wwPDB EM Validation Summary Report (i)

Aug 6, 2026 – 06:14 AM JST

PDB ID	:	7F0L / pdb_00007f0l
EMDB ID	:	EMD-31400
Title	:	STRUCTURE OF PHOTOSYNTHETIC LH1-RC SUPER-COMPLEX OF RHODOBACTER SPHAEROIDES MONOMER
Authors	:	Tani, K.; Nagashima, V.P.; Kanno, R.; Kawamura, S.; Kikuchi, R.; Ji, X.-C.; Hall, M.; Yu, L.-J.; Kimura, Y.; Madigan, M.T.; Mizoguchi, A.; Humbel, B.M.; Wang-Otomo, Z.-Y.
Deposited on	:	2021-06-05
Resolution	:	2.94 Å(reported)
Based on initial model	:	5Y5S

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:

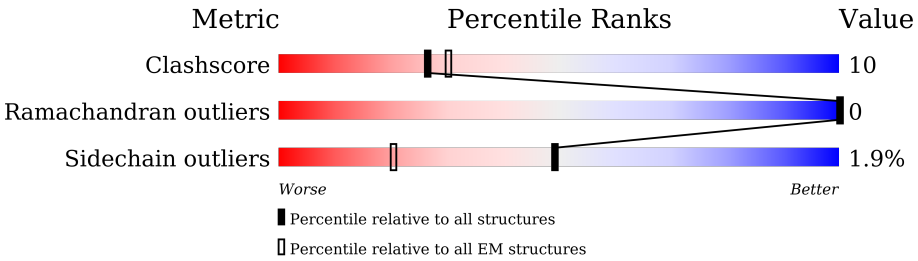
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using 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)

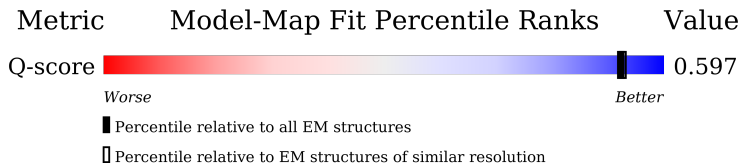
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.94 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	13068 (2.44 - 3.44)

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	78% 20% •
2	M	308	77% 21% ••
3	H	260	• 80% 15% 5%

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Validation Pipeline (wwPDB-VP) : 2.50

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Mol	Chain	Length	Quality of chain
4	1	54	87% 13%
4	3	54	7% 94%
4	A	54	59% 24% 17%
4	D	54	78% 22%
4	F	54	89% 9%
4	I	54	81% 19%
4	K	54	80% 19%
4	O	54	76% 20%
4	Q	54	7% 67% 33%
4	S	54	6% 80% 20%
4	V	54	72% 26%
4	Y	54	76% 22%
5	2	49	6% 84% 14%
5	4	49	8% 76% 12% 12%
5	6	49	10% 76% 10% 14%
5	8	49	27% 63% 14% 22%
5	B	49	78% 12% 10%
5	E	49	73% 14% 12%
5	G	49	6% 84% 8% 8%
5	J	49	78% 10% 12%
5	N	49	76% 10% 12%
5	P	49	8% 73% 14% 12%
5	R	49	78% 10% 12%
5	T	49	78% 10% 12%
5	W	49	10% 63% 24% 12%

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Mol	Chain	Length	Quality of chain
5	Z	49	12% 78% 8% • 12%
6	5	54	6% 80% 19% •
6	7	54	26% 80% 15% 6%
7	X	82	• 51% 13% 35%
8	U	53	9% 83% 11% 6%

2 Entry composition (i)

There are 17 unique types of molecules in this entry. The entry contains 23458 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 Photosynthetic reaction center L subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	L	281	2233	1508	355	362	8	0	0

- 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	2437	1627	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	246	1864	1197	314	343	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	D	54	455	309	73	70	3	0	0
4	F	54	457	311	73	70	3	0	0
4	I	54	457	311	73	70	3	0	0
4	K	54	457	311	73	70	3	0	0
4	O	54	453	308	72	70	3	0	0
4	Q	54	457	311	73	70	3	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	S	54	454	309	73	70	2	0	0
			Total	C	N	O	S		
4	V	54	457	311	73	70	3	0	0
			Total	C	N	O	S		
4	Y	54	457	311	73	70	3	0	0
			Total	C	N	O	S		
4	1	54	457	311	73	70	3	0	0
			Total	C	N	O	S		
4	3	54	457	311	73	70	3	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	B	44	359	240	56	62	1	0	0
			Total	C	N	O	S		
5	E	43	351	236	55	59	1	0	0
			Total	C	N	O	S		
5	G	45	365	243	57	64	1	0	0
			Total	C	N	O	S		
5	J	43	351	236	55	59	1	0	0
			Total	C	N	O	S		
5	N	43	351	236	55	59	1	0	0
			Total	C	N	O	S		
5	P	43	351	236	55	59	1	0	0
			Total	C	N	O	S		
5	R	43	347	234	55	57	1	0	0
			Total	C	N	O	S		
5	T	43	351	236	55	59	1	0	0
			Total	C	N	O	S		
5	W	43	347	234	55	57	1	0	0
			Total	C	N	O	S		
5	Z	43	351	236	55	59	1	0	0
			Total	C	N	O	S		
5	2	42	343	230	54	58	1	0	0
			Total	C	N	O	S		
5	4	43	351	236	55	59	1	0	0
			Total	C	N	O	S		
5	6	42	332	222	54	55	1	0	0
			Total	C	N	O	S		
5	8	38	296	202	49	44	1	0	0

- Molecule 6 is a protein called Light-harvesting protein B-875 alpha chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	5	53	447	305	72	68	2	0	0
6	7	51	415	281	68	64	2	0	0

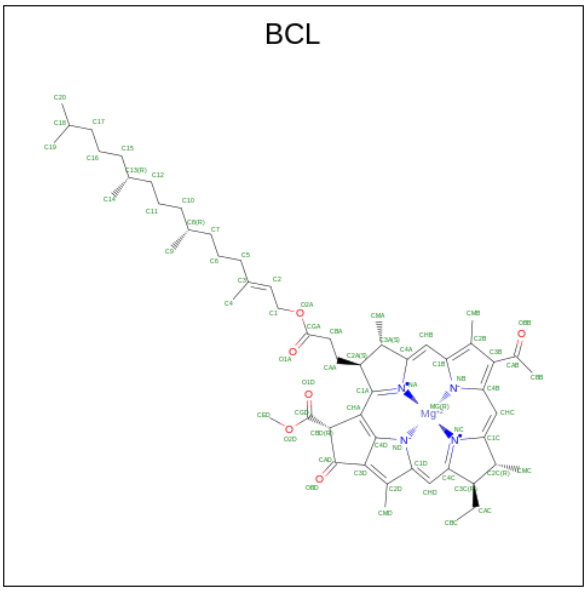
- Molecule 7 is a protein called PufX.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	X	53	405	269	69	64	3	0	0

- Molecule 8 is a protein called protein-U.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	U	50	369	252	57	57	3	0	0

- Molecule 9 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	
9	L	1	66	55	1	4	6	0
9	L	1	66	55	1	4	6	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
9	L	1	66	55	1	4	6	0
9	M	1	66	55	1	4	6	0
9	A	1	61	50	1	4	6	0
9	B	1	66	55	1	4	6	0
9	D	1	66	55	1	4	6	0
9	E	1	66	55	1	4	6	0
9	F	1	66	55	1	4	6	0
9	G	1	66	55	1	4	6	0
9	I	1	66	55	1	4	6	0
9	J	1	66	55	1	4	6	0
9	K	1	66	55	1	4	6	0
9	N	1	66	55	1	4	6	0
9	O	1	66	55	1	4	6	0
9	P	1	66	55	1	4	6	0
9	Q	1	66	55	1	4	6	0
9	R	1	66	55	1	4	6	0
9	S	1	66	55	1	4	6	0
9	T	1	66	55	1	4	6	0
9	V	1	66	55	1	4	6	0
9	W	1	66	55	1	4	6	0
9	Y	1	66	55	1	4	6	0

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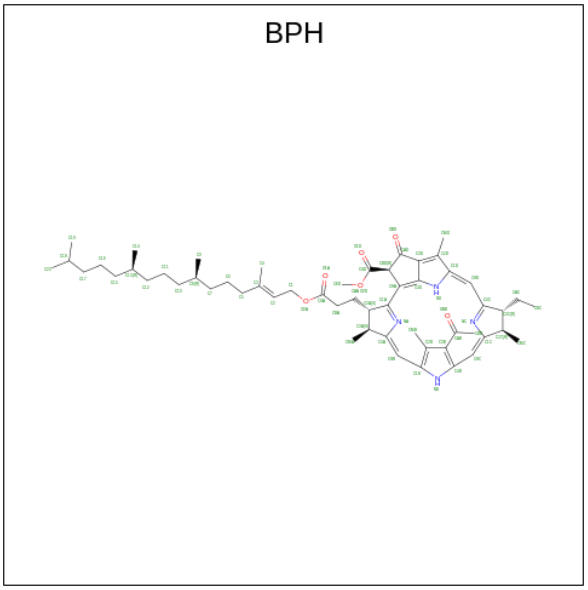
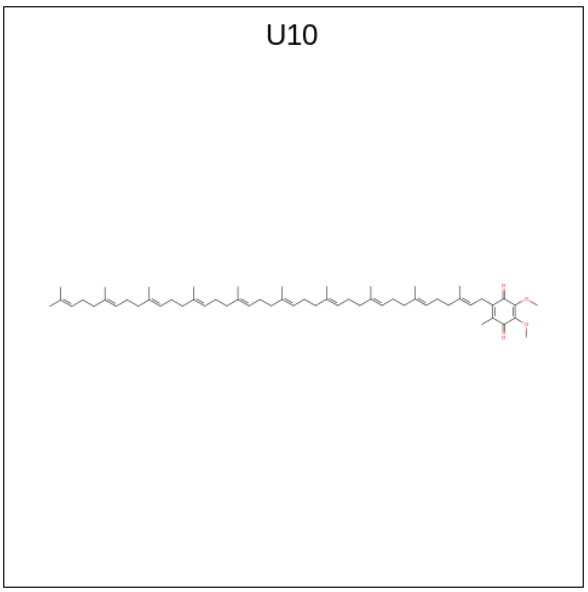
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
9	Z	1	66	55	1	4	6	0
9	1	1	66	55	1	4	6	0
9	2	1	66	55	1	4	6	0
9	3	1	66	55	1	4	6	0
9	4	1	66	55	1	4	6	0
9	5	1	66	55	1	4	6	0
9	6	1	66	55	1	4	6	0
9	7	1	66	55	1	4	6	0
9	8	1	60	49	1	4	6	0

- Molecule 10 is BACTERIOPHEOPHYTIN A (CCD ID: BPH) (formula: $C_{55}H_{76}N_4O_6$).



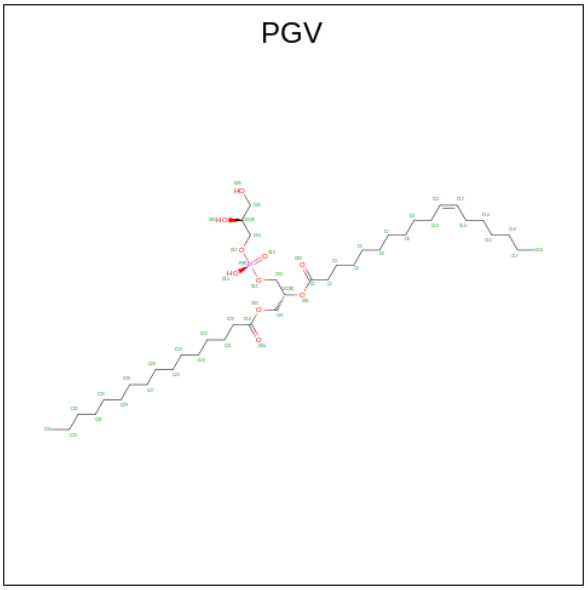
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
10	L	1	65	55	4	6	0
10	M	1	65	55	4	6	0

- Molecule 11 is UBIQUINONE-10 (CCD ID: U10) (formula: $C_{59}H_{90}O_4$).



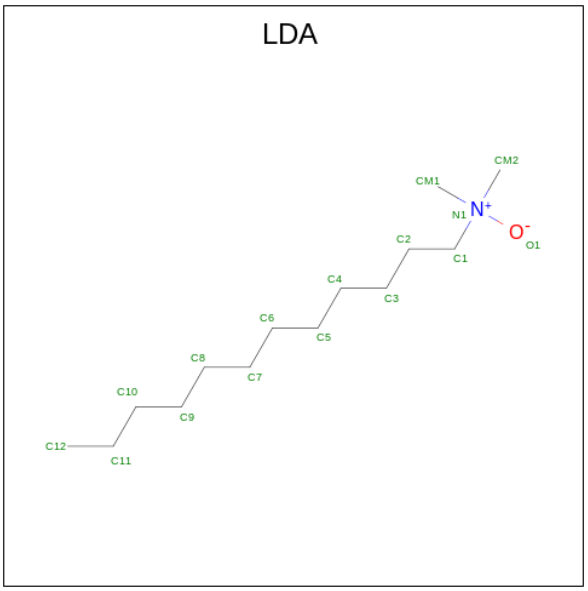
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
11	L	1	35	31	4	0
			Total	C	O	
11	L	1	35	31	4	0
			Total	C	O	
11	M	1	48	44	4	0

- Molecule 12 is (1R)-2-{[{[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (CCD ID: PGV) (formula: $C_{40}H_{77}O_{10}P$).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
12	L	1	39	28	10	1	0
			Total	C	O	P	
12	L	1	33	22	10	1	0
			Total	C	O	P	
12	L	1	45	36	8	1	0
			Total	C	O	P	
12	M	1	47	36	10	1	0
			Total	C	O	P	
12	M	1	38	27	10	1	0
			Total	C	O	P	
12	H	1	34	25	8	1	0
			Total	C	O	P	
12	H	1	40	29	10	1	0
			Total	C	O	P	
12	H	1	47	36	10	1	0
			Total	C	O	P	
12	K	1	41	34	6	1	0
			Total	C	O	P	
12	Q	1	39	28	10	1	0
			Total	C	O	P	
12	Y	1	43	32	10	1	0
			Total	C	O	P	
12	3	1	51	40	10	1	0
			Total	C	O	P	
12	X	1	39	28	10	1	0

- Molecule 13 is LAURYL DIMETHYLAMINE-N-OXIDE (CCD ID: LDA) (formula: $C_{14}H_{31}NO$).

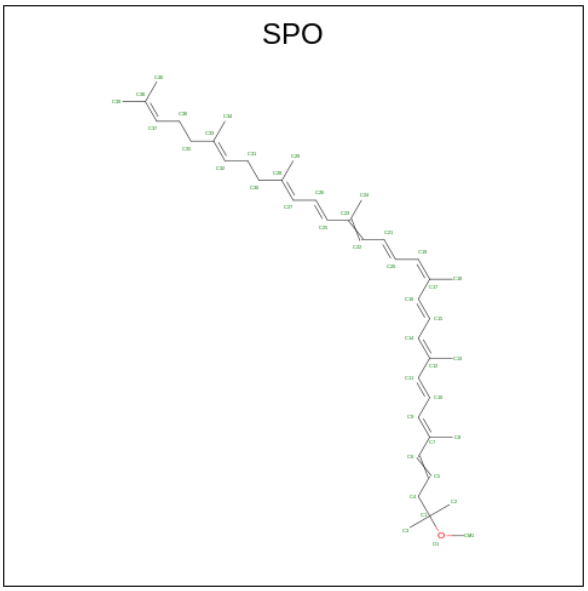


Mol	Chain	Residues	Atoms				AltConf
13	L	1	Total	C	N	O	0
			16	14	1	1	
13	L	1	Total	C	N	O	0
			16	14	1	1	
13	M	1	Total	C	N	O	0
			16	14	1	1	
13	Y	1	Total	C	N	O	0
			12	10	1	1	
13	X	1	Total	C	N	O	0
			13	11	1	1	
13	X	1	Total	C	N	O	0
			16	14	1	1	

- Molecule 14 is FE (III) ION (CCD ID: FE) (formula: Fe).

