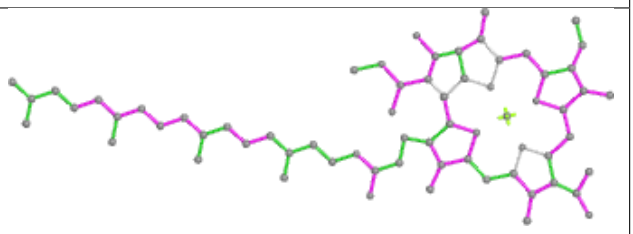
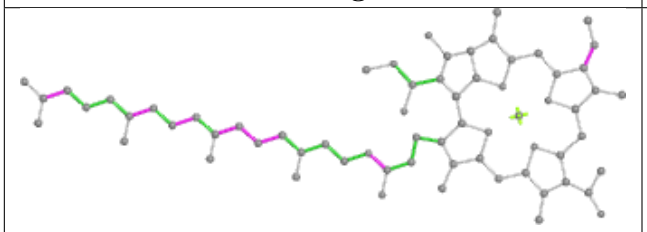
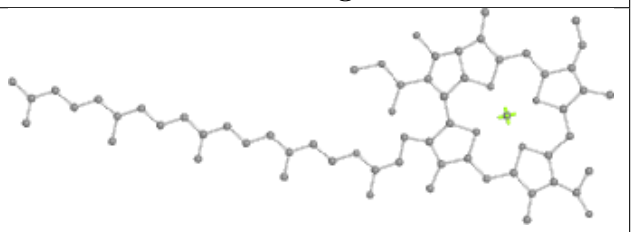
Bond angles

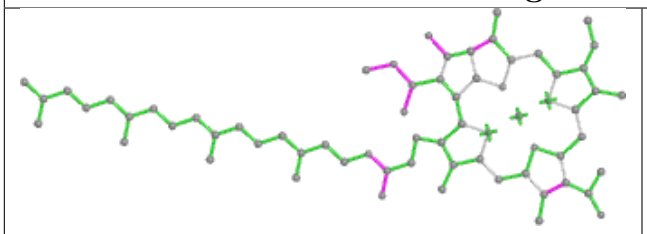
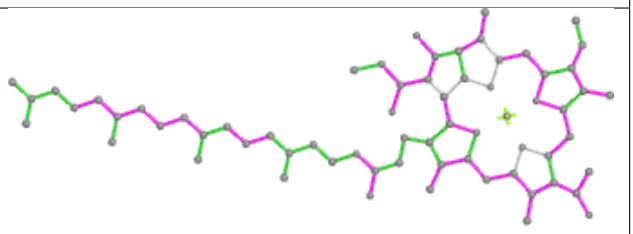
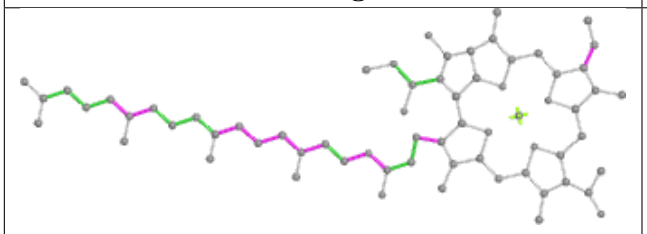
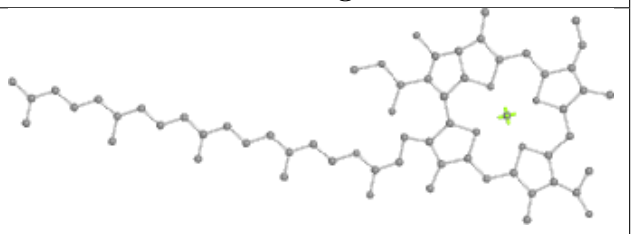


Torsions



Rings

Ligand BCL A 806	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCL A 811	
 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.

