wwPDB EM Validation Summary Report (i)

Oct 8, 2022 – 01:15 PM EDT

PDB ID	:	7UEA
EMDB ID	:	EMD-26469
Title	:	Photosynthetic assembly of Chlorobaculum tepidum (RC-FMO1)
Authors	:	Puskar, R.; Truong, C.D.; Swain, K.; Li, S.; Cheng, K.-W.; Wang, T.Y.; Poh, Y.-P.; Liu, H.; Chou, T.-F.; Nannenga, B.; Chiu, P.-L.
Deposited on	:	2022-03-21
Resolution	:	3.49 Å(reported)
Based on initial model	:	6M32

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 (i)) were used in the production of this report:

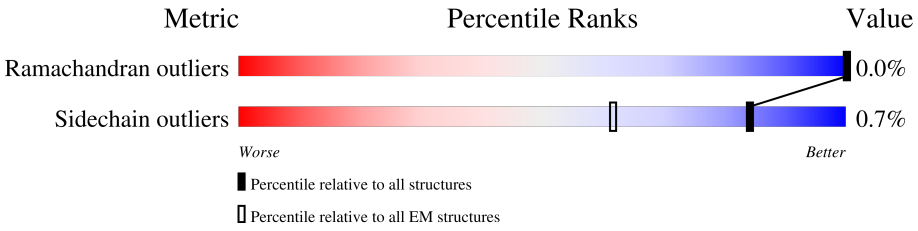
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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 3.49 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	A	731	8% 88% · 12%
1	a	731	8% 86% · 13%
2	B	231	14% 48% 52%
3	C	206	35% 55% · 43%
3	c	206	24% 50% 49%
4	D	143	40% 69% · 30%
5	U	366	10% 99% ·
5	V	366	11% 98% ·
5	W	366	15% 97% · ·

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
13	G2O	A	824	X	-	-	-
13	G2O	a	801	X	-	-	-
13	G2O	a	802	X	-	-	-
13	G2O	a	805	X	-	-	-
6	GS0	A	801	X	-	-	-
6	GS0	a	804	X	-	-	-
9	F26	a	820	-	X	-	-

2 Entry composition (i)

There are 14 unique types of molecules in this entry. The entry contains 26313 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 Photosystem P840 reaction center, large subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	645	Total	C	N	O	S	0	0
			5167	3449	821	871	26		
1	a	633	Total	C	N	O	S	0	0
			5079	3398	804	852	25		

- Molecule 2 is a protein called Photosystem P840 reaction center iron-sulfur protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	110	Total	C	N	O	S	0	0
			855	545	143	158	9		

- Molecule 3 is a protein called Cytochrome c.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	117	Total	C	N	O	S	0	0
			916	617	142	150	7		
3	c	105	Total	C	N	O	S	0	0
			839	565	130	138	6		

- Molecule 4 is a protein called P840 reaction center 17 kDa protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	100	Total	C	N	O	S	0	0
			817	520	144	149	4		

- Molecule 5 is a protein called Bacteriochlorophyll a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	U	364	Total	C	N	O	S	0	0
			2834	1798	503	526	7		
5	V	360	Total	C	N	O	S	0	0
			2805	1778	499	521	7		

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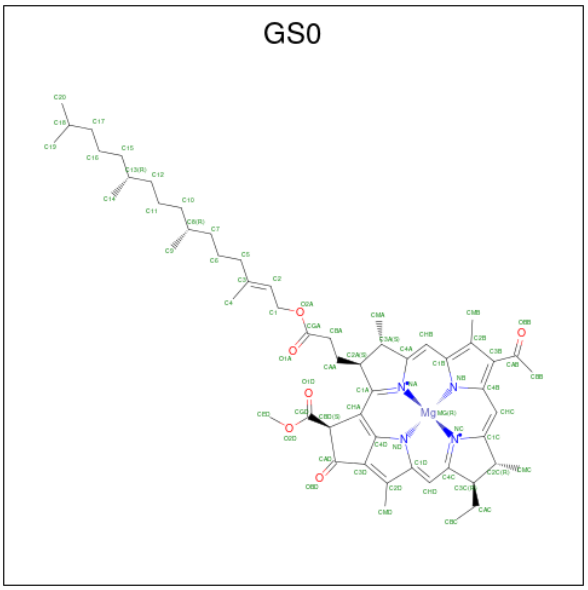
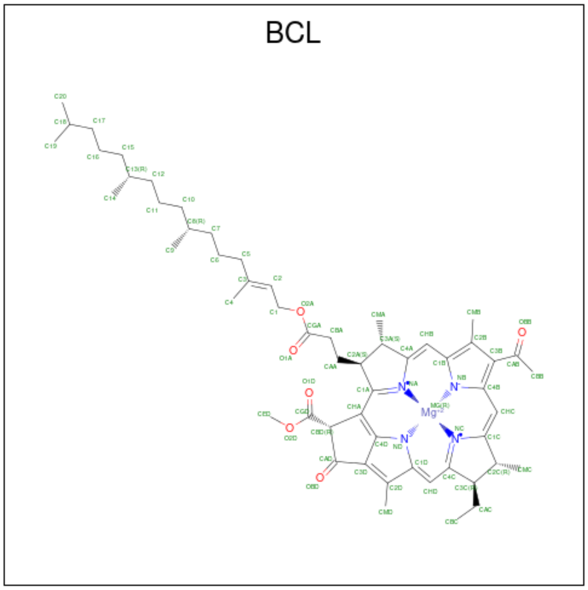
Mol	Chain	Residues	Atoms					AltConf	Trace
5	W	359	Total	C	N	O	S	0	0
			2797	1774	497	519	7		

- Molecule 6 is Bacteriochlorophyll A isomer (three-letter code: GS0) (formula: $C_{55}H_{74}MgN_4O_6$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 7 is BACTERIOCHLOROPHYLL A (three-letter code: BCL) (formula: $C_{55}H_{74}MgN_4O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
7	A	1	Total C Mg N O 791 659 12 48 72	0
7	A	1	Total C Mg N O 791 659 12 48 72	0
7	A	1	Total C Mg N O 791 659 12 48 72	0
7	A	1	Total C Mg N O 791 659 12 48 72	0
7	A	1	Total C Mg N O 791 659 12 48 72	0
7	A	1	Total C Mg N O 791 659 12 48 72	0
7	A	1	Total C Mg N O 791 659 12 48 72	0
7	A	1	Total C Mg N O 791 659 12 48 72	0
7	A	1	Total C Mg N O 791 659 12 48 72	0
7	A	1	Total C Mg N O 791 659 12 48 72	0
7	A	1	Total C Mg N O 791 659 12 48 72	0
7	A	1	Total C Mg N O 791 659 12 48 72	0
7	a	1	Total C Mg N O 772 640 12 48 72	0
7	a	1	Total C Mg N O 772 640 12 48 72	0

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Mol	Chain	Residues	Atoms					AltConf
7	a	1	Total 772	C 640	Mg 12	N 48	O 72	0
7	a	1	Total 772	C 640	Mg 12	N 48	O 72	0
7	a	1	Total 772	C 640	Mg 12	N 48	O 72	0
7	a	1	Total 772	C 640	Mg 12	N 48	O 72	0
7	a	1	Total 772	C 640	Mg 12	N 48	O 72	0
7	a	1	Total 772	C 640	Mg 12	N 48	O 72	0
7	a	1	Total 772	C 640	Mg 12	N 48	O 72	0
7	a	1	Total 772	C 640	Mg 12	N 48	O 72	0
7	a	1	Total 772	C 640	Mg 12	N 48	O 72	0
7	a	1	Total 772	C 640	Mg 12	N 48	O 72	0
7	U	1	Total 574	C 475	Mg 9	N 36	O 54	0
7	U	1	Total 574	C 475	Mg 9	N 36	O 54	0
7	U	1	Total 574	C 475	Mg 9	N 36	O 54	0
7	U	1	Total 574	C 475	Mg 9	N 36	O 54	0
7	U	1	Total 574	C 475	Mg 9	N 36	O 54	0
7	U	1	Total 574	C 475	Mg 9	N 36	O 54	0
7	U	1	Total 574	C 475	Mg 9	N 36	O 54	0
7	U	1	Total 574	C 475	Mg 9	N 36	O 54	1
7	U	1	Total 574	C 475	Mg 9	N 36	O 54	0
7	V	1	Total 508	C 420	Mg 8	N 32	O 48	0
7	V	1	Total 508	C 420	Mg 8	N 32	O 48	0

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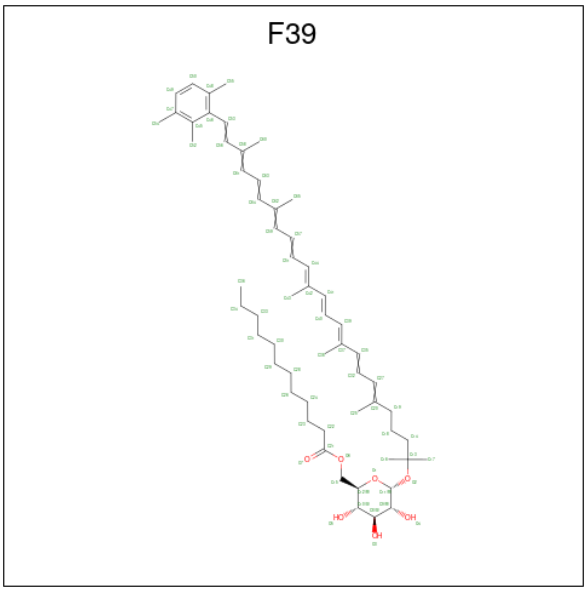
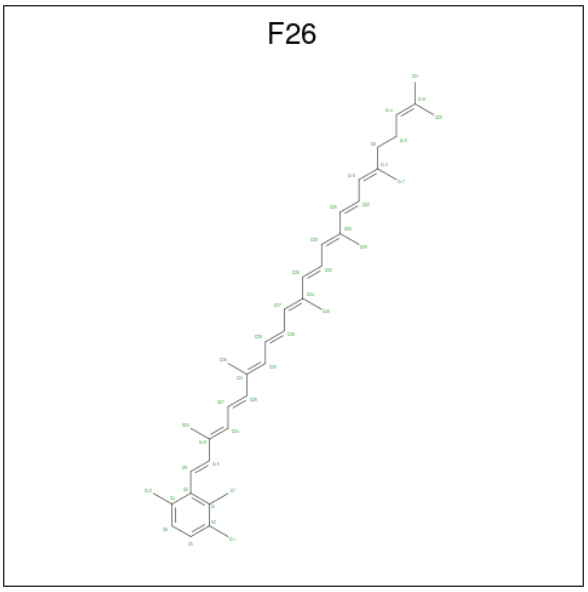
Mol	Chain	Residues	Atoms					AltConf
7	V	1	Total 508	C 420	Mg 8	N 32	O 48	0
7	V	1	Total 508	C 420	Mg 8	N 32	O 48	0
7	V	1	Total 508	C 420	Mg 8	N 32	O 48	0
7	V	1	Total 508	C 420	Mg 8	N 32	O 48	0
7	V	1	Total 508	C 420	Mg 8	N 32	O 48	0
7	V	1	Total 508	C 420	Mg 8	N 32	O 48	1
7	W	1	Total 442	C 365	Mg 7	N 28	O 42	0
7	W	1	Total 442	C 365	Mg 7	N 28	O 42	0
7	W	1	Total 442	C 365	Mg 7	N 28	O 42	0
7	W	1	Total 442	C 365	Mg 7	N 28	O 42	0
7	W	1	Total 442	C 365	Mg 7	N 28	O 42	0
7	W	1	Total 442	C 365	Mg 7	N 28	O 42	0
7	W	1	Total 442	C 365	Mg 7	N 28	O 42	1

- Molecule 8 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: $C_{58}H_{86}O_{7}$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 9 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: $C_{40}H_{52}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
9	A	1	Total C 40 40	0

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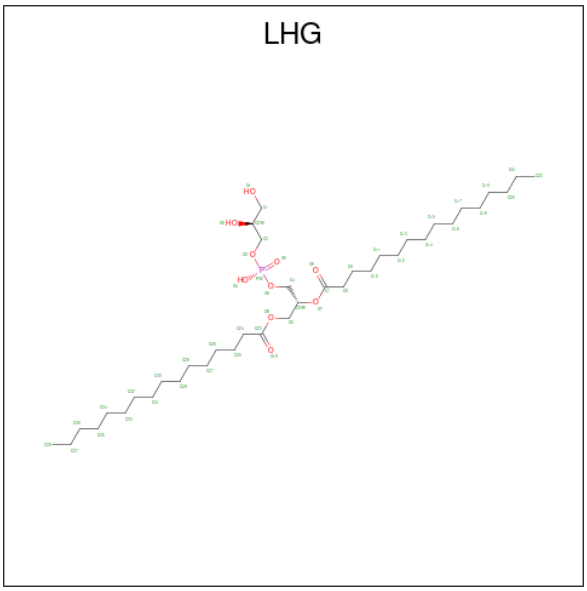
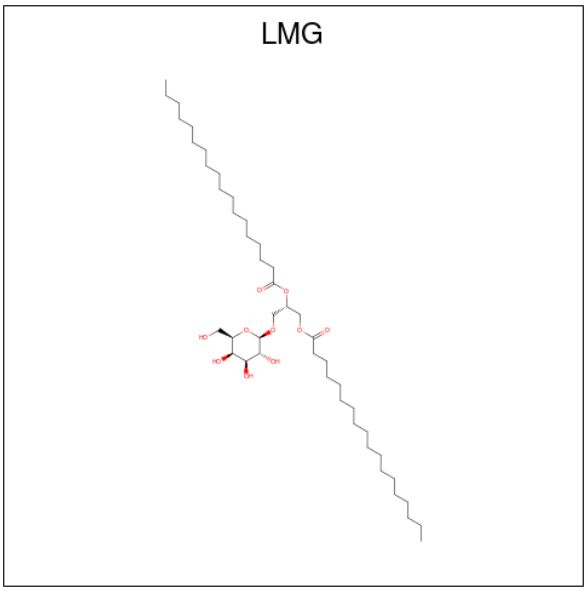
Mol	Chain	Residues	Atoms	AltConf
9	a	1	Total C 80 80	0
9	a	1	Total C 80 80	0

- Molecule 10 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: $C_{38}H_{75}O_{10}P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
10	A	1	Total C O P 67 45 20 2	0
10	A	1	Total C O P 67 45 20 2	0
10	a	1	Total C O P 99 66 30 3	0
10	a	1	Total C O P 99 66 30 3	0
10	a	1	Total C O P 99 66 30 3	0
10	C	1	Total C O P 34 23 10 1	0

- Molecule 11 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: $C_{45}H_{86}O_{10}$) (labeled as "Ligand of Interest" by depositor).

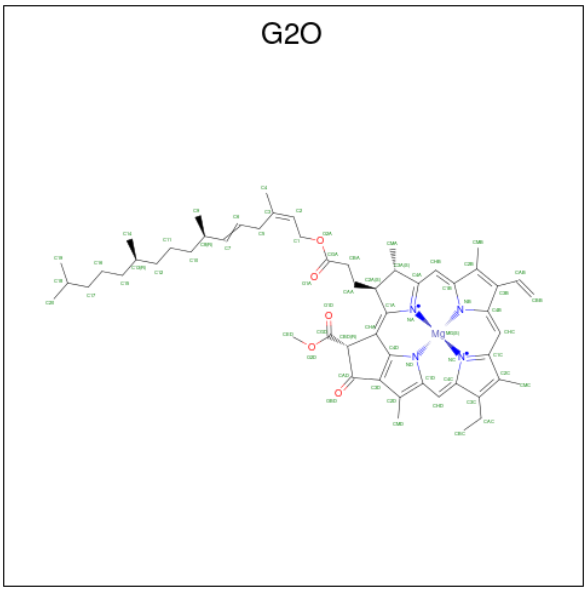


Mol	Chain	Residues	Atoms	AltConf
11	A	1	Total C O 174 124 50	0
11	A	1	Total C O 174 124 50	0
11	A	1	Total C O 174 124 50	0
11	A	1	Total C O 174 124 50	0
11	A	1	Total C O 174 124 50	0
11	a	1	Total C O 40 30 10	0
11	C	1	Total C O 35 25 10	0

- Molecule 12 is CALCIUM ION (three-letter code: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

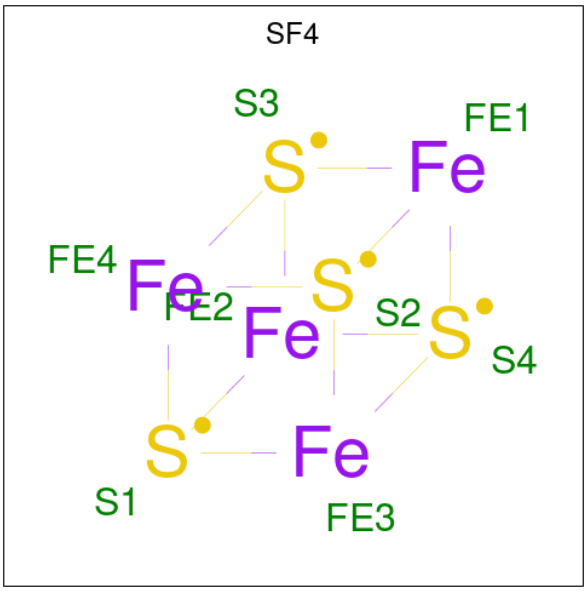
Mol	Chain	Residues	Atoms	AltConf
12	A	1	Total Ca 1 1	0
12	a	1	Total Ca 1 1	0

- Molecule 13 is Chlorophyll A ester (three-letter code: G2O) (formula: $C_{55}H_{70}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
13	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			195	165	3	12	15	
13	a	1	Total	C	Mg	N	O	0
			195	165	3	12	15	
13	a	1	Total	C	Mg	N	O	0
			195	165	3	12	15	

- Molecule 14 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).

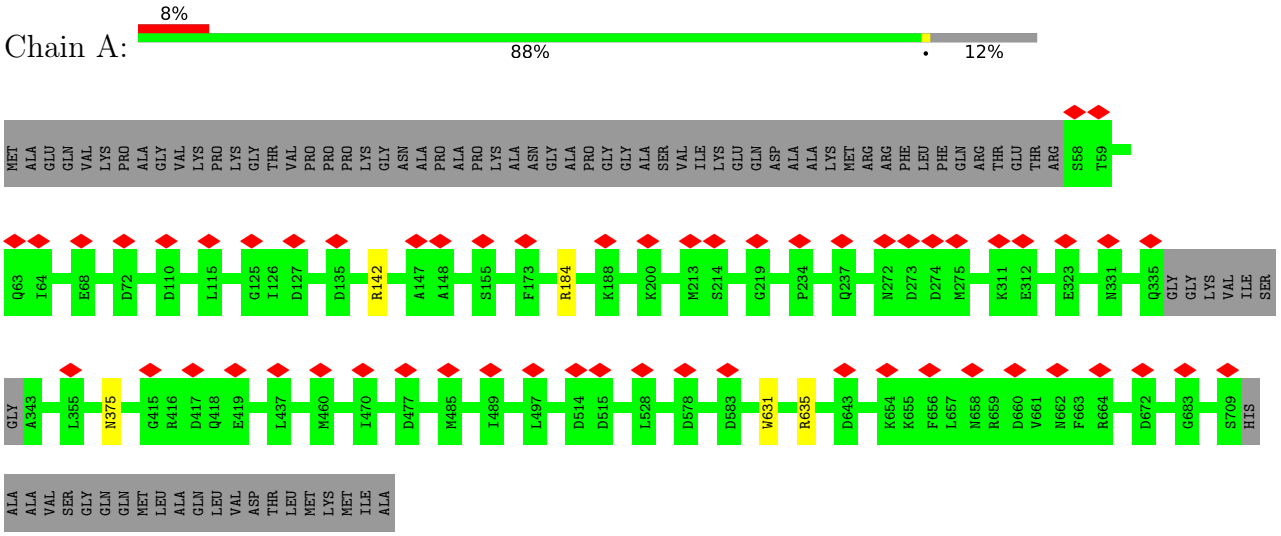


Mol	Chain	Residues	Atoms	AltConf
14	a	1	Total Fe S 8 4 4	0
14	B	1	Total Fe S 16 8 8	0
14	B	1	Total Fe S 16 8 8	0

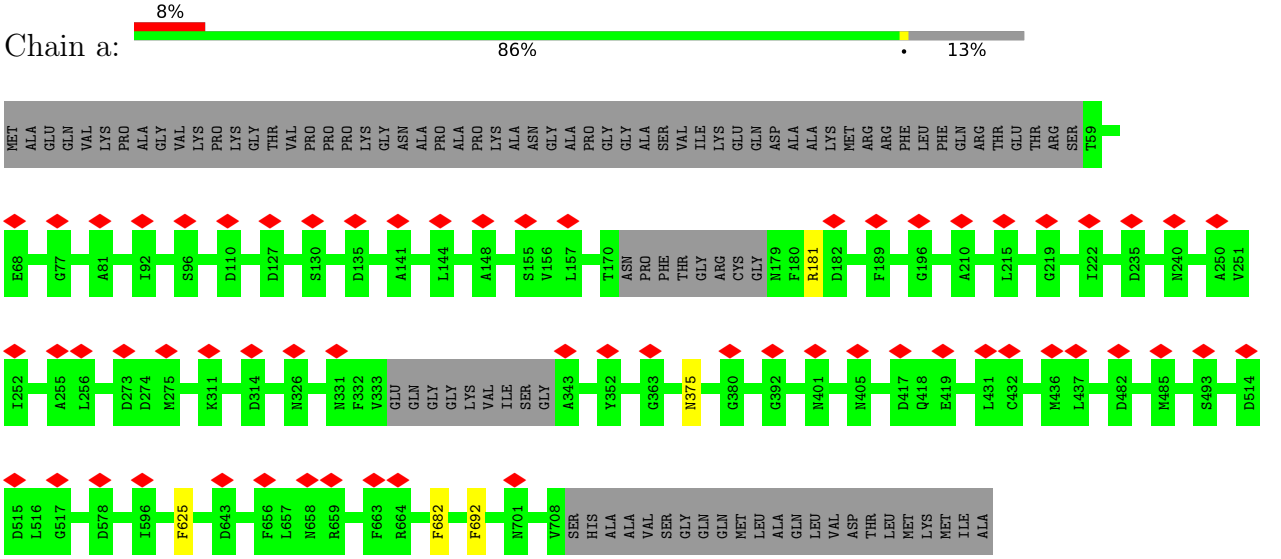
3 Residue-property plots (i)

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: Photosystem P840 reaction center, large subunit

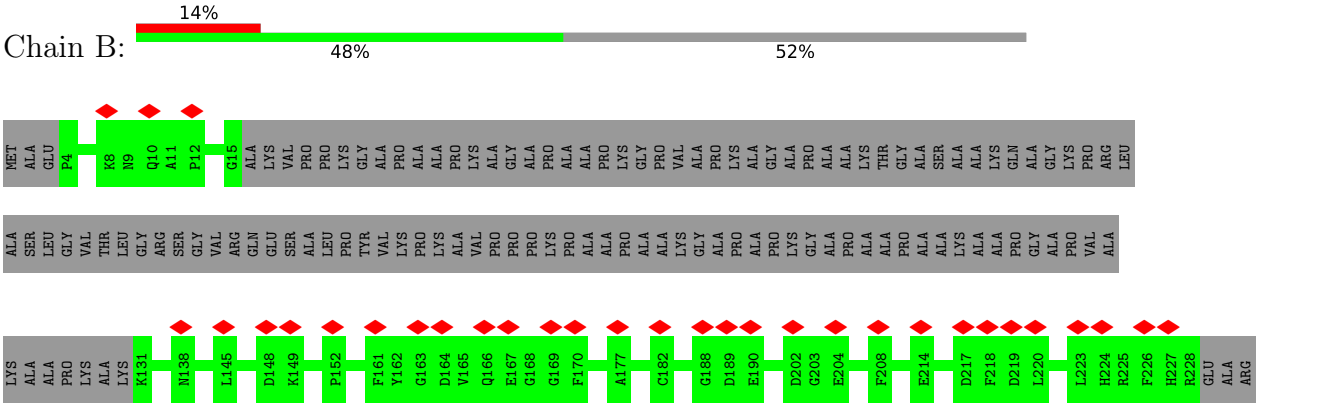


• Molecule 1: Photosystem P840 reaction center, large subunit



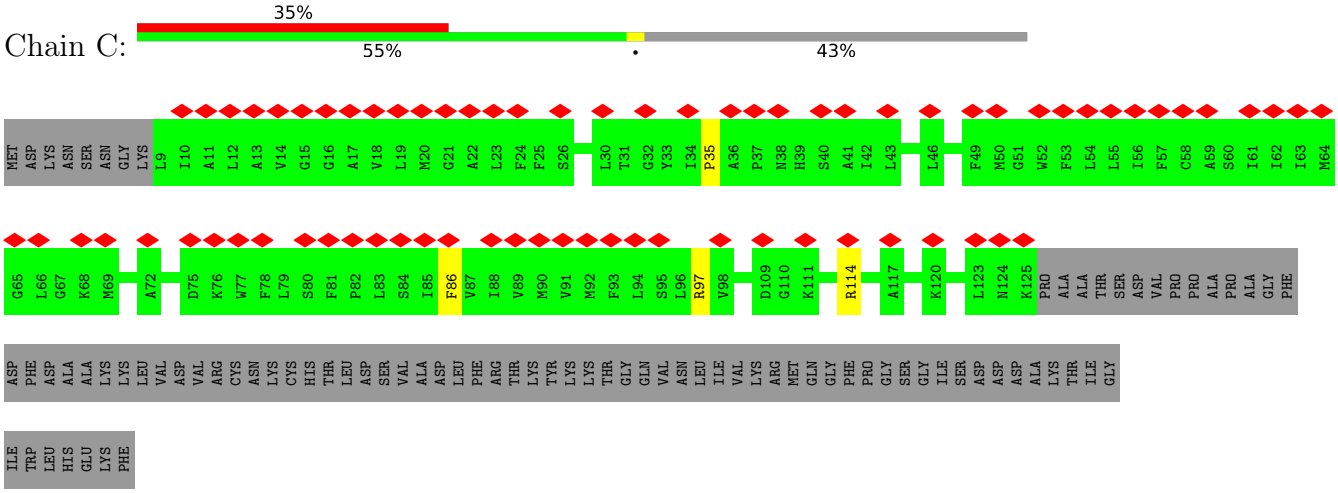
• Molecule 2: Photosystem P840 reaction center iron-sulfur protein

Chain B:



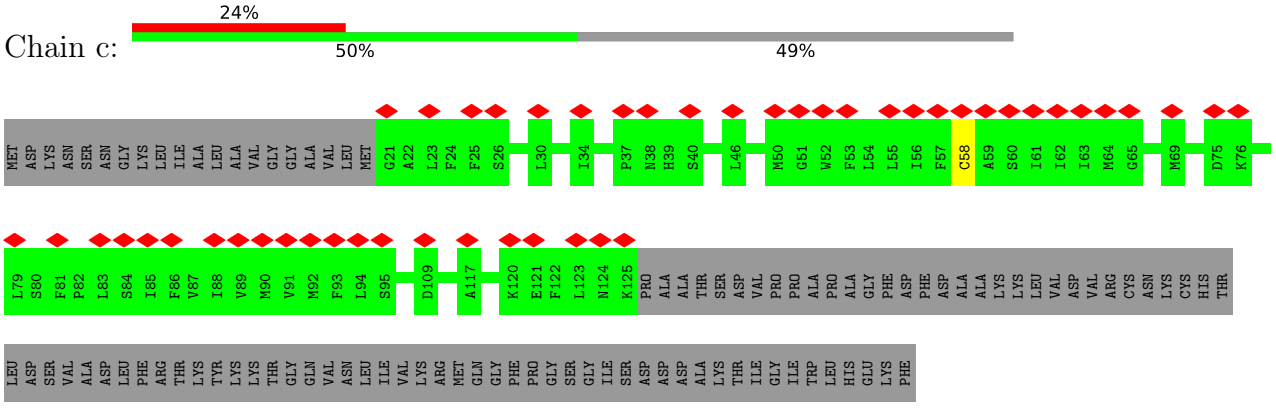
• Molecule 3: Cytochrome c

Chain C:



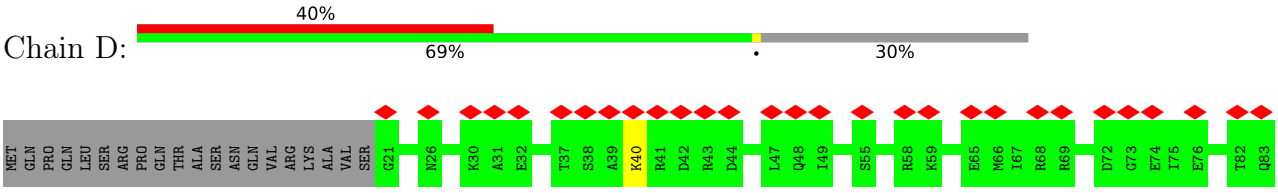
• Molecule 3: Cytochrome c

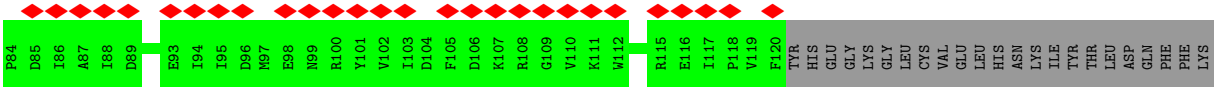
Chain c:



• Molecule 4: P840 reaction center 17 kDa protein

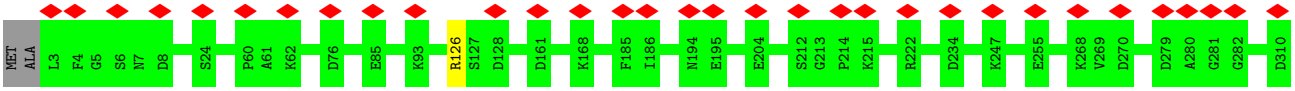
Chain D:

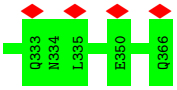




• Molecule 5: Bacteriochlorophyll a protein

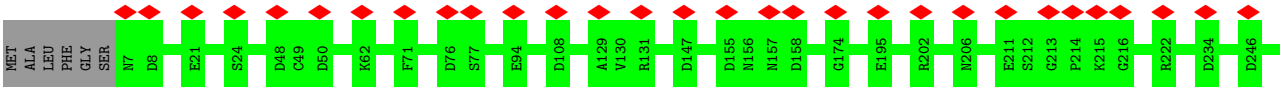
Chain U:

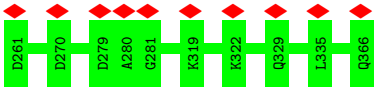




• Molecule 5: Bacteriochlorophyll a protein

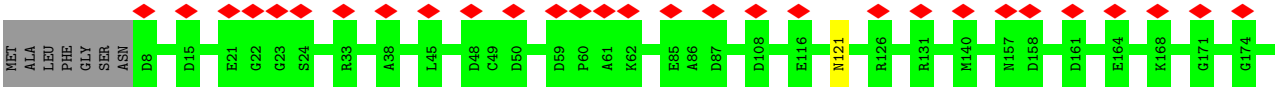
Chain V:

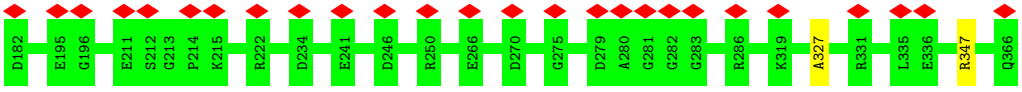




• Molecule 5: Bacteriochlorophyll a protein

Chain W:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	142020	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	45.4	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	47259	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	8.114	Depositor
Minimum map value	-3.718	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.090	Depositor
Recommended contour level	0.352	Depositor
Map size (Å)	374.4, 374.4, 374.4	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.04, 1.04, 1.04	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, BCL, G2O, F26, SF4, GS0, LMG, F39, LHG

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	0.28	0/5348	0.44	0/7288
1	a	0.29	0/5257	0.44	0/7164
2	B	0.30	0/878	0.49	0/1187
3	C	0.26	0/940	0.50	0/1272
3	c	0.26	0/863	0.49	0/1167
4	D	0.25	0/833	0.55	0/1122
5	U	0.29	0/2905	0.53	0/3937
5	V	0.29	0/2875	0.53	0/3897
5	W	0.29	0/2867	0.53	0/3886
All	All	0.29	0/22766	0.49	0/30920