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

- Molecule 15 is SPHEROIDENE (CCD ID: SPO) (formula: $C_{41}H_{60}O$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
15	M	1	42	41	1	0
15	D	1	42	41	1	0
15	E	1	42	41	1	0
15	F	1	42	41	1	0
15	F	1	42	41	1	0
15	G	1	42	41	1	0
15	G	1	42	41	1	0
15	K	1	42	41	1	0
15	N	1	42	41	1	0
15	O	1	42	41	1	0
15	O	1	42	41	1	0
15	P	1	42	41	1	0
15	R	1	42	41	1	0
15	S	1	42	41	1	0

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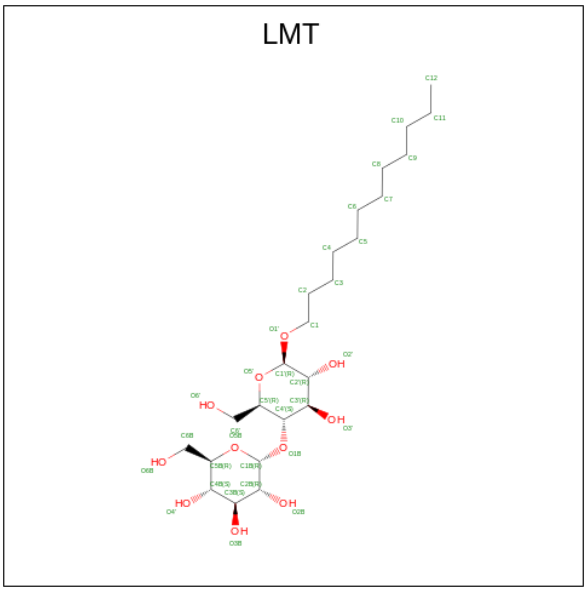
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
15	S	1	42	41	1	0
15	T	1	42	41	1	0
15	V	1	42	41	1	0
15	V	1	42	41	1	0
15	W	1	42	41	1	0
15	1	1	42	41	1	0
15	1	1	42	41	1	0
15	1	1	42	41	1	0
15	3	1	42	41	1	0
15	5	1	42	41	1	0
15	5	1	42	41	1	0
15	8	1	42	41	1	0
15	X	1	42	41	1	0

- Molecule 16 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: $C_{24}H_{46}O_{11}$).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
16	M	1	27	20	7	0
			Total	C	O	
16	M	1	35	24	11	0
			Total	C	O	
16	M	1	33	22	11	0
			Total	C	O	
16	H	1	35	24	11	0
			Total	C	O	
16	H	1	30	19	11	0
			Total	C	O	
16	A	1	35	24	11	0
			Total	C	O	
16	A	1	35	24	11	0
			Total	C	O	
16	A	1	27	16	11	0
			Total	C	O	
16	D	1	27	16	11	0
			Total	C	O	
16	F	1	26	16	10	0
			Total	C	O	
16	F	1	17	11	6	0
			Total	C	O	
16	I	1	27	16	11	0
			Total	C	O	
16	K	1	35	24	11	0
			Total	C	O	
16	Q	1	24	18	6	0

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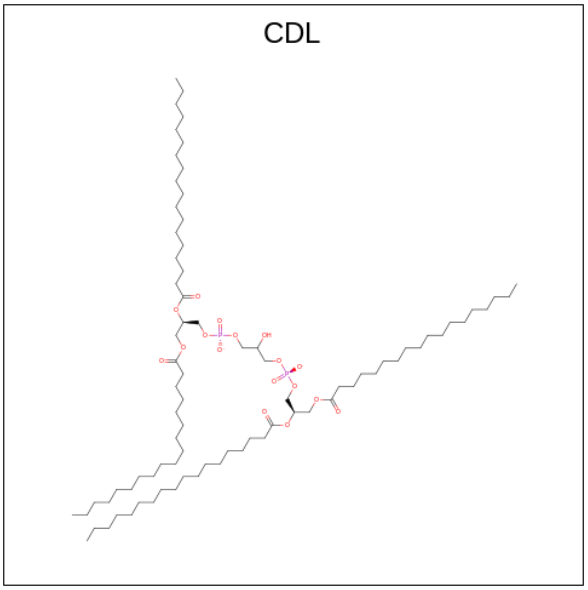
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O		
16	Q	1	19	13	6		0
			Total	C	O		
16	S	1	25	19	6		0
			Total	C	O		
16	S	1	30	19	11		0
			Total	C	O		
16	1	1	24	15	9		0
			Total	C	O		
16	3	1	35	24	11		0
			Total	C	O		
16	4	1	27	16	11		0
			Total	C	O		
16	5	1	33	22	11		0
			Total	C	O		
16	X	1	31	20	11		0
			Total	C	O		
16	U	1	32	21	11		0
			Total	C	O		
16	U	1	35	24	11		0

- Molecule 17 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
17	M	1	79	60	17	2	0

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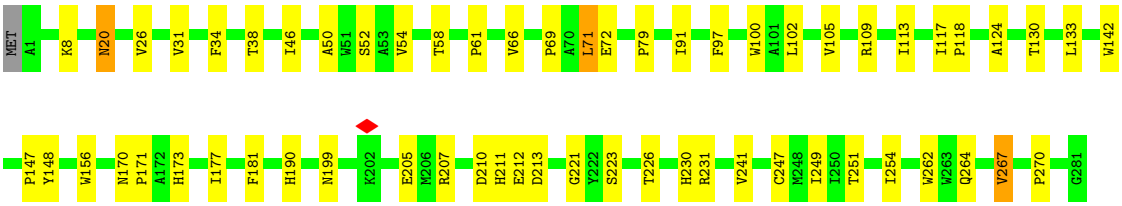
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
17	H	1	61	42	17	2	0
			Total	C	O	P	
17	H	1	37	20	15	2	0
			Total	C	O	P	
17	Y	1	48	30	16	2	0

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.

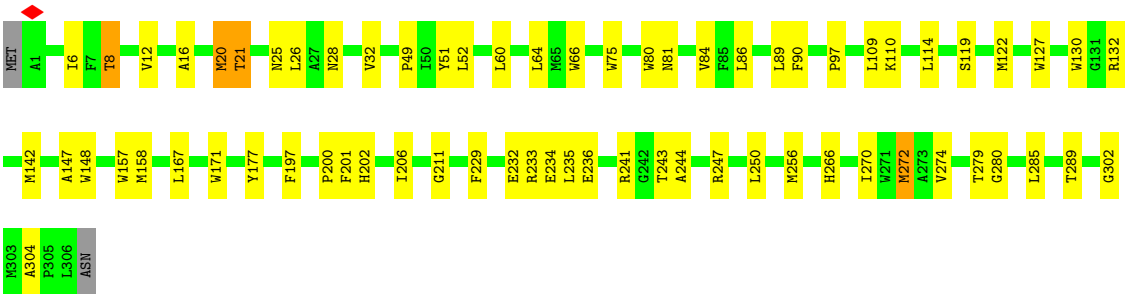
• Molecule 1: Photosynthetic reaction center L subunit

Chain L: 78% 20%



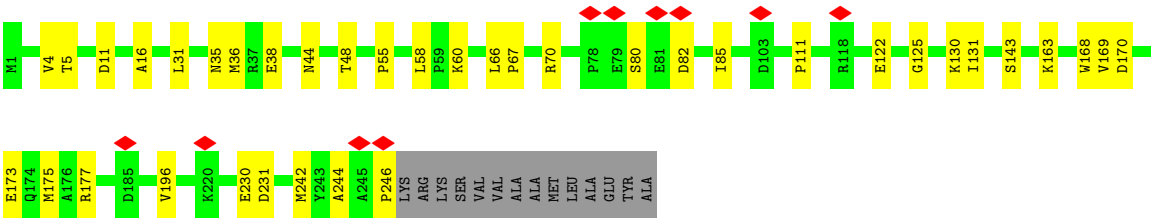
• Molecule 2: Reaction center protein M chain

Chain M: 77% 21%



• Molecule 3: Reaction center protein H chain

Chain H: 80% 15% 5%

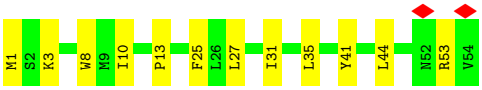


• Molecule 4: Light-harvesting protein B-875 alpha chain

Chain A: 59% 24% 17%

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

Chain D: 78% 22%

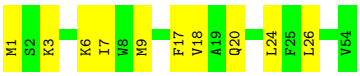


• Molecule 4: Light-harvesting protein B-875 alpha chain

Chain F: 89% 9%

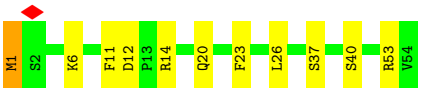
• Molecule 4: Light-harvesting protein B-875 alpha chain

Chain I: 81% 19%



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

Chain K: 80% 19%

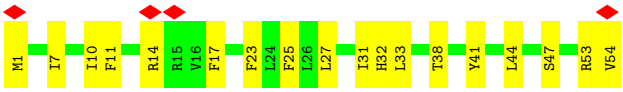


• Molecule 4: Light-harvesting protein B-875 alpha chain

Chain O: 76% 20%

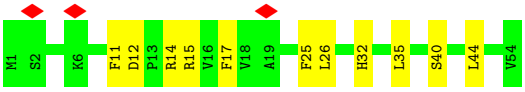
• Molecule 4: Light-harvesting protein B-875 alpha chain

Chain Q: 7% 67% 33%



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

Chain S:

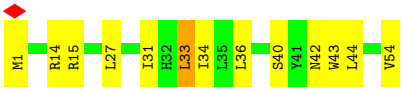


• Molecule 4: Light-harvesting protein B-875 alpha chain

Chain V:

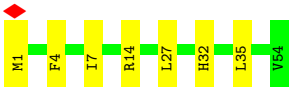
• Molecule 4: Light-harvesting protein B-875 alpha chain

Chain Y:



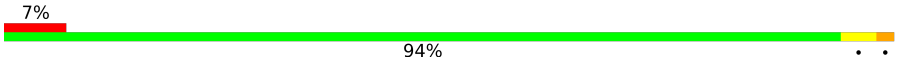
• Molecule 4: Light-harvesting protein B-875 alpha chain

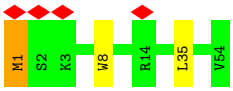
Chain 1:



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

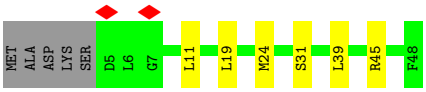
Chain 3:





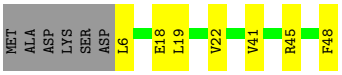
• Molecule 5: Antenna pigment protein beta chain

Chain B:



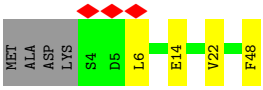
• Molecule 5: Antenna pigment protein beta chain

Chain E:



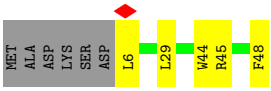
• Molecule 5: Antenna pigment protein beta chain

Chain G:



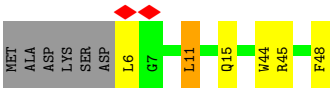
• Molecule 5: Antenna pigment protein beta chain

Chain J:



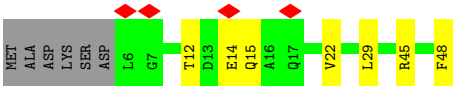
• Molecule 5: Antenna pigment protein beta chain

Chain N:



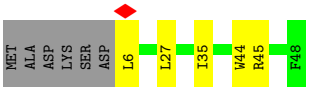
• Molecule 5: Antenna pigment protein beta chain

Chain P:



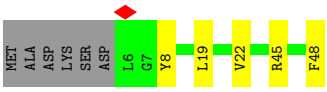
• Molecule 5: Antenna pigment protein beta chain

Chain R:



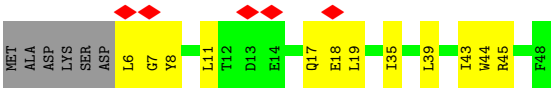
• Molecule 5: Antenna pigment protein beta chain

Chain T:



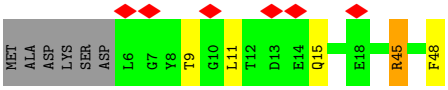
• Molecule 5: Antenna pigment protein beta chain

Chain W:



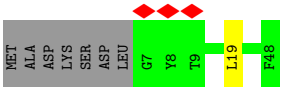
• Molecule 5: Antenna pigment protein beta chain

Chain Z:



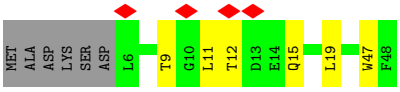
• Molecule 5: Antenna pigment protein beta chain

Chain 2:



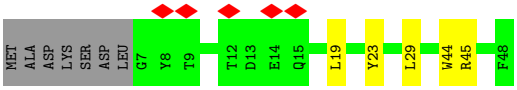
• Molecule 5: Antenna pigment protein beta chain

Chain 4:



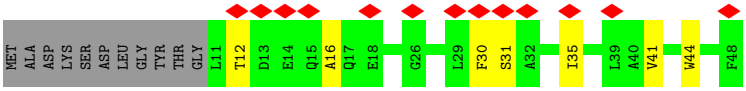
• Molecule 5: Antenna pigment protein beta chain

Chain 6:



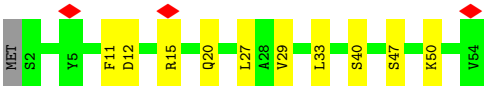
• Molecule 5: Antenna pigment protein beta chain

Chain 8:



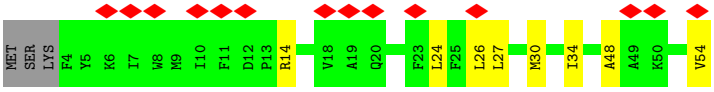
• Molecule 6: Light-harvesting protein B-875 alpha chain

Chain 5:



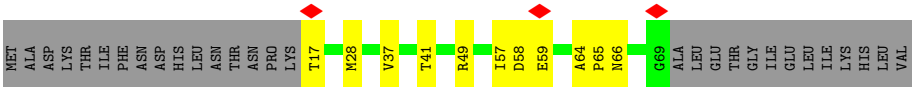
- Molecule 6: Light-harvesting protein B-875 alpha chain

Chain 7:



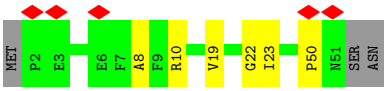
- Molecule 7: PufX

Chain X:



- Molecule 8: protein-U

Chain U:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	160448	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	42	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.466	Depositor
Minimum map value	-0.288	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.016	Depositor
Recommended contour level	0.064	Depositor
Map size (Å)	306.32, 306.32, 306.32	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.094, 1.094, 1.094	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: LMT, FME, CDL, LDA, BCL, BPH, U10, PGV, FE, SPO

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	0.24	0/2321	0.29	0/3177
2	M	0.24	0/2530	0.31	0/3455
3	H	0.19	0/1914	0.29	0/2607
4	1	0.19	0/461	0.26	0/625
4	3	0.17	0/461	0.23	0/625
4	A	0.19	0/389	0.24	0/528
4	D	0.19	0/459	0.27	0/622
4	F	0.21	0/461	0.25	0/625
4	I	0.21	0/461	0.26	0/625
4	K	0.20	0/461	0.25	0/625
4	O	0.21	0/457	0.26	0/621
4	Q	0.20	0/461	0.27	0/625
4	S	0.19	0/461	0.25	0/625
4	V	0.20	0/461	0.25	0/625
4	Y	0.20	0/461	0.25	0/625
5	2	0.16	0/356	0.23	0/488
5	4	0.16	0/364	0.30	0/499
5	6	0.12	0/344	0.22	0/472
5	8	0.11	0/308	0.21	0/424
5	B	0.18	0/372	0.26	0/510
5	E	0.20	0/364	0.23	0/499
5	G	0.18	0/378	0.24	0/518
5	J	0.17	0/364	0.24	0/499
5	N	0.17	0/364	0.21	0/499
5	P	0.17	0/364	0.27	0/499
5	R	0.18	0/360	0.25	0/494
5	T	0.17	0/364	0.22	0/499
5	W	0.17	0/360	0.22	0/494
5	Z	0.16	0/364	0.21	0/499
6	5	0.16	0/461	0.24	0/625
6	7	0.12	0/427	0.24	0/582
7	X	0.16	0/417	0.27	0/566

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
8	U	0.14	0/381	0.25	0/516
All	All	0.20	0/18931	0.26	0/25817

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	2233	0	2189	47	0
2	M	2437	0	2355	56	0
3	H	1864	0	1862	26	0
4	1	457	0	476	7	0
4	3	457	0	476	3	0
4	A	386	0	400	15	0
4	D	455	0	469	10	0
4	F	457	0	476	6	0
4	I	457	0	476	10	0
4	K	457	0	476	9	0
4	O	453	0	465	14	0
4	Q	457	0	476	16	0
4	S	454	0	469	12	0
4	V	457	0	476	16	0
4	Y	457	0	476	13	0
5	2	343	0	325	1	0
5	4	351	0	336	5	0
5	6	332	0	314	5	0
5	8	296	0	273	6	0
5	B	359	0	340	5	0
5	E	351	0	336	8	0
5	G	365	0	345	4	0
5	J	351	0	336	9	0
5	N	351	0	336	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	P	351	0	336	7	0
5	R	347	0	332	5	0
5	T	351	0	336	5	0
5	W	347	0	332	11	0
5	Z	351	0	336	5	0
6	5	447	0	465	11	0
6	7	415	0	422	6	0
7	X	405	0	412	8	0
8	U	369	0	366	7	0
9	1	66	0	74	4	0
9	2	66	0	74	4	0
9	3	66	0	74	3	0
9	4	66	0	74	3	0
9	5	66	0	74	6	0
9	6	66	0	74	3	0
9	7	66	0	74	6	0
9	8	60	0	58	6	0
9	A	61	0	61	2	0
9	B	66	0	74	8	0
9	D	66	0	74	4	0
9	E	66	0	74	6	0
9	F	66	0	74	2	0
9	G	66	0	74	2	0
9	I	66	0	74	6	0
9	J	66	0	74	3	0
9	K	66	0	74	5	0
9	L	198	0	222	14	0
9	M	66	0	74	3	0
9	N	66	0	74	1	0
9	O	66	0	74	4	0
9	P	66	0	74	2	0
9	Q	66	0	74	1	0
9	R	66	0	74	3	0
9	S	66	0	74	4	0
9	T	66	0	74	5	0
9	V	66	0	74	7	0
9	W	66	0	74	6	0
9	Y	66	0	74	6	0
9	Z	66	0	74	2	0
10	L	65	0	76	5	0
10	M	65	0	76	6	0
11	L	70	0	86	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	M	48	0	63	2	0
12	3	51	0	76	1	0
12	H	121	0	149	6	0
12	K	41	0	60	3	0
12	L	117	0	147	8	0
12	M	85	0	110	6	0
12	Q	39	0	48	1	0
12	X	39	0	48	3	0
12	Y	43	0	54	7	0
13	L	32	0	62	2	0
13	M	16	0	31	0	0
13	X	29	0	53	3	0
13	Y	12	0	20	5	0
14	M	1	0	0	0	0
15	1	126	0	180	14	0
15	3	42	0	60	2	0
15	5	84	0	120	11	0
15	8	42	0	60	5	0
15	D	42	0	60	3	0
15	E	42	0	60	3	0
15	F	84	0	120	6	0
15	G	84	0	120	15	0
15	K	42	0	60	6	0
15	M	42	0	60	4	0
15	N	42	0	60	8	0
15	O	84	0	120	12	0
15	P	42	0	60	2	0
15	R	42	0	60	6	0
15	S	84	0	120	11	0
15	T	42	0	60	10	0
15	V	84	0	120	8	0
15	W	42	0	60	4	0
15	X	42	0	60	4	0
16	1	24	0	21	0	0
16	3	35	0	46	4	0
16	4	27	0	27	0	0
16	5	33	0	39	2	0
16	A	97	0	119	7	0
16	D	27	0	27	0	0
16	F	43	0	40	0	0
16	H	65	0	79	5	0
16	I	27	0	27	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	K	35	0	46	2	0
16	M	95	0	121	6	0
16	Q	43	0	55	4	0
16	S	55	0	68	2	0
16	U	67	0	83	2	0
16	X	31	0	35	0	0
17	H	98	0	92	6	0
17	M	79	0	105	6	0
17	Y	48	0	46	2	0
All	All	23458	0	24489	480	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 10.