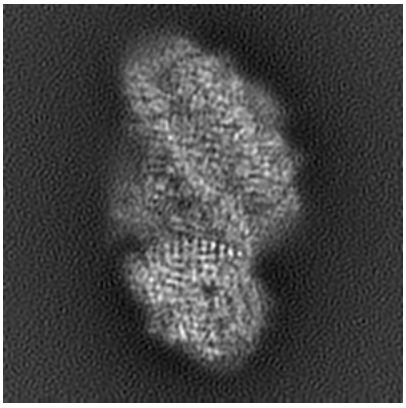
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-30069. These allow visual inspection of the internal detail of the map and identification of artifacts.

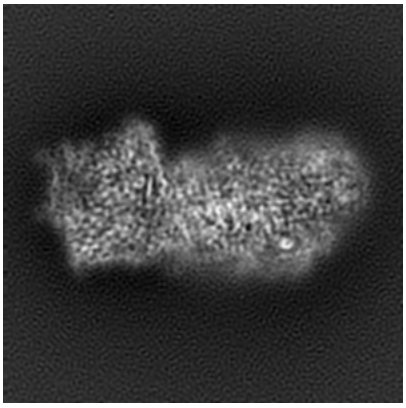
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

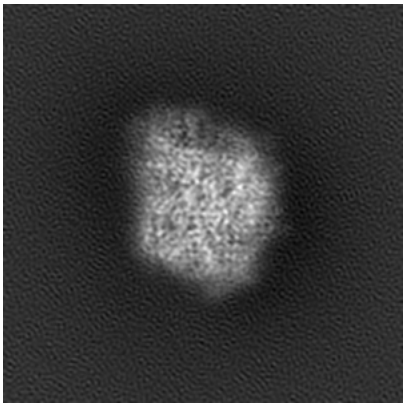
6.1.1 Primary map



X



Y

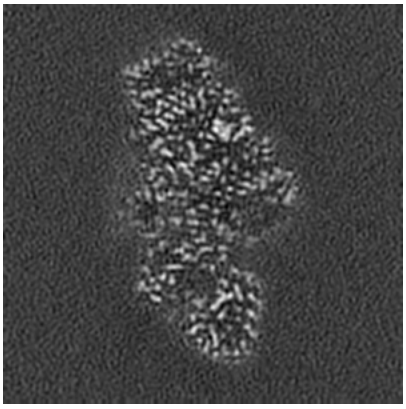


Z

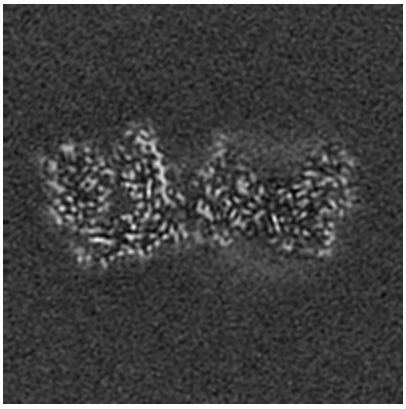
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