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
4	D	0	1
5	W	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	D	40	LYS	Peptide
5	W	327	ALA	Peptide

5.2 Too-close contacts

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

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	A	641/731 (88%)	620 (97%)	21 (3%)	0	100	100
1	a	627/731 (86%)	600 (96%)	27 (4%)	0	100	100
2	B	106/231 (46%)	99 (93%)	7 (7%)	0	100	100
3	C	115/206 (56%)	110 (96%)	4 (4%)	1 (1%)	17	56
3	c	103/206 (50%)	102 (99%)	1 (1%)	0	100	100
4	D	98/143 (68%)	84 (86%)	14 (14%)	0	100	100
5	U	362/366 (99%)	348 (96%)	14 (4%)	0	100	100
5	V	358/366 (98%)	351 (98%)	7 (2%)	0	100	100
5	W	357/366 (98%)	344 (96%)	13 (4%)	0	100	100
All	All	2767/3346 (83%)	2658 (96%)	108 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	35	PRO

5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	A	536/599 (90%)	531 (99%)	5 (1%)	78 90
1	a	526/599 (88%)	521 (99%)	5 (1%)	76 88
2	B	93/162 (57%)	93 (100%)	0	100 100
3	C	99/173 (57%)	96 (97%)	3 (3%)	41 71
3	c	92/173 (53%)	91 (99%)	1 (1%)	73 88
4	D	89/128 (70%)	89 (100%)	0	100 100
5	U	301/302 (100%)	300 (100%)	1 (0%)	92 97
5	V	298/302 (99%)	298 (100%)	0	100 100
5	W	297/302 (98%)	295 (99%)	2 (1%)	84 93
All	All	2331/2740 (85%)	2314 (99%)	17 (1%)	84 93

5 of 17 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	U	126	ARG
5	W	347	ARG
1	a	625	PHE
1	a	682	PHE
1	a	692	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
5	U	144	GLN
5	U	146	HIS
5	W	121	ASN
5	V	333	GLN
2	B	155	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 77 ligands modelled in this entry, 2 are monoatomic - leaving 75 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	$\#\|Z\| > 2$
7	BCL	U	402	-	58,74,74	1.18	3 (5%)	69,115,115	1.35	9 (13%)
7	BCL	a	813	-	58,74,74	1.19	3 (5%)	69,115,115	1.44	12 (17%)
7	BCL	U	409	-	58,74,74	1.16	3 (5%)	69,115,115	1.38	10 (14%)
7	BCL	A	803	-	58,74,74	1.22	3 (5%)	69,115,115	1.39	10 (14%)
7	BCL	V	408[B]	5	38,54,74	1.41	3 (7%)	45,91,115	1.59	10 (22%)
7	BCL	W	406	-	58,74,74	1.11	2 (3%)	69,115,115	1.38	11 (15%)
9	F26	A	815	-	40,40,40	1.79	10 (25%)	46,50,50	2.10	16 (34%)
7	BCL	A	806	-	58,74,74	1.15	3 (5%)	69,115,115	1.44	9 (13%)
7	BCL	W	402	-	58,74,74	1.13	4 (6%)	69,115,115	1.50	10 (14%)
11	LMG	A	821	-	27,27,55	1.03	0	35,35,63	1.23	5 (14%)
10	LHG	a	823	-	39,39,48	0.66	0	42,45,54	0.98	2 (4%)
7	BCL	a	815	-	58,74,74	1.20	4 (6%)	69,115,115	1.39	10 (14%)
7	BCL	U	408[B]	5	38,54,74	1.38	4 (10%)	45,91,115	1.55	9 (20%)
14	SF4	a	803	1	0,12,12	-	-	-		
10	LHG	A	816	-	25,25,48	0.83	1 (4%)	28,31,54	0.94	1 (3%)
7	BCL	a	808	-	58,74,74	1.20	2 (3%)	69,115,115	1.56	11 (15%)
7	BCL	A	811	-	58,74,74	1.16	3 (5%)	69,115,115	1.48	12 (17%)
7	BCL	a	809	-	58,74,74	1.16	4 (6%)	69,115,115	1.89	16 (23%)
7	BCL	a	812	-	58,74,74	1.16	4 (6%)	69,115,115	1.39	9 (13%)
13	G2O	a	805	-	67,73,73	4.13	39 (58%)	75,113,113	2.94	21 (28%)
9	F26	a	819	-	40,40,40	1.68	10 (25%)	46,50,50	2.22	15 (32%)
6	GS0	A	801	-	64,74,74	2.34	11 (17%)	78,115,115	2.88	30 (38%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
7	BCL	V	401	-	58,74,74	1.17	3 (5%)	69,115,115	1.51	14 (20%)
13	G2O	A	824	-	67,73,73	4.26	41 (61%)	75,113,113	3.02	22 (29%)
8	F39	a	818	-	66,66,66	2.81	21 (31%)	79,85,85	2.15	22 (27%)
7	BCL	A	804	-	58,74,74	1.15	3 (5%)	69,115,115	1.47	10 (14%)
7	BCL	U	401	-	58,74,74	1.18	4 (6%)	69,115,115	1.49	13 (18%)
7	BCL	A	813	-	57,73,74	1.17	2 (3%)	67,113,115	1.52	12 (17%)
7	BCL	A	807	-	58,74,74	1.17	3 (5%)	69,115,115	1.42	9 (13%)
13	G2O	a	801	-	67,73,73	4.14	40 (59%)	75,113,113	3.11	20 (26%)
14	SF4	B	301	2	0,12,12	-	-	-		
7	BCL	a	816	-	58,74,74	1.17	4 (6%)	69,115,115	1.37	9 (13%)
7	BCL	a	811	1	38,54,74	1.33	3 (7%)	45,91,115	1.83	11 (24%)
7	BCL	V	405	-	58,74,74	1.13	4 (6%)	69,115,115	1.42	8 (11%)
7	BCL	A	810	-	58,74,74	1.16	4 (6%)	69,115,115	1.52	11 (15%)
7	BCL	U	407	-	58,74,74	1.17	4 (6%)	69,115,115	1.37	11 (15%)
10	LHG	A	817	-	40,40,48	0.68	1 (2%)	43,46,54	1.00	2 (4%)
11	LMG	a	824	-	40,40,55	0.83	1 (2%)	48,48,63	1.18	4 (8%)
7	BCL	a	810	-	58,74,74	1.13	3 (5%)	69,115,115	1.45	12 (17%)
11	LMG	C	302	-	35,35,55	0.90	1 (2%)	43,43,63	1.16	3 (6%)
7	BCL	U	404	-	58,74,74	1.16	3 (5%)	69,115,115	1.58	14 (20%)
7	BCL	a	814	-	58,74,74	1.14	4 (6%)	69,115,115	1.56	10 (14%)
7	BCL	A	808	-	58,74,74	1.16	4 (6%)	69,115,115	1.47	11 (15%)
7	BCL	V	404	-	58,74,74	1.12	3 (5%)	69,115,115	1.42	11 (15%)
7	BCL	a	807	-	58,74,74	1.24	3 (5%)	69,115,115	1.33	8 (11%)
7	BCL	A	805	-	58,74,74	1.15	4 (6%)	69,115,115	1.62	13 (18%)
11	LMG	A	820	-	36,36,55	0.92	0	44,44,63	1.12	4 (9%)
11	LMG	A	818	-	42,42,55	0.80	0	50,50,63	1.17	5 (10%)
8	F39	A	814	-	66,66,66	2.79	20 (30%)	79,85,85	2.19	24 (30%)
7	BCL	a	817	-	58,74,74	1.15	3 (5%)	69,115,115	1.38	8 (11%)
7	BCL	V	406	-	58,74,74	1.18	3 (5%)	69,115,115	1.52	12 (17%)
7	BCL	W	401	-	58,74,74	1.19	4 (6%)	69,115,115	1.62	11 (15%)
7	BCL	U	403	-	58,74,74	1.16	3 (5%)	69,115,115	1.44	10 (14%)
6	GS0	a	804	-	64,74,74	2.39	14 (21%)	78,115,115	2.84	29 (37%)
9	F26	a	820	-	40,40,40	1.74	10 (25%)	46,50,50	2.13	15 (32%)
7	BCL	V	403	-	58,74,74	1.14	3 (5%)	69,115,115	1.47	9 (13%)
7	BCL	U	405	5	58,74,74	1.17	3 (5%)	69,115,115	1.45	10 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
10	LHG	a	822	-	25,25,48	0.82	1 (4%)	28,31,54	0.95	1 (3%)
14	SF4	B	302	2	0,12,12	-	-	-		
10	LHG	a	821	-	32,32,48	0.74	1 (3%)	35,38,54	1.03	2 (5%)
11	LMG	A	822	-	30,30,55	0.96	0	38,38,63	1.28	5 (13%)
7	BCL	W	404	5	58,74,74	1.16	3 (5%)	69,115,115	1.46	13 (18%)
7	BCL	W	405	-	58,74,74	1.13	3 (5%)	69,115,115	1.56	12 (17%)
13	G2O	a	802	-	67,73,73	4.15	40 (59%)	75,113,113	3.03	20 (26%)
7	BCL	U	406	-	58,74,74	1.18	3 (5%)	69,115,115	1.41	9 (13%)
7	BCL	A	812	-	58,74,74	1.15	3 (5%)	69,115,115	1.30	9 (13%)
7	BCL	A	809	-	58,74,74	1.16	4 (6%)	69,115,115	1.41	10 (14%)
7	BCL	V	402	-	58,74,74	1.18	4 (6%)	69,115,115	1.45	12 (17%)
7	BCL	W	407[B]	5	38,54,74	1.39	3 (7%)	45,91,115	1.48	10 (22%)
7	BCL	W	403	-	58,74,74	1.12	3 (5%)	69,115,115	1.46	12 (17%)
10	LHG	C	301	-	33,33,48	0.73	1 (3%)	36,39,54	0.99	2 (5%)
7	BCL	V	407	-	58,74,74	1.13	3 (5%)	69,115,115	1.41	11 (15%)
7	BCL	a	806	-	58,74,74	1.17	3 (5%)	69,115,115	1.40	11 (15%)
11	LMG	A	819	-	39,39,55	0.83	0	47,47,63	1.13	5 (10%)
7	BCL	A	802	-	58,74,74	1.18	3 (5%)	69,115,115	1.53	12 (17%)

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
7	BCL	U	402	-	-	7/37/137/137	-
7	BCL	a	813	-	-	13/37/137/137	-
7	BCL	U	409	-	-	8/37/137/137	-
7	BCL	A	803	-	-	11/37/137/137	-
7	BCL	V	408[B]	5	-	2/13/113/137	-
7	BCL	W	406	-	-	9/37/137/137	-
9	F26	A	815	-	-	15/36/36/36	0/1/1/1
7	BCL	A	806	-	-	9/37/137/137	-
7	BCL	W	402	-	-	10/37/137/137	-
11	LMG	A	821	-	-	12/22/42/70	0/1/1/1
10	LHG	a	823	-	-	19/44/44/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	BCL	a	815	-	-	7/37/137/137	-
7	BCL	U	408[B]	5	-	4/13/113/137	-
14	SF4	a	803	1	-	-	0/6/5/5
10	LHG	A	816	-	-	12/30/30/53	-
7	BCL	A	811	-	-	7/37/137/137	-
13	G2O	a	805	-	3/3/15/22	23/39/115/115	-
7	BCL	a	808	-	-	7/37/137/137	-
7	BCL	a	809	-	-	11/37/137/137	-
7	BCL	a	812	-	-	12/37/137/137	-
9	F26	a	819	-	-	17/36/36/36	0/1/1/1
6	GS0	A	801	-	2/2/21/25	23/37/137/137	-
13	G2O	A	824	-	3/3/15/22	21/39/115/115	-
7	BCL	V	401	-	-	8/37/137/137	-
8	F39	a	818	-	-	25/58/78/78	0/2/2/2
7	BCL	A	804	-	-	8/37/137/137	-
7	BCL	U	401	-	-	7/37/137/137	-
13	G2O	a	801	-	4/4/15/22	24/39/115/115	-
7	BCL	A	807	-	-	3/37/137/137	-
7	BCL	A	813	-	-	15/36/136/137	-
14	SF4	B	301	2	-	-	0/6/5/5
7	BCL	a	816	-	-	12/37/137/137	-
7	BCL	a	811	1	-	7/13/113/137	-
7	BCL	V	405	-	-	7/37/137/137	-
7	BCL	A	810	-	-	8/37/137/137	-
7	BCL	U	407	-	-	4/37/137/137	-
10	LHG	A	817	-	-	19/45/45/53	-
11	LMG	a	824	-	-	15/35/55/70	0/1/1/1
7	BCL	a	810	-	-	11/37/137/137	-
11	LMG	C	302	-	-	16/30/50/70	0/1/1/1
7	BCL	U	404	-	-	8/37/137/137	-
7	BCL	a	814	-	-	11/37/137/137	-
7	BCL	A	808	-	-	10/37/137/137	-
7	BCL	V	404	-	-	10/37/137/137	-
7	BCL	a	807	-	-	8/37/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	BCL	A	805	-	-	16/37/137/137	-
11	LMG	A	820	-	-	14/31/51/70	0/1/1/1
11	LMG	A	818	-	-	20/37/57/70	0/1/1/1
8	F39	A	814	-	-	29/58/78/78	0/2/2/2
7	BCL	a	817	-	-	7/37/137/137	-
7	BCL	V	406	-	-	7/37/137/137	-
7	BCL	W	401	-	-	7/37/137/137	-
7	BCL	U	403	-	-	11/37/137/137	-
6	GS0	a	804	-	2/2/21/25	25/37/137/137	-
9	F26	a	820	-	-	26/36/36/36	0/1/1/1
7	BCL	V	403	-	-	10/37/137/137	-
7	BCL	U	405	5	-	8/37/137/137	-
10	LHG	a	822	-	-	17/30/30/53	-
14	SF4	B	302	2	-	-	0/6/5/5
10	LHG	a	821	-	-	15/37/37/53	-
11	LMG	A	822	-	-	11/24/44/70	0/1/1/1
7	BCL	W	404	5	-	10/37/137/137	-
7	BCL	W	405	-	-	9/37/137/137	-
13	G2O	a	802	-	3/3/15/22	17/39/115/115	-
7	BCL	U	406	-	-	5/37/137/137	-
7	BCL	A	812	-	-	12/37/137/137	-
7	BCL	A	809	-	-	10/37/137/137	-
7	BCL	V	402	-	-	3/37/137/137	-
7	BCL	W	407[B]	5	-	4/13/113/137	-
7	BCL	W	403	-	-	6/37/137/137	-
10	LHG	C	301	-	-	19/38/38/53	-
7	BCL	V	407	-	-	7/37/137/137	-
7	BCL	a	806	-	-	16/37/137/137	-
11	LMG	A	819	-	-	19/34/54/70	0/1/1/1
7	BCL	A	802	-	-	10/37/137/137	-

The worst 5 of 420 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	824	G2O	MG-NA	14.77	2.41	2.06
13	a	805	G2O	MG-NA	12.75	2.36	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	a	801	G2O	MG-NC	12.01	2.34	2.06
13	A	824	G2O	C1D-ND	11.50	1.45	1.35
13	a	802	G2O	MG-NC	11.41	2.33	2.06

The worst 5 of 791 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	a	801	G2O	C1A-NA-C4A	20.39	115.87	106.71
13	a	802	G2O	C1A-NA-C4A	19.69	115.56	106.71
13	a	805	G2O	C1A-NA-C4A	17.74	114.68	106.71
13	A	824	G2O	C1A-NA-C4A	17.57	114.60	106.71
6	A	801	GS0	C4A-NA-C1A	12.63	112.38	106.71

5 of 17 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	A	801	GS0	CBD
6	A	801	GS0	C13
6	a	804	GS0	CBD
6	a	804	GS0	C3C
13	A	824	G2O	CBD

5 of 865 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	801	GS0	C1-C2-C3-C4
6	A	801	GS0	C1A-C2A-CAA-CBA
6	A	801	GS0	C3A-C2A-CAA-CBA
6	A	801	GS0	C4-C3-C5-C6
6	A	801	GS0	C2C-C3C-CAC-CBC

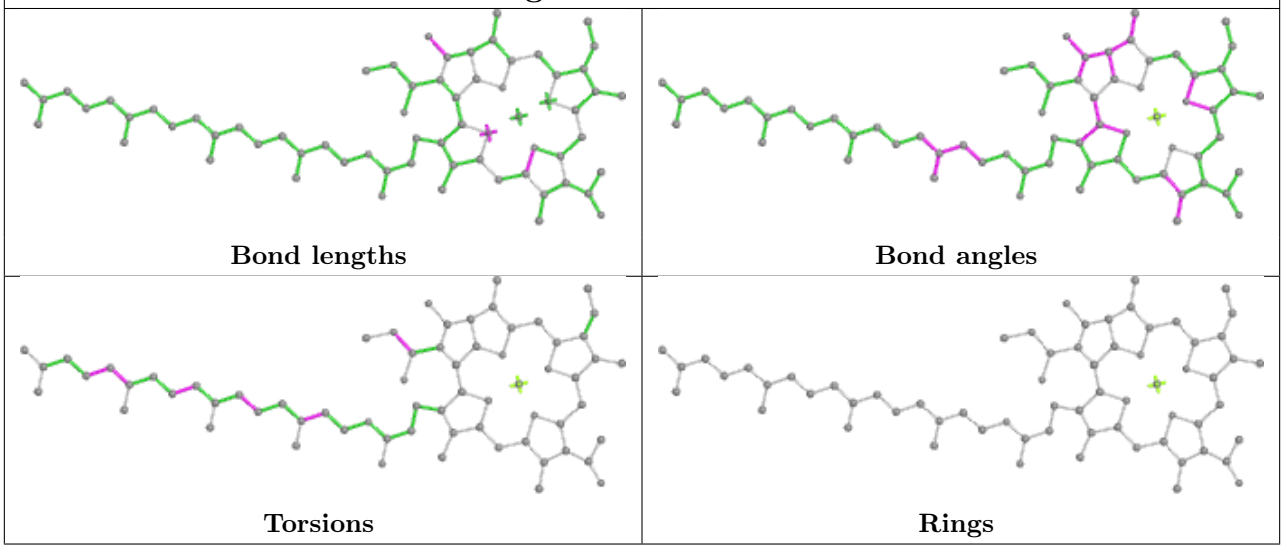
There are no ring outliers.

No monomer is involved in short contacts.

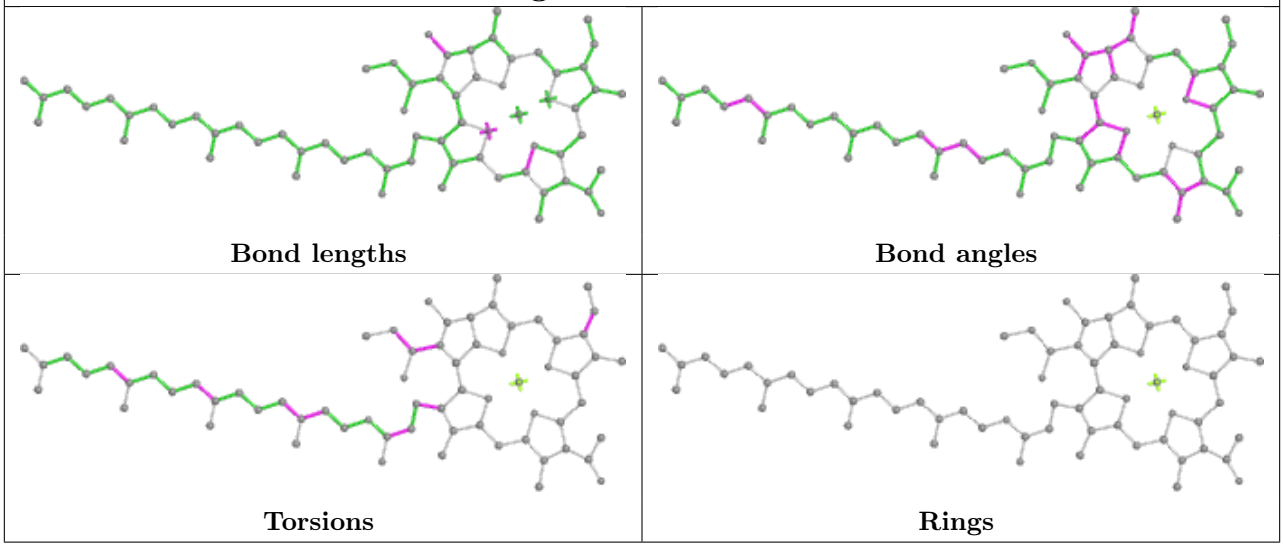
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

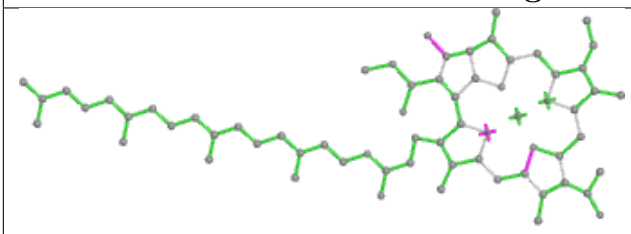
Ligand BCL U 402



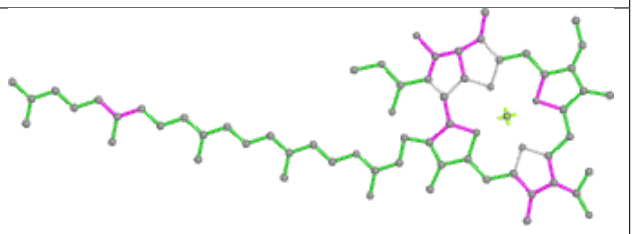
Ligand BCL a 813



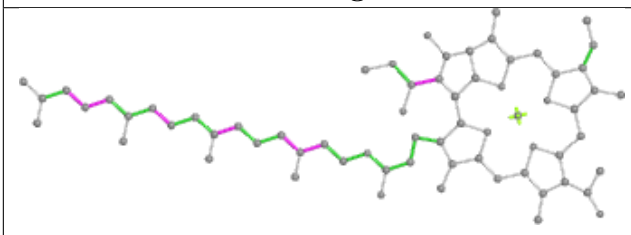
Ligand BCL U 409



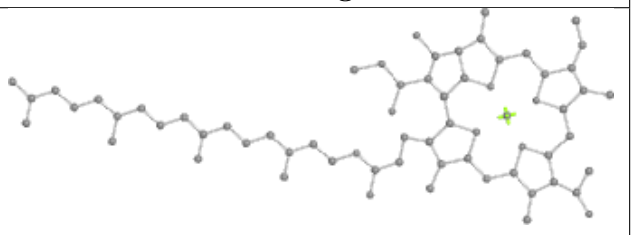
Bond lengths



Bond angles

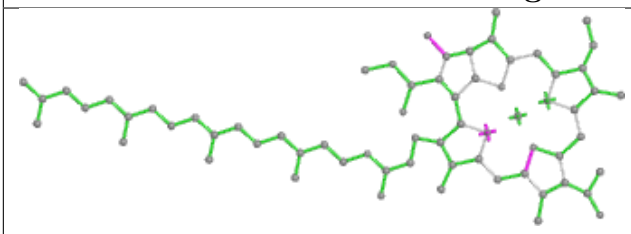


Torsions

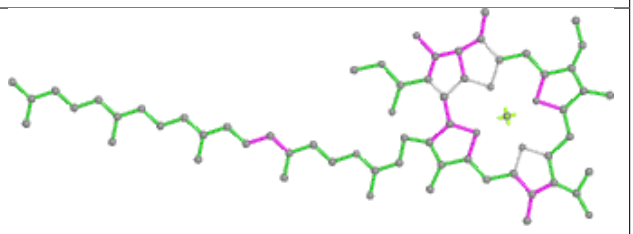


Rings

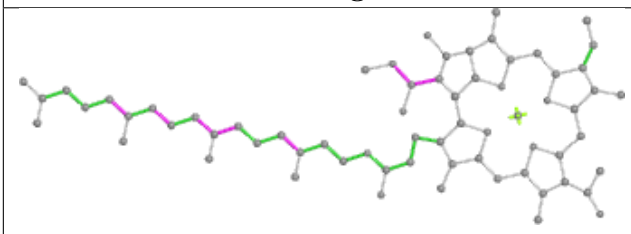
Ligand BCL A 803



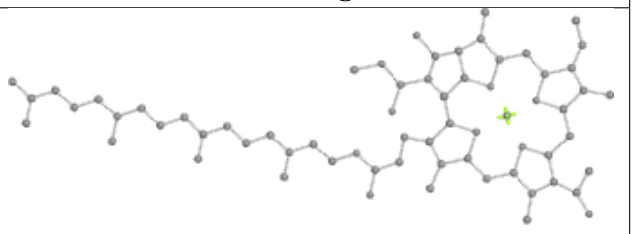
Bond lengths



Bond angles

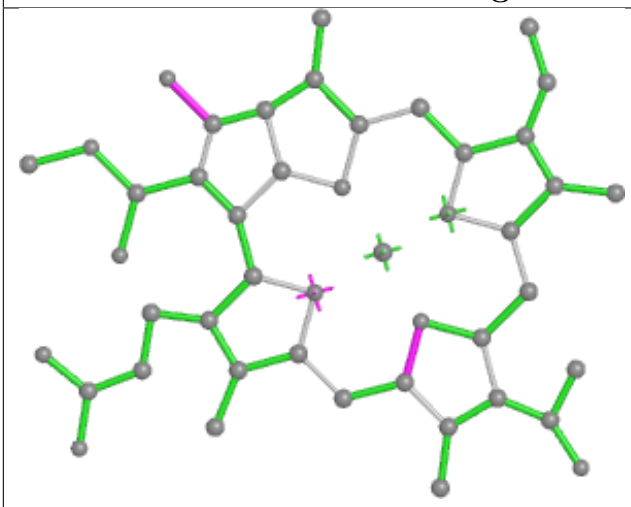


Torsions

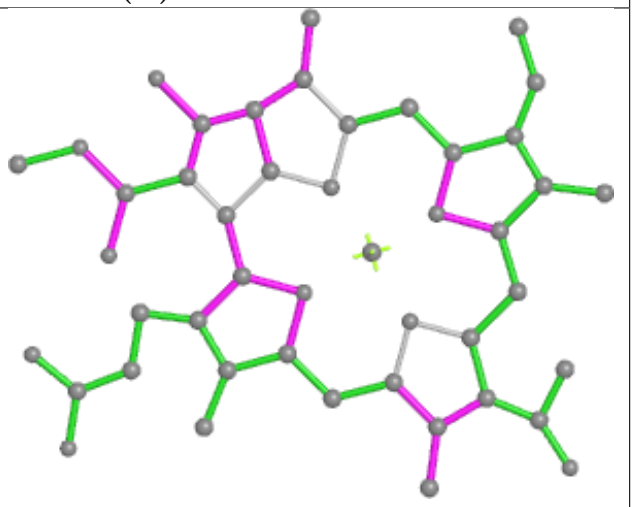


Rings

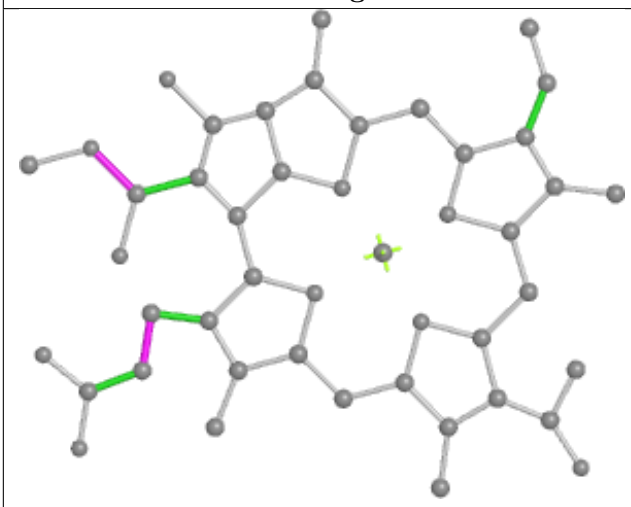
Ligand BCL V 408 (B)