The worst 5 of 480 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:231:ARG:HH12	2:M:8:THR:HG22	1.49	0.77
16:H:302:LMT:H5'	4:O:38:THR:HG22	1.65	0.76
2:M:75:TRP:HE1	15:M:807:SPO:HM12	1.50	0.76
2:M:247:ARG:NH2	3:H:111:PRO:O	2.20	0.74
4:A:40:SER:O	5:B:45:ARG:NH1	2.21	0.74

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%)	267 (96%)	12 (4%)	0	100	100
2	M	304/308 (99%)	293 (96%)	11 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	H	244/260 (94%)	231 (95%)	13 (5%)	0	100	100
4	1	52/54 (96%)	48 (92%)	4 (8%)	0	100	100
4	3	52/54 (96%)	51 (98%)	1 (2%)	0	100	100
4	A	43/54 (80%)	43 (100%)	0	0	100	100
4	D	52/54 (96%)	51 (98%)	1 (2%)	0	100	100
4	F	52/54 (96%)	52 (100%)	0	0	100	100
4	I	52/54 (96%)	50 (96%)	2 (4%)	0	100	100
4	K	52/54 (96%)	51 (98%)	1 (2%)	0	100	100
4	O	52/54 (96%)	52 (100%)	0	0	100	100
4	Q	52/54 (96%)	51 (98%)	1 (2%)	0	100	100
4	S	52/54 (96%)	52 (100%)	0	0	100	100
4	V	52/54 (96%)	47 (90%)	5 (10%)	0	100	100
4	Y	52/54 (96%)	51 (98%)	1 (2%)	0	100	100
5	2	40/49 (82%)	39 (98%)	1 (2%)	0	100	100
5	4	41/49 (84%)	39 (95%)	2 (5%)	0	100	100
5	6	40/49 (82%)	39 (98%)	1 (2%)	0	100	100
5	8	36/49 (74%)	36 (100%)	0	0	100	100
5	B	42/49 (86%)	42 (100%)	0	0	100	100
5	E	41/49 (84%)	41 (100%)	0	0	100	100
5	G	43/49 (88%)	42 (98%)	1 (2%)	0	100	100
5	J	41/49 (84%)	41 (100%)	0	0	100	100
5	N	41/49 (84%)	41 (100%)	0	0	100	100
5	P	41/49 (84%)	37 (90%)	4 (10%)	0	100	100
5	R	41/49 (84%)	41 (100%)	0	0	100	100
5	T	41/49 (84%)	41 (100%)	0	0	100	100
5	W	41/49 (84%)	41 (100%)	0	0	100	100
5	Z	41/49 (84%)	40 (98%)	1 (2%)	0	100	100
6	5	51/54 (94%)	50 (98%)	1 (2%)	0	100	100
6	7	49/54 (91%)	49 (100%)	0	0	100	100
7	X	51/82 (62%)	48 (94%)	3 (6%)	0	100	100
8	U	48/53 (91%)	47 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	2211/2427 (91%)	2144 (97%)	67 (3%)	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	220/221 (100%)	212 (96%)	8 (4%)	31	56
2	M	239/241 (99%)	231 (97%)	8 (3%)	33	58
3	H	197/208 (95%)	194 (98%)	3 (2%)	57	75
4	1	48/48 (100%)	48 (100%)	0	100	100
4	3	48/48 (100%)	48 (100%)	0	100	100
4	A	41/48 (85%)	41 (100%)	0	100	100
4	D	47/48 (98%)	47 (100%)	0	100	100
4	F	48/48 (100%)	48 (100%)	0	100	100
4	I	48/48 (100%)	48 (100%)	0	100	100
4	K	48/48 (100%)	46 (96%)	2 (4%)	26	52
4	O	47/48 (98%)	45 (96%)	2 (4%)	26	51
4	Q	48/48 (100%)	47 (98%)	1 (2%)	47	70
4	S	48/48 (100%)	48 (100%)	0	100	100
4	V	48/48 (100%)	46 (96%)	2 (4%)	26	52
4	Y	48/48 (100%)	46 (96%)	2 (4%)	26	52
5	2	34/40 (85%)	34 (100%)	0	100	100
5	4	35/40 (88%)	35 (100%)	0	100	100
5	6	32/40 (80%)	32 (100%)	0	100	100
5	8	26/40 (65%)	26 (100%)	0	100	100
5	B	36/40 (90%)	35 (97%)	1 (3%)	38	63
5	E	35/40 (88%)	34 (97%)	1 (3%)	37	62

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	G	37/40 (92%)	36 (97%)	1 (3%)	39	64
5	J	35/40 (88%)	35 (100%)	0	100	100
5	N	35/40 (88%)	34 (97%)	1 (3%)	37	62
5	P	35/40 (88%)	35 (100%)	0	100	100
5	R	34/40 (85%)	34 (100%)	0	100	100
5	T	35/40 (88%)	35 (100%)	0	100	100
5	W	34/40 (85%)	33 (97%)	1 (3%)	37	62
5	Z	35/40 (88%)	34 (97%)	1 (3%)	37	62
6	5	48/49 (98%)	48 (100%)	0	100	100
6	7	43/49 (88%)	42 (98%)	1 (2%)	44	68
7	X	40/66 (61%)	39 (98%)	1 (2%)	42	66
8	U	34/37 (92%)	34 (100%)	0	100	100
All	All	1866/2007 (93%)	1830 (98%)	36 (2%)	49	71

5 of 36 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	V	7	ILE
7	X	17	THR
4	V	10	ILE
4	Y	54	VAL
2	M	197	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
4	Y	42	ASN
7	X	26	GLN
8	U	51	ASN
7	X	60	ASN
3	H	44	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	3	1	4	8,9,10	0.49	0	7,9,11	0.95	1 (14%)
4	FME	I	1	4	8,9,10	0.51	0	7,9,11	0.96	1 (14%)
4	FME	K	1	4	8,9,10	0.50	0	7,9,11	0.98	1 (14%)
4	FME	O	1	4	8,9,10	0.51	0	7,9,11	1.04	1 (14%)
4	FME	F	1	4	8,9,10	0.53	0	7,9,11	0.91	1 (14%)
4	FME	Q	1	4	8,9,10	0.51	0	7,9,11	0.97	1 (14%)
4	FME	D	1	4	8,9,10	0.49	0	7,9,11	1.05	1 (14%)
4	FME	V	1	4	8,9,10	0.52	0	7,9,11	1.03	1 (14%)
4	FME	1	1	4	8,9,10	0.51	0	7,9,11	0.99	1 (14%)
4	FME	A	1	4	8,9,10	0.50	0	7,9,11	0.88	1 (14%)
4	FME	S	1	4	5,6,10	0.79	0	3,6,11	0.67	0
4	FME	Y	1	4	8,9,10	0.50	0	7,9,11	0.98	1 (14%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	FME	3	1	4	-	0/7/9/11	-
4	FME	I	1	4	-	1/7/9/11	-
4	FME	K	1	4	-	1/7/9/11	-
4	FME	O	1	4	-	1/7/9/11	-
4	FME	F	1	4	-	1/7/9/11	-
4	FME	Q	1	4	-	0/7/9/11	-
4	FME	D	1	4	-	0/7/9/11	-
4	FME	V	1	4	-	1/7/9/11	-
4	FME	1	1	4	-	0/7/9/11	-
4	FME	A	1	4	-	3/7/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	FME	S	1	4	-	1/2/5/11	-
4	FME	Y	1	4	-	1/7/9/11	-

There are no bond length outliers.

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	O	1	FME	O-C-CA	-2.53	118.14	124.78
4	D	1	FME	O-C-CA	-2.53	118.14	124.78
4	I	1	FME	O-C-CA	-2.49	118.26	124.78
4	Y	1	FME	O-C-CA	-2.48	118.28	124.78
4	1	1	FME	O-C-CA	-2.47	118.31	124.78

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

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

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	3	1	FME	1	0
4	K	1	FME	1	0
4	O	1	FME	1	0
4	F	1	FME	1	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 112 ligands modelled in this entry, 1 is monoatomic - leaving 111 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	$\#\|Z\| > 2$
15	SPO	O	102	-	40,41,41	0.66	0	47,50,50	1.82	12 (25%)
15	SPO	V	102	-	40,41,41	0.65	0	47,50,50	1.71	12 (25%)
12	PGV	X	101	-	38,38,50	1.04	2 (5%)	41,44,56	1.10	3 (7%)
9	BCL	8	102	5	63,68,74	1.94	17 (26%)	75,107,115	2.51	19 (25%)
15	SPO	K	103	-	40,41,41	0.66	0	47,50,50	1.81	10 (21%)
12	PGV	L	305	-	38,38,50	1.05	2 (5%)	41,44,56	1.07	3 (7%)
9	BCL	Z	101	5	69,74,74	1.79	19 (27%)	83,115,115	2.44	26 (31%)
12	PGV	M	801	-	46,46,50	0.94	2 (4%)	49,52,56	1.17	4 (8%)
10	BPH	L	302	-	59,70,70	0.80	3 (5%)	61,101,101	0.92	3 (4%)
15	SPO	8	101	-	40,41,41	0.65	0	47,50,50	2.13	13 (27%)
9	BCL	L	308	1	69,74,74	1.78	18 (26%)	83,115,115	2.53	26 (31%)
9	BCL	V	101	4	69,74,74	1.77	18 (26%)	83,115,115	2.49	24 (28%)
12	PGV	Q	103	-	38,38,50	1.05	2 (5%)	41,44,56	1.04	2 (4%)
16	LMT	M	808	-	27,27,36	0.46	0	32,33,47	0.64	1 (3%)
12	PGV	H	307	-	46,46,50	0.95	2 (4%)	49,52,56	1.02	3 (6%)
15	SPO	W	102	-	40,41,41	0.67	0	47,50,50	1.72	14 (29%)
9	BCL	A	703	4	64,69,74	1.85	17 (26%)	77,109,115	2.57	23 (29%)
15	SPO	P	101	-	40,41,41	0.64	0	47,50,50	1.76	12 (25%)
12	PGV	H	306	-	39,39,50	1.07	2 (5%)	42,45,56	1.22	3 (7%)
12	PGV	K	104	-	38,40,50	1.02	2 (5%)	40,42,56	1.16	3 (7%)
17	CDL	Y	102	-	47,47,99	1.16	3 (6%)	52,58,111	1.07	3 (5%)
15	SPO	V	103	-	40,41,41	0.68	0	47,50,50	1.82	14 (29%)
9	BCL	1	101	4	69,74,74	1.78	18 (26%)	83,115,115	2.68	29 (34%)
16	LMT	5	101	-	34,34,36	0.39	0	45,45,47	0.73	0
12	PGV	H	303	-	33,33,50	1.14	2 (6%)	36,38,56	1.15	4 (11%)
9	BCL	L	309	2	69,74,74	1.80	17 (24%)	83,115,115	2.44	23 (27%)
15	SPO	1	105	-	40,41,41	0.66	0	47,50,50	1.77	13 (27%)
9	BCL	F	102	4	69,74,74	1.78	18 (26%)	83,115,115	2.54	28 (33%)
16	LMT	H	301	-	36,36,36	0.37	0	47,47,47	0.92	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
16	LMT	A	704	-	28,28,36	0.45	0	39,39,47	0.75	1 (2%)
9	BCL	E	102	5	69,74,74	1.82	18 (26%)	83,115,115	2.47	27 (32%)
15	SPO	G	102	-	40,41,41	0.64	0	47,50,50	1.80	12 (25%)
9	BCL	Q	104	4	69,74,74	1.76	17 (24%)	83,115,115	2.54	25 (30%)
13	LDA	X	103	-	9,12,15	2.43	1 (11%)	11,14,17	0.49	0
15	SPO	F	104	-	40,41,41	0.64	0	47,50,50	1.86	13 (27%)
16	LMT	Q	102	-	19,19,36	0.49	0	24,24,47	0.55	0
16	LMT	3	101	-	36,36,36	0.42	0	47,47,47	0.91	3 (6%)
16	LMT	S	101	-	25,25,36	0.46	0	30,30,47	0.81	0
13	LDA	L	311	-	12,15,15	2.09	1 (8%)	14,17,17	0.53	0
9	BCL	6	101	5	69,74,74	1.81	17 (24%)	83,115,115	2.38	21 (25%)
16	LMT	K	101	-	36,36,36	0.41	0	47,47,47	0.96	2 (4%)
16	LMT	S	105	-	31,31,36	0.45	0	42,42,47	0.67	0
16	LMT	X	105	-	32,32,36	0.40	0	43,43,47	0.80	1 (2%)
15	SPO	F	103	-	40,41,41	0.64	0	47,50,50	1.66	12 (25%)
10	BPH	M	804	-	59,70,70	0.75	2 (3%)	61,101,101	0.95	3 (4%)
9	BCL	I	101	4	69,74,74	1.78	19 (27%)	83,115,115	2.61	26 (31%)
15	SPO	5	103	-	40,41,41	0.66	0	47,50,50	1.97	15 (31%)
9	BCL	L	301	1	69,74,74	1.80	18 (26%)	83,115,115	2.57	29 (34%)
16	LMT	D	103	-	28,28,36	0.43	0	39,39,47	0.67	1 (2%)
9	BCL	5	102	6	69,74,74	1.79	19 (27%)	83,115,115	2.59	26 (31%)
15	SPO	G	103	-	40,41,41	0.64	0	47,50,50	2.14	14 (29%)
9	BCL	R	102	5	69,74,74	1.79	17 (24%)	83,115,115	2.49	26 (31%)
16	LMT	M	809	-	36,36,36	0.37	0	47,47,47	0.69	1 (2%)
9	BCL	M	803	2	69,74,74	1.82	18 (26%)	83,115,115	2.61	24 (28%)
15	SPO	N	101	-	40,41,41	0.65	0	47,50,50	2.11	16 (34%)
15	SPO	O	103	-	40,41,41	0.67	0	47,50,50	1.83	14 (29%)
9	BCL	B	101	5	69,74,74	1.80	18 (26%)	83,115,115	2.40	25 (30%)
15	SPO	S	103	-	40,41,41	0.67	0	47,50,50	1.98	15 (31%)
15	SPO	X	102	-	40,41,41	0.66	0	47,50,50	1.81	11 (23%)
15	SPO	3	104	-	40,41,41	0.64	0	47,50,50	2.02	16 (34%)
16	LMT	M	810	-	34,34,36	0.42	0	45,45,47	1.15	4 (8%)
13	LDA	L	307	-	12,15,15	2.08	1 (8%)	14,17,17	0.50	0
16	LMT	A	701	-	36,36,36	0.34	0	47,47,47	0.71	0
15	SPO	R	101	-	40,41,41	0.68	0	47,50,50	2.32	15 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
11	U10	L	303	-	35,35,63	0.81	2 (5%)	42,45,79	0.67	0
15	SPO	T	102	-	40,41,41	0.69	0	47,50,50	1.84	13 (27%)
9	BCL	7	101	6	69,74,74	1.79	18 (26%)	83,115,115	2.59	25 (30%)
16	LMT	U	102	-	36,36,36	0.35	0	47,47,47	0.73	1 (2%)
17	CDL	H	305	-	35,35,99	1.38	3 (8%)	42,44,111	1.31	6 (14%)
9	BCL	N	102	5	69,74,74	1.79	18 (26%)	83,115,115	2.53	24 (28%)
11	U10	L	304	-	35,35,63	0.77	2 (5%)	42,45,79	0.67	0
11	U10	M	806	-	48,48,63	0.71	2 (4%)	58,61,79	0.58	0
13	LDA	M	802	-	12,15,15	2.08	1 (8%)	14,17,17	0.57	0
16	LMT	U	101	-	33,33,36	0.38	0	44,44,47	0.78	1 (2%)
16	LMT	H	302	-	31,31,36	0.45	0	42,42,47	1.09	3 (7%)
15	SPO	S	104	-	40,41,41	0.66	0	47,50,50	1.66	16 (34%)
9	BCL	D	101	4	69,74,74	1.78	17 (24%)	83,115,115	2.60	27 (32%)
13	LDA	Y	101	-	8,11,15	2.55	1 (12%)	10,13,17	0.45	0
17	CDL	M	811	-	78,78,99	1.03	4 (5%)	84,90,111	1.20	6 (7%)
9	BCL	W	101	5	69,74,74	1.78	19 (27%)	83,115,115	2.48	25 (30%)
16	LMT	F	101	-	27,27,36	0.48	0	38,38,47	0.88	2 (5%)
15	SPO	1	102	-	40,41,41	0.65	0	47,50,50	2.02	14 (29%)
9	BCL	K	102	4	69,74,74	1.80	19 (27%)	83,115,115	2.54	23 (27%)
15	SPO	M	807	-	40,41,41	0.63	0	47,50,50	1.67	10 (21%)
15	SPO	E	101	-	40,41,41	0.63	0	47,50,50	1.71	12 (25%)
9	BCL	T	101	5	69,74,74	1.81	19 (27%)	83,115,115	2.44	23 (27%)
15	SPO	5	104	-	40,41,41	0.63	0	47,50,50	1.93	11 (23%)
12	PGV	Y	104	-	42,42,50	0.98	2 (4%)	44,48,56	1.09	3 (6%)
16	LMT	4	102	-	28,28,36	0.46	0	39,39,47	0.77	1 (2%)
12	PGV	L	306	-	32,32,50	1.10	2 (6%)	35,38,56	1.18	3 (8%)
16	LMT	Q	101	-	24,24,36	0.44	0	29,29,47	0.97	1 (3%)
9	BCL	G	101	5	69,74,74	1.80	18 (26%)	83,115,115	2.35	21 (25%)
9	BCL	J	101	5	69,74,74	1.82	19 (27%)	83,115,115	2.47	24 (28%)
15	SPO	1	103	-	40,41,41	0.66	0	47,50,50	1.97	17 (36%)
12	PGV	M	812	-	37,37,50	1.05	2 (5%)	40,43,56	1.18	4 (10%)
9	BCL	Y	103	4	69,74,74	1.77	18 (26%)	83,115,115	2.56	26 (31%)
15	SPO	D	102	-	40,41,41	0.65	0	47,50,50	1.84	15 (31%)
12	PGV	3	102	-	50,50,50	0.90	2 (4%)	53,56,56	1.05	3 (5%)
16	LMT	I	102	-	28,28,36	0.43	0	39,39,47	0.71	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
16	LMT	A	702	-	36,36,36	0.39	0	47,47,47	0.74	1 (2%)
13	LDA	X	104	-	12,15,15	2.13	1 (8%)	14,17,17	0.50	0
17	CDL	H	304	-	60,60,99	1.18	4 (6%)	66,72,111	1.17	4 (6%)
9	BCL	4	101	5	69,74,74	1.82	17 (24%)	83,115,115	2.46	22 (26%)
9	BCL	S	102	4	69,74,74	1.79	18 (26%)	83,115,115	2.69	26 (31%)
9	BCL	P	102	5	69,74,74	1.77	19 (27%)	83,115,115	2.51	24 (28%)
12	PGV	L	310	-	44,44,50	1.00	2 (4%)	48,49,56	1.13	4 (8%)
9	BCL	3	103	4	69,74,74	1.80	18 (26%)	83,115,115	2.59	22 (26%)
16	LMT	F	105	-	17,17,36	0.45	0	22,22,47	0.57	0
16	LMT	1	104	-	24,25,36	0.61	1 (4%)	31,34,47	0.82	1 (3%)
9	BCL	2	101	5	69,74,74	1.78	18 (26%)	83,115,115	2.49	23 (27%)
9	BCL	O	101	4	69,74,74	1.77	17 (24%)	83,115,115	2.54	22 (26%)

