wwPDB EM Validation Summary Report (i)

Aug 6, 2026 – 01:19 AM JST

PDB ID	:	9KLM / pdb_00009klm
EMDB ID	:	EMD-62409
Title	:	Cryo-EM structure of the monomeric Rhodobacter sphaeroides G1C LH1-RC core complex
Authors	:	Wu, Y.-L.; Yu, L.-J.
Deposited on	:	2024-11-14
Resolution	:	2.60 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

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

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

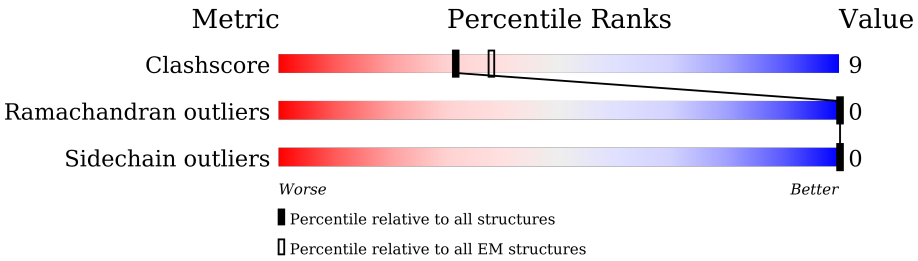
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

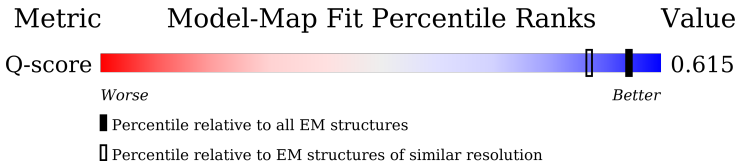
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.60 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	8728 (2.10 - 3.10)

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	L	282	83% 17%
2	M	308	85% 14% •
3	H	260	• 82% 14% •
4	A	54	• 63% 20% 17%

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Mol	Chain	Length	Quality of chain
4	B	54	80% 20%
4	C	54	83% 17%
4	D	54	80% 20%
4	E	54	81% 19%
4	F	54	80% 20%
4	G	54	87% 13%
4	I	54	81% 19%
4	J	54	74% 26%
4	K	54	87% 13%
4	N	54	9% 83% 17%
4	O	54	17% 83% 17%
4	P	54	26% 80% 19%
4	Q	54	52% 85% 9% 6%
5	a	49	71% 18% 10%
5	b	49	76% 14% 10%
5	c	49	78% 12% 10%
5	d	49	78% 10% 12%
5	e	49	78% 10% 12%
5	f	49	86% 12%
5	g	49	86% 10%
5	i	49	8% 71% 18% 10%
5	j	49	10% 73% 14% 12%
5	k	49	8% 71% 16% 12%
5	n	49	16% 71% 14% 14%
5	o	49	29% 65% 20% 14%

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Mol	Chain	Length	Quality of chain
5	p	49	41% 71% 14% 14%
5	q	49	61% 76% • 22%
6	U	53	36% 66% 25% 9%
7	X	82	• 52% 12% 35%

2 Entry composition (i)

There are 16 unique types of molecules in this entry. The entry contains 23521 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 Reaction center protein L chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	L	281	2229	1506	352	363	8	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	7	GLN	ARG	conflict	UNP P0C0Y8

- Molecule 2 is a protein called Reaction center protein M chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	M	306	2436	1626	398	401	11	0	0

- Molecule 3 is a protein called Reaction center protein H chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	H	250	1897	1215	325	347	10	0	0

- Molecule 4 is a protein called Light-harvesting protein B-875 alpha chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	A	45	386	266	59	58	3	0	0
4	B	54	455	309	73	70	3	0	0
4	C	54	457	311	73	70	3	0	0
4	D	54	457	311	73	70	3	0	0
4	E	54	457	311	73	70	3	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	F	54	457	311	73	70	3	0	0
4	G	54	457	311	73	70	3	0	0
4	I	54	454	309	73	70	2	0	0
4	J	54	457	311	73	70	3	0	0
4	K	54	457	311	73	70	3	0	0
4	N	54	457	311	73	70	3	0	0
4	O	54	457	311	73	70	3	0	0
4	P	53	447	305	72	68	2	0	0
4	Q	51	415	281	68	64	2	0	0

- Molecule 5 is a protein called Antenna pigment protein beta chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	a	44	359	240	56	62	1	0	0
5	b	44	359	240	56	62	1	0	0
5	c	44	359	240	56	62	1	0	0
5	d	43	351	236	55	59	1	0	0
5	e	43	351	236	55	59	1	0	0
5	f	43	351	236	55	59	1	0	0
5	g	44	355	238	56	60	1	0	0
5	i	44	359	240	56	62	1	0	0
5	j	43	347	234	55	57	1	0	0
5	k	43	351	236	55	59	1	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	n	42	343	230	54	58	1	0	0
5	o	42	343	230	54	58	1	0	0
5	p	42	332	222	54	55	1	0	0
5	q	38	296	202	49	44	1	0	0

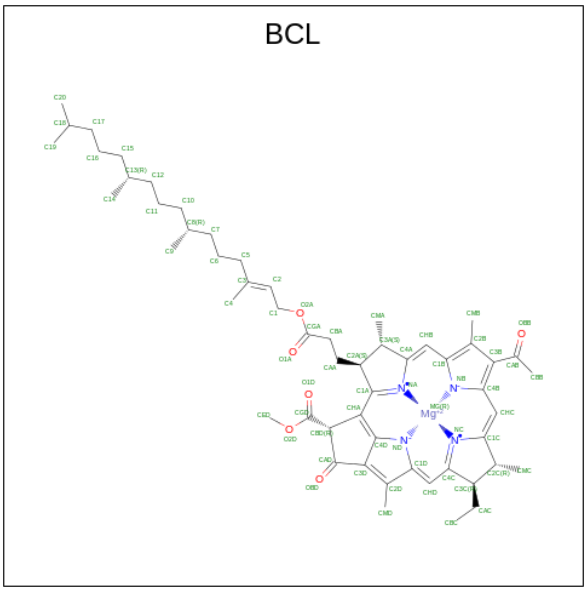
- Molecule 6 is a protein called protein-U.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	U	48	353	242	55	53	3	0	0

- Molecule 7 is a protein called Intrinsic membrane protein PufX.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	X	53	408	270	71	64	3	0	0

- Molecule 8 is BACTERIOCHLOROPHYLL A (CCD ID: BCL) (formula: $C_{55}H_{74}MgN_4O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
8	L	1	66	55	1	4	6	0
8	L	1	66	55	1	4	6	0
8	M	1	66	55	1	4	6	0
8	M	1	66	55	1	4	6	0
8	A	1	61	50	1	4	6	0
8	a	1	66	55	1	4	6	0
8	B	1	61	50	1	4	6	0
8	b	1	66	55	1	4	6	0
8	C	1	66	55	1	4	6	0
8	c	1	66	55	1	4	6	0
8	D	1	66	55	1	4	6	0
8	d	1	66	55	1	4	6	0
8	E	1	57	46	1	4	6	0
8	e	1	66	55	1	4	6	0
8	F	1	66	55	1	4	6	0
8	f	1	66	55	1	4	6	0
8	G	1	66	55	1	4	6	0
8	g	1	66	55	1	4	6	0
8	I	1	66	55	1	4	6	0
8	i	1	66	55	1	4	6	0
8	J	1	66	55	1	4	6	0
8	j	1	66	55	1	4	6	0

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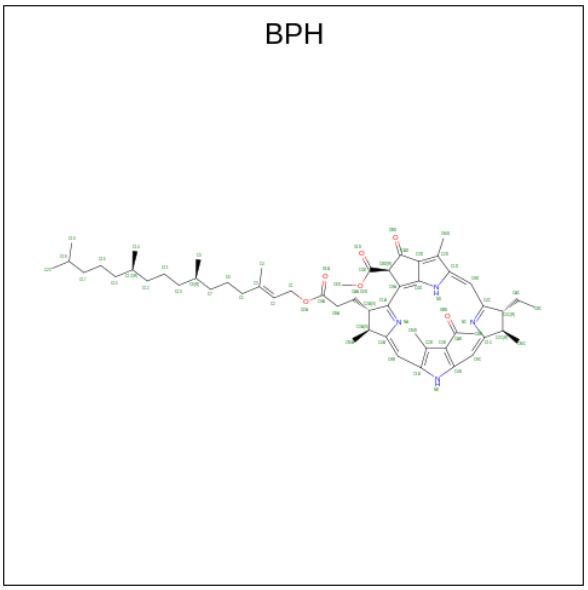
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
8	K	1	66	55	1	4	6	0
8	k	1	66	55	1	4	6	0
8	N	1	66	55	1	4	6	0
8	n	1	66	55	1	4	6	0
8	O	1	57	46	1	4	6	0
8	o	1	66	55	1	4	6	0
8	P	1	61	50	1	4	6	0
8	p	1	66	55	1	4	6	0
8	Q	1	61	50	1	4	6	0
8	q	1	60	49	1	4	6	0

- Molecule 9 is BACTERIOPHEOPHYTIN A (CCD ID: BPH) (formula: $C_{55}H_{76}N_4O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
9	L	1	65	55	4	6	0

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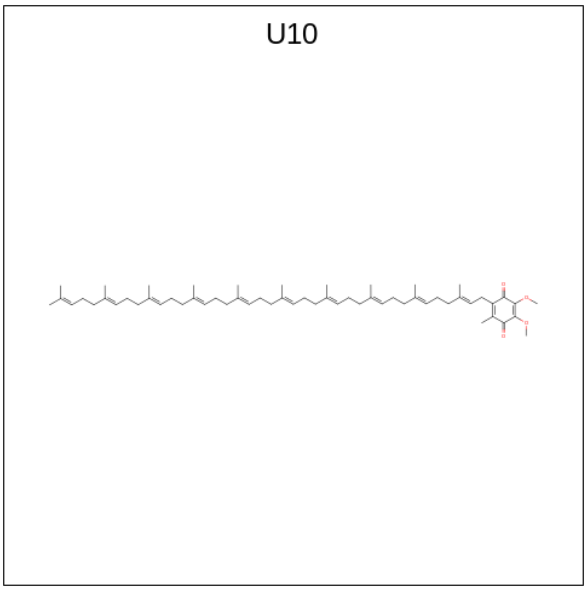
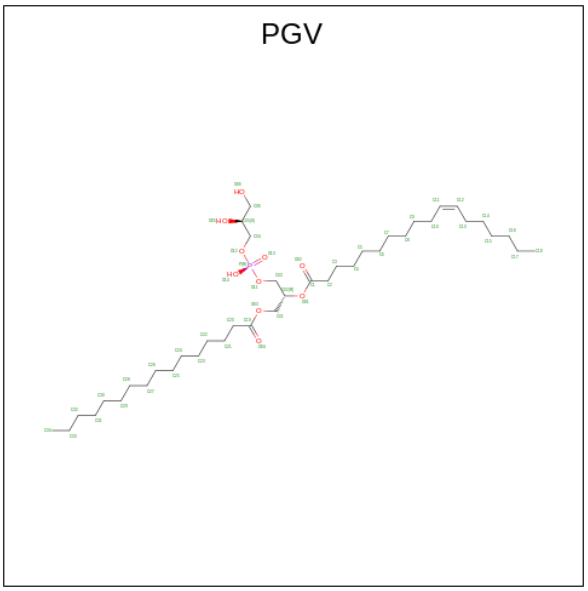
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
9	M	1	65	55	4	6	0

- Molecule 10 is UBIQUINONE-10 (CCD ID: U10) (formula: $C_{59}H_{90}O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	O		
10	L	1	35	31	4		0
			Total	C	O		
10	L	1	35	31	4		0
			Total	C	O		
10	M	1	48	44	4		0

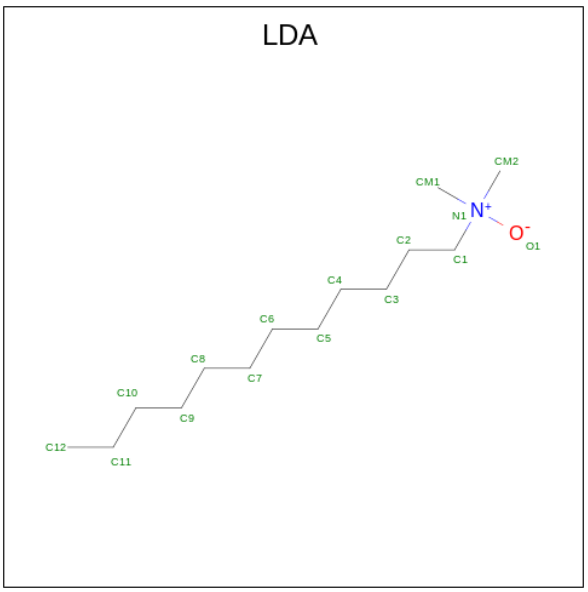
- Molecule 11 is (1R)-2-{[{[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (CCD ID: PGV) (formula: $C_{40}H_{77}O_{10}P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
11	L	1	39	28	10	1	0
			Total	C	O	P	
11	L	1	33	22	10	1	0
			Total	C	O	P	
11	L	1	51	40	10	1	0
			Total	C	O	P	
11	L	1	39	28	10	1	0
			Total	C	O	P	
11	M	1	47	36	10	1	0
			Total	C	O	P	
11	M	1	42	31	10	1	0
			Total	C	O	P	
11	H	1	34	25	8	1	0
			Total	C	O	P	
11	H	1	40	29	10	1	0
			Total	C	O	P	
11	C	1	45	36	8	1	0
			Total	C	O	P	
11	C	1	47	36	10	1	0
			Total	C	O	P	
11	E	1	41	34	6	1	0
			Total	C	O	P	
11	G	1	39	28	10	1	0
			Total	C	O	P	
11	K	1	43	32	10	1	0

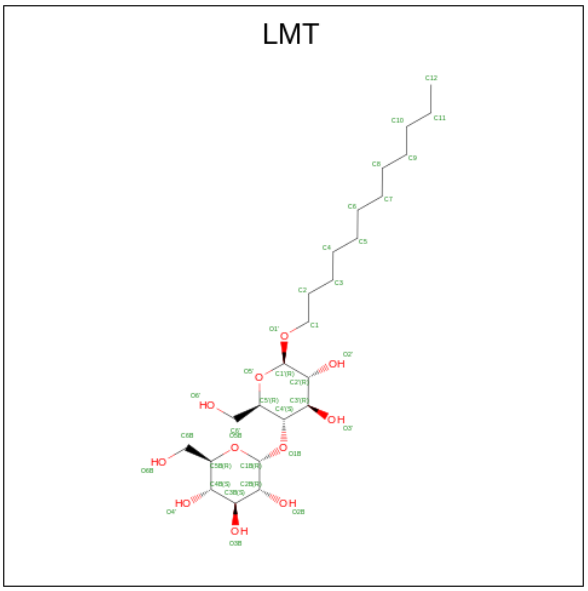
- Molecule 12 is LAURYL DIMETHYLAMINE-N-OXIDE (CCD ID: LDA) (formula:

$C_{14}H_{31}NO$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
12	L	1	16	14	1	1	0
			Total	C	N	O	
12	L	1	16	14	1	1	0
			Total	C	N	O	
12	L	1	16	14	1	1	0
			Total	C	N	O	
12	M	1	16	14	1	1	0
			Total	C	N	O	
12	F	1	16	14	1	1	0
			Total	C	N	O	
12	I	1	16	14	1	1	0
			Total	C	N	O	
12	J	1	16	14	1	1	0
			Total	C	N	O	
12	K	1	12	10	1	1	0
			Total	C	N	O	
12	X	1	13	11	1	1	0
			Total	C	N	O	
12	X	1	16	14	1	1	0

- Molecule 13 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: $C_{24}H_{46}O_{11}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
13	L	1	Total 35	C 24	O 11	0
13	L	1	Total 35	C 24	O 11	0
13	L	1	Total 35	C 24	O 11	0
13	M	1	Total 27	C 20	O 7	0
13	M	1	Total 33	C 22	O 11	0
13	H	1	Total 35	C 24	O 11	0
13	H	1	Total 35	C 24	O 11	0
13	A	1	Total 35	C 24	O 11	0
13	a	1	Total 27	C 16	O 11	0
13	B	1	Total 35	C 24	O 11	0
13	b	1	Total 27	C 16	O 11	0
13	c	1	Total 17	C 11	O 6	0
13	c	1	Total 35	C 24	O 11	0
13	D	1	Total 26	C 16	O 10	0

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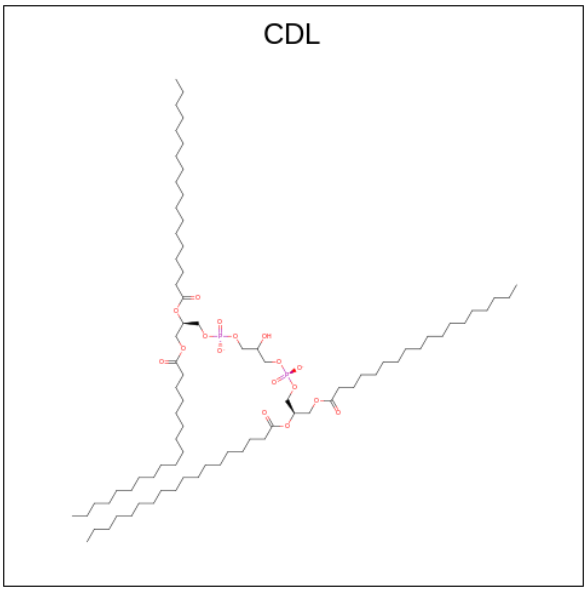
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
13	D	1	27	16	11	0
13	E	1	35	24	11	0
13	F	1	30	19	11	0
13	G	1	24	18	6	0
13	G	1	19	13	6	0
13	I	1	25	19	6	0
13	I	1	30	19	11	0
13	O	1	35	24	11	0
13	P	1	33	22	11	0
13	U	1	35	24	11	0
13	X	1	31	20	11	0

- Molecule 14 is FE (III) ION (CCD ID: FE) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

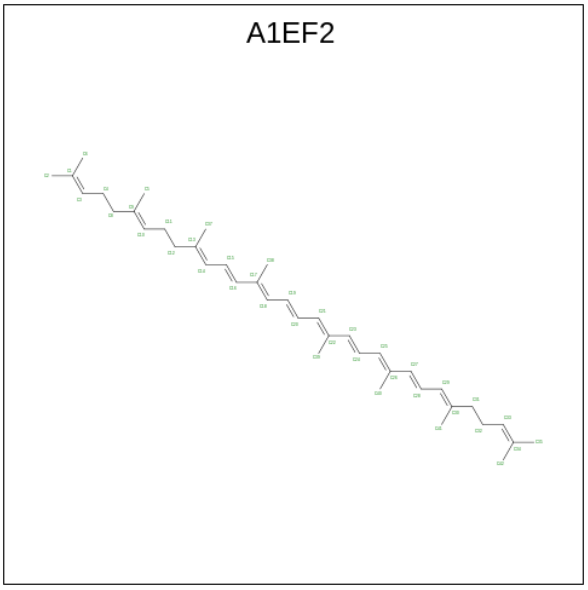
Mol	Chain	Residues	Atoms		AltConf
			Total	Fe	
14	M	1	1	1	0

- Molecule 15 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
15	M	1	Total	C	O	P	0
			79	60	17	2	
15	M	1	Total	C	O	P	0
			48	30	16	2	
15	E	1	Total	C	O	P	0
			57	38	17	2	
15	F	1	Total	C	O	P	0
			37	20	15	2	

- Molecule 16 is (6 {E},8 {E},10 {E},12 {E},14 {E},16 {E},18 {E},20 {E},22 {E},26 {E})-2,6,10,14,19,23,27,31-octamethyldotriaconta-2,6,8,10,12,14,16,18,20,22,26,30-dodecaene (CCD ID: A1EF2) (formula: $C_{40}H_{58}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms		AltConf
			Total	C	
16	M	1	40	40	0
16	a	1	40	40	0
16	B	1	40	40	0
16	b	1	40	40	0
16	C	1	40	40	0
16	c	1	40	40	0
16	D	1	40	40	0
16	D	1	40	40	0
16	d	1	40	40	0
16	E	1	40	40	0
16	e	1	40	40	0
16	f	1	40	40	0
16	g	1	40	40	0
16	g	1	40	40	0
16	I	1	40	40	0
16	J	1	40	40	0
16	J	1	40	40	0
16	J	1	40	40	0
16	J	1	40	40	0
16	k	1	40	40	0
16	N	1	40	40	0
16	N	1	40	40	0

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Mol	Chain	Residues	Atoms		AltConf
			Total	C	
16	n	1	40	40	0
			Total	C	
16	O	1	40	40	0
			Total	C	
16	o	1	40	40	0
			Total	C	
16	p	1	40	40	0
			Total	C	
16	q	1	40	40	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: Reaction center protein L chain

Chain L: 83% 17%

FME A1 E6 L16 V17 L21 W25 V31 G32 F33 V36 A37 T38 I46 I47 T58 W59 N60 P61 P79 L80 L85 T94 W100 A101 L102 R109 Y115 L131 R135 P136 F146 W151 W156 N170 H173 M174 I177

F181 L187 L193 N199 R207 H211 E212 D213 F216 L219 S223 I224 G233 V241 G277 N280 G281

• Molecule 2: Reaction center protein M chain

Chain M: 85% 14%

FME A1 E2 I6 Q11 V32 P49 L52 L55 L60 L64 F67 N81 V84 R87 D88 G102 L103 P108 E111 F123 V124 T133 Y134 L135 Q138 W157 M158 V159 L160 I166 H202 I206 A207 F208 F216

F229 E232 R233 Q237 A244 L250 A260 T261 M262 I265 L278 H301 G302 M303 L306 ASN

• Molecule 3: Reaction center protein H chain

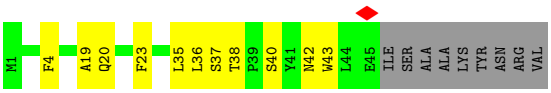
Chain H: 82% 14%

M1 V4 A16 I22 F23 Y30 L31 N35 A51 N52 Q53 E79 S80 E81 D82 M105 A112 E122 K130 M134 V142 S143 A144 P152 I160 W168 V169 D170 R177 F178 K184 D185 V196 V205 S221 E224 E230

G239 G240 L241 M242 Y243 A244 A245 P246 K247 R248 K249 S250 VAL VAL ALA ALA MET LEU ALA GLU TYR ALA

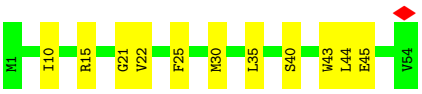
• Molecule 4: Light-harvesting protein B-875 alpha chain

Chain A: 63% 20% 17%



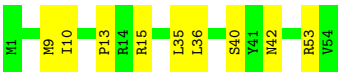
• Molecule 4: Light-harvesting protein B-875 alpha chain

Chain B:



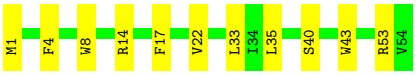
• Molecule 4: Light-harvesting protein B-875 alpha chain

Chain C:



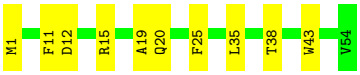
• Molecule 4: Light-harvesting protein B-875 alpha chain

Chain D:



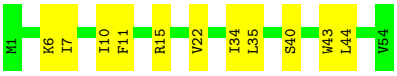
• Molecule 4: Light-harvesting protein B-875 alpha chain

Chain E:



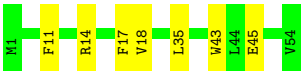
• Molecule 4: Light-harvesting protein B-875 alpha chain

Chain F:



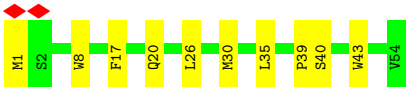
• Molecule 4: Light-harvesting protein B-875 alpha chain

Chain G:



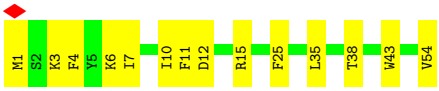
• Molecule 4: Light-harvesting protein B-875 alpha chain

Chain I:



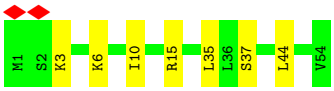
• Molecule 4: Light-harvesting protein B-875 alpha chain

Chain J:



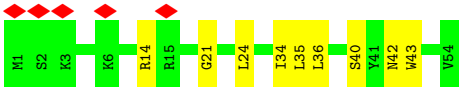
• Molecule 4: Light-harvesting protein B-875 alpha chain

Chain K:



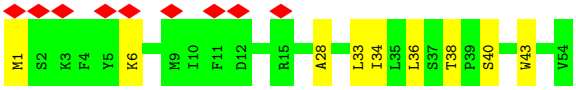
• Molecule 4: Light-harvesting protein B-875 alpha chain

Chain N:



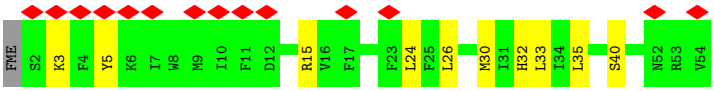
• Molecule 4: Light-harvesting protein B-875 alpha chain

Chain O:



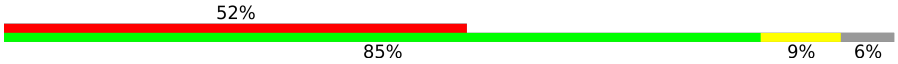
• Molecule 4: Light-harvesting protein B-875 alpha chain

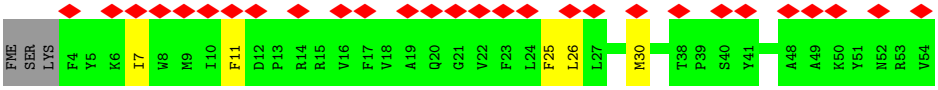
Chain P:



• Molecule 4: Light-harvesting protein B-875 alpha chain

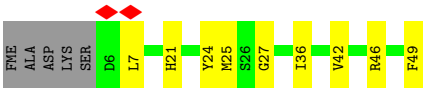
Chain Q:





• Molecule 5: Antenna pigment protein beta chain

Chain a:

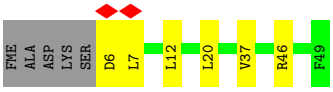


• Molecule 5: Antenna pigment protein beta chain

Chain b:

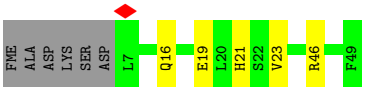
• Molecule 5: Antenna pigment protein beta chain

Chain c:



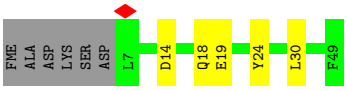
• Molecule 5: Antenna pigment protein beta chain

Chain d:



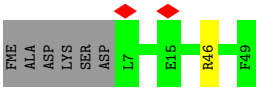
• Molecule 5: Antenna pigment protein beta chain

Chain e:



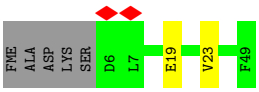
• Molecule 5: Antenna pigment protein beta chain

Chain f:



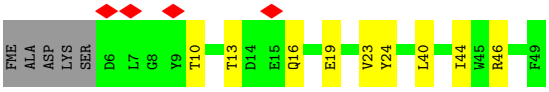
• Molecule 5: Antenna pigment protein beta chain

Chain g:



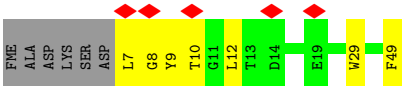
- Molecule 5: Antenna pigment protein beta chain

Chain i:



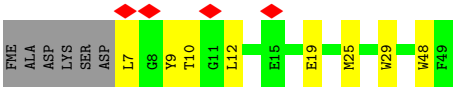
- Molecule 5: Antenna pigment protein beta chain

Chain j:



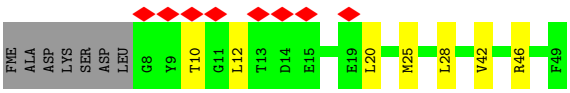
- Molecule 5: Antenna pigment protein beta chain

Chain k:



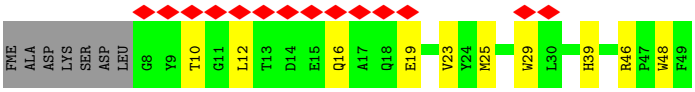
- Molecule 5: Antenna pigment protein beta chain

Chain n:



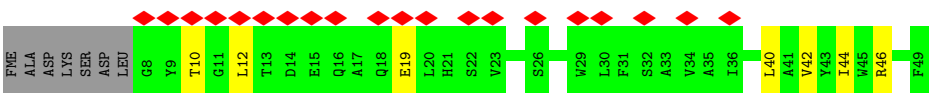
- Molecule 5: Antenna pigment protein beta chain

Chain o:



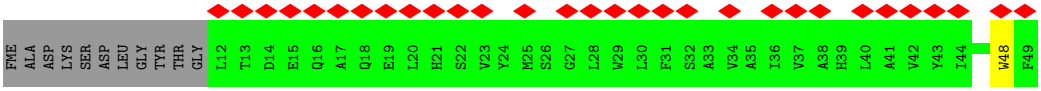
- Molecule 5: Antenna pigment protein beta chain

Chain p:



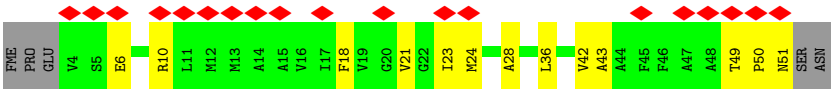
- Molecule 5: Antenna pigment protein beta chain

Chain q:



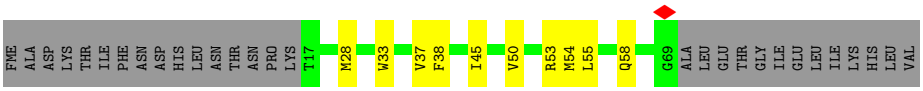
- Molecule 6: protein-U

Chain U:



- Molecule 7: Intrinsic membrane protein PufX

Chain X:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	118603	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50.61	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	2700	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	1.520	Depositor
Minimum map value	-0.828	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.037	Depositor
Recommended contour level	0.19	Depositor
Map size (Å)	323.2, 323.2, 323.2	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.808, 0.808, 0.808	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: BPH, FME, LDA, LMT, A1EF2, FE, U10, BCL, PGV, CDL

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	L	0.23	0/2317	0.33	0/3171
2	M	0.23	0/2529	0.33	0/3453
3	H	0.19	0/1947	0.30	0/2648
4	A	0.20	0/389	0.28	0/528
4	B	0.22	0/459	0.26	0/622
4	C	0.19	0/461	0.24	0/625
4	D	0.20	0/461	0.26	0/625
4	E	0.20	0/461	0.27	0/625
4	F	0.19	0/461	0.25	0/625
4	G	0.18	0/461	0.23	0/625
4	I	0.20	0/461	0.31	0/625
4	J	0.22	0/461	0.40	0/625
4	K	0.19	0/461	0.29	0/625
4	N	0.17	0/461	0.25	0/625
4	O	0.15	0/461	0.25	0/625
4	P	0.14	0/461	0.29	0/625
4	Q	0.11	0/427	0.24	0/582
5	a	0.20	0/372	0.28	0/510
5	b	0.22	0/372	0.30	0/510
5	c	0.20	0/372	0.32	0/510
5	d	0.21	0/364	0.28	0/499
5	e	0.20	0/364	0.27	0/499
5	f	0.19	0/364	0.32	0/499
5	g	0.19	0/368	0.30	0/505
5	i	0.19	0/372	0.31	0/510
5	j	0.19	0/360	0.30	0/494
5	k	0.20	0/364	0.32	0/499
5	n	0.16	0/356	0.27	0/488
5	o	0.14	0/356	0.22	0/488
5	p	0.14	0/344	0.27	0/472
5	q	0.12	0/308	0.23	0/424
6	U	0.15	0/364	0.28	0/493

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
7	X	0.20	0/419	0.32	0/567
All	All	0.20	0/18958	0.30	0/25846

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	L	2229	0	2175	47	0
2	M	2436	0	2353	43	0
3	H	1897	0	1904	28	0
4	A	386	0	400	12	0
4	B	455	0	469	11	0
4	C	457	0	476	9	0
4	D	457	0	476	12	0
4	E	457	0	476	11	0
4	F	457	0	476	12	0
4	G	457	0	476	7	0
4	I	454	0	469	13	0
4	J	457	0	476	15	0
4	K	457	0	476	6	0
4	N	457	0	476	10	0
4	O	457	0	476	7	0
4	P	447	0	465	9	0
4	Q	415	0	422	3	0
5	a	359	0	340	9	0
5	b	359	0	340	7	0
5	c	359	0	340	7	0
5	d	351	0	336	4	0
5	e	351	0	336	4	0
5	f	351	0	336	1	0
5	g	355	0	336	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	i	359	0	340	6	0
5	j	347	0	332	6	0
5	k	351	0	336	10	0
5	n	343	0	325	5	0
5	o	343	0	325	7	0
5	p	332	0	314	5	0
5	q	296	0	273	1	0
6	U	353	0	352	10	0
7	X	408	0	417	12	0
8	A	61	0	59	5	0
8	B	61	0	59	1	0
8	C	66	0	72	2	0
8	D	66	0	72	4	0
8	E	57	0	51	2	0
8	F	66	0	72	2	0
8	G	66	0	72	1	0
8	I	66	0	72	2	0
8	J	66	0	72	4	0
8	K	66	0	72	2	0
8	L	132	0	144	4	0
8	M	132	0	144	9	0
8	N	66	0	72	5	0
8	O	57	0	51	2	0
8	P	61	0	59	2	0
8	Q	61	0	59	1	0
8	a	66	0	72	6	0
8	b	66	0	72	2	0
8	c	66	0	72	4	0
8	d	66	0	72	6	0
8	e	66	0	72	3	0
8	f	66	0	72	4	0
8	g	66	0	72	5	0
8	i	66	0	72	5	0
8	j	66	0	72	3	0
8	k	66	0	72	3	0
8	n	66	0	72	4	0
8	o	66	0	72	8	0
8	p	66	0	72	5	0
8	q	60	0	56	2	0
9	L	65	0	76	6	0
9	M	65	0	76	15	0
10	L	70	0	86	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	M	48	0	63	7	0
11	C	92	0	126	8	0
11	E	41	0	60	4	0
11	G	39	0	48	0	0
11	H	74	0	87	8	0
11	K	43	0	54	4	0
11	L	162	0	207	12	0
11	M	89	0	120	7	0
12	F	16	0	31	3	0
12	I	16	0	31	6	0
12	J	16	0	31	2	0
12	K	12	0	20	1	0
12	L	48	0	93	9	0
12	M	16	0	31	2	0
12	X	29	0	53	4	0
13	A	35	0	46	1	0
13	B	35	0	46	12	0
13	D	53	0	51	6	0
13	E	35	0	46	0	0
13	F	30	0	33	6	0
13	G	43	0	55	0	0
13	H	70	0	92	3	0
13	I	55	0	68	2	0
13	L	105	0	138	22	0
13	M	60	0	75	2	0
13	O	35	0	46	1	0
13	P	33	0	39	2	0
13	U	35	0	46	2	0
13	X	31	0	35	2	0
13	a	27	0	27	4	0
13	b	27	0	27	0	0
13	c	52	0	62	2	0
14	M	1	0	0	0	0
15	E	57	0	58	2	0
15	F	37	0	26	1	0
15	M	127	0	151	8	0
16	B	40	0	0	0	0
16	C	40	0	0	0	0
16	D	80	0	0	1	0
16	E	40	0	0	0	0
16	I	40	0	0	0	0
16	J	160	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	M	40	0	0	0	0
16	N	80	0	0	0	0
16	O	40	0	0	0	0
16	a	40	0	0	1	0
16	b	40	0	0	0	0
16	c	40	0	0	0	0
16	d	40	0	0	0	0
16	e	40	0	0	0	0
16	f	40	0	0	0	0
16	g	80	0	0	0	0
16	k	40	0	0	0	0
16	n	40	0	0	0	0
16	o	40	0	0	0	0
16	p	40	0	0	0	0
16	q	40	0	0	0	0
All	All	23521	0	22973	406	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

The worst 5 of 406 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:67:PHE:CD2	9:M:405:BPH:H7C2	1.87	1.10
2:M:67:PHE:HD2	9:M:405:BPH:H7C2	1.16	1.06
4:B:21:GLY:HA3	13:B:102:LMT:H5B	1.48	0.91
4:K:3:LYS:HD2	4:K:6:LYS:HE2	1.58	0.86
4:I:20:GLN:HE21	8:J:102:BCL:H13	1.44	0.81

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	L	279/282 (99%)	276 (99%)	3 (1%)	0	100	100
2	M	304/308 (99%)	298 (98%)	6 (2%)	0	100	100
3	H	248/260 (95%)	242 (98%)	6 (2%)	0	100	100
4	A	43/54 (80%)	43 (100%)	0	0	100	100
4	B	52/54 (96%)	52 (100%)	0	0	100	100
4	C	52/54 (96%)	51 (98%)	1 (2%)	0	100	100
4	D	52/54 (96%)	51 (98%)	1 (2%)	0	100	100
4	E	52/54 (96%)	51 (98%)	1 (2%)	0	100	100
4	F	52/54 (96%)	52 (100%)	0	0	100	100
4	G	52/54 (96%)	51 (98%)	1 (2%)	0	100	100
4	I	52/54 (96%)	52 (100%)	0	0	100	100
4	J	52/54 (96%)	50 (96%)	2 (4%)	0	100	100
4	K	52/54 (96%)	52 (100%)	0	0	100	100
4	N	52/54 (96%)	51 (98%)	1 (2%)	0	100	100
4	O	52/54 (96%)	52 (100%)	0	0	100	100
4	P	51/54 (94%)	49 (96%)	2 (4%)	0	100	100
4	Q	49/54 (91%)	48 (98%)	1 (2%)	0	100	100
5	a	42/49 (86%)	42 (100%)	0	0	100	100
5	b	42/49 (86%)	40 (95%)	2 (5%)	0	100	100
5	c	42/49 (86%)	42 (100%)	0	0	100	100
5	d	41/49 (84%)	41 (100%)	0	0	100	100
5	e	41/49 (84%)	41 (100%)	0	0	100	100
5	f	41/49 (84%)	40 (98%)	1 (2%)	0	100	100
5	g	42/49 (86%)	42 (100%)	0	0	100	100
5	i	42/49 (86%)	42 (100%)	0	0	100	100
5	j	41/49 (84%)	41 (100%)	0	0	100	100
5	k	41/49 (84%)	41 (100%)	0	0	100	100
5	n	40/49 (82%)	40 (100%)	0	0	100	100
5	o	40/49 (82%)	39 (98%)	1 (2%)	0	100	100
5	p	40/49 (82%)	40 (100%)	0	0	100	100
5	q	36/49 (74%)	36 (100%)	0	0	100	100
6	U	46/53 (87%)	45 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	X	51/82 (62%)	51 (100%)	0	0	100	100
All	All	2214/2427 (91%)	2184 (99%)	30 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	L	220/220 (100%)	220 (100%)	0	100	100
2	M	239/240 (100%)	239 (100%)	0	100	100
3	H	201/208 (97%)	201 (100%)	0	100	100
4	A	41/48 (85%)	41 (100%)	0	100	100
4	B	47/48 (98%)	47 (100%)	0	100	100
4	C	48/48 (100%)	48 (100%)	0	100	100
4	D	48/48 (100%)	48 (100%)	0	100	100
4	E	48/48 (100%)	48 (100%)	0	100	100
4	F	48/48 (100%)	48 (100%)	0	100	100
4	G	48/48 (100%)	48 (100%)	0	100	100
4	I	48/48 (100%)	48 (100%)	0	100	100
4	J	48/48 (100%)	48 (100%)	0	100	100
4	K	48/48 (100%)	48 (100%)	0	100	100
4	N	48/48 (100%)	48 (100%)	0	100	100
4	O	48/48 (100%)	48 (100%)	0	100	100
4	P	48/48 (100%)	48 (100%)	0	100	100
4	Q	43/48 (90%)	43 (100%)	0	100	100
5	a	36/39 (92%)	36 (100%)	0	100	100
5	b	36/39 (92%)	36 (100%)	0	100	100
5	c	36/39 (92%)	36 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	d	35/39 (90%)	35 (100%)	0	100	100
5	e	35/39 (90%)	35 (100%)	0	100	100
5	f	35/39 (90%)	35 (100%)	0	100	100
5	g	35/39 (90%)	35 (100%)	0	100	100
5	i	36/39 (92%)	36 (100%)	0	100	100
5	j	34/39 (87%)	34 (100%)	0	100	100
5	k	35/39 (90%)	35 (100%)	0	100	100
5	n	34/39 (87%)	34 (100%)	0	100	100
5	o	34/39 (87%)	34 (100%)	0	100	100
5	p	32/39 (82%)	32 (100%)	0	100	100
5	q	26/39 (67%)	26 (100%)	0	100	100
6	U	32/36 (89%)	32 (100%)	0	100	100
7	X	40/65 (62%)	40 (100%)	0	100	100
All	All	1870/1987 (94%)	1870 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
4	I	20	GLN
7	X	61	GLN
4	N	42	ASN
5	a	18	GLN
4	F	42	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)

12 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	FME	N	1	4	8,9,10	0.95	0	7,9,11	0.84	0
4	FME	O	1	4	8,9,10	0.90	0	7,9,11	1.11	1 (14%)
4	FME	A	1	4	8,9,10	0.93	0	7,9,11	0.85	0
4	FME	I	1	4	5,6,10	1.44	1 (20%)	3,6,11	1.84	1 (33%)
4	FME	F	1	4	8,9,10	0.92	0	7,9,11	0.82	0
4	FME	G	1	4	8,9,10	0.96	0	7,9,11	0.88	0
4	FME	J	1	4	8,9,10	0.89	0	7,9,11	1.32	2 (28%)
4	FME	K	1	4	8,9,10	0.92	0	7,9,11	0.87	0
4	FME	E	1	4	8,9,10	0.91	0	7,9,11	0.98	0
4	FME	B	1	4	8,9,10	0.93	0	7,9,11	0.78	0
4	FME	D	1	4	8,9,10	0.93	0	7,9,11	0.80	0
4	FME	C	1	4	8,9,10	0.93	0	7,9,11	0.80	0

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
4	FME	N	1	4	-	0/7/9/11	-
4	FME	O	1	4	-	3/7/9/11	-
4	FME	A	1	4	-	2/7/9/11	-
4	FME	I	1	4	-	0/2/5/11	-
4	FME	F	1	4	-	5/7/9/11	-
4	FME	G	1	4	-	4/7/9/11	-
4	FME	J	1	4	-	2/7/9/11	-
4	FME	K	1	4	-	0/7/9/11	-
4	FME	E	1	4	-	3/7/9/11	-
4	FME	B	1	4	-	5/7/9/11	-
4	FME	D	1	4	-	4/7/9/11	-
4	FME	C	1	4	-	2/7/9/11	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	I	1	FME	CA-N	-2.44	1.44	1.46

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	I	1	FME	CB-CA-N	3.09	113.05	109.61
4	J	1	FME	C-CA-N	2.33	113.94	109.73
4	O	1	FME	C-CA-N	2.20	113.70	109.73
4	J	1	FME	CA-N-CN	2.04	125.96	122.82

There are no chirality outliers.