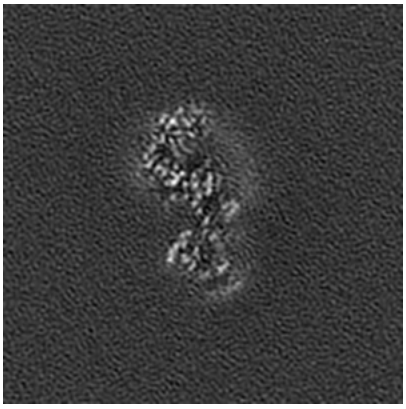
6.2.1 Primary map



X Index: 80



Y Index: 80

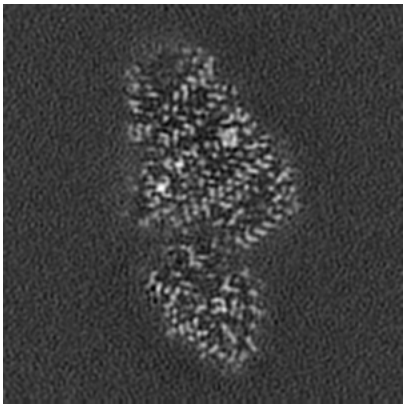


Z Index: 80

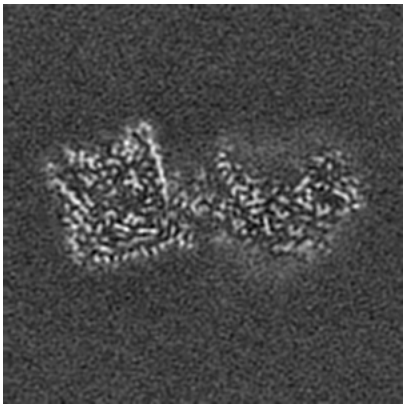
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

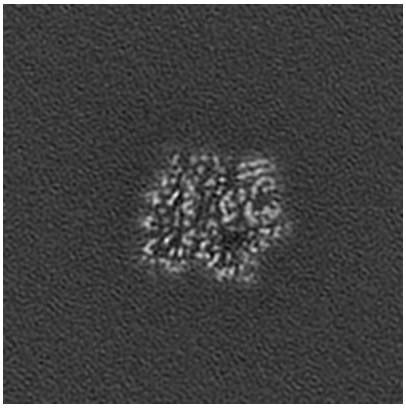
6.3.1 Primary map



X Index: 77



Y Index: 76



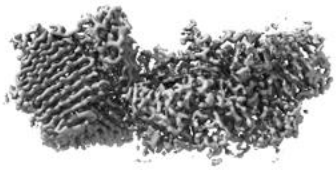
Z Index: 50

The images above show the largest variance slices of the map in three orthogonal directions.

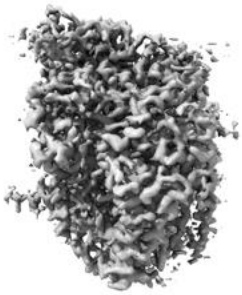
6.4 Orthogonal surface views (i)

6.4.1 Primary map

X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0341. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