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
15	SPO	O	102	-	-	5/47/47/47	-
15	SPO	V	102	-	-	3/47/47/47	-
12	PGV	X	101	-	-	8/43/43/55	-
9	BCL	8	102	5	-	14/33/129/137	-
15	SPO	K	103	-	-	4/47/47/47	-
12	PGV	L	305	-	-	13/43/43/55	-
9	BCL	Z	101	5	-	12/41/137/137	-
12	PGV	M	801	-	-	14/51/51/55	-
10	BPH	L	302	-	-	3/37/105/105	0/5/6/6
15	SPO	8	101	-	-	2/47/47/47	-
9	BCL	L	308	1	-	7/41/137/137	-
9	BCL	V	101	4	-	15/41/137/137	-
12	PGV	Q	103	-	-	9/43/43/55	-
16	LMT	M	808	-	-	2/19/39/61	0/1/1/2
12	PGV	H	307	-	-	13/51/51/55	-
15	SPO	W	102	-	-	10/47/47/47	-
9	BCL	A	703	4	-	12/35/131/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	SPO	P	101	-	-	8/47/47/47	-
12	PGV	H	306	-	-	14/44/44/55	-
12	PGV	K	104	-	-	14/40/42/55	-
17	CDL	Y	102	-	-	16/56/56/110	-
15	SPO	V	103	-	-	5/47/47/47	-
9	BCL	1	101	4	-	12/41/137/137	-
16	LMT	5	101	-	-	5/19/59/61	0/2/2/2
12	PGV	H	303	-	-	3/35/35/55	-
9	BCL	L	309	2	-	12/41/137/137	-
15	SPO	1	105	-	-	6/47/47/47	-
9	BCL	F	102	4	-	9/41/137/137	-
16	LMT	H	301	-	-	4/21/61/61	0/2/2/2
16	LMT	A	704	-	-	0/13/53/61	0/2/2/2
9	BCL	E	102	5	-	13/41/137/137	-
15	SPO	G	102	-	-	7/47/47/47	-
9	BCL	Q	104	4	-	17/41/137/137	-
13	LDA	X	103	-	-	1/10/10/13	-
15	SPO	F	104	-	-	1/47/47/47	-
16	LMT	Q	102	-	-	2/11/31/61	0/1/1/2
16	LMT	3	101	-	-	7/21/61/61	0/2/2/2
16	LMT	S	101	-	-	4/17/37/61	0/1/1/2
13	LDA	L	311	-	-	2/13/13/13	-
9	BCL	6	101	5	-	16/41/137/137	-
16	LMT	K	101	-	-	2/21/61/61	0/2/2/2
16	LMT	S	105	-	-	5/16/56/61	0/2/2/2
16	LMT	X	105	-	-	4/17/57/61	0/2/2/2
15	SPO	F	103	-	-	4/47/47/47	-
10	BPH	M	804	-	-	6/37/105/105	0/5/6/6
9	BCL	I	101	4	-	10/41/137/137	-
15	SPO	5	103	-	-	5/47/47/47	-
9	BCL	L	301	1	-	20/41/137/137	-
16	LMT	D	103	-	-	2/13/53/61	0/2/2/2
9	BCL	5	102	6	-	12/41/137/137	-
15	SPO	G	103	-	-	6/47/47/47	-
9	BCL	R	102	5	-	13/41/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	LMT	M	809	-	-	8/21/61/61	0/2/2/2
9	BCL	M	803	2	-	10/41/137/137	-
15	SPO	N	101	-	-	9/47/47/47	-
15	SPO	O	103	-	-	10/47/47/47	-
9	BCL	B	101	5	-	7/41/137/137	-
15	SPO	S	103	-	-	6/47/47/47	-
15	SPO	X	102	-	-	4/47/47/47	-
15	SPO	3	104	-	-	4/47/47/47	-
16	LMT	M	810	-	-	7/19/59/61	0/2/2/2
13	LDA	L	307	-	-	4/13/13/13	-
16	LMT	A	701	-	-	5/21/61/61	0/2/2/2
15	SPO	R	101	-	-	7/47/47/47	-
11	U10	L	303	-	-	9/30/54/87	0/1/1/1
15	SPO	T	102	-	-	7/47/47/47	-
9	BCL	7	101	6	-	15/41/137/137	-
16	LMT	U	102	-	-	3/21/61/61	0/2/2/2
17	CDL	H	305	-	-	8/37/37/110	-
9	BCL	N	102	5	-	14/41/137/137	-
11	U10	L	304	-	-	5/30/54/87	0/1/1/1
11	U10	M	806	-	-	1/45/69/87	0/1/1/1
13	LDA	M	802	-	-	2/13/13/13	-
16	LMT	U	101	-	-	1/18/58/61	0/2/2/2
16	LMT	H	302	-	-	6/16/56/61	0/2/2/2
15	SPO	S	104	-	-	10/47/47/47	-
9	BCL	D	101	4	-	9/41/137/137	-
13	LDA	Y	101	-	-	1/9/9/13	-
17	CDL	M	811	-	-	30/89/89/110	-
9	BCL	W	101	5	-	19/41/137/137	-
16	LMT	F	101	-	-	5/11/51/61	0/2/2/2
15	SPO	1	102	-	-	5/47/47/47	-
9	BCL	K	102	4	-	11/41/137/137	-
15	SPO	M	807	-	-	8/47/47/47	-
15	SPO	E	101	-	-	6/47/47/47	-
9	BCL	T	101	5	-	13/41/137/137	-
15	SPO	5	104	-	-	8/47/47/47	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	PGV	Y	104	-	-	13/47/47/55	-
16	LMT	4	102	-	-	2/13/53/61	0/2/2/2
12	PGV	L	306	-	-	13/37/37/55	-
16	LMT	Q	101	-	-	2/15/35/61	0/1/1/2
9	BCL	G	101	5	-	15/41/137/137	-
9	BCL	J	101	5	-	14/41/137/137	-
15	SPO	1	103	-	-	4/47/47/47	-
12	PGV	M	812	-	-	19/42/42/55	-
9	BCL	Y	103	4	-	15/41/137/137	-
15	SPO	D	102	-	-	2/47/47/47	-
12	PGV	3	102	-	-	10/55/55/55	-
16	LMT	I	102	-	-	3/13/53/61	0/2/2/2
16	LMT	A	702	-	-	6/21/61/61	0/2/2/2
13	LDA	X	104	-	-	0/13/13/13	-
17	CDL	H	304	-	-	23/71/71/110	-
9	BCL	4	101	5	-	9/41/137/137	-
9	BCL	S	102	4	-	15/41/137/137	-
9	BCL	P	102	5	-	15/41/137/137	-
12	PGV	L	310	-	-	7/46/46/55	-
9	BCL	3	103	4	-	11/41/137/137	-
16	LMT	F	105	-	-	1/9/29/61	0/1/1/2
16	LMT	1	104	-	-	2/11/44/61	0/2/2/2
9	BCL	2	101	5	-	15/41/137/137	-
9	BCL	O	101	4	-	12/41/137/137	-

The worst 5 of 633 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	X	104	LDA	O1-N1	-7.33	1.25	1.42
13	X	103	LDA	O1-N1	-7.27	1.25	1.42
13	L	311	LDA	O1-N1	-7.19	1.25	1.42
13	L	307	LDA	O1-N1	-7.19	1.25	1.42
13	Y	101	LDA	O1-N1	-7.18	1.25	1.42

The worst 5 of 1240 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	7	101	BCL	C2B-C1B-NB	11.02	117.62	110.23
9	5	102	BCL	C2B-C1B-NB	10.99	117.60	110.23
9	O	101	BCL	C2B-C1B-NB	10.77	117.45	110.23
9	I	101	BCL	C2B-C1B-NB	10.74	117.43	110.23
9	3	103	BCL	C2B-C1B-NB	10.58	117.32	110.23

There are no chirality outliers.

5 of 918 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	L	301	BCL	C2C-C3C-CAC-CBC
9	L	301	BCL	C4C-C3C-CAC-CBC
9	A	703	BCL	C2A-CAA-CBA-CGA
9	B	101	BCL	C1A-C2A-CAA-CBA
9	B	101	BCL	C3A-C2A-CAA-CBA

There are no ring outliers.

99 monomers are involved in 325 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	O	102	SPO	8	0
15	V	102	SPO	4	0
12	X	101	PGV	3	0
9	8	102	BCL	6	0
15	K	103	SPO	6	0
12	L	305	PGV	4	0
9	Z	101	BCL	2	0
12	M	801	PGV	2	0
10	L	302	BPH	5	0
15	8	101	SPO	5	0
9	L	308	BCL	6	0
9	V	101	BCL	7	0
12	Q	103	PGV	1	0
16	M	808	LMT	2	0
12	H	307	PGV	3	0
15	W	102	SPO	4	0
9	A	703	BCL	2	0
15	P	101	SPO	2	0
12	H	306	PGV	3	0
12	K	104	PGV	3	0
17	Y	102	CDL	2	0
15	V	103	SPO	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	1	101	BCL	4	0
16	5	101	LMT	2	0
9	L	309	BCL	3	0
15	1	105	SPO	7	0
9	F	102	BCL	2	0
16	H	301	LMT	1	0
16	A	704	LMT	1	0
9	E	102	BCL	6	0
15	G	102	SPO	7	0
9	Q	104	BCL	1	0
13	X	103	LDA	2	0
15	F	104	SPO	3	0
16	Q	102	LMT	1	0
16	3	101	LMT	4	0
16	S	101	LMT	1	0
13	L	311	LDA	2	0
9	6	101	BCL	3	0
16	K	101	LMT	2	0
16	S	105	LMT	1	0
15	F	103	SPO	4	0
10	M	804	BPH	6	0
9	I	101	BCL	6	0
15	5	103	SPO	5	0
9	L	301	BCL	7	0
9	5	102	BCL	6	0
15	G	103	SPO	8	0
9	R	102	BCL	3	0
16	M	809	LMT	2	0
9	M	803	BCL	3	0
15	N	101	SPO	8	0
15	O	103	SPO	4	0
9	B	101	BCL	8	0
15	S	103	SPO	6	0
15	X	102	SPO	4	0
15	3	104	SPO	2	0
16	M	810	LMT	2	0
16	A	701	LMT	1	0
15	R	101	SPO	6	0
11	L	303	U10	3	0
15	T	102	SPO	10	0
9	7	101	BCL	6	0
16	U	102	LMT	2	0

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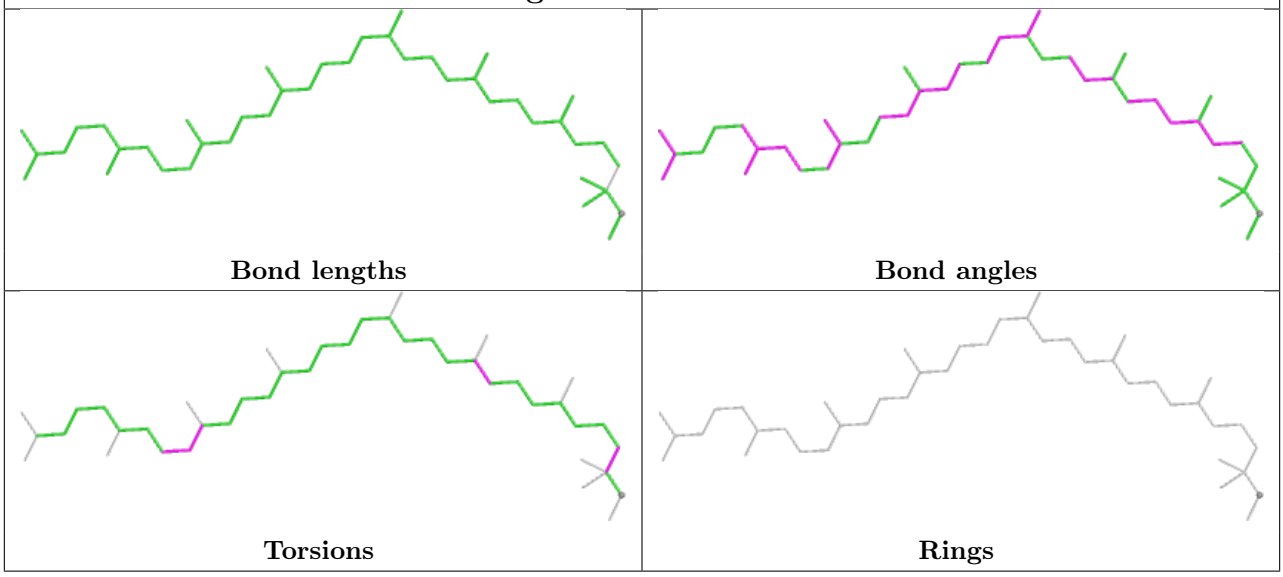
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	N	102	BCL	1	0
11	L	304	U10	4	0
11	M	806	U10	2	0
16	H	302	LMT	4	0
15	S	104	SPO	5	0
9	D	101	BCL	4	0
13	Y	101	LDA	5	0
17	M	811	CDL	6	0
9	W	101	BCL	6	0
15	1	102	SPO	3	0
9	K	102	BCL	5	0
15	M	807	SPO	4	0
15	E	101	SPO	3	0
9	T	101	BCL	5	0
15	5	104	SPO	7	0
12	Y	104	PGV	7	0
12	L	306	PGV	3	0
16	Q	101	LMT	3	0
9	G	101	BCL	2	0
9	J	101	BCL	3	0
15	1	103	SPO	4	0
12	M	812	PGV	4	0
9	Y	103	BCL	6	0
15	D	102	SPO	3	0
12	3	102	PGV	1	0
16	A	702	LMT	5	0
13	X	104	LDA	1	0
17	H	304	CDL	6	0
9	4	101	BCL	3	0
9	S	102	BCL	4	0
9	P	102	BCL	2	0
12	L	310	PGV	1	0
9	3	103	BCL	3	0
9	2	101	BCL	4	0
9	O	101	BCL	4	0

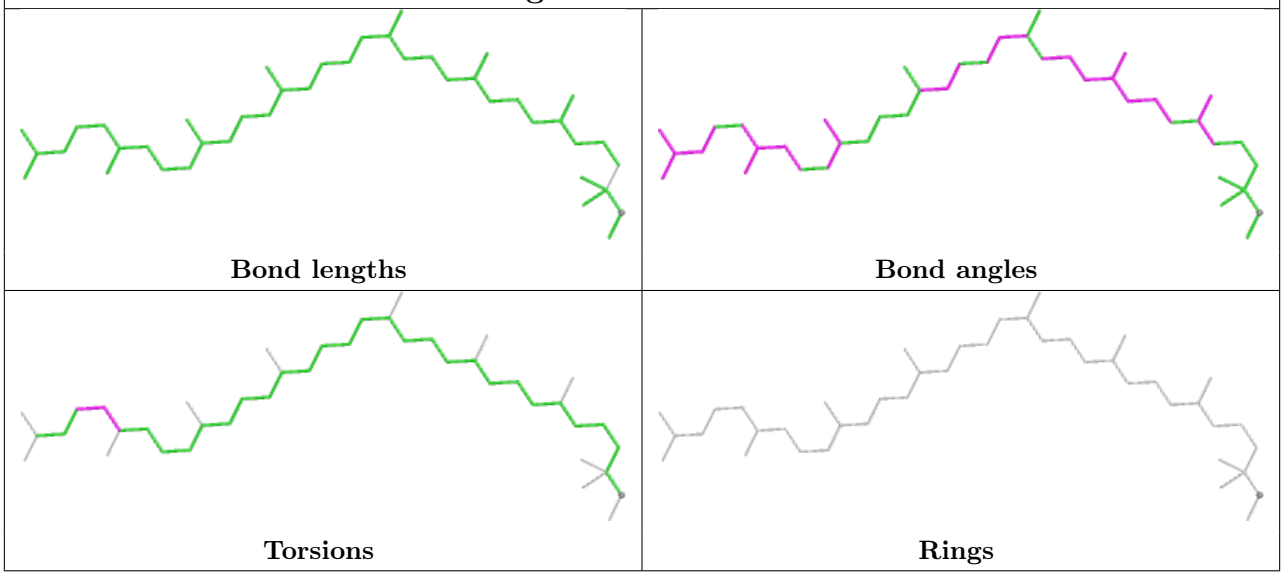
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