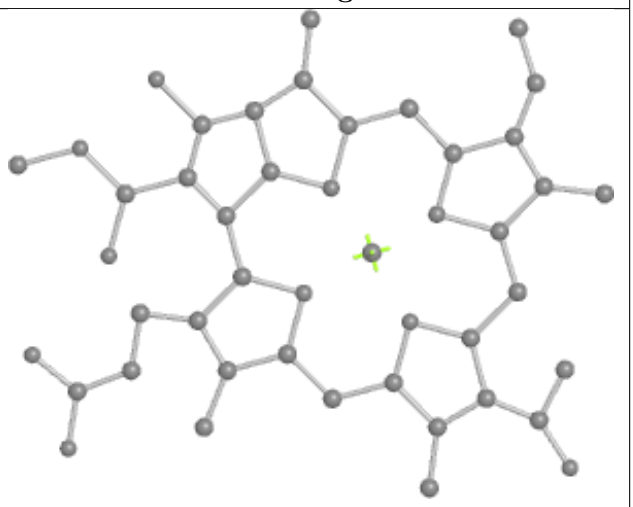
Bond lengths



Bond angles

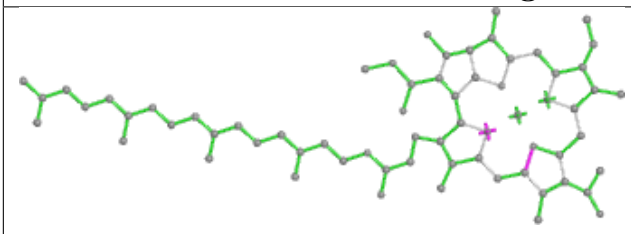


Torsions

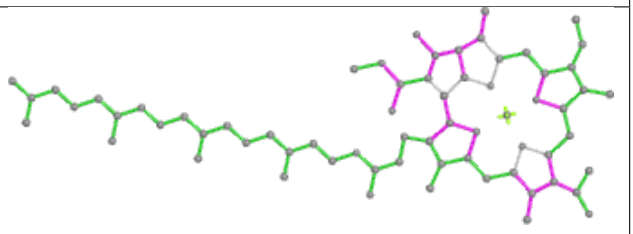


Rings

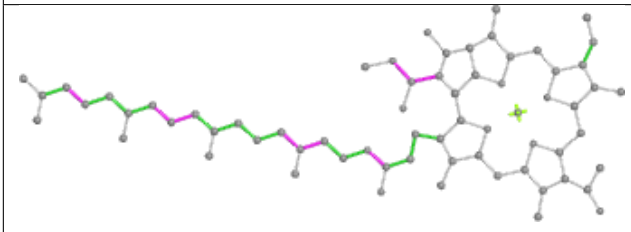
Ligand BCL W 406



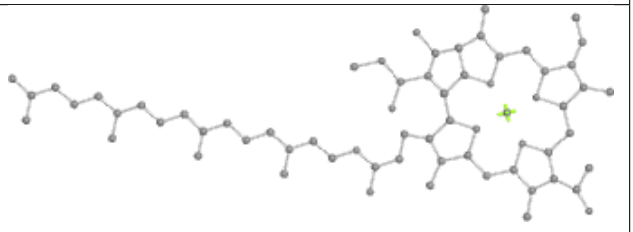
Bond lengths



Bond angles

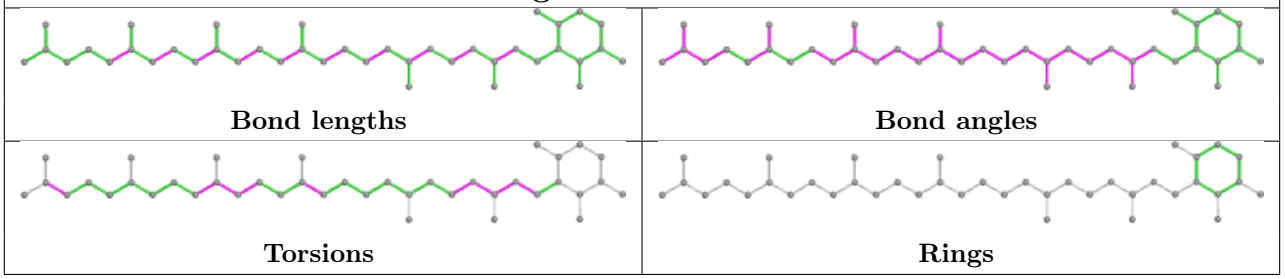


Torsions

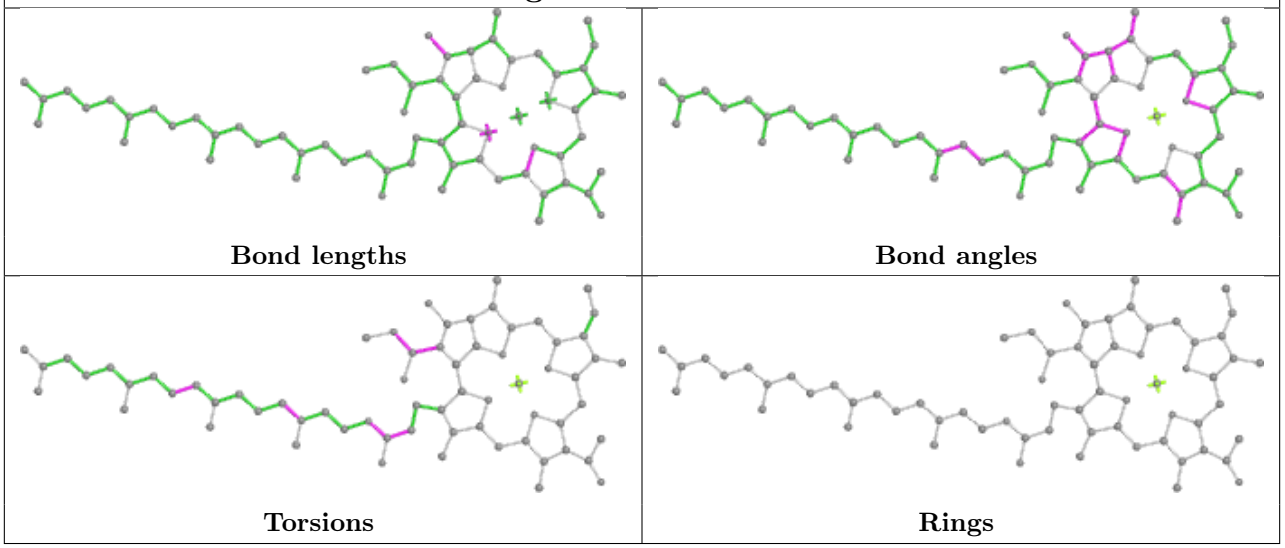


Rings

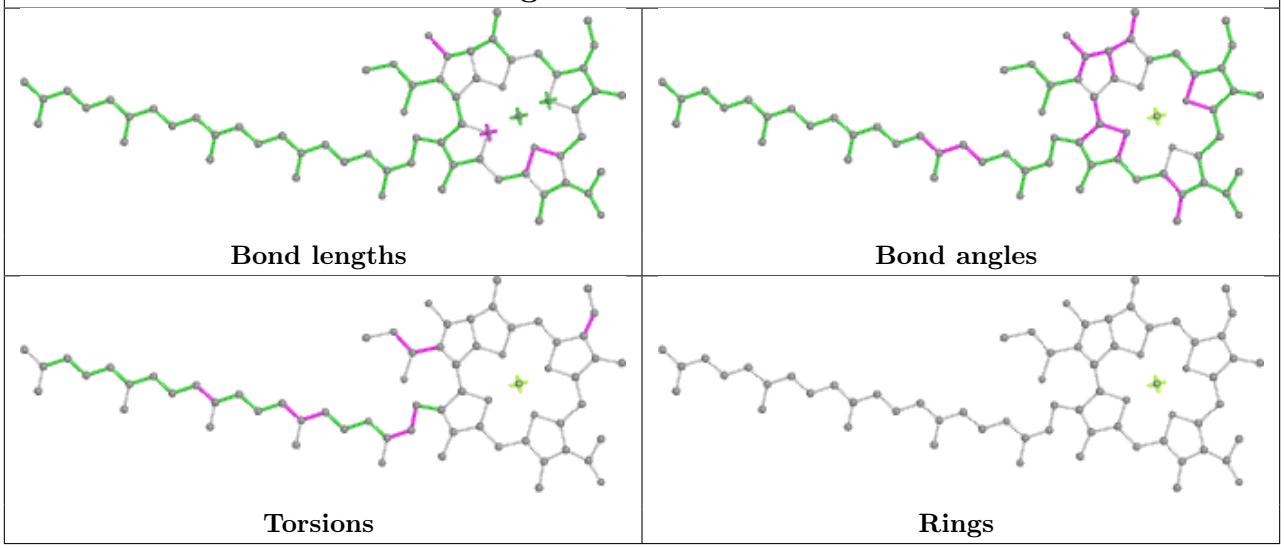
Ligand F26 A 815



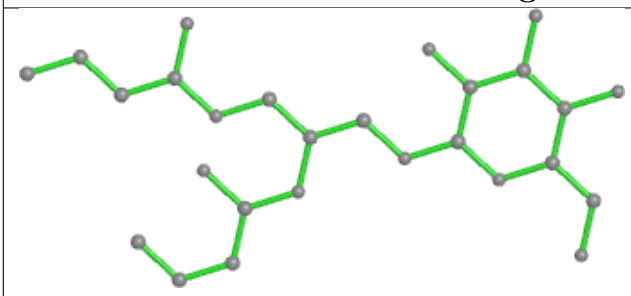
Ligand BCL A 806



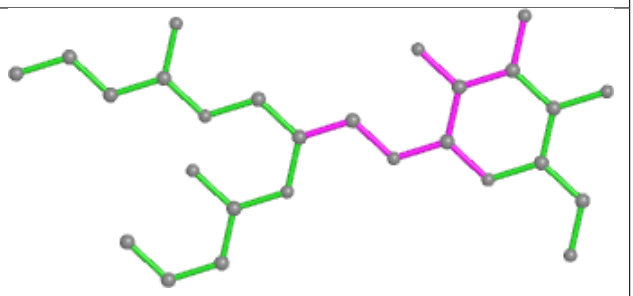
Ligand BCL W 402



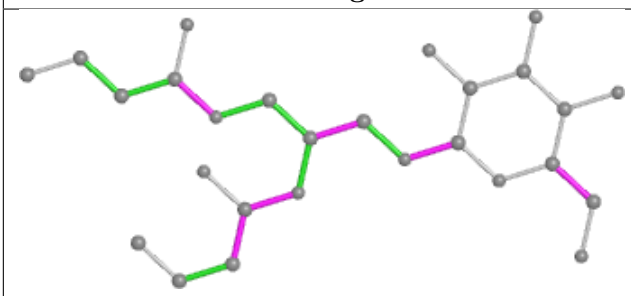
Ligand LMG A 821



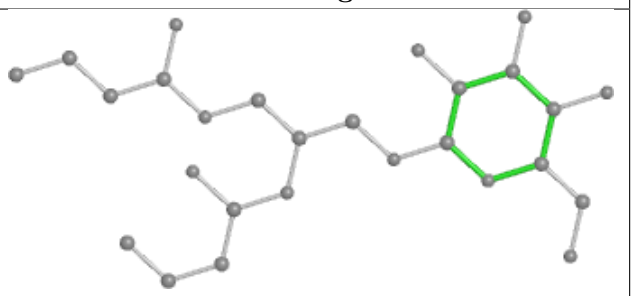
Bond lengths



Bond angles

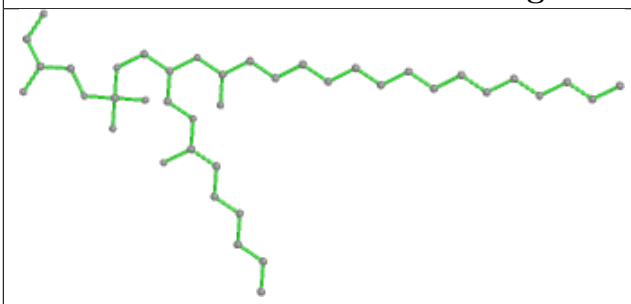


Torsions

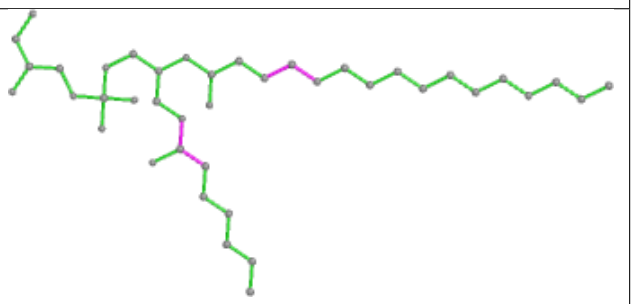


Rings

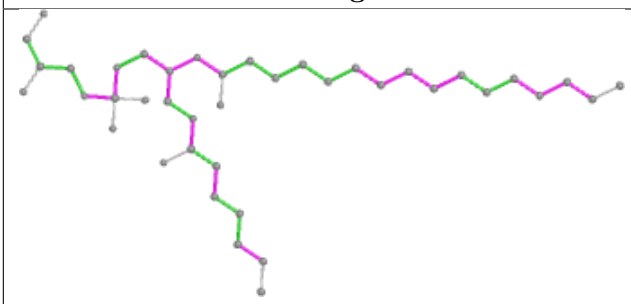
Ligand LHG a 823



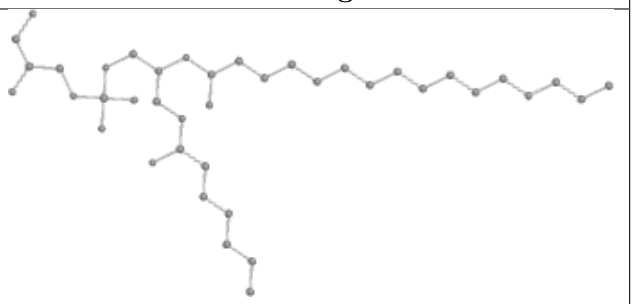
Bond lengths



Bond angles

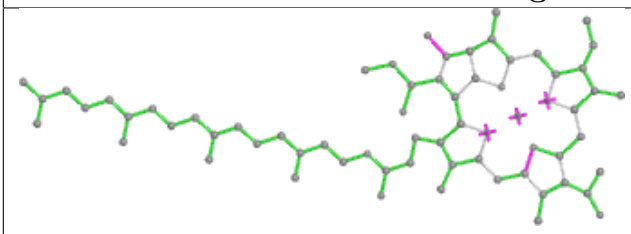


Torsions

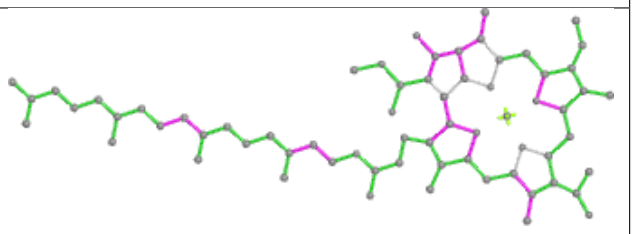


Rings

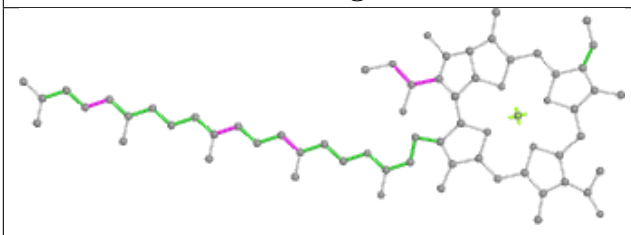
Ligand BCL a 815



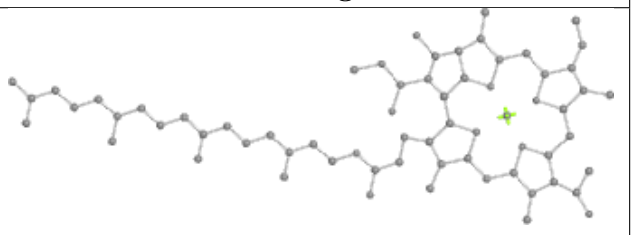
Bond lengths



Bond angles

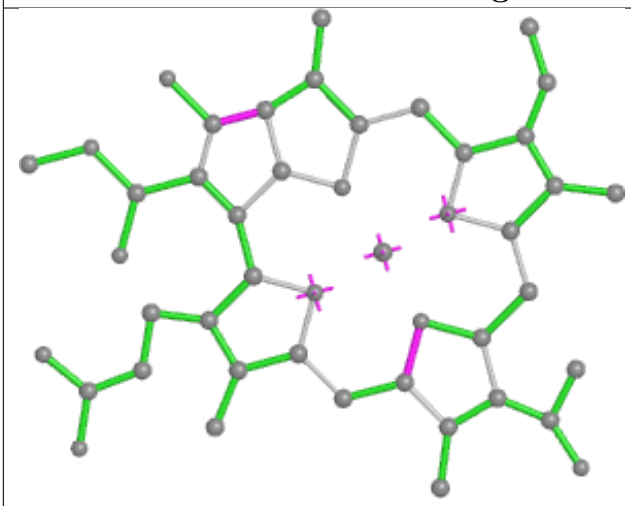


Torsions

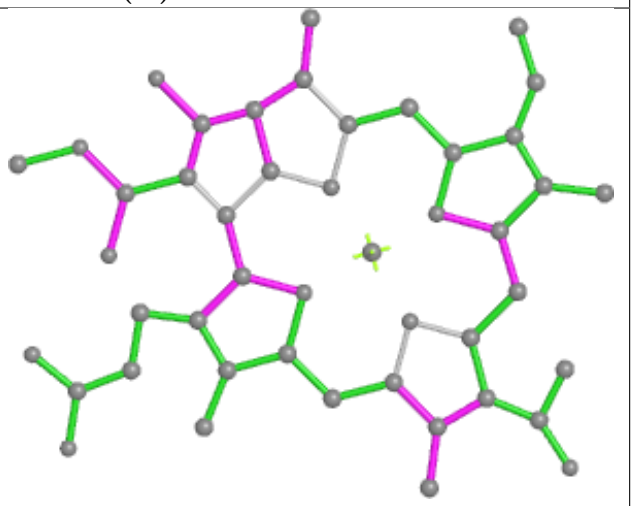


Rings

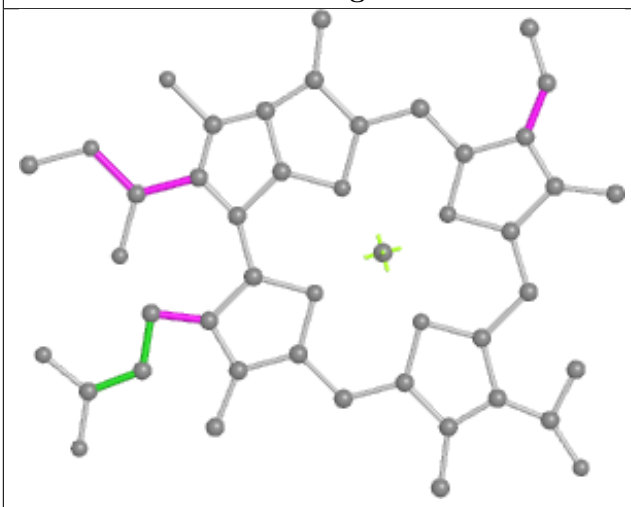
Ligand BCL U 408 (B)



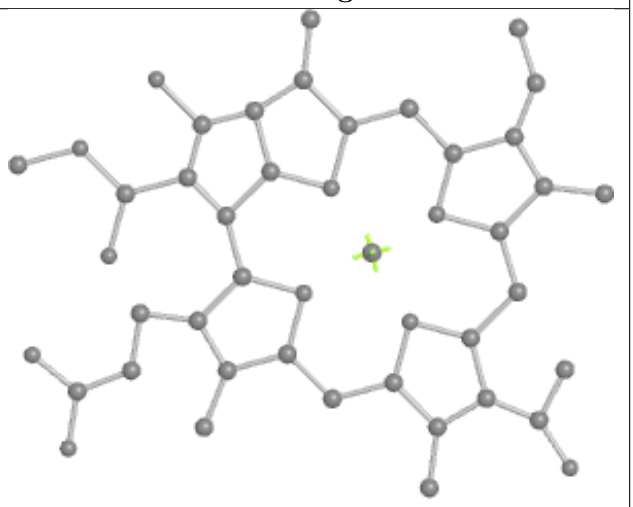
Bond lengths



Bond angles

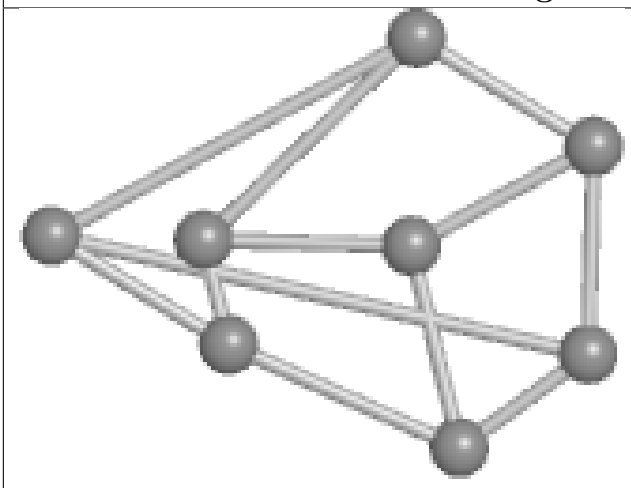


Torsions

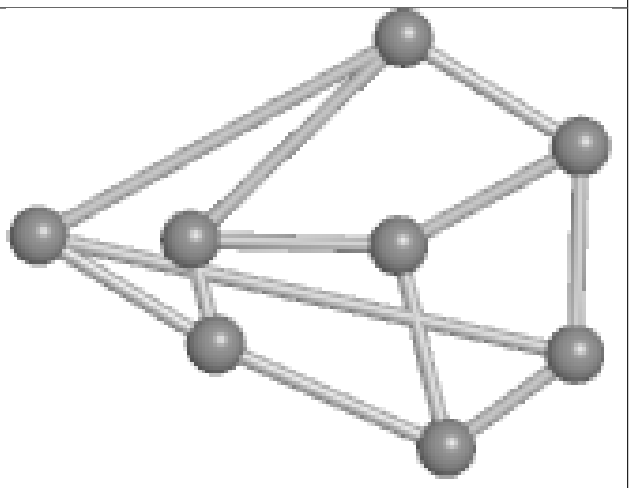


Rings

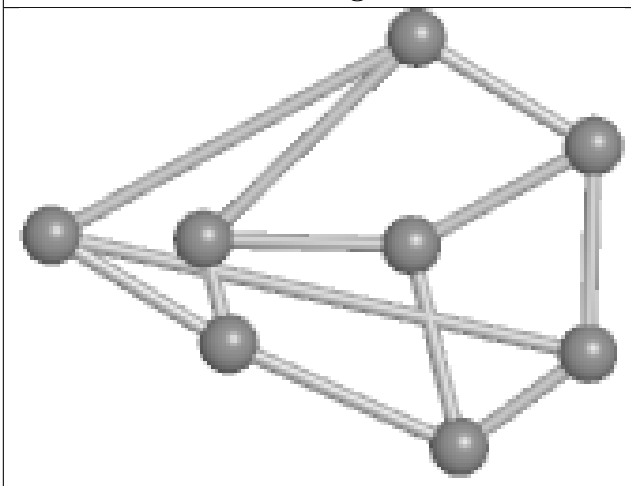
Ligand SF4 a 803



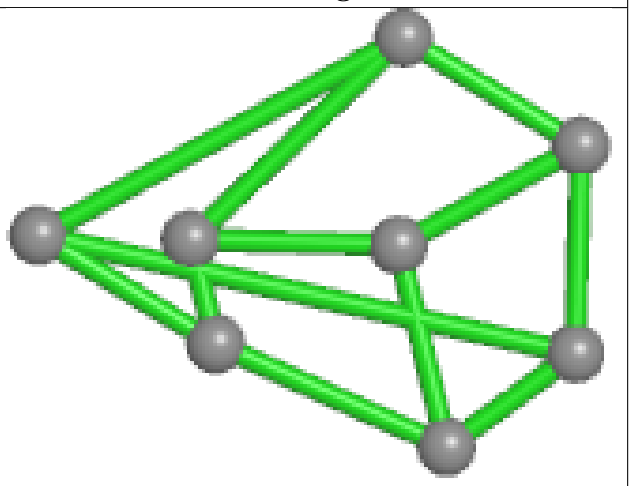
Bond lengths



Bond angles

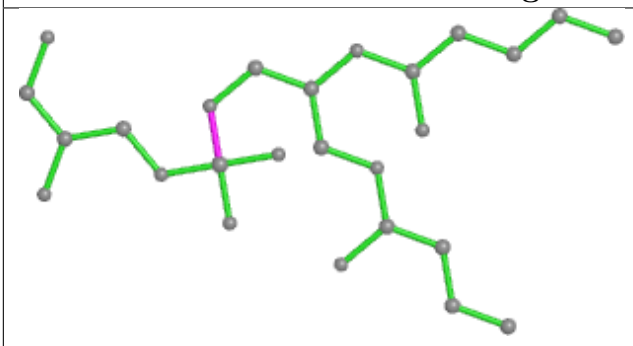


Torsions

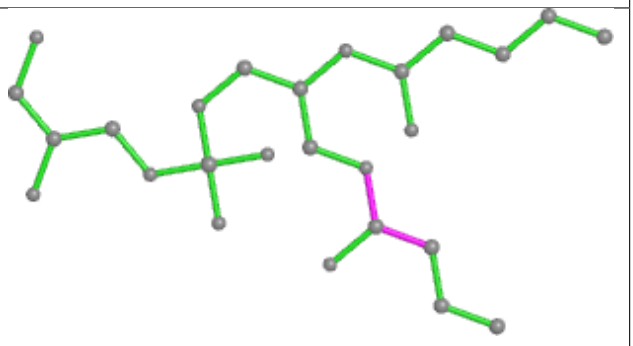


Rings

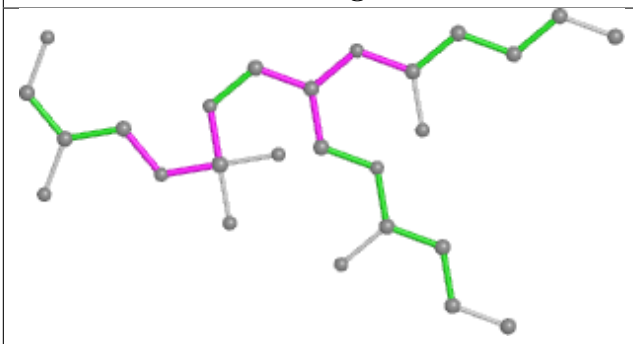
Ligand LHG A 816



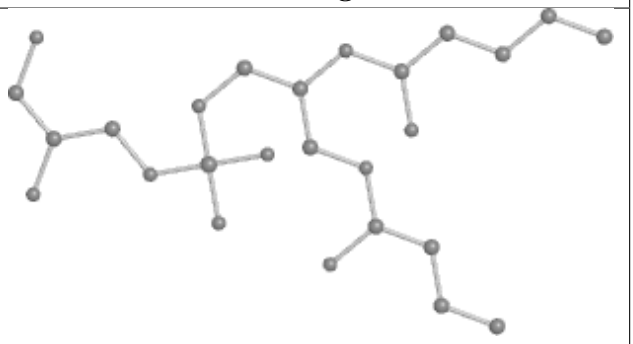
Bond lengths



Bond angles

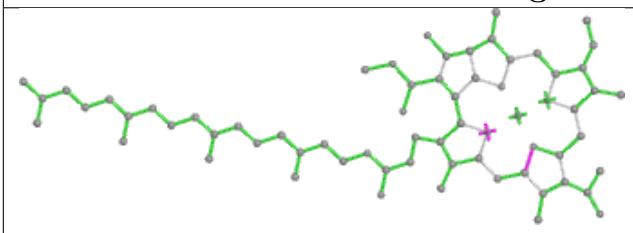


Torsions

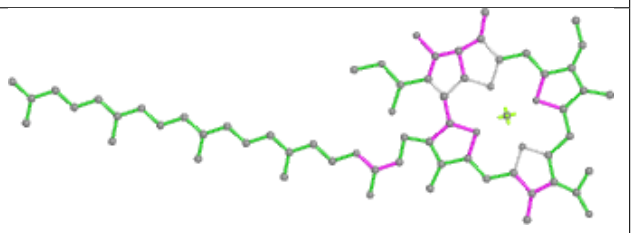


Rings

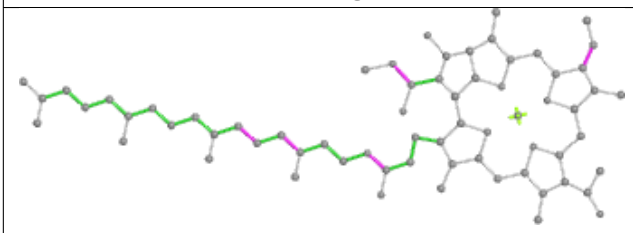
Ligand BCL a 808



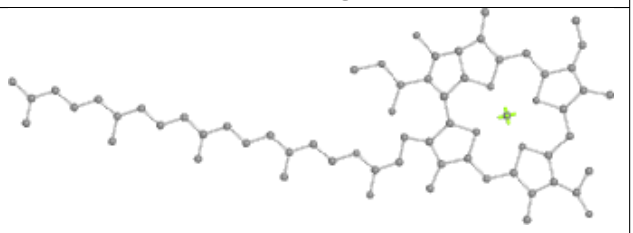
Bond lengths



Bond angles

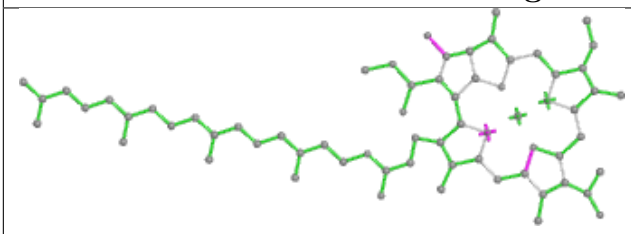


Torsions

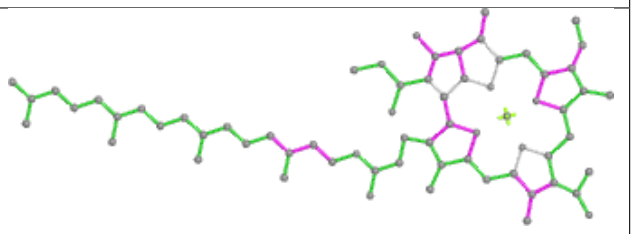


Rings

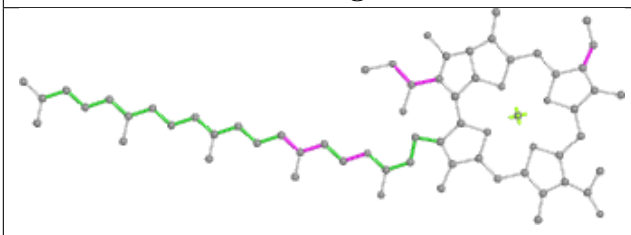
Ligand BCL A 811



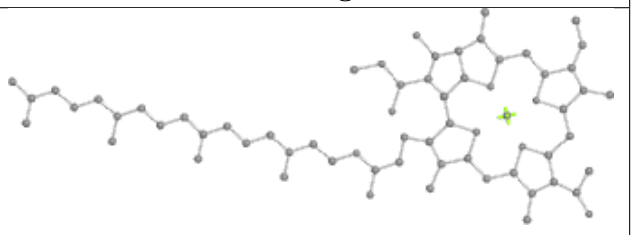
Bond lengths



Bond angles

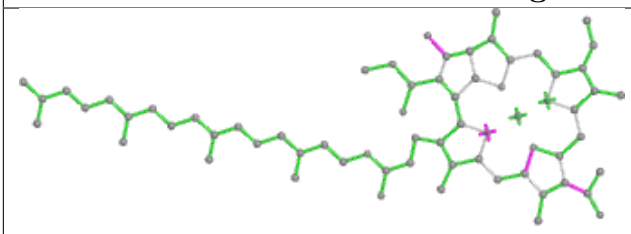


Torsions

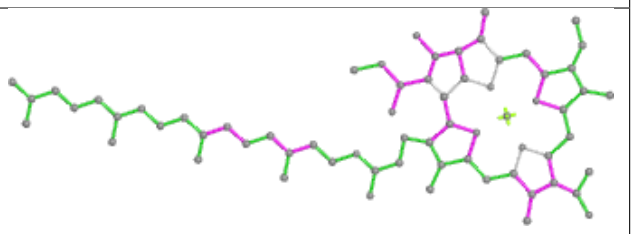


Rings

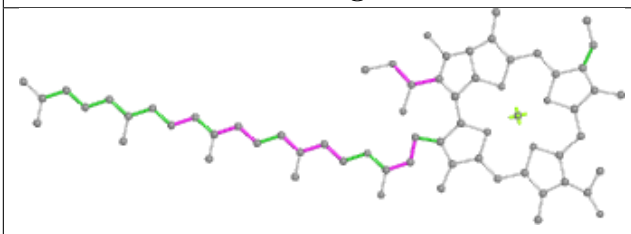
Ligand BCL a 809



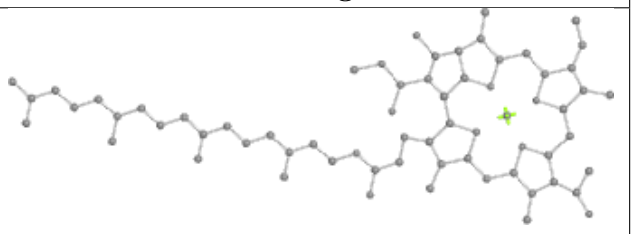
Bond lengths



Bond angles

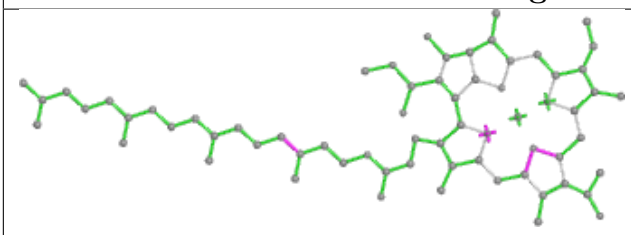


Torsions

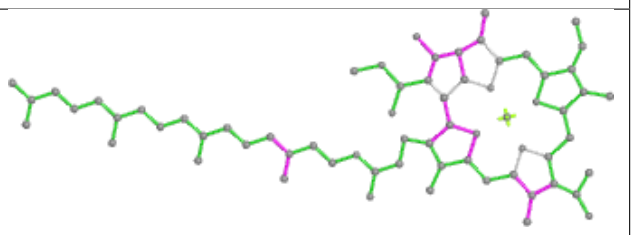


Rings

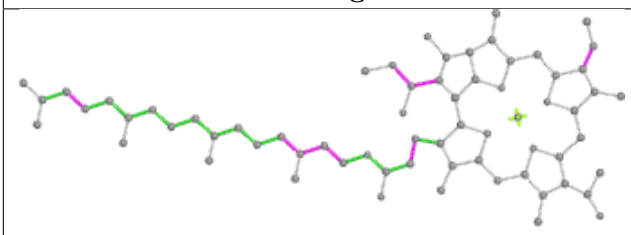
Ligand BCL a 812



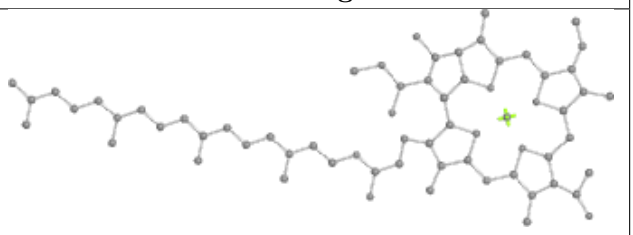
Bond lengths



Bond angles

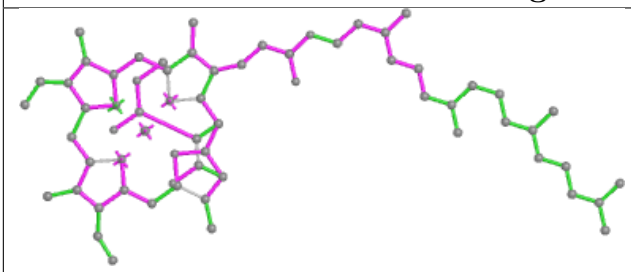


Torsions

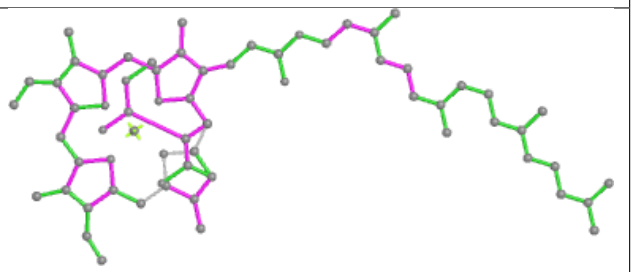


Rings

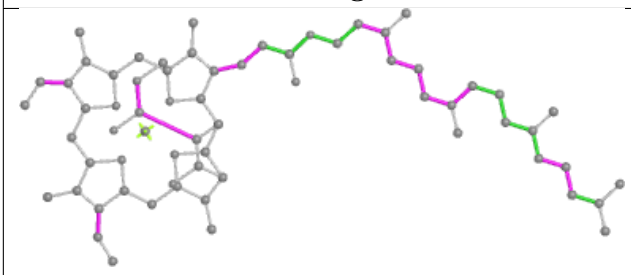
Ligand G2O a 805



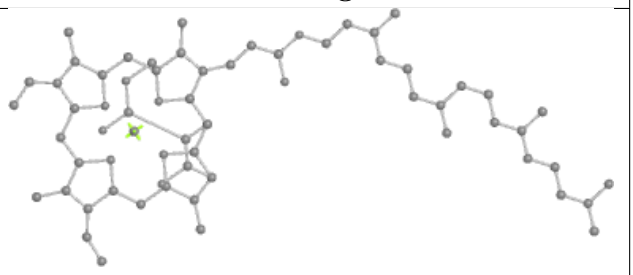
Bond lengths



Bond angles

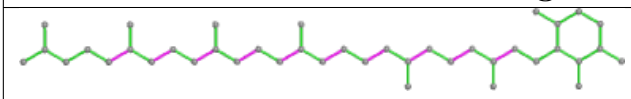


Torsions

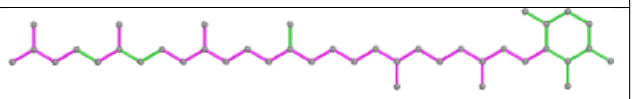


Rings

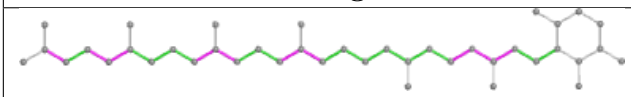
Ligand F26 a 819



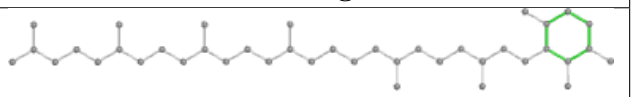
Bond lengths



Bond angles

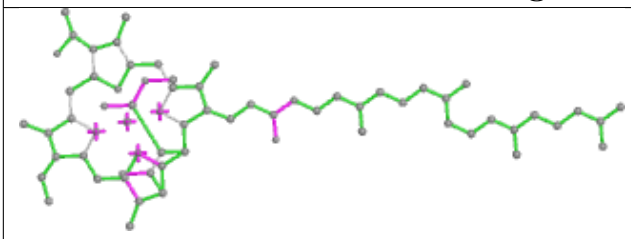


Torsions



Rings

Ligand GS0 A 801



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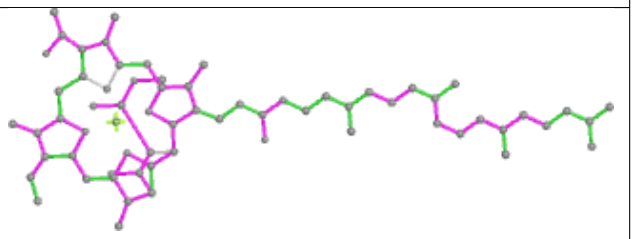
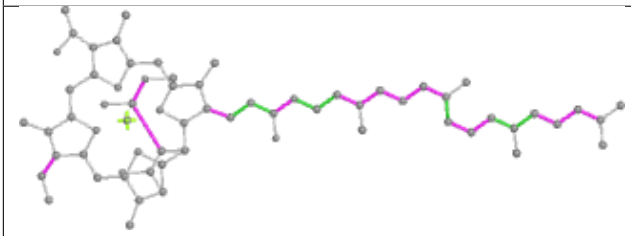