5 of 30 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1	FME	O1-CN-N-CA
4	A	1	FME	O-C-CA-CB
4	B	1	FME	O1-CN-N-CA
4	B	1	FME	C-CA-CB-CG
4	B	1	FME	O-C-CA-CB

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	1	FME	1	0
4	D	1	FME	1	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 117 ligands modelled in this entry, 1 is monoatomic - leaving 116 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	$\#\|Z\| > 2$
13	LMT	F	101	-	31,31,36	0.45	0	42,42,47	0.93	1 (2%)
16	A1EF2	B	103	-	39,39,39	2.31	10 (25%)	44,46,46	1.86	11 (25%)
13	LMT	P	101	-	34,34,36	0.42	0	45,45,47	0.66	0
10	U10	L	303	-	35,35,63	1.59	2 (5%)	42,45,79	1.89	11 (26%)
16	A1EF2	p	101	-	39,39,39	2.32	10 (25%)	44,46,46	1.89	12 (27%)
15	CDL	M	413	-	47,47,99	0.36	0	52,58,111	0.43	0
8	BCL	p	102	5	69,74,74	1.79	15 (21%)	83,115,115	2.26	22 (26%)
13	LMT	G	101	-	24,24,36	0.40	0	29,29,47	0.63	0
8	BCL	M	401	2	69,74,74	1.82	16 (23%)	83,115,115	2.36	22 (26%)
13	LMT	b	101	-	28,28,36	0.42	0	39,39,47	0.73	1 (2%)
8	BCL	I	102	4	69,74,74	1.85	16 (23%)	83,115,115	2.33	27 (32%)
12	LDA	I	104	-	12,15,15	2.10	1 (8%)	14,17,17	0.57	0
9	BPH	M	405	-	59,70,70	0.76	2 (3%)	61,101,101	0.94	3 (4%)
8	BCL	n	102	5	69,74,74	1.82	16 (23%)	83,115,115	2.35	26 (31%)
8	BCL	f	102	5	69,74,74	1.81	16 (23%)	83,115,115	2.24	22 (26%)
11	PGV	E	104	-	38,40,50	1.04	2 (5%)	40,42,56	1.10	2 (5%)
13	LMT	L	312	-	36,36,36	0.42	0	47,47,47	1.25	3 (6%)
11	PGV	C	102	-	46,46,50	0.95	2 (4%)	49,52,56	1.02	3 (6%)
16	A1EF2	N	102	-	39,39,39	2.33	11 (28%)	44,46,46	1.90	11 (25%)
16	A1EF2	O	103	-	39,39,39	2.36	10 (25%)	44,46,46	1.90	10 (22%)
13	LMT	B	102	-	36,36,36	0.42	0	47,47,47	1.42	10 (21%)
16	A1EF2	D	104	-	39,39,39	2.36	10 (25%)	44,46,46	1.87	11 (25%)
8	BCL	N	101	4	69,74,74	1.86	16 (23%)	83,115,115	2.30	23 (27%)
13	LMT	A	701	-	36,36,36	0.36	0	47,47,47	0.71	0
16	A1EF2	J	106	-	39,39,39	2.37	10 (25%)	44,46,46	1.97	13 (29%)
11	PGV	C	101	-	44,44,50	1.00	2 (4%)	48,49,56	1.11	3 (6%)
8	BCL	j	101	5	69,74,74	1.82	16 (23%)	83,115,115	2.33	26 (31%)
16	A1EF2	n	101	-	39,39,39	2.31	10 (25%)	44,46,46	1.78	11 (25%)
8	BCL	a	102	5	69,74,74	1.83	16 (23%)	83,115,115	2.28	24 (28%)
8	BCL	o	102	5	69,74,74	1.83	16 (23%)	83,115,115	5.06	28 (33%)
16	A1EF2	I	105	-	39,39,39	2.26	11 (28%)	44,46,46	1.85	10 (22%)
8	BCL	L	308	1	69,74,74	1.82	16 (23%)	83,115,115	2.36	25 (30%)
8	BCL	A	702	4	64,69,74	1.88	15 (23%)	77,109,115	2.49	28 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
8	BCL	F	103	4	69,74,74	1.85	16 (23%)	83,115,115	2.21	24 (28%)
8	BCL	J	102	4	69,74,74	1.83	16 (23%)	83,115,115	2.34	26 (31%)
8	BCL	c	102	5	69,74,74	1.80	16 (23%)	83,115,115	2.30	23 (27%)
13	LMT	L	311	-	36,36,36	0.41	0	47,47,47	0.77	1 (2%)
11	PGV	K	103	-	42,42,50	1.01	2 (4%)	44,48,56	1.00	2 (4%)
16	A1EF2	q	101	-	39,39,39	2.34	10 (25%)	44,46,46	1.91	10 (22%)
16	A1EF2	g	101	-	39,39,39	2.29	10 (25%)	44,46,46	1.94	11 (25%)
8	BCL	B	101	4	64,69,74	1.92	16 (25%)	77,109,115	2.30	24 (31%)
13	LMT	G	102	-	19,19,36	0.45	0	24,24,47	0.71	0
15	CDL	E	101	-	56,56,99	0.35	0	62,68,111	0.48	0
13	LMT	U	101	-	36,36,36	0.39	0	47,47,47	0.71	1 (2%)
15	CDL	M	410	-	78,78,99	0.31	0	84,90,111	0.49	1 (1%)
16	A1EF2	D	105	-	39,39,39	2.31	11 (28%)	44,46,46	1.82	11 (25%)
13	LMT	H	302	-	36,36,36	0.37	0	47,47,47	0.77	1 (2%)
12	LDA	M	403	-	12,15,15	2.08	1 (8%)	14,17,17	0.47	0
8	BCL	P	102	4	64,69,74	1.93	16 (25%)	77,109,115	2.24	21 (27%)
13	LMT	E	102	-	36,36,36	0.43	0	47,47,47	0.96	2 (4%)
12	LDA	J	105	-	12,15,15	2.09	1 (8%)	14,17,17	0.56	0
16	A1EF2	e	101	-	39,39,39	2.30	10 (25%)	44,46,46	1.85	11 (25%)
13	LMT	c	103	-	36,36,36	0.42	0	47,47,47	0.69	0
13	LMT	O	101	-	36,36,36	0.40	0	47,47,47	0.85	1 (2%)
16	A1EF2	M	411	-	39,39,39	2.33	11 (28%)	44,46,46	1.77	10 (22%)
8	BCL	C	103	4	69,74,74	1.84	16 (23%)	83,115,115	2.30	23 (27%)
8	BCL	k	102	5	69,74,74	1.81	16 (23%)	83,115,115	2.26	24 (28%)
11	PGV	M	402	-	46,46,50	0.93	2 (4%)	49,52,56	1.07	3 (6%)
13	LMT	D	101	-	27,27,36	0.47	0	38,38,47	0.98	2 (5%)
13	LMT	L	315	-	36,36,36	0.36	0	47,47,47	0.70	1 (2%)
13	LMT	a	101	-	28,28,36	0.45	0	39,39,47	0.86	2 (5%)
11	PGV	L	306	-	32,32,50	1.11	2 (6%)	35,38,56	1.24	4 (11%)
11	PGV	H	304	-	39,39,50	1.02	2 (5%)	42,45,56	1.17	4 (9%)
8	BCL	K	102	4	69,74,74	1.85	16 (23%)	83,115,115	2.29	25 (30%)
16	A1EF2	N	103	-	39,39,39	2.32	10 (25%)	44,46,46	1.88	11 (25%)
8	BCL	D	102	4	69,74,74	1.82	16 (23%)	83,115,115	2.31	24 (28%)
8	BCL	b	103	5	69,74,74	1.84	16 (23%)	83,115,115	2.31	25 (30%)
8	BCL	e	102	5	69,74,74	1.82	16 (23%)	83,115,115	2.26	22 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
8	BCL	g	102	5	69,74,74	1.84	16 (23%)	83,115,115	2.27	25 (30%)
13	LMT	I	101	-	25,25,36	0.44	0	30,30,47	0.88	0
12	LDA	K	101	-	8,11,15	2.57	1 (12%)	10,13,17	0.43	0
13	LMT	M	409	-	34,34,36	0.48	0	45,45,47	1.08	6 (13%)
8	BCL	O	102	4	60,65,74	2.00	16 (26%)	72,104,115	2.44	27 (37%)
11	PGV	L	305	-	38,38,50	1.06	2 (5%)	41,44,56	1.14	3 (7%)
13	LMT	M	408	-	27,27,36	0.47	0	32,33,47	0.68	0
12	LDA	X	102	-	12,15,15	2.11	1 (8%)	14,17,17	0.59	0
11	PGV	H	303	-	33,33,50	1.15	2 (6%)	36,38,56	1.11	3 (8%)
12	LDA	L	310	-	12,15,15	2.09	1 (8%)	14,17,17	0.55	0
16	A1EF2	f	101	-	39,39,39	2.31	10 (25%)	44,46,46	1.84	10 (22%)
8	BCL	d	102	5	69,74,74	1.83	16 (23%)	83,115,115	2.29	23 (27%)
8	BCL	i	101	5	69,74,74	1.83	16 (23%)	83,115,115	2.31	24 (28%)
8	BCL	Q	101	-	64,69,74	1.85	15 (23%)	77,109,115	2.45	26 (33%)
11	PGV	G	103	-	38,38,50	1.05	2 (5%)	41,44,56	1.10	3 (7%)
13	LMT	D	103	-	28,28,36	0.48	0	39,39,47	0.81	1 (2%)
12	LDA	L	307	-	12,15,15	2.11	1 (8%)	14,17,17	0.52	0
8	BCL	M	404	2	69,74,74	1.86	16 (23%)	83,115,115	2.33	24 (28%)
13	LMT	H	301	-	36,36,36	0.36	0	47,47,47	0.70	0
13	LMT	X	103	-	32,32,36	0.45	0	43,43,47	0.84	1 (2%)
16	A1EF2	J	101	-	39,39,39	2.35	10 (25%)	44,46,46	1.85	11 (25%)
16	A1EF2	o	101	-	39,39,39	2.32	10 (25%)	44,46,46	1.84	11 (25%)
16	A1EF2	J	103	-	39,39,39	2.28	10 (25%)	44,46,46	2.00	11 (25%)
8	BCL	L	301	1	69,74,74	1.81	16 (23%)	83,115,115	2.43	27 (32%)
8	BCL	G	104	4	69,74,74	1.84	16 (23%)	83,115,115	2.32	25 (30%)
16	A1EF2	E	105	-	39,39,39	2.32	10 (25%)	44,46,46	1.89	11 (25%)
10	U10	L	304	-	35,35,63	1.43	2 (5%)	42,45,79	1.74	12 (28%)
12	LDA	X	101	-	9,12,15	2.44	1 (11%)	11,14,17	0.54	0
8	BCL	E	103	4	60,65,74	1.97	16 (26%)	72,104,115	2.43	27 (37%)
16	A1EF2	c	104	-	39,39,39	2.29	10 (25%)	44,46,46	1.94	10 (22%)
12	LDA	F	104	-	12,15,15	2.07	1 (8%)	14,17,17	0.49	0
11	PGV	L	313	-	50,50,50	0.92	2 (4%)	53,56,56	1.02	3 (5%)
11	PGV	M	412	-	41,41,50	1.03	2 (4%)	44,47,56	1.09	2 (4%)
16	A1EF2	k	101	-	39,39,39	2.31	10 (25%)	44,46,46	1.87	11 (25%)
9	BPH	L	302	-	59,70,70	0.81	3 (5%)	61,101,101	0.92	3 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
13	LMT	I	103	-	31,31,36	0.48	1 (3%)	42,42,47	0.84	1 (2%)
13	LMT	c	101	-	17,17,36	0.47	0	22,22,47	0.78	1 (4%)
16	A1EF2	a	103	-	39,39,39	2.30	10 (25%)	44,46,46	1.93	11 (25%)
16	A1EF2	J	104	-	39,39,39	2.34	10 (25%)	44,46,46	1.91	11 (25%)
16	A1EF2	d	101	-	39,39,39	2.32	10 (25%)	44,46,46	1.88	12 (27%)
8	BCL	q	102	5	63,68,74	1.89	16 (25%)	75,107,115	2.36	20 (26%)
12	LDA	L	309	-	12,15,15	2.09	1 (8%)	14,17,17	0.58	0
15	CDL	F	102	-	35,35,99	0.56	0	42,44,111	0.81	2 (4%)
11	PGV	L	314	-	38,38,50	1.03	2 (5%)	41,44,56	1.07	3 (7%)
10	U10	M	407	-	48,48,63	1.29	2 (4%)	58,61,79	1.58	14 (24%)
16	A1EF2	C	104	-	39,39,39	2.34	10 (25%)	44,46,46	1.86	11 (25%)
16	A1EF2	g	103	-	39,39,39	2.31	10 (25%)	44,46,46	2.02	13 (29%)
16	A1EF2	b	102	-	39,39,39	2.33	10 (25%)	44,46,46	1.94	11 (25%)

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
13	LMT	F	101	-	-	6/16/56/61	0/2/2/2
16	A1EF2	B	103	-	-	10/43/43/43	-
13	LMT	P	101	-	-	3/19/59/61	0/2/2/2
10	U10	L	303	-	-	7/30/54/87	0/1/1/1
16	A1EF2	p	101	-	-	4/43/43/43	-
15	CDL	M	413	-	-	11/56/56/110	-
8	BCL	p	102	5	-	15/41/137/137	-
13	LMT	G	101	-	-	5/15/35/61	0/1/1/2
8	BCL	M	401	2	-	13/41/137/137	-
13	LMT	b	101	-	-	1/13/53/61	0/2/2/2
8	BCL	I	102	4	-	15/41/137/137	-
12	LDA	I	104	-	-	3/13/13/13	-
9	BPH	M	405	-	-	6/37/105/105	0/5/6/6
8	BCL	n	102	5	-	18/41/137/137	-
8	BCL	f	102	5	-	16/41/137/137	-
11	PGV	E	104	-	-	6/40/42/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	LMT	L	312	-	-	10/21/61/61	0/2/2/2
11	PGV	C	102	-	-	19/51/51/55	-
16	A1EF2	N	102	-	-	9/43/43/43	-
16	A1EF2	O	103	-	-	8/43/43/43	-
13	LMT	B	102	-	-	11/21/61/61	0/2/2/2
16	A1EF2	D	104	-	-	11/43/43/43	-
8	BCL	N	101	4	-	17/41/137/137	-
13	LMT	A	701	-	-	5/21/61/61	0/2/2/2
16	A1EF2	J	106	-	-	9/43/43/43	-
11	PGV	C	101	-	-	13/46/46/55	-
8	BCL	j	101	5	-	13/41/137/137	-
16	A1EF2	n	101	-	-	7/43/43/43	-
8	BCL	a	102	5	-	18/41/137/137	-
8	BCL	o	102	5	-	17/41/137/137	-
16	A1EF2	I	105	-	-	5/43/43/43	-
8	BCL	L	308	1	-	7/41/137/137	-
8	BCL	A	702	4	-	10/35/131/137	-
8	BCL	F	103	4	-	12/41/137/137	-
8	BCL	J	102	4	-	17/41/137/137	-
8	BCL	c	102	5	-	15/41/137/137	-
13	LMT	L	311	-	-	8/21/61/61	0/2/2/2
11	PGV	K	103	-	-	12/47/47/55	-
16	A1EF2	q	101	-	-	6/43/43/43	-
16	A1EF2	g	101	-	-	8/43/43/43	-
8	BCL	B	101	4	-	6/35/131/137	-
13	LMT	G	102	-	-	3/11/31/61	0/1/1/2
15	CDL	E	101	-	-	15/67/67/110	-
13	LMT	U	101	-	-	3/21/61/61	0/2/2/2
15	CDL	M	410	-	-	14/89/89/110	-
16	A1EF2	D	105	-	-	7/43/43/43	-
13	LMT	H	302	-	-	2/21/61/61	0/2/2/2
12	LDA	M	403	-	-	1/13/13/13	-
8	BCL	P	102	4	-	11/35/131/137	-
13	LMT	E	102	-	-	5/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	LDA	J	105	-	-	2/13/13/13	-
16	A1EF2	e	101	-	-	7/43/43/43	-
13	LMT	c	103	-	-	5/21/61/61	0/2/2/2
13	LMT	O	101	-	-	7/21/61/61	0/2/2/2
16	A1EF2	M	411	-	-	6/43/43/43	-
8	BCL	C	103	4	-	13/41/137/137	-
8	BCL	k	102	5	-	14/41/137/137	-
11	PGV	M	402	-	-	15/51/51/55	-
13	LMT	D	101	-	-	4/11/51/61	0/2/2/2
13	LMT	L	315	-	-	4/21/61/61	0/2/2/2
13	LMT	a	101	-	-	2/13/53/61	0/2/2/2
11	PGV	L	306	-	-	15/37/37/55	-
11	PGV	H	304	-	-	18/44/44/55	-
8	BCL	K	102	4	-	15/41/137/137	-
16	A1EF2	N	103	-	-	8/43/43/43	-
8	BCL	D	102	4	-	8/41/137/137	-
8	BCL	b	103	5	-	18/41/137/137	-
8	BCL	e	102	5	-	16/41/137/137	-
8	BCL	g	102	5	-	19/41/137/137	-
13	LMT	I	101	-	-	6/17/37/61	0/1/1/2
12	LDA	K	101	-	-	0/9/9/13	-
13	LMT	M	409	-	-	8/19/59/61	0/2/2/2
8	BCL	O	102	4	-	9/31/127/137	-
11	PGV	L	305	-	-	14/43/43/55	-
13	LMT	M	408	-	-	5/19/39/61	0/1/1/2
12	LDA	X	102	-	-	5/13/13/13	-
11	PGV	H	303	-	-	9/35/35/55	-
12	LDA	L	310	-	-	4/13/13/13	-
16	A1EF2	f	101	-	-	7/43/43/43	-
8	BCL	d	102	5	-	17/41/137/137	-
8	BCL	i	101	5	-	18/41/137/137	-
8	BCL	Q	101	-	-	11/35/131/137	-
11	PGV	G	103	-	-	16/43/43/55	-
13	LMT	D	103	-	-	8/13/53/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	LDA	L	307	-	-	2/13/13/13	-
8	BCL	M	404	2	-	7/41/137/137	-
13	LMT	H	301	-	-	1/21/61/61	0/2/2/2
13	LMT	X	103	-	-	1/17/57/61	0/2/2/2
16	A1EF2	J	101	-	-	6/43/43/43	-
16	A1EF2	o	101	-	-	4/43/43/43	-
16	A1EF2	J	103	-	-	7/43/43/43	-
8	BCL	L	301	1	-	8/41/137/137	-
8	BCL	G	104	4	-	17/41/137/137	-
16	A1EF2	E	105	-	-	6/43/43/43	-
10	U10	L	304	-	-	5/30/54/87	0/1/1/1
12	LDA	X	101	-	-	1/10/10/13	-
8	BCL	E	103	4	-	7/31/127/137	-
16	A1EF2	c	104	-	-	7/43/43/43	-
12	LDA	F	104	-	-	4/13/13/13	-
11	PGV	L	313	-	-	10/55/55/55	-
11	PGV	M	412	-	-	16/46/46/55	-
16	A1EF2	k	101	-	-	8/43/43/43	-
9	BPH	L	302	-	-	3/37/105/105	0/5/6/6
13	LMT	I	103	-	-	2/16/56/61	0/2/2/2
13	LMT	c	101	-	-	1/9/29/61	0/1/1/2
16	A1EF2	a	103	-	-	8/43/43/43	-
16	A1EF2	J	104	-	-	12/43/43/43	-
16	A1EF2	d	101	-	-	8/43/43/43	-
8	BCL	q	102	5	-	12/33/129/137	-
12	LDA	L	309	-	-	1/13/13/13	-
15	CDL	F	102	-	-	11/37/37/110	-
11	PGV	L	314	-	-	10/43/43/55	-
10	U10	M	407	-	-	7/45/69/87	0/1/1/1
16	A1EF2	C	104	-	-	8/43/43/43	-
16	A1EF2	g	103	-	-	11/43/43/43	-
16	A1EF2	b	102	-	-	8/43/43/43	-

The worst 5 of 831 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	L	303	U10	C6-C1	8.56	1.50	1.35
10	M	407	U10	C6-C1	7.79	1.49	1.35
10	L	304	U10	C6-C1	7.36	1.48	1.35
12	X	101	LDA	O1-N1	-7.31	1.25	1.42
12	L	307	LDA	O1-N1	-7.28	1.25	1.42

The worst 5 of 1199 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	o	102	BCL	O2D-CGD-CBD	27.34	159.85	111.27
8	o	102	BCL	O1D-CGD-CBD	-22.50	78.45	124.48
8	o	102	BCL	O2D-CGD-O1D	-21.71	81.40	123.84
8	M	401	BCL	C2B-C1B-NB	9.05	116.30	110.23
8	Q	101	BCL	C2B-C1B-NB	8.85	116.16	110.23

There are no chirality outliers.

5 of 1025 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	L	301	BCL	C2C-C3C-CAC-CBC
8	L	301	BCL	C4C-C3C-CAC-CBC
8	L	308	BCL	C4C-C3C-CAC-CBC
8	M	401	BCL	C4C-C3C-CAC-CBC
8	M	404	BCL	CBD-CGD-O2D-CED

There are no ring outliers.

83 monomers are involved in 265 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	F	101	LMT	6	0
13	P	101	LMT	2	0
10	L	303	U10	4	0
15	M	413	CDL	1	0
8	p	102	BCL	5	0
8	M	401	BCL	5	0
8	I	102	BCL	2	0
12	I	104	LDA	6	0
9	M	405	BPH	15	0
8	n	102	BCL	4	0
8	f	102	BCL	4	0
11	E	104	PGV	4	0
13	L	312	LMT	12	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	C	102	PGV	3	0
13	B	102	LMT	12	0
8	N	101	BCL	5	0
13	A	701	LMT	1	0
11	C	101	PGV	5	0
8	j	101	BCL	3	0
8	a	102	BCL	6	0
8	o	102	BCL	8	0
8	L	308	BCL	3	0
8	A	702	BCL	5	0
8	F	103	BCL	2	0
8	J	102	BCL	4	0
8	c	102	BCL	4	0
13	L	311	LMT	5	0
11	K	103	PGV	4	0
8	B	101	BCL	1	0
15	E	101	CDL	2	0
13	U	101	LMT	2	0
15	M	410	CDL	7	0
16	D	105	A1EF2	1	0
13	H	302	LMT	2	0
12	M	403	LDA	2	0
8	P	102	BCL	2	0
12	J	105	LDA	2	0
13	c	103	LMT	2	0
13	O	101	LMT	1	0
8	C	103	BCL	2	0
8	k	102	BCL	3	0
11	M	402	PGV	2	0
13	D	101	LMT	2	0
13	L	315	LMT	5	0
13	a	101	LMT	4	0
11	H	304	PGV	6	0
8	K	102	BCL	2	0
8	D	102	BCL	4	0
8	b	103	BCL	2	0
8	e	102	BCL	3	0
8	g	102	BCL	5	0
13	I	101	LMT	1	0
12	K	101	LDA	1	0
13	M	409	LMT	1	0
8	O	102	BCL	2	0

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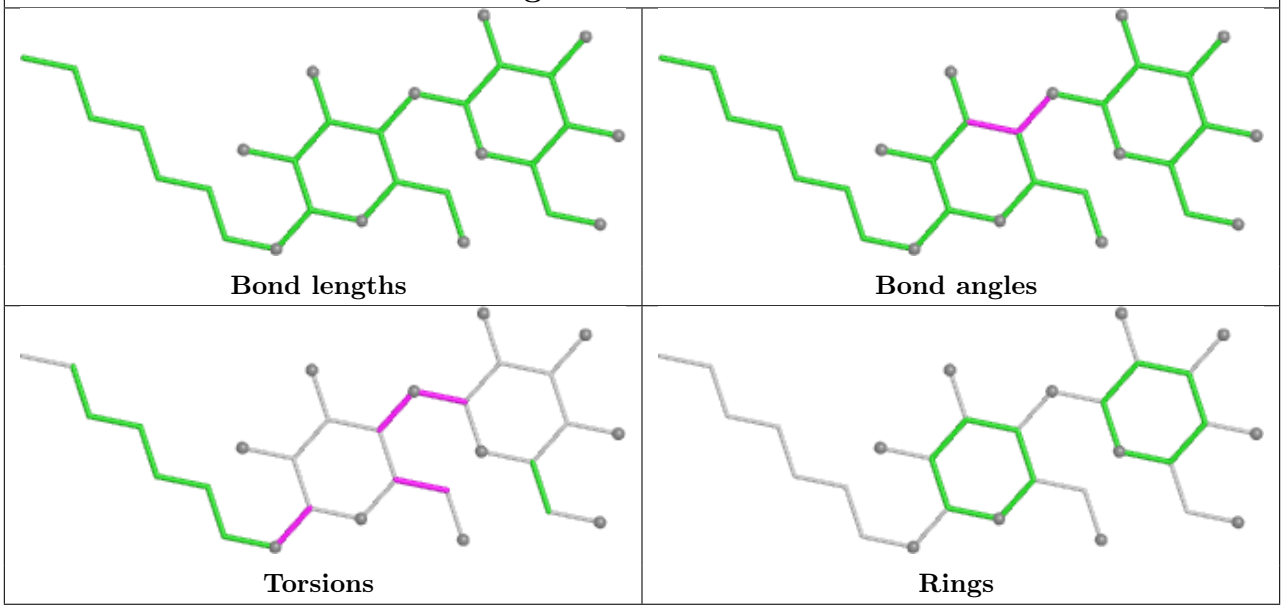
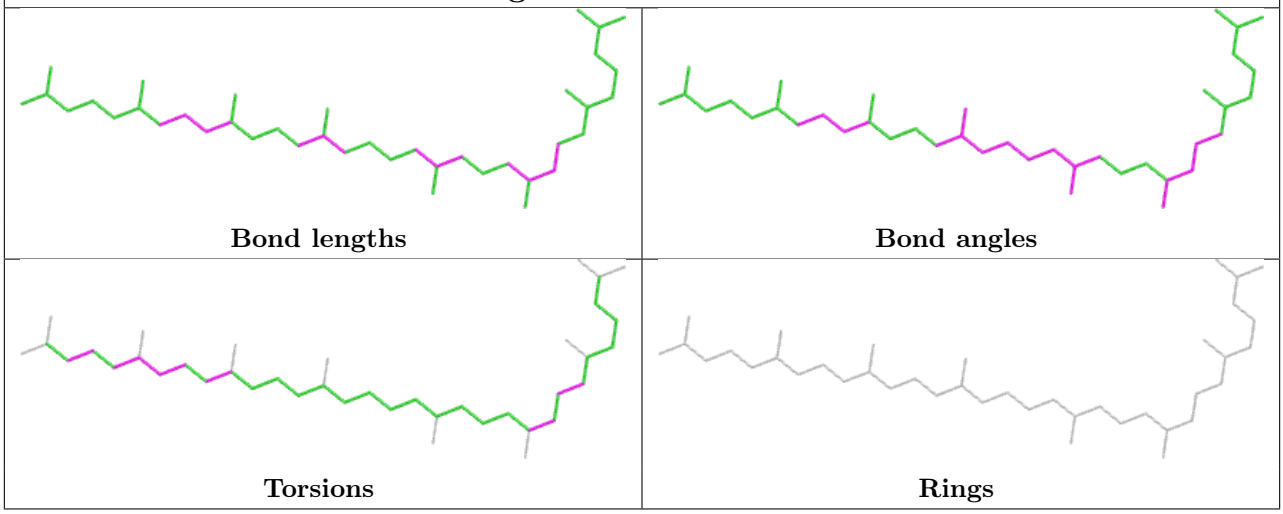
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	L	305	PGV	5	0
13	M	408	LMT	1	0
11	H	303	PGV	2	0
12	L	310	LDA	3	0
8	d	102	BCL	6	0
8	i	101	BCL	5	0
8	Q	101	BCL	1	0
13	D	103	LMT	4	0
12	L	307	LDA	1	0
8	M	404	BCL	5	0
13	H	301	LMT	1	0
13	X	103	LMT	2	0
8	L	301	BCL	1	0
8	G	104	BCL	1	0
10	L	304	U10	2	0
12	X	101	LDA	4	0
8	E	103	BCL	2	0
12	F	104	LDA	3	0
11	L	313	PGV	6	0
11	M	412	PGV	5	0
9	L	302	BPH	6	0
13	I	103	LMT	1	0
16	a	103	A1EF2	1	0
8	q	102	BCL	2	0
12	L	309	LDA	6	0
15	F	102	CDL	1	0
11	L	314	PGV	1	0
10	M	407	U10	7	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

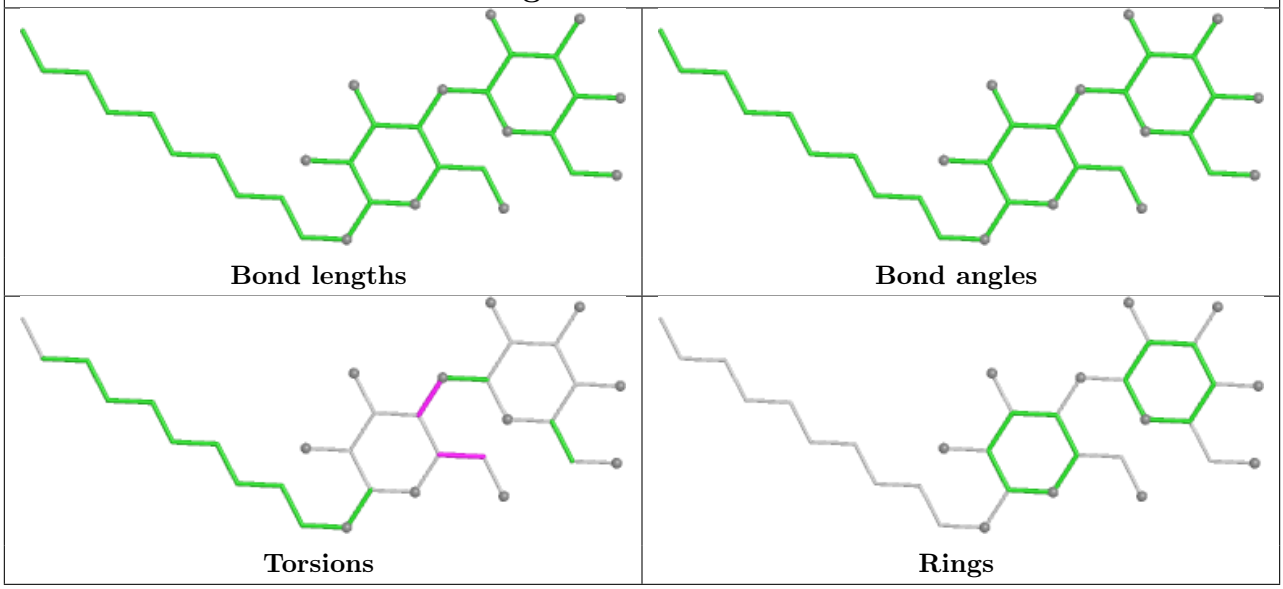
Ligand LMT F 101



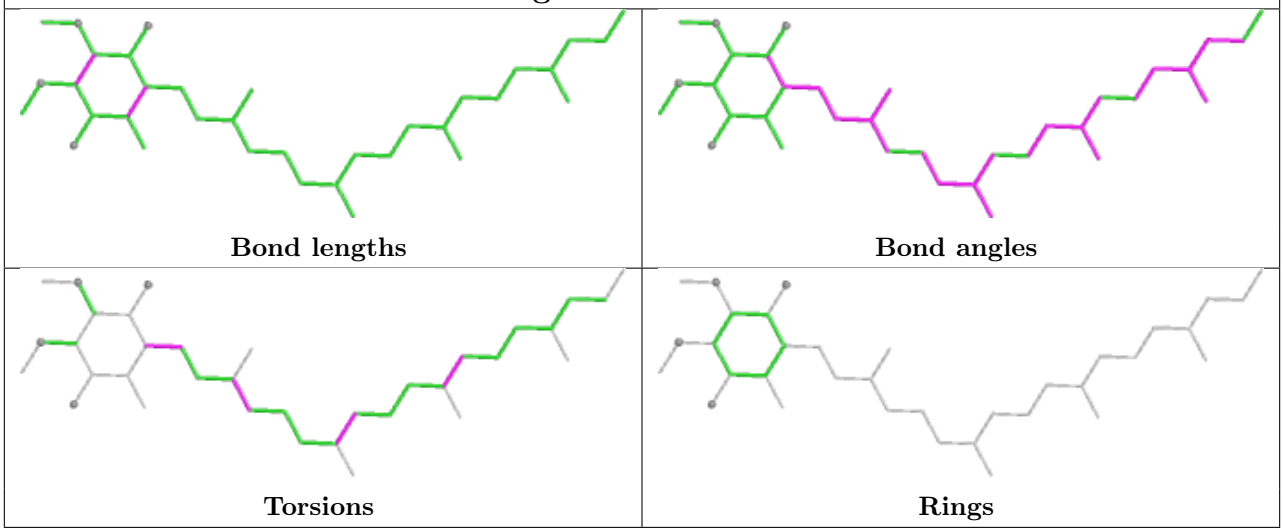
Ligand A1EF2 B 103



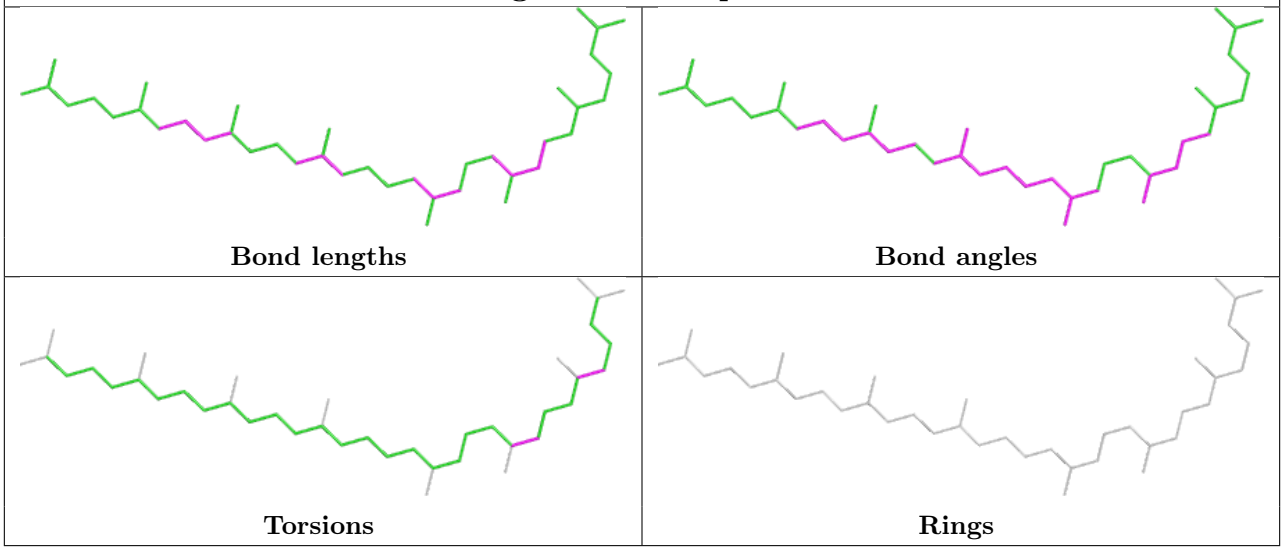
Ligand LMT P 101



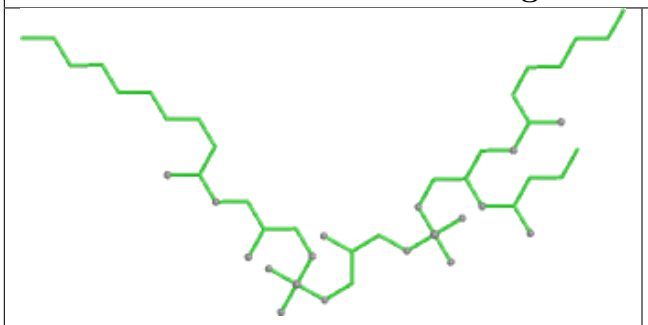
Ligand U10 L 303



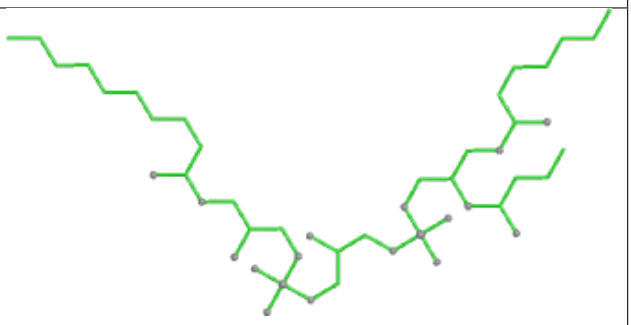
Ligand A1EF2 p 101



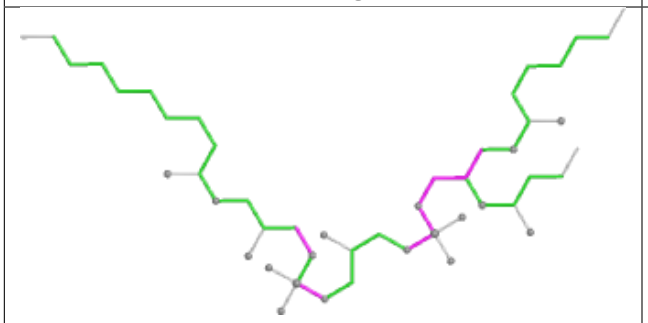
Ligand CDL M 413



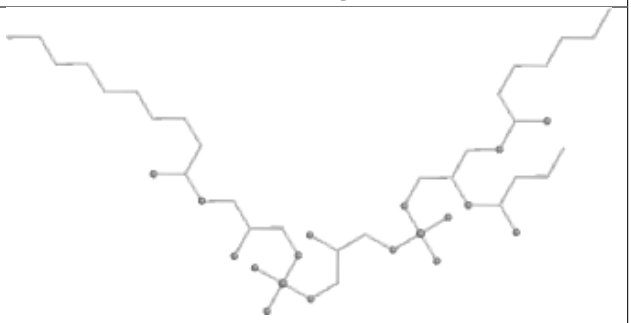
Bond lengths



Bond angles

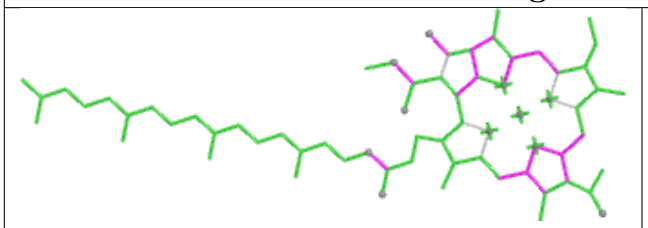


Torsions

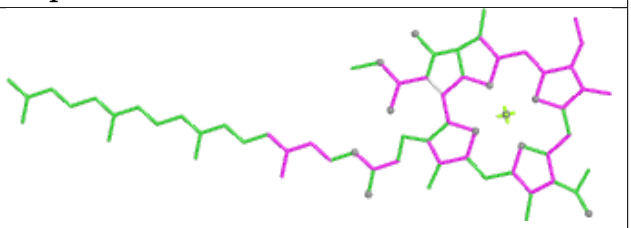


Rings

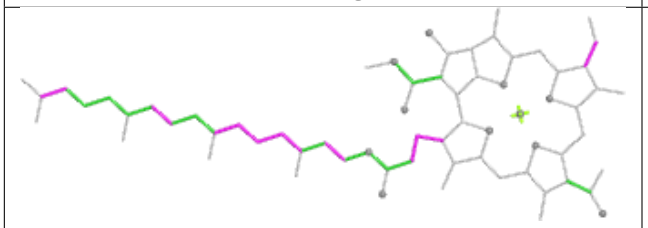
Ligand BCL p 102



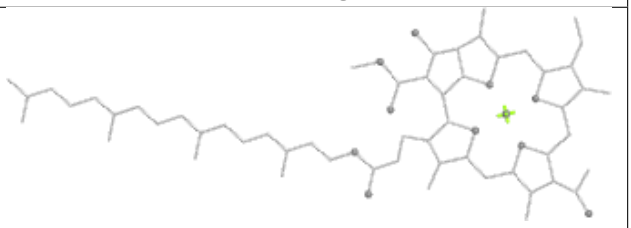
Bond lengths



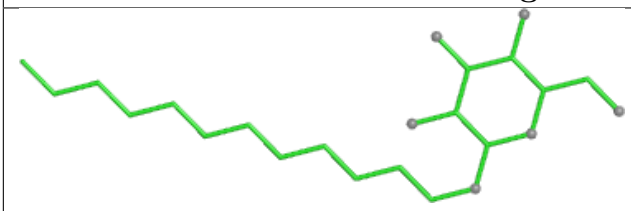
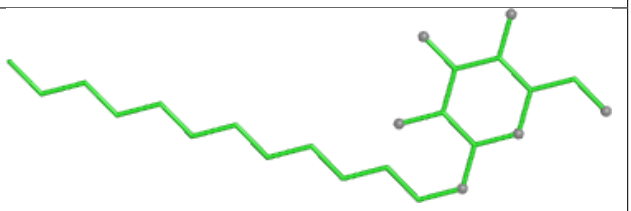
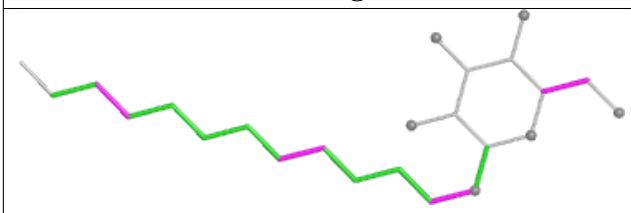
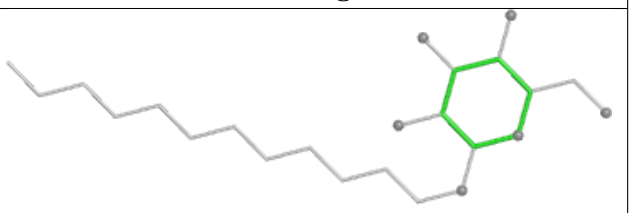
Bond angles

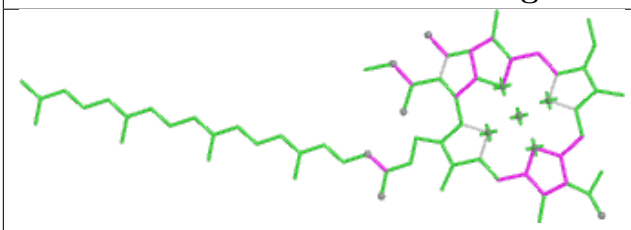
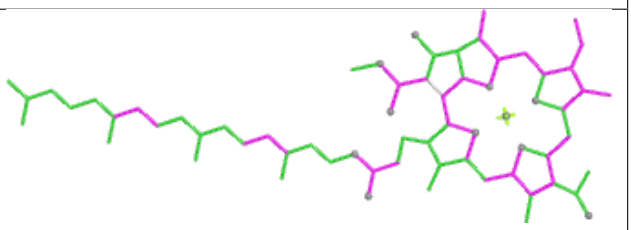
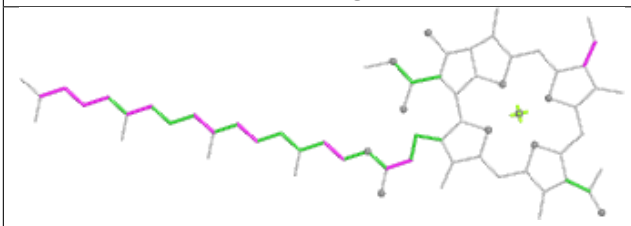
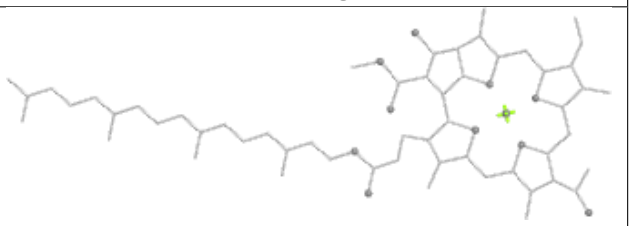


Torsions

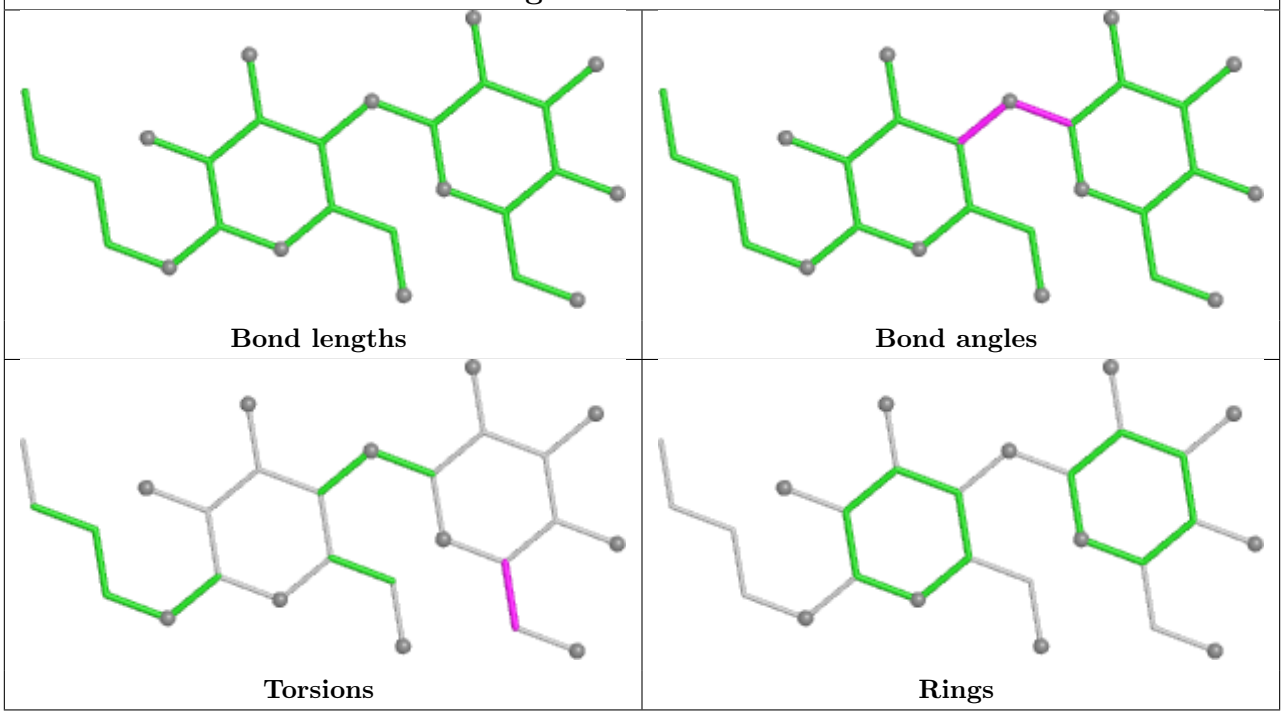


Rings

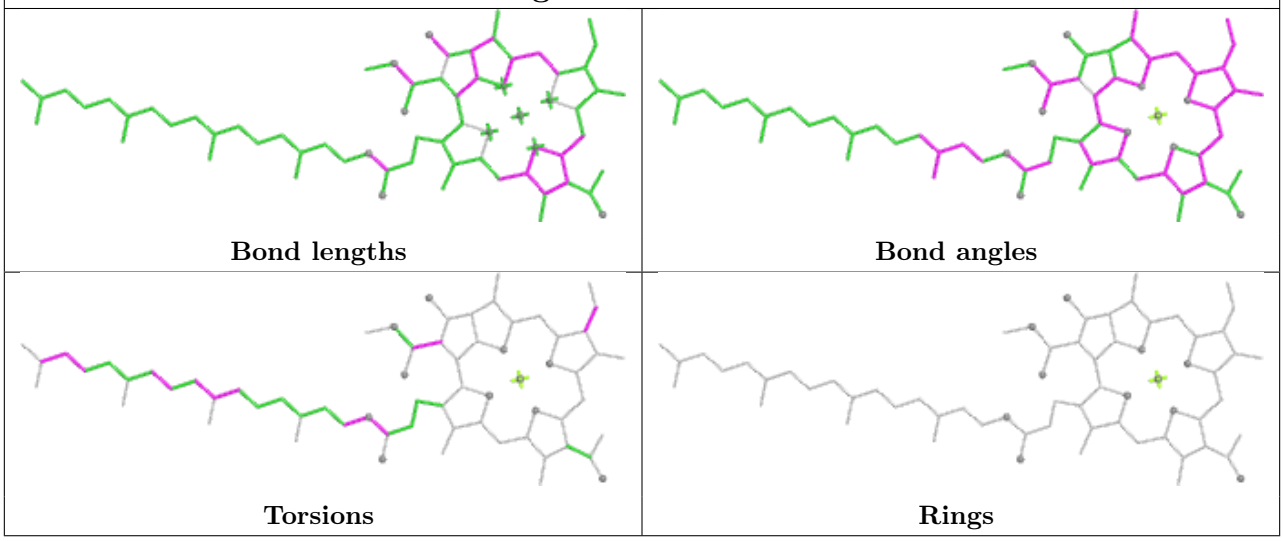
Ligand LMT G 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCL M 401	
 Bond lengths	 Bond angles
 Torsions	 Rings