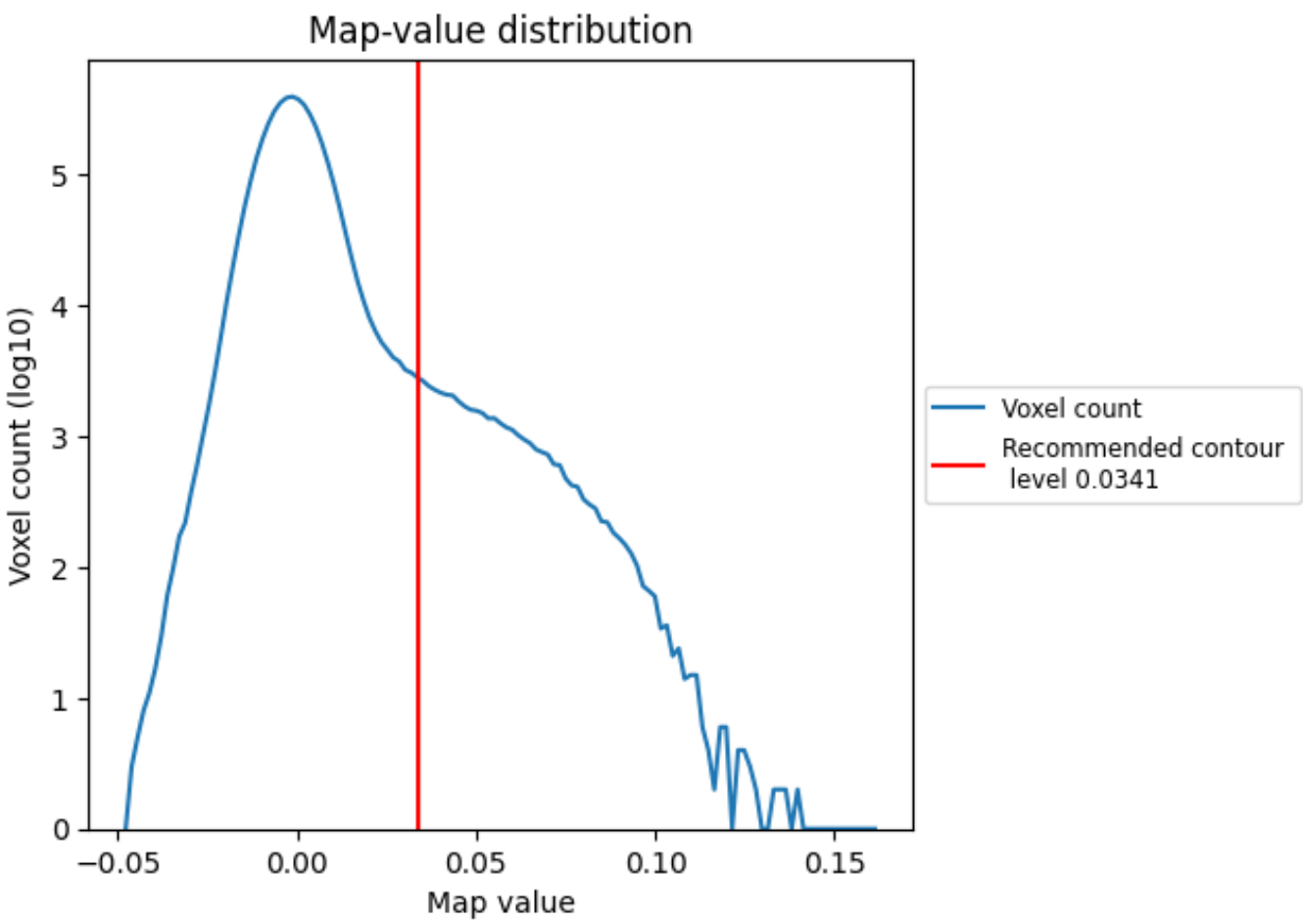
6.5 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis (i)