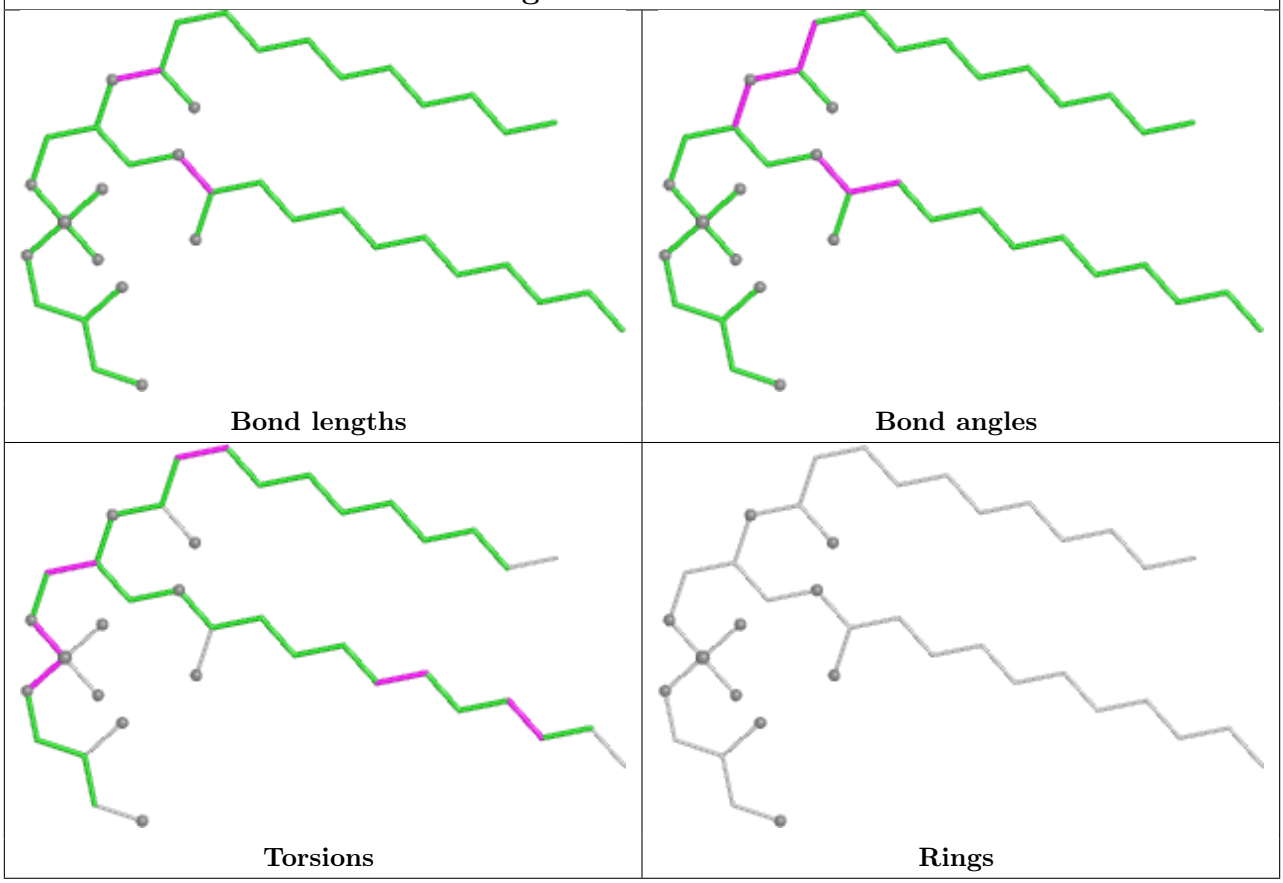
Ligand SPO O 102



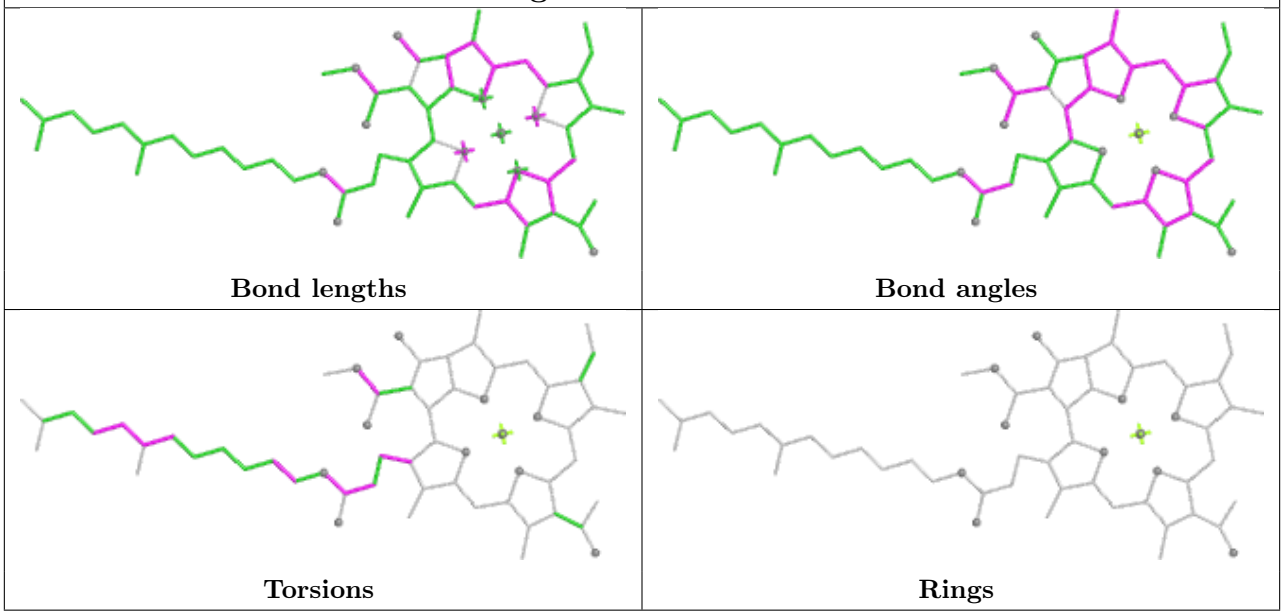
Ligand SPO V 102



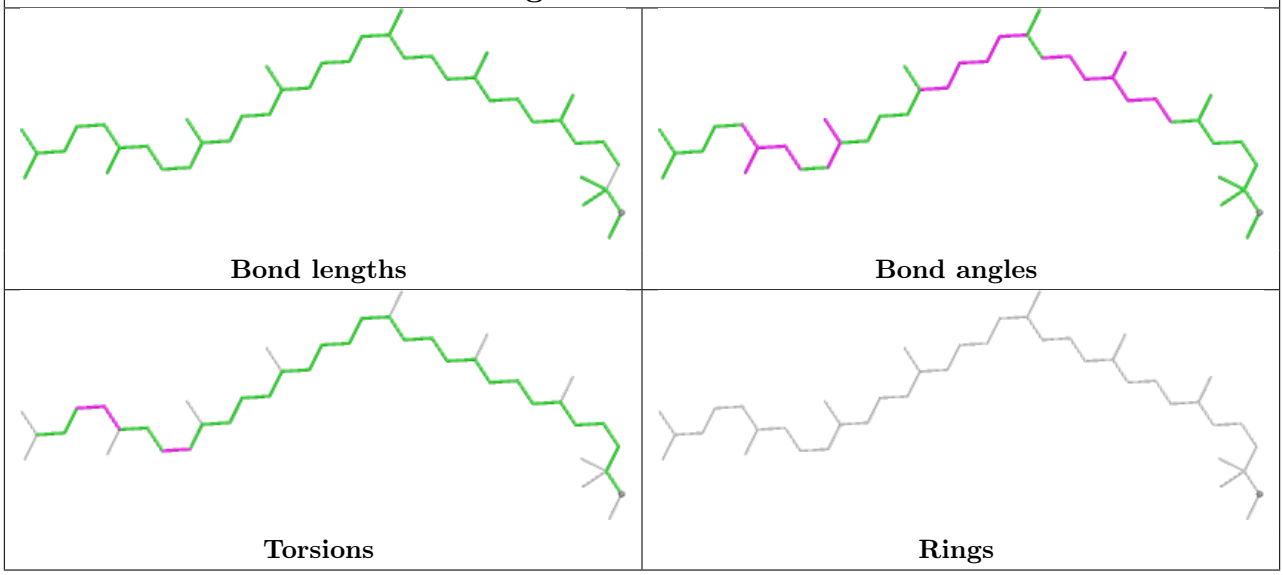
Ligand PGV X 101



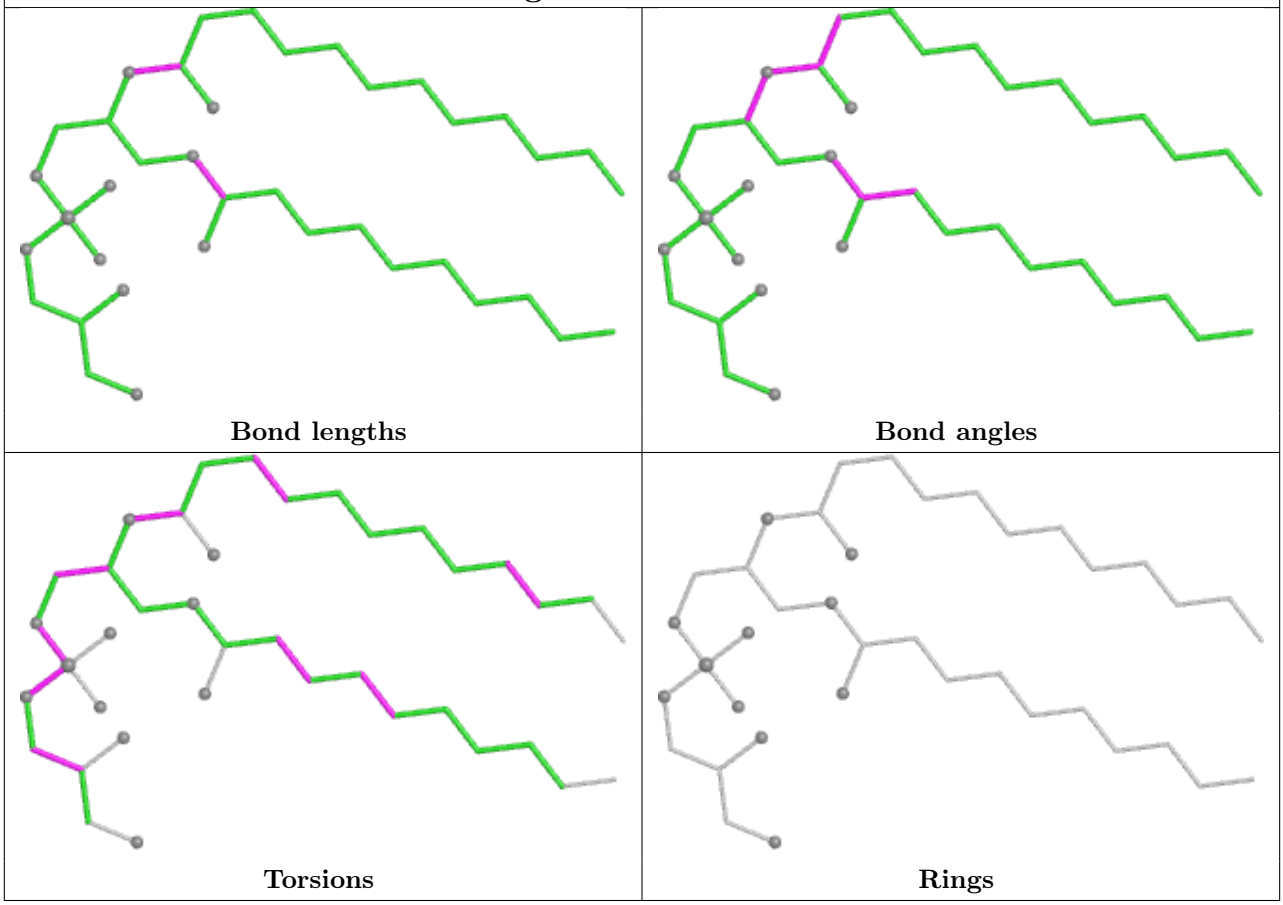
Ligand BCL 8 102

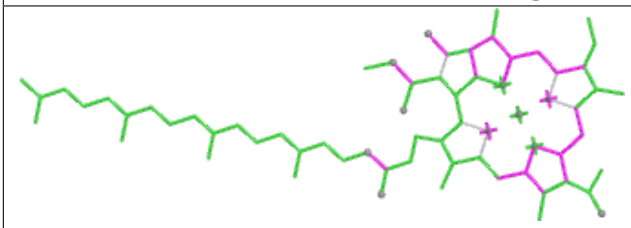
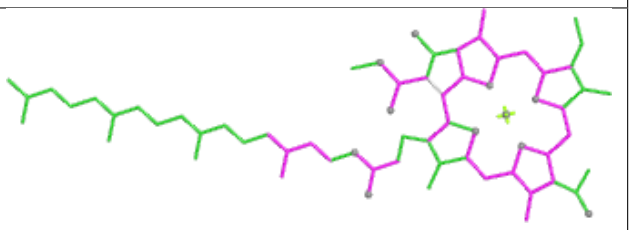
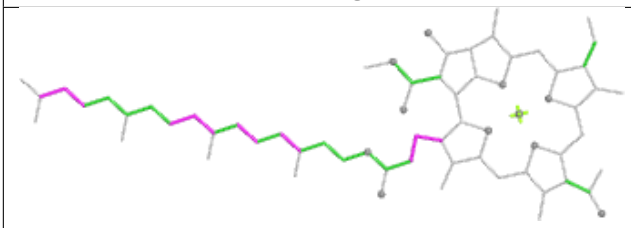
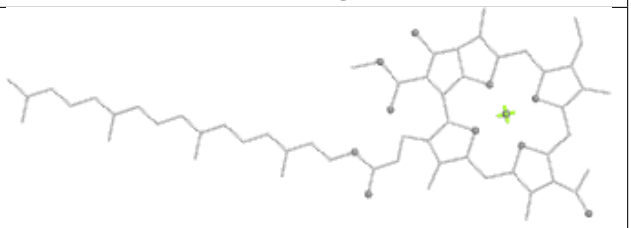


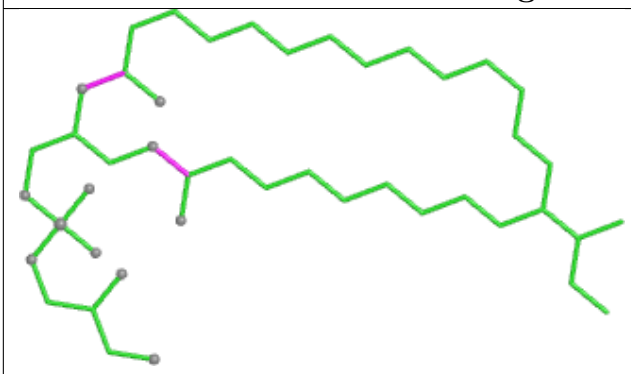
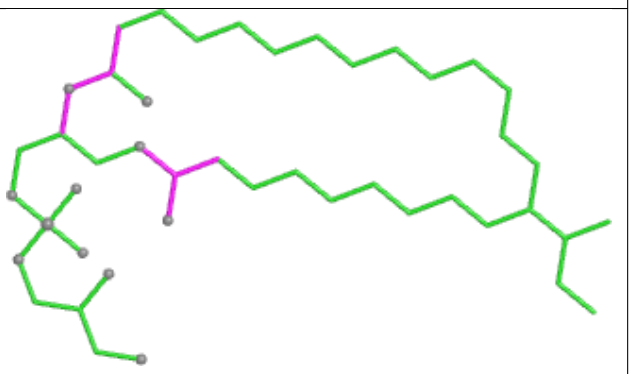
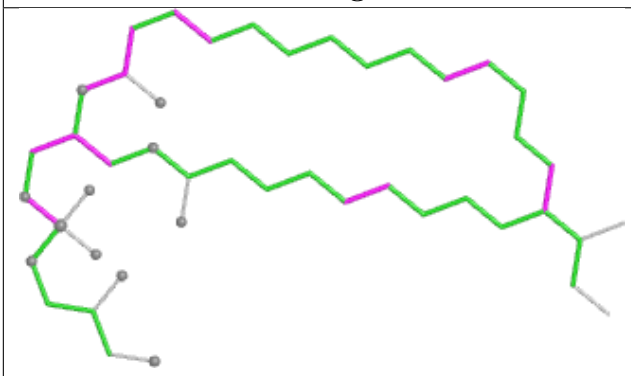
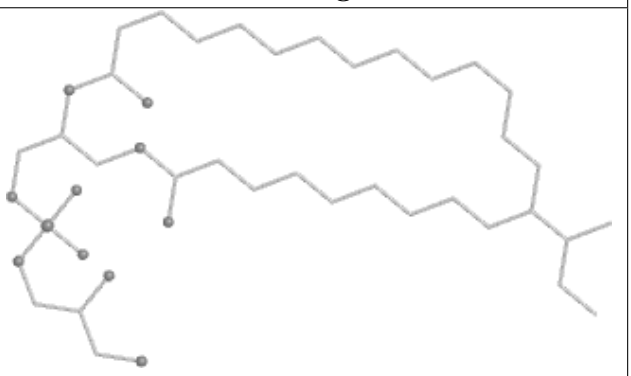
Ligand SPO K 103



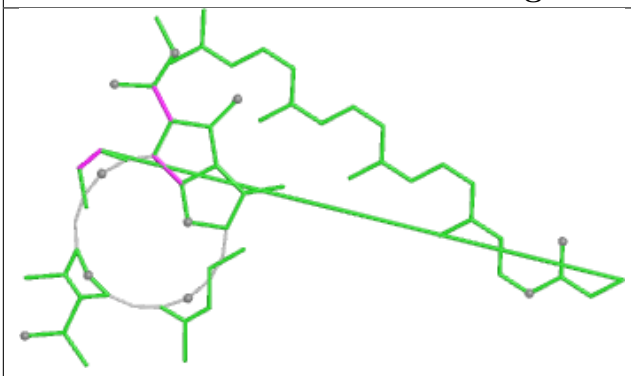
Ligand PGV L 305



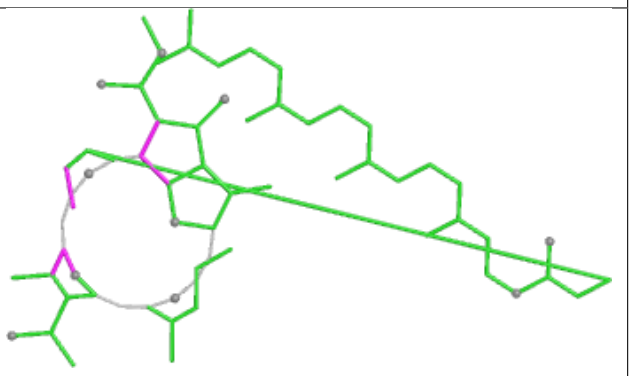
Ligand BCL Z 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PGV M 801	
 Bond lengths	 Bond angles
 Torsions	 Rings

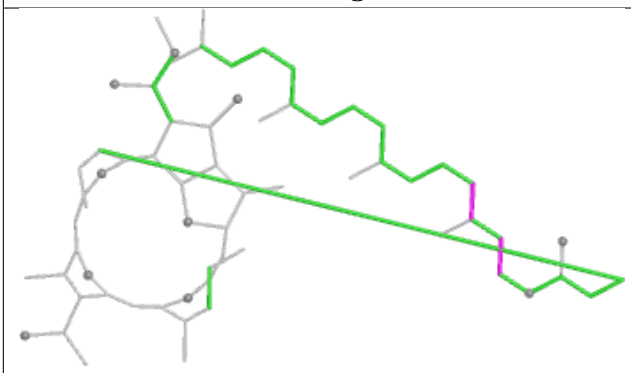
Ligand BPH L 302



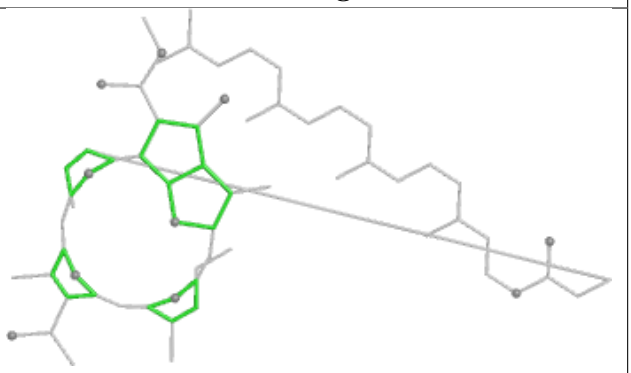
Bond lengths



Bond angles

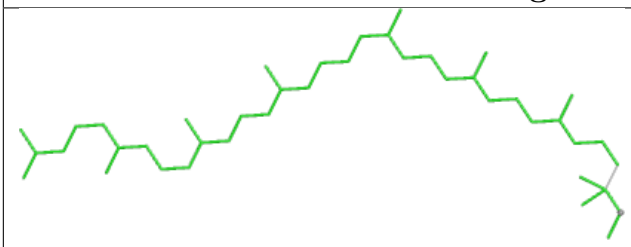


Torsions



Rings

Ligand SPO 8 101



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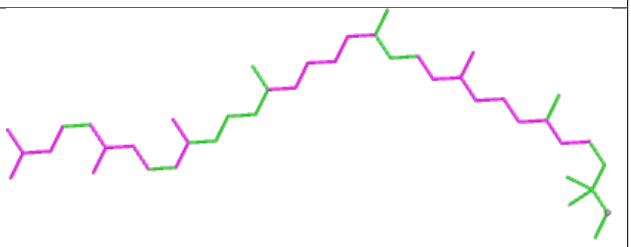