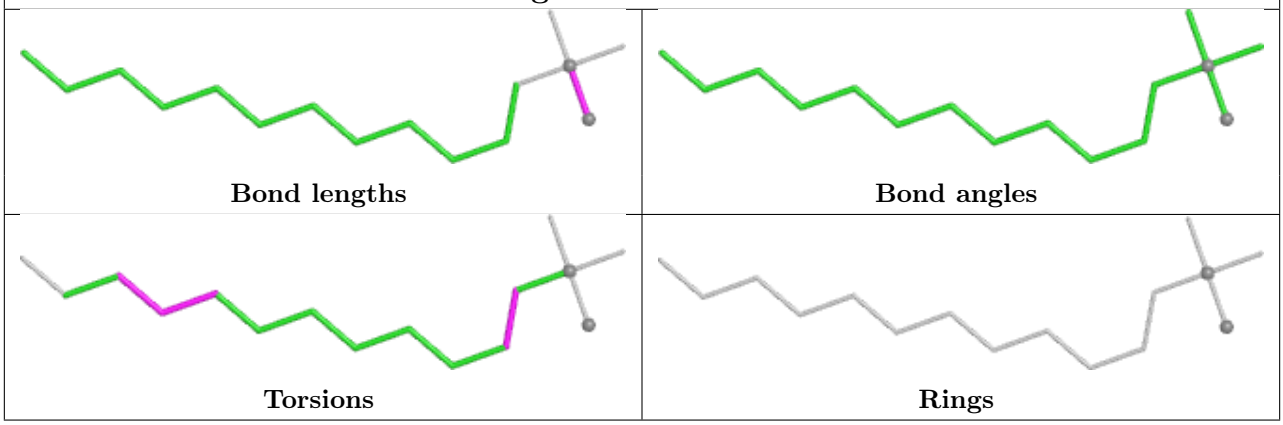
Ligand LMT b 101



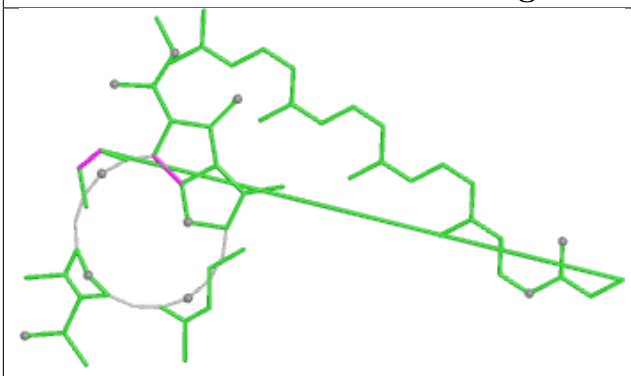
Ligand BCL I 102



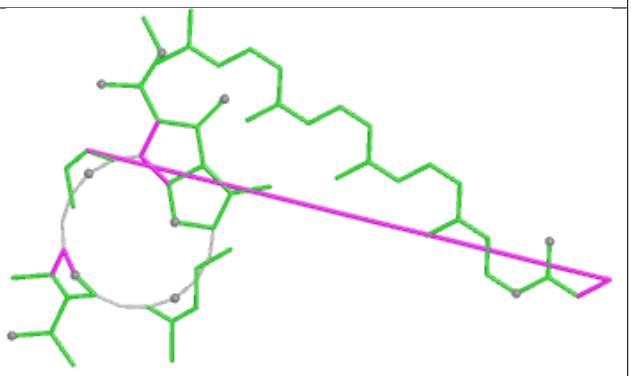
Ligand LDA I 104



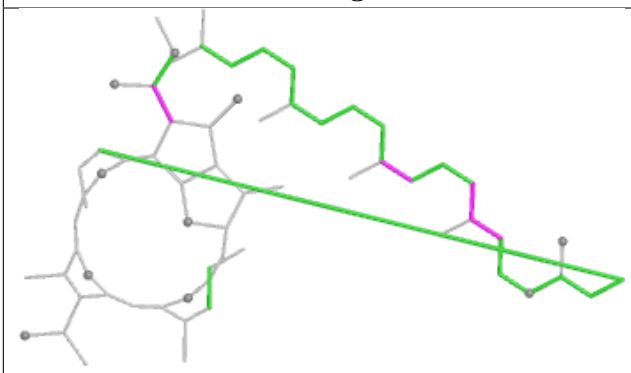
Ligand BPH M 405



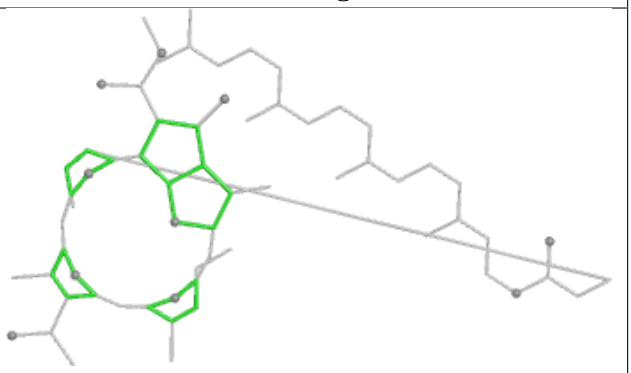
Bond lengths



Bond angles

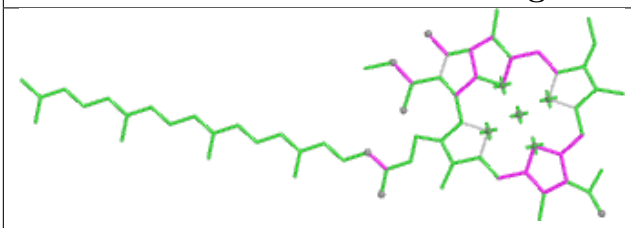


Torsions

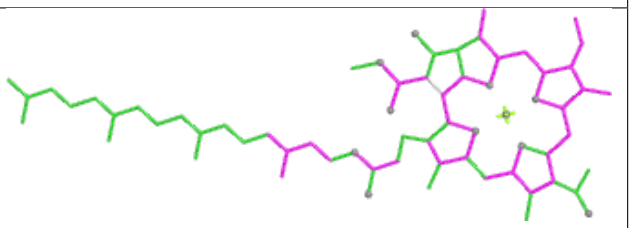


Rings

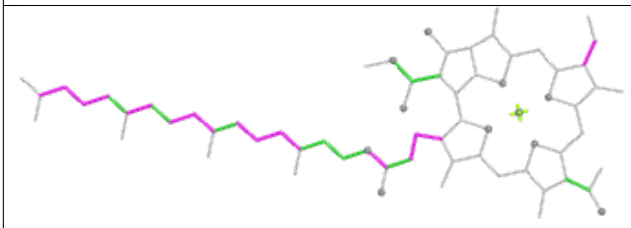
Ligand BCL n 102



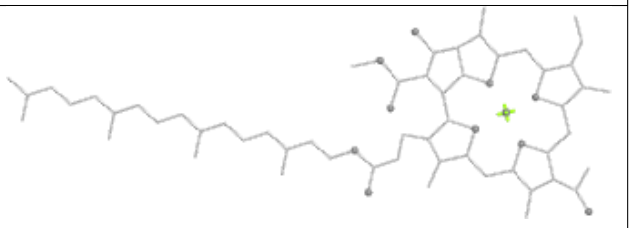
Bond lengths



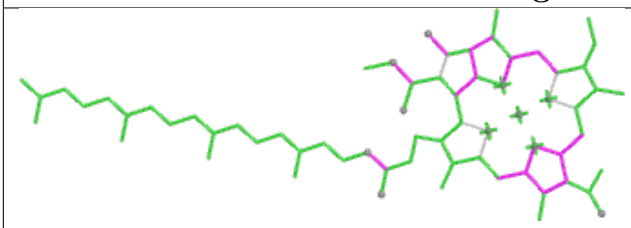
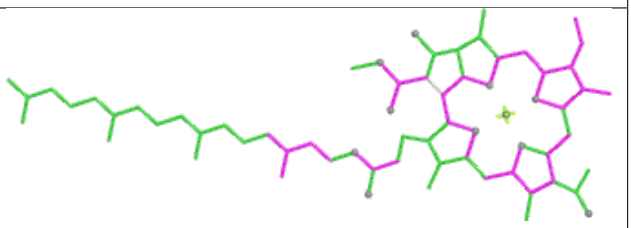
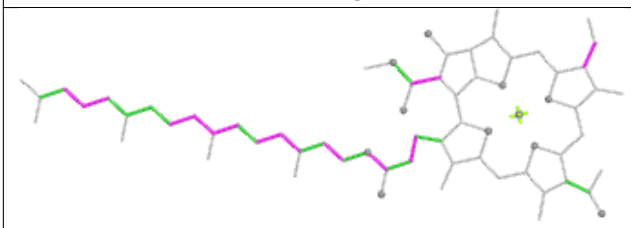
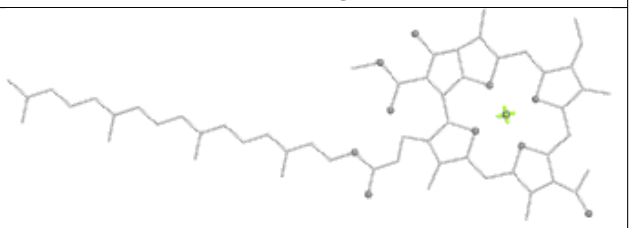
Bond angles

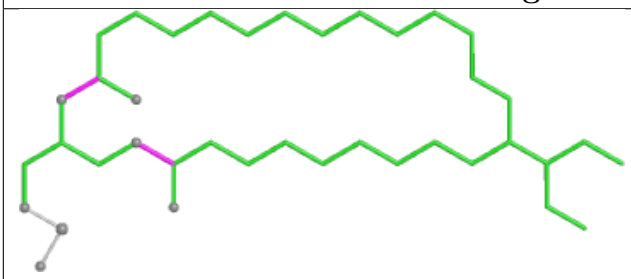
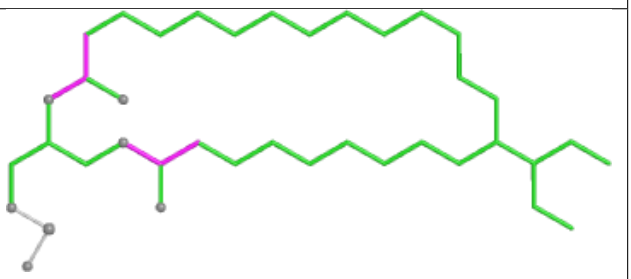
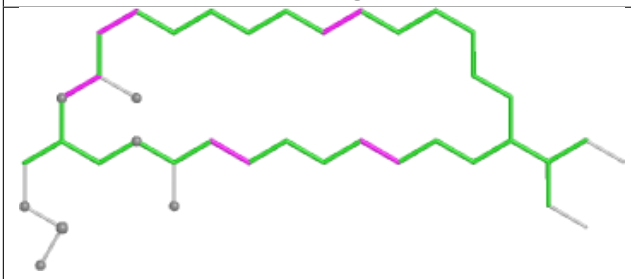
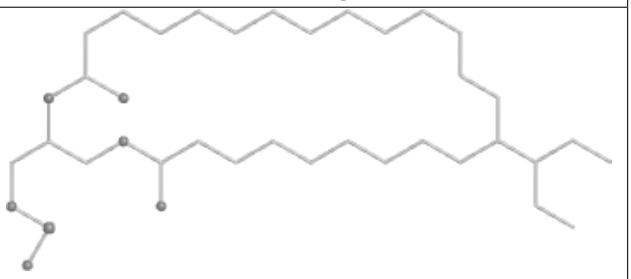


Torsions

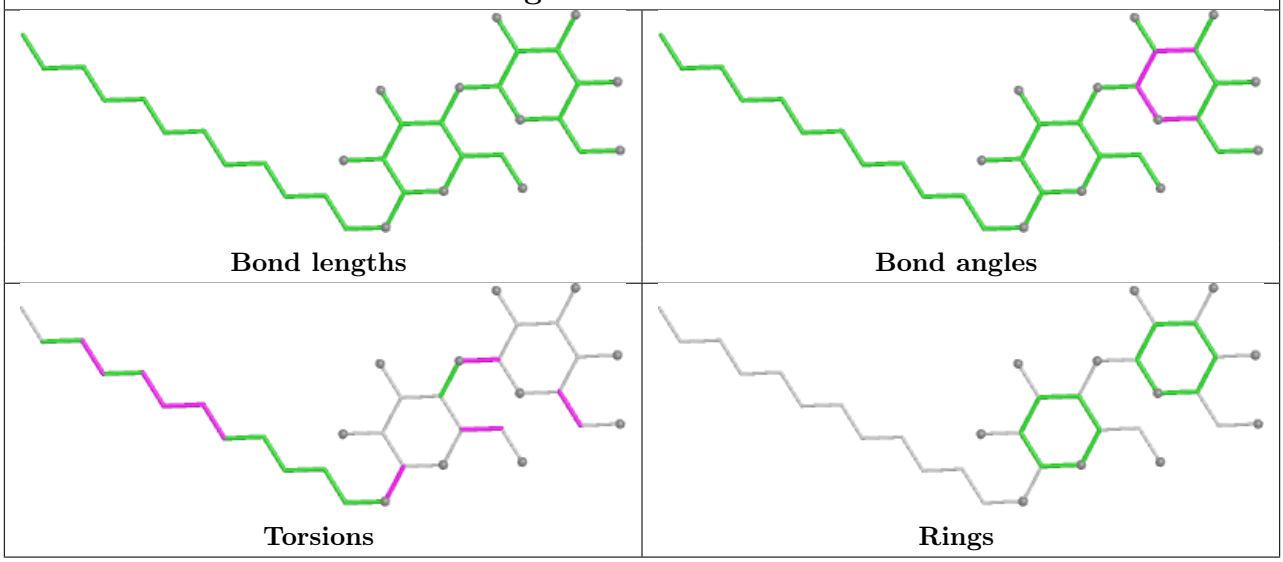


Rings

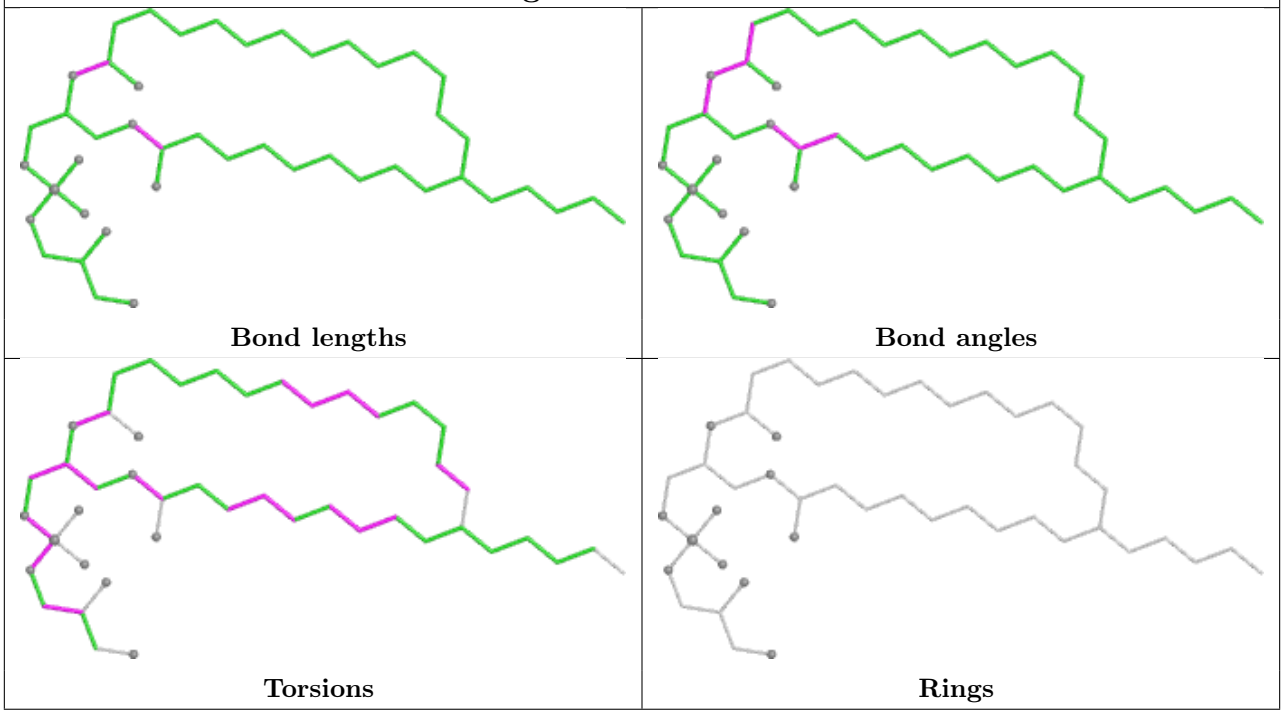
Ligand BCL f 102	
 Bond lengths	 Bond angles
 Torsions	 Rings

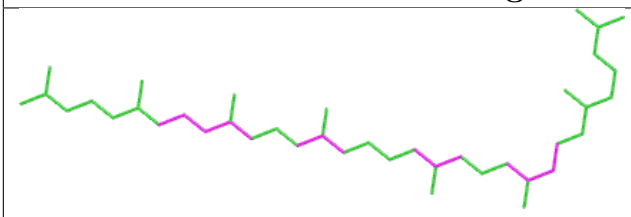
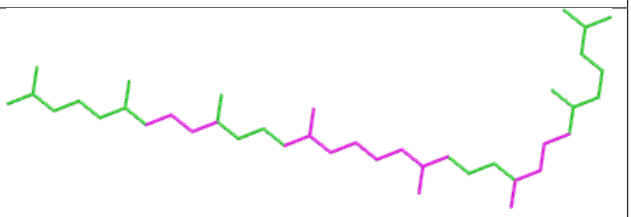
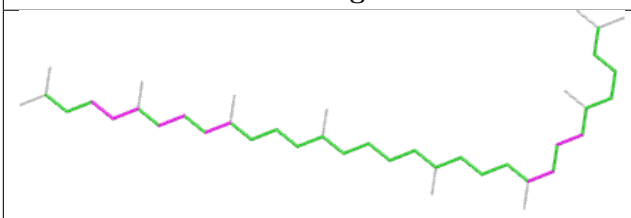
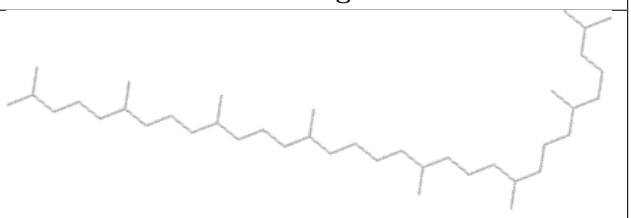
Ligand PGV E 104	
 Bond lengths	 Bond angles
 Torsions	 Rings

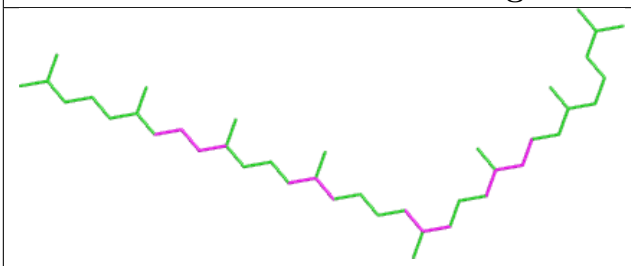
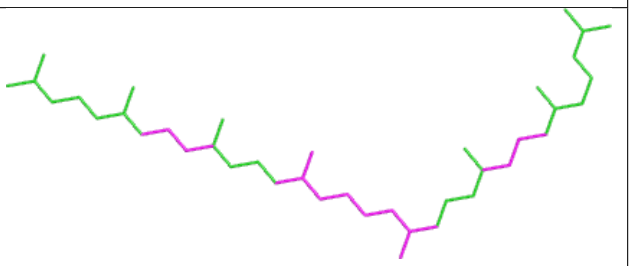
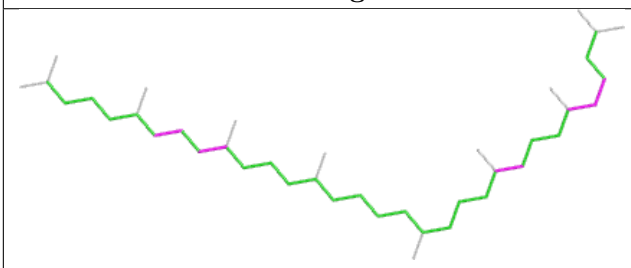
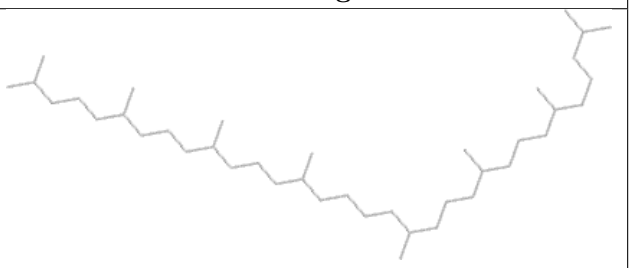
Ligand LMT L 312



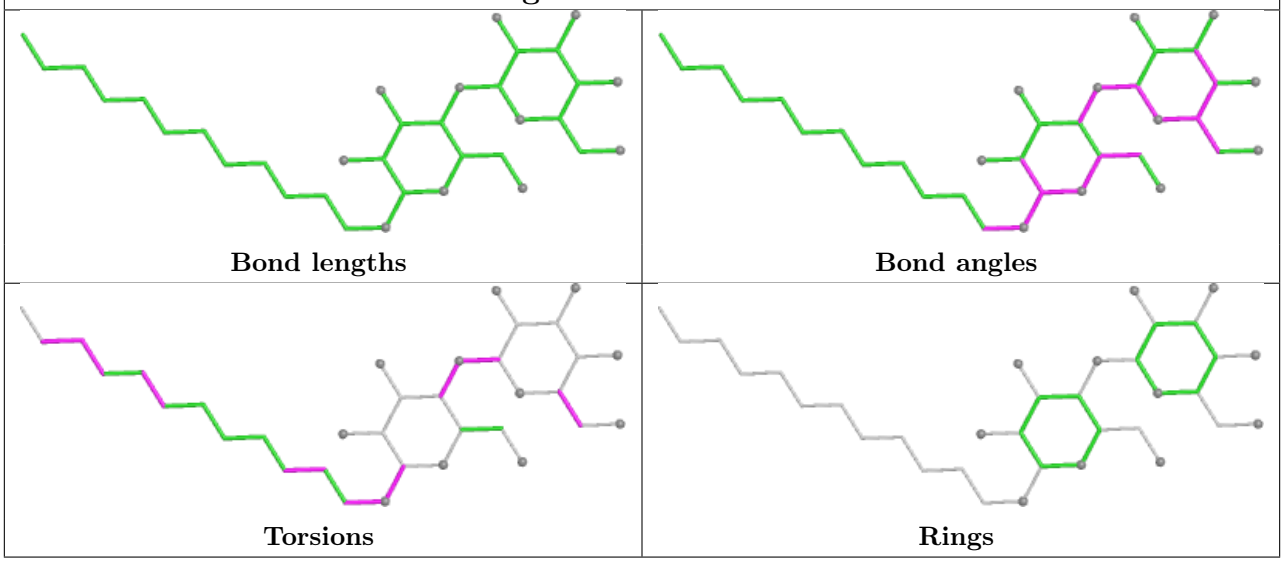
Ligand PGV C 102



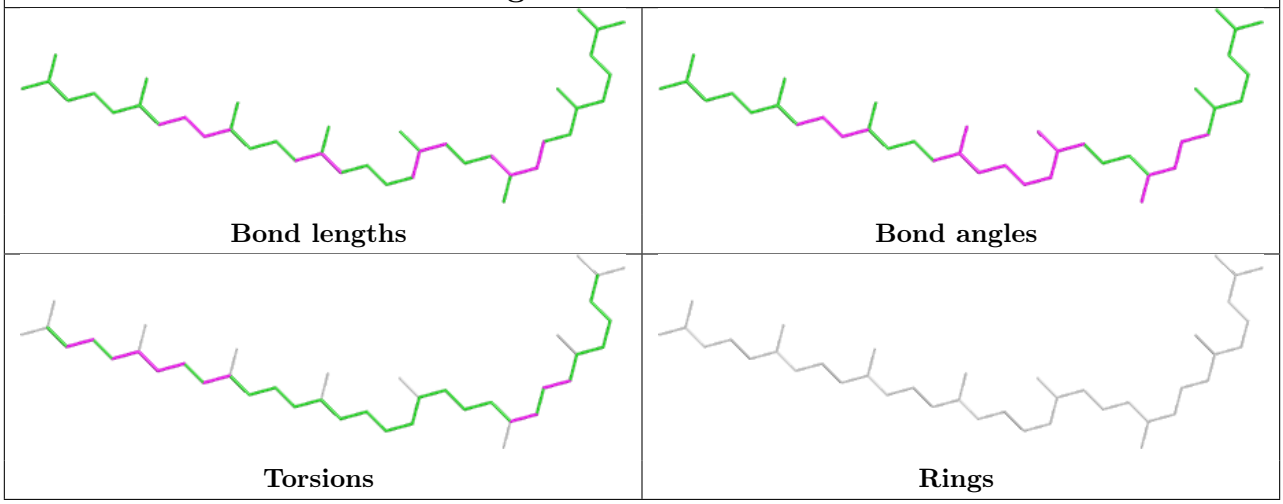
Ligand A1EF2 N 102	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand A1EF2 O 103	
 Bond lengths	 Bond angles
 Torsions	 Rings

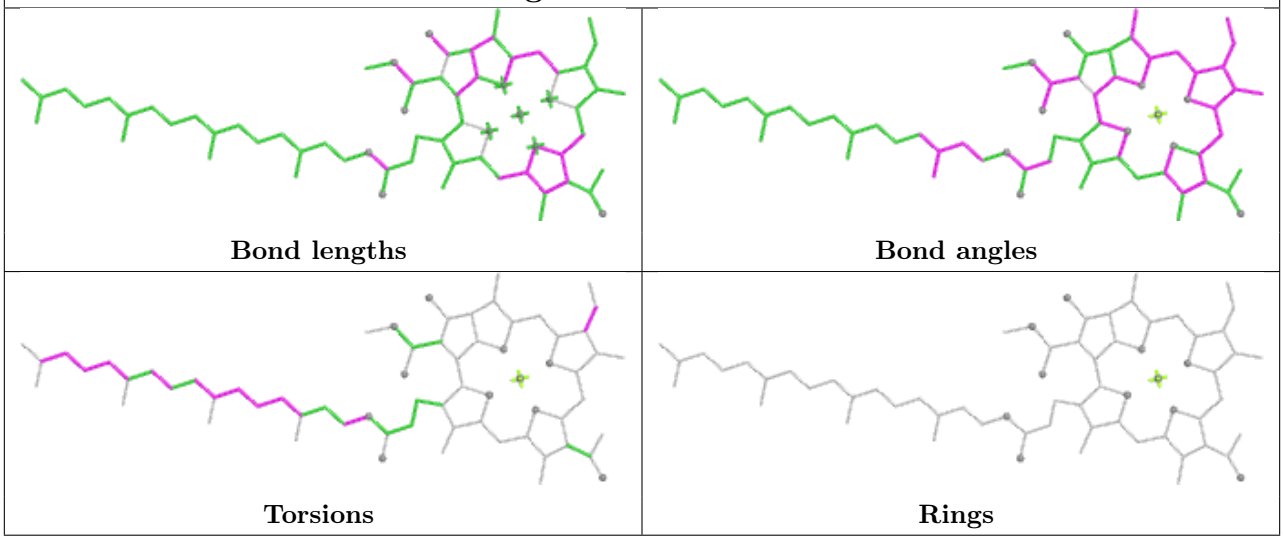
Ligand LMT B 102



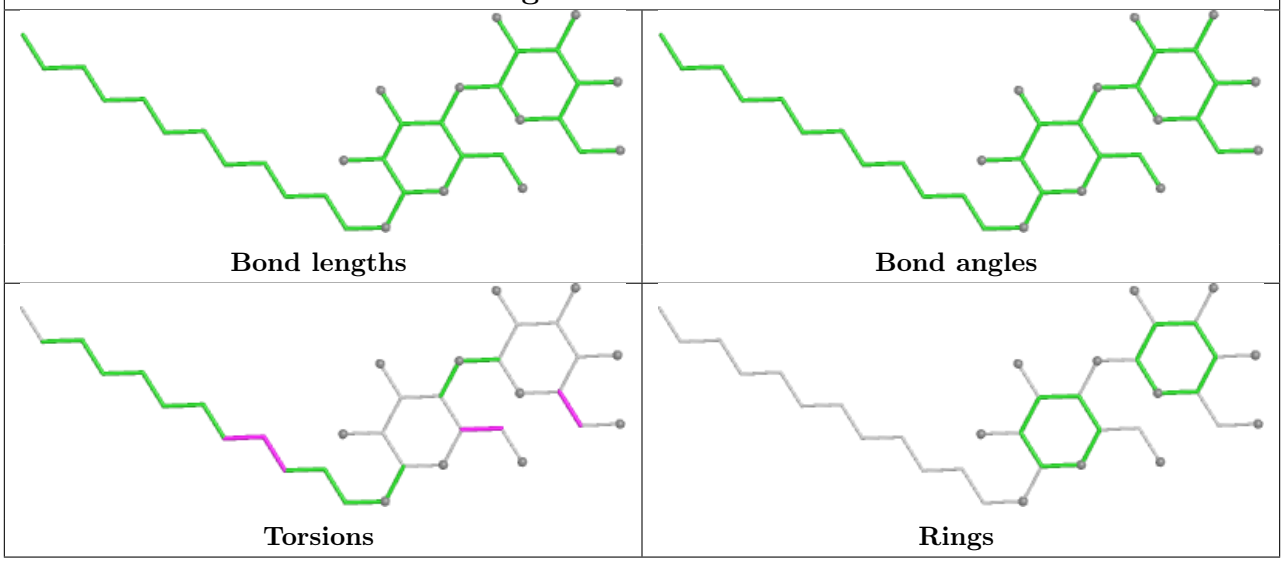
Ligand A1EF2 D 104



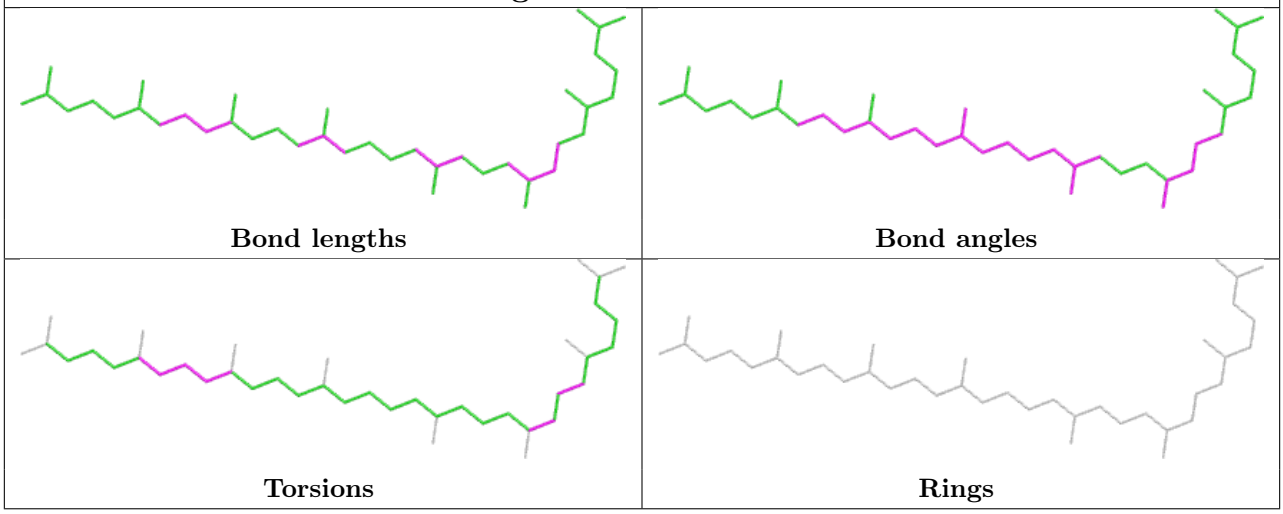
Ligand BCL N 101



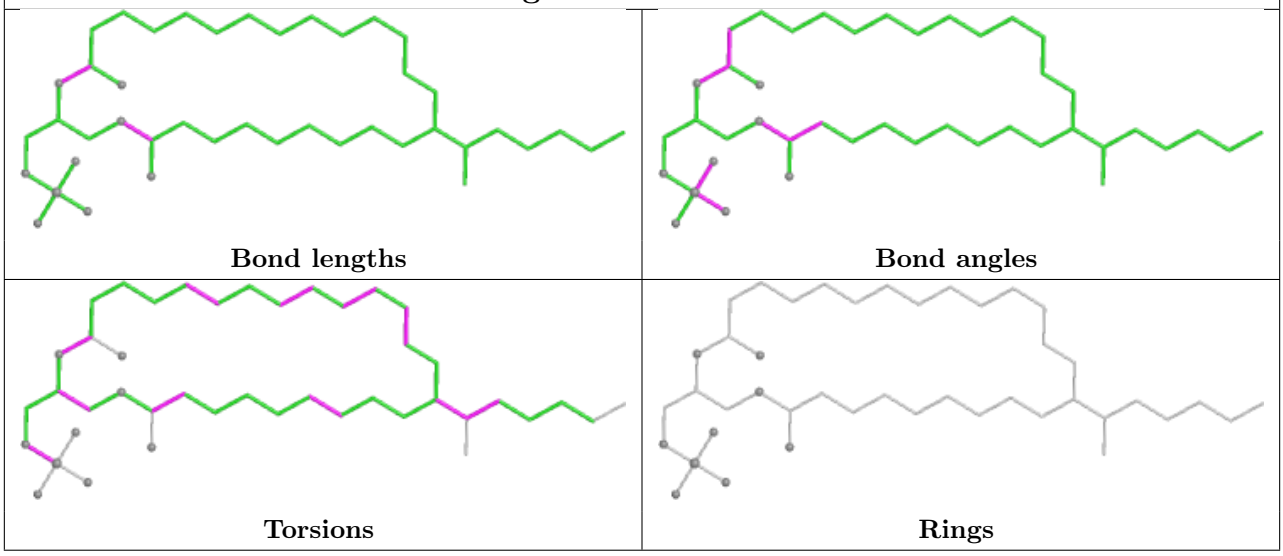
Ligand LMT A 701

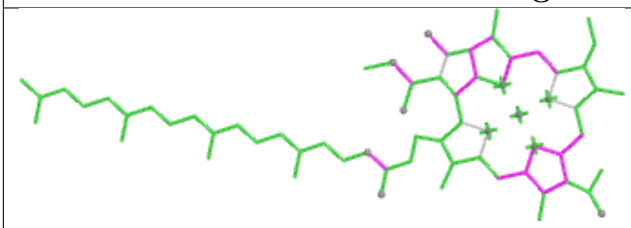
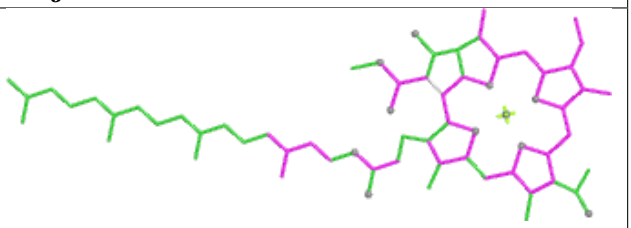
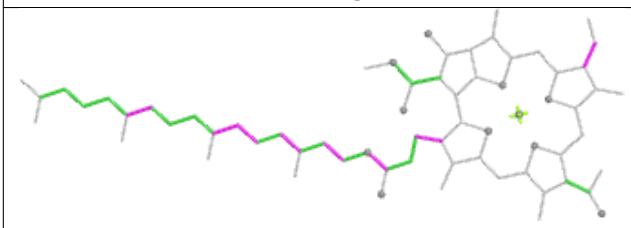
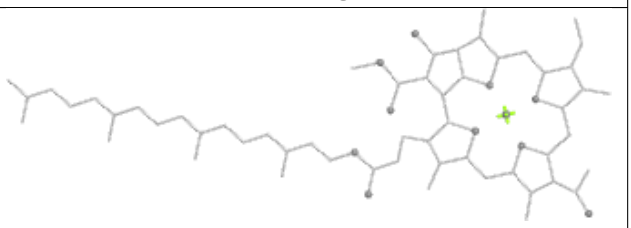


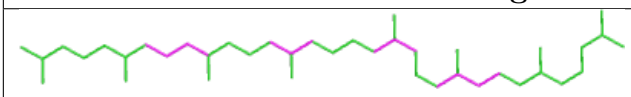
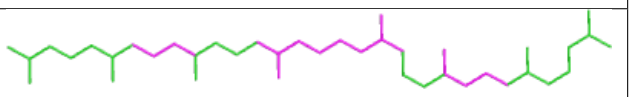
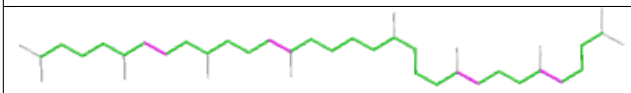
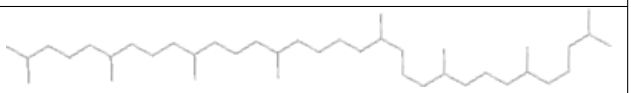
Ligand A1EF2 J 106

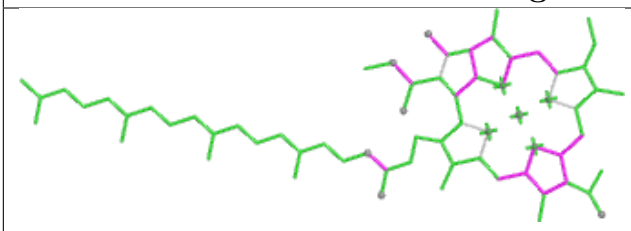
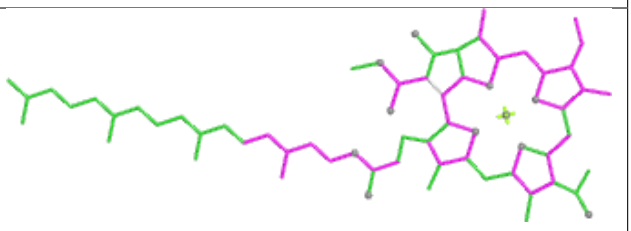
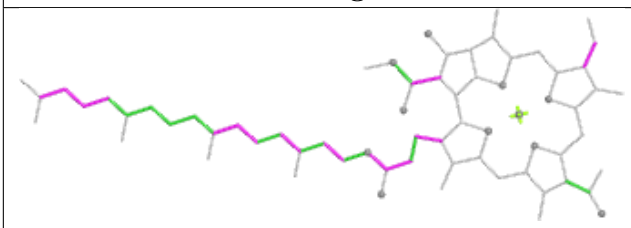
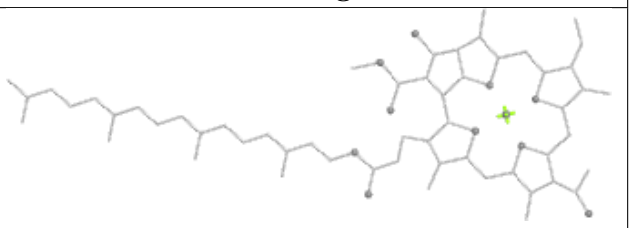


Ligand PGV C 101

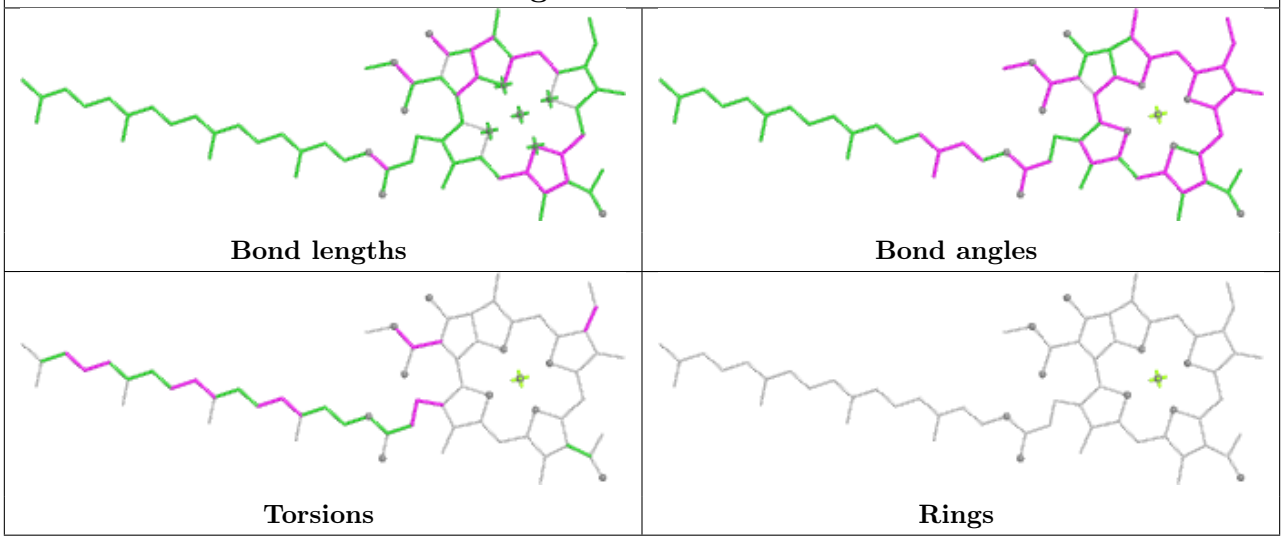


Ligand BCL j 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

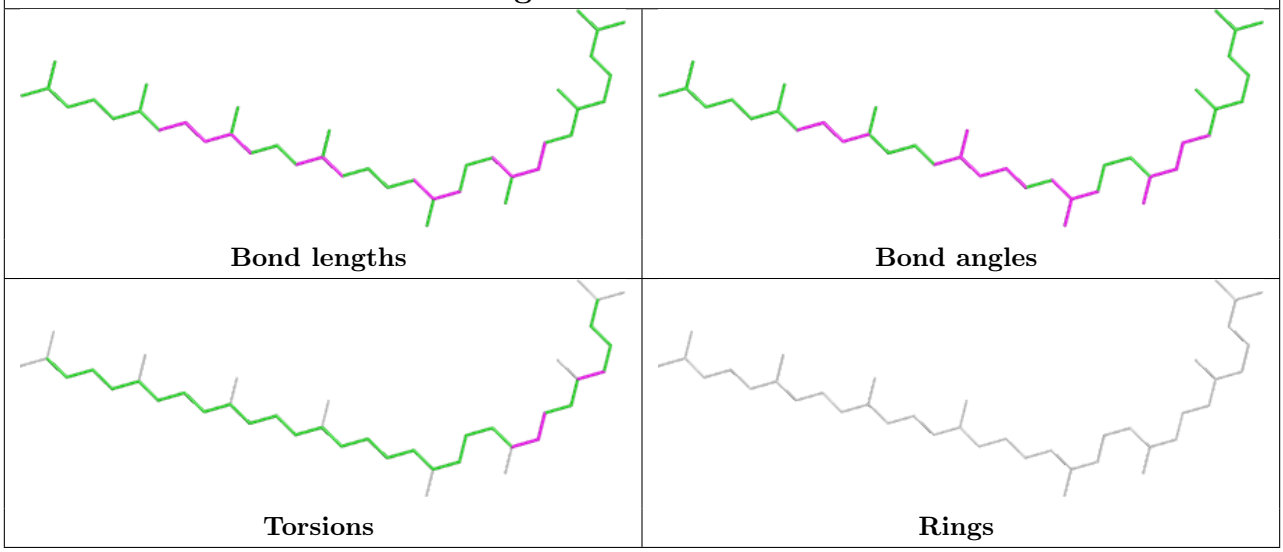
Ligand A1EF2 n 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCL a 102	
 Bond lengths	 Bond angles
 Torsions	 Rings

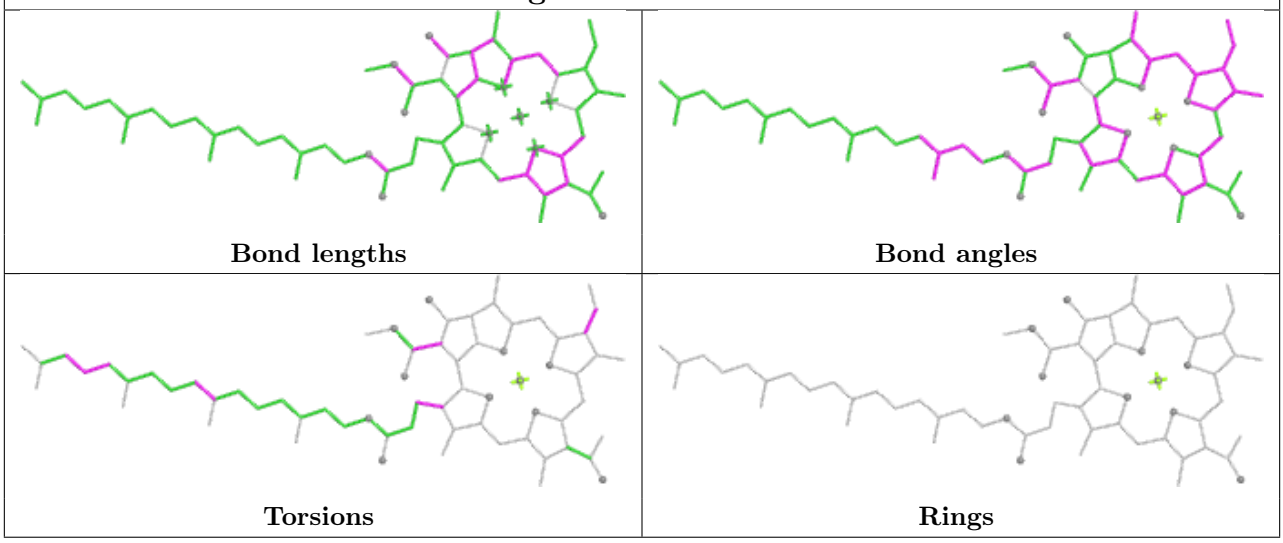
Ligand BCL o 102



Ligand A1EF2 I 105



Ligand BCL L 308



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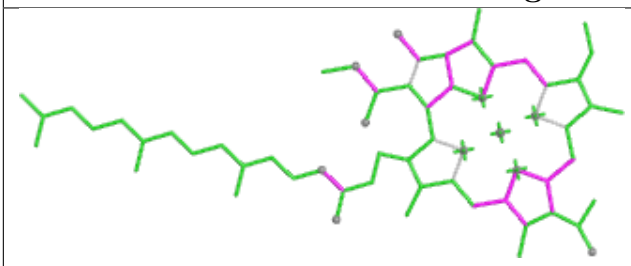
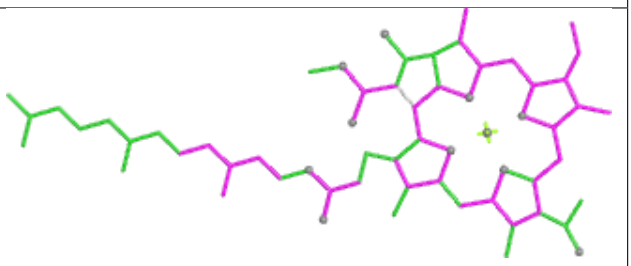
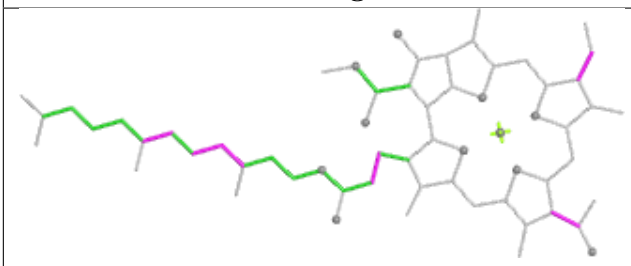
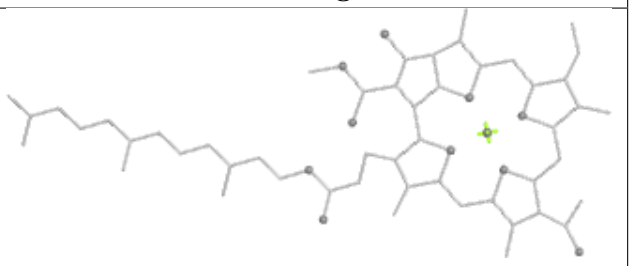
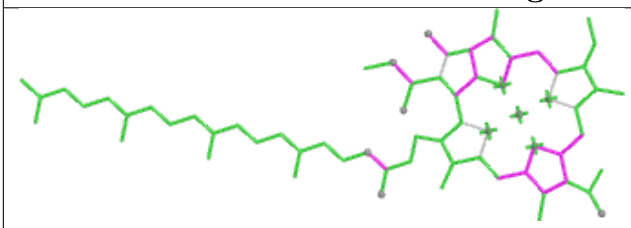
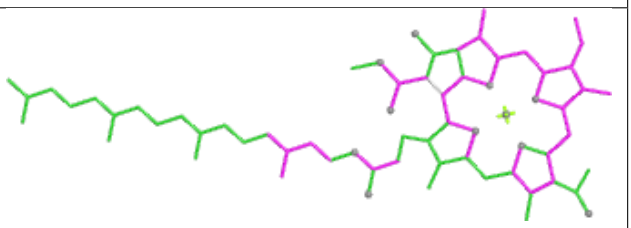
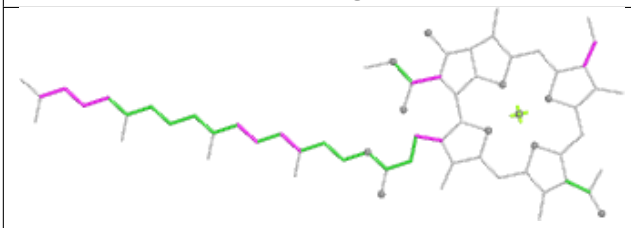
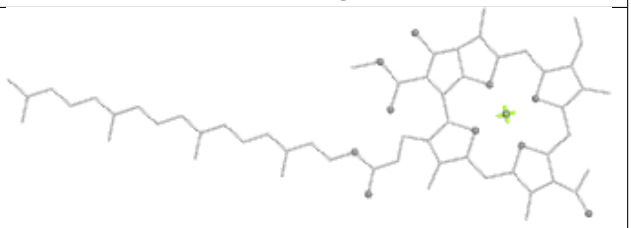
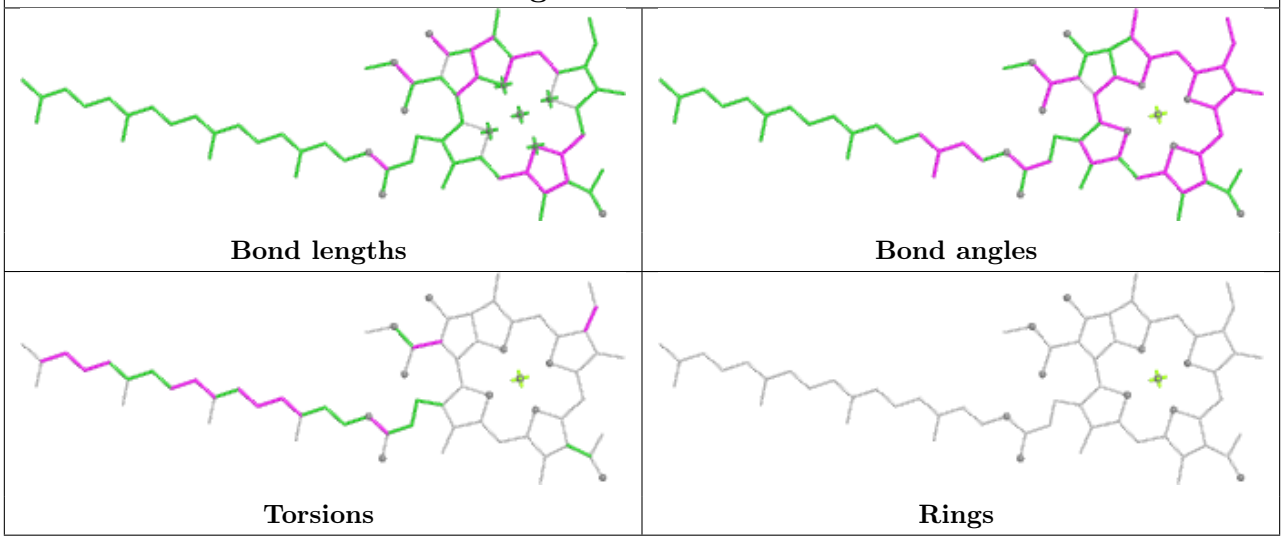
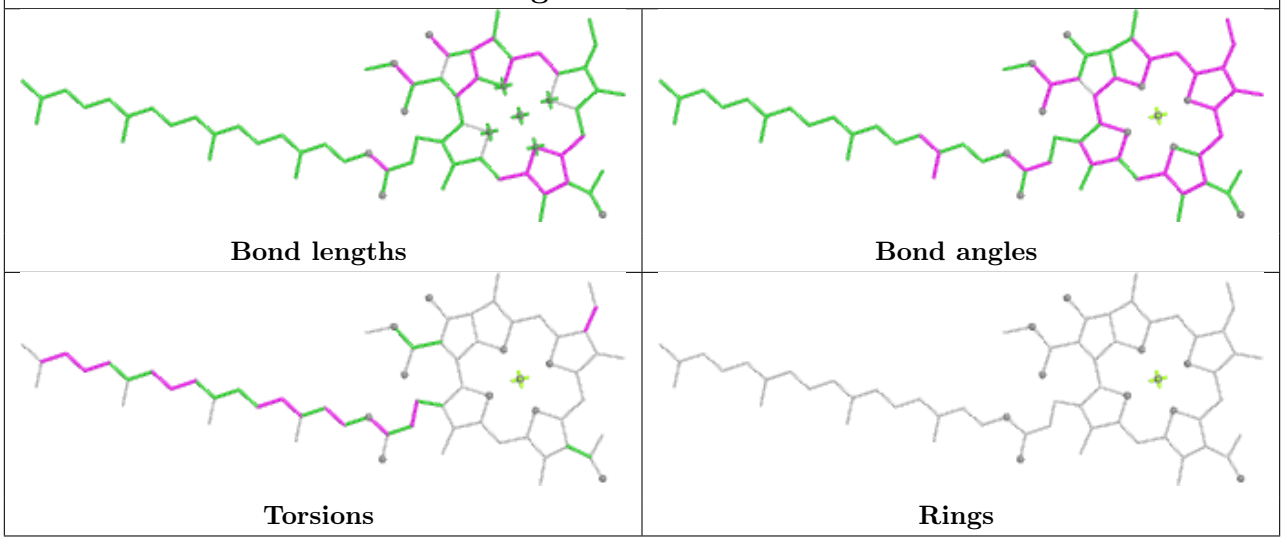
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCL F 103	
 Bond lengths	 Bond angles
 Torsions	 Rings