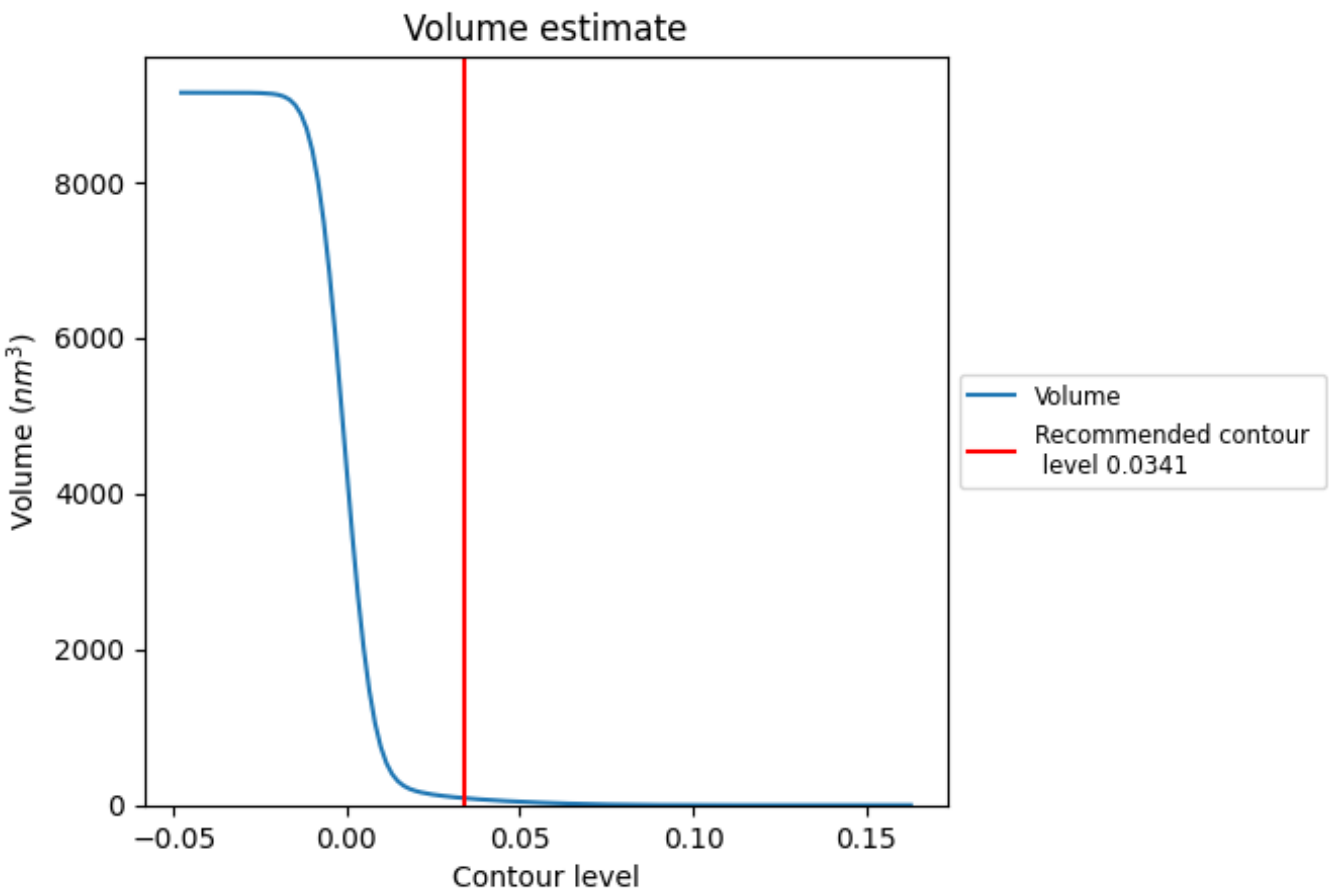
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