Bond angles



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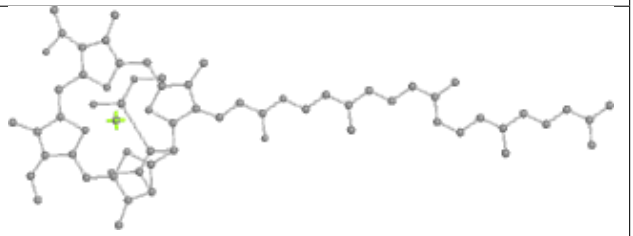
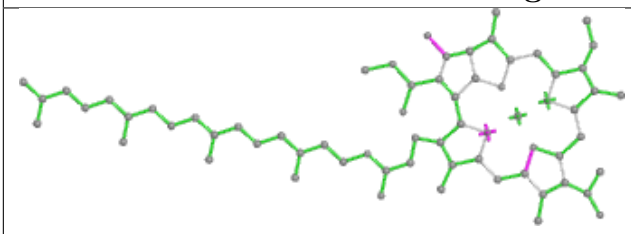


Rings

Ligand BCL V 401



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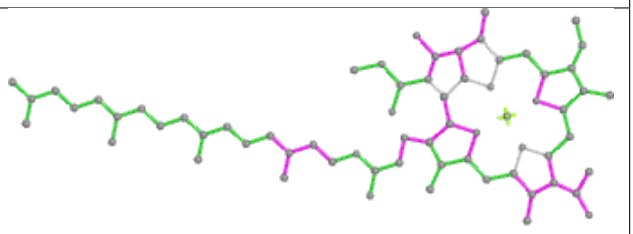
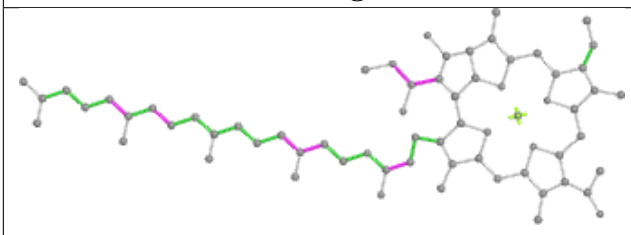
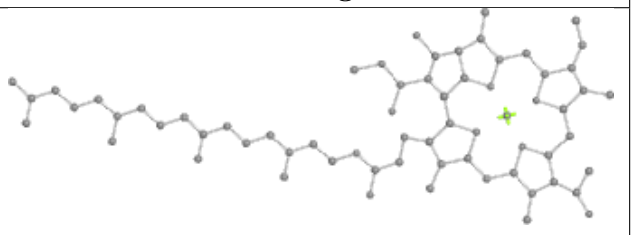


Bond angles

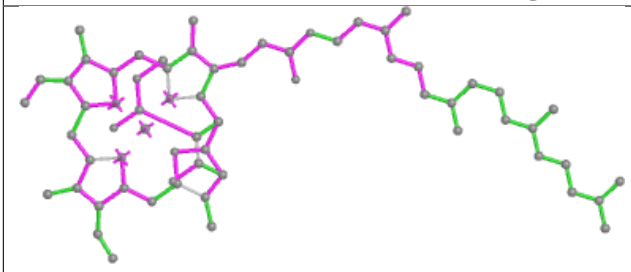


Torsions



Rings

Ligand G2O A 824



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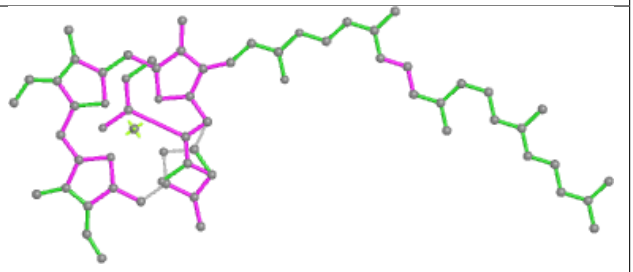
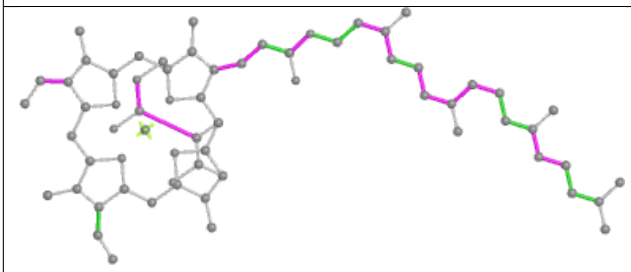
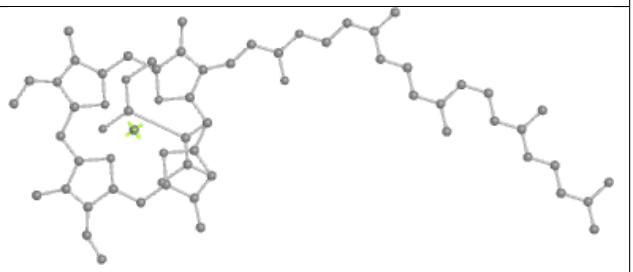