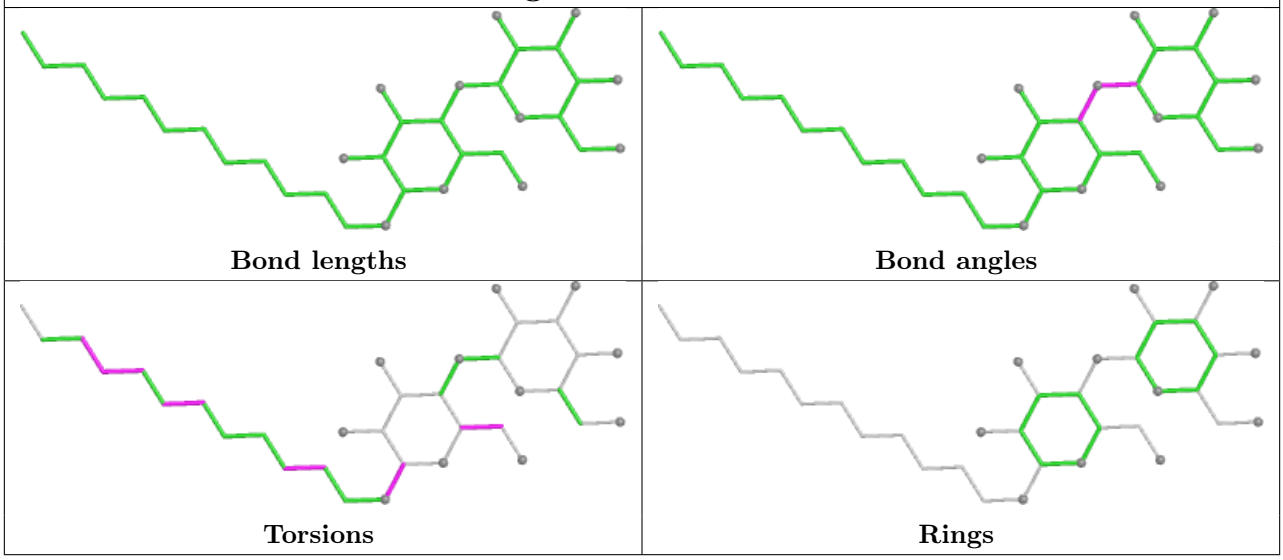
Ligand BCL J 102



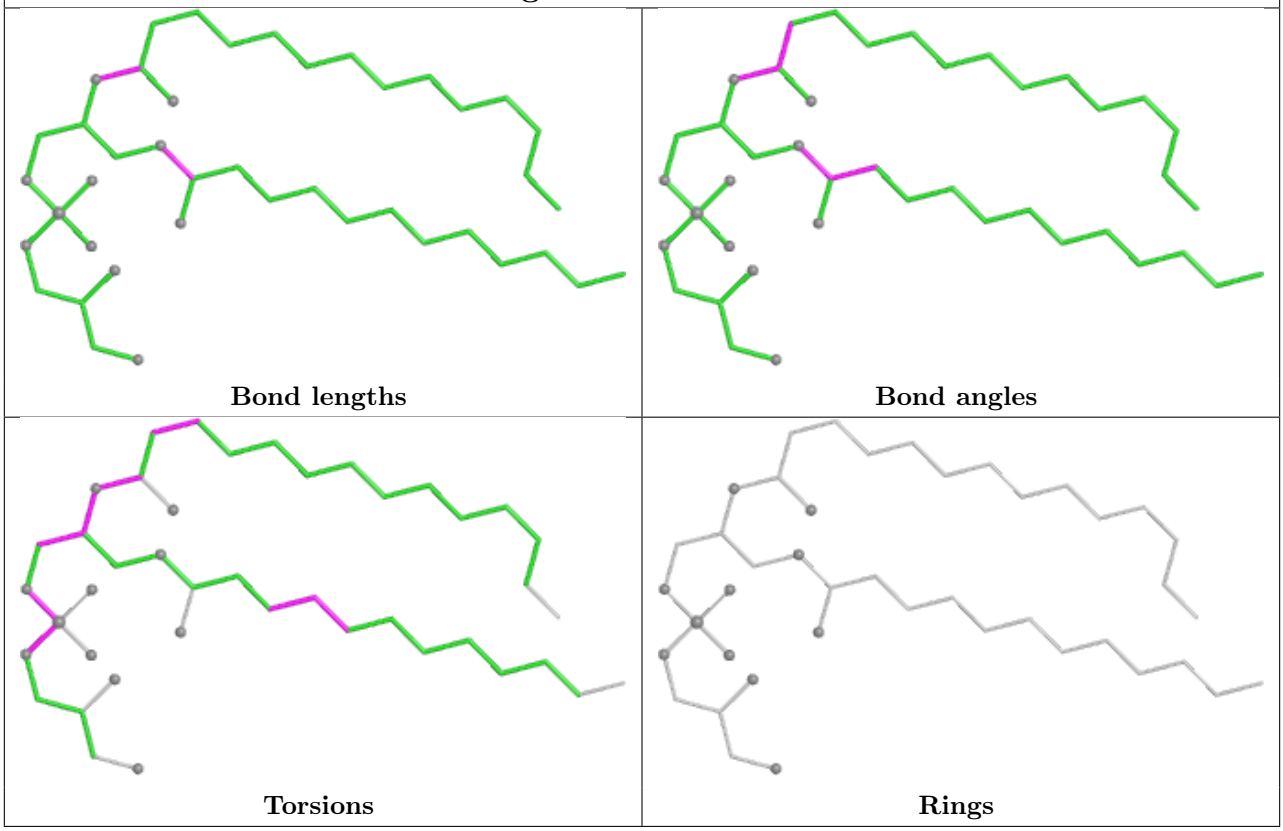
Ligand BCL c 102



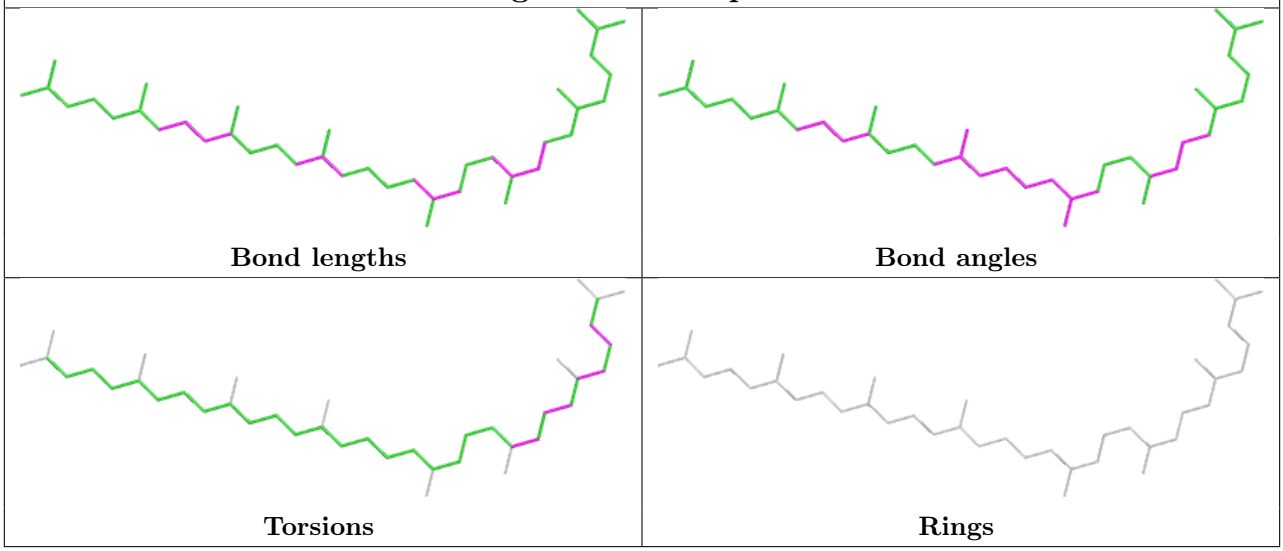
Ligand LMT L 311



Ligand PGV K 103



Ligand A1EF2 q 101



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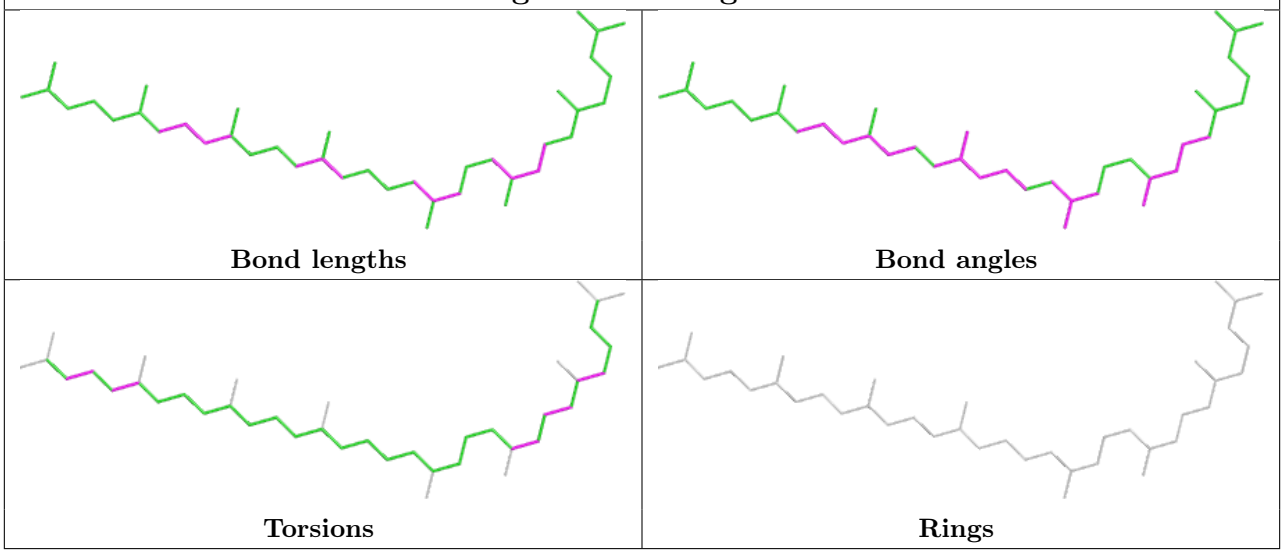

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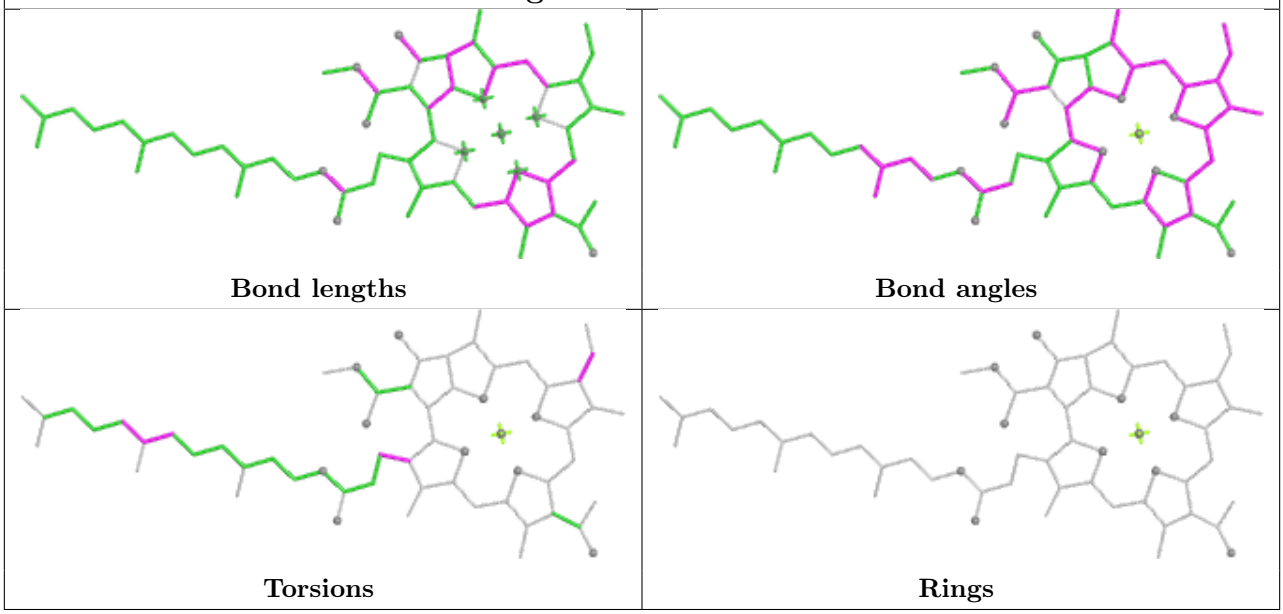

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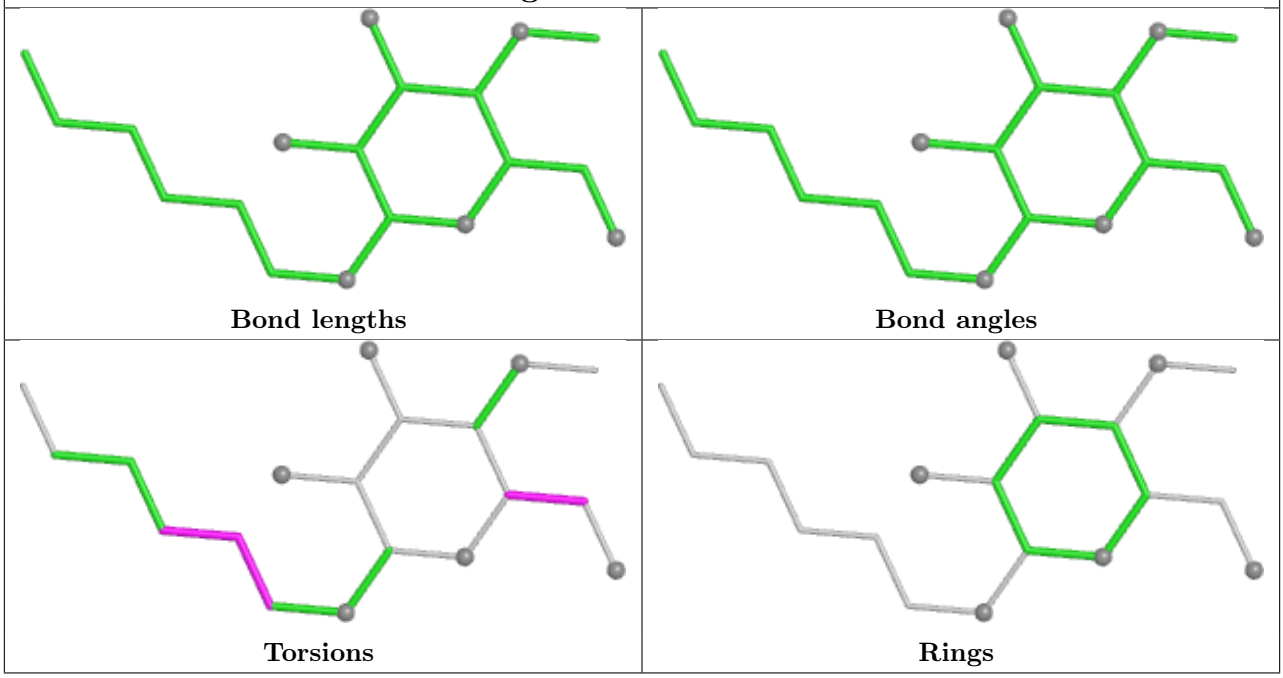
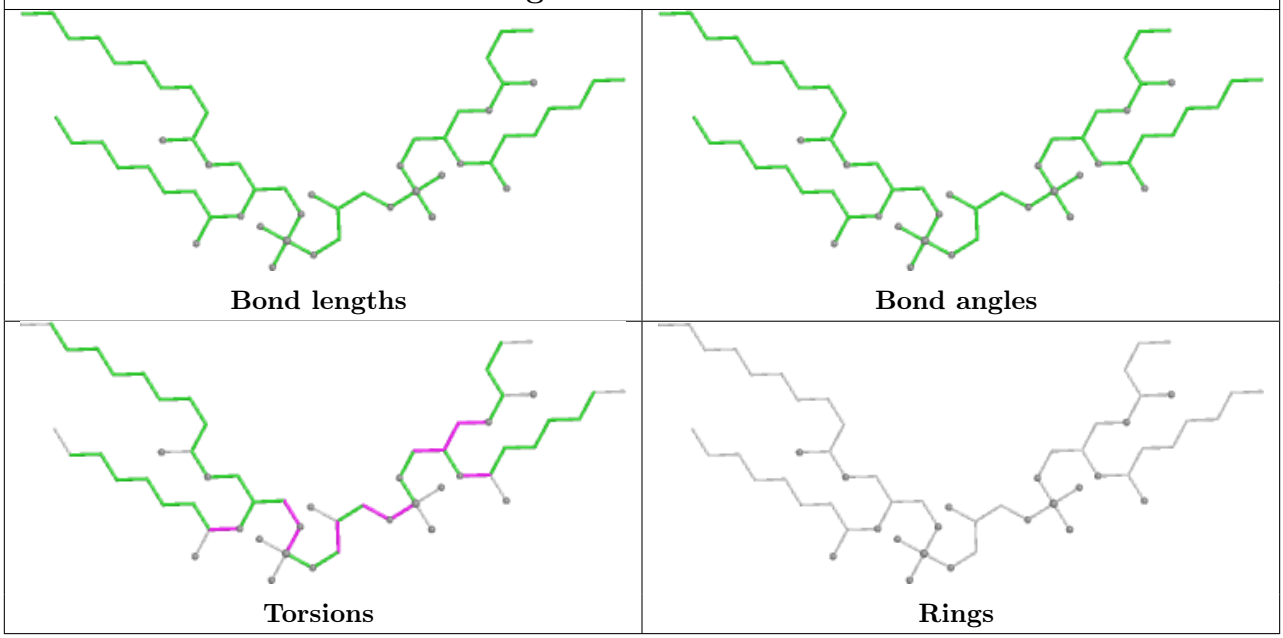


Ligand CDL E 101



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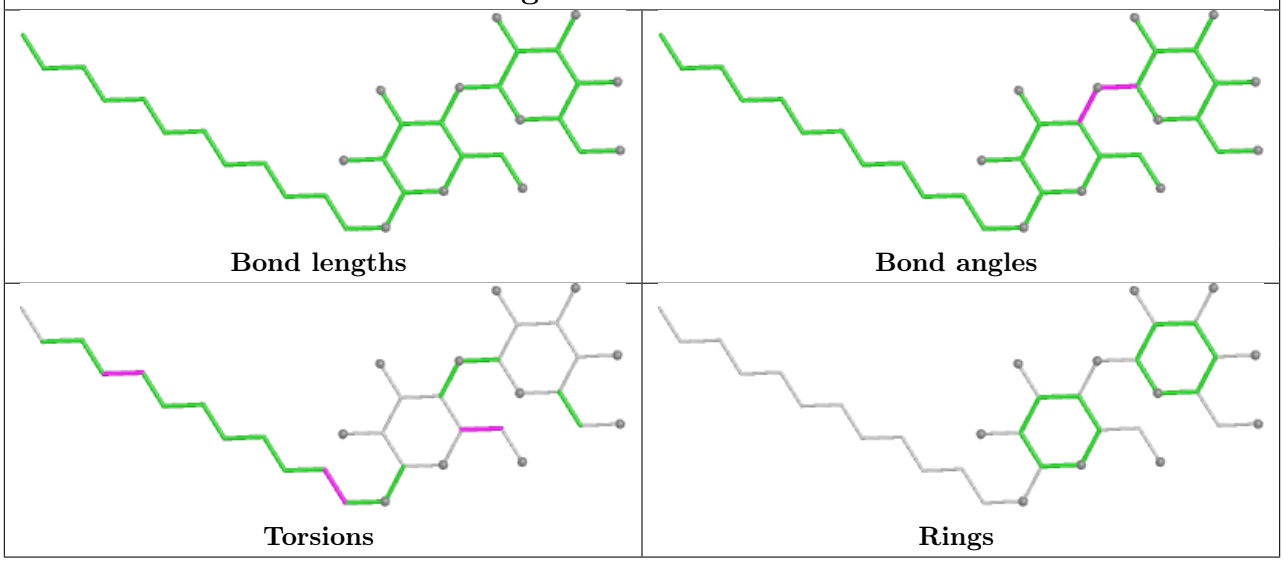
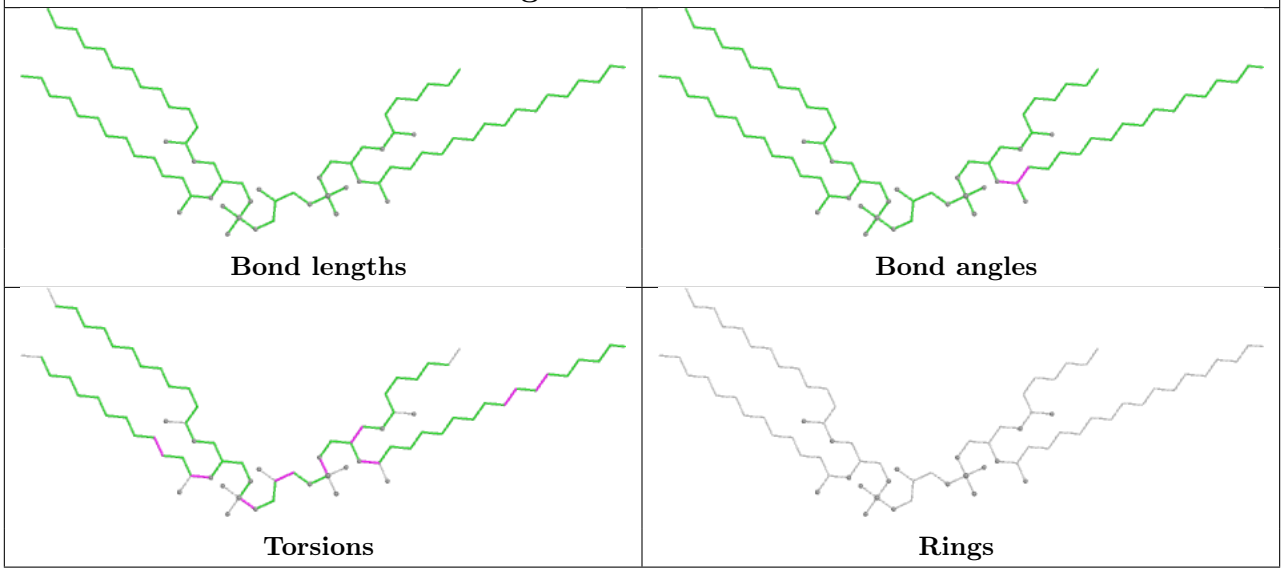
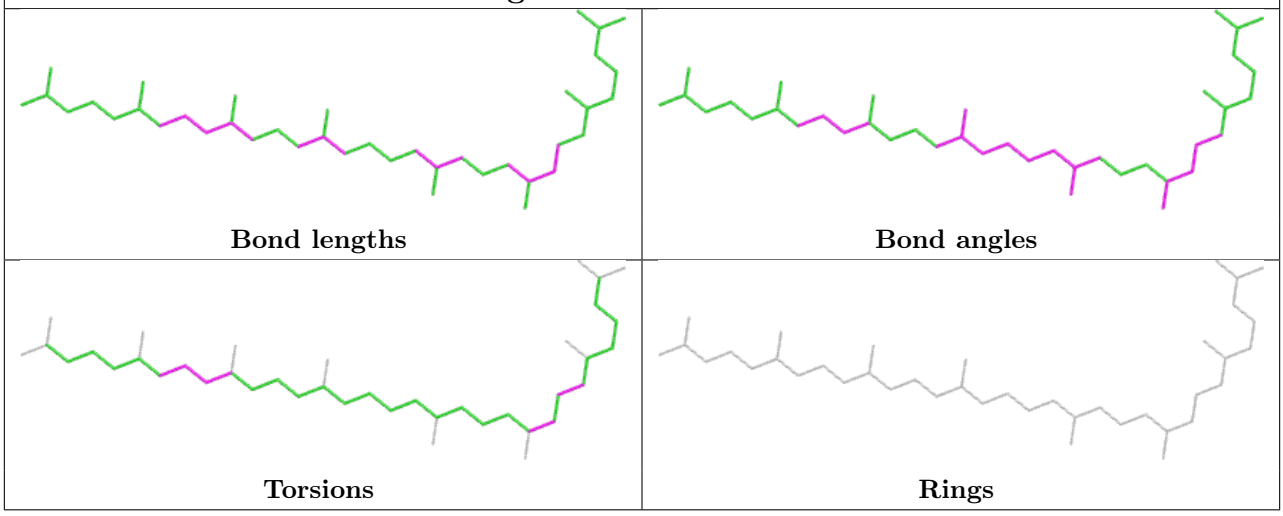


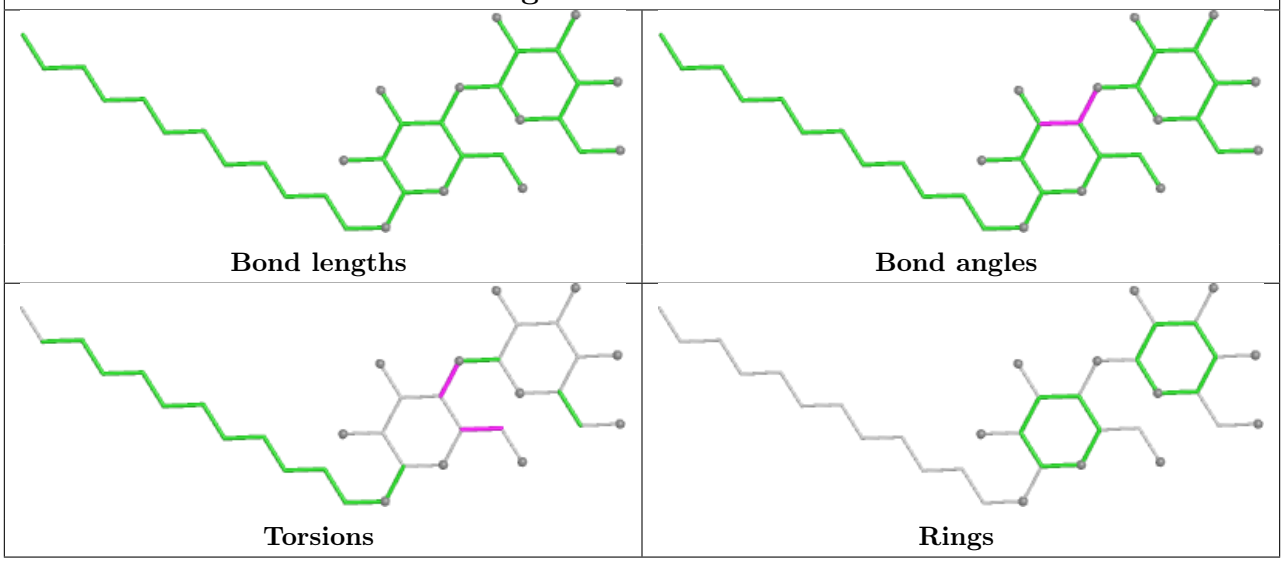
Ligand CDL M 410



Ligand A1EF2 D 105



Ligand LMT H 302



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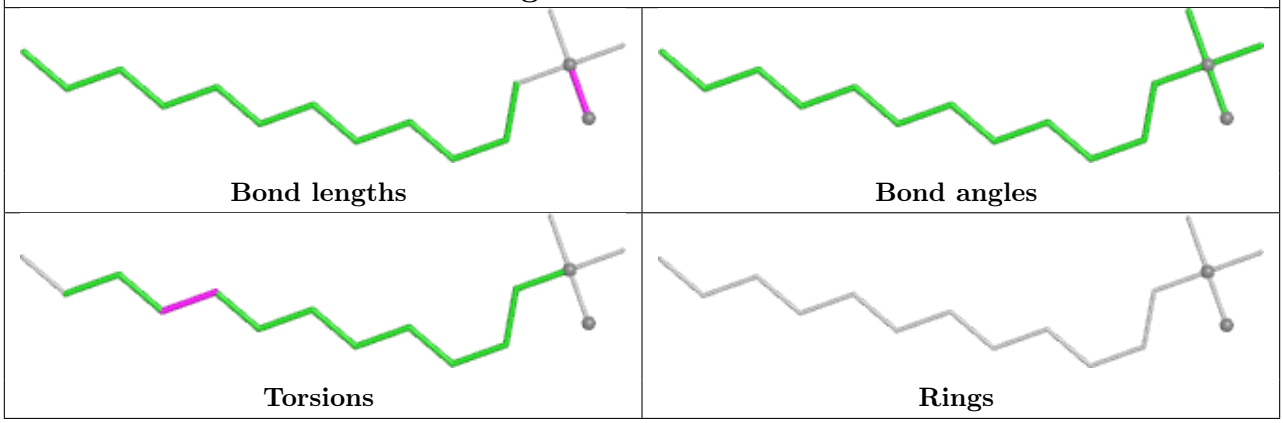
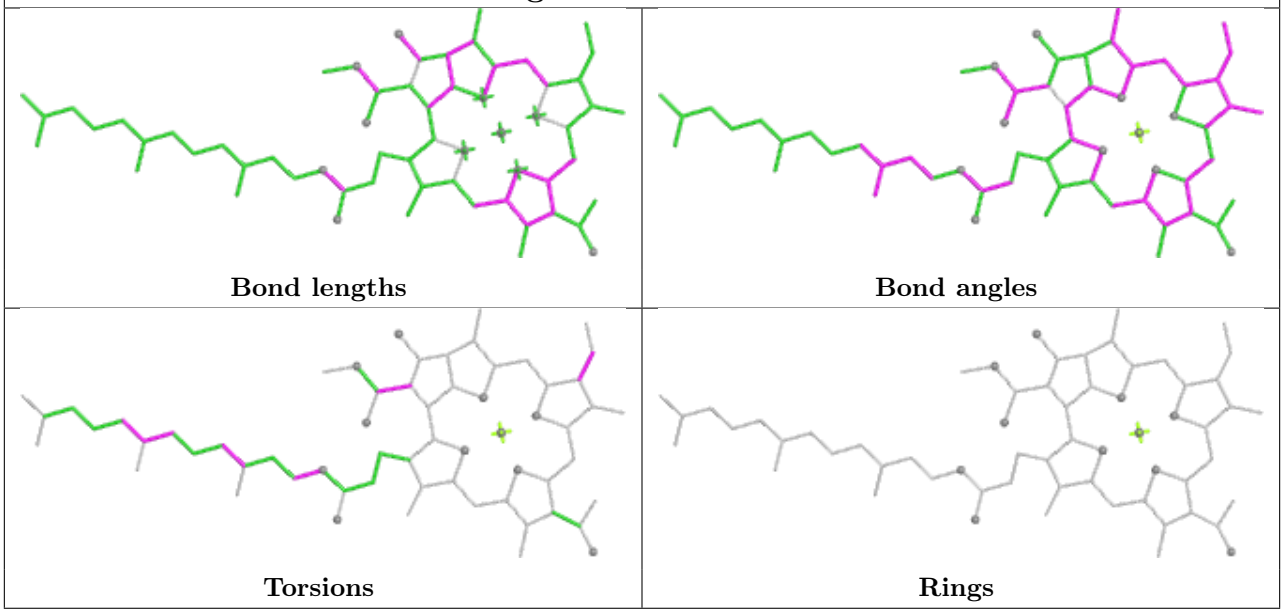


Ligand BCL P 102



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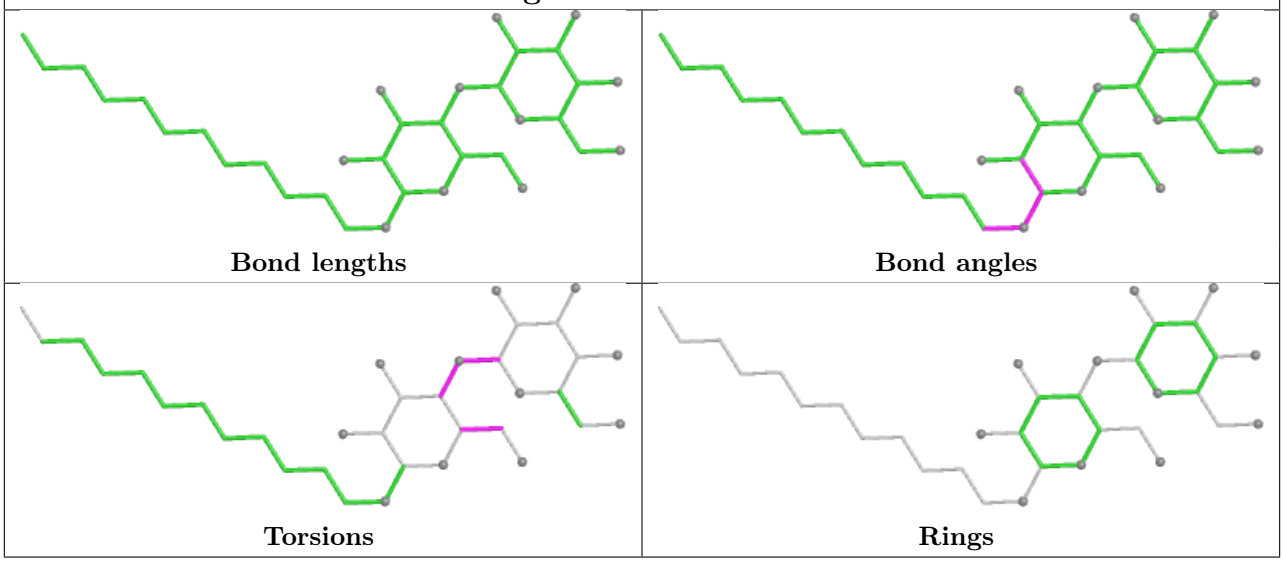

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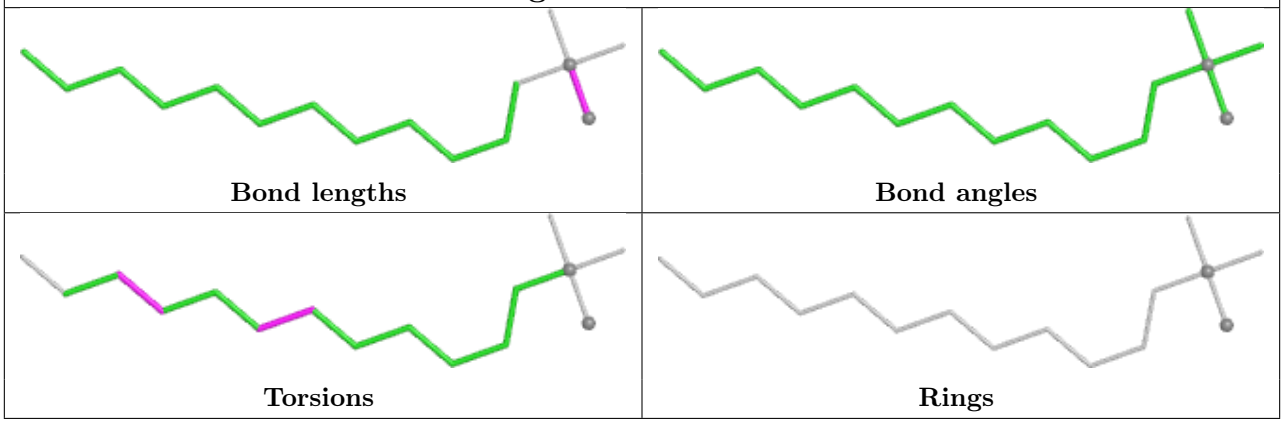
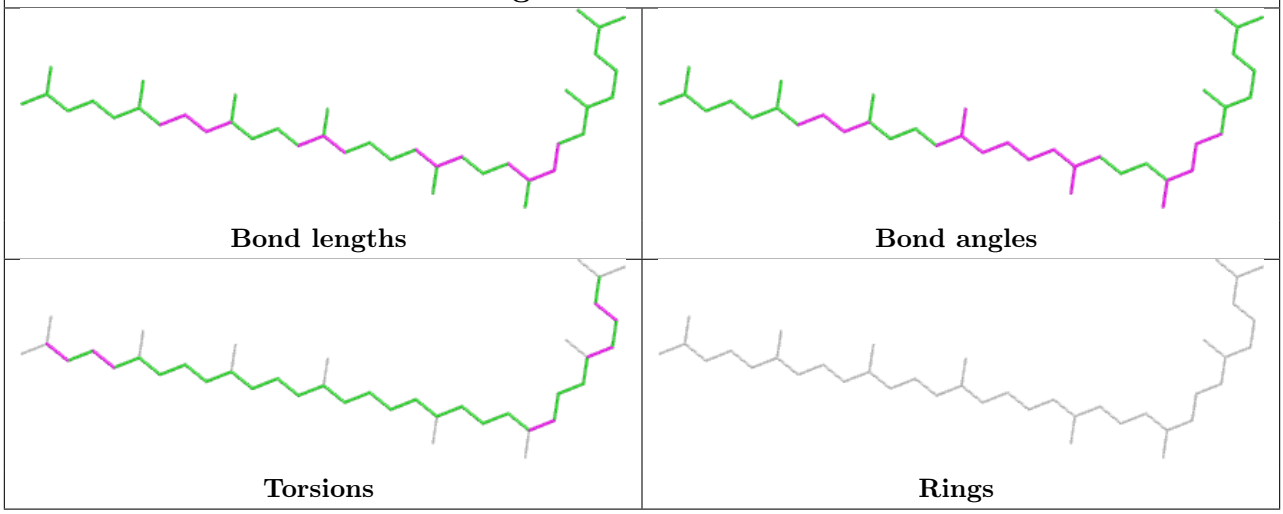
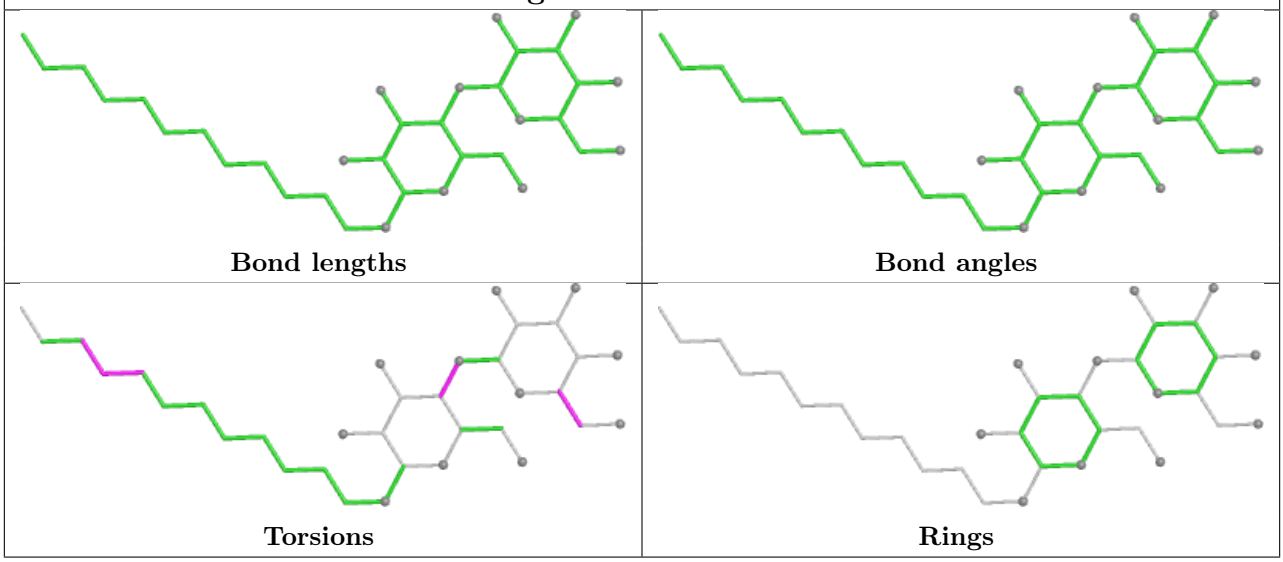