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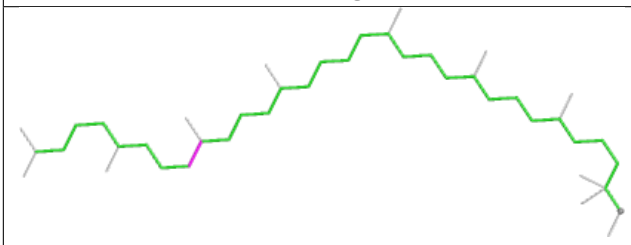

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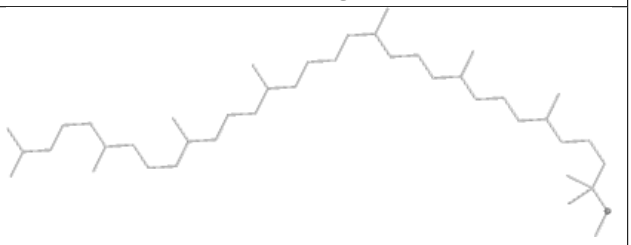
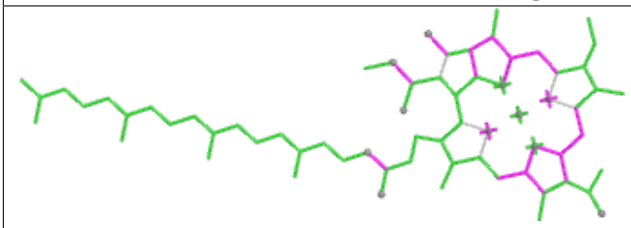
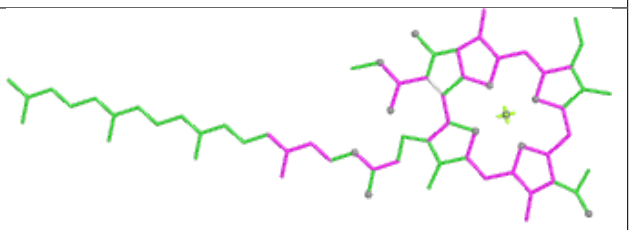
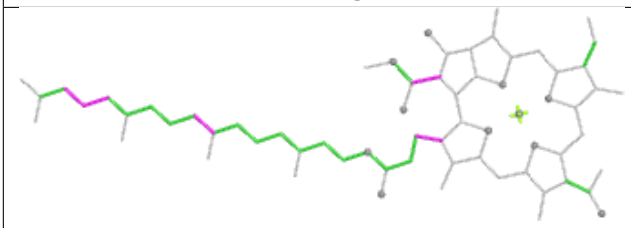
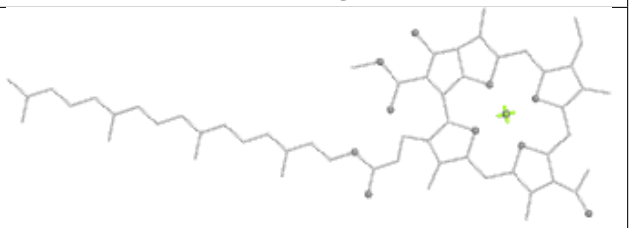
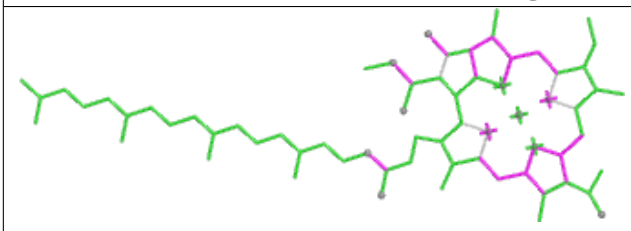
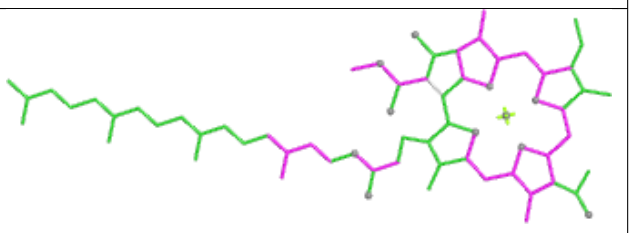
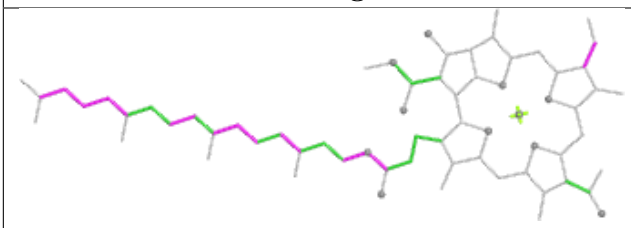
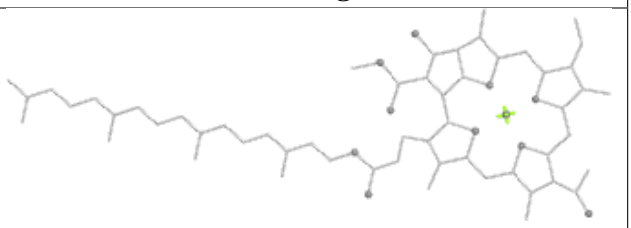
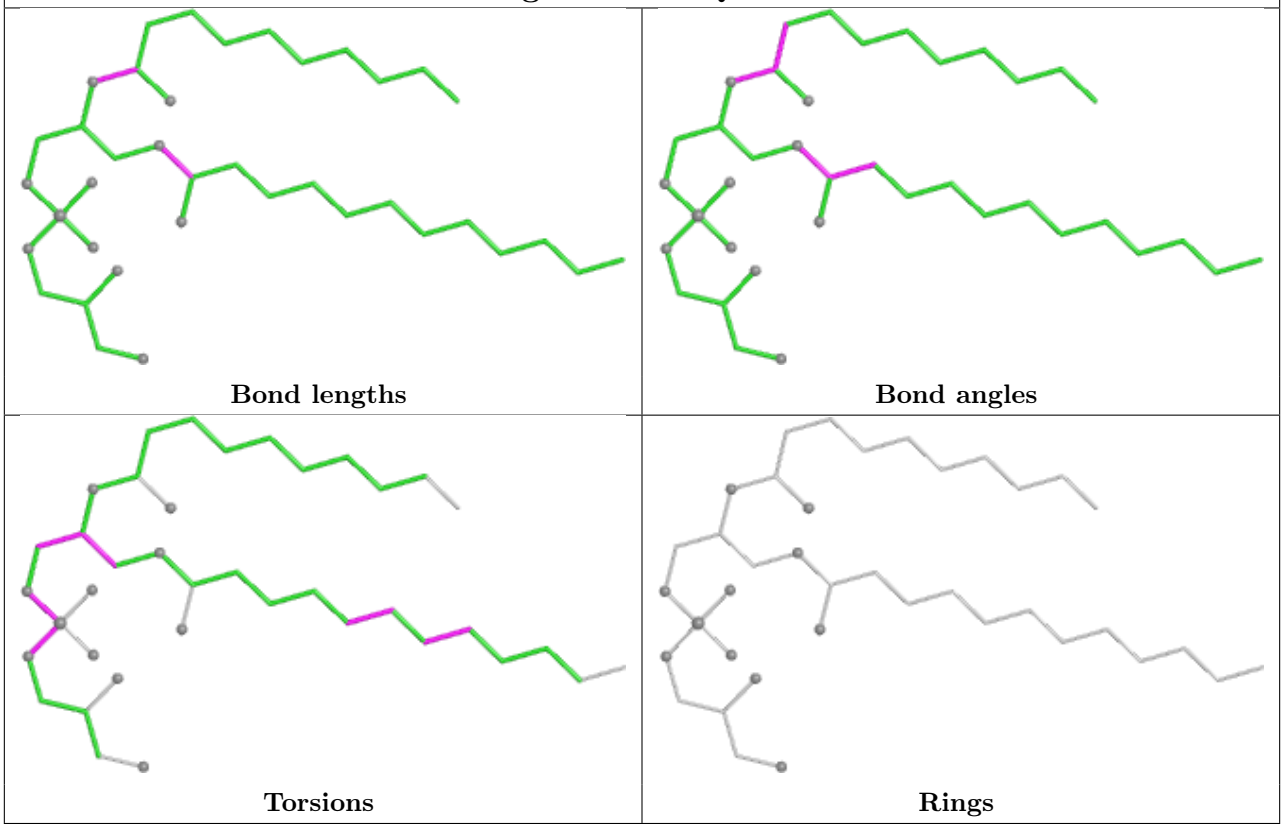


Rings

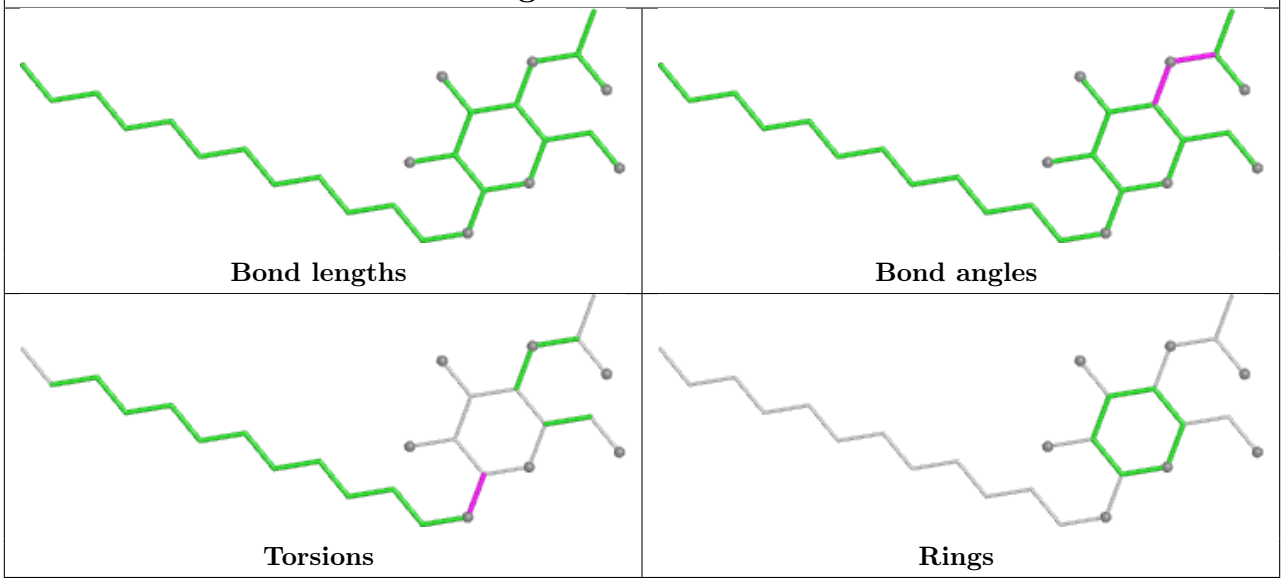
Ligand BCL L 308	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCL V 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