Bond angles

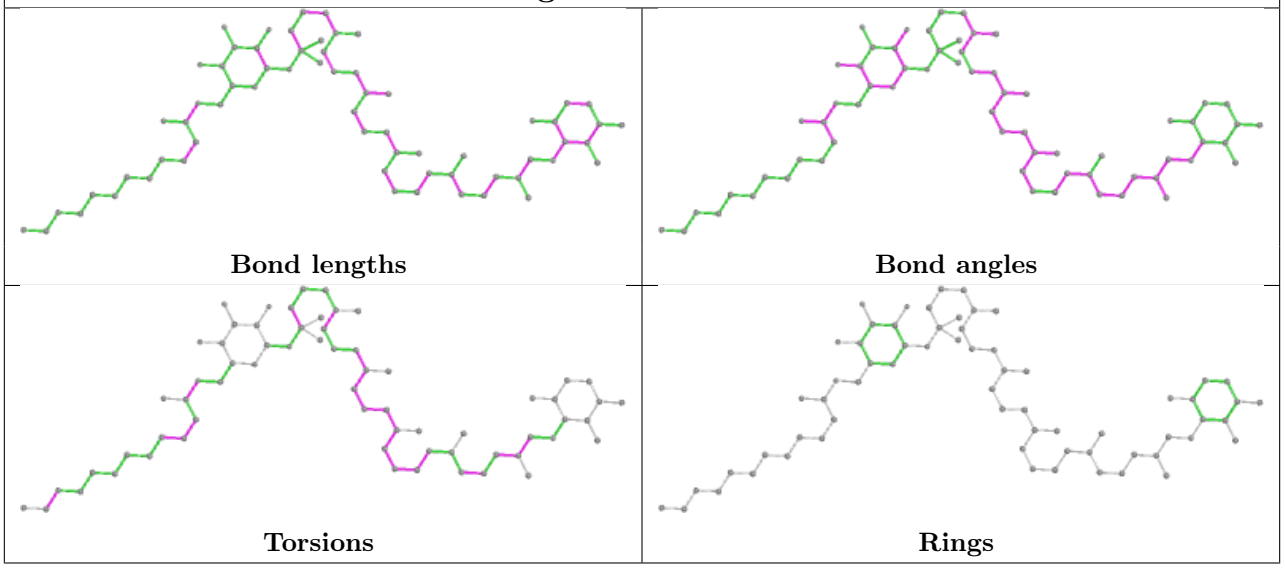


Torsions

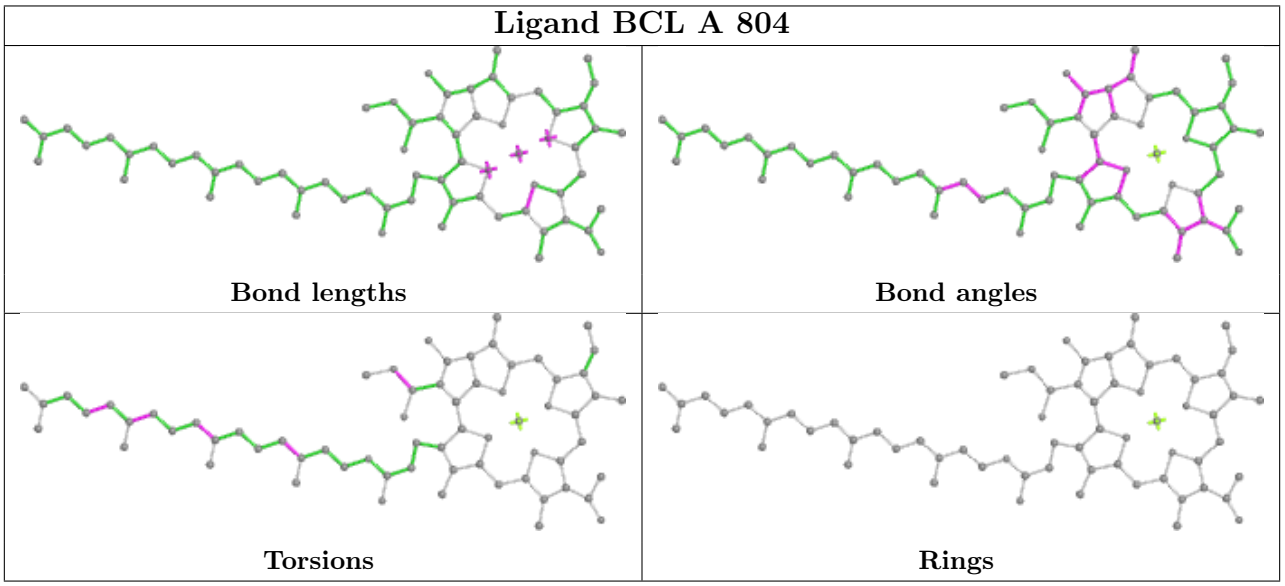


Rings

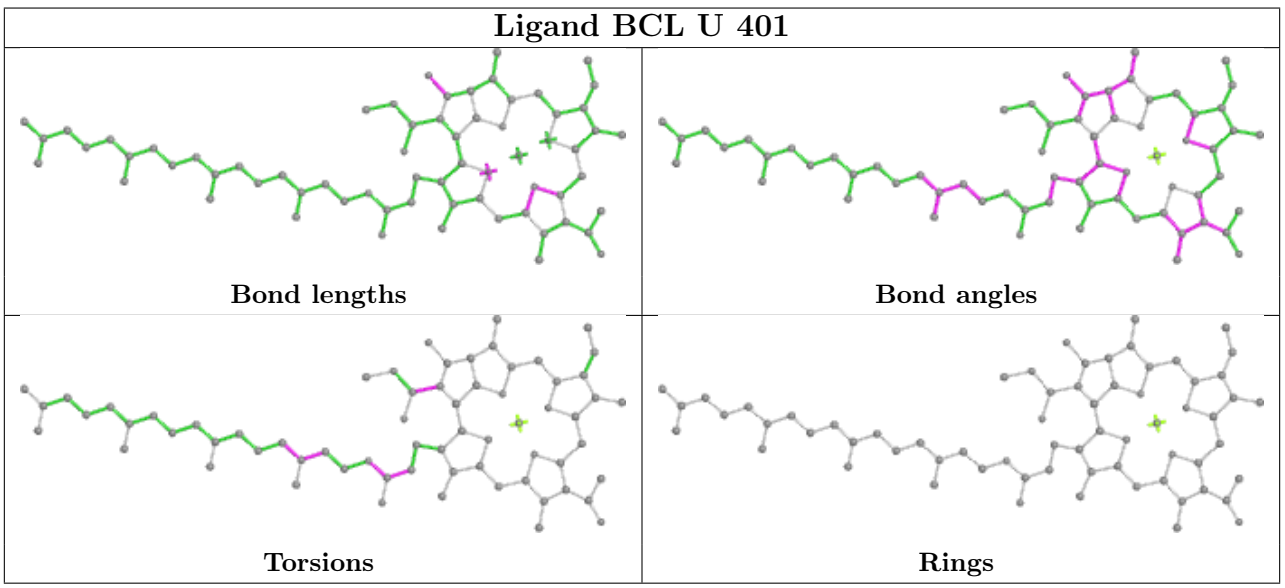
Ligand F39 a 818



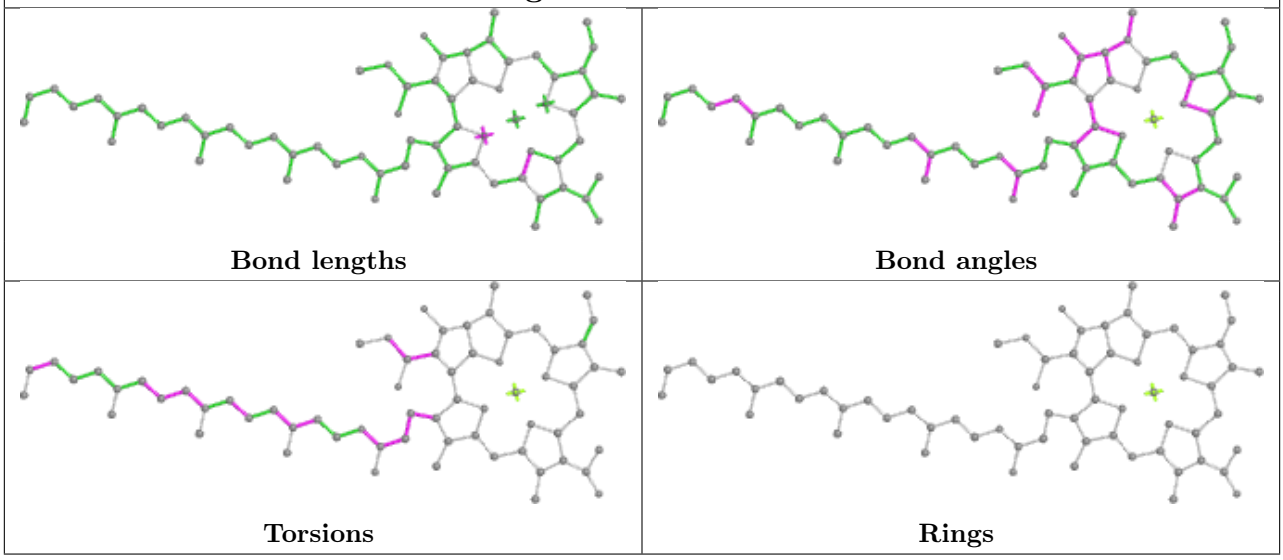
Ligand BCL A 804



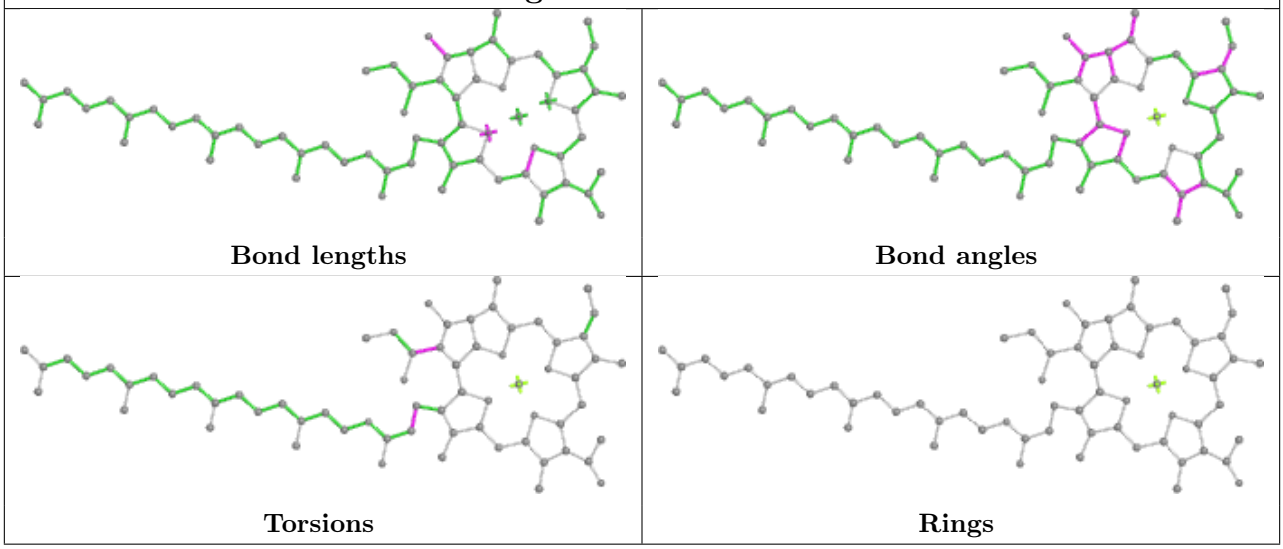
Ligand BCL U 401



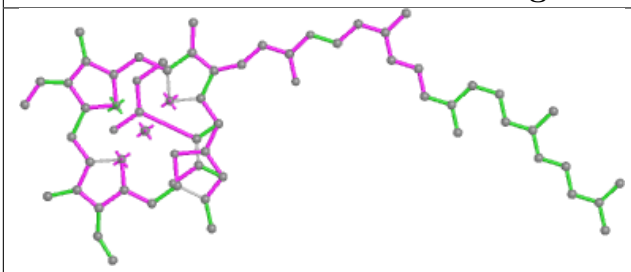
Ligand BCL A 813



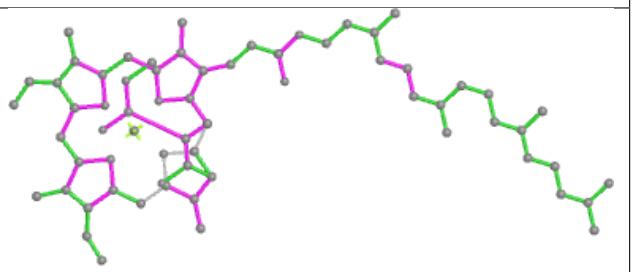
Ligand BCL A 807



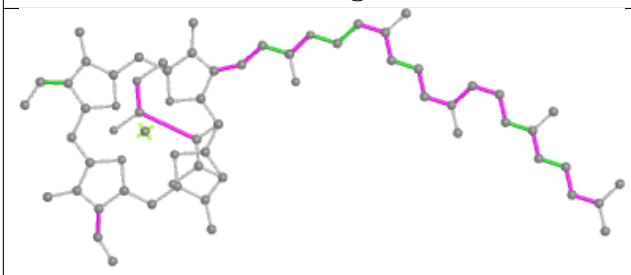
Ligand G2O a 801



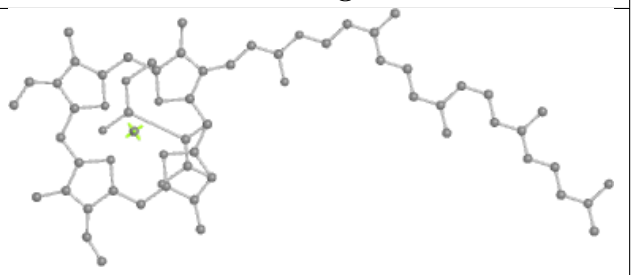
Bond lengths



Bond angles

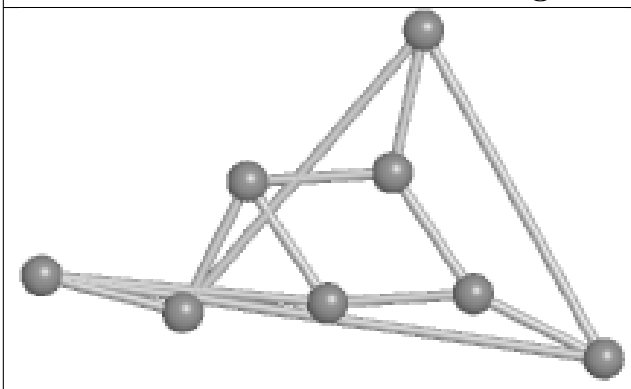


Torsions

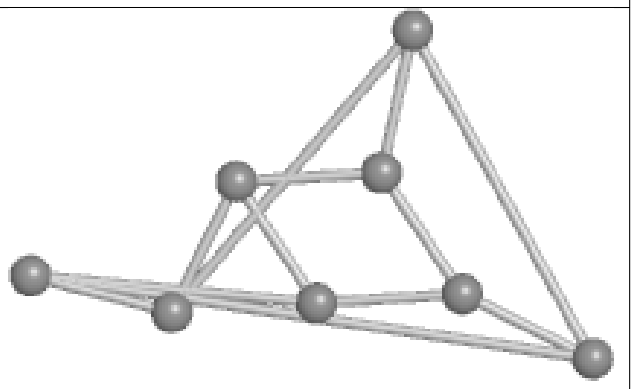


Rings

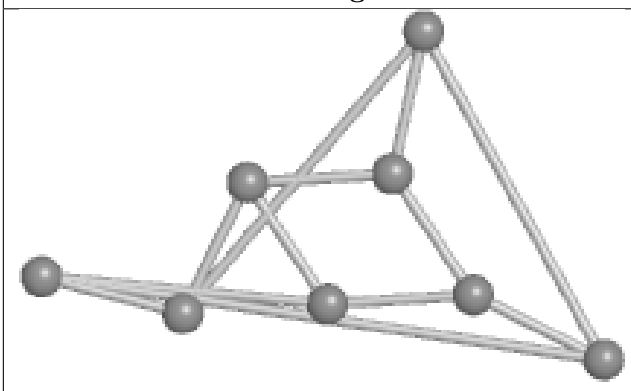
Ligand SF4 B 301



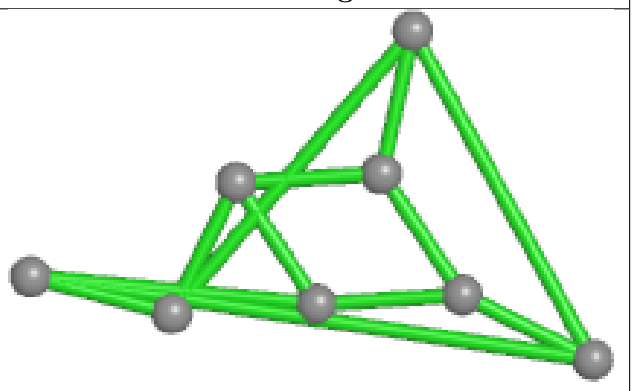
Bond lengths



Bond angles

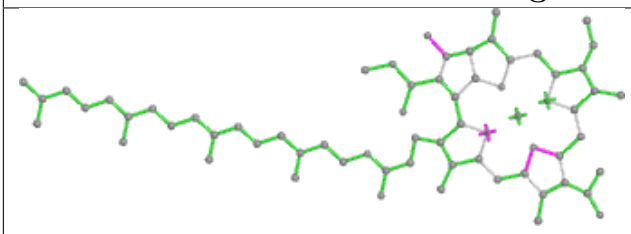


Torsions

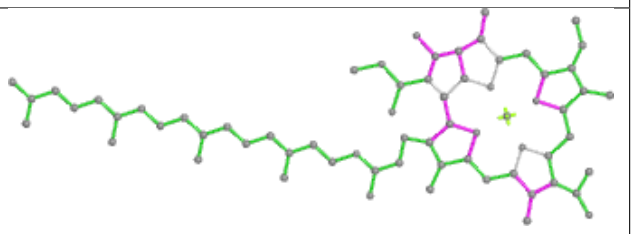


Rings

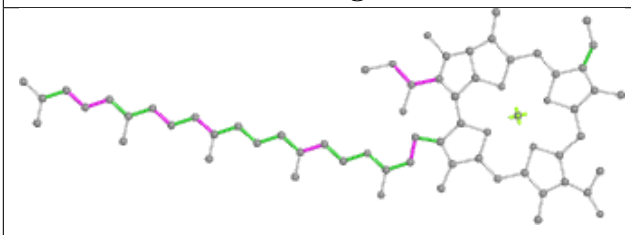
Ligand BCL a 816



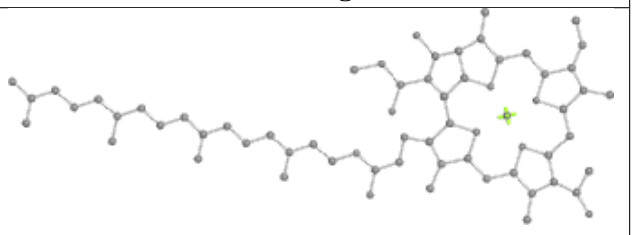
Bond lengths



Bond angles

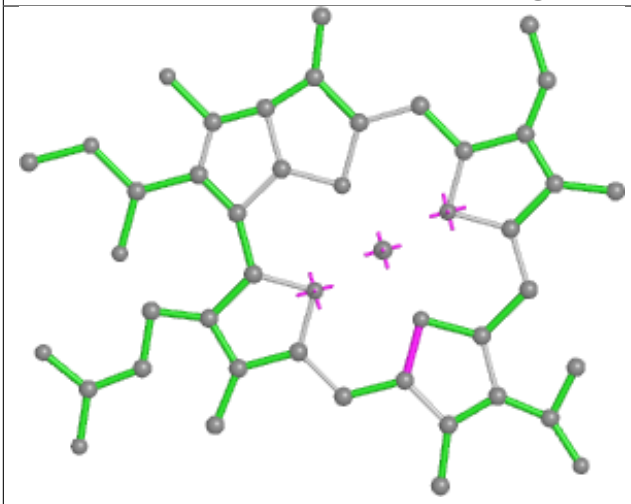


Torsions

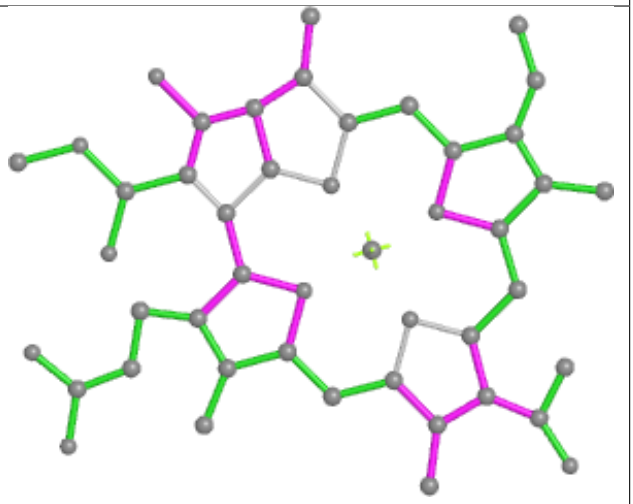


Rings

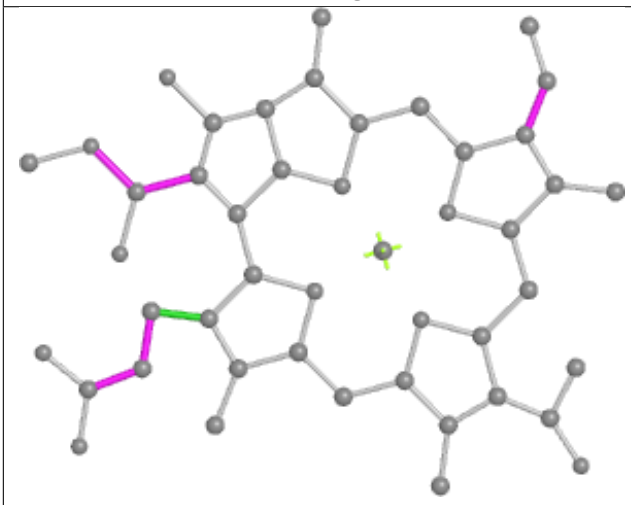
Ligand BCL a 811



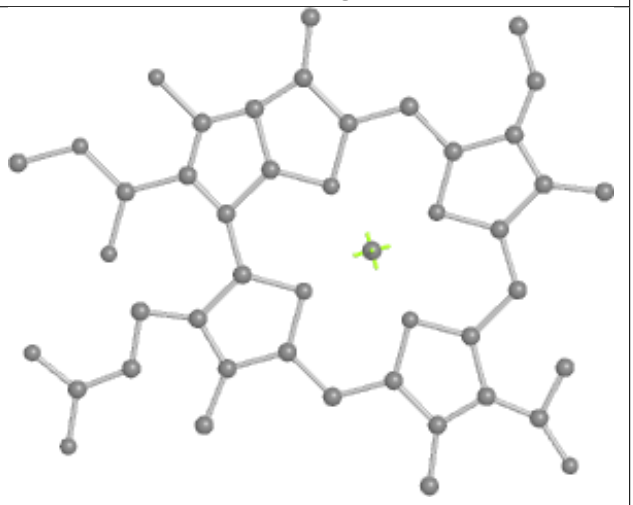
Bond lengths



Bond angles

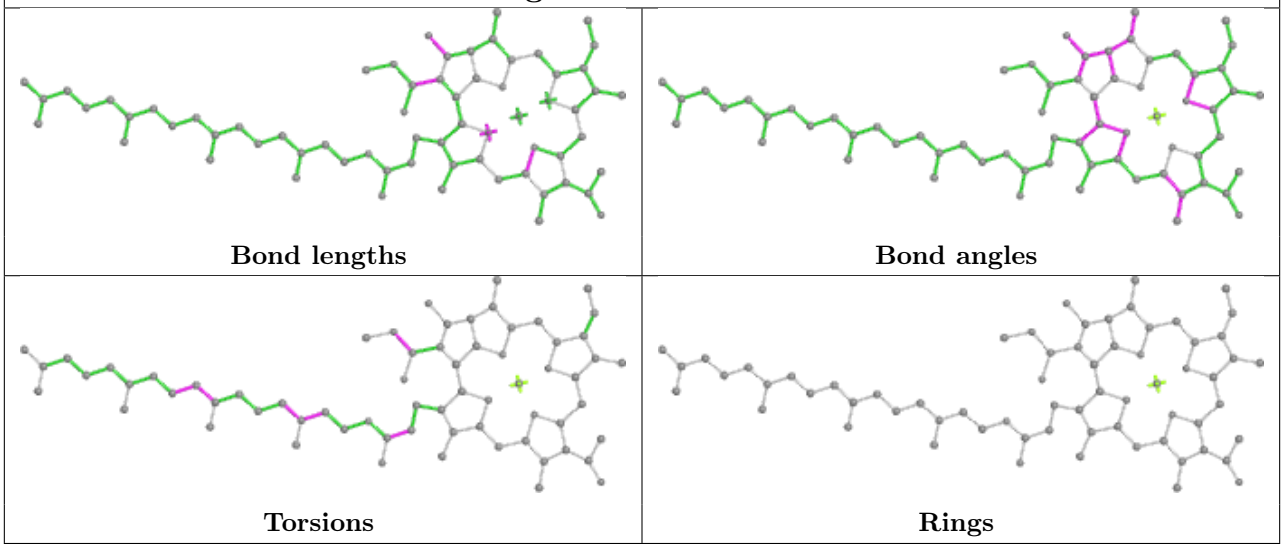


Torsions

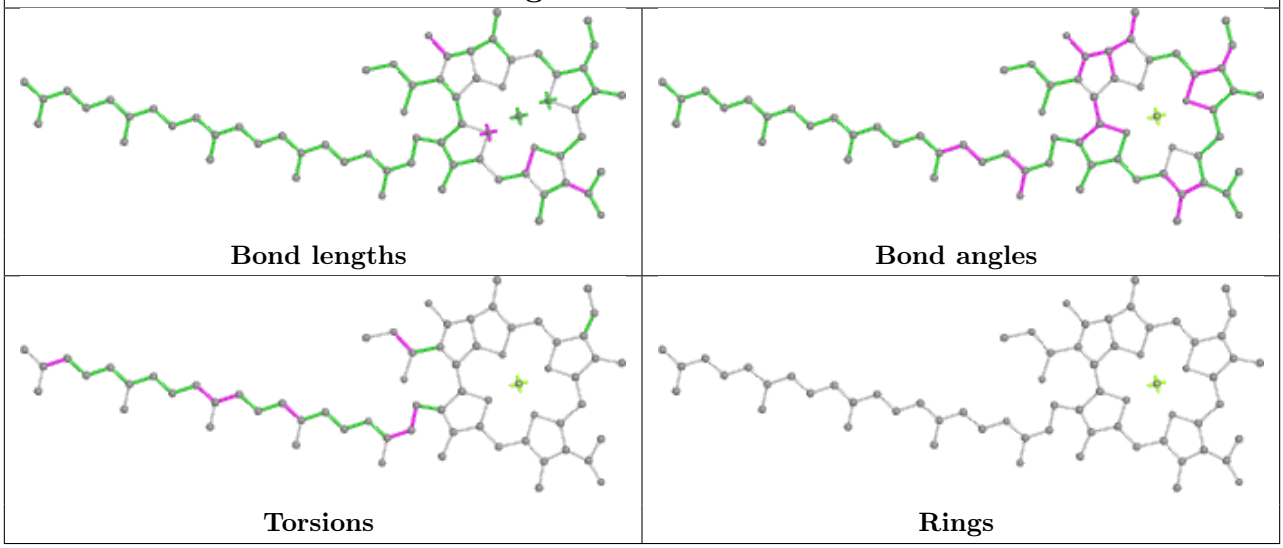


Rings

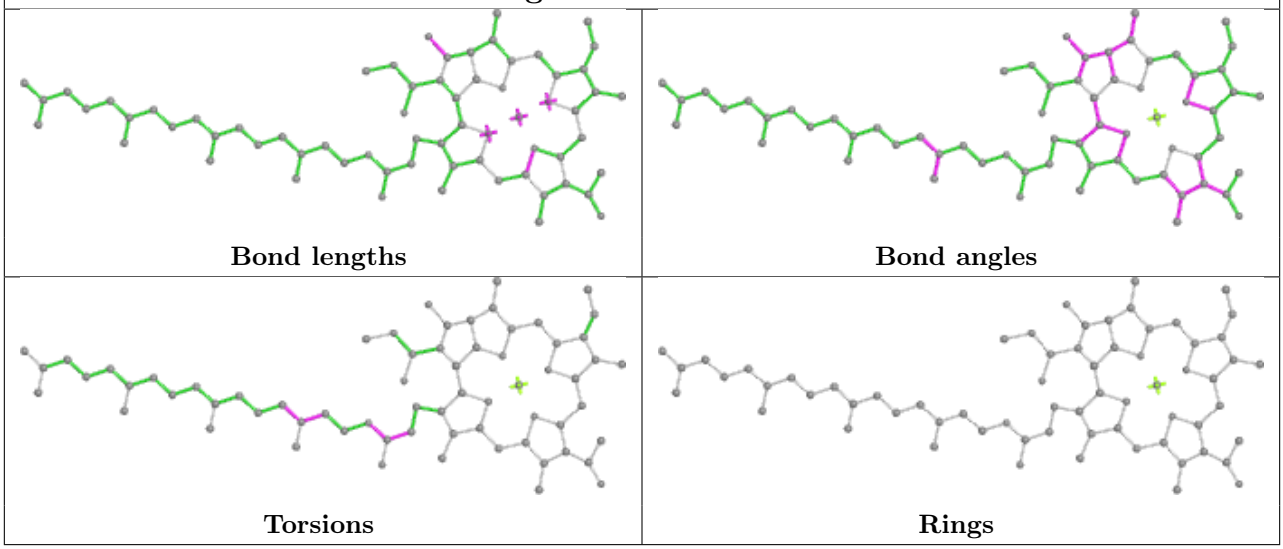
Ligand BCL V 405



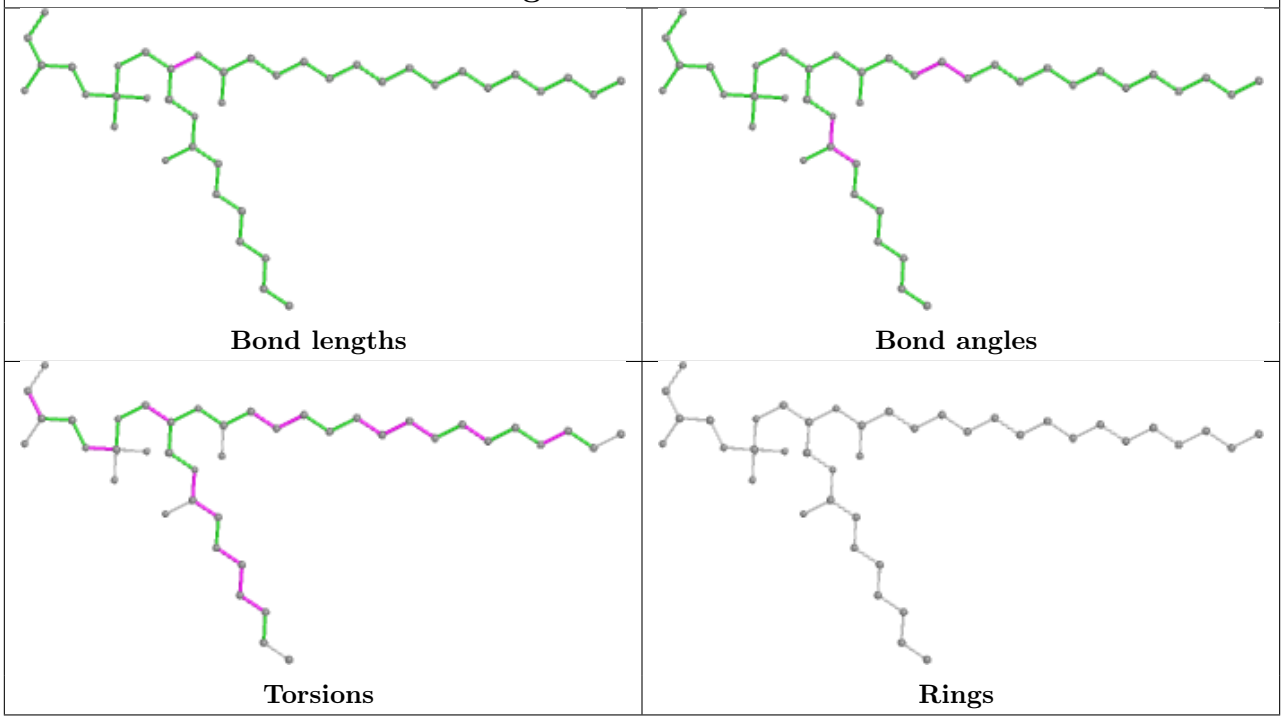
Ligand BCL A 810



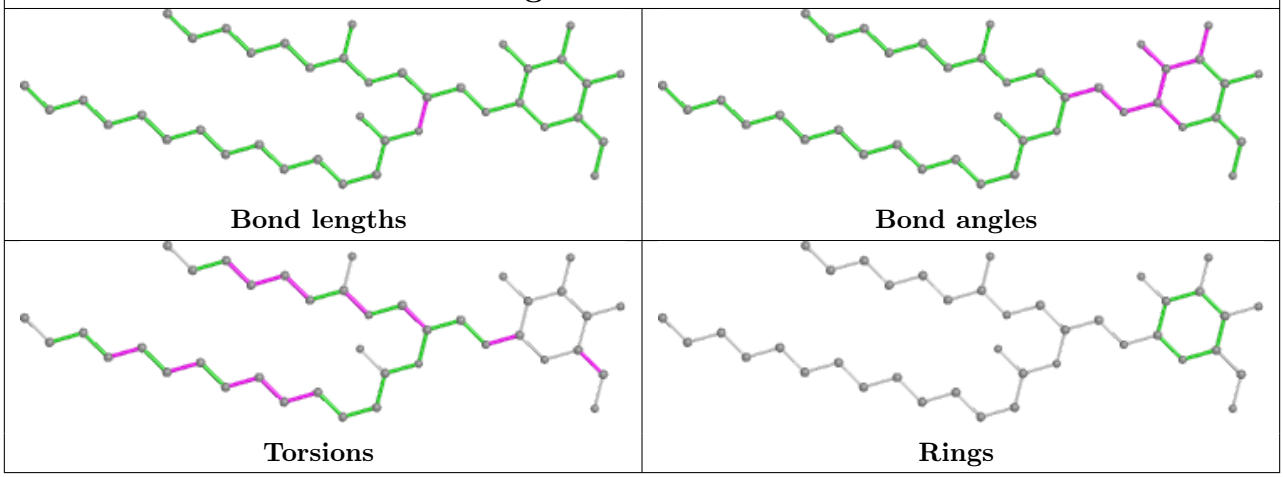
Ligand BCL U 407



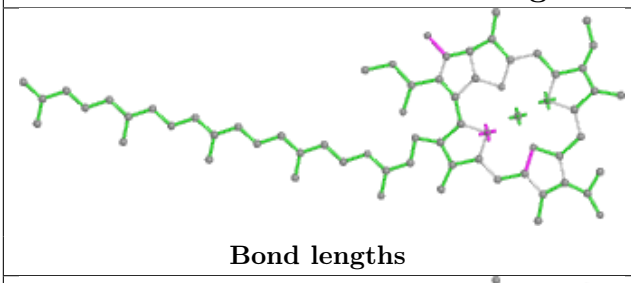
Ligand LHG A 817

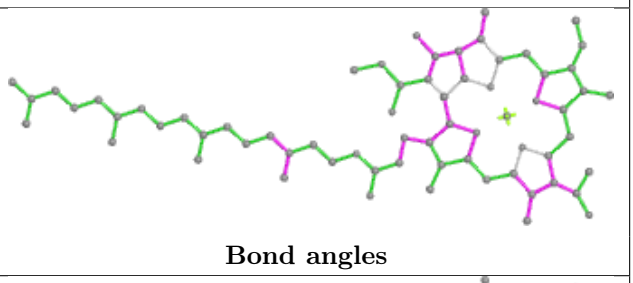


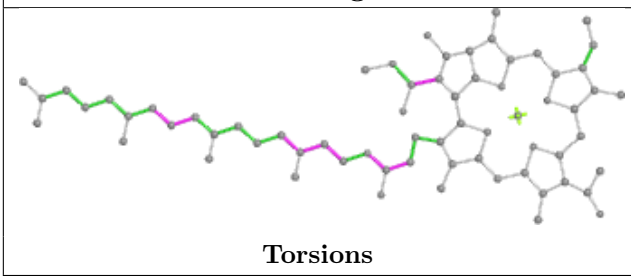
Ligand LMG a 824

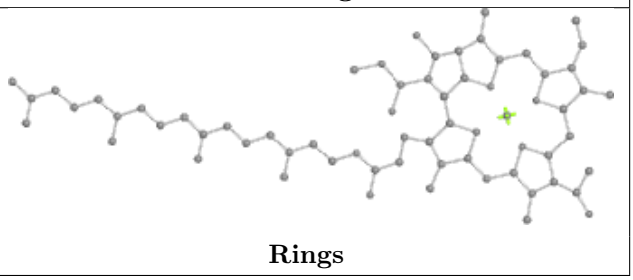


Ligand BCL a 810

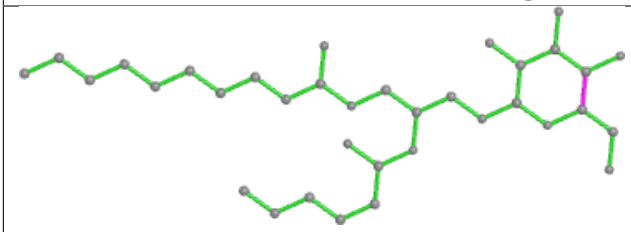

Bond lengths

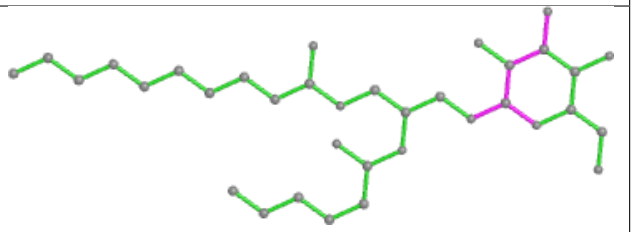

Bond angles

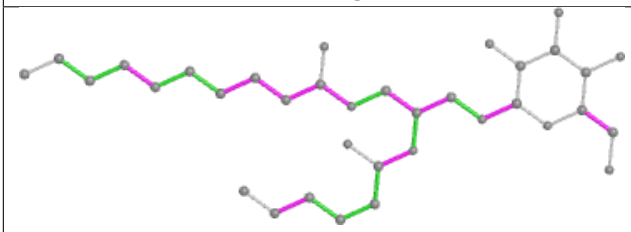

Torsions

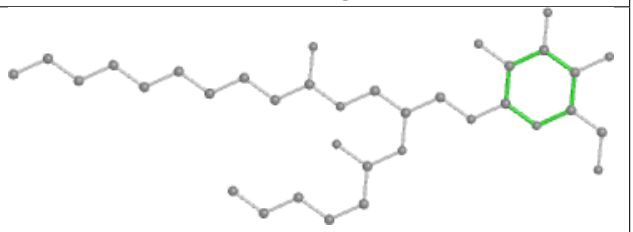

Rings

Ligand LMG C 302

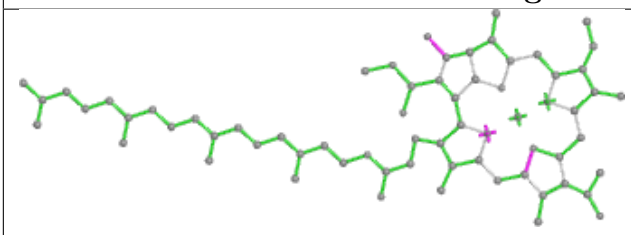

Bond lengths


Bond angles


Torsions


Rings

Ligand BCL U 404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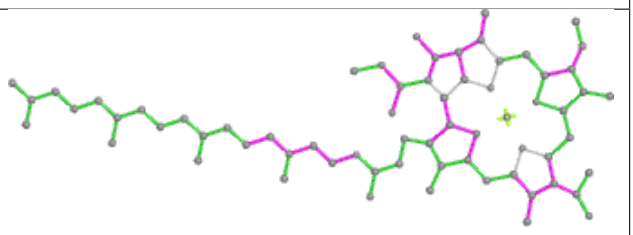
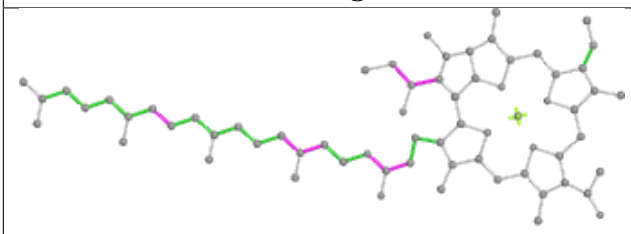
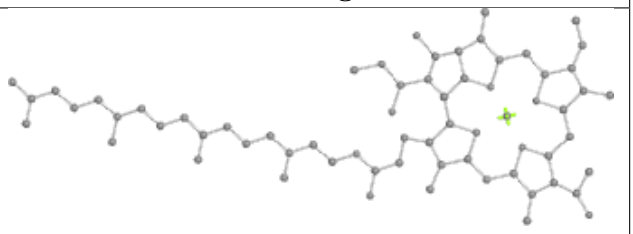
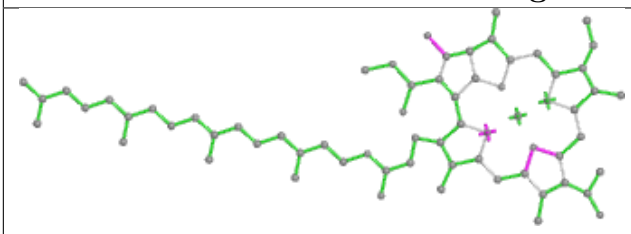

Bond angles


Torsions


Rings

Ligand BCL a 814



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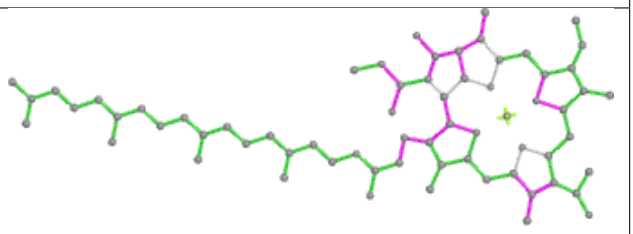
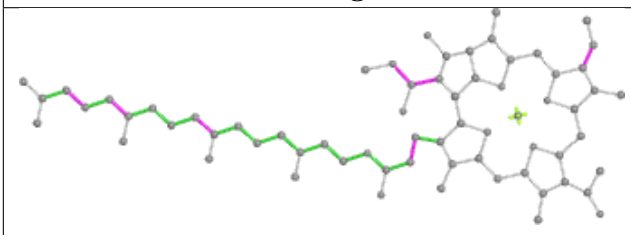
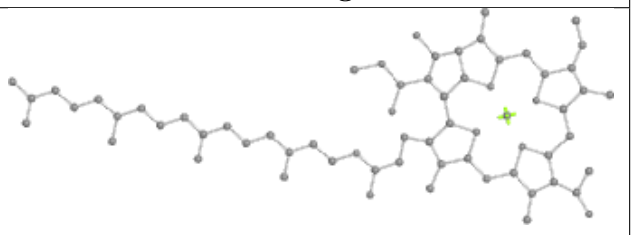