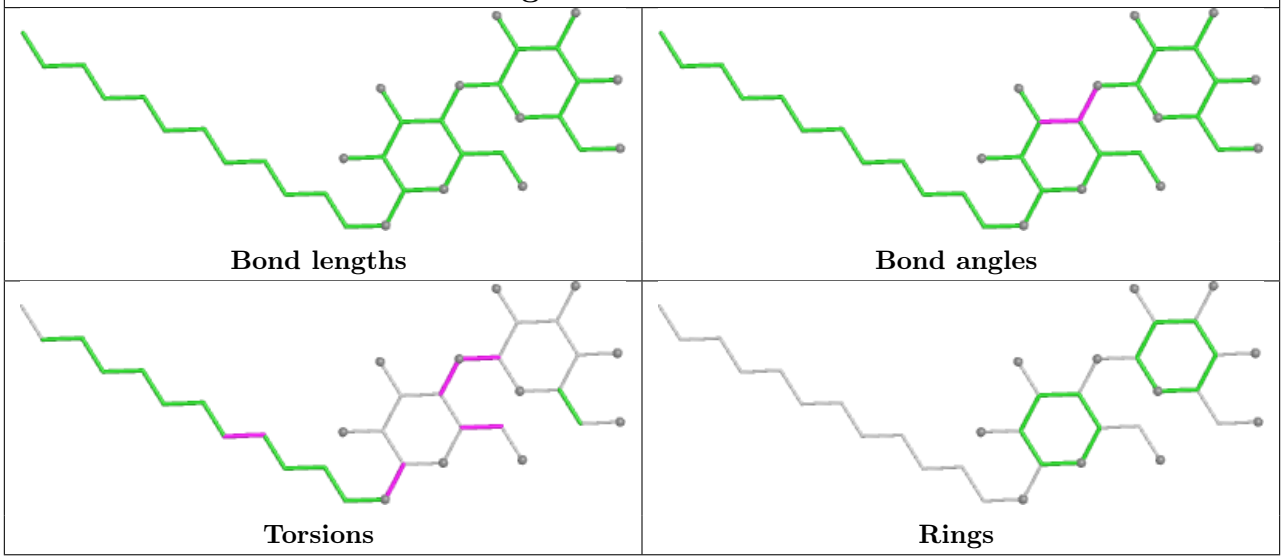
Ligand A1EF2 e 101



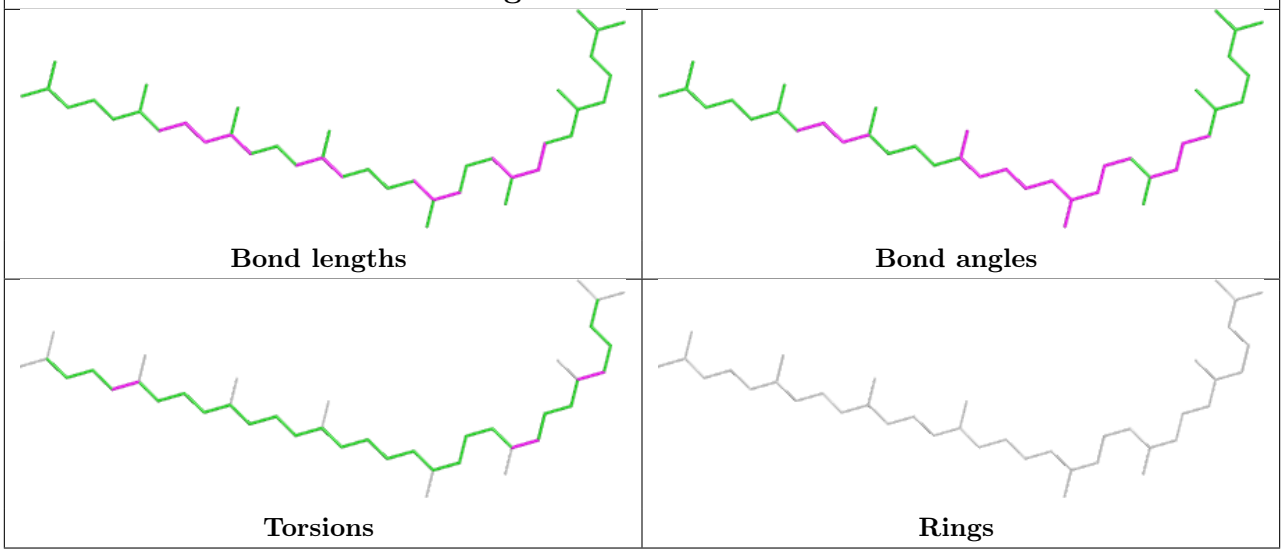
Ligand LMT c 103

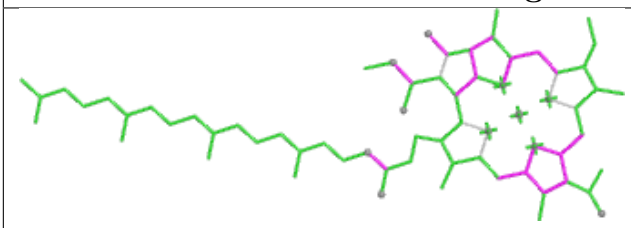
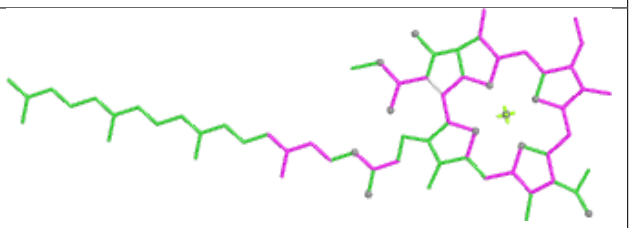
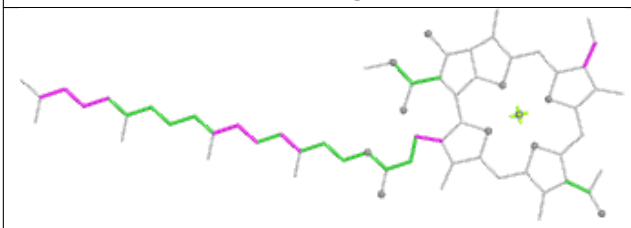
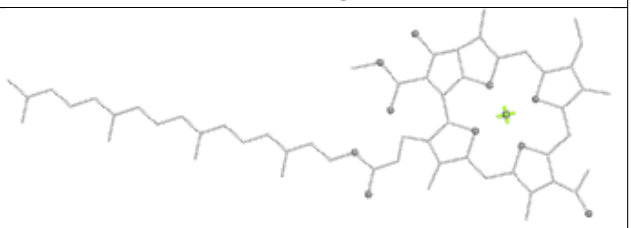


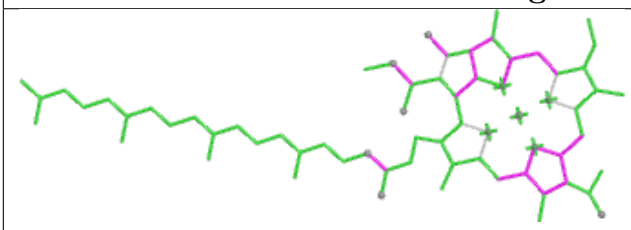
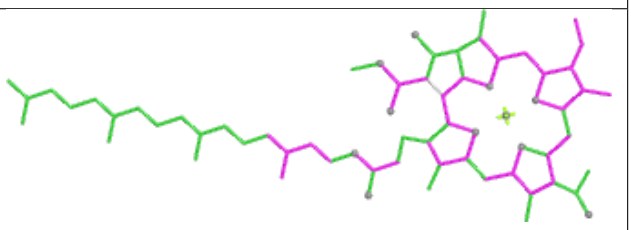
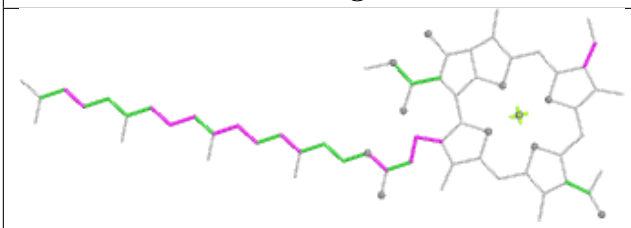
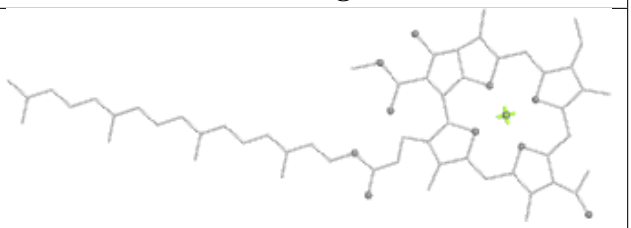
Ligand LMT O 101



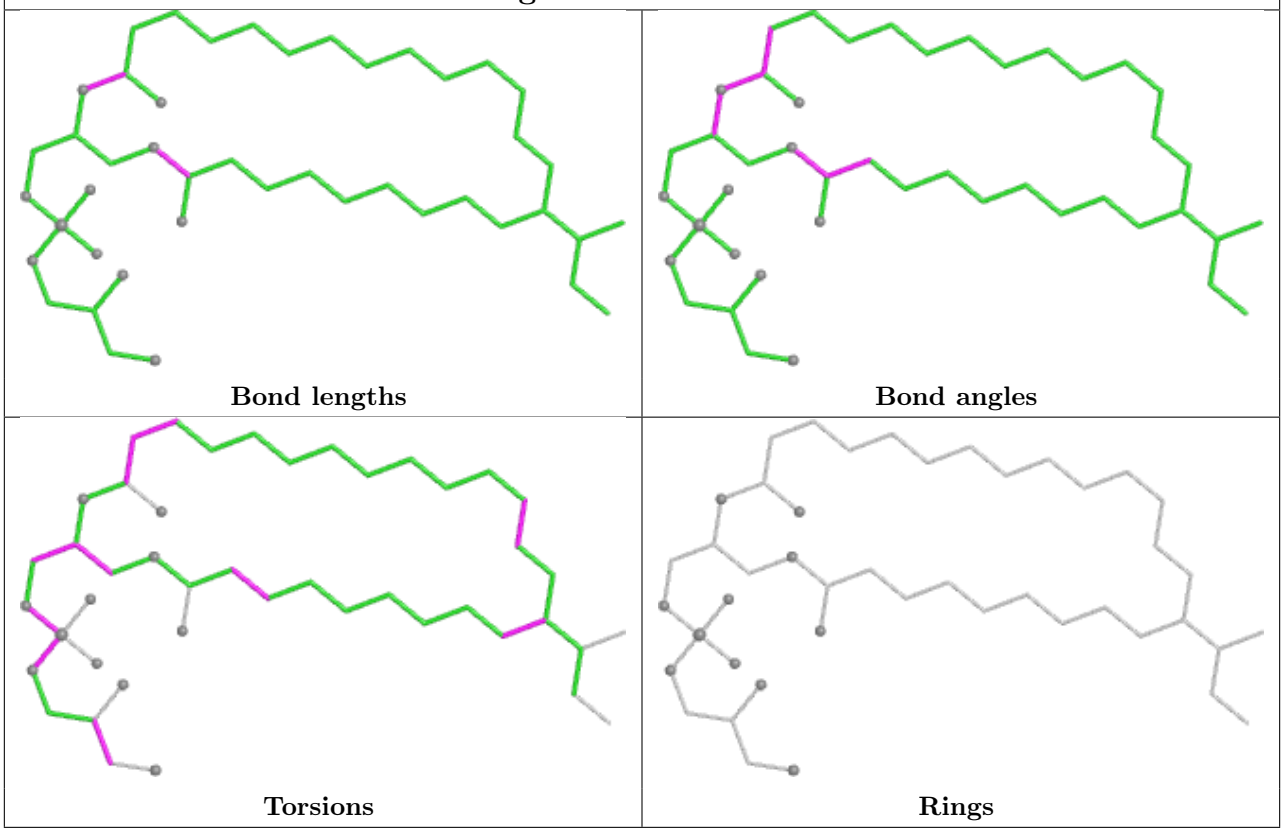
Ligand A1EF2 M 411



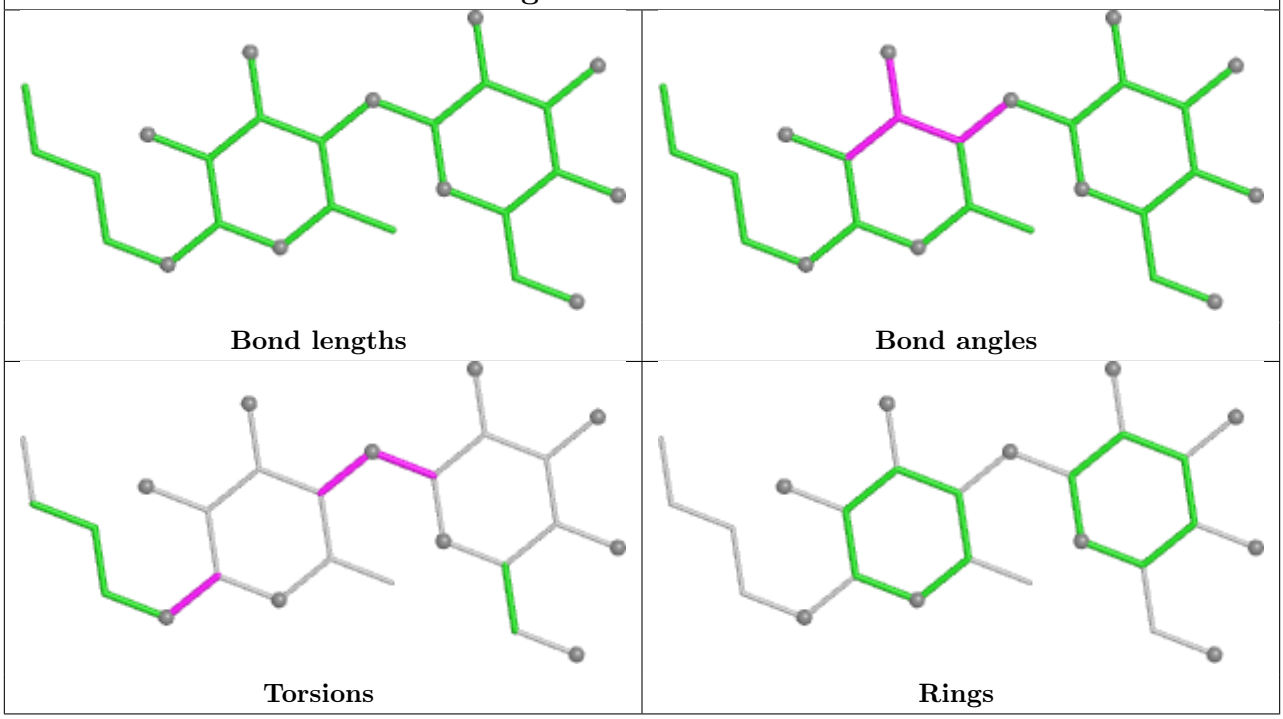
Ligand BCL C 103	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCL k 102	
 Bond lengths	 Bond angles
 Torsions	 Rings

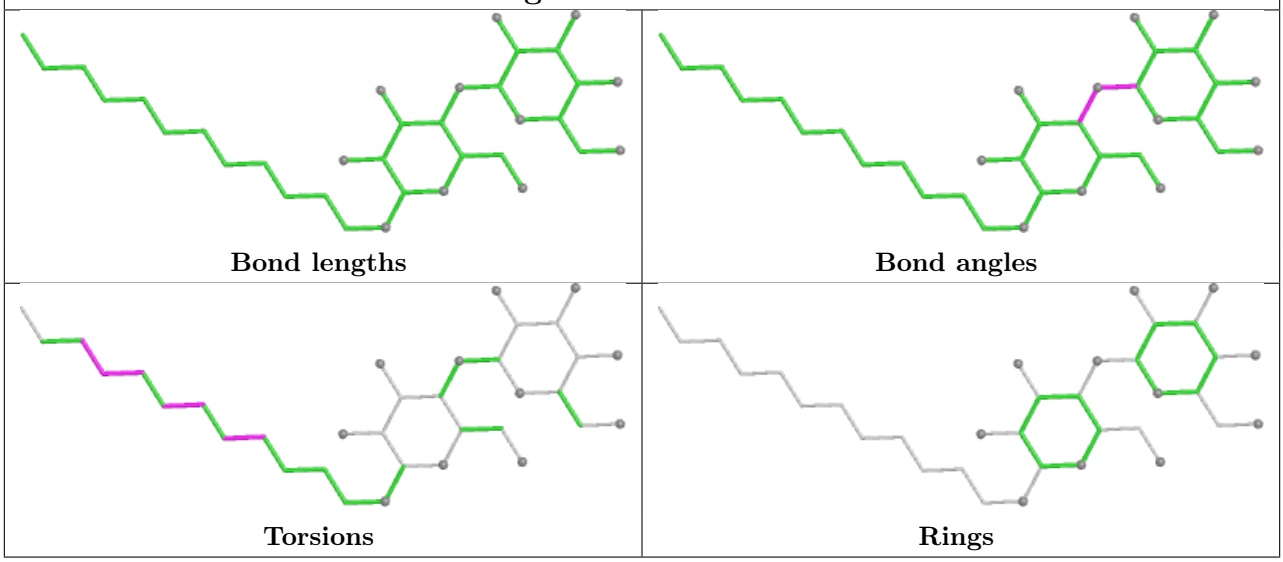
Ligand PGV M 402



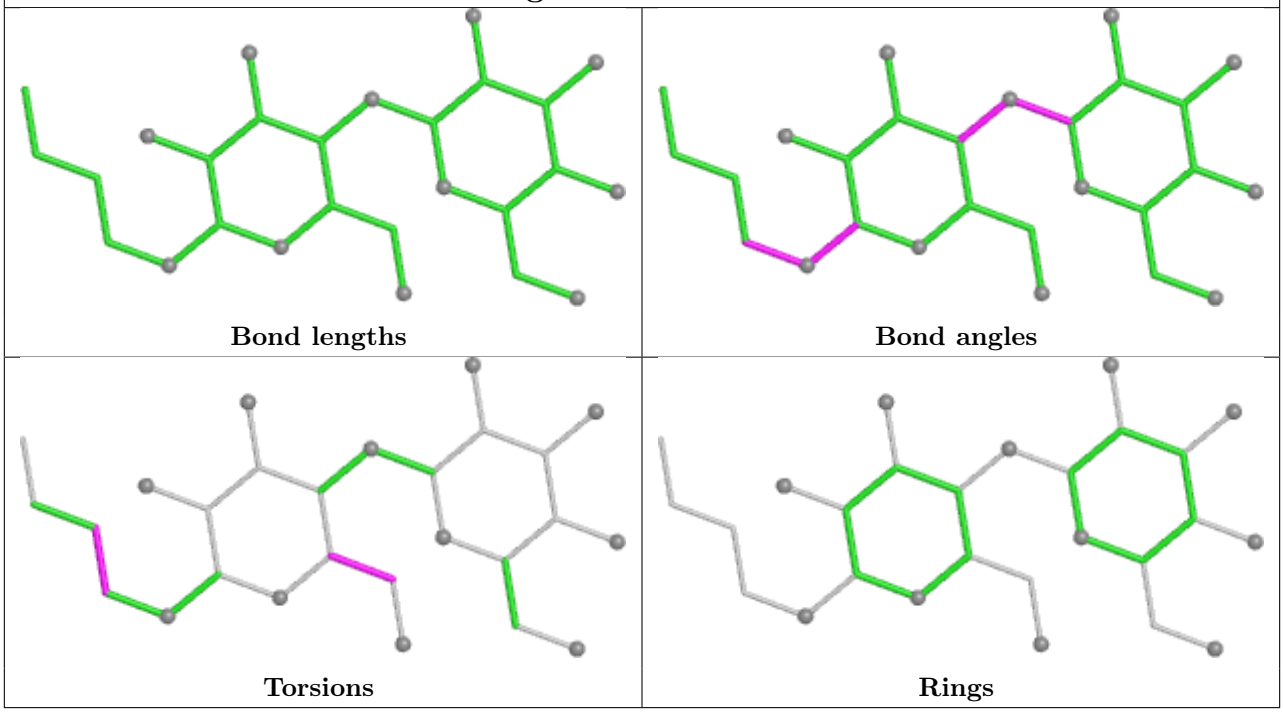
Ligand LMT D 101

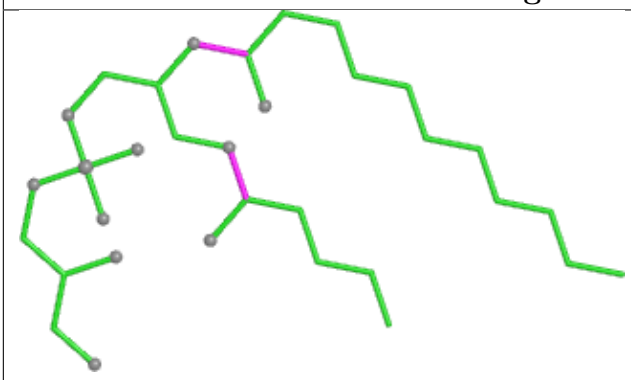
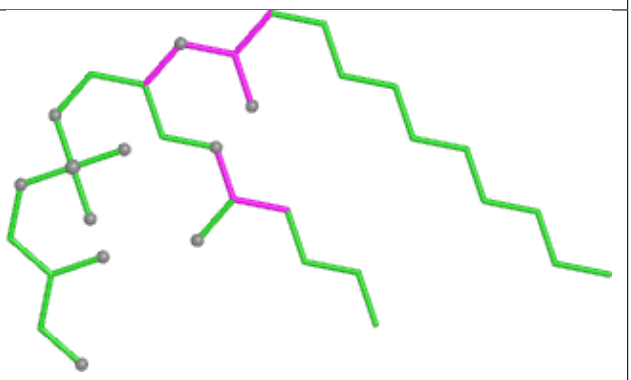
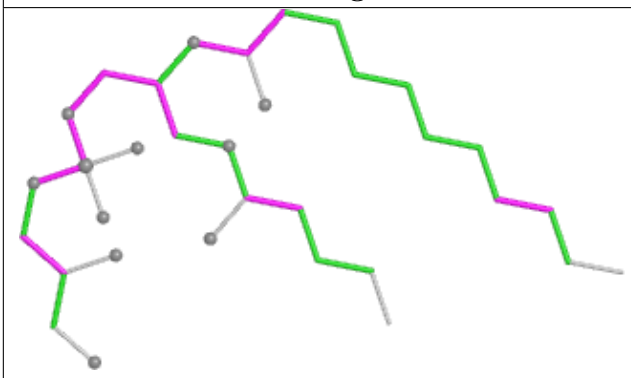
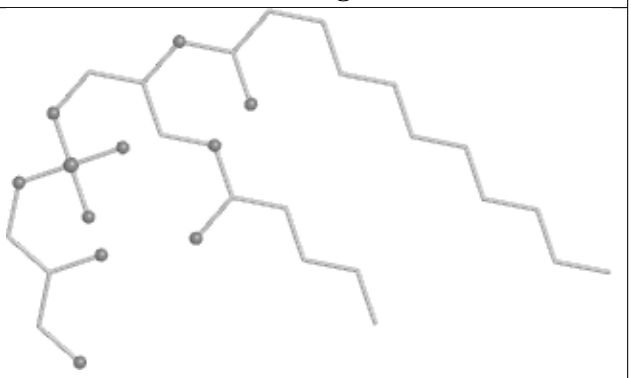


Ligand LMT L 315

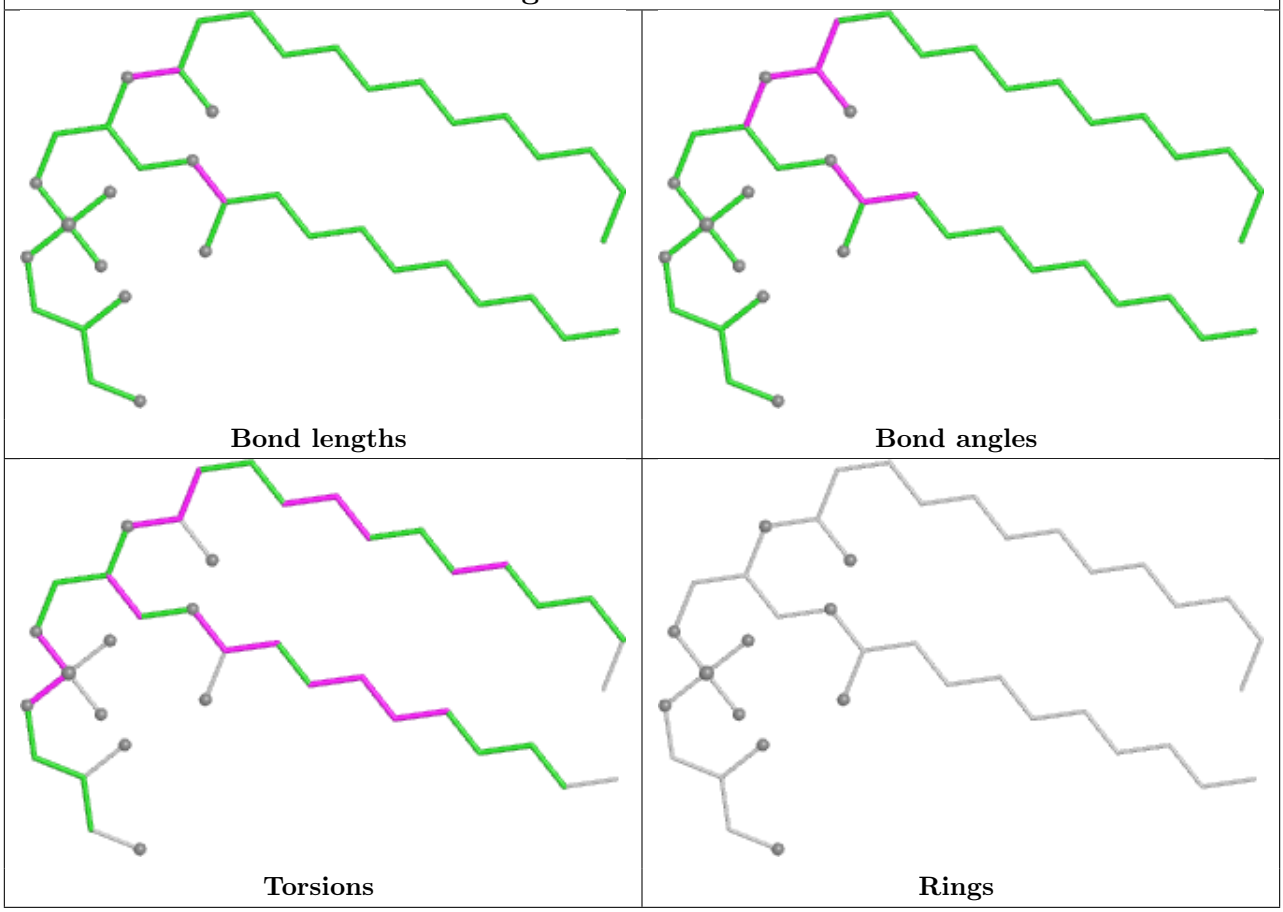


Ligand LMT a 101

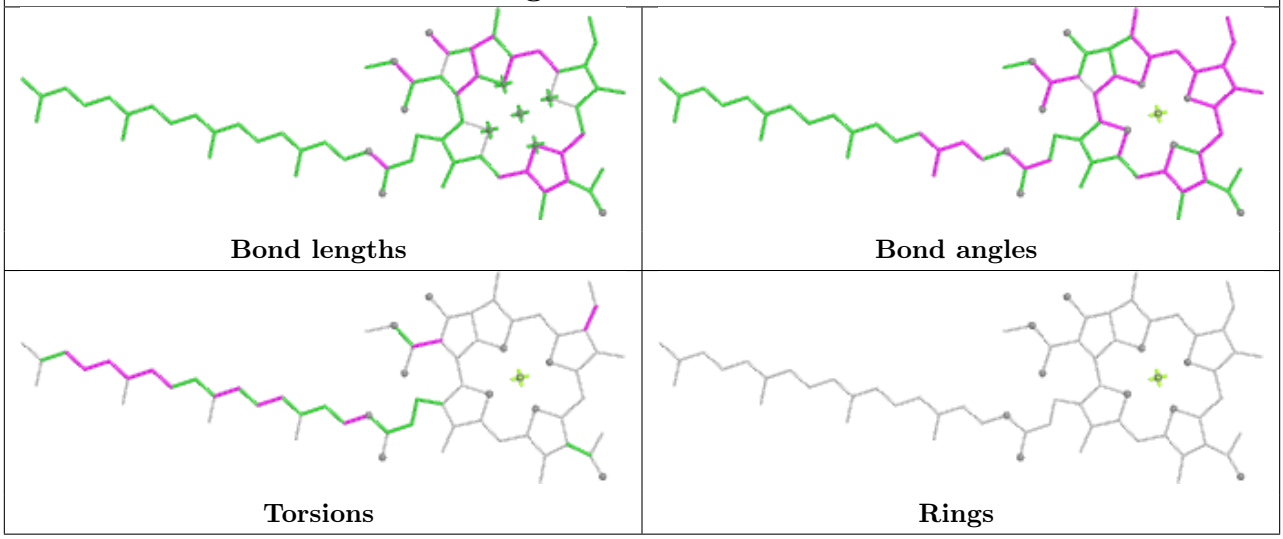


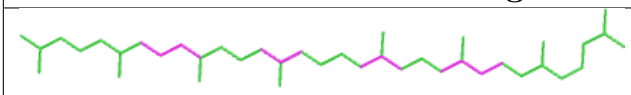
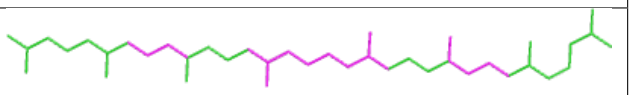
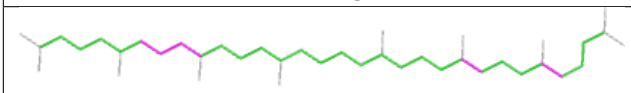
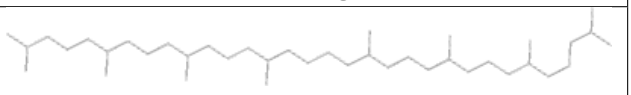
Ligand PGV L 306	
 Bond lengths	 Bond angles
 Torsions	 Rings

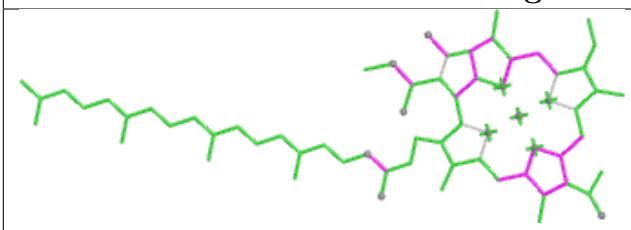
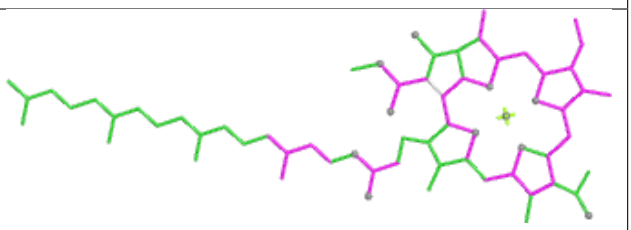
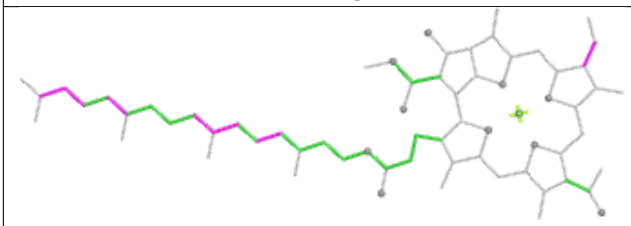
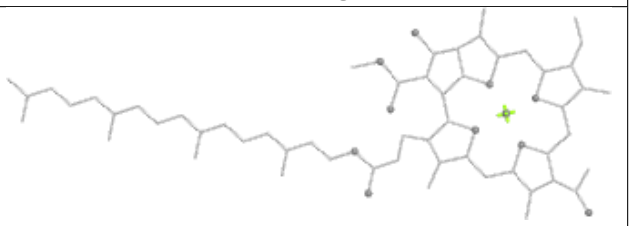
Ligand PGV H 304



Ligand BCL K 102



Ligand A1EF2 N 103	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCL D 102	
 Bond lengths	 Bond angles
 Torsions	 Rings

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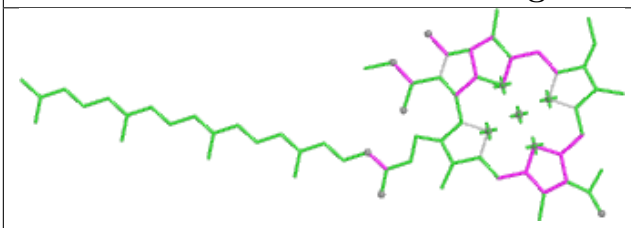
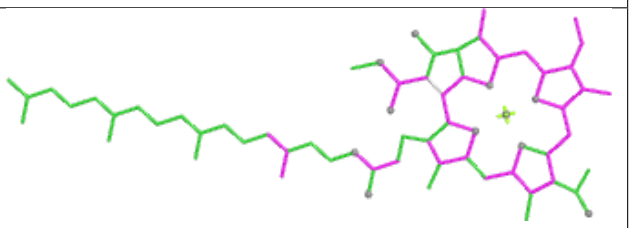
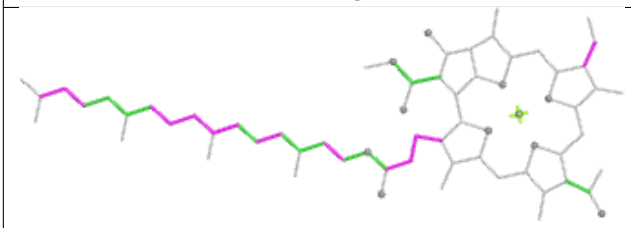
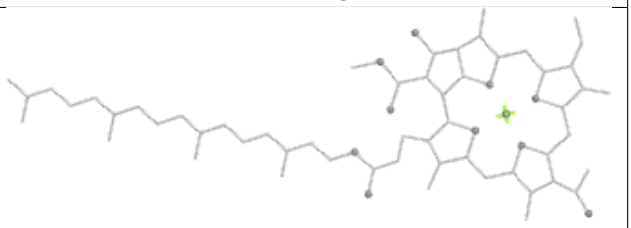
 Bond lengths	 Bond angles
 Torsions	 Rings

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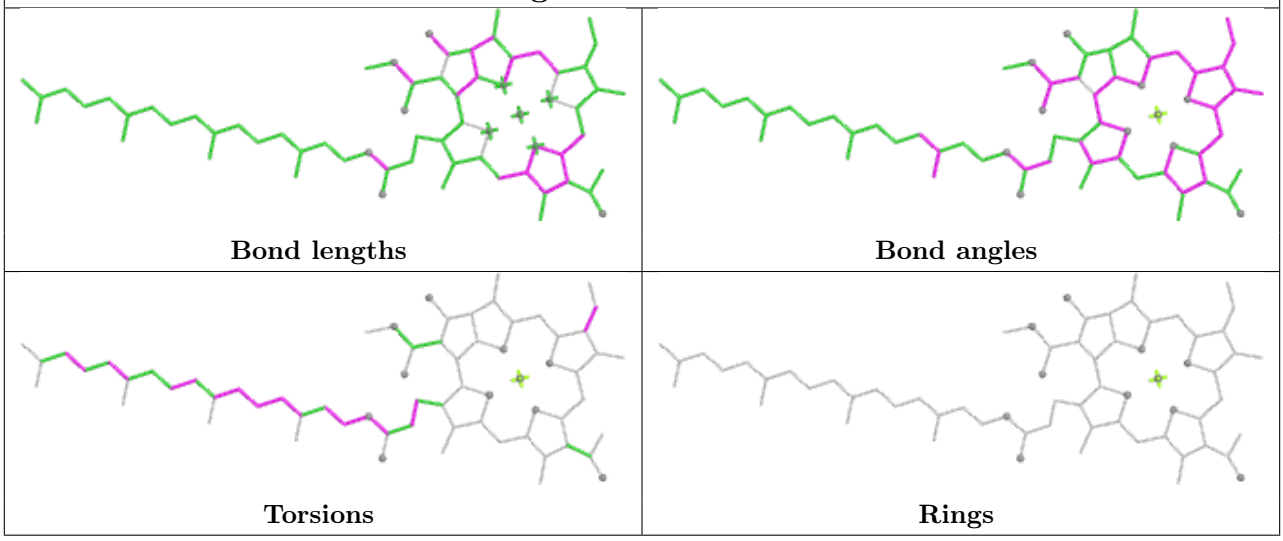

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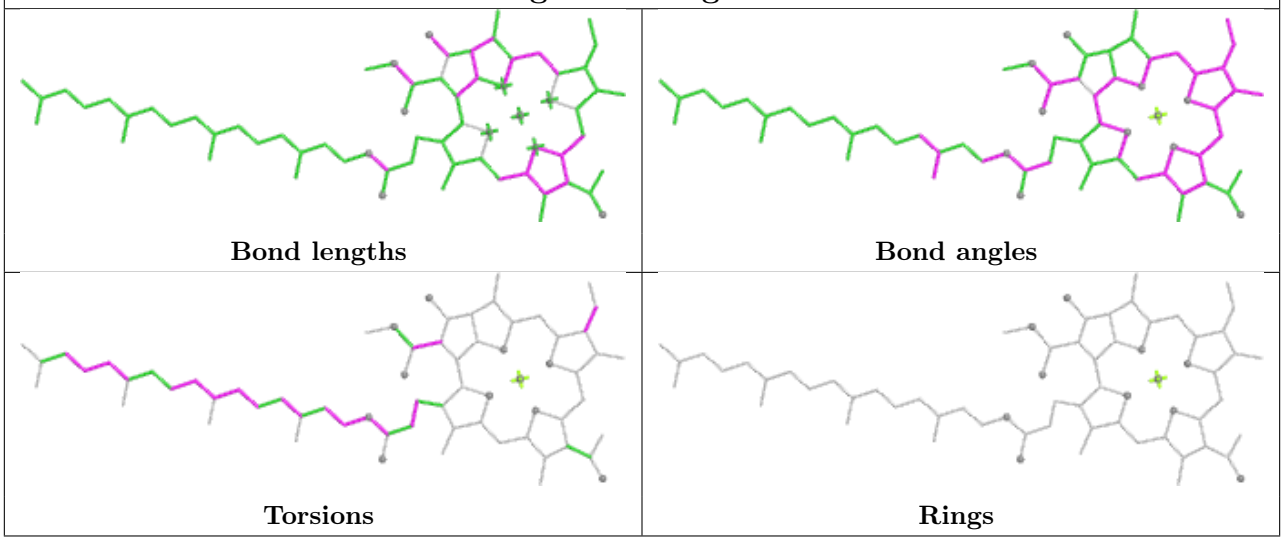
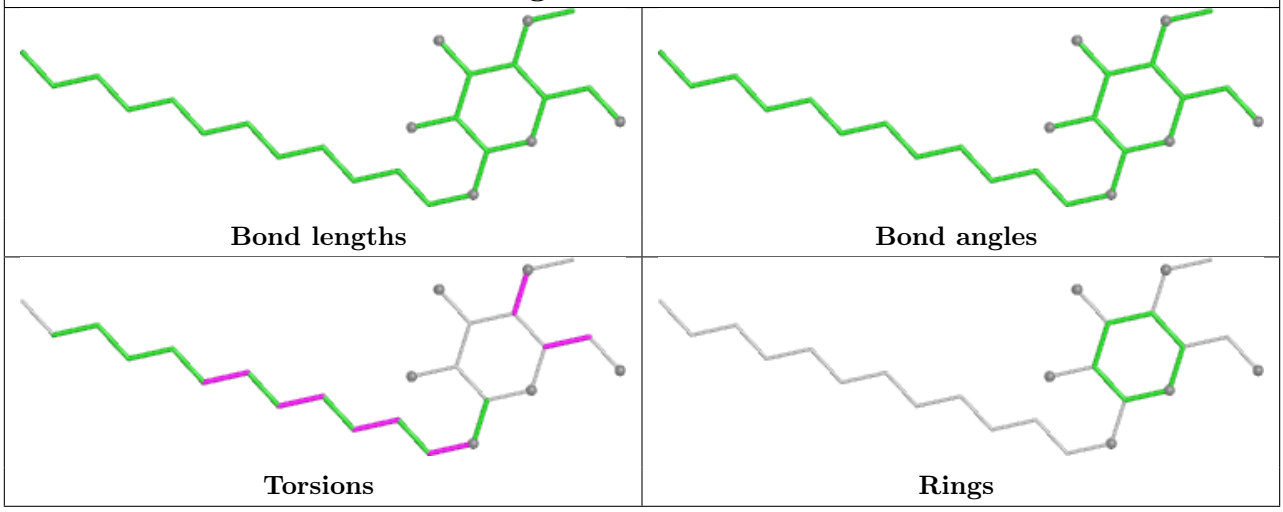
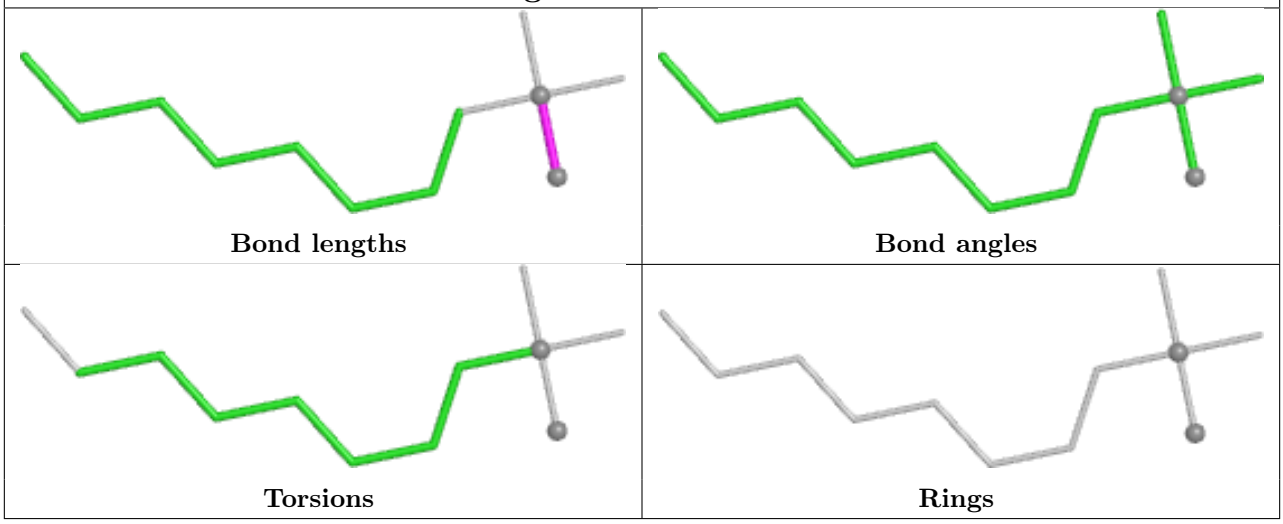