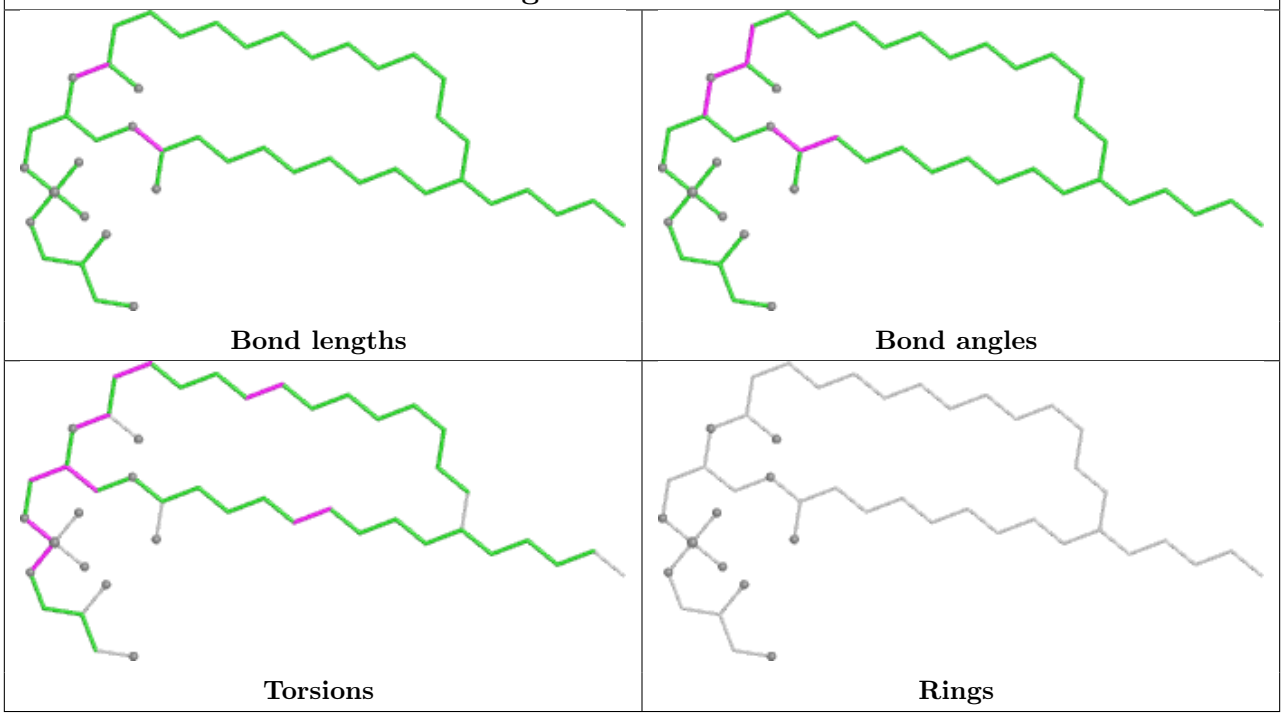
Ligand PGV Q 103



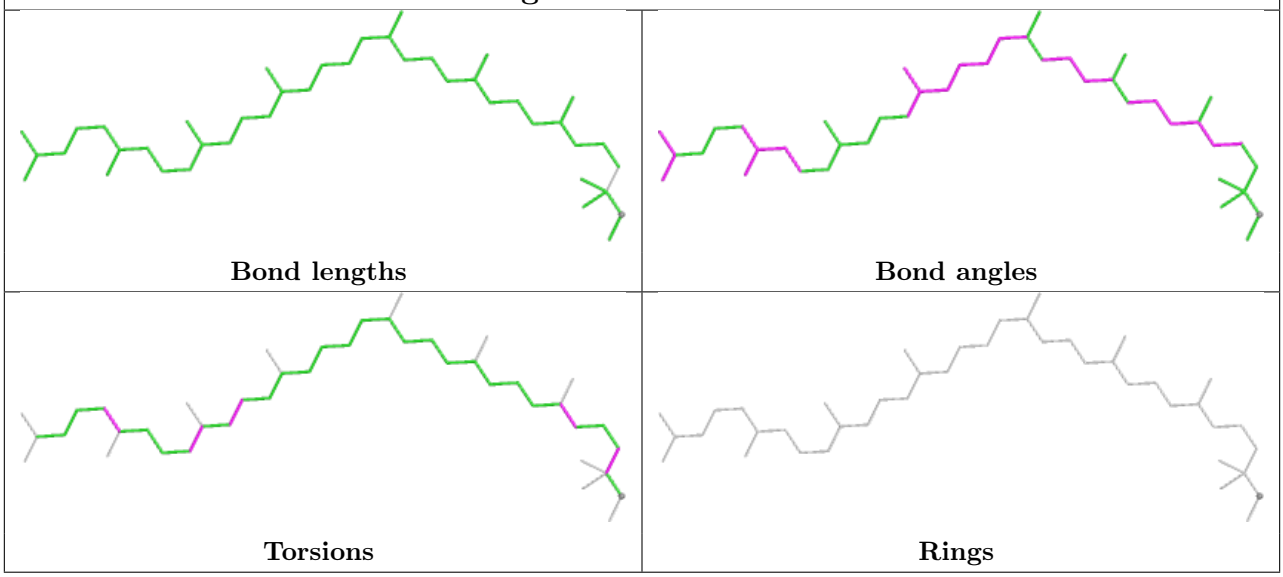
Ligand LMT M 808



Ligand PGV H 307



Ligand SPO W 102



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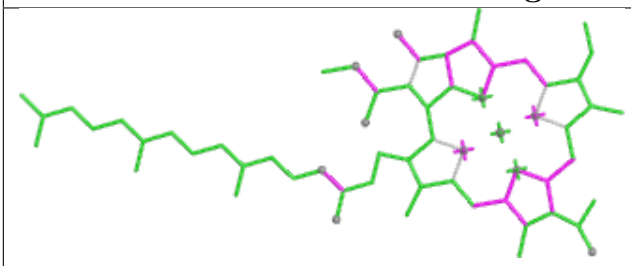
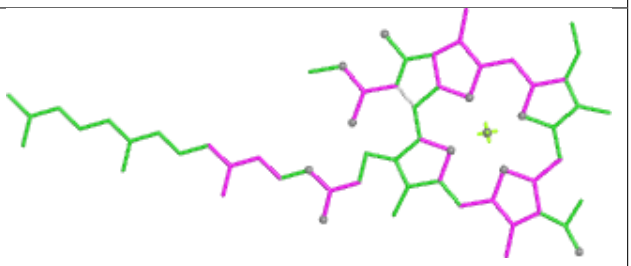
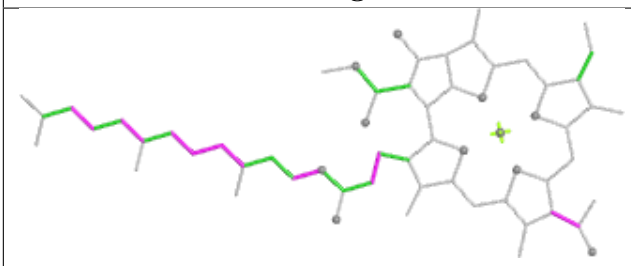
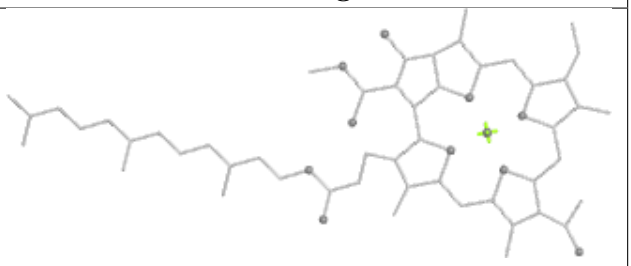
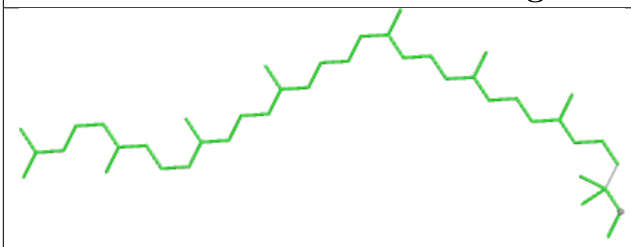
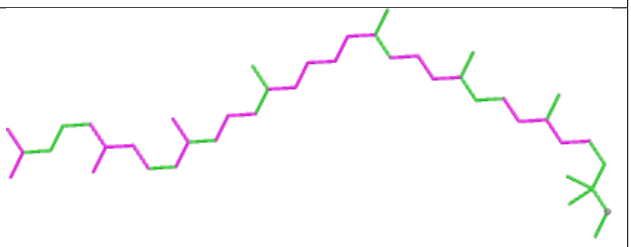
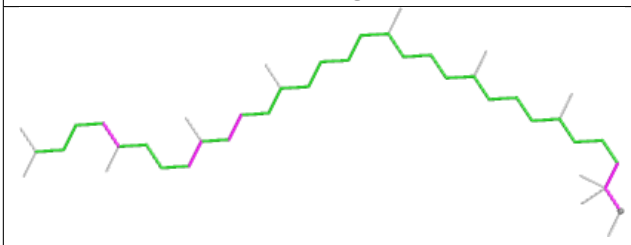
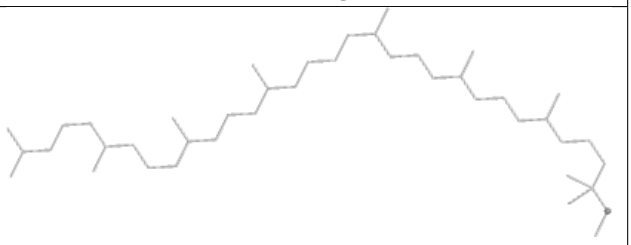
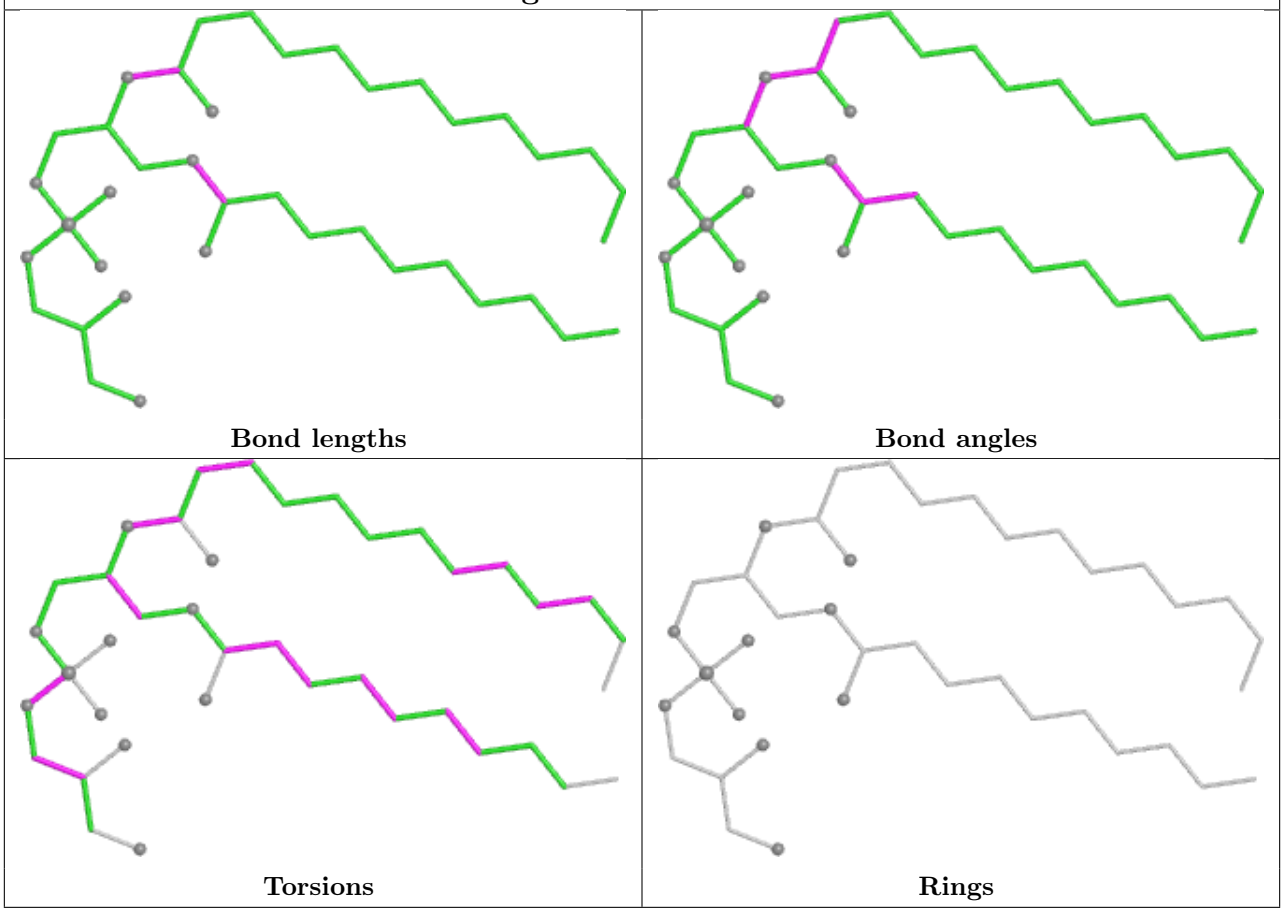
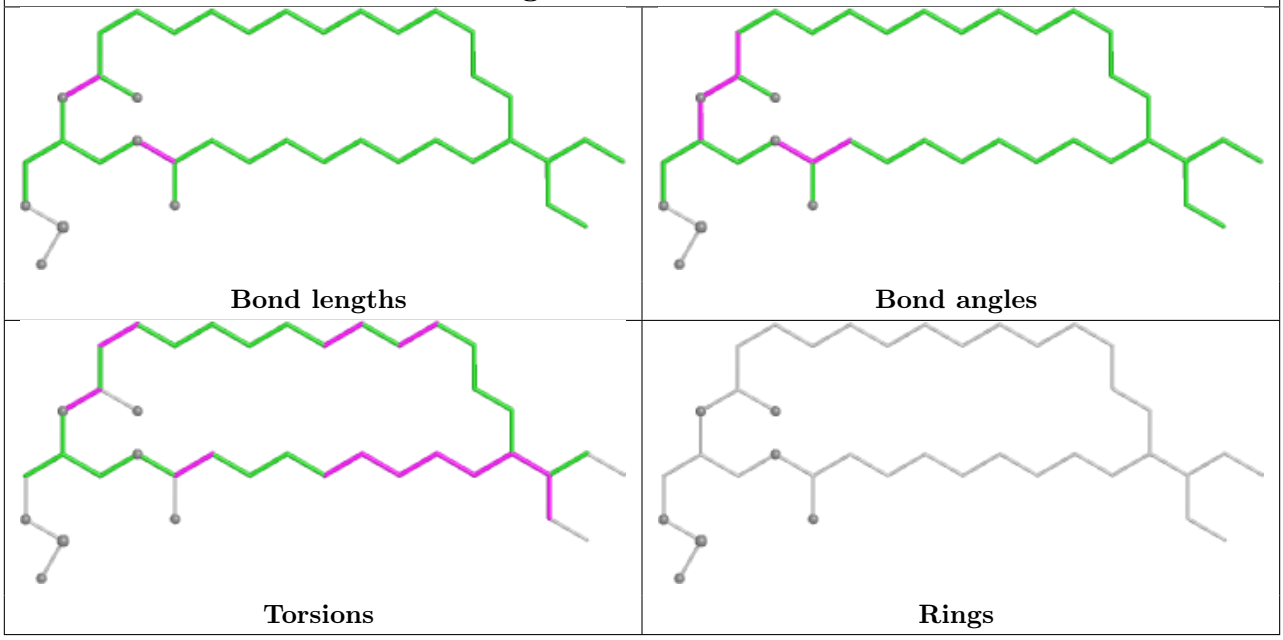
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand SPO P 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

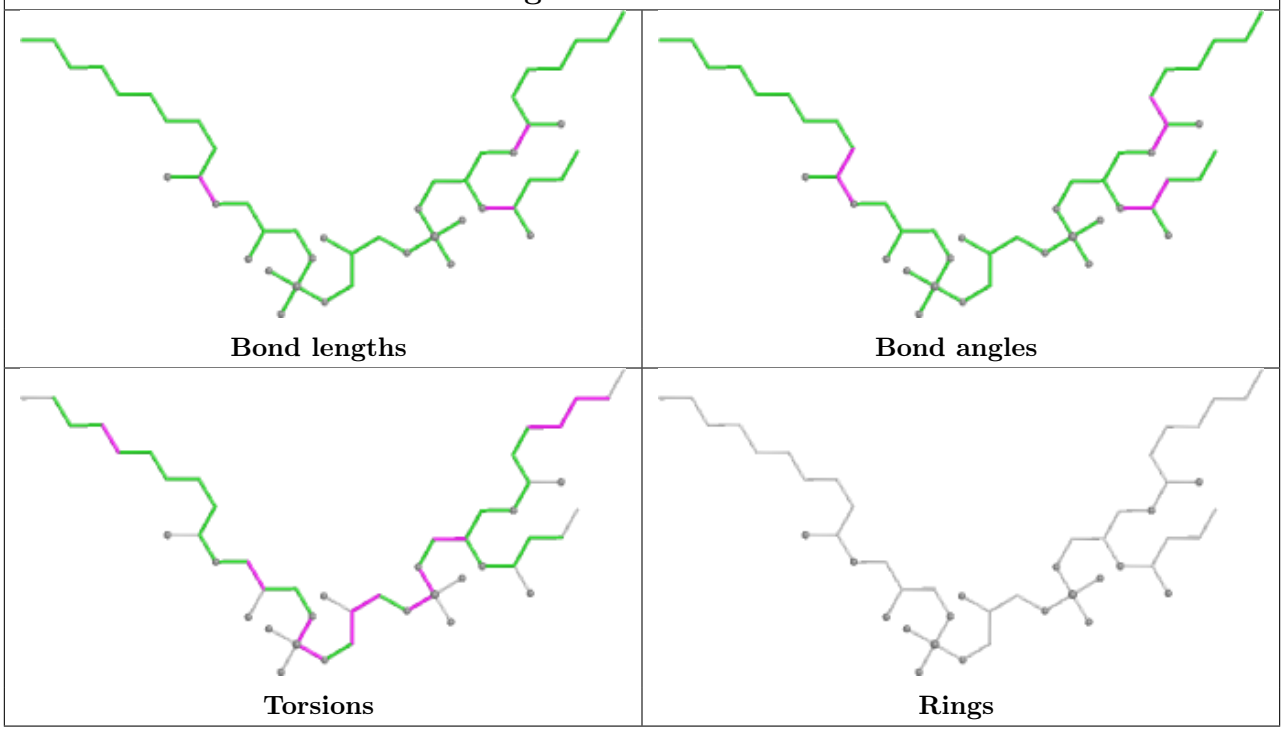
Ligand PGV H 306



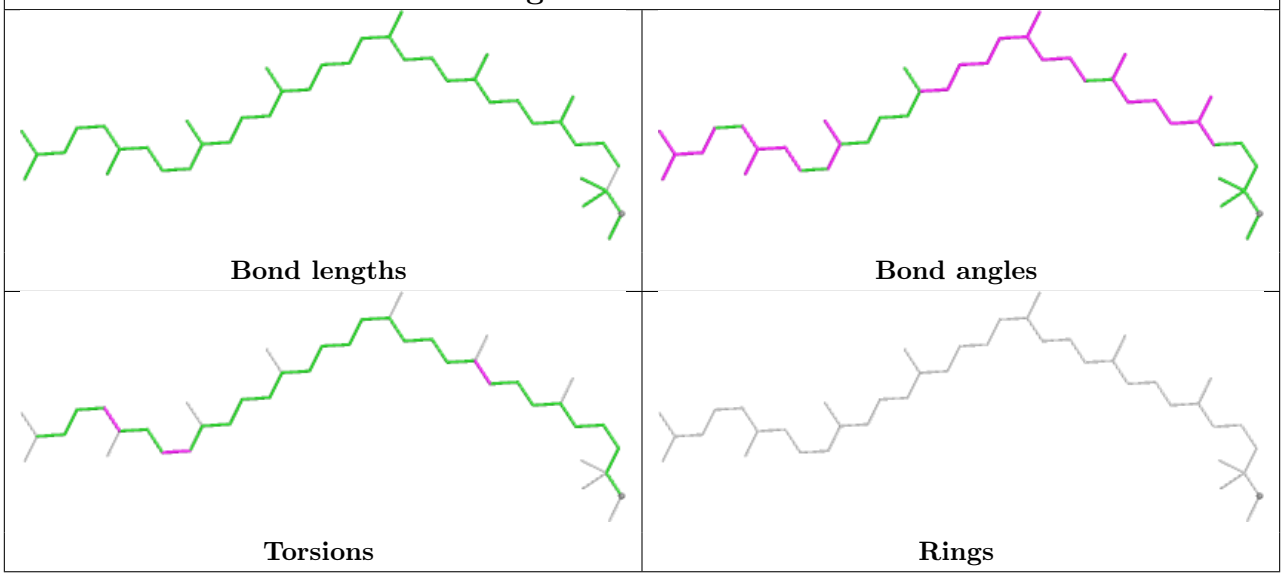
Ligand PGV K 104



Ligand CDL Y 102



Ligand SPO V 103



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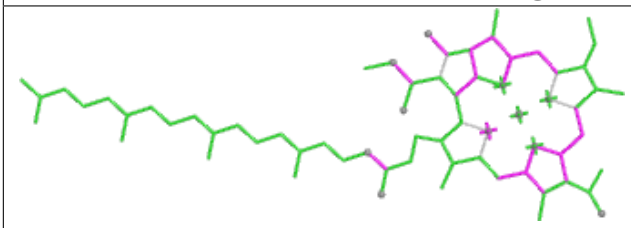
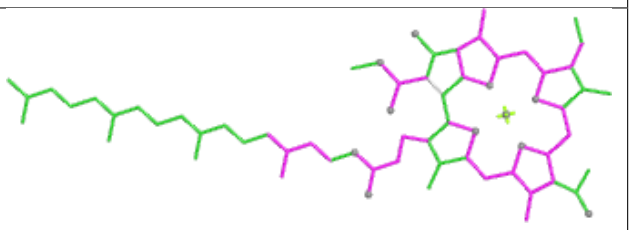
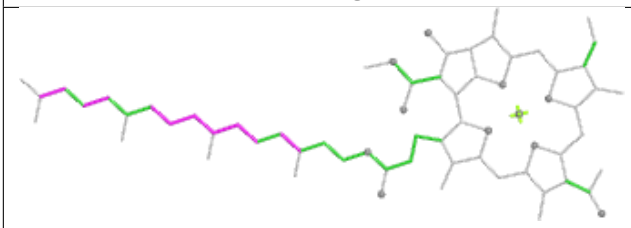
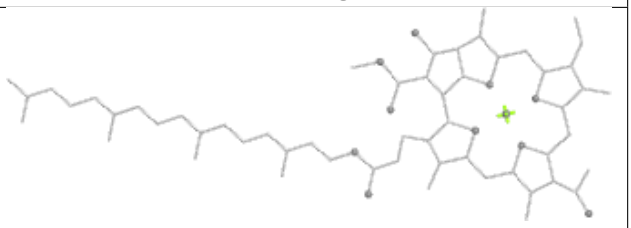
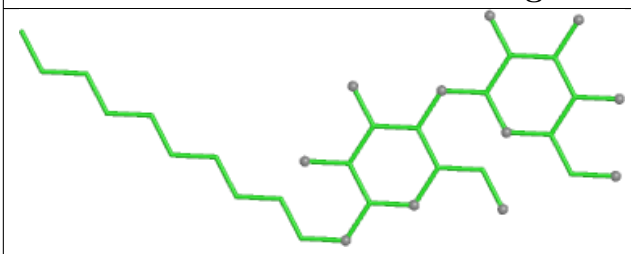
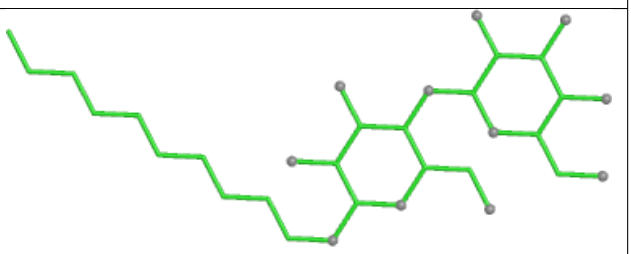
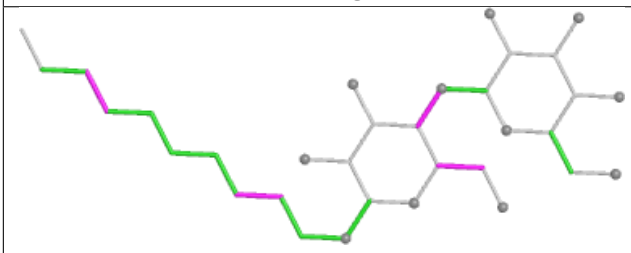
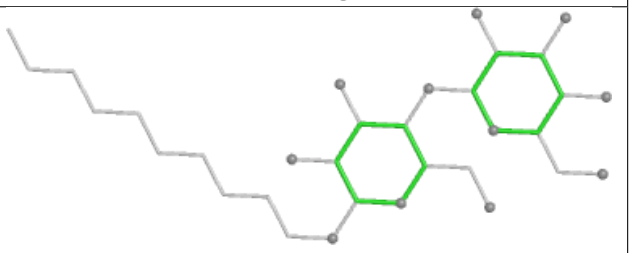
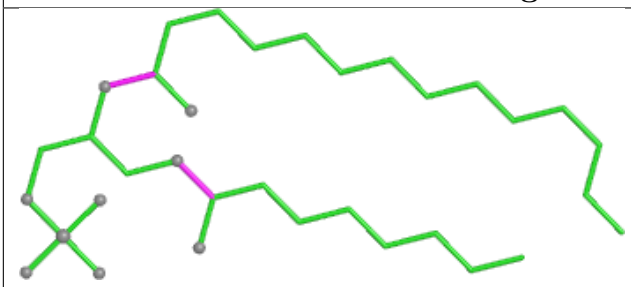
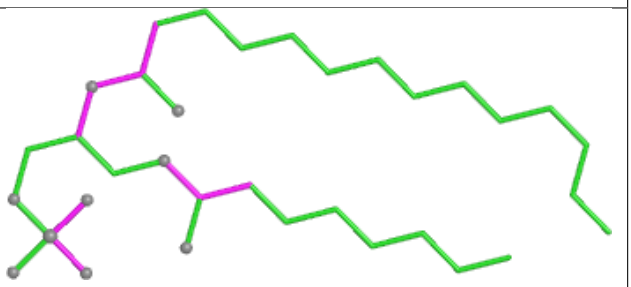
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LMT 5 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