Bond angles

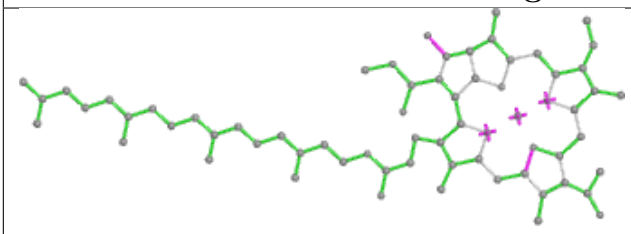


Torsions

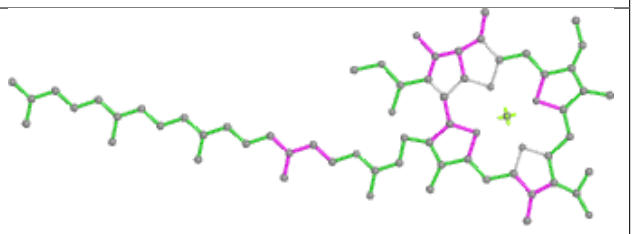


Rings

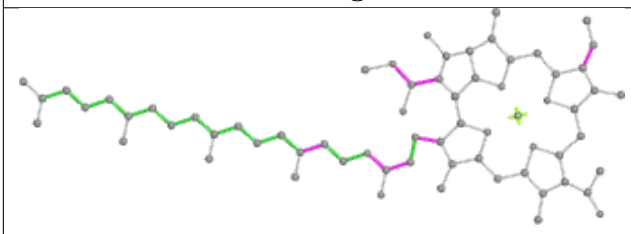
Ligand BCL A 808



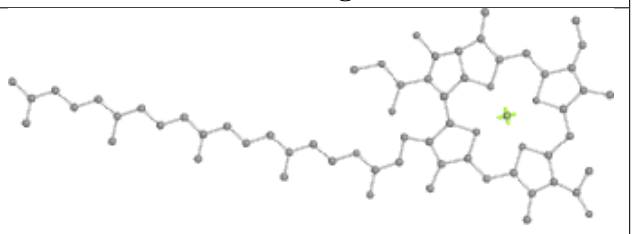
Bond lengths



Bond angles

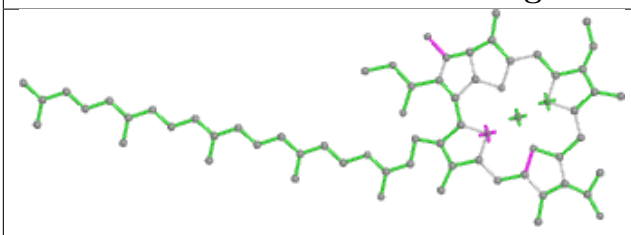


Torsions

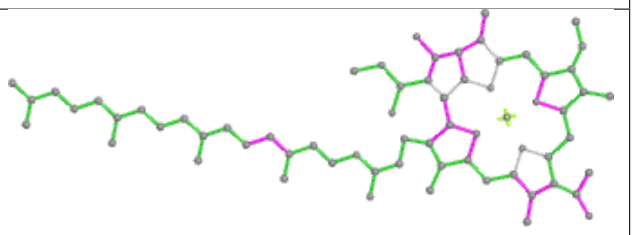


Rings

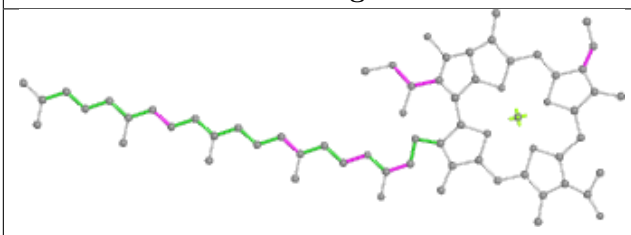
Ligand BCL V 404



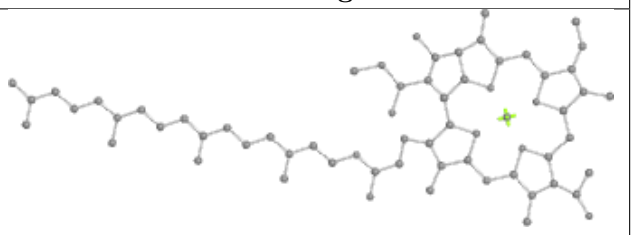
Bond lengths



Bond angles

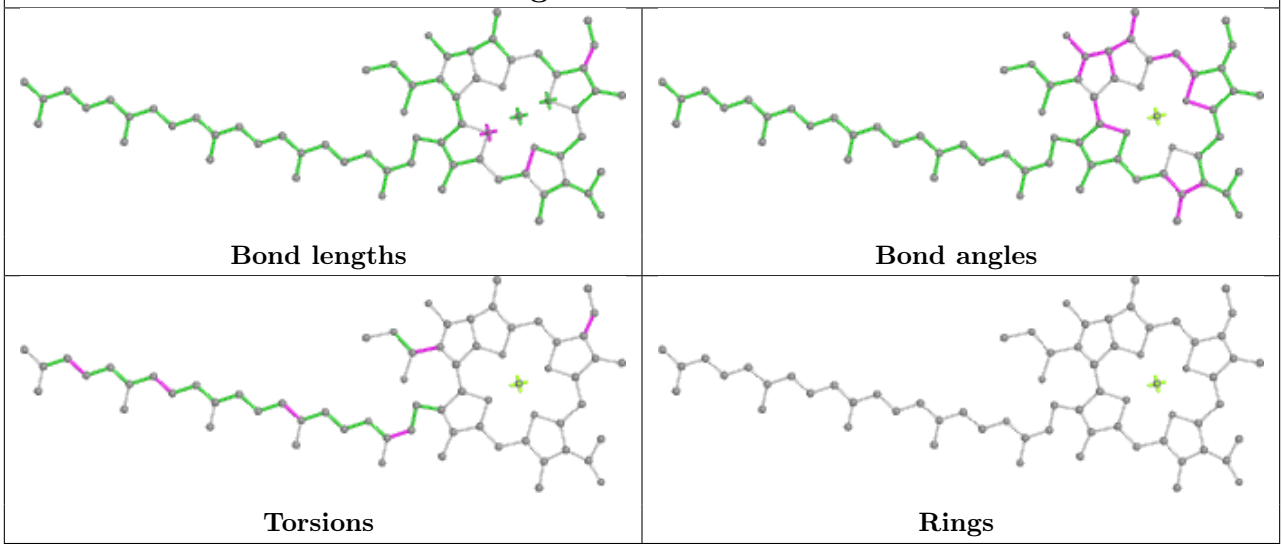


Torsions

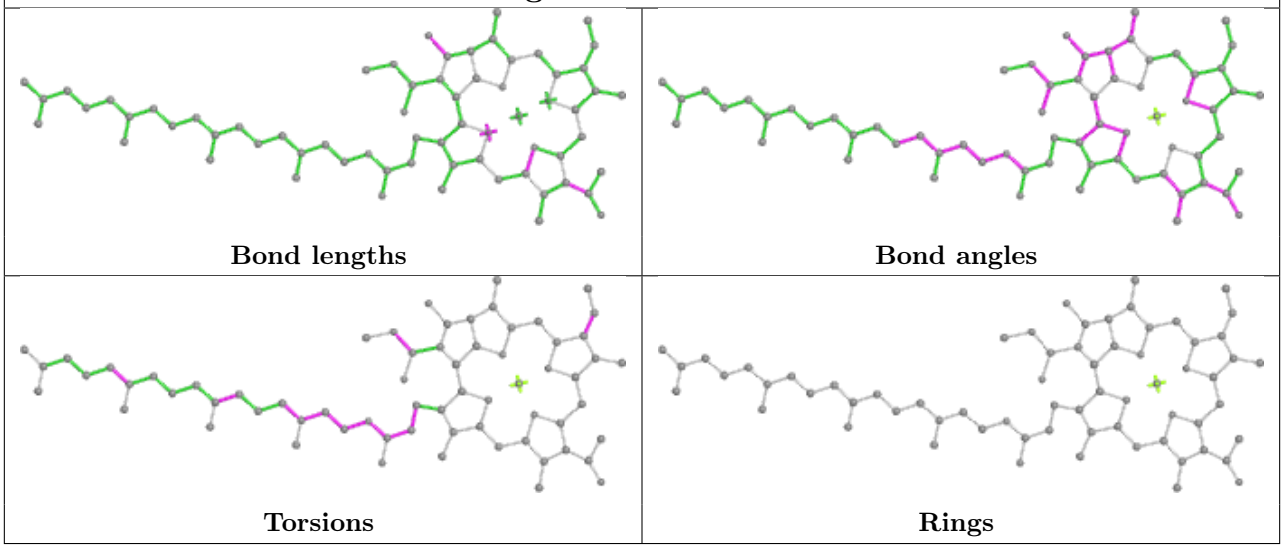


Rings

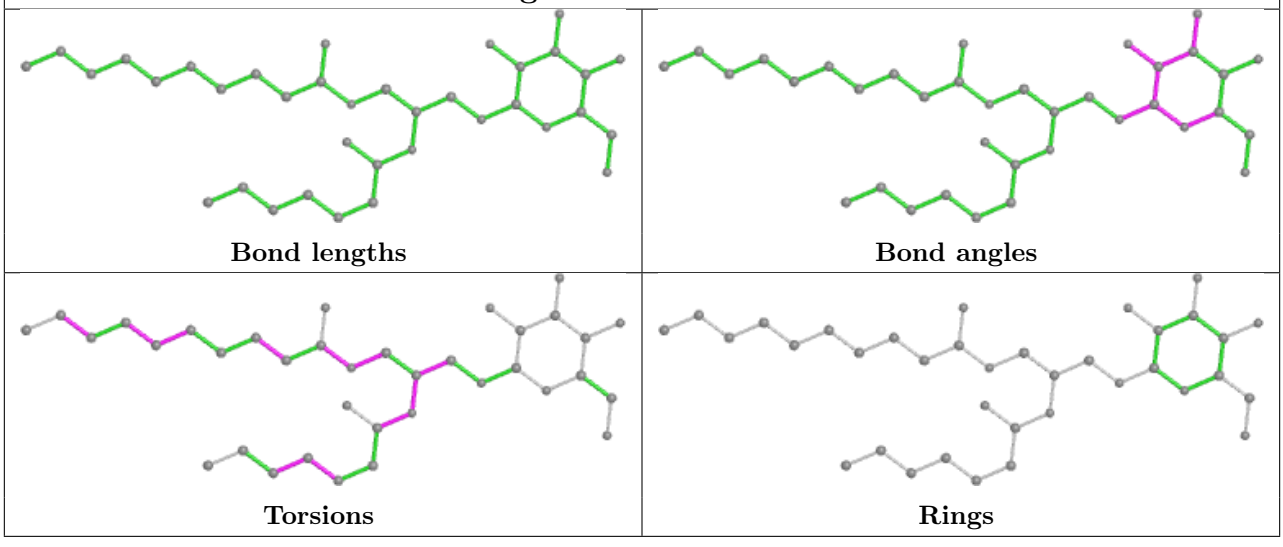
Ligand BCL a 807



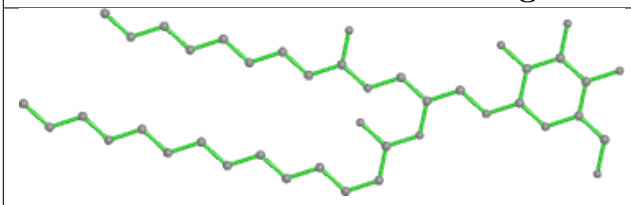
Ligand BCL A 805

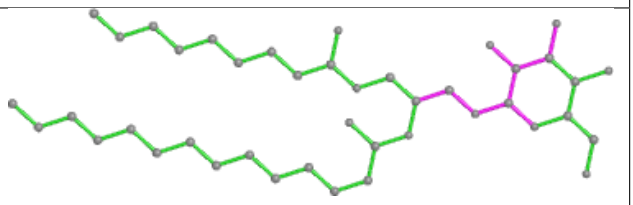


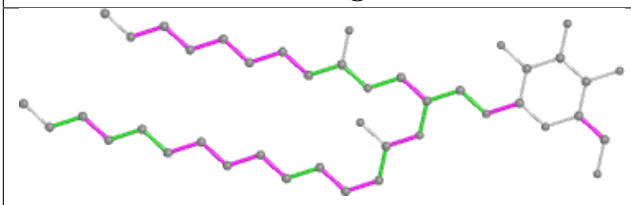
Ligand LMG A 820

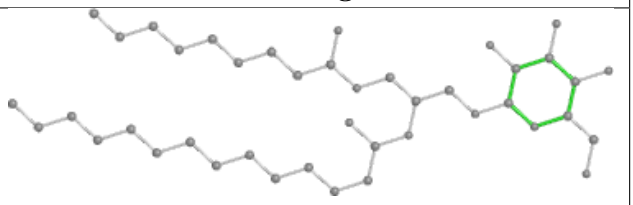


Ligand LMG A 818

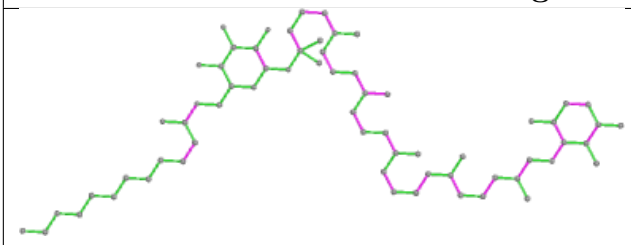

Bond lengths

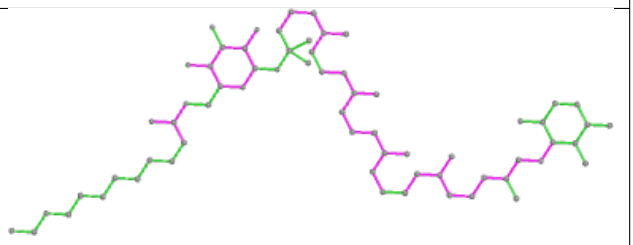

Bond angles

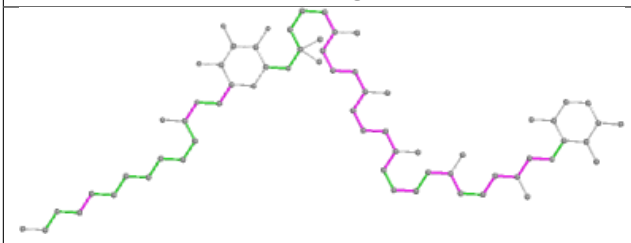

Torsions

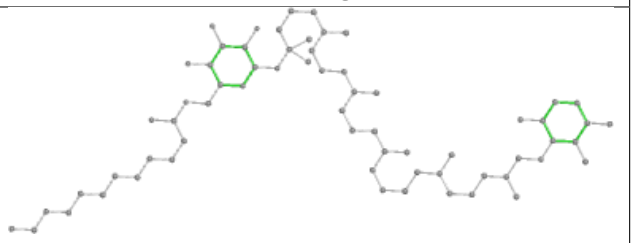

Rings

Ligand F39 A 814

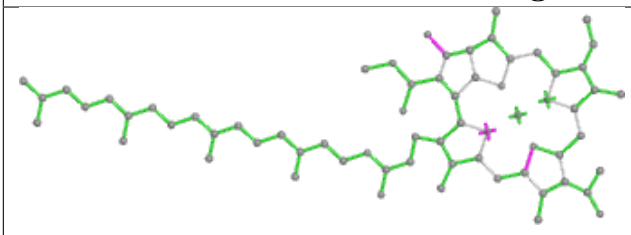

Bond lengths

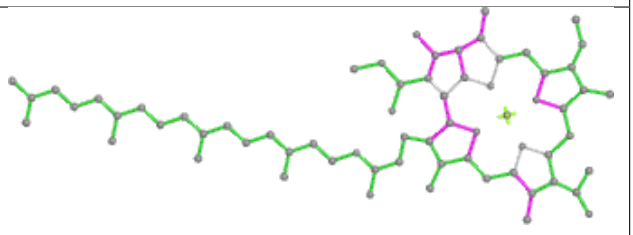

Bond angles

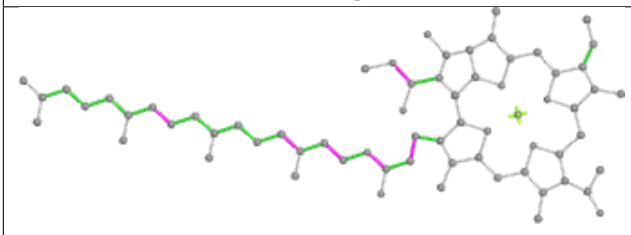

Torsions

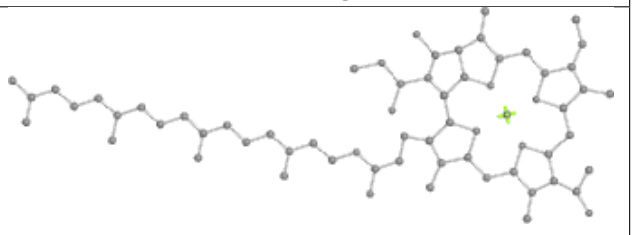

Rings

Ligand BCL a 817

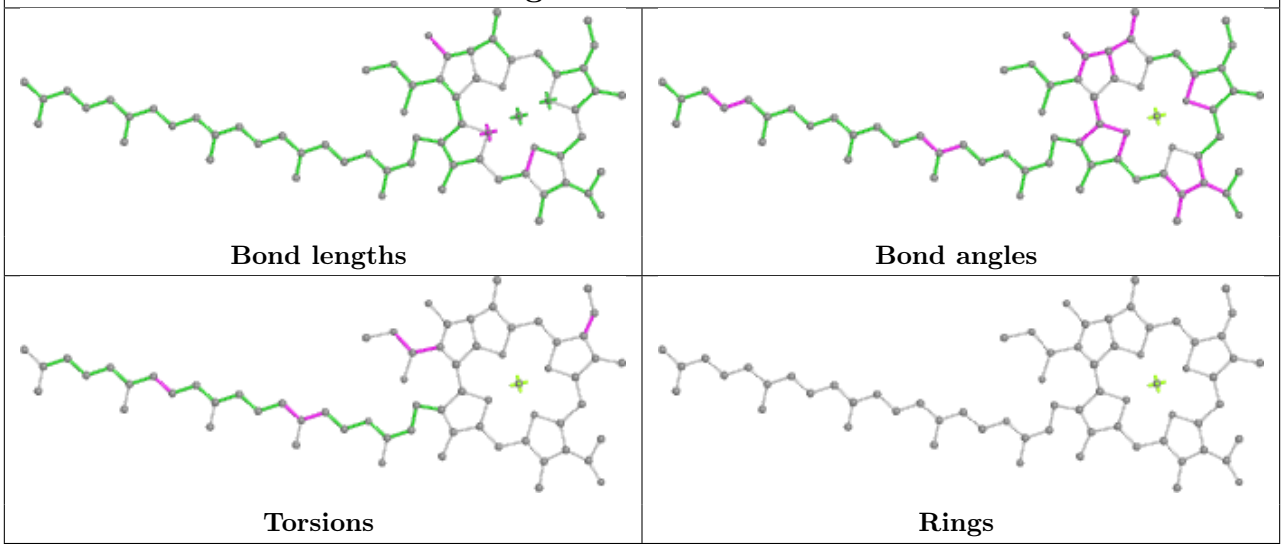

Bond lengths


Bond angles

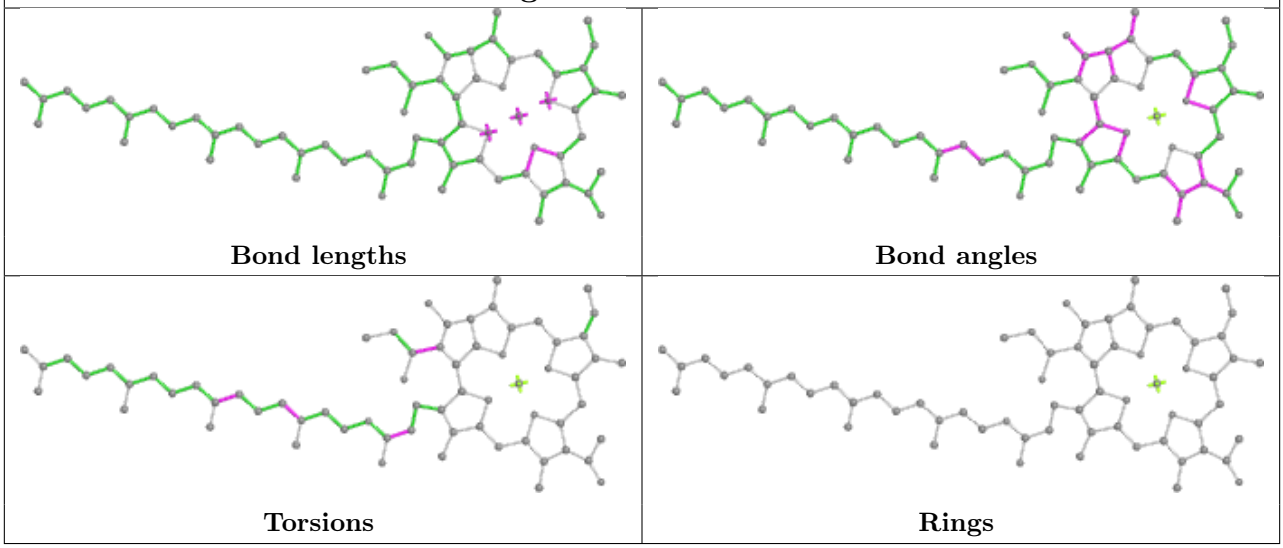

Torsions


Rings

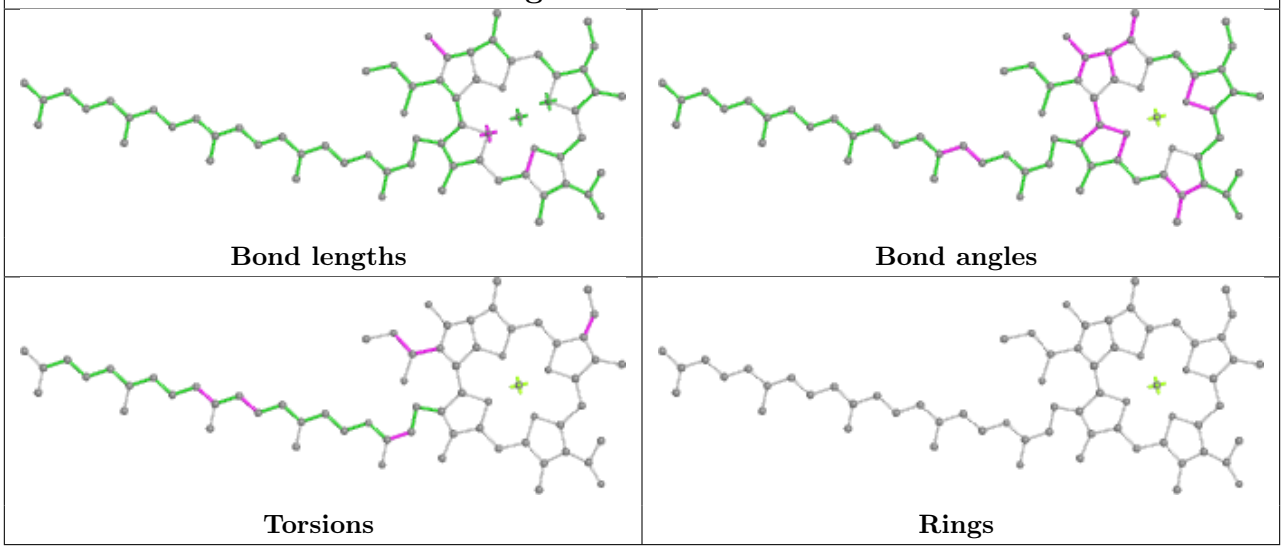
Ligand BCL V 406



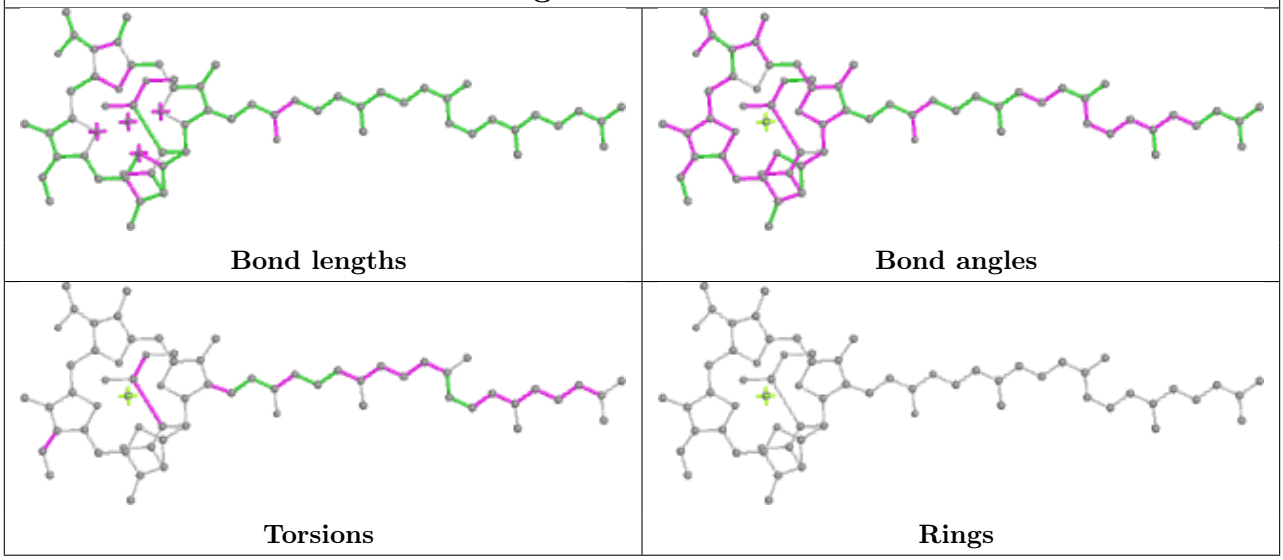
Ligand BCL W 401



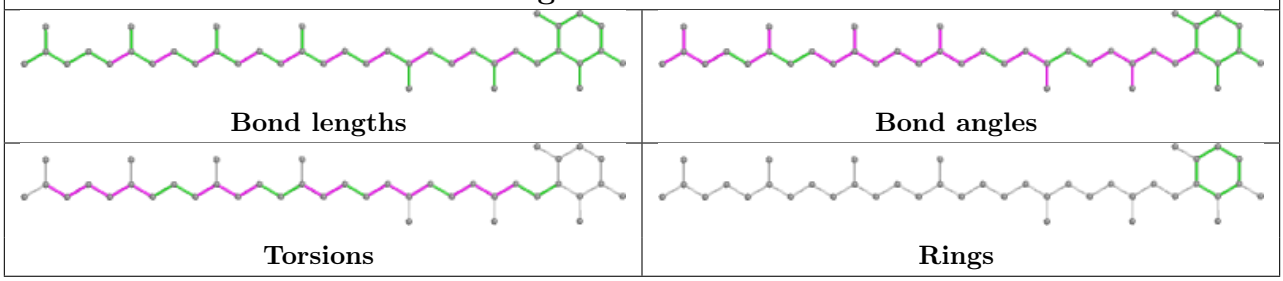
Ligand BCL U 403



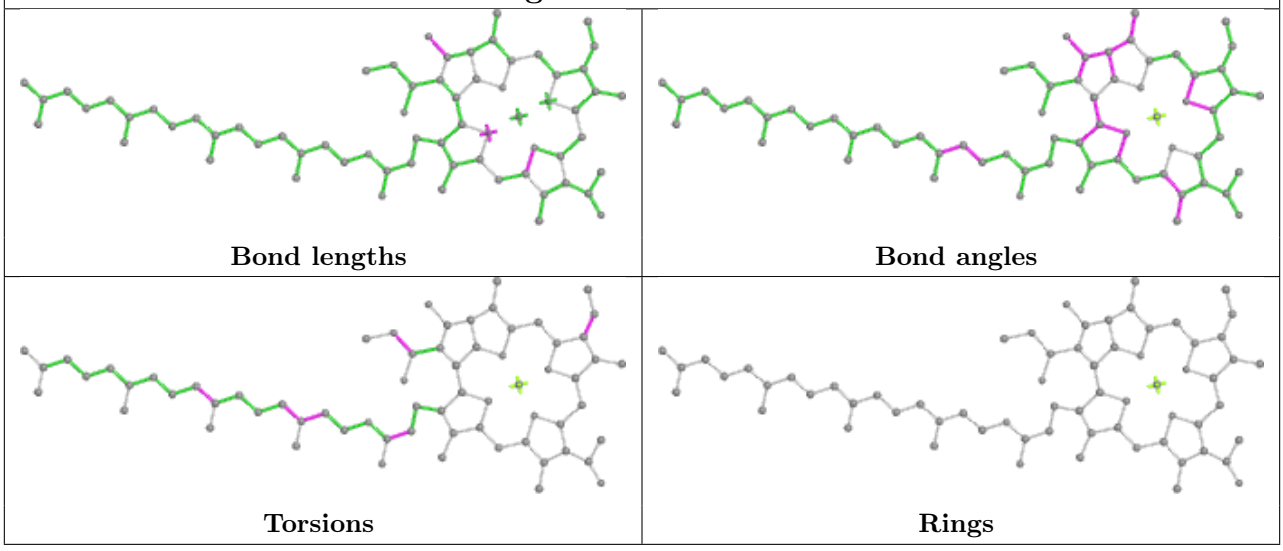
Ligand GS0 a 804



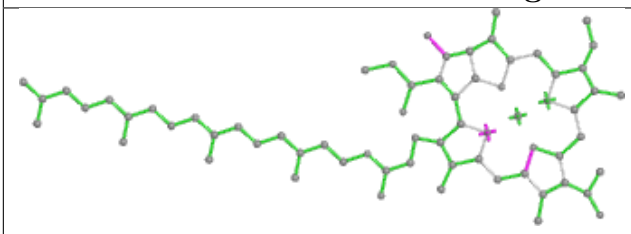
Ligand F26 a 820



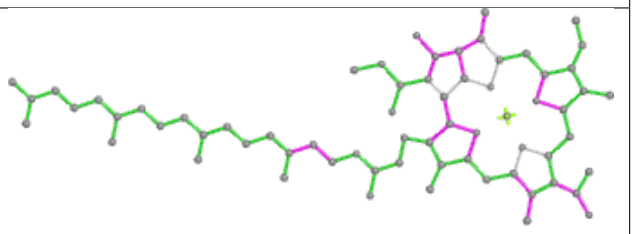
Ligand BCL V 403



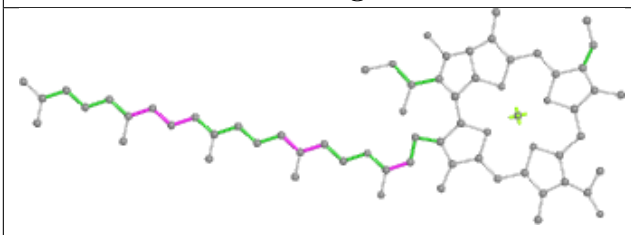
Ligand BCL U 405



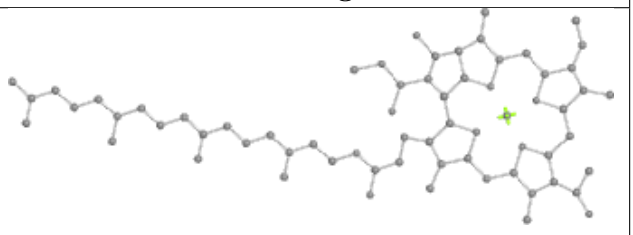
Bond lengths



Bond angles

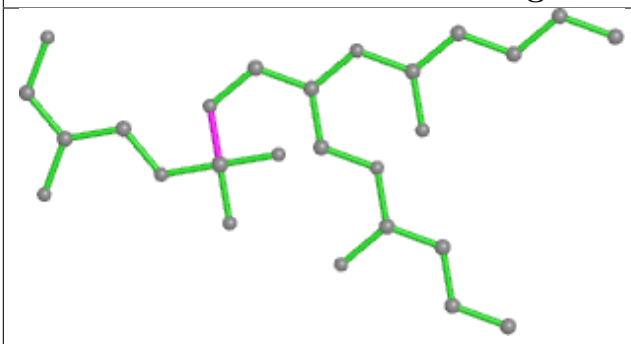


Torsions

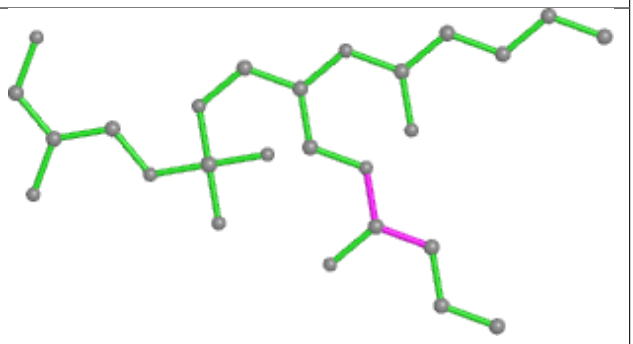


Rings

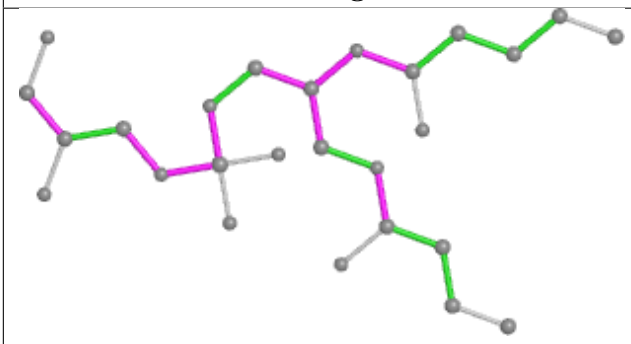
Ligand LHG a 822



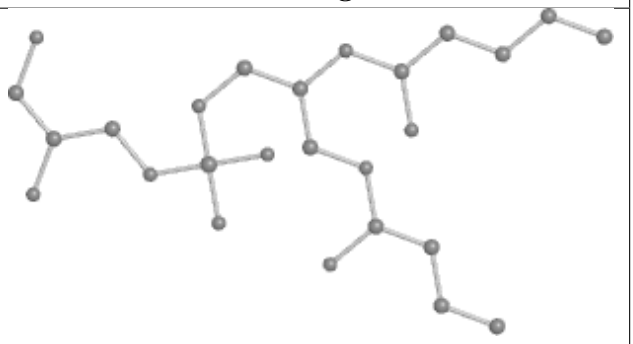
Bond lengths



Bond angles

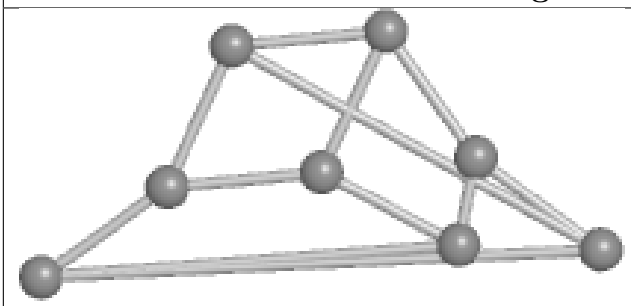


Torsions

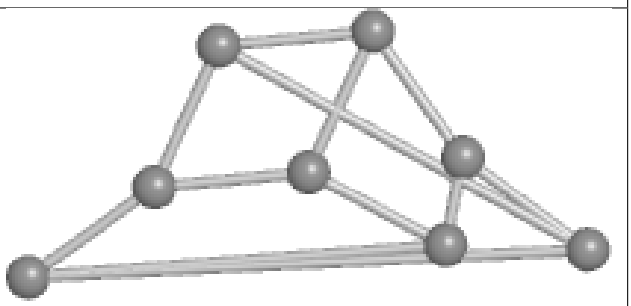