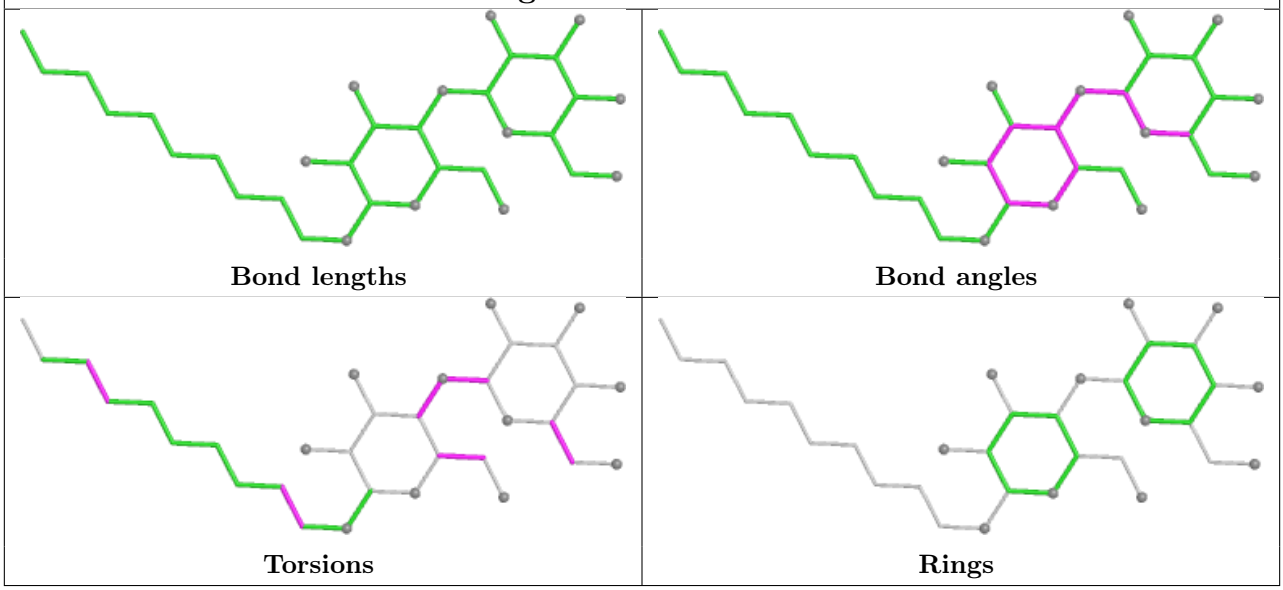
Ligand LMT I 101



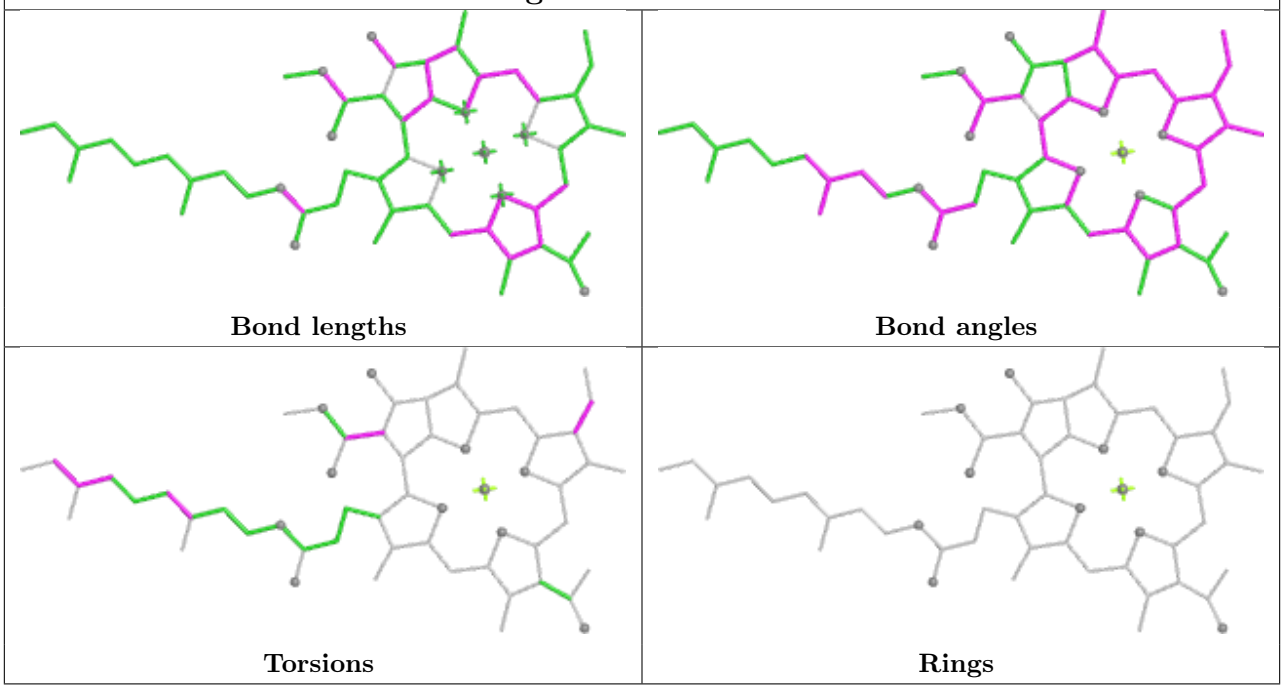
Ligand LDA K 101



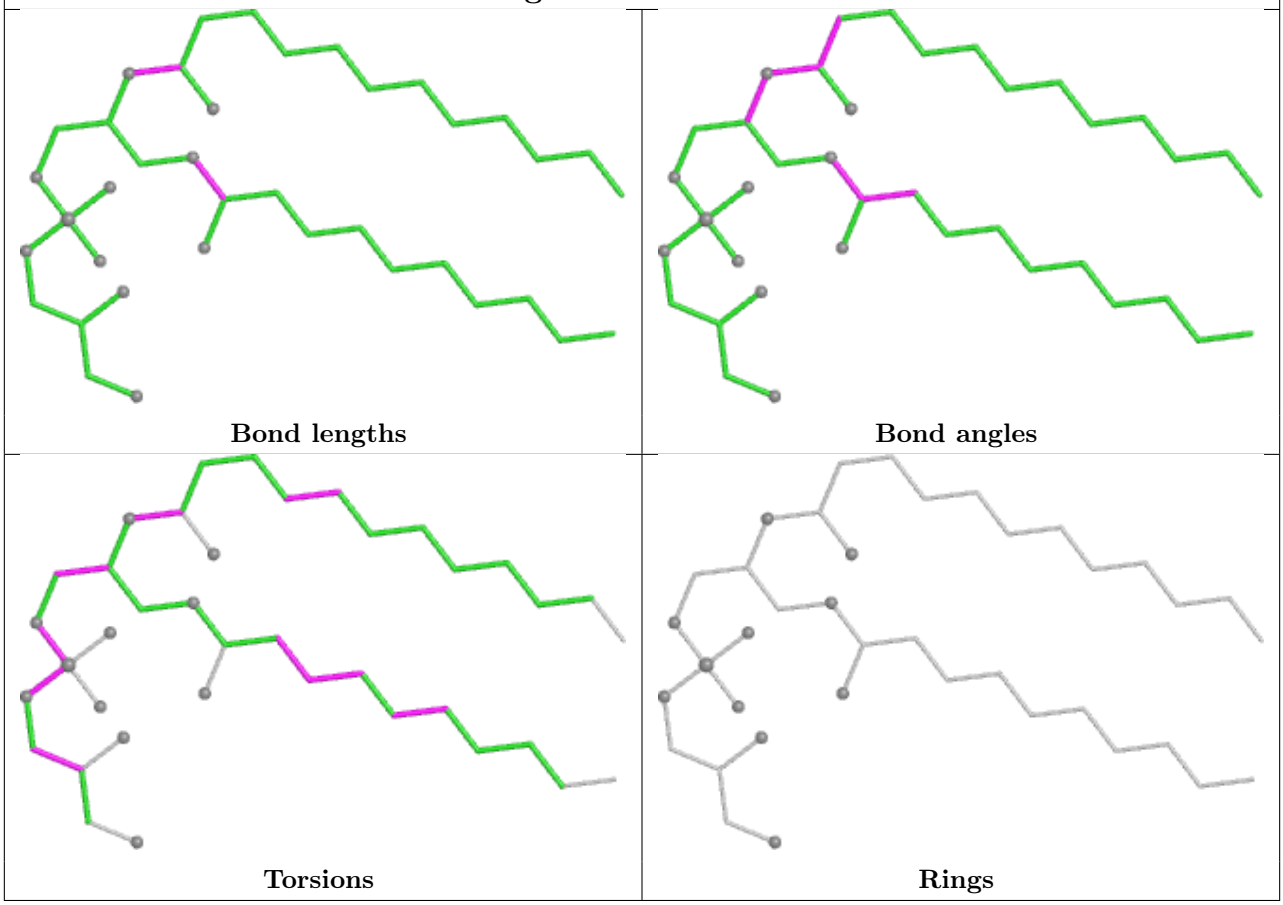
Ligand LMT M 409



Ligand BCL O 102



Ligand PGV L 305



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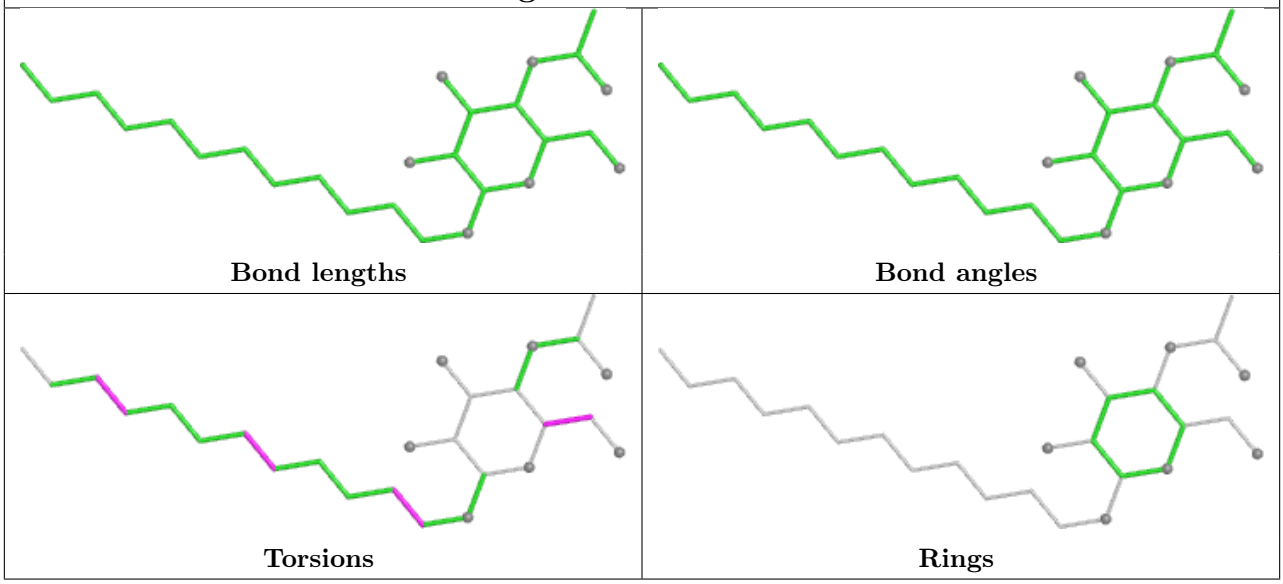
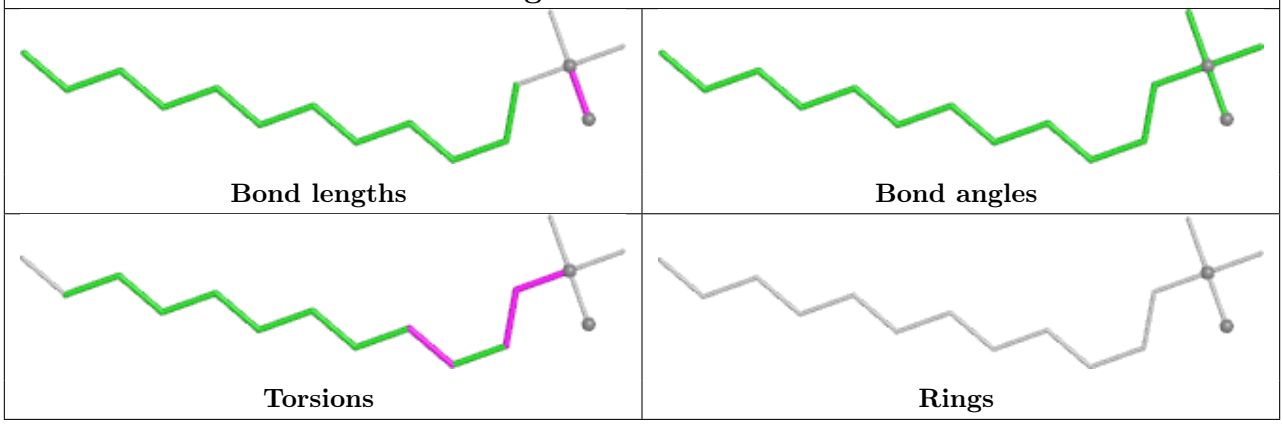
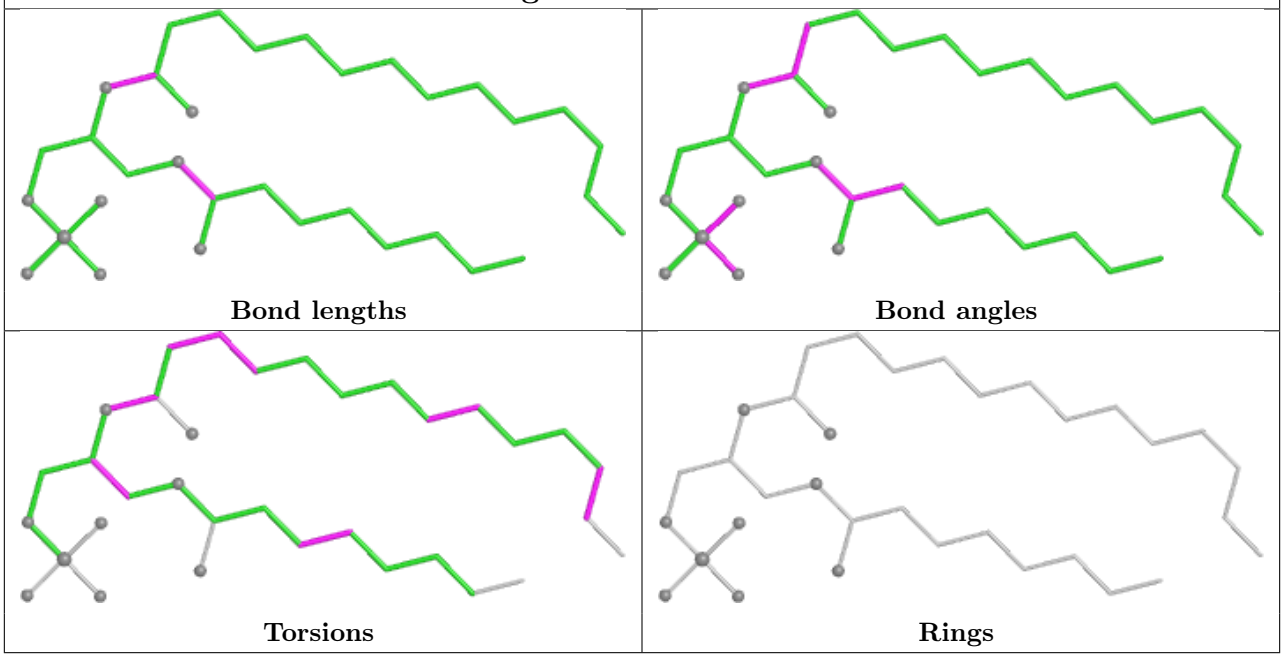


Ligand LDA X 102



Ligand PGV H 303



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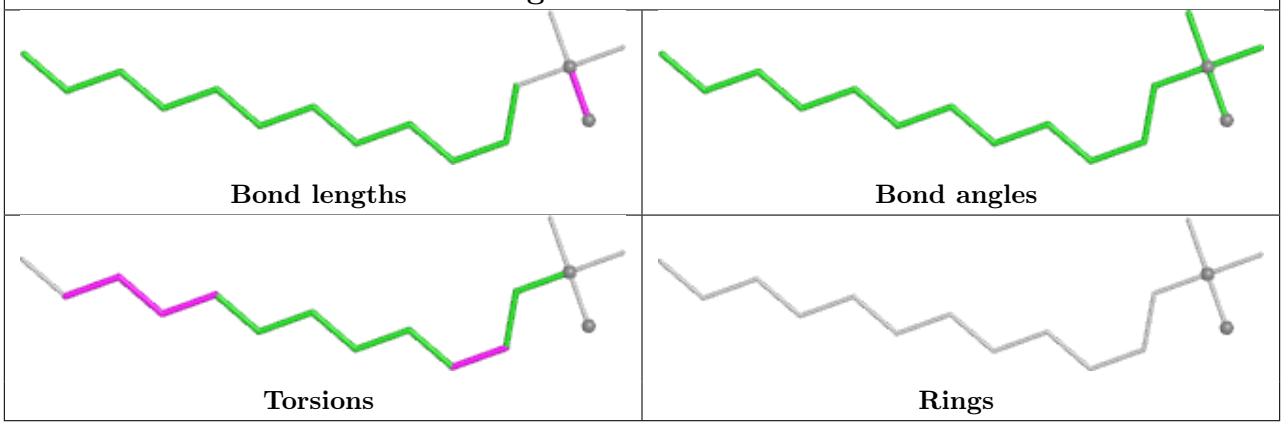
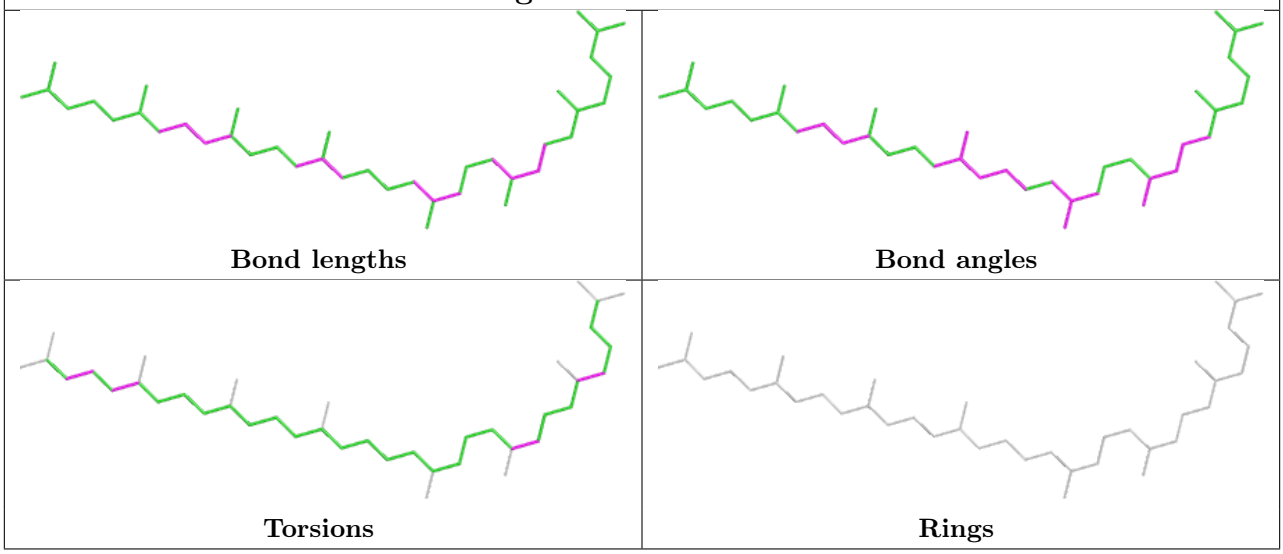
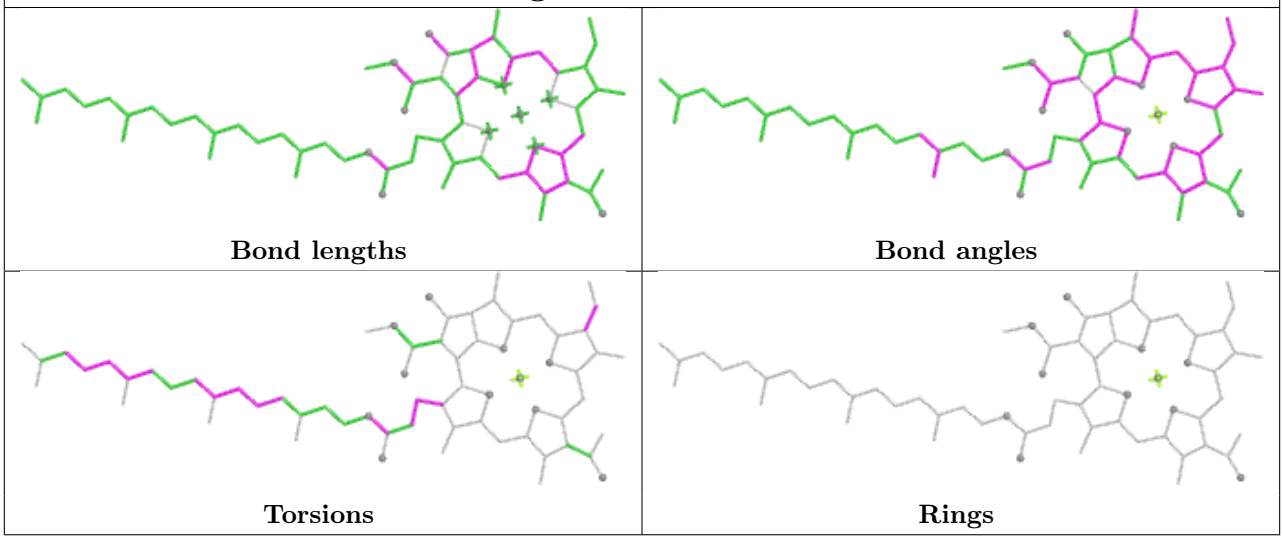


Ligand A1EF2 f 101



Ligand BCL d 102



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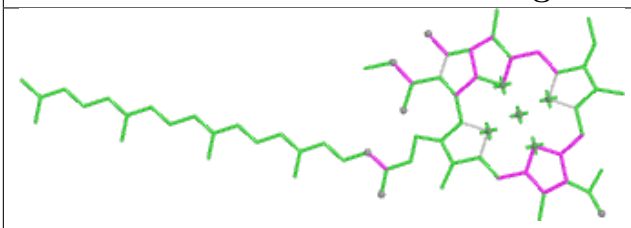
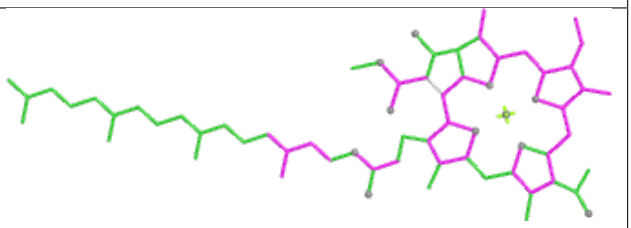
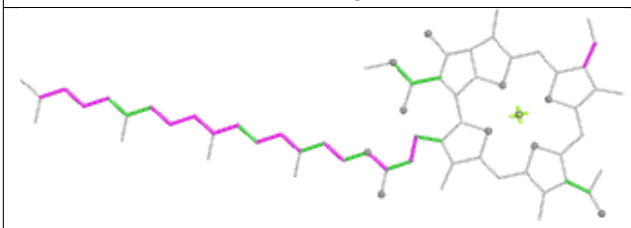
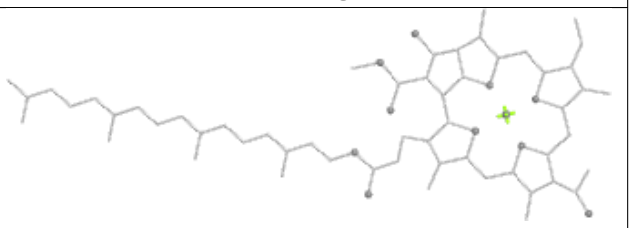
 Bond lengths	 Bond angles
 Torsions	 Rings

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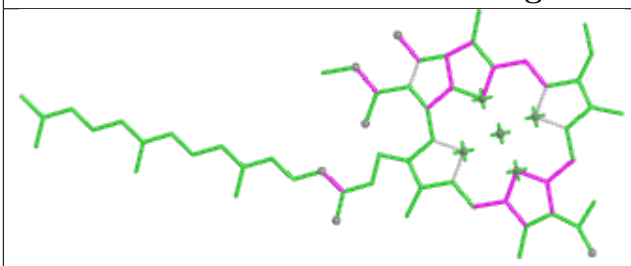
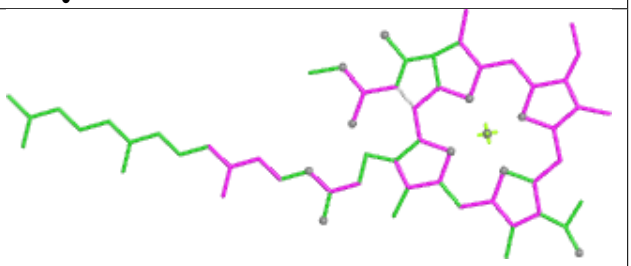
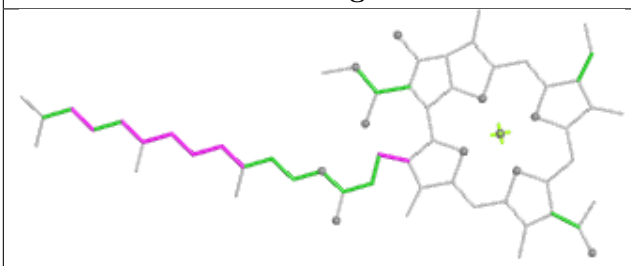
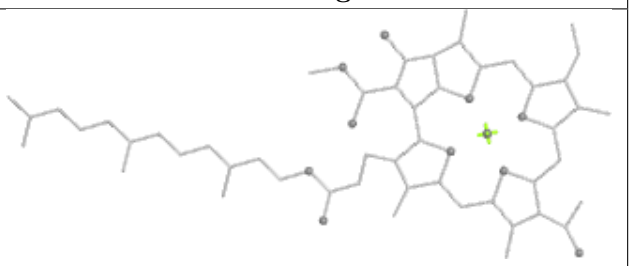
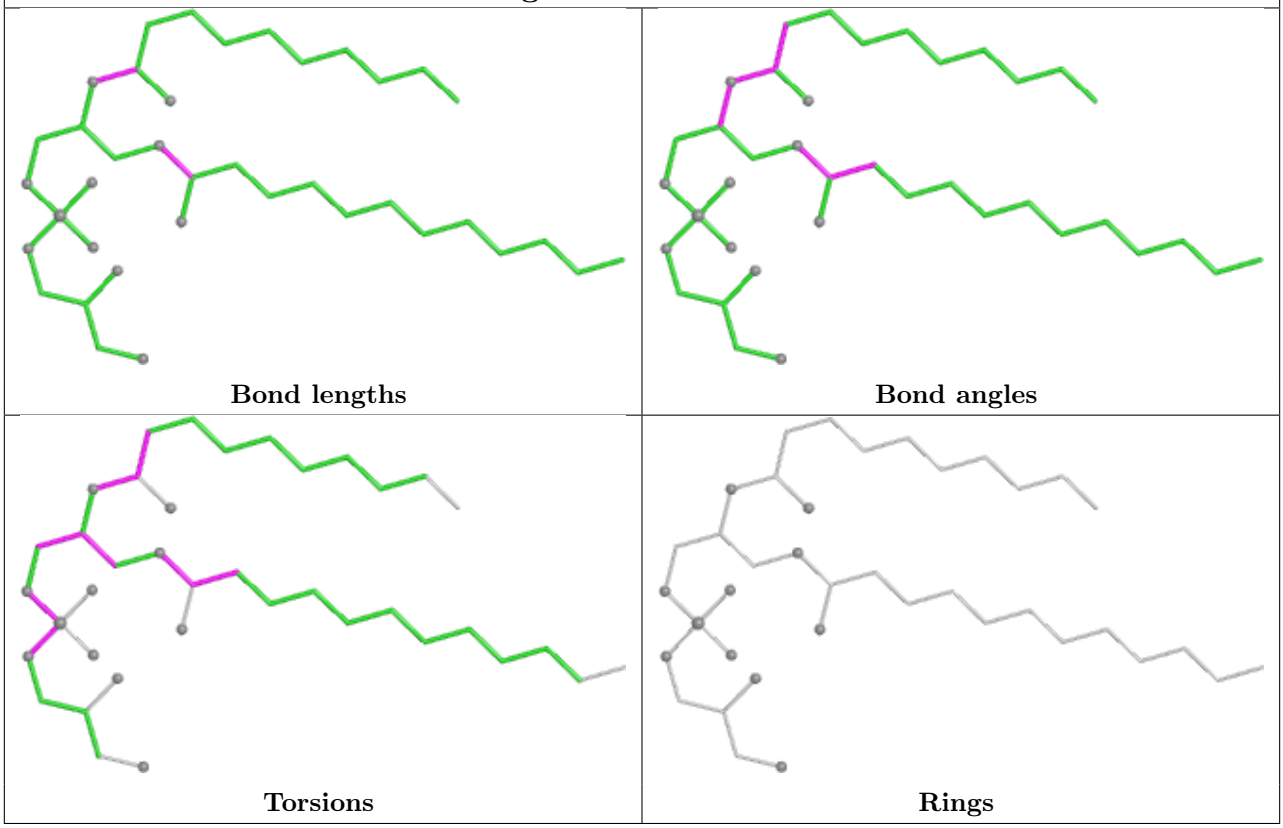
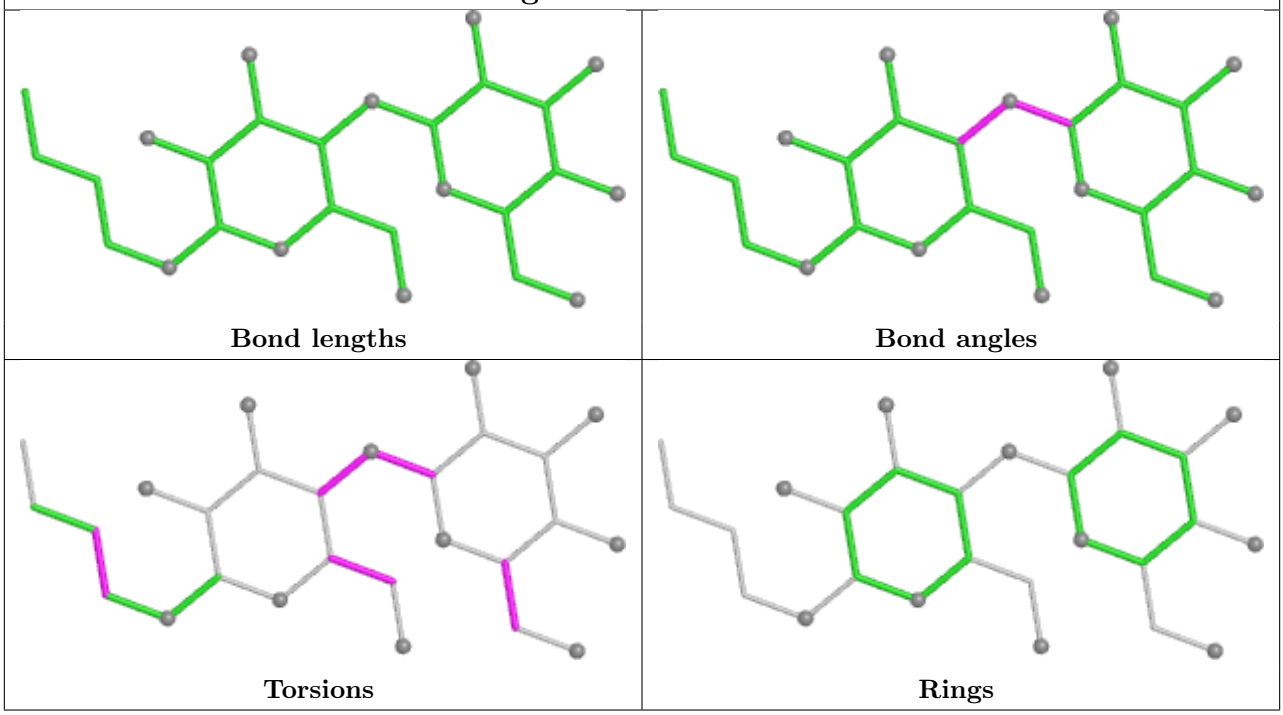
 Bond lengths	 Bond angles
 Torsions	 Rings