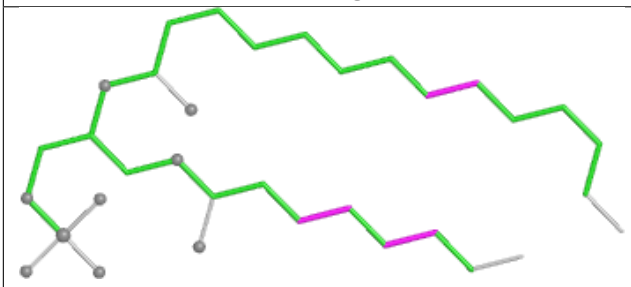
Ligand PGV H 303



Bond lengths



Bond angles



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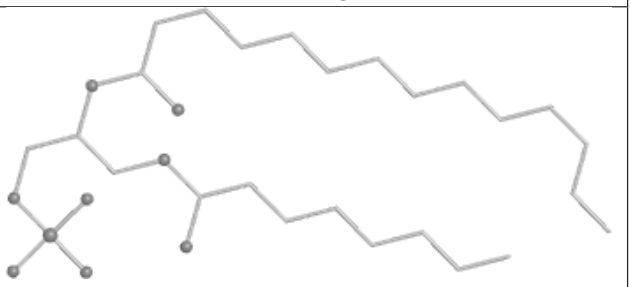
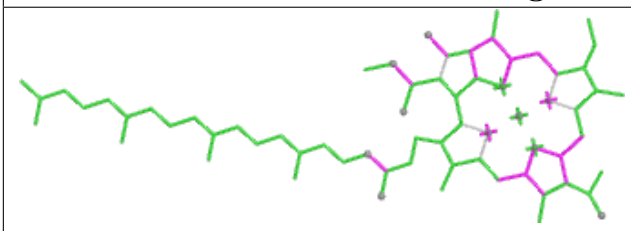


Rings

Ligand BCL L 309



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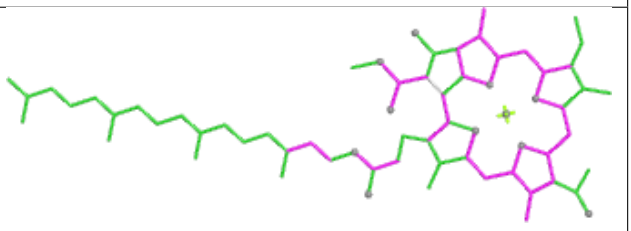
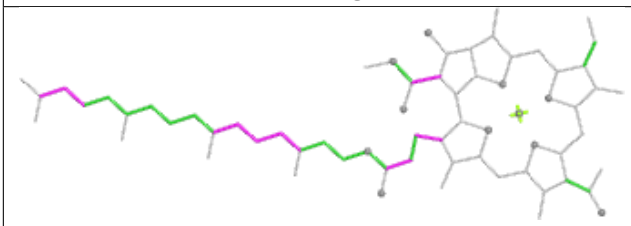


Bond angles



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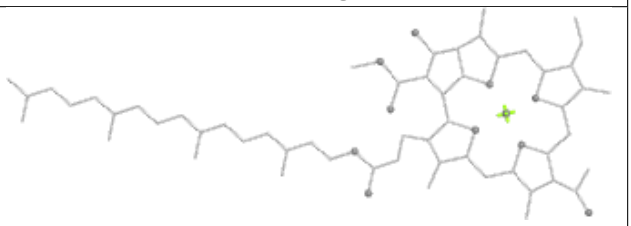
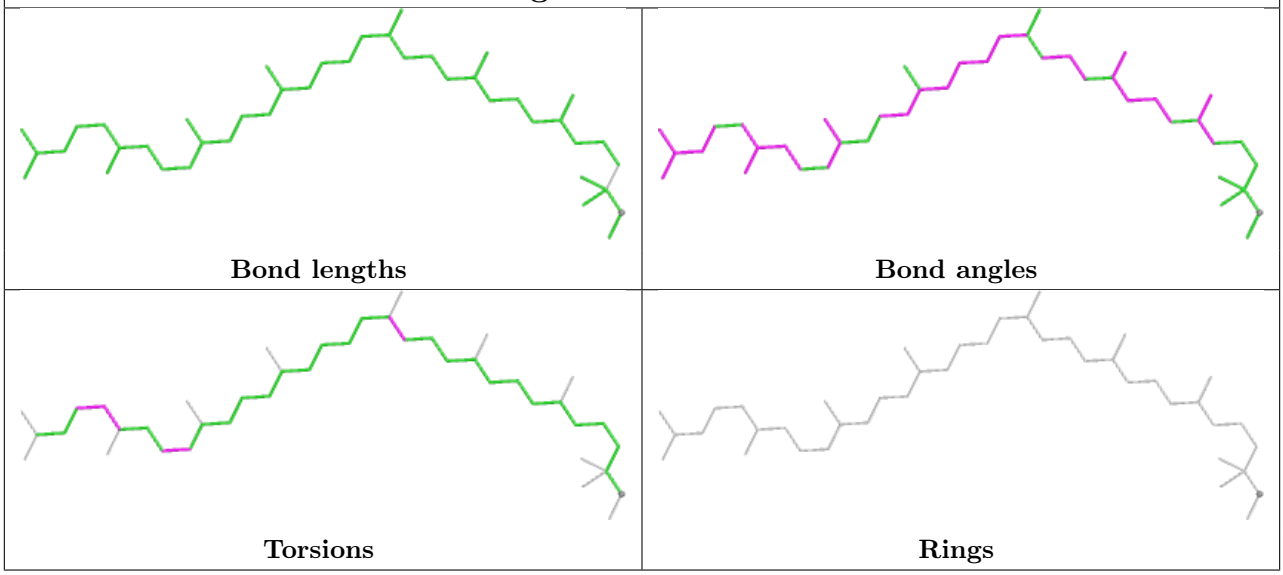
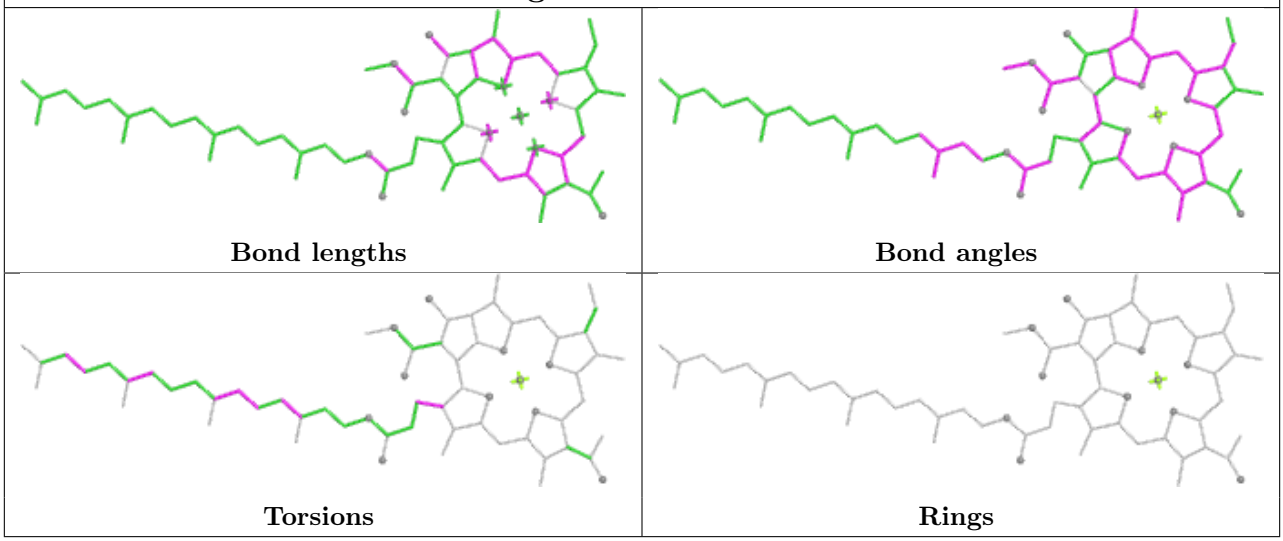


Rings

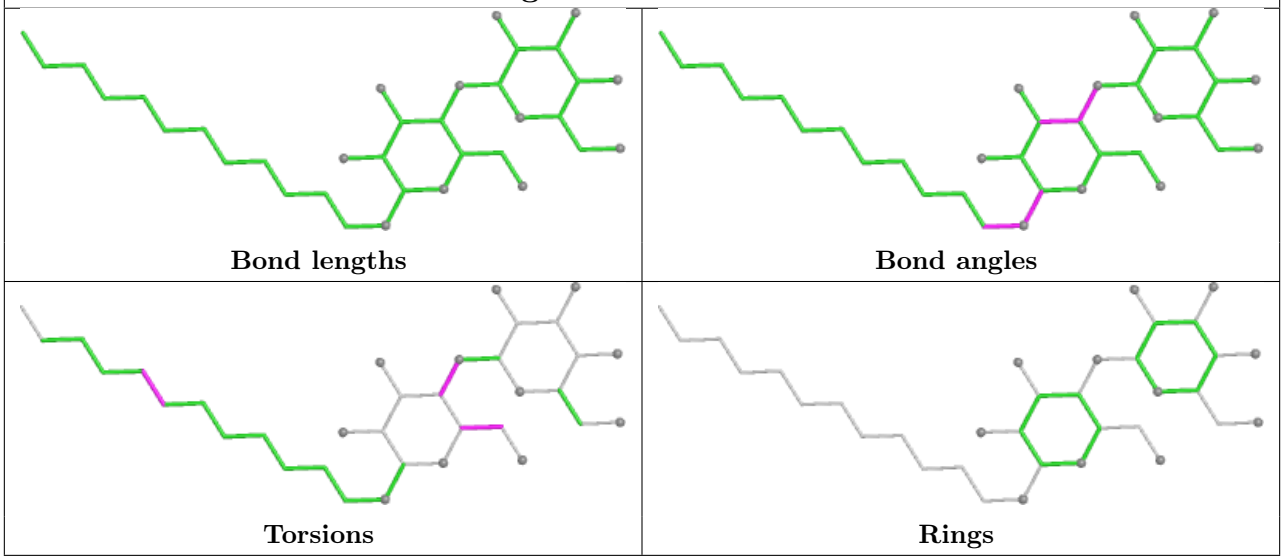
Ligand SPO 1 105



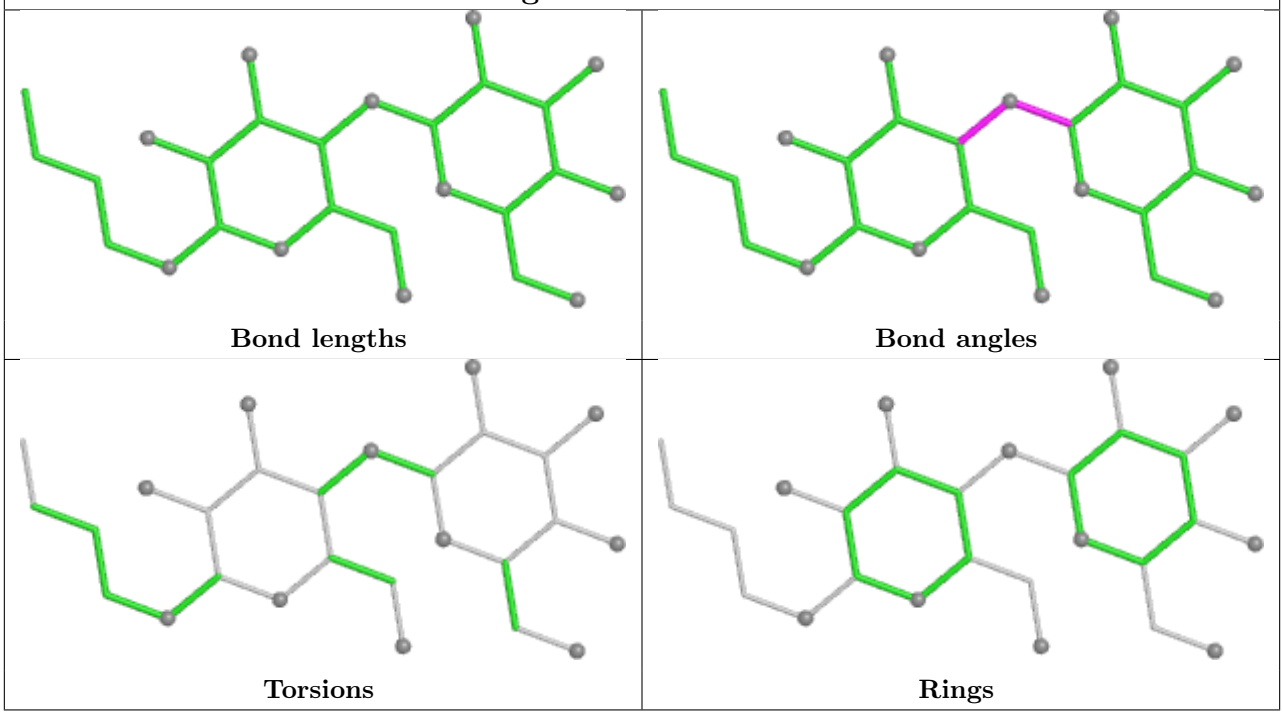
Ligand BCL F 102



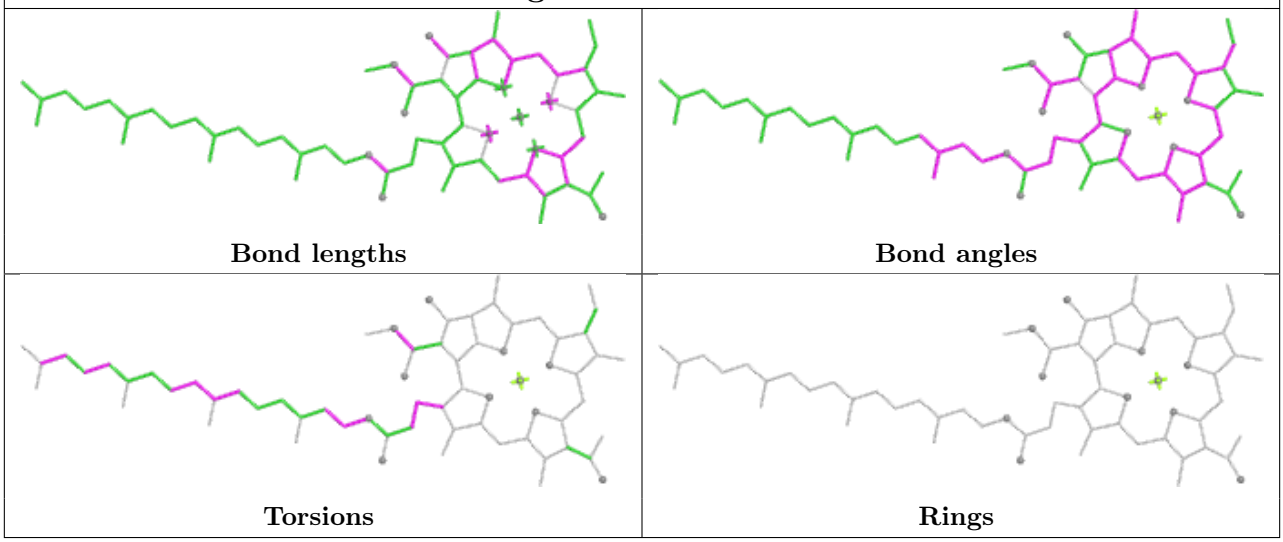
Ligand LMT H 301

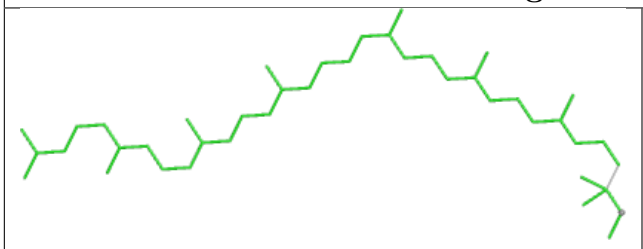
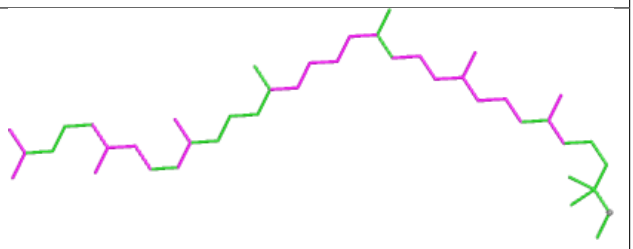
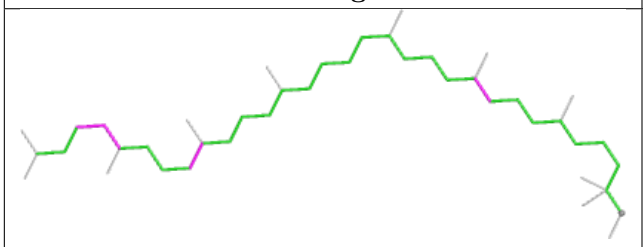
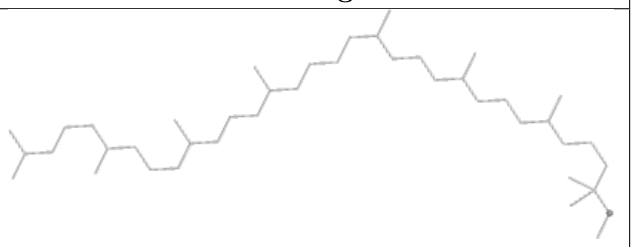


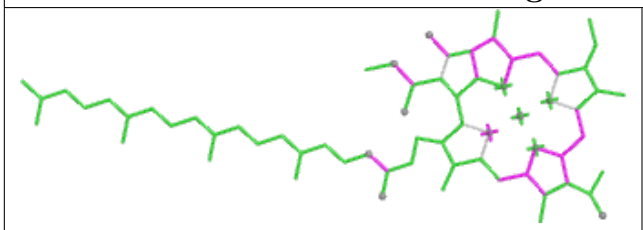
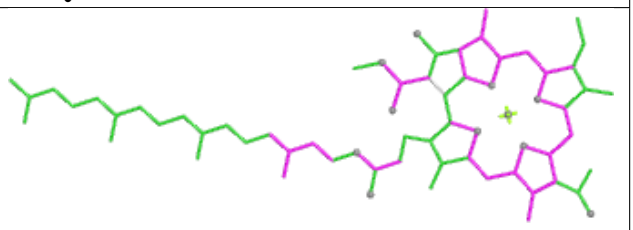
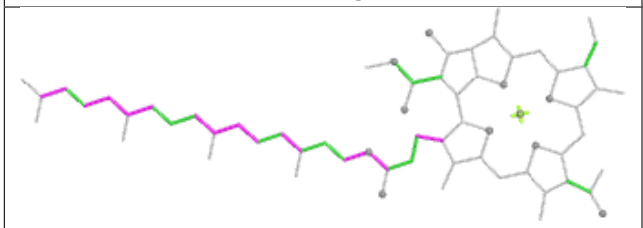