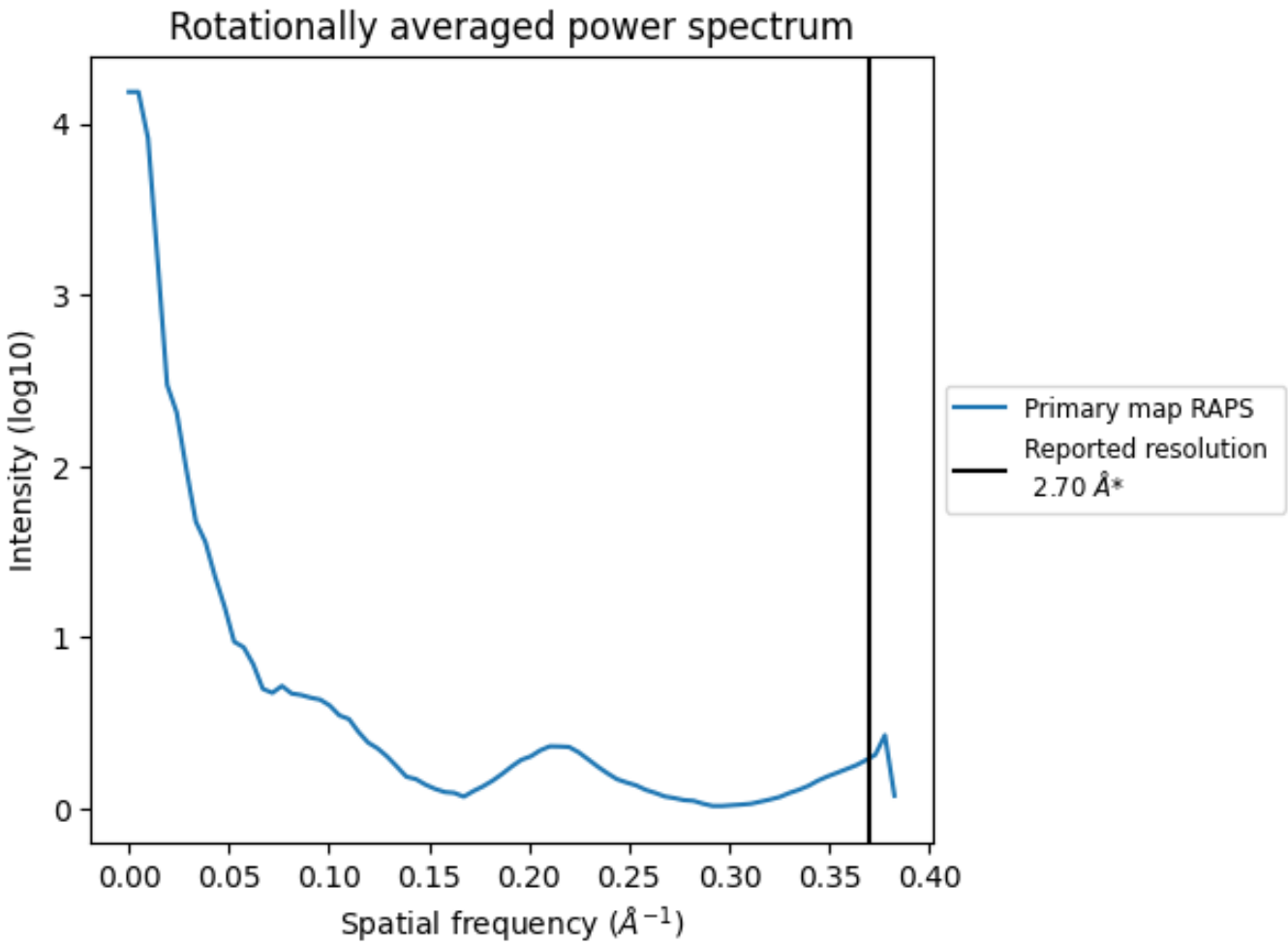
7.2 Volume estimate (i)



The volume at the recommended contour level is 90 nm^3; this corresponds to an approximate mass of 81 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.370 Å^{-1}

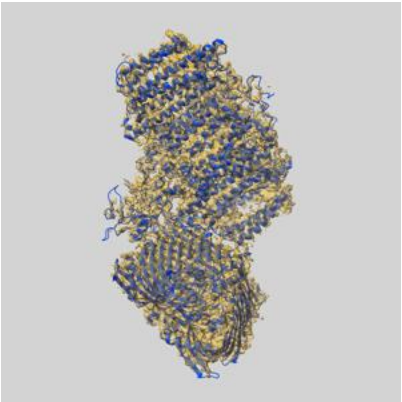
8 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.

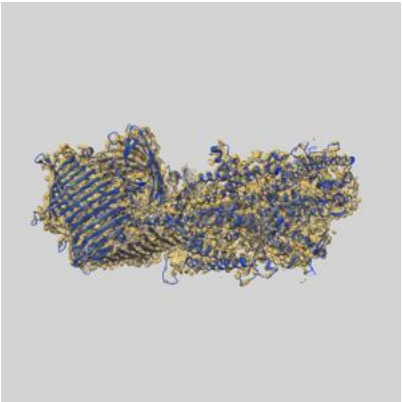
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-30069 and PDB model 6M32. Per-residue inclusion information can be found in section 3 on page 13.