Rings

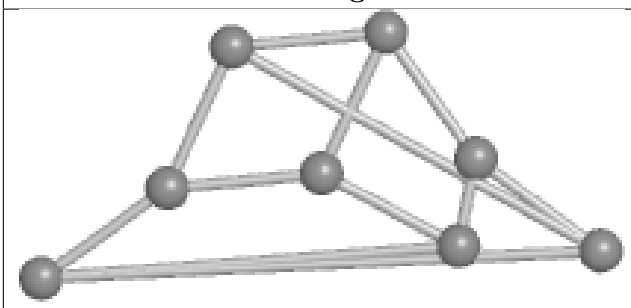
Ligand SF4 B 302



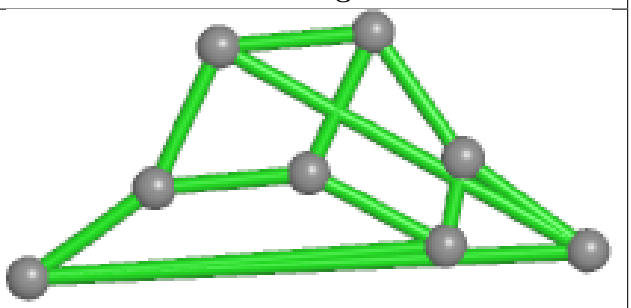
Bond lengths



Bond angles

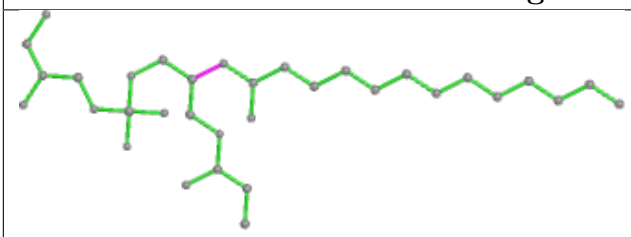


Torsions

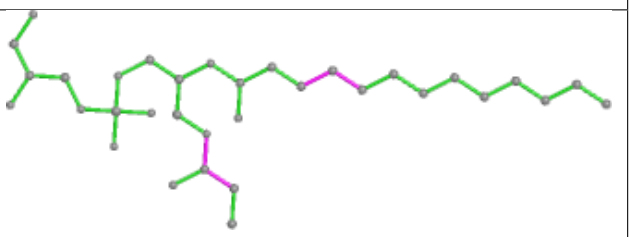


Rings

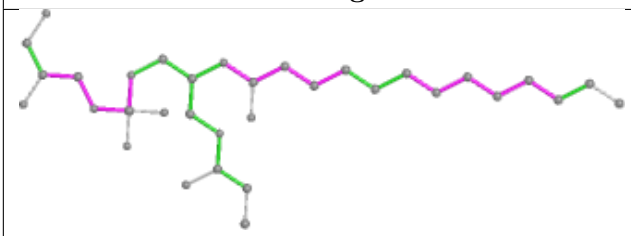
Ligand LHG a 821



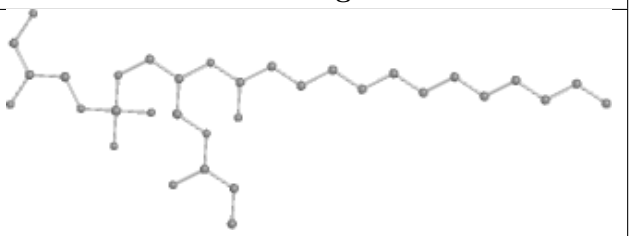
Bond lengths



Bond angles

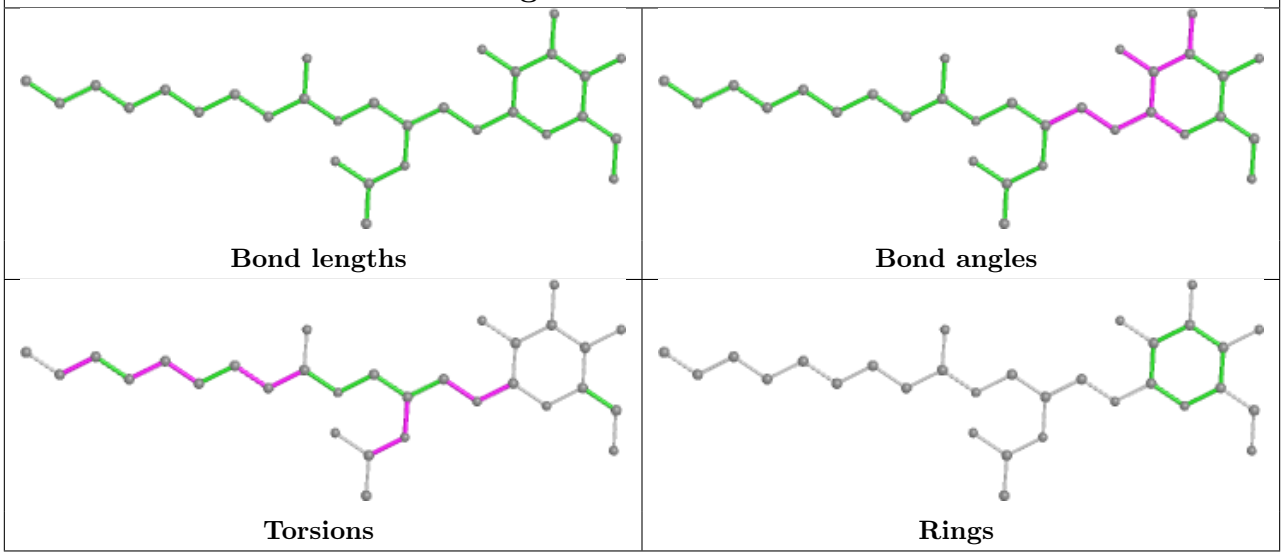


Torsions

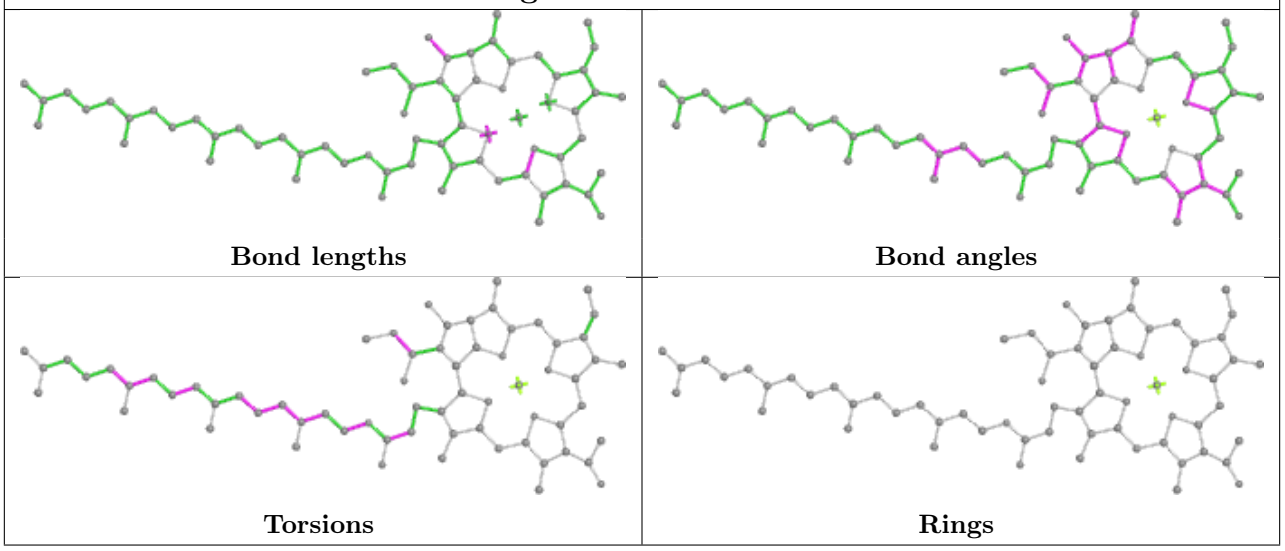


Rings

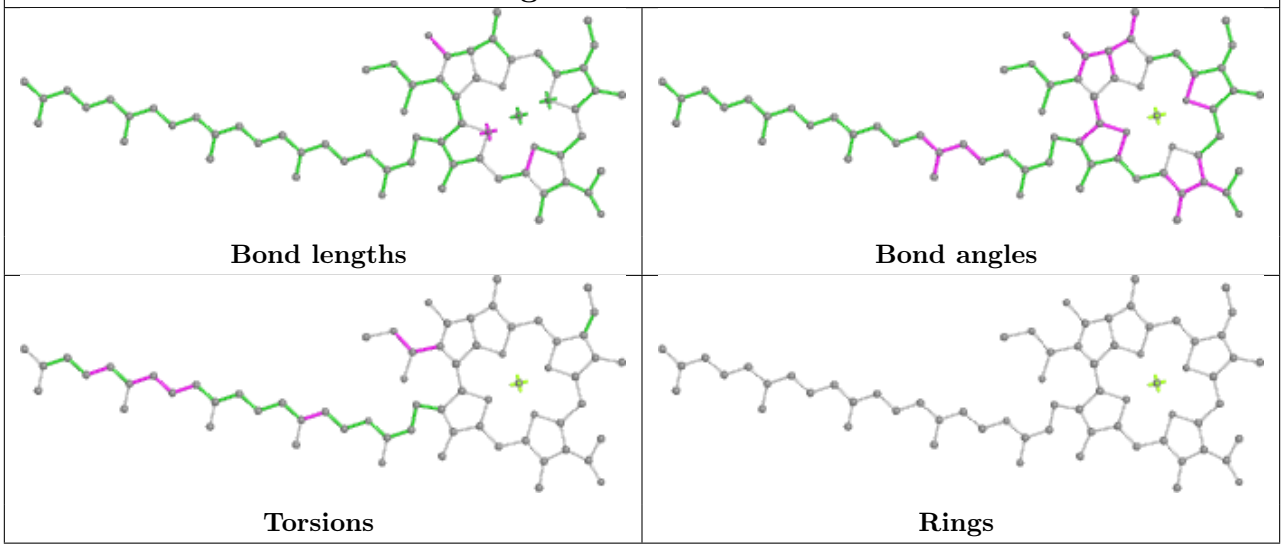
Ligand LMG A 822



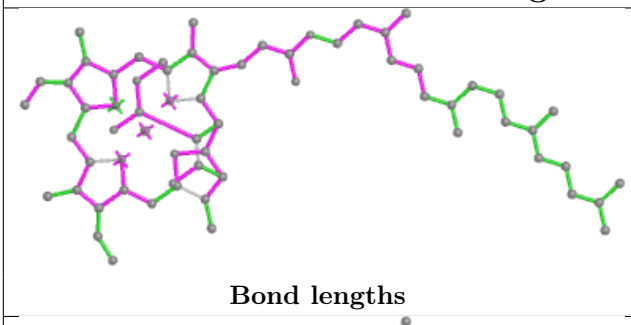
Ligand BCL W 404



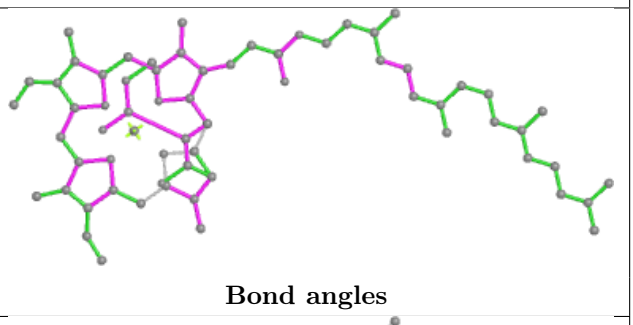
Ligand BCL W 405



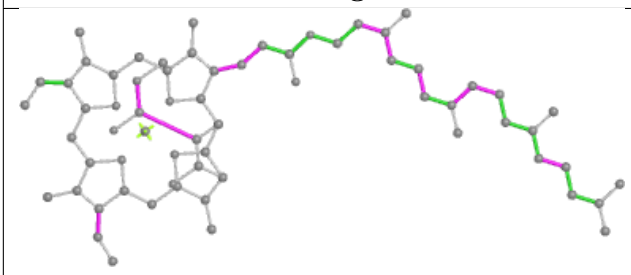
Ligand G2O a 802



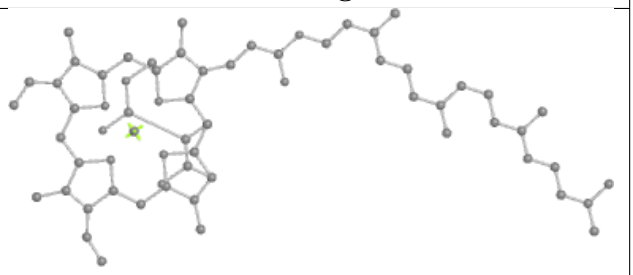
Bond lengths



Bond angles

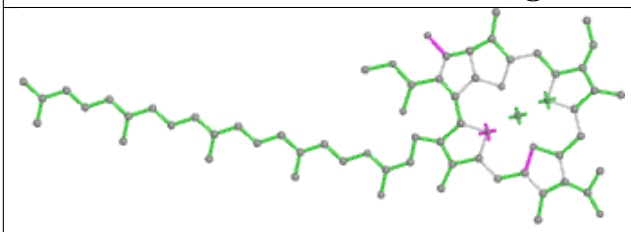


Torsions

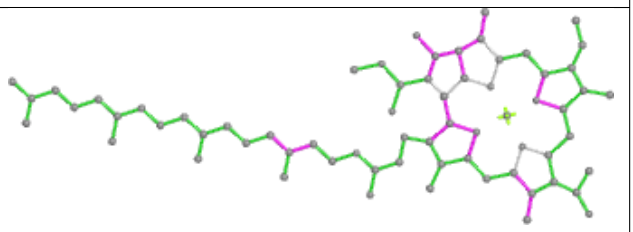


Rings

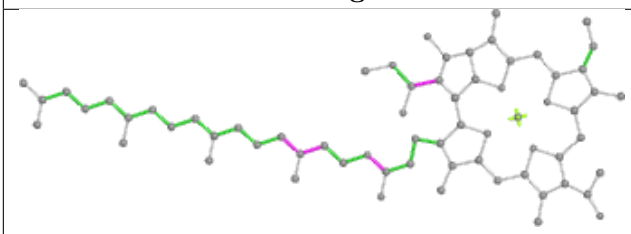
Ligand BCL U 406



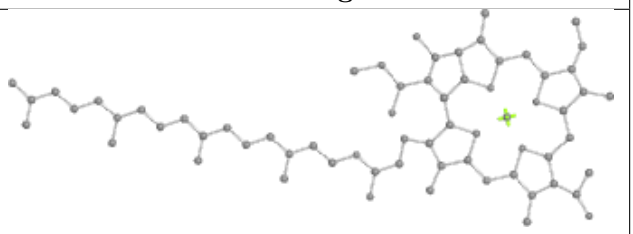
Bond lengths



Bond angles

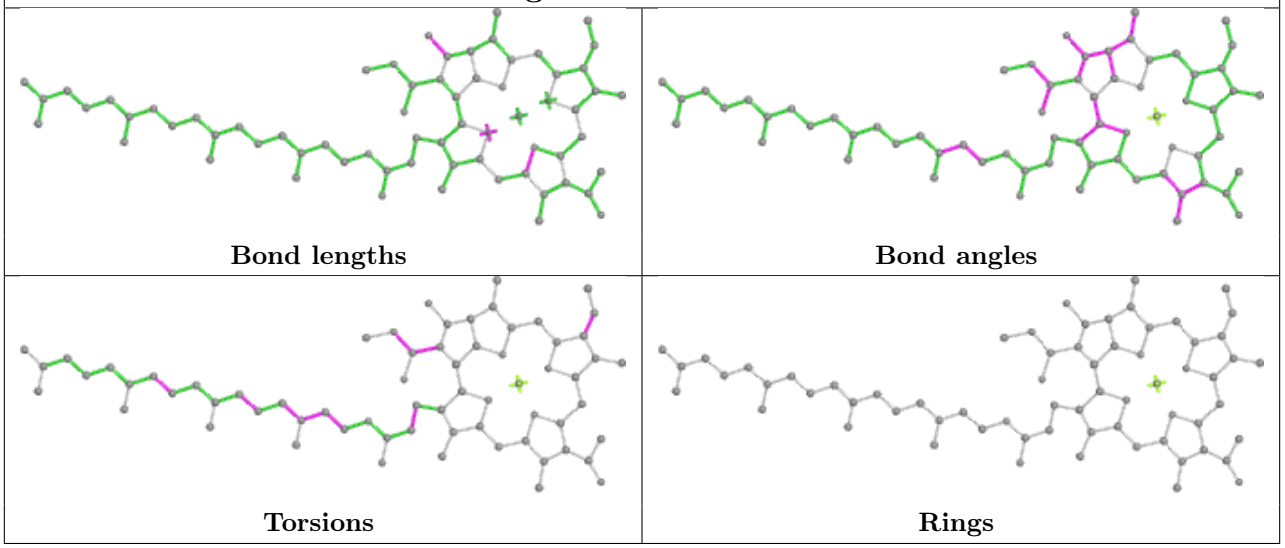


Torsions

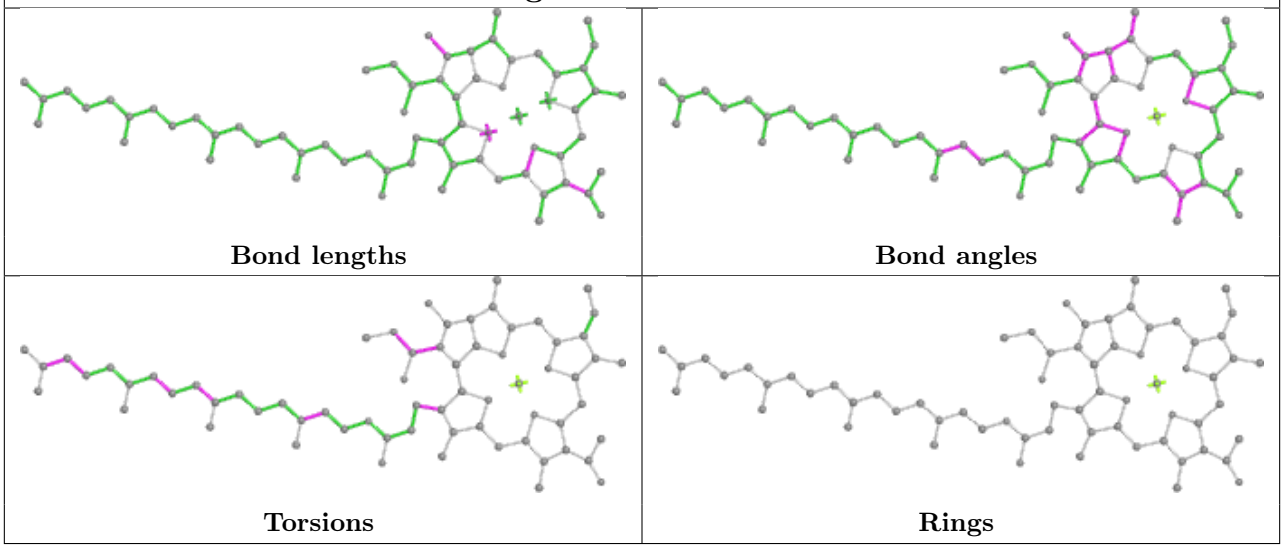


Rings

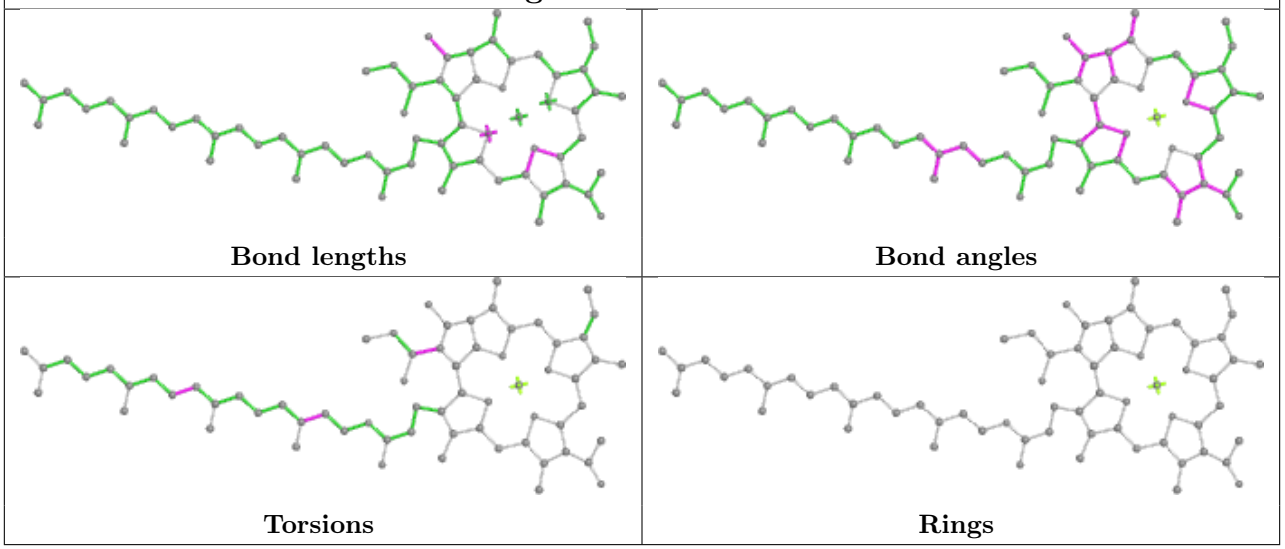
Ligand BCL A 812



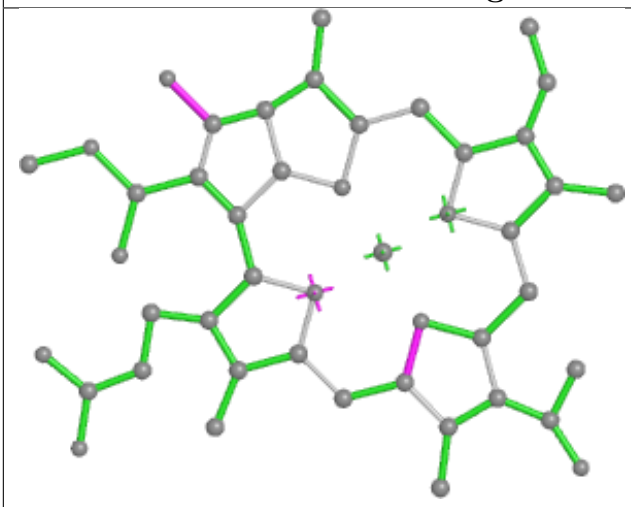
Ligand BCL A 809



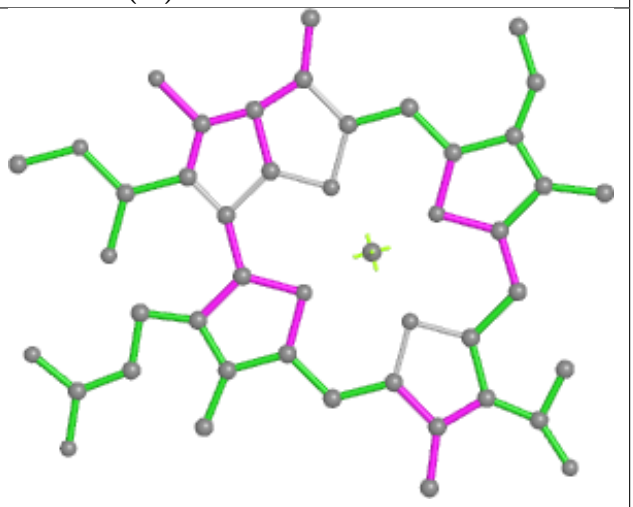
Ligand BCL V 402



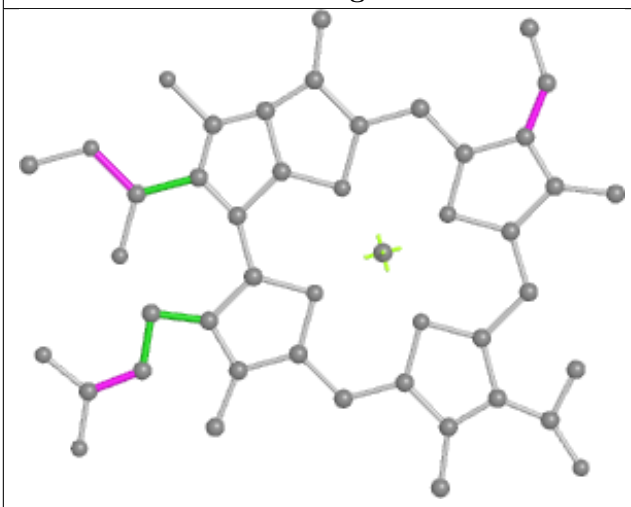
Ligand BCL W 407 (B)



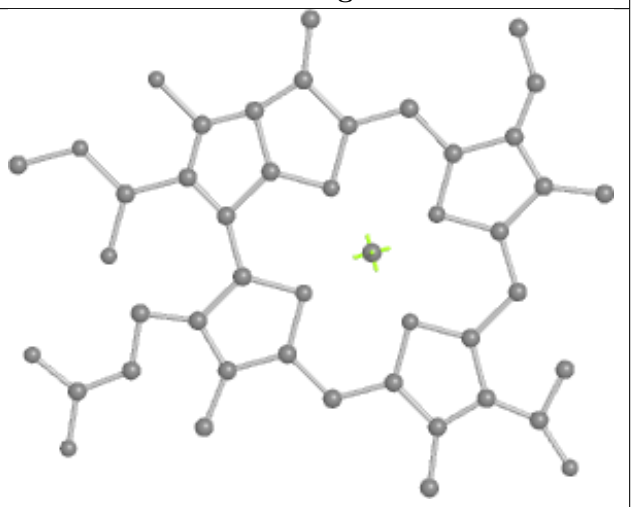
Bond lengths



Bond angles

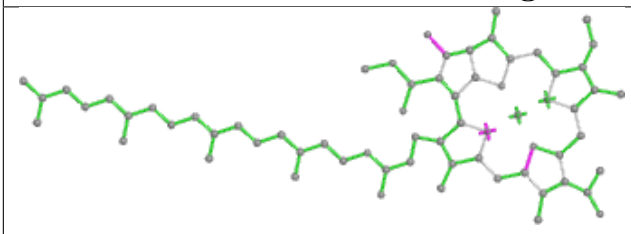


Torsions

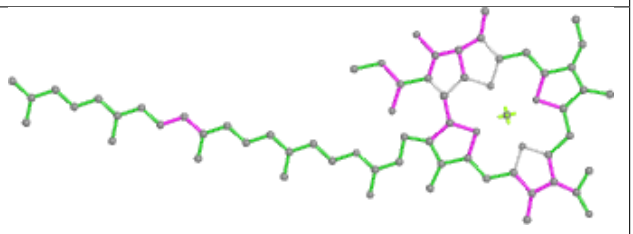


Rings

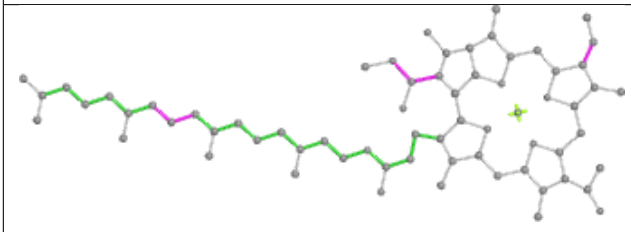
Ligand BCL W 403



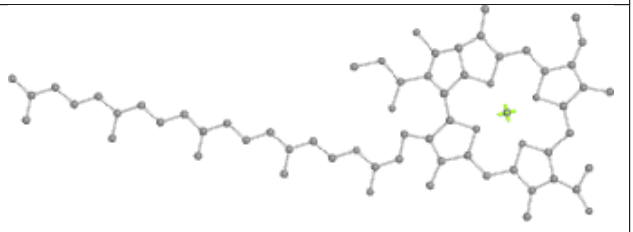
Bond lengths



Bond angles

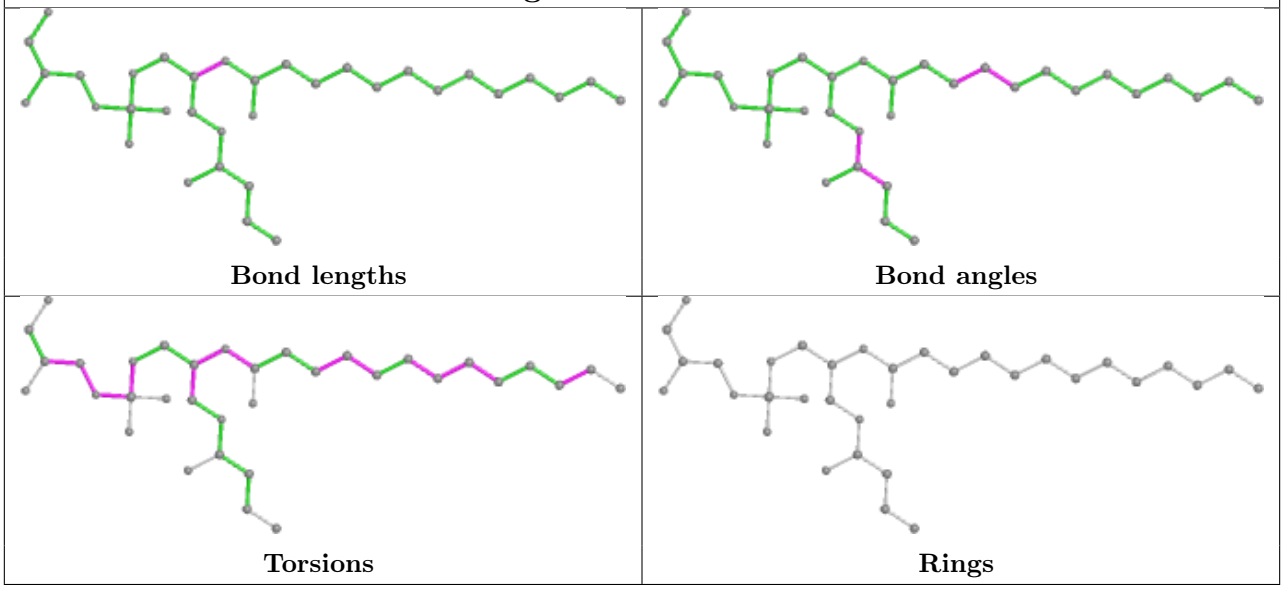


Torsions

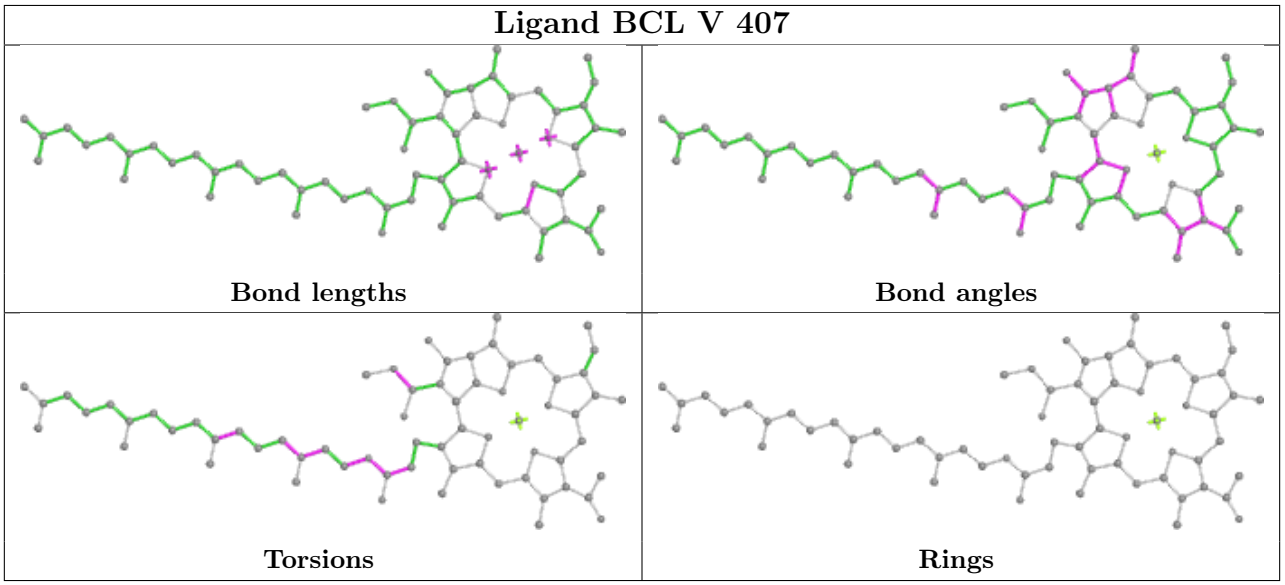


Rings

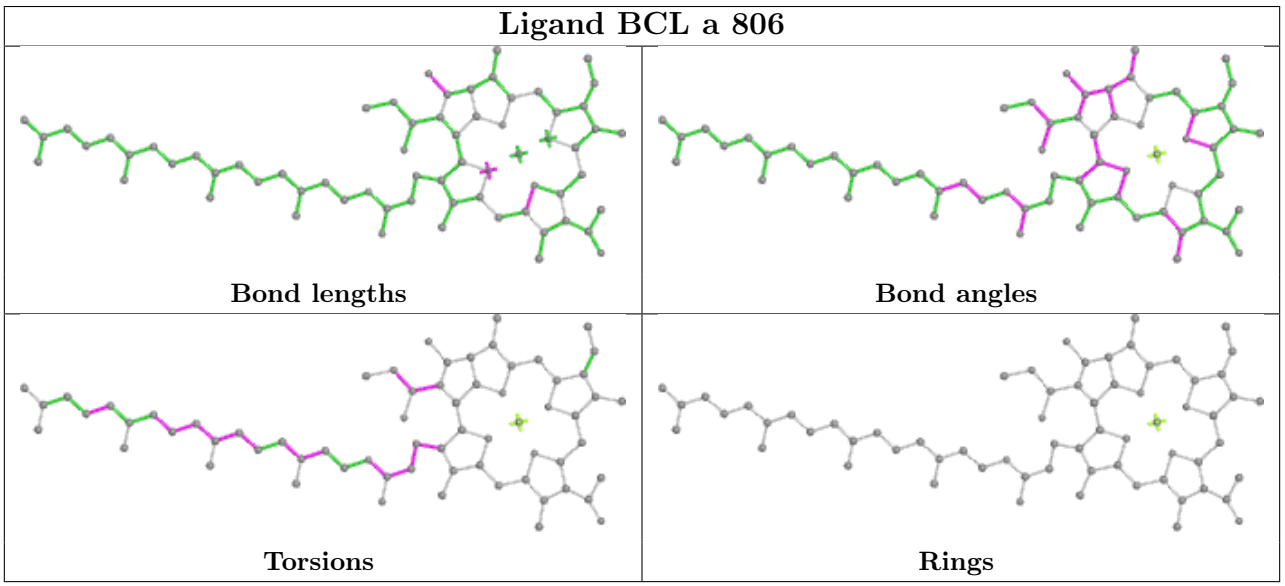
Ligand LHG C 301



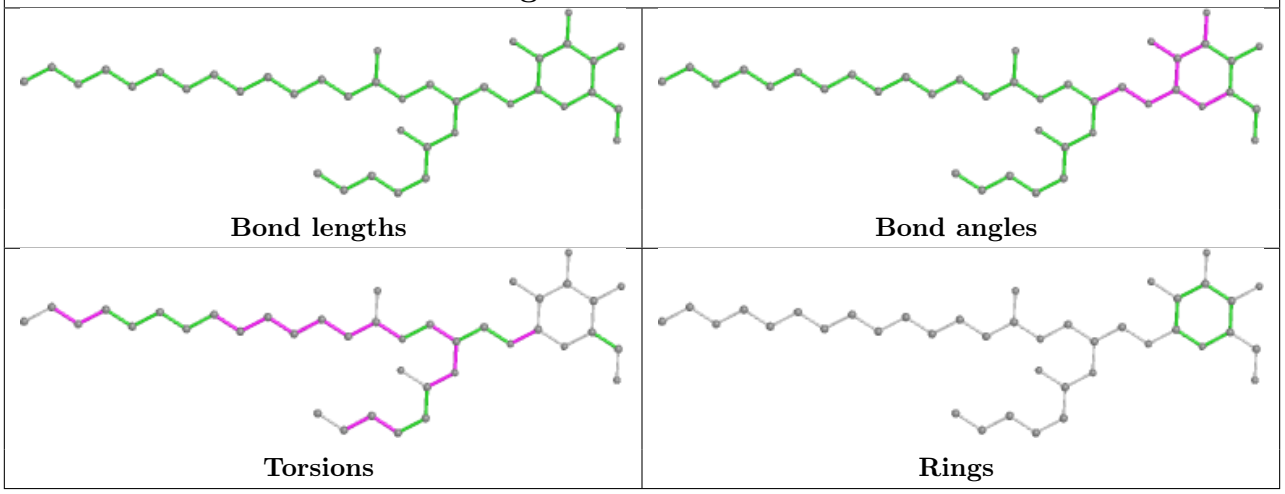
Ligand BCL V 407



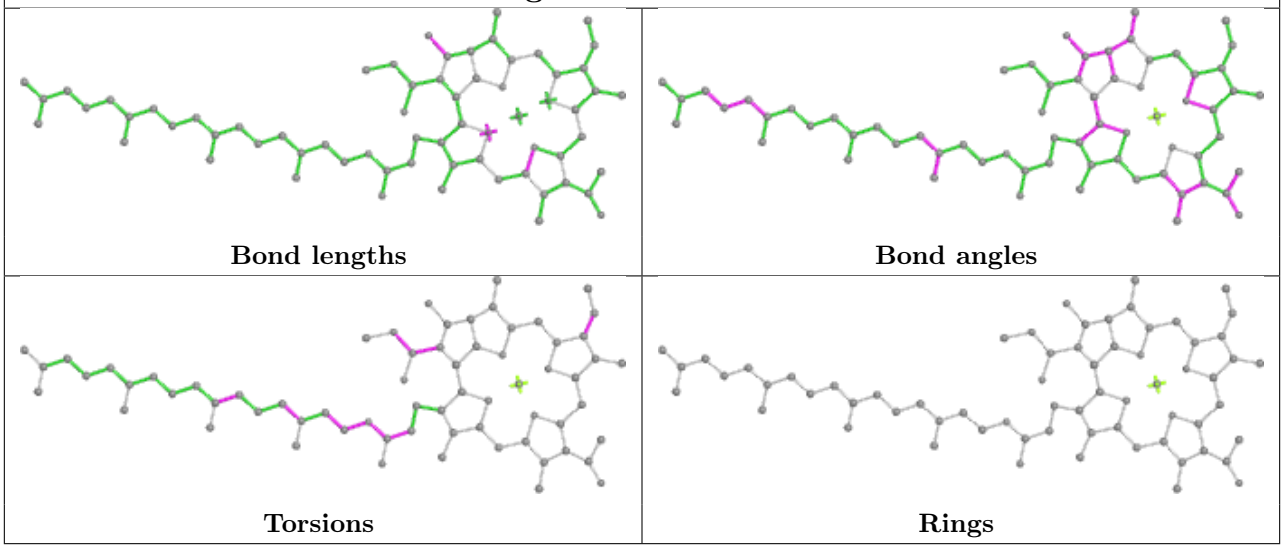
Ligand BCL a 806



Ligand LMG A 819



Ligand BCL A 802



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.

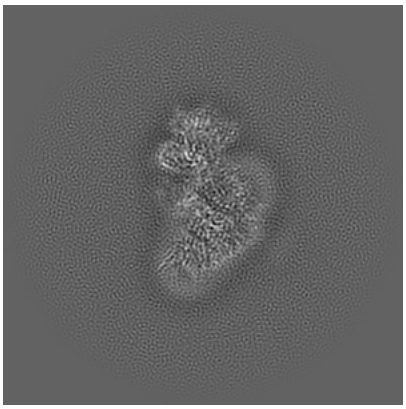
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-26469. These allow visual inspection of the internal detail of the map and identification of artifacts.