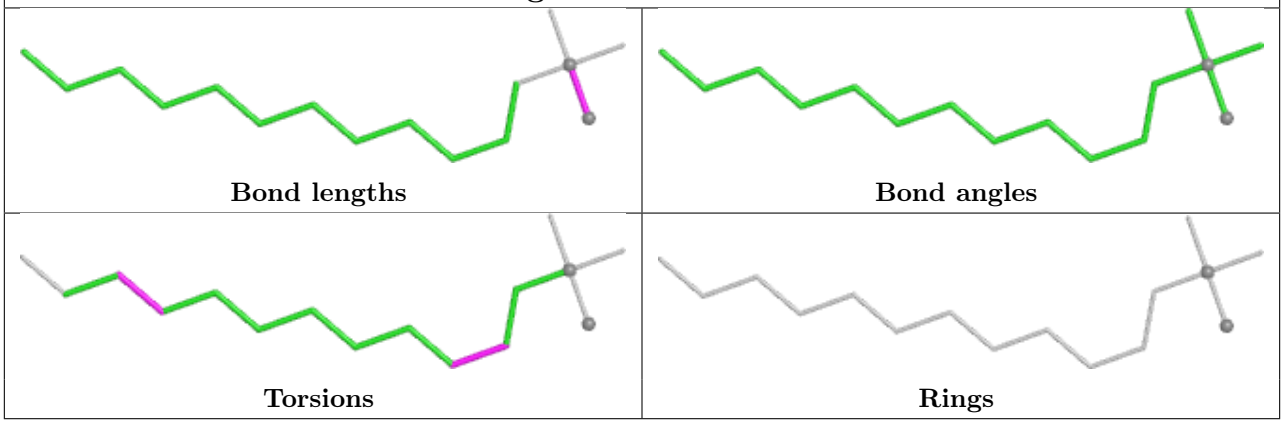
Ligand PGV G 103



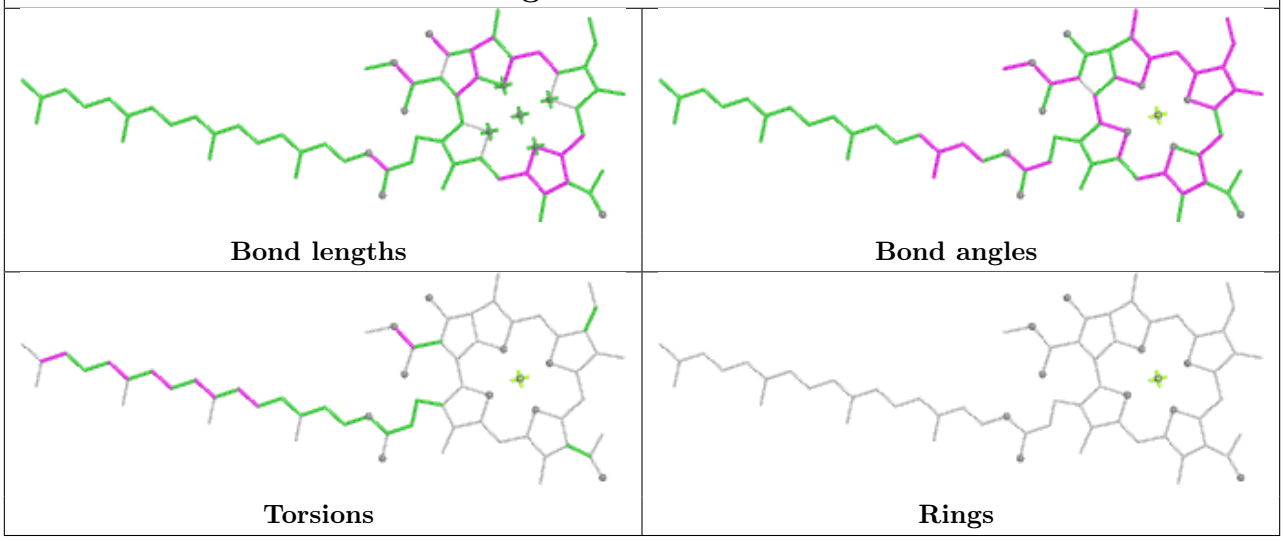
Ligand LMT D 103



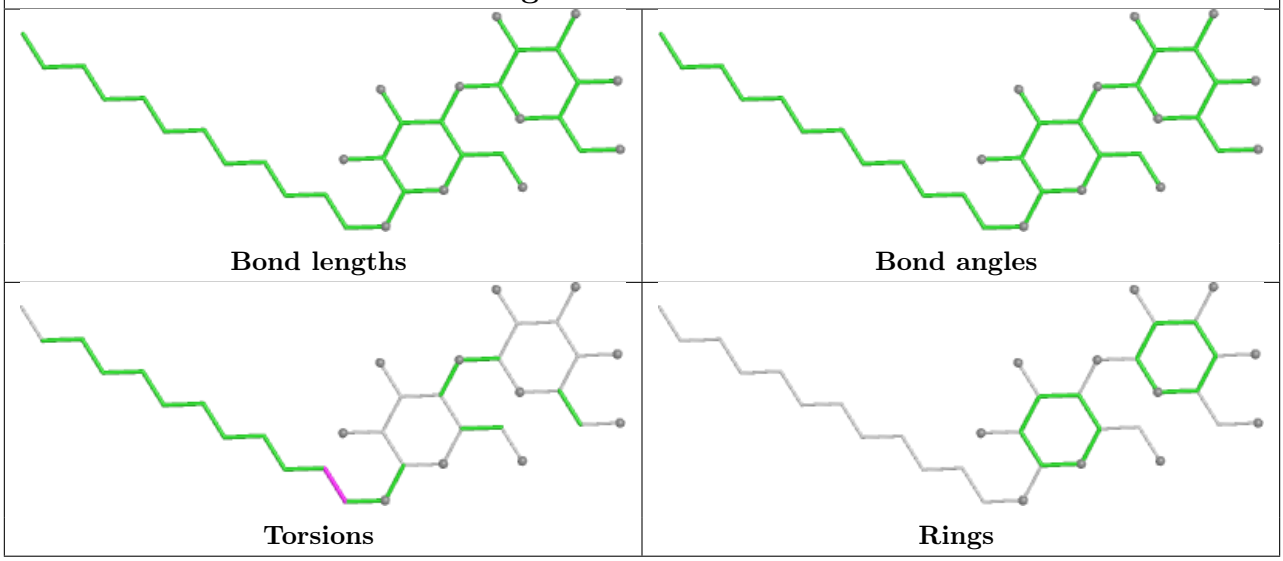
Ligand LDA L 307



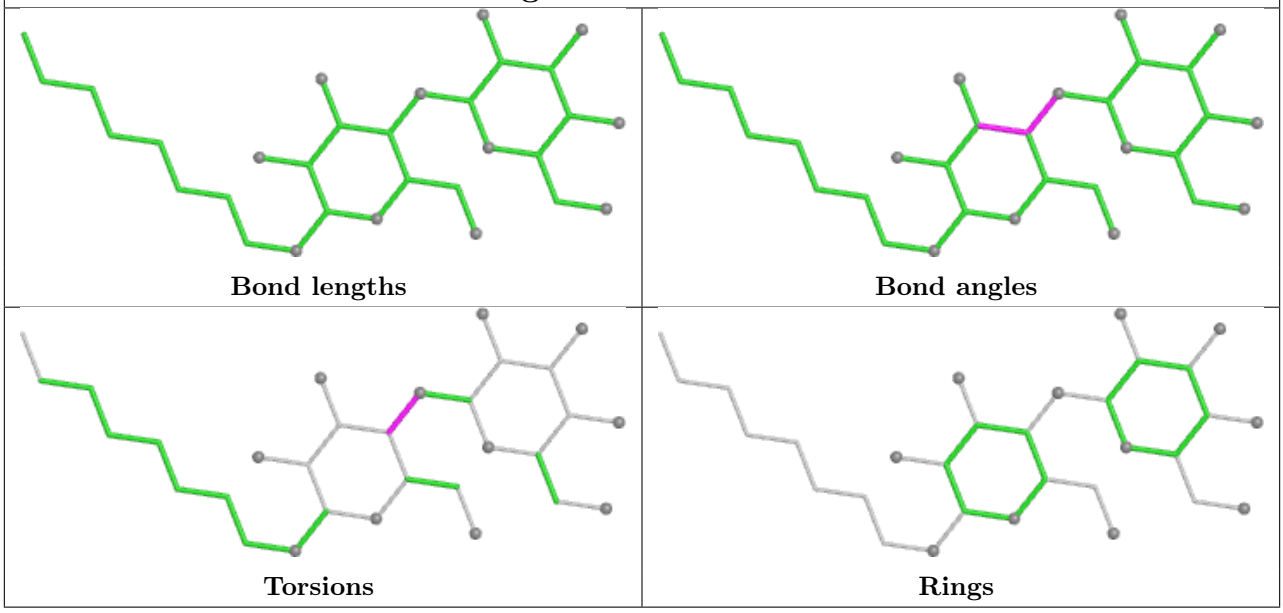
Ligand BCL M 404



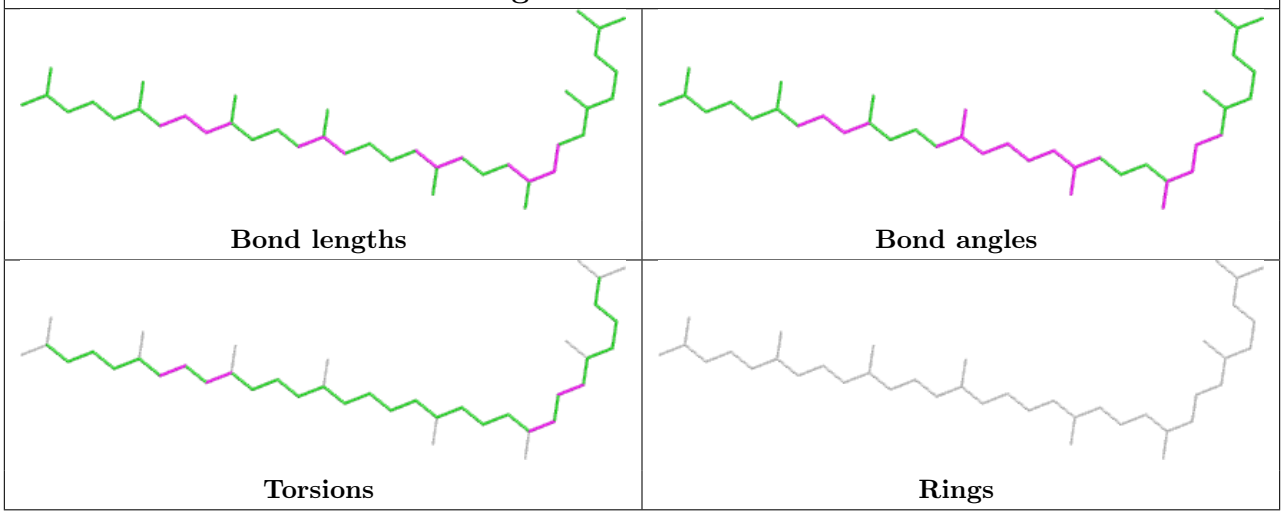
Ligand LMT H 301



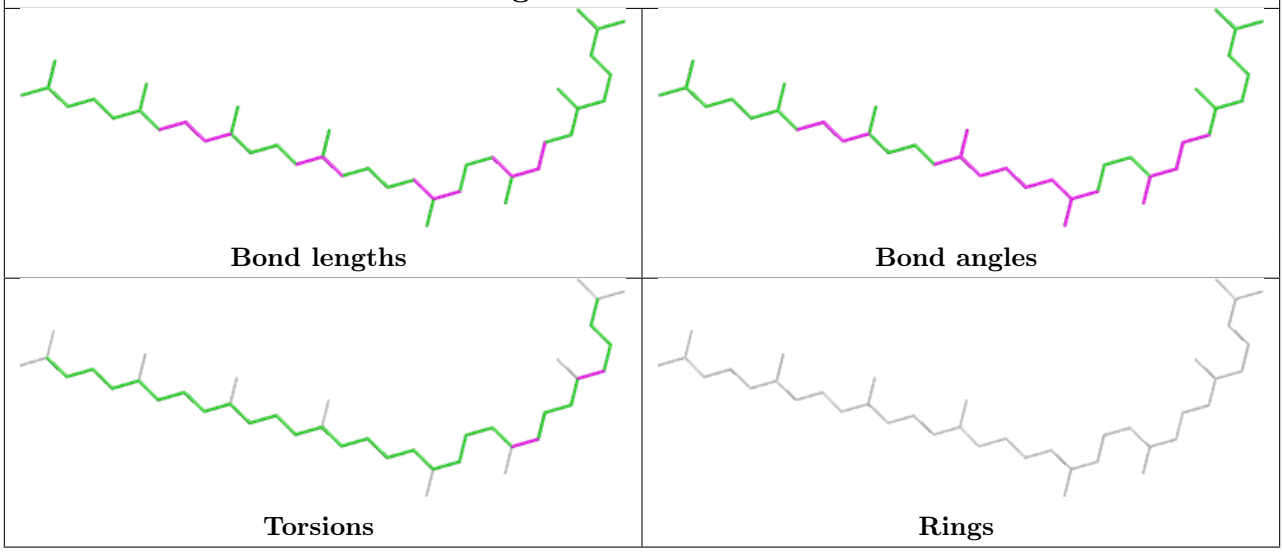
Ligand LMT X 103



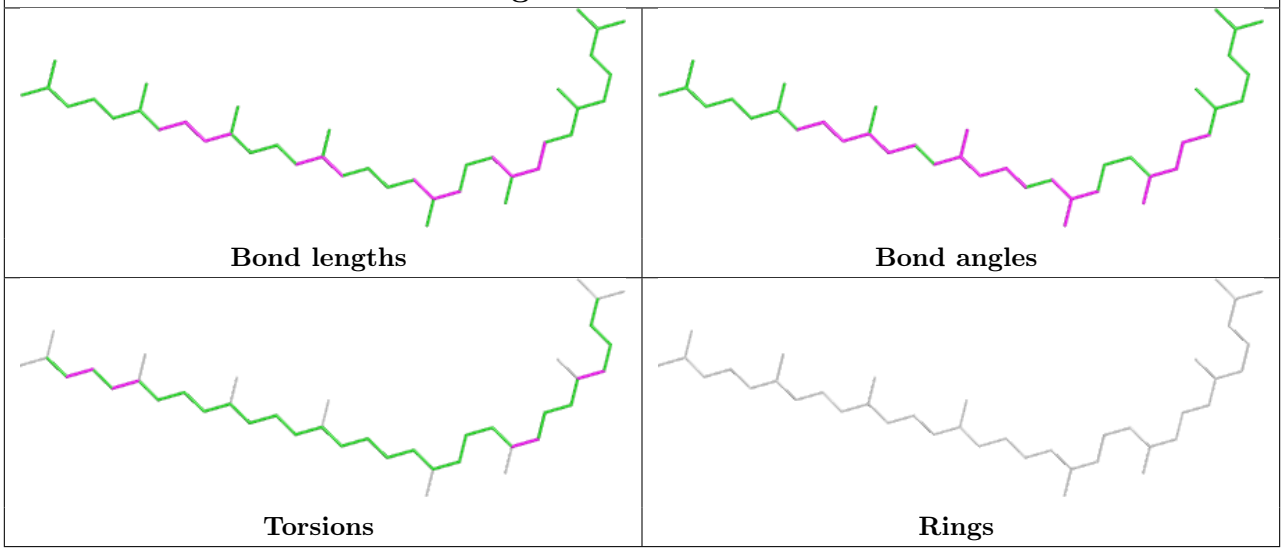
Ligand A1EF2 J 101



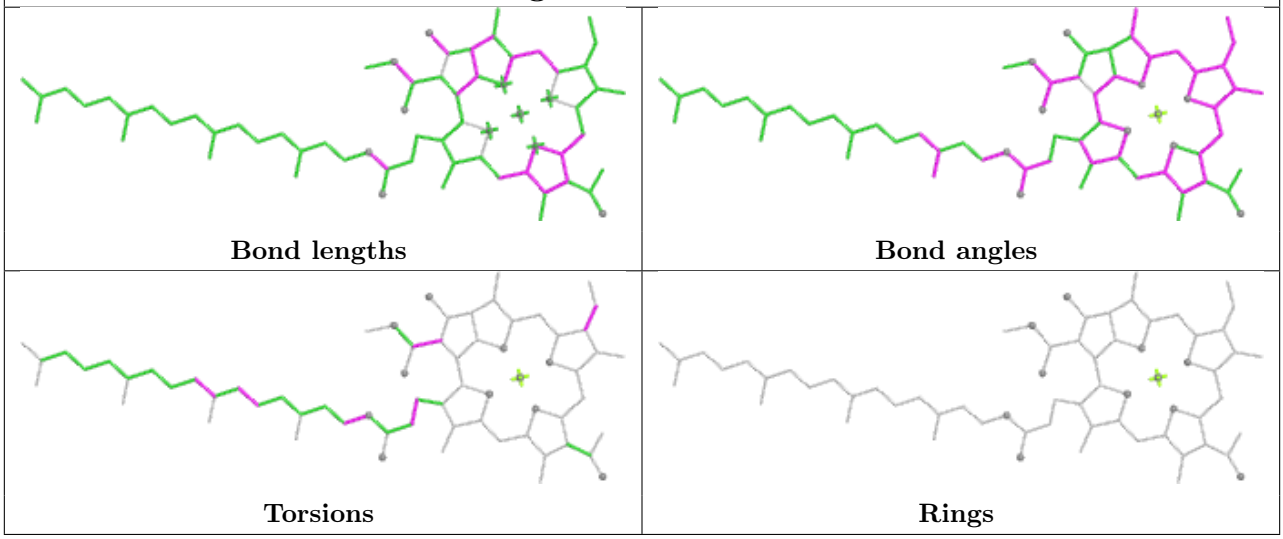
Ligand A1EF2 o 101



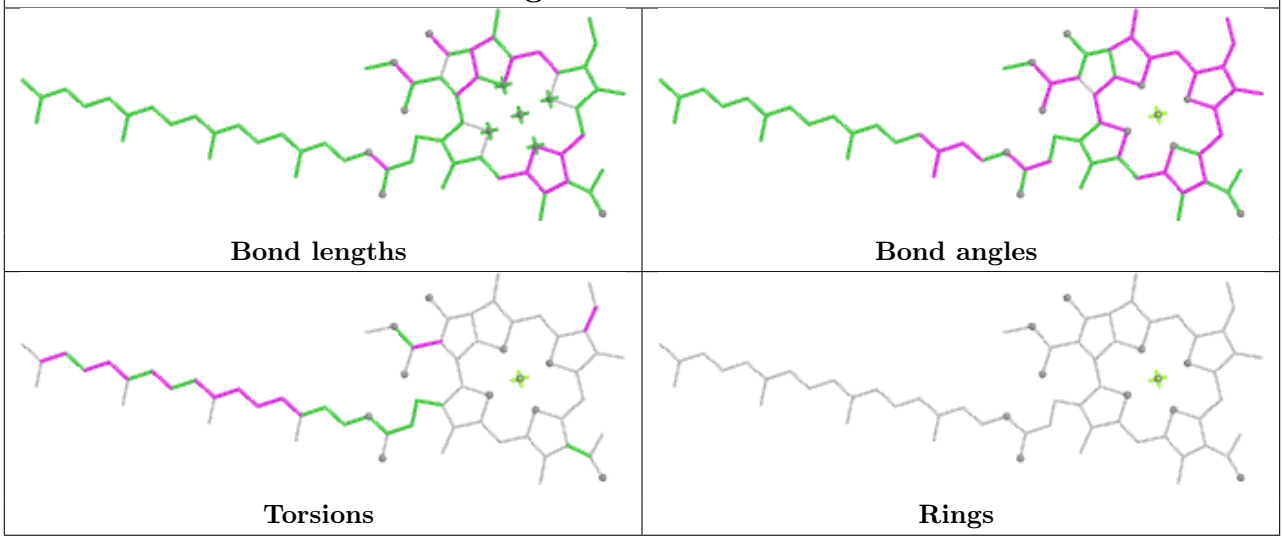
Ligand A1EF2 J 103



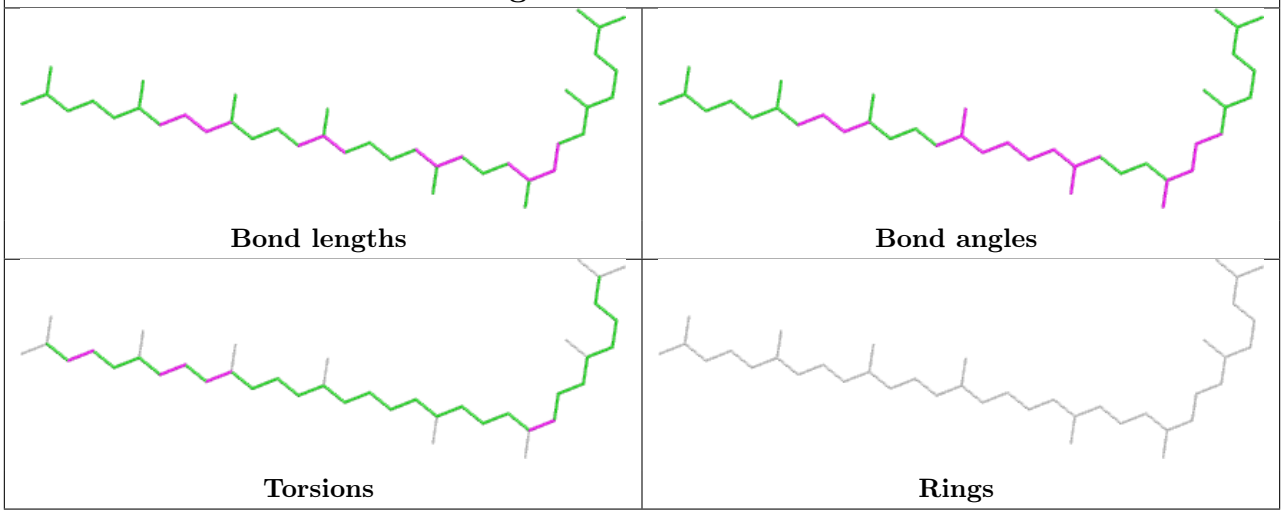
Ligand BCL L 301



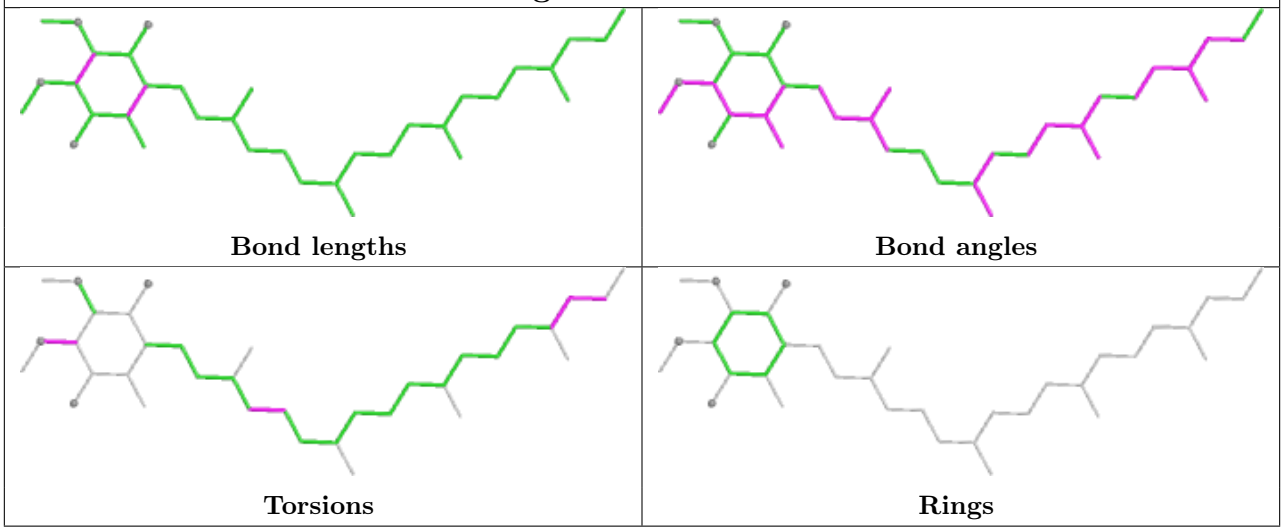
Ligand BCL G 104



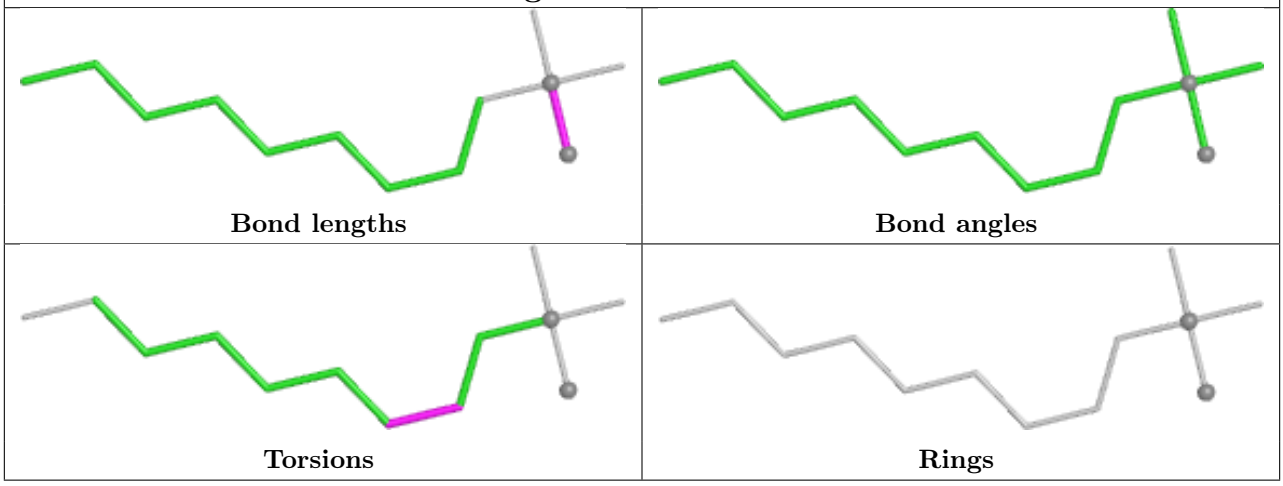
Ligand A1EF2 E 105



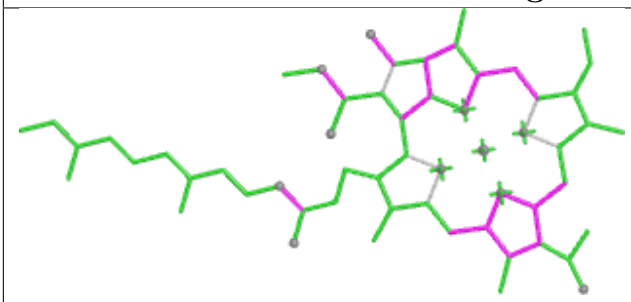
Ligand U10 L 304



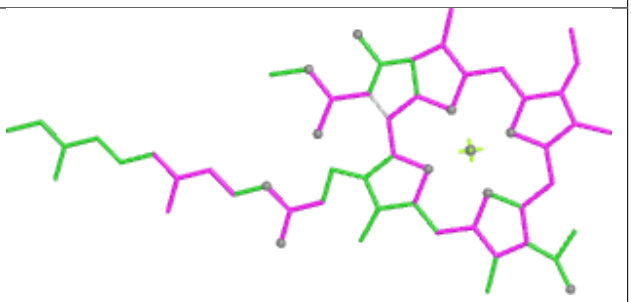
Ligand LDA X 101



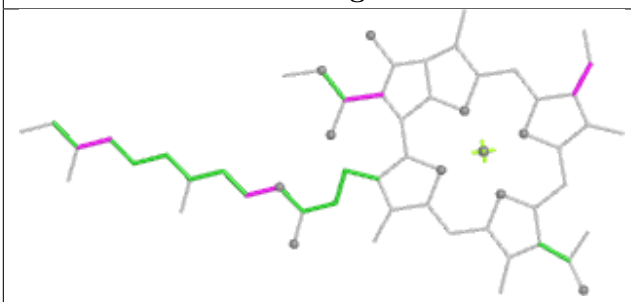
Ligand BCL E 103



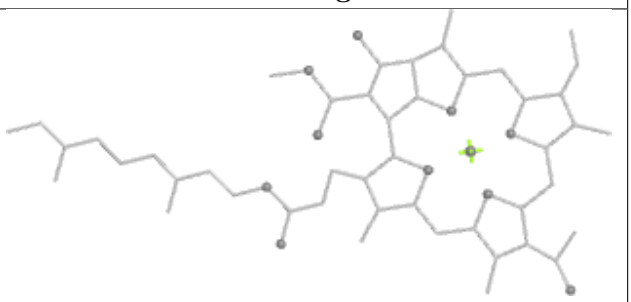
Bond lengths



Bond angles

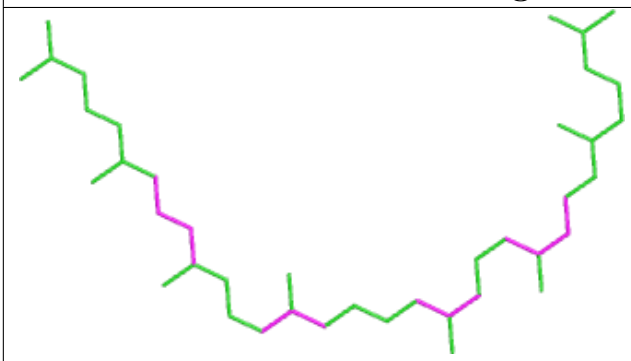


Torsions

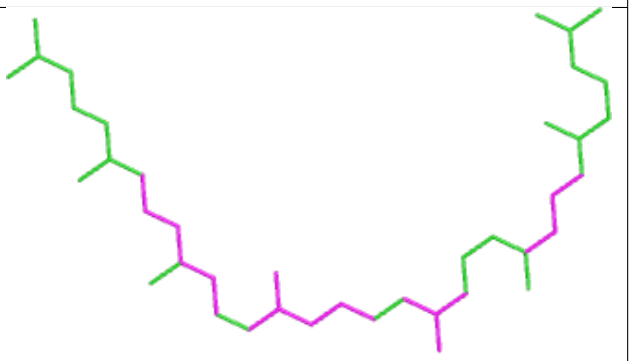


Rings

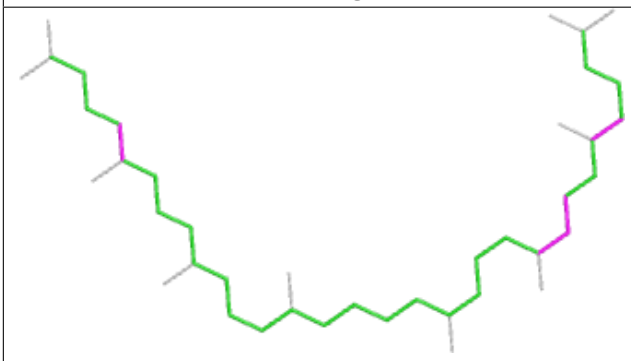
Ligand A1EF2 c 104



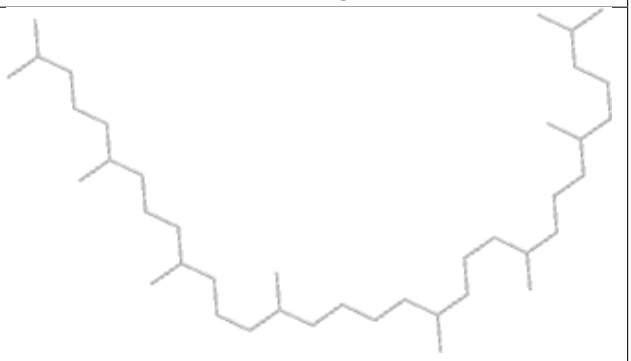
Bond lengths



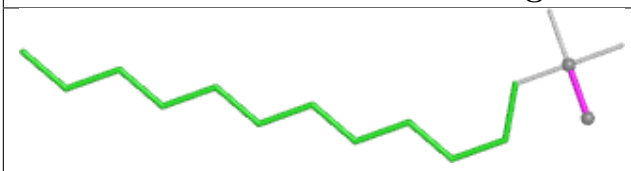
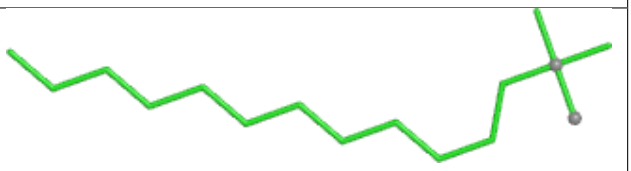
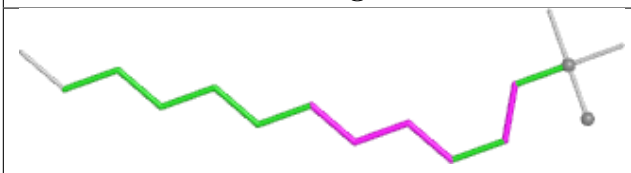
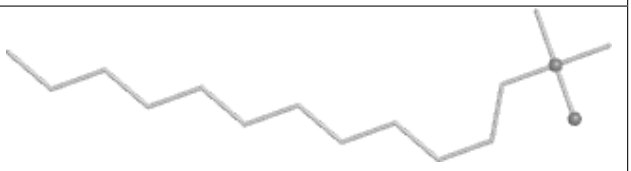
Bond angles

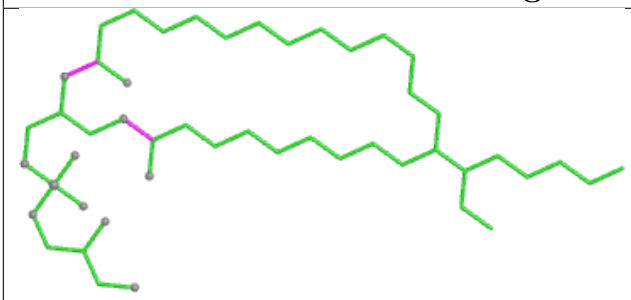
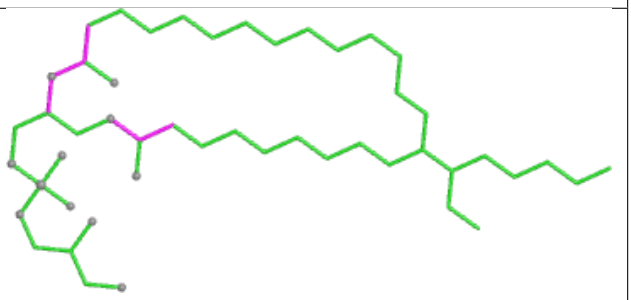
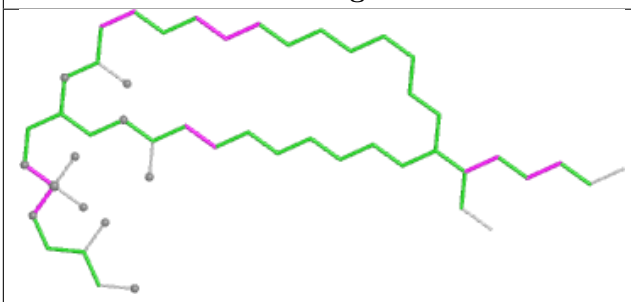
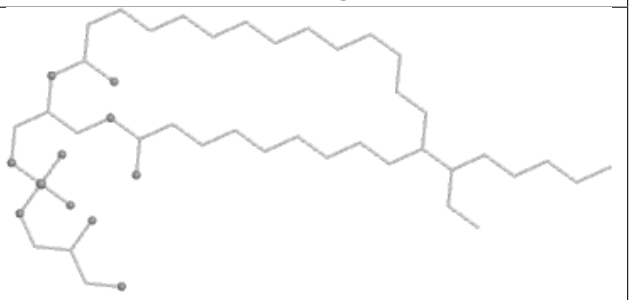


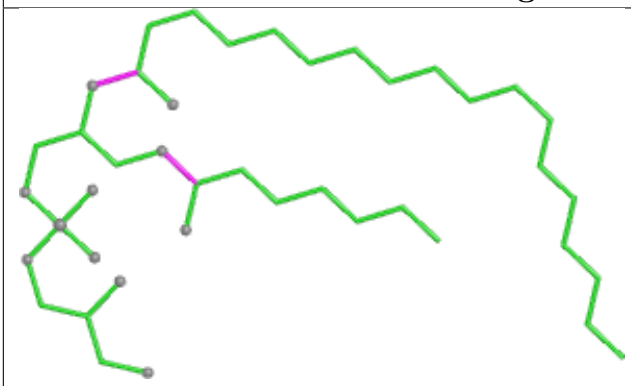
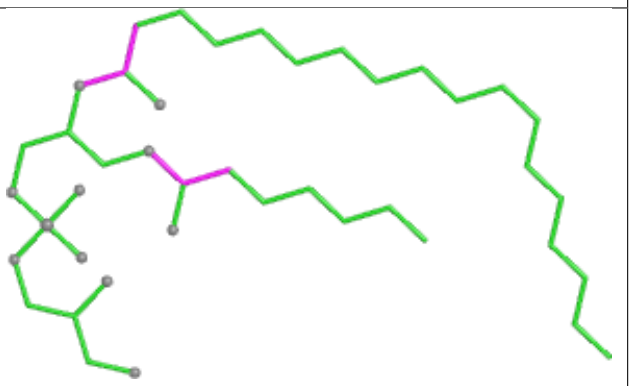
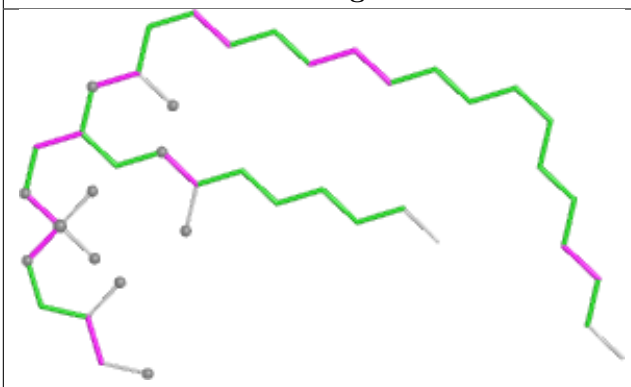
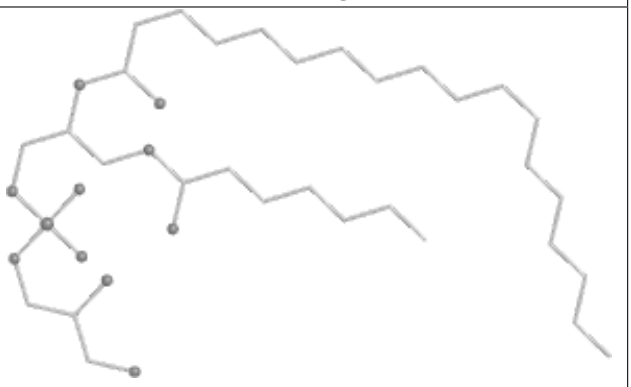
Torsions

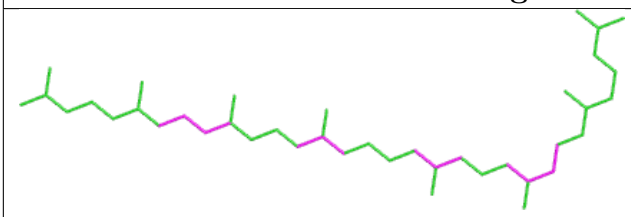
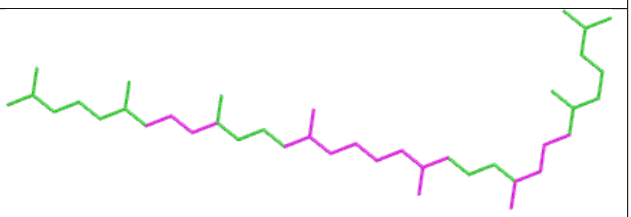
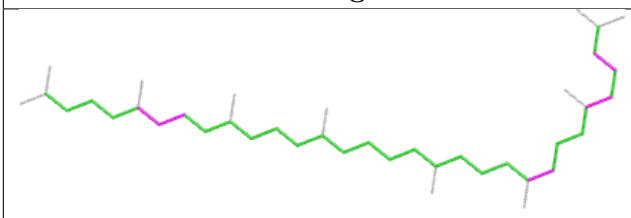
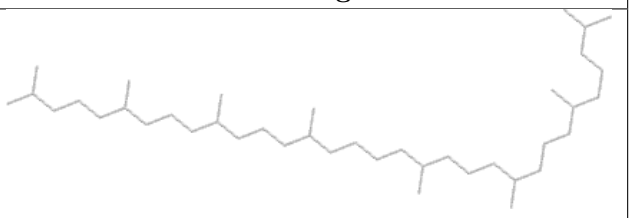


Rings

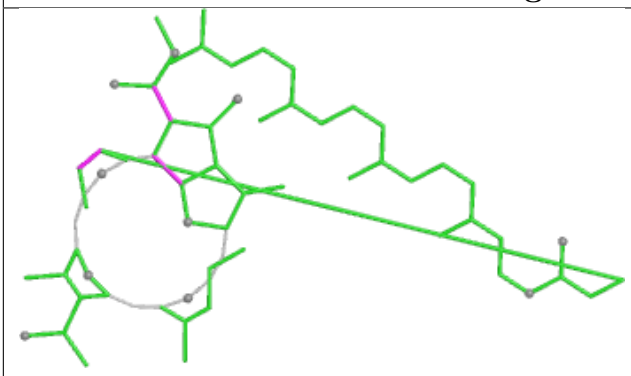
Ligand LDA F 104	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PGV L 313	
 Bond lengths	 Bond angles
 Torsions	 Rings

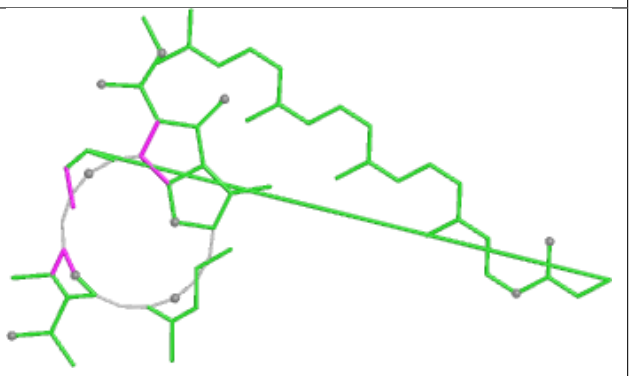
Ligand PGV M 412	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand A1EF2 k 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

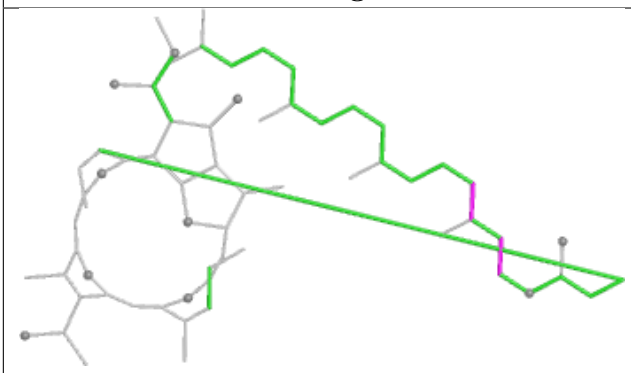
Ligand BPH L 302



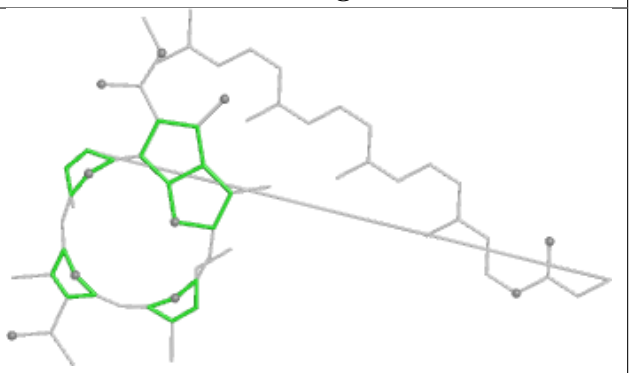
Bond lengths



Bond angles

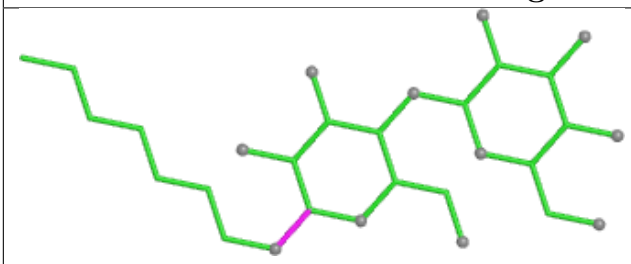


Torsions

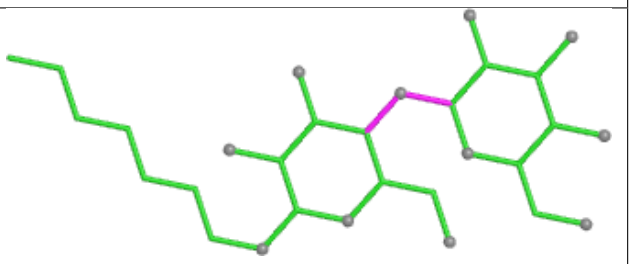


Rings

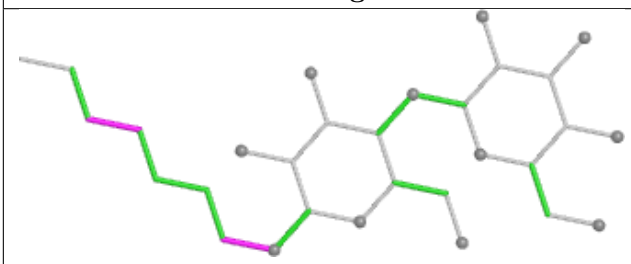
Ligand LMT I 103



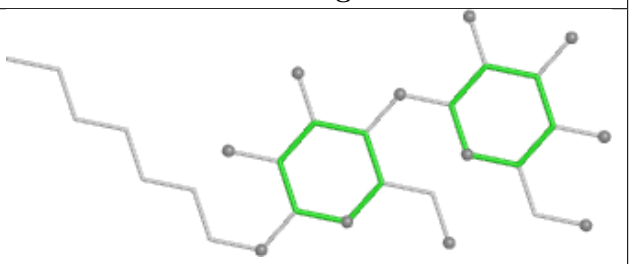
Bond lengths



Bond angles

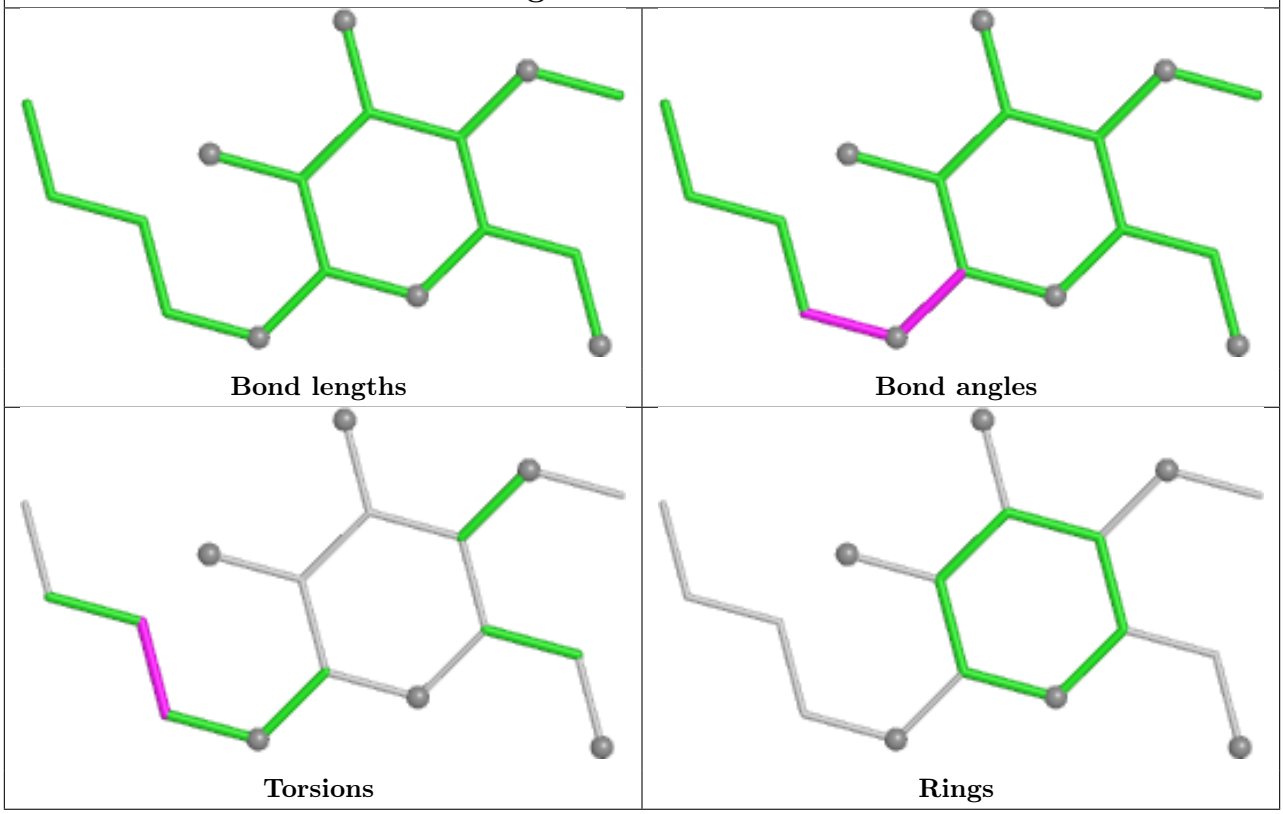


Torsions

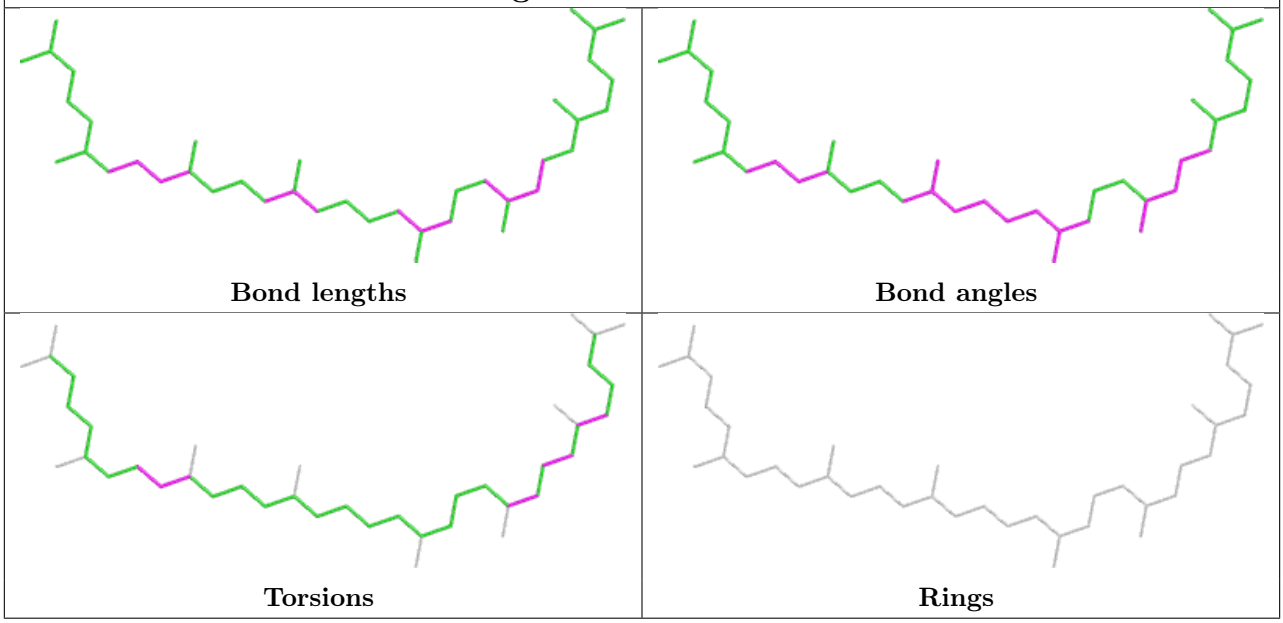


Rings

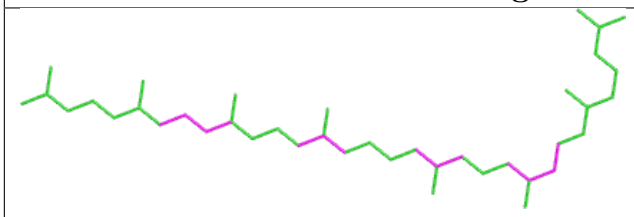
Ligand LMT c 101



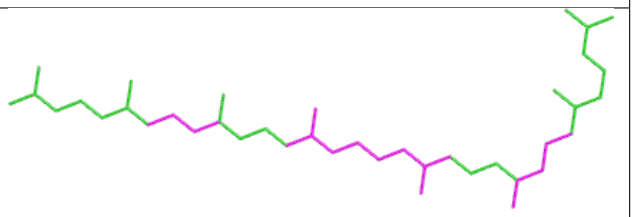
Ligand A1EF2 a 103



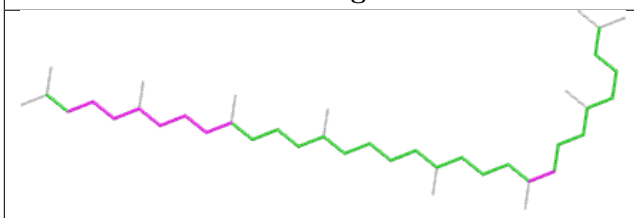
Ligand A1EF2 J 104



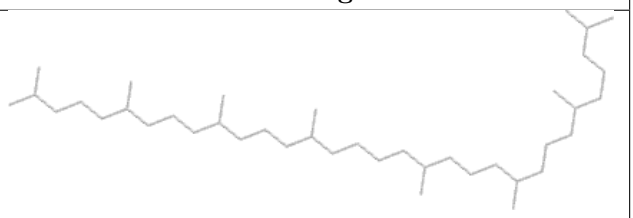
Bond lengths



Bond angles

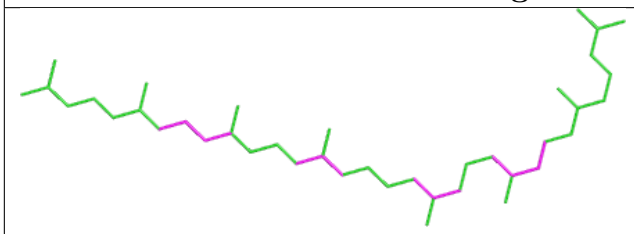


Torsions

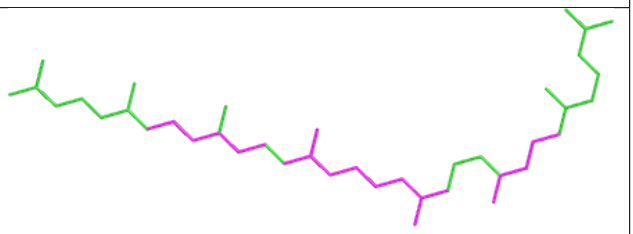


Rings

Ligand A1EF2 d 101

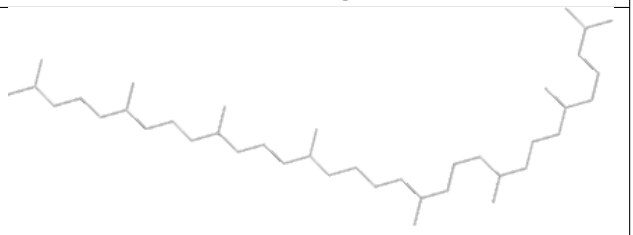


Bond lengths



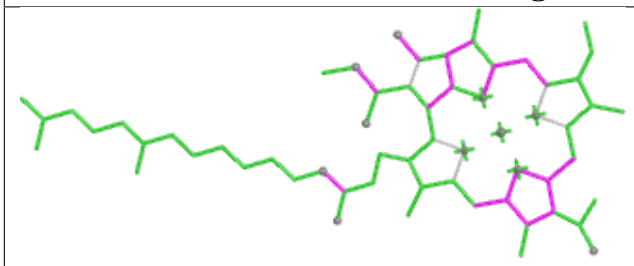
Bond angles

Torsions

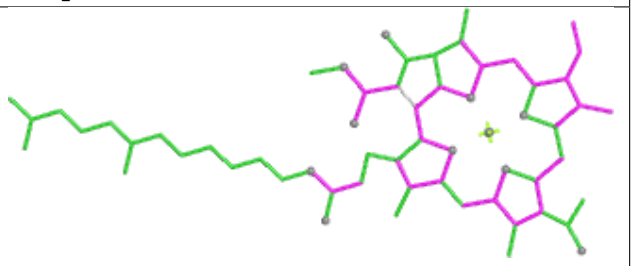


Rings

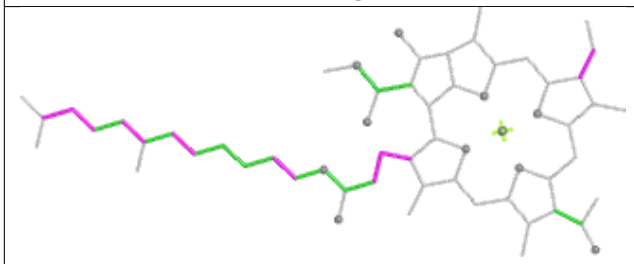
Ligand BCL q 102



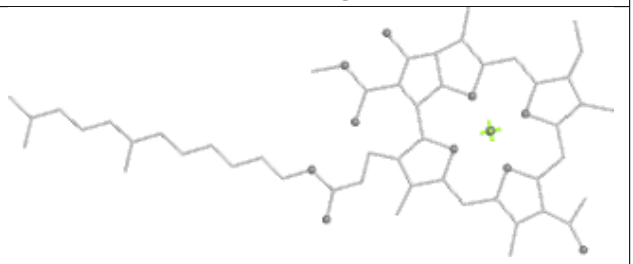
Bond lengths



Bond angles

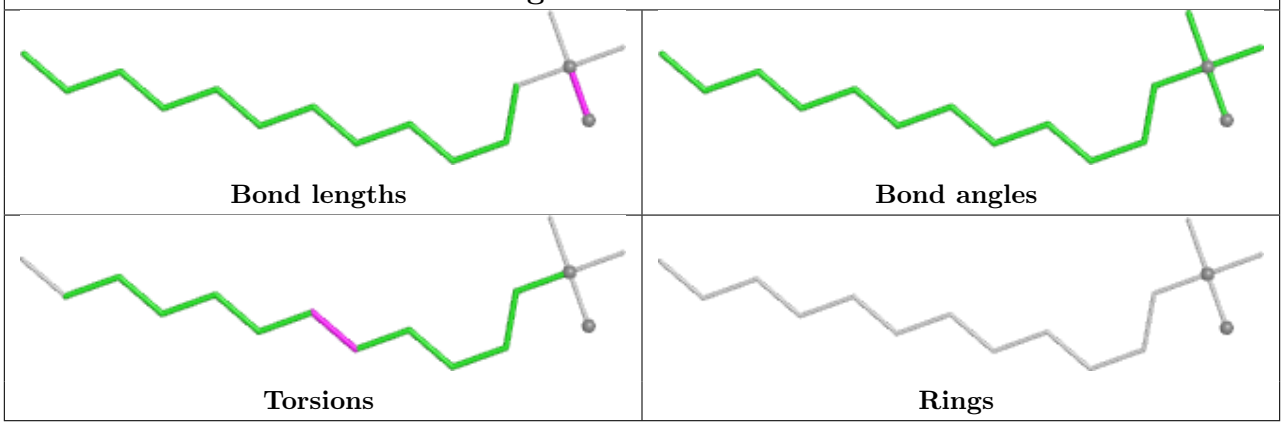


Torsions

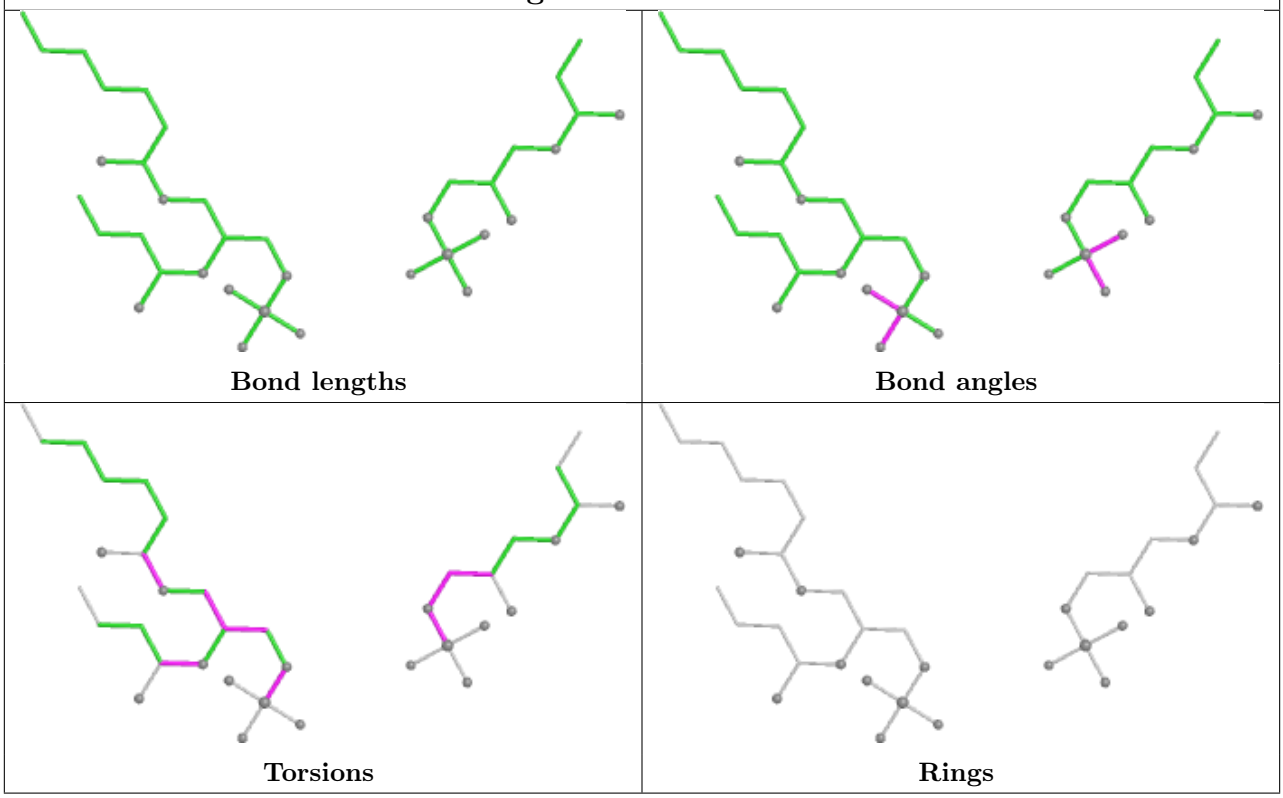


Rings

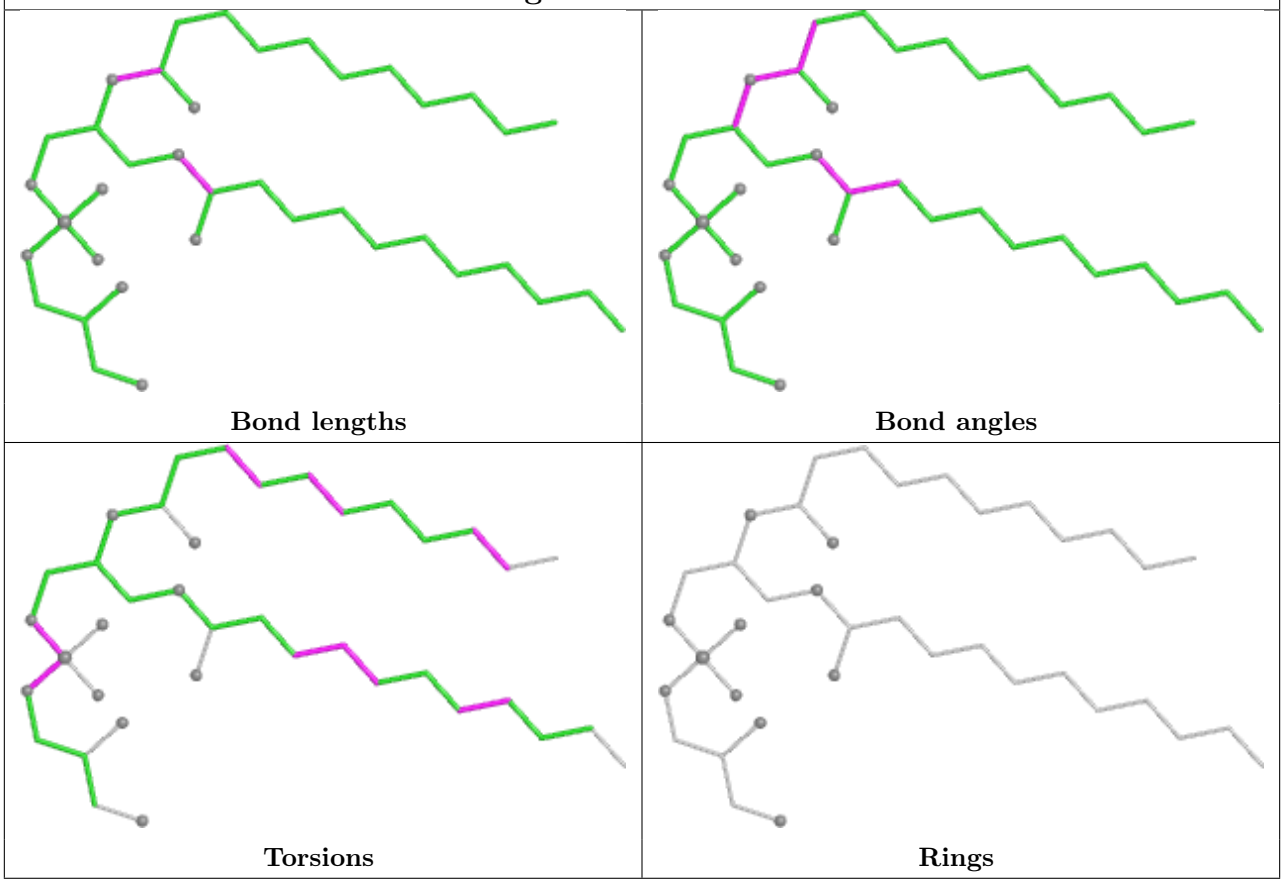
Ligand LDA L 309



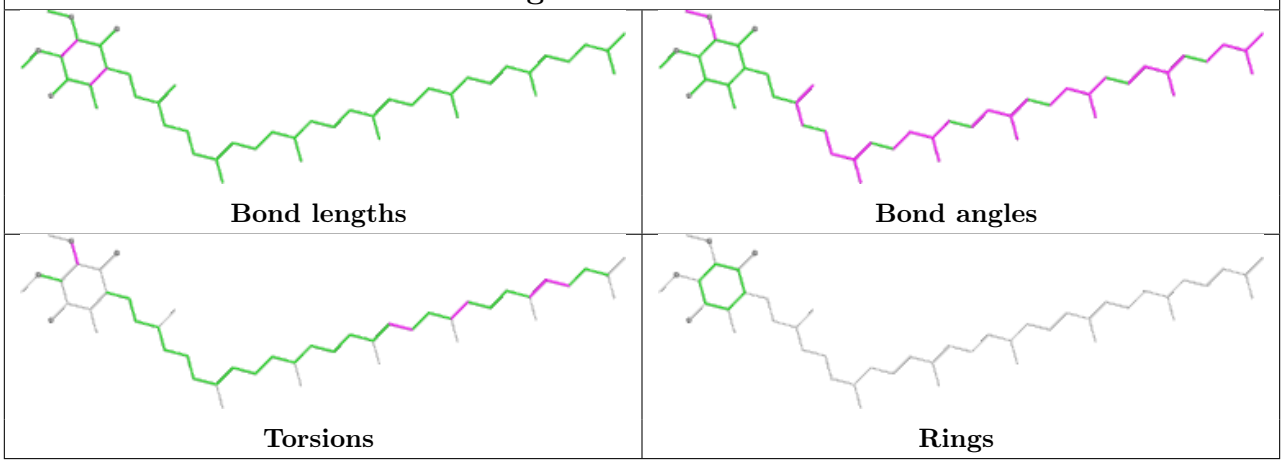
Ligand CDL F 102



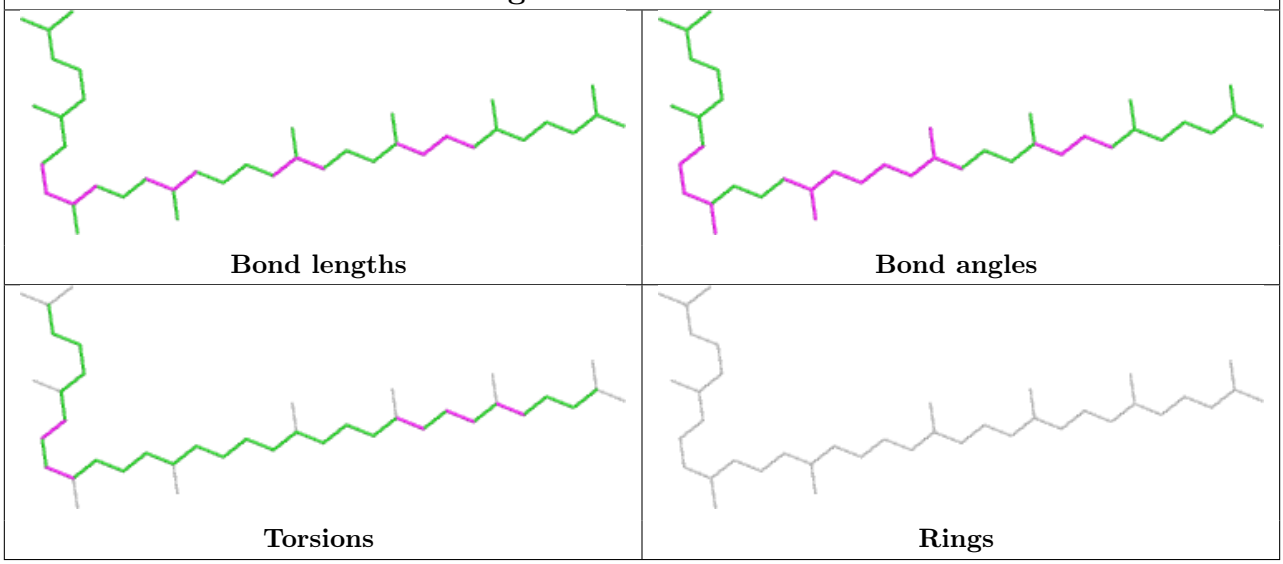
Ligand PGV L 314



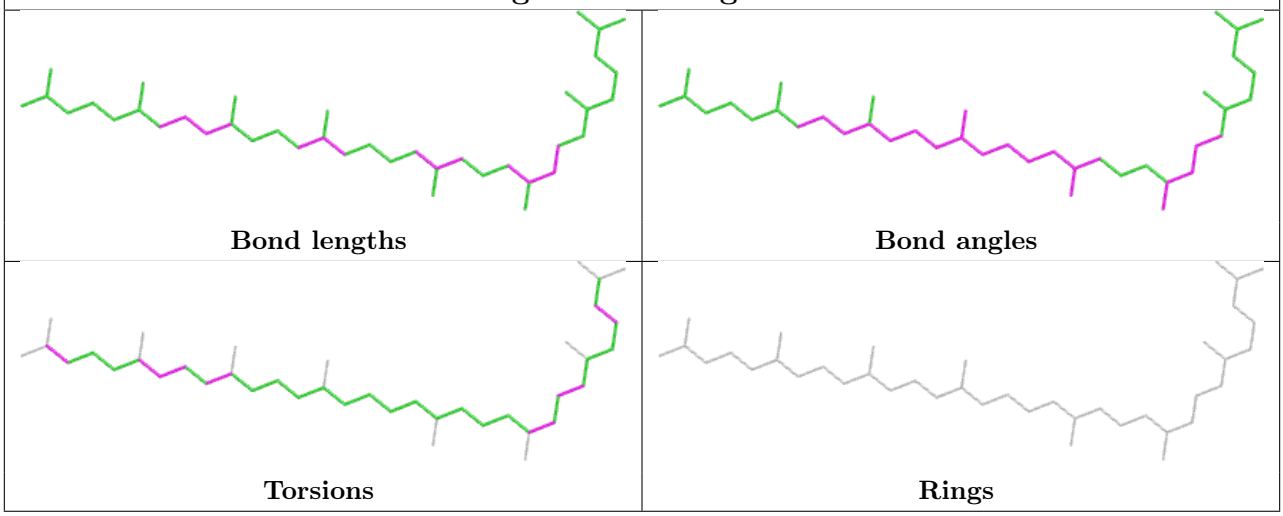
Ligand U10 M 407



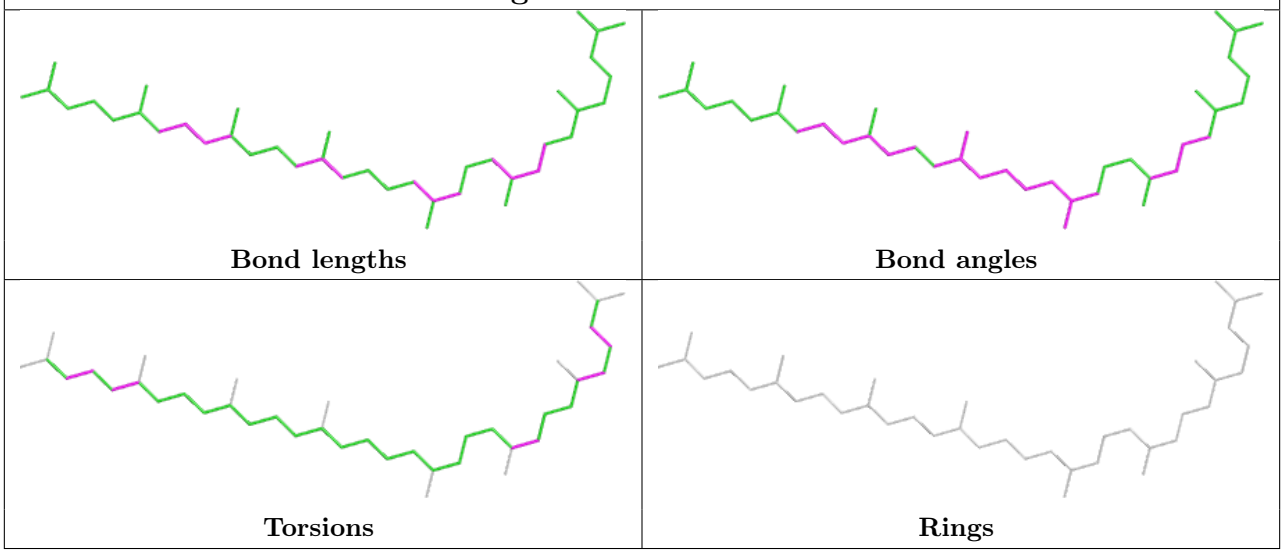
Ligand A1EF2 C 104



Ligand A1EF2 g 103



Ligand A1EF2 b 102



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

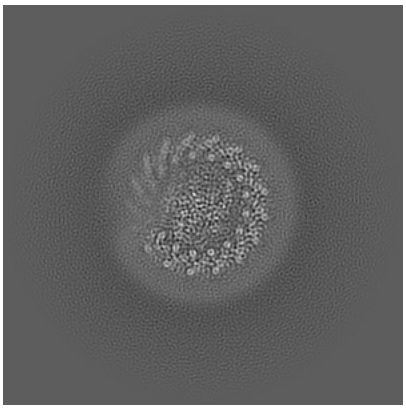
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-62409. These allow visual inspection of the internal detail of the map and identification of artifacts.