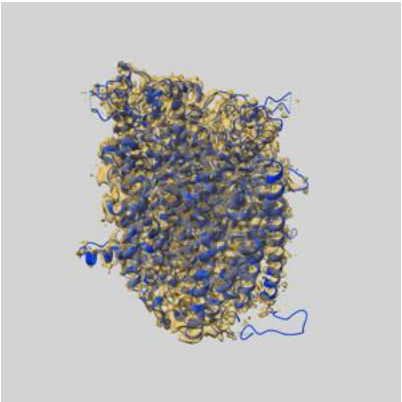
9.1 Map-model overlay (i)



X



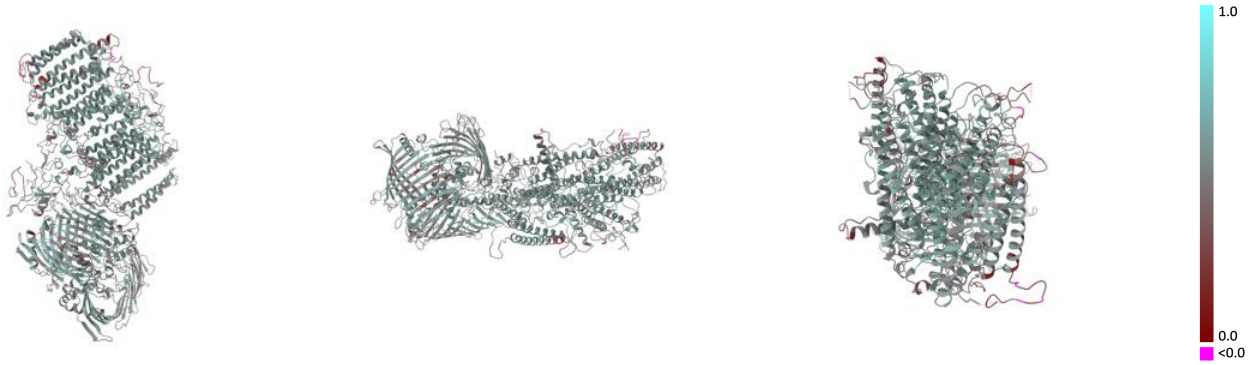
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0341 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

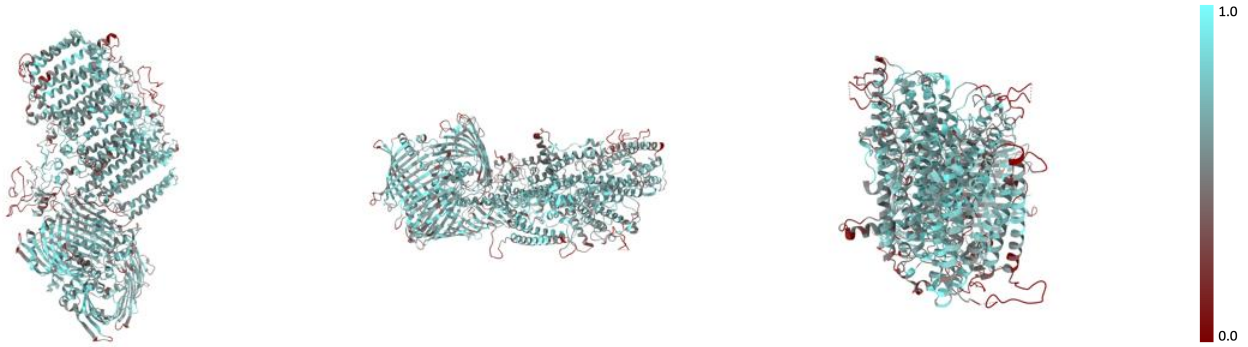
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