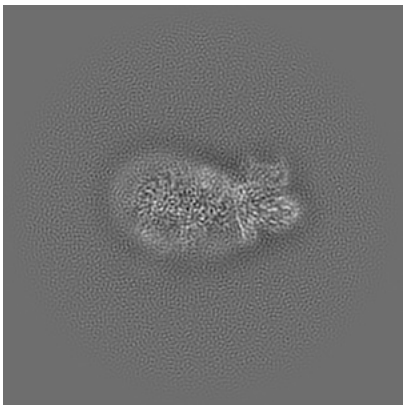
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

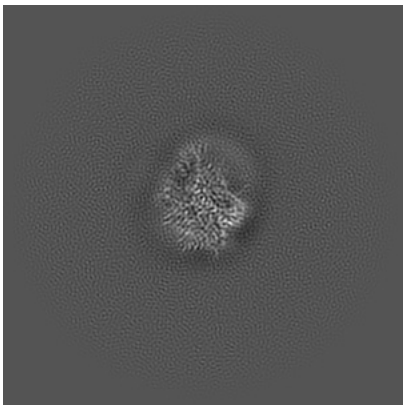
6.1.1 Primary map



X

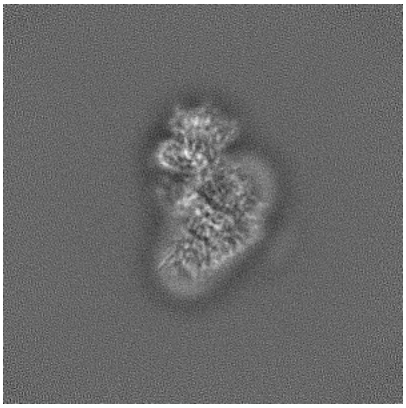


Y

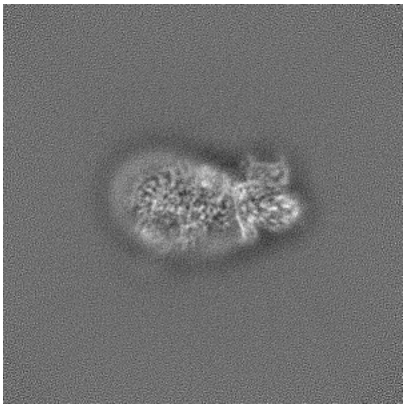


Z

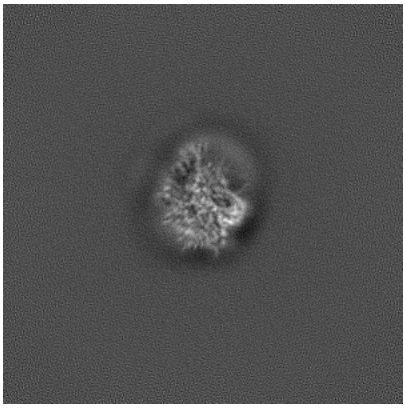
6.1.2 Raw map



X



Y

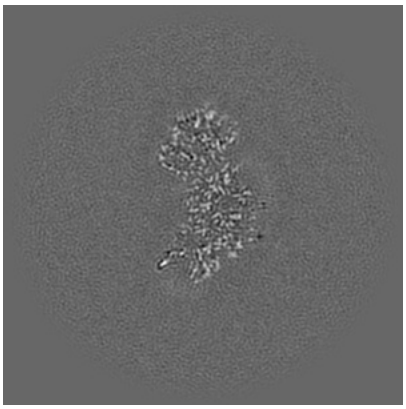


Z

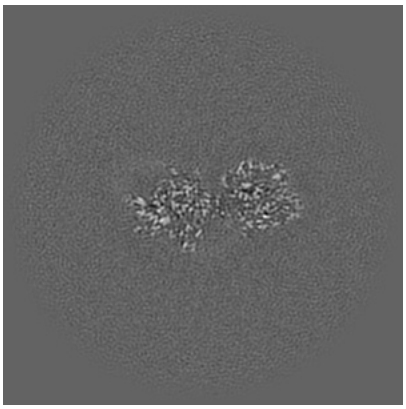
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

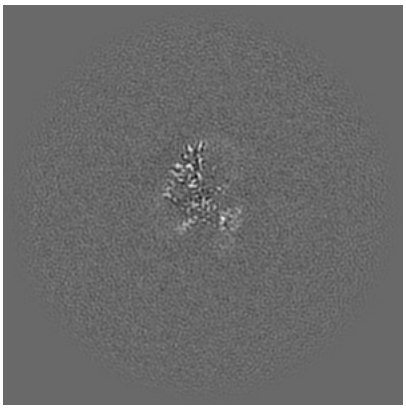
6.2.1 Primary map



X Index: 180

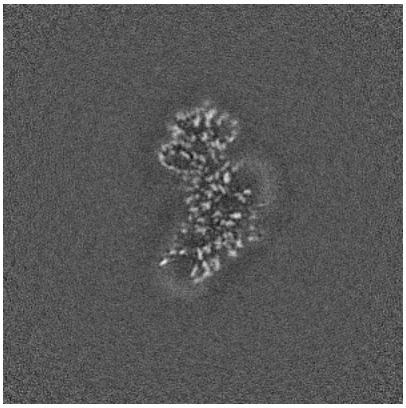


Y Index: 180

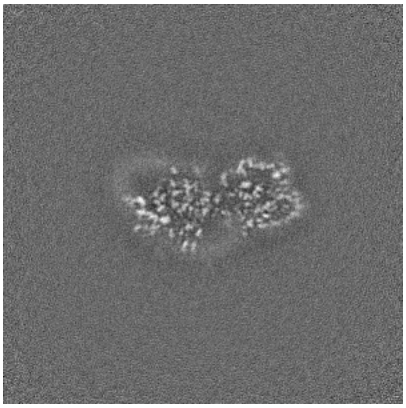


Z Index: 180

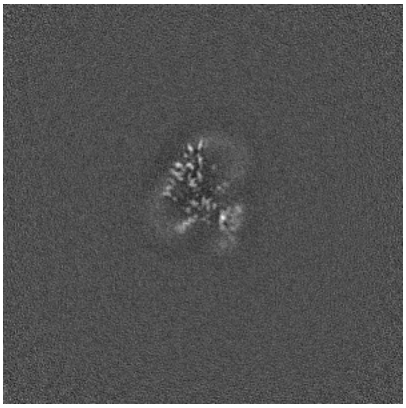
6.2.2 Raw map



X Index: 180



Y Index: 180

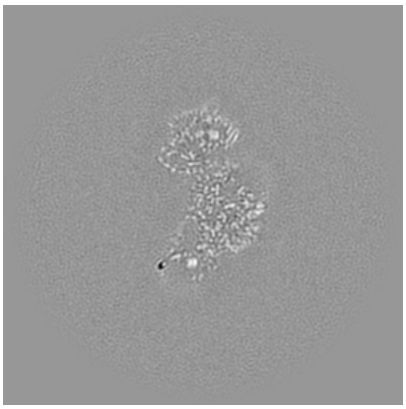


Z Index: 180

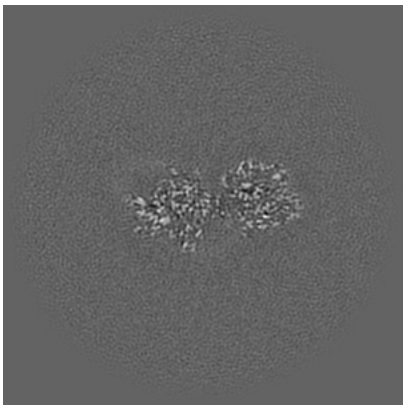
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

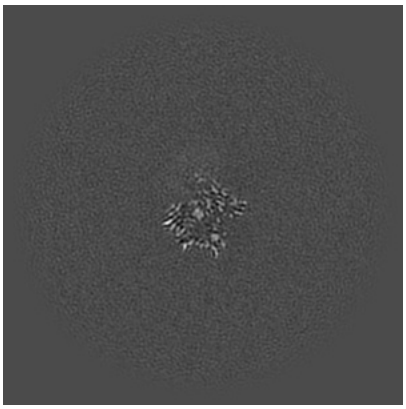
6.3.1 Primary map



X Index: 176

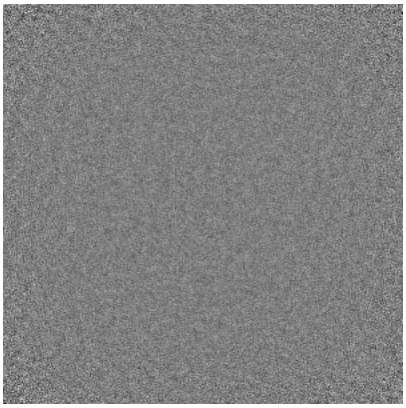


Y Index: 180

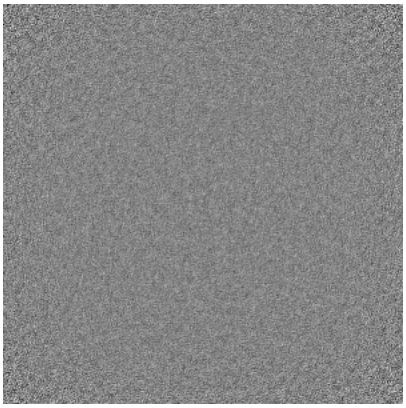


Z Index: 217

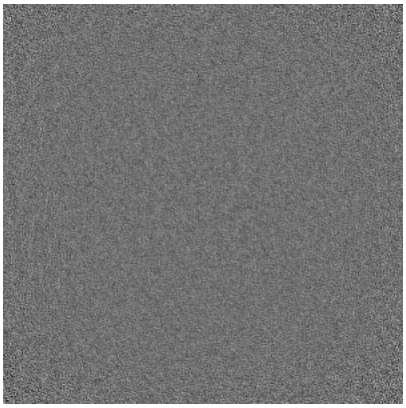
6.3.2 Raw map



X Index: 0



Y Index: 0



Z Index: 359

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 0.352. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map

X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

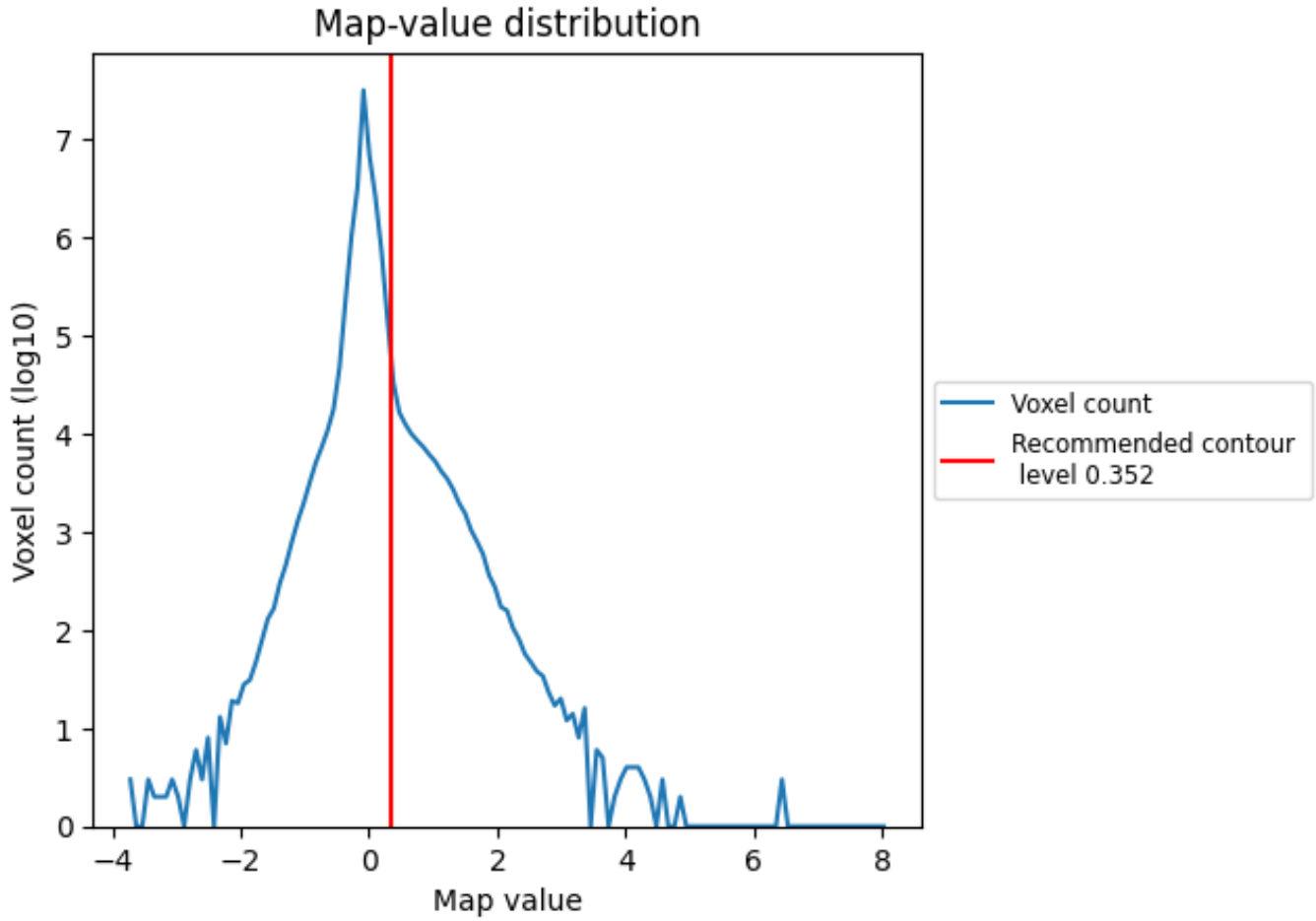
6.5 Mask visualisation (i)

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

7 Map analysis

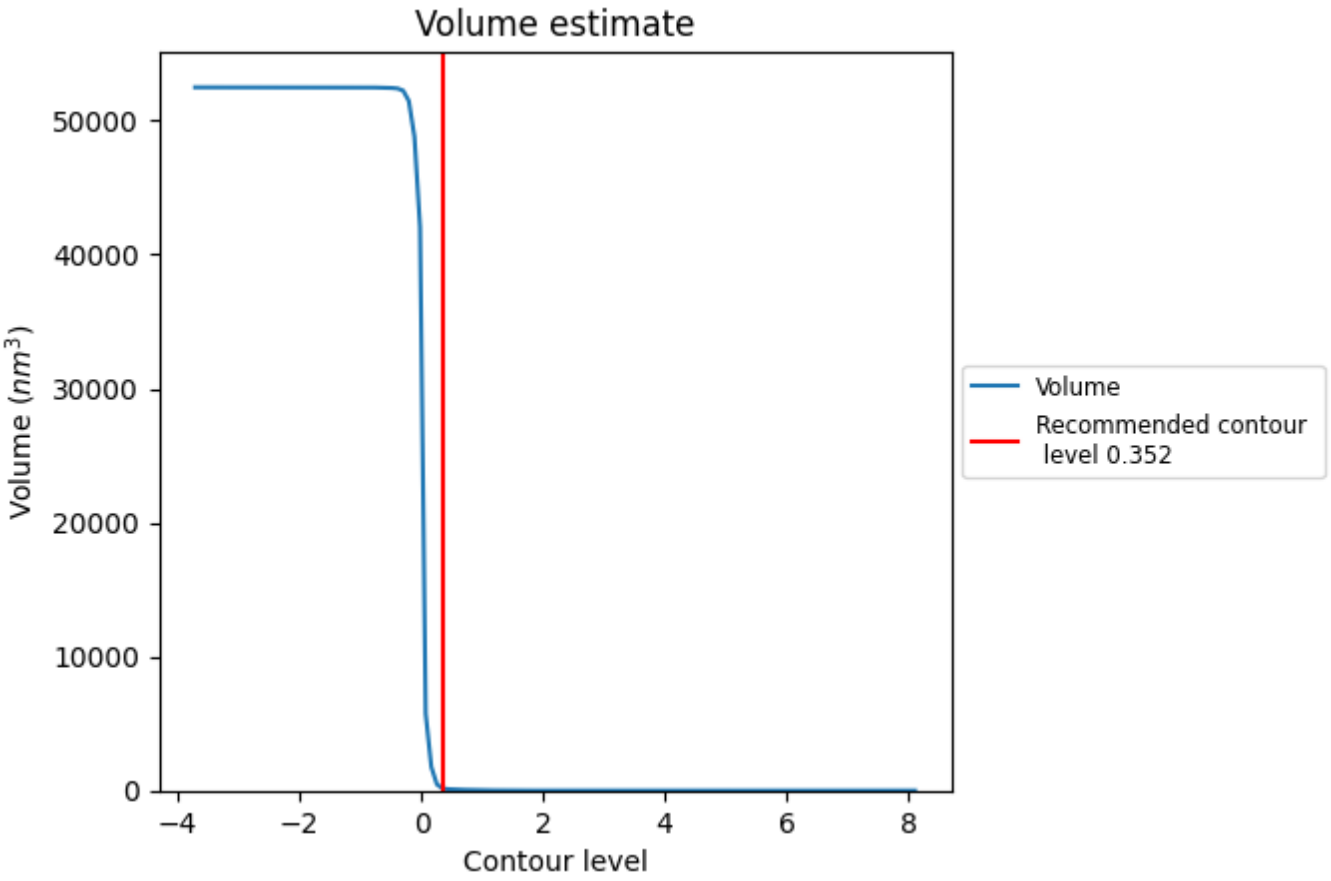
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

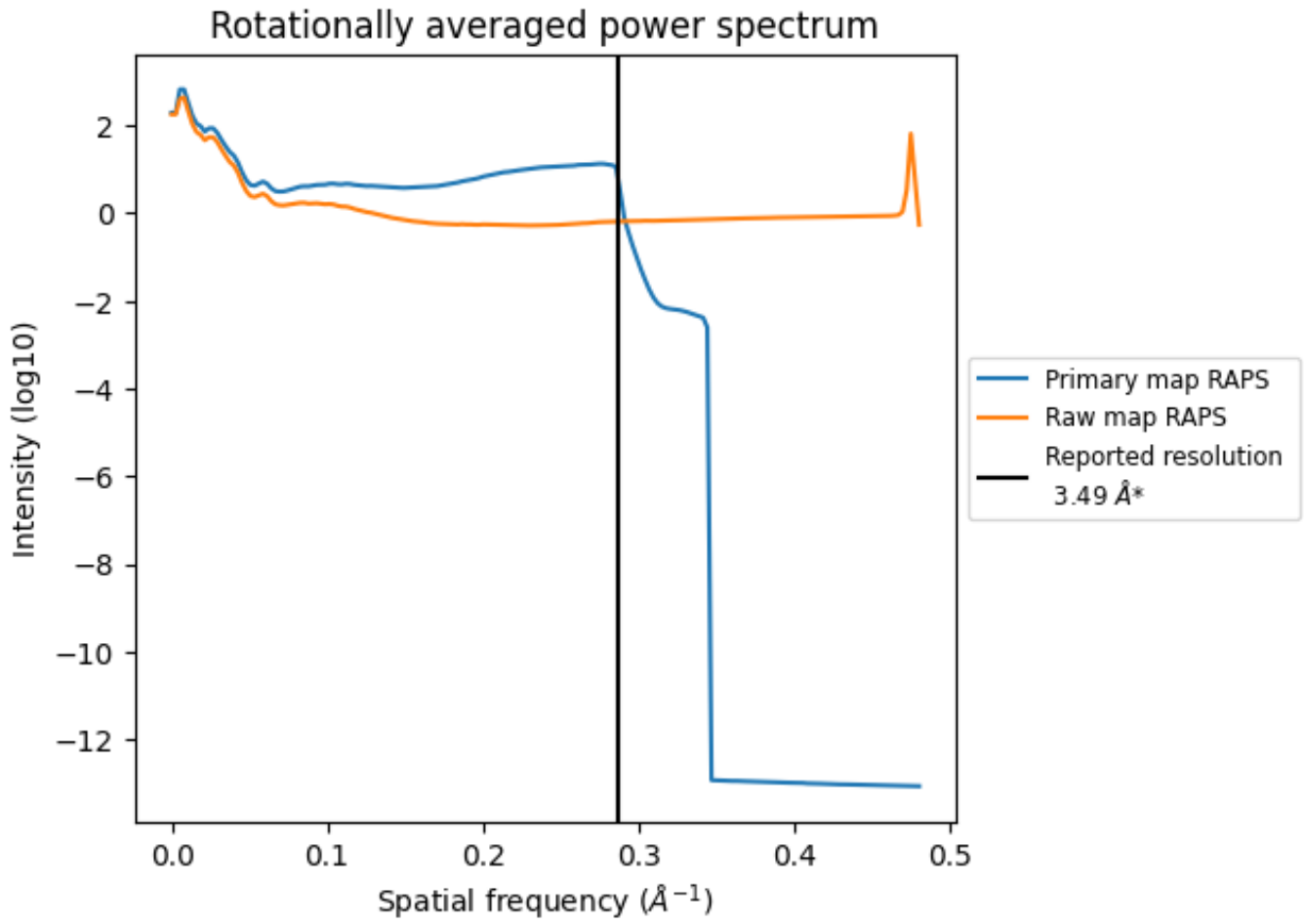
7.2 Volume estimate (i)



The volume at the recommended contour level is 160 nm^3; this corresponds to an approximate mass of 145 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)

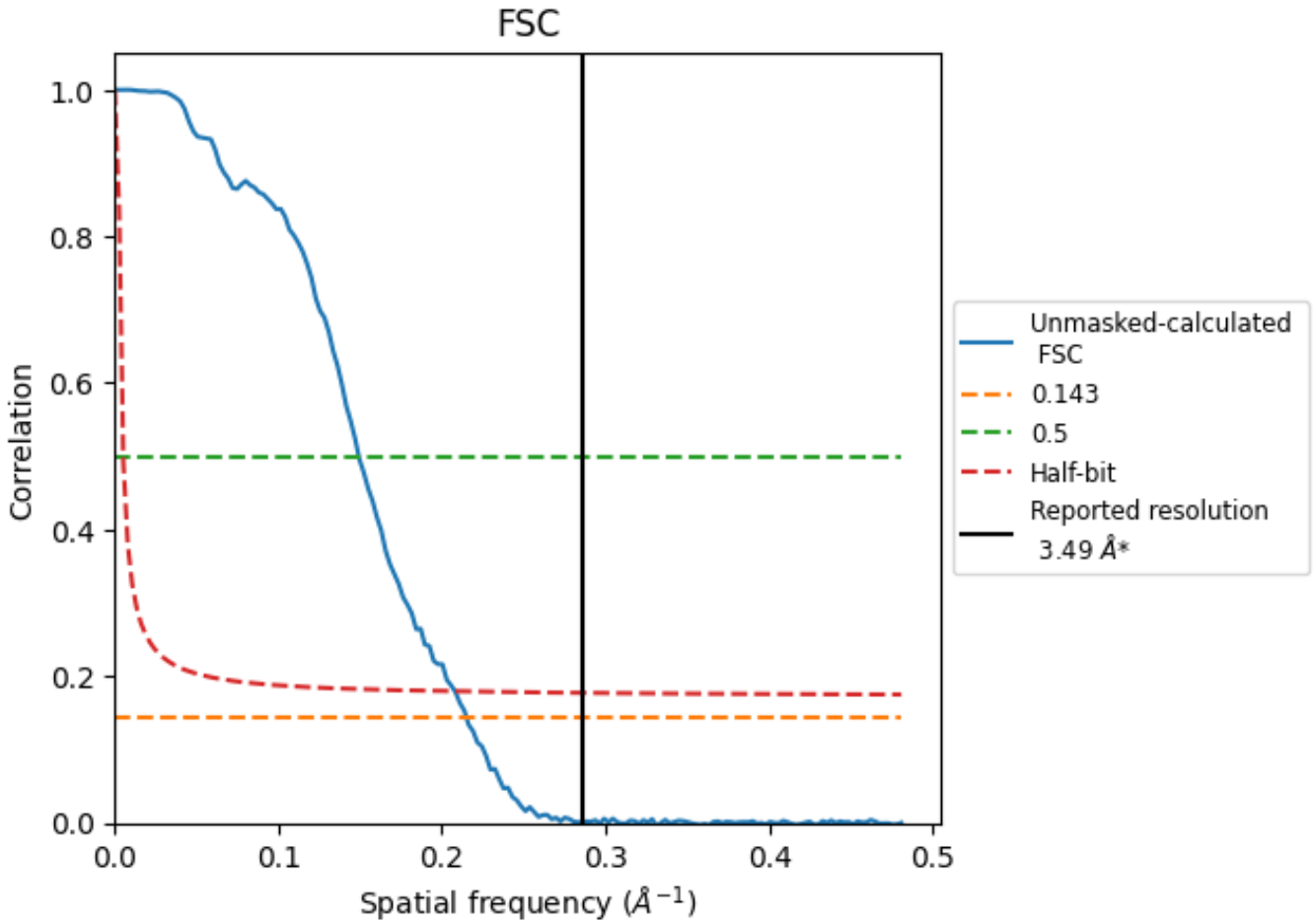


*Reported resolution corresponds to spatial frequency of 0.287 Å^{-1}

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.287 Å^{-1}

8.2 Resolution estimates (i)

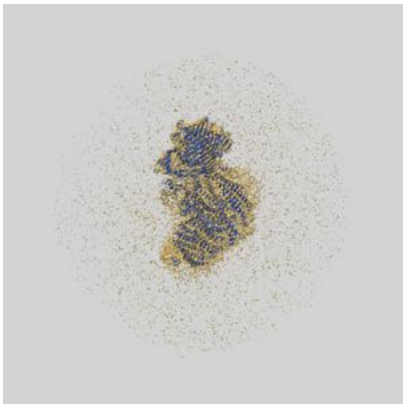
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.49	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.65	6.71	4.81

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.65 differs from the reported value 3.49 by more than 10 %

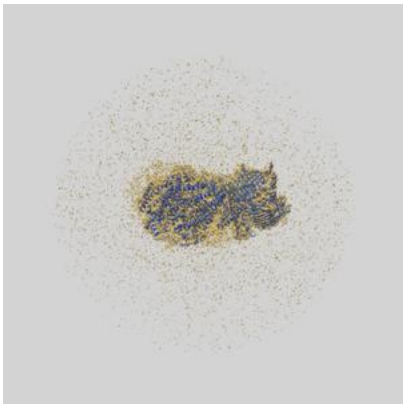
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-26469 and PDB model 7UEA. Per-residue inclusion information can be found in section 3 on page 14.

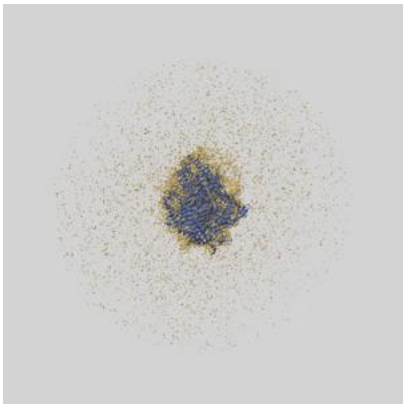
9.1 Map-model overlay



X



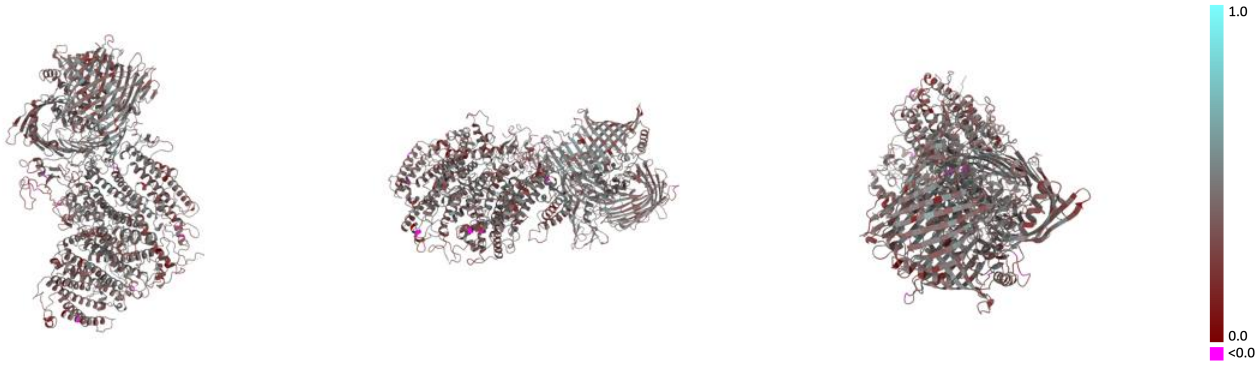
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.352 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.

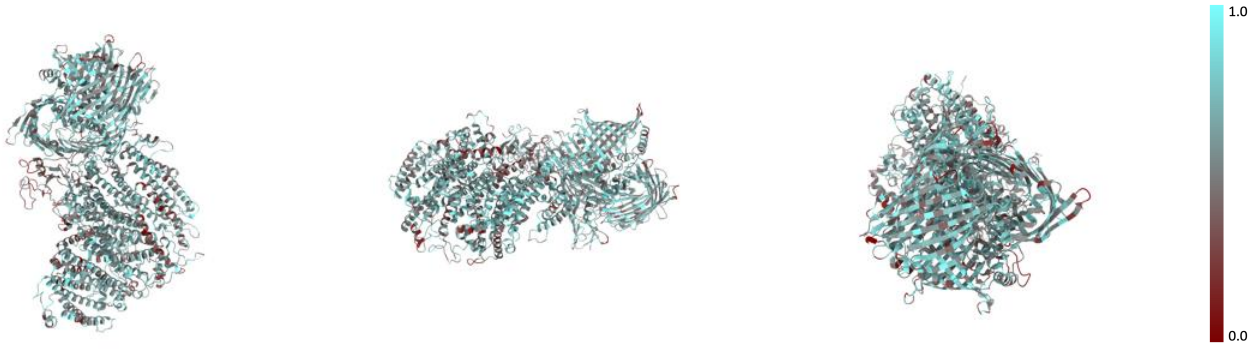
9.2 Q-score mapped to coordinate model (i)



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.

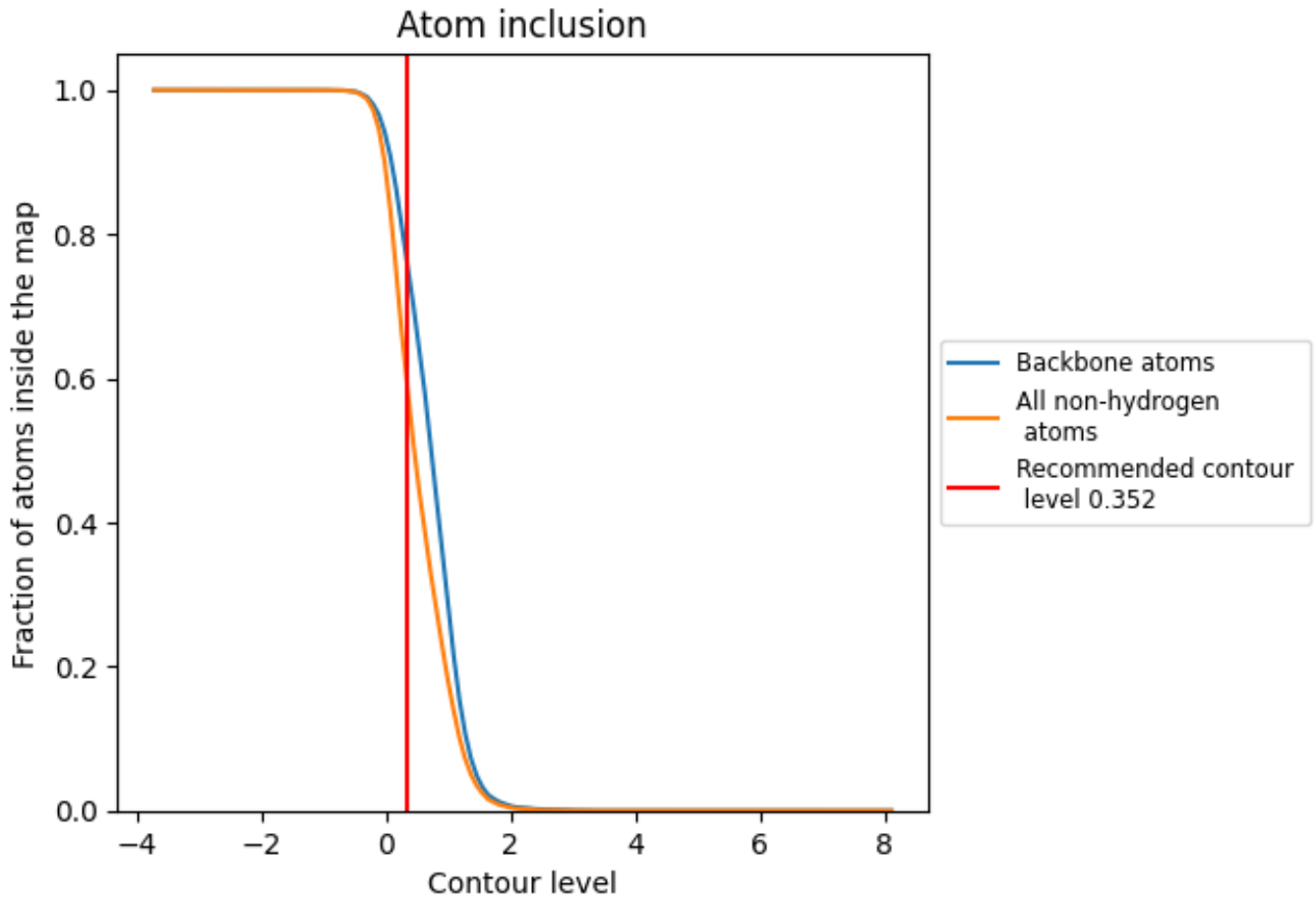
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.352).

9.4 Atom inclusion (i)



At the recommended contour level, 76% of all backbone atoms, 58% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.352) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5814	0.4060
A	0.6165	0.4250
B	0.5292	0.3720
C	0.3460	0.2920
D	0.3514	0.3080
U	0.6053	0.4160
V	0.6157	0.4350
W	0.6012	0.4070
a	0.5982	0.4080
c	0.4388	0.3370