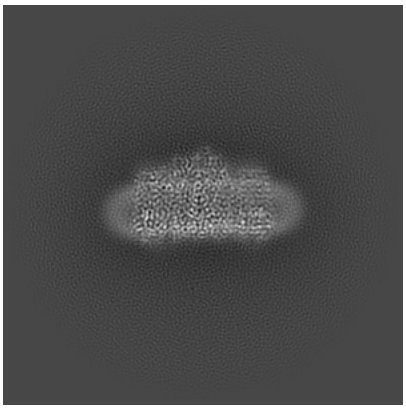
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

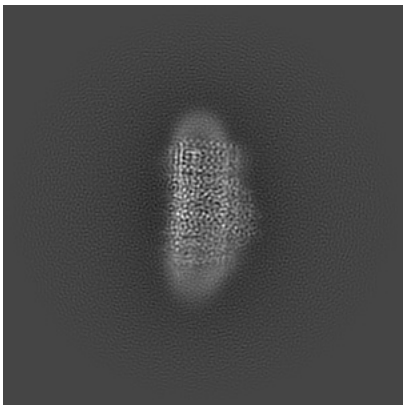
6.1.1 Primary map



X

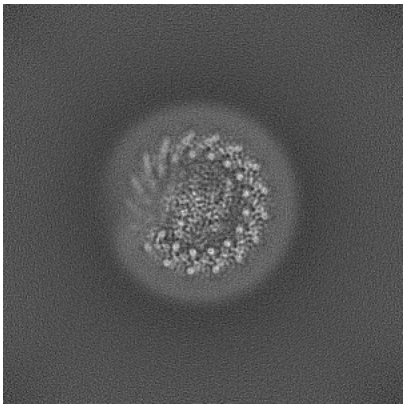


Y

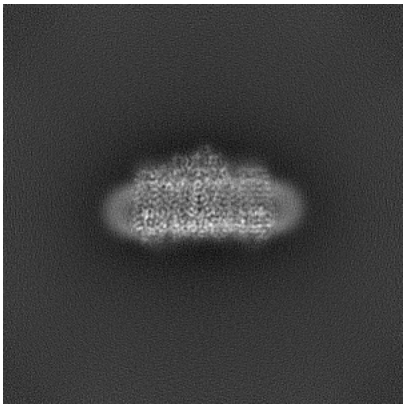


Z

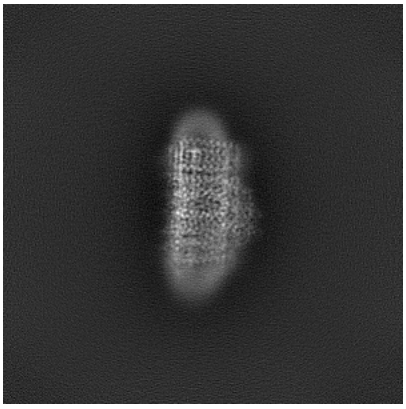
6.1.2 Raw map



X



Y

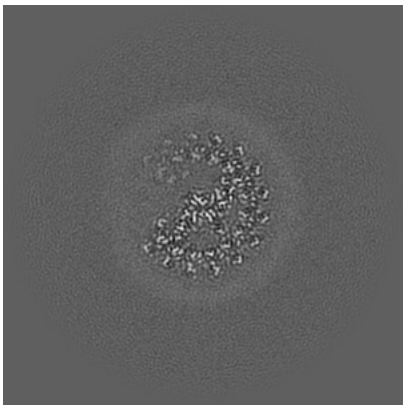


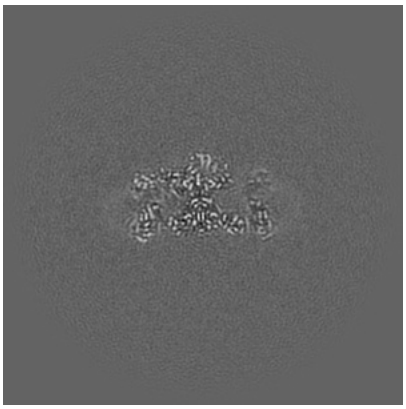
Z

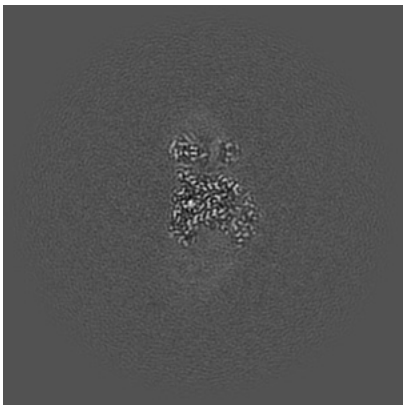
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

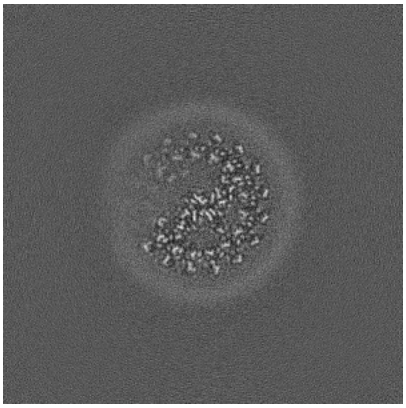
6.2.1 Primary map

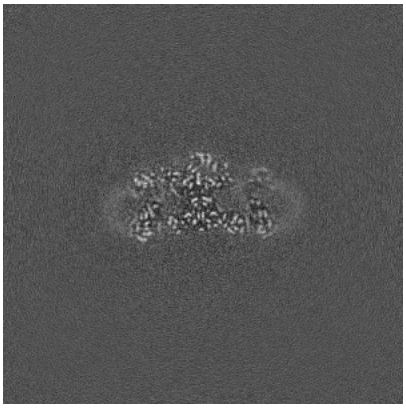

X Index: 200

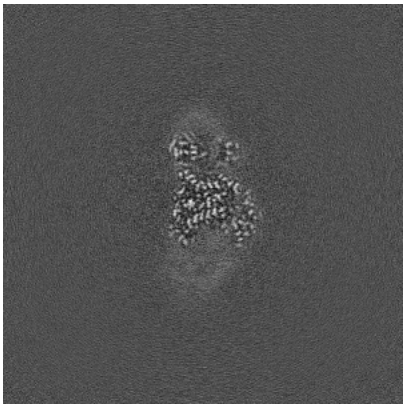

Y Index: 200


Z Index: 200

6.2.2 Raw map


X Index: 200

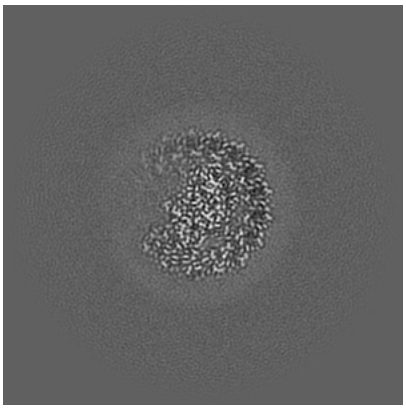

Y Index: 200

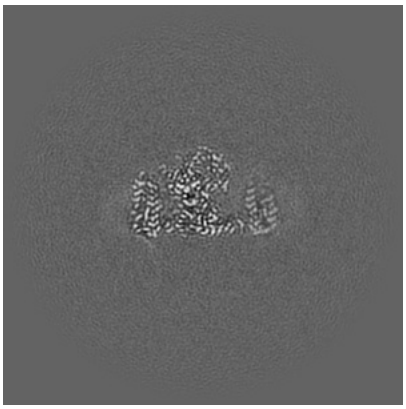

Z Index: 200

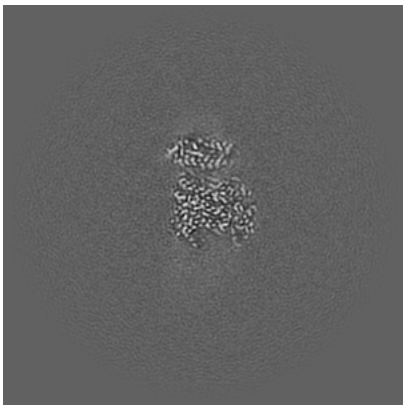
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

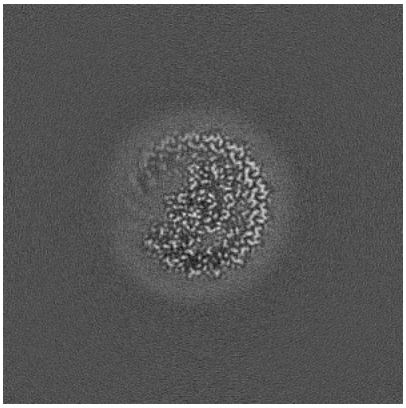
6.3.1 Primary map

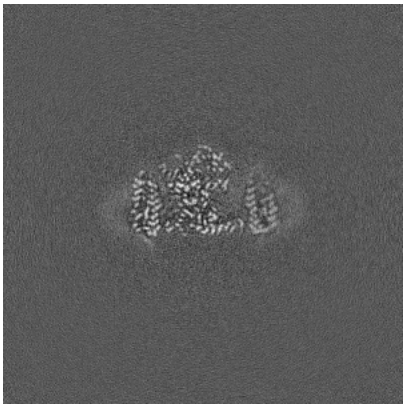

X Index: 181

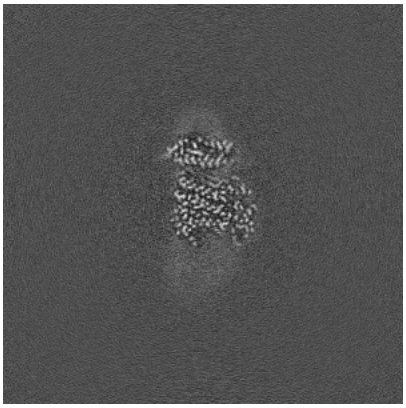

Y Index: 190


Z Index: 191

6.3.2 Raw map


X Index: 178

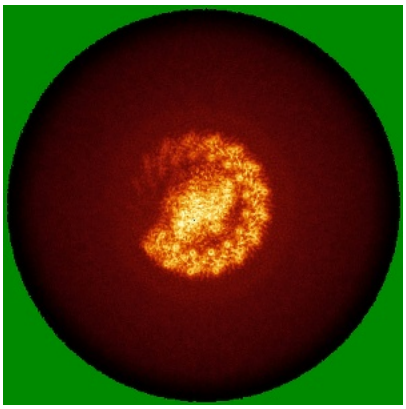

Y Index: 190

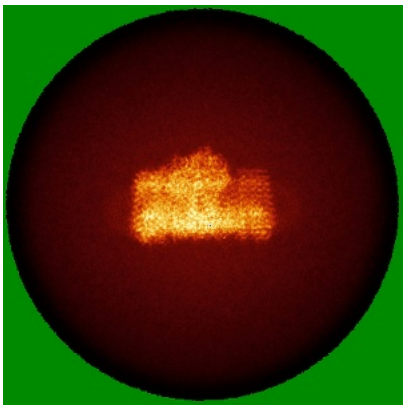

Z Index: 191

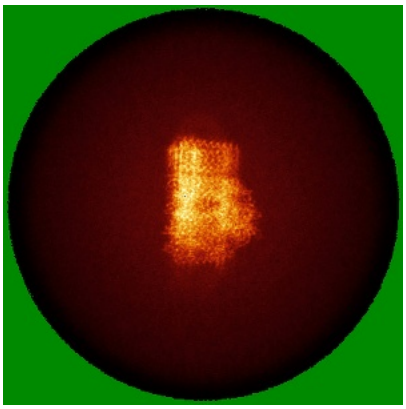
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

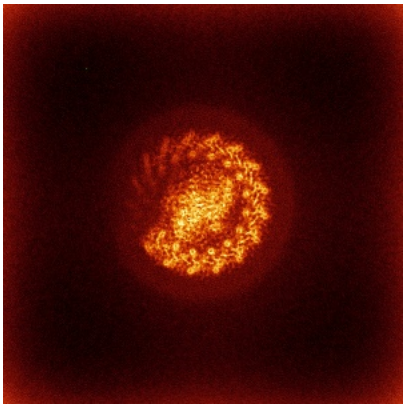
6.4.1 Primary map

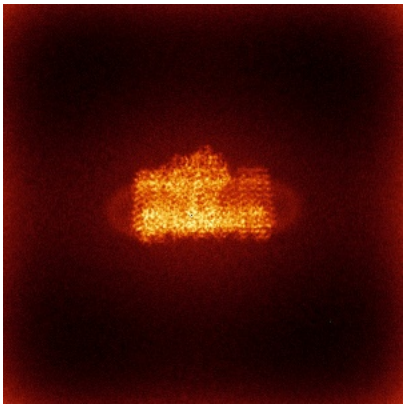

X

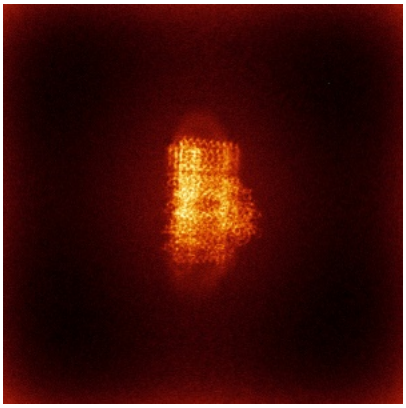

Y


Z

6.4.2 Raw map


X

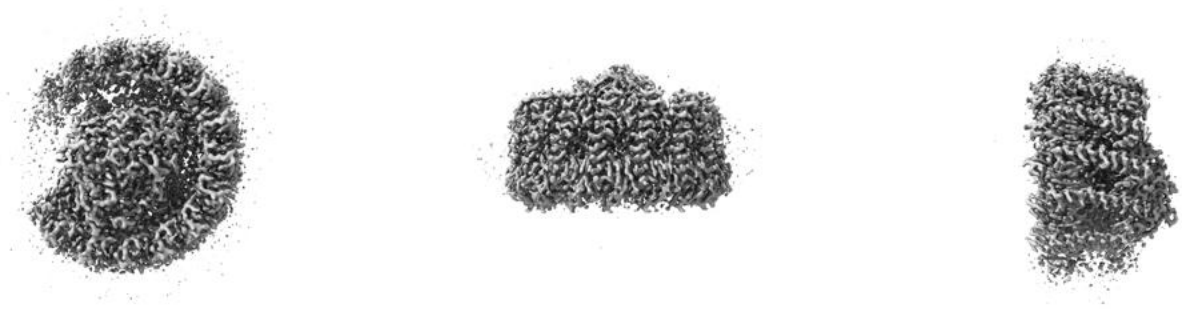

Y


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

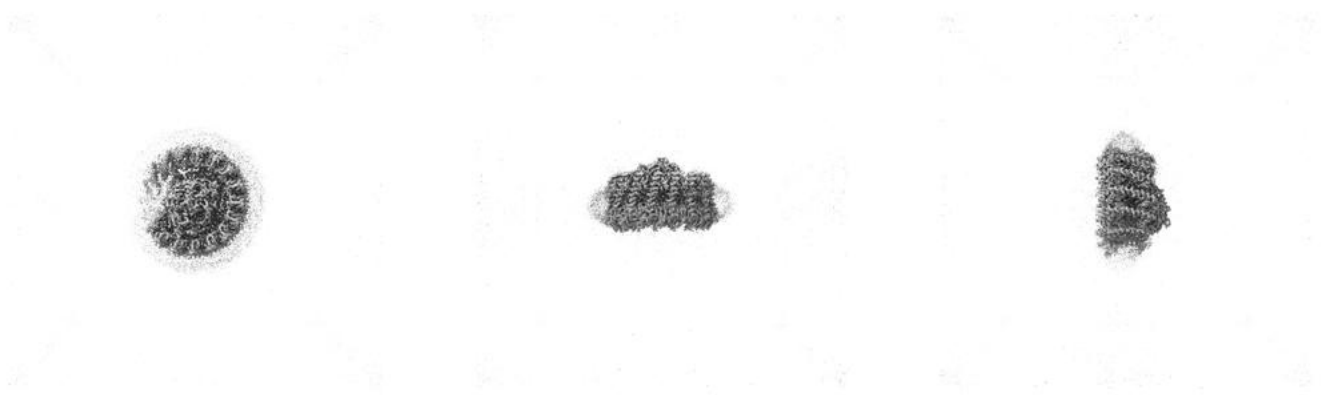
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.19. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 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.

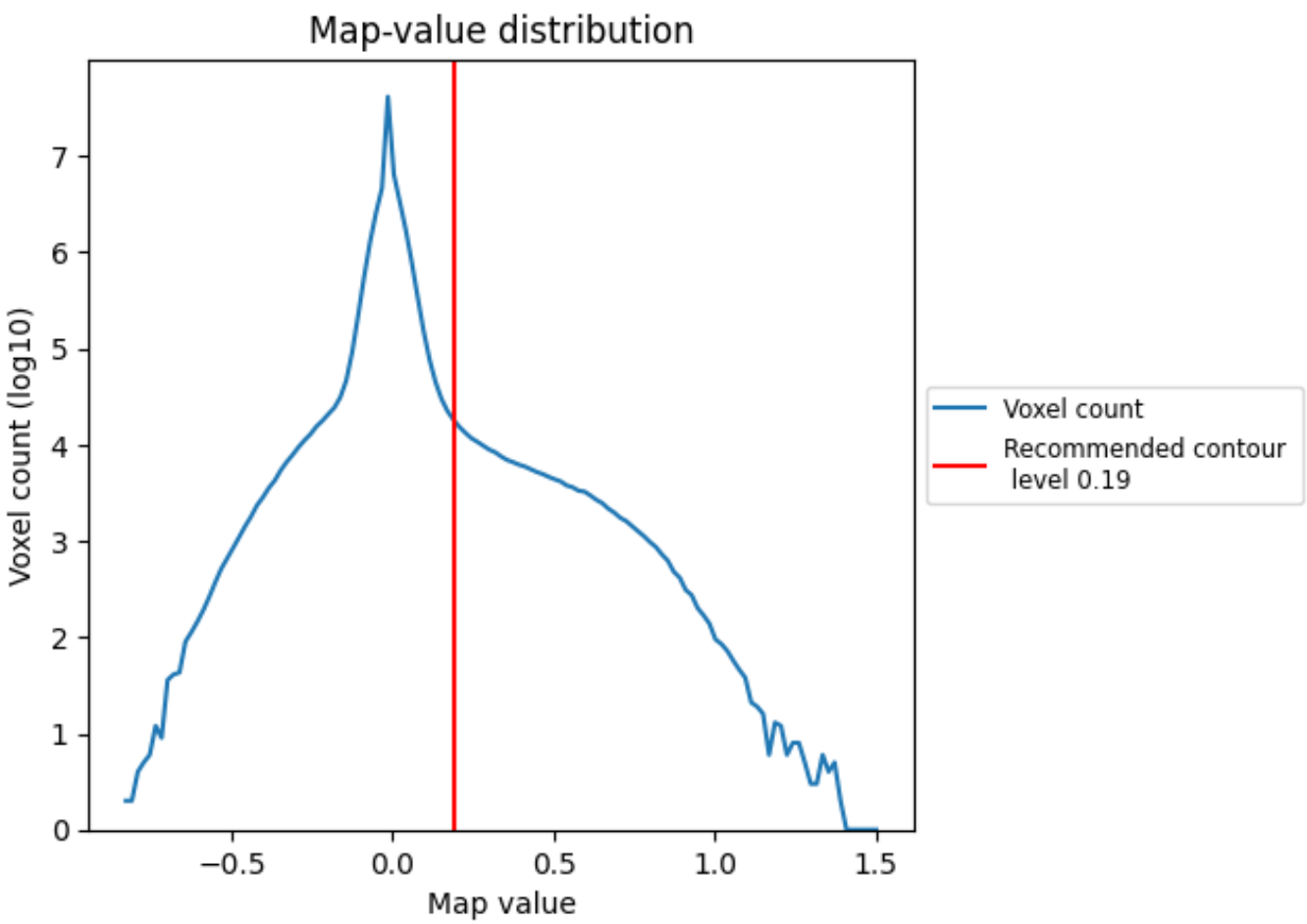
6.6 Mask visualisation (i)

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

7 Map analysis (i)

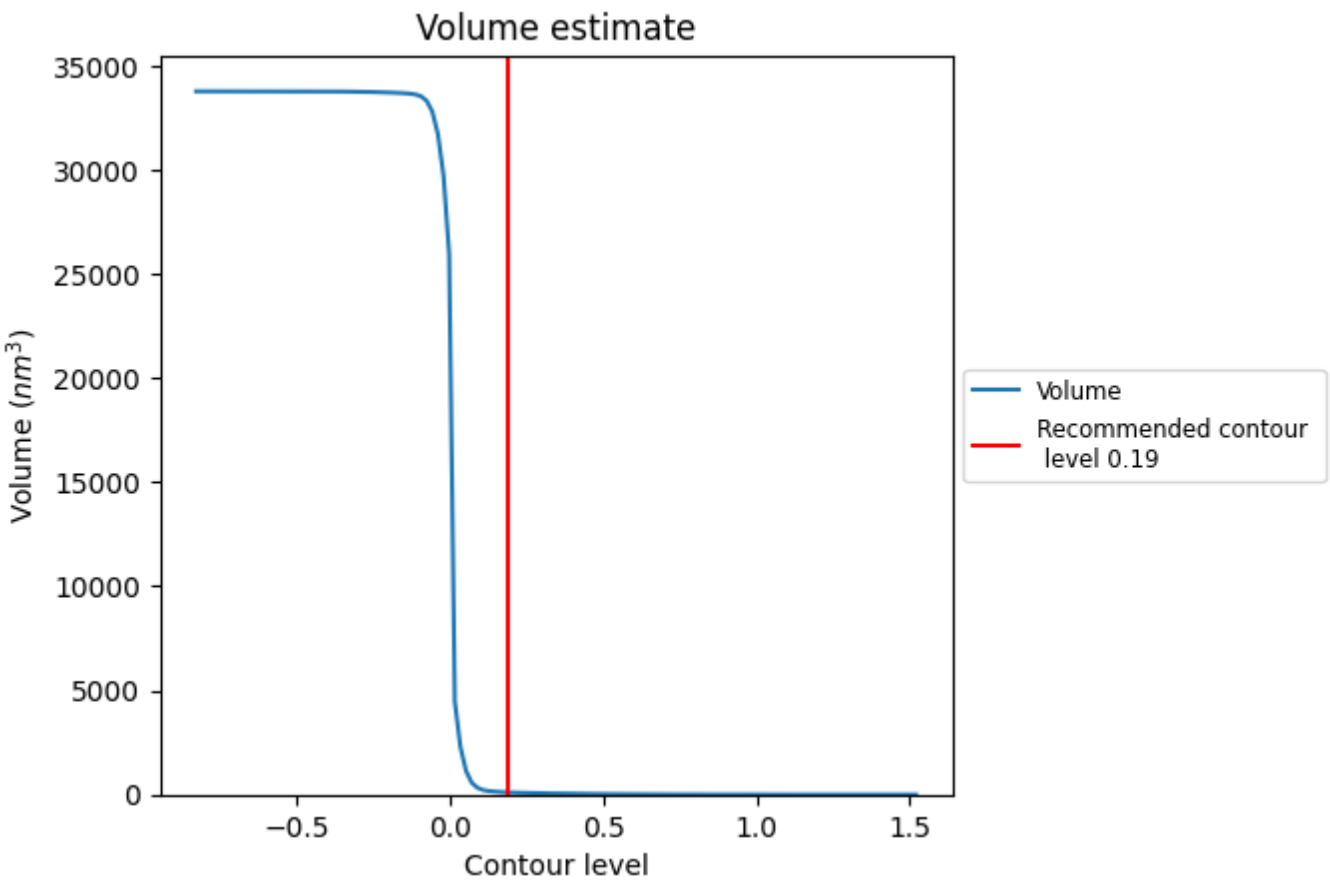
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

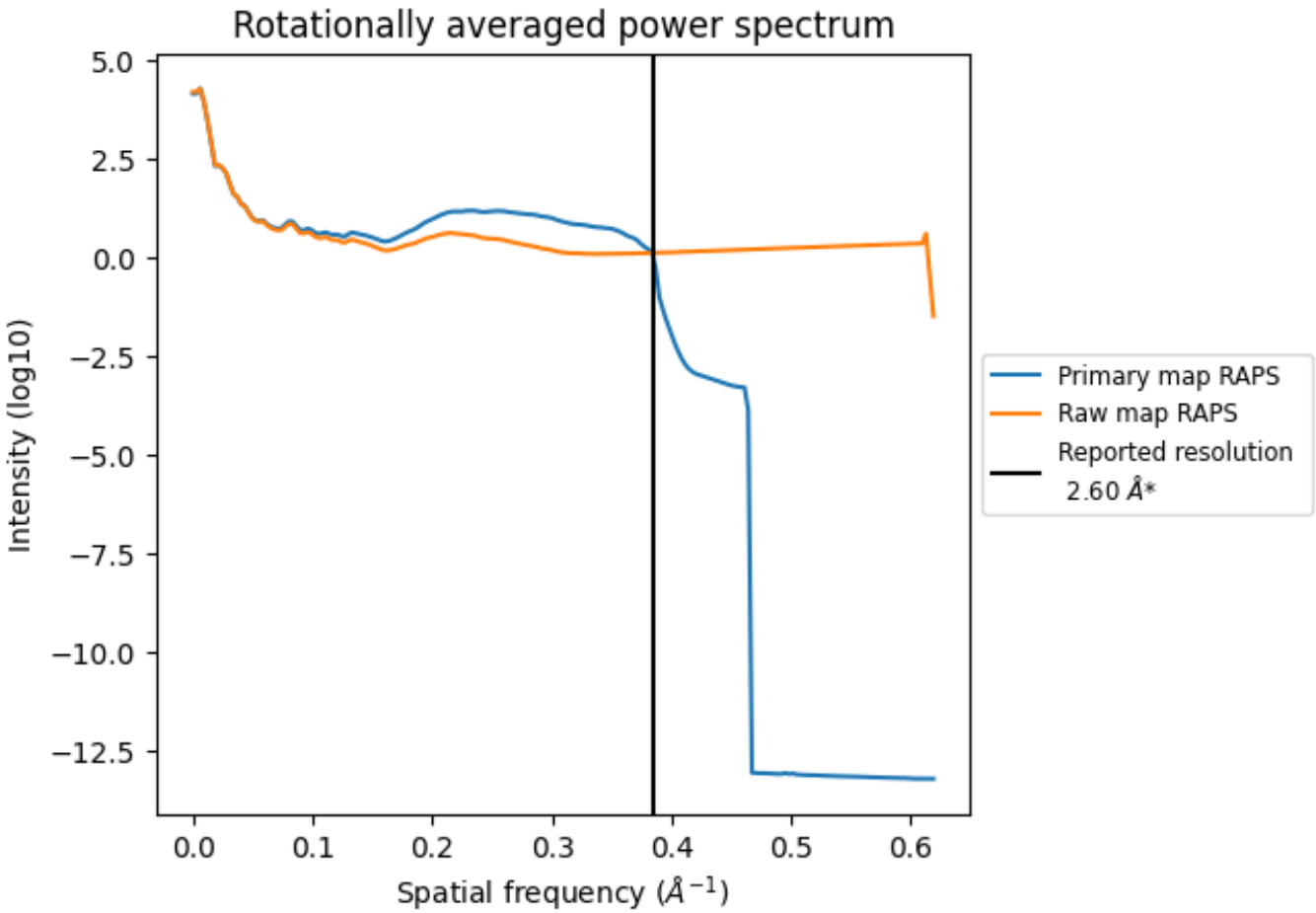
7.2 Volume estimate (i)



The volume at the recommended contour level is 104 nm^3; this corresponds to an approximate mass of 94 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)

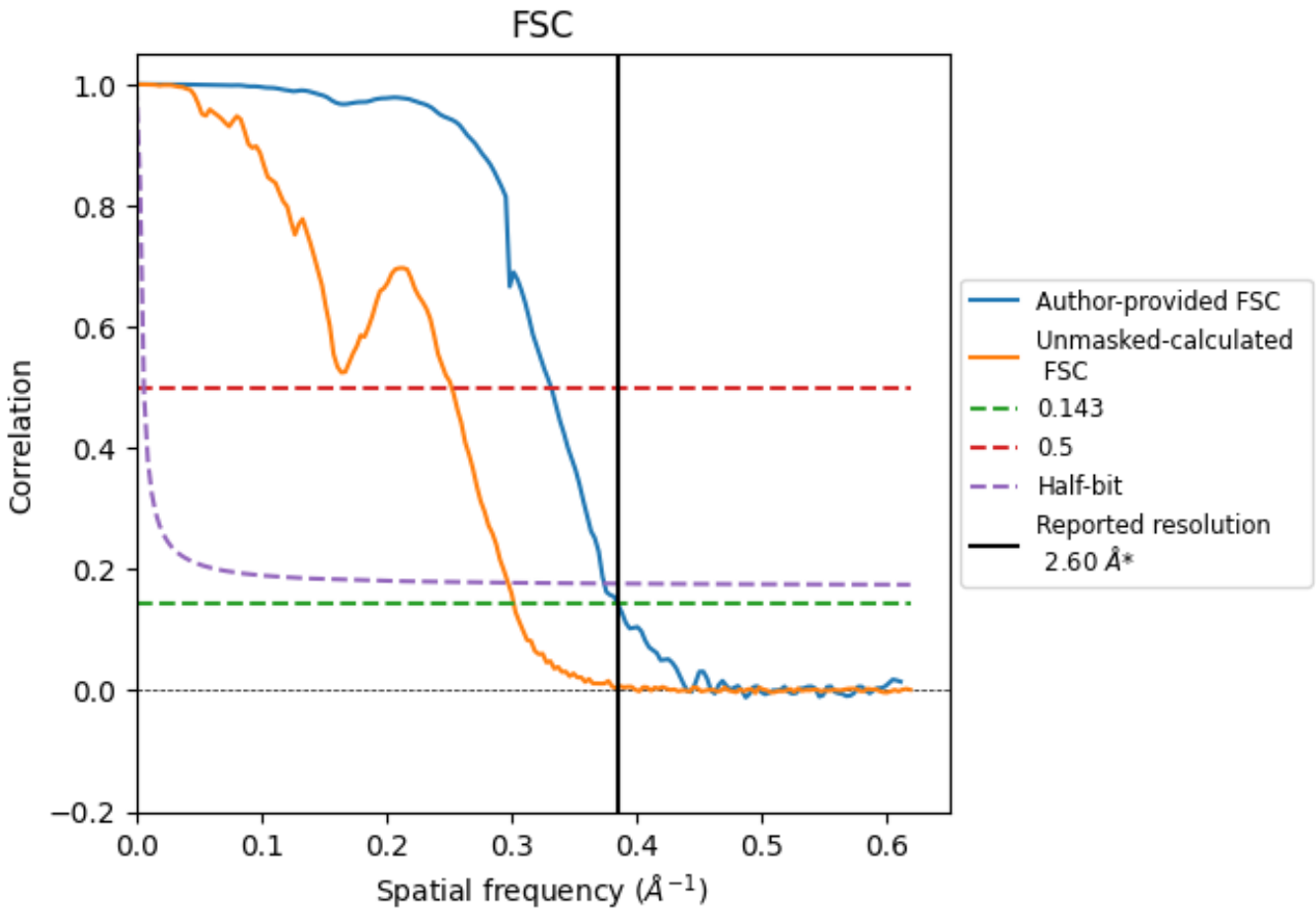


*Reported resolution corresponds to spatial frequency of 0.385 Å^{-1}

8 Fourier-Shell correlation (i)

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 (i)



*Reported resolution corresponds to spatial frequency of 0.385 Å^{-1}

8.2 Resolution estimates (i)

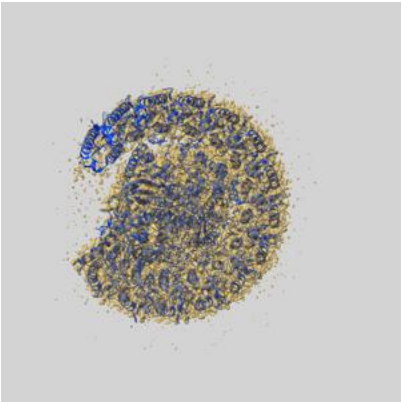
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.60	-	-
Author-provided FSC curve	2.60	3.02	2.67
Unmasked-calculated*	3.31	3.97	3.36

*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 3.31 differs from the reported value 2.6 by more than 10 %

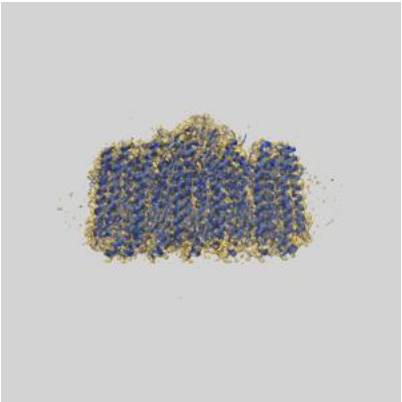
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-62409 and PDB model 9KLM. Per-residue inclusion information can be found in section 3 on page 18.

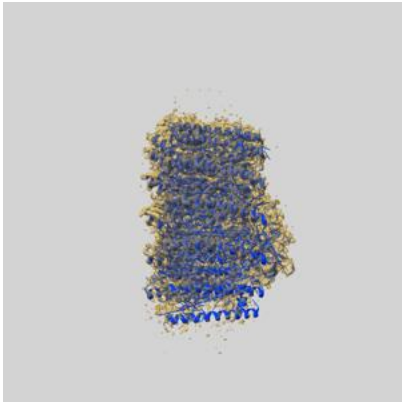
9.1 Map-model overlay (i)



X



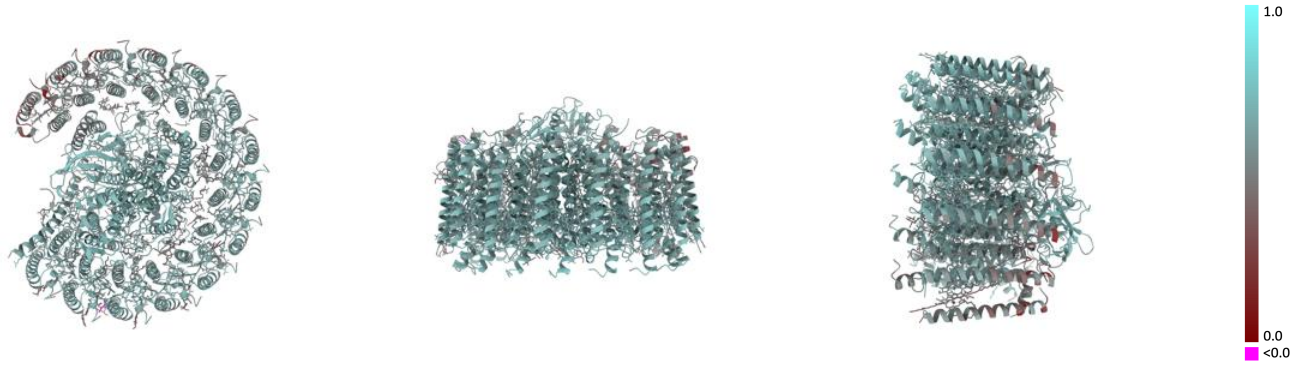
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.19 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.

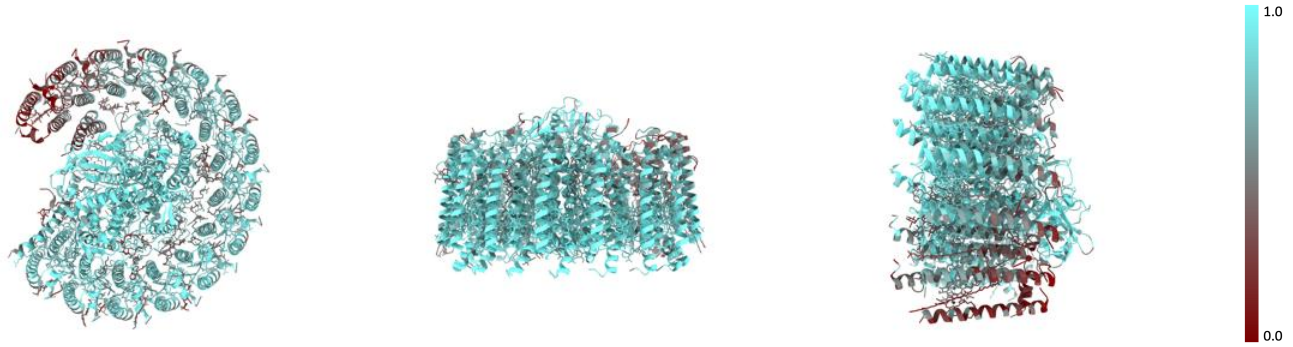
9.2 Q-score mapped to coordinate model (i)



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.

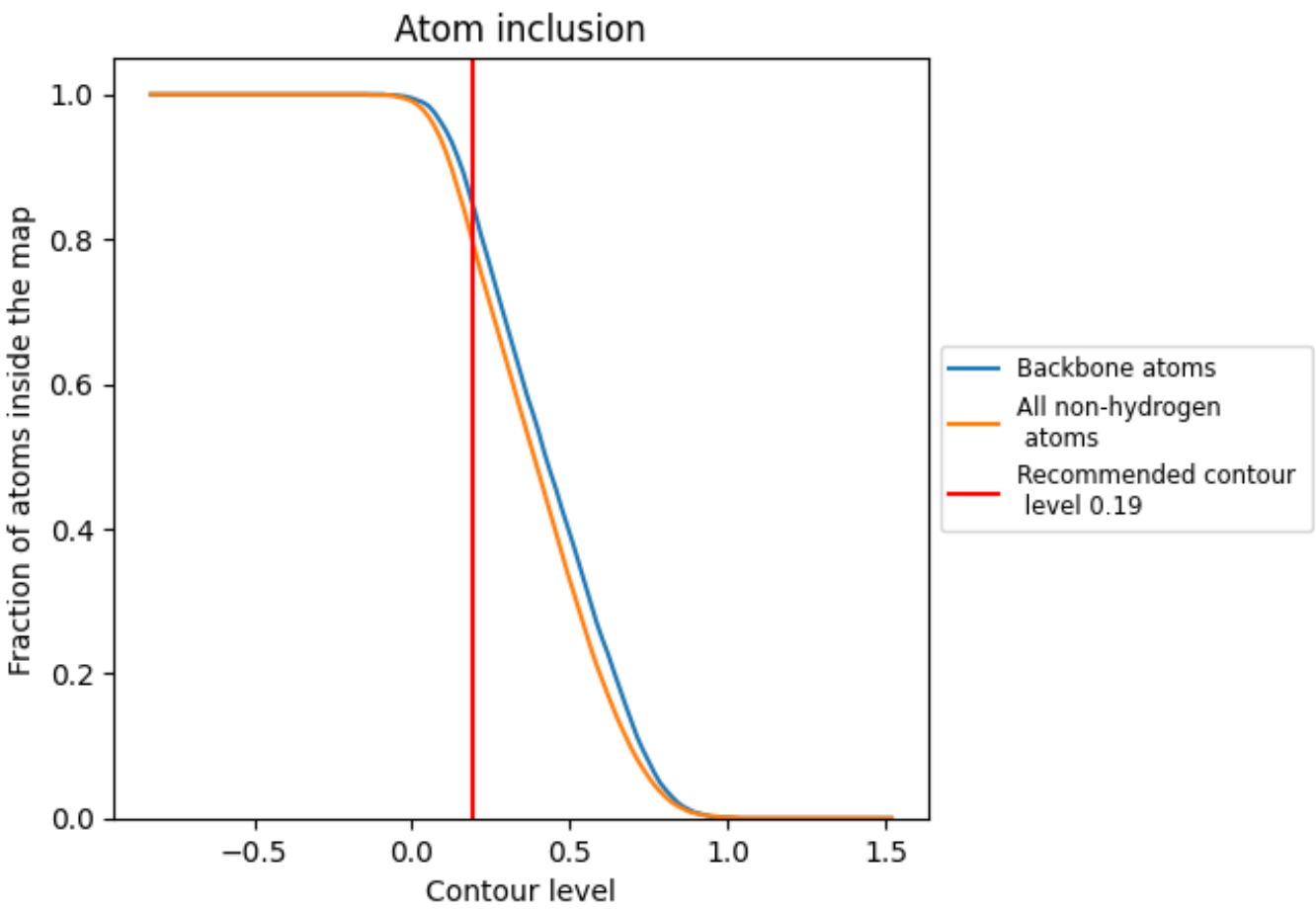
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.19).

9.4 Atom inclusion (i)



At the recommended contour level, 85% of all backbone atoms, 80% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.19) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8000	0.6150
A	0.8680	0.6330
B	0.9100	0.6480
C	0.8360	0.6270
D	0.8580	0.6340
E	0.8270	0.6150
F	0.8170	0.6150
G	0.8320	0.6230
H	0.8710	0.6370
I	0.7950	0.6040
J	0.8350	0.6270
K	0.8030	0.6190
L	0.9080	0.6520
M	0.9250	0.6570
N	0.7580	0.5950
O	0.6290	0.5620
P	0.5380	0.5310
Q	0.4130	0.5140
U	0.4390	0.5540
X	0.7650	0.6060
a	0.7980	0.6110
b	0.8270	0.6070
c	0.7800	0.6000
d	0.8490	0.6230
e	0.8520	0.6180
f	0.8140	0.6110
g	0.8220	0.6130
i	0.8140	0.6180
j	0.8180	0.6200
k	0.8000	0.5990
n	0.7320	0.5830
o	0.5560	0.5340
p	0.4170	0.5100
q	0.2360	0.4520