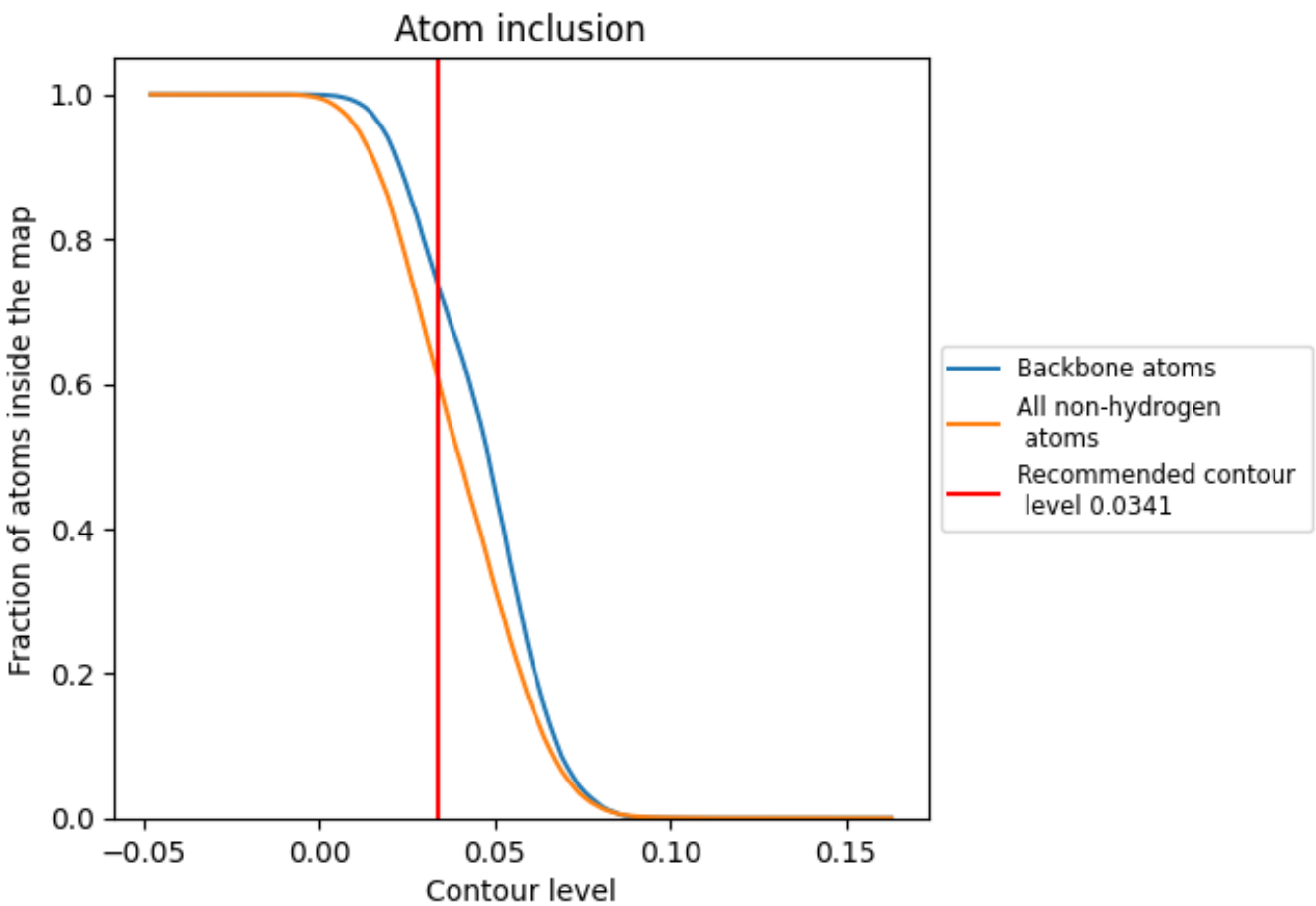
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0341).

9.4 Atom inclusion (i)



At the recommended contour level, 73% of all backbone atoms, 60% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.0341) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6032	0.5250
A	0.6034	0.5350
B	0.5747	0.4900
D	0.3096	0.4350
E	0.6448	0.5350
F	0.6387	0.5260
G	0.6612	0.5420
a	0.5709	0.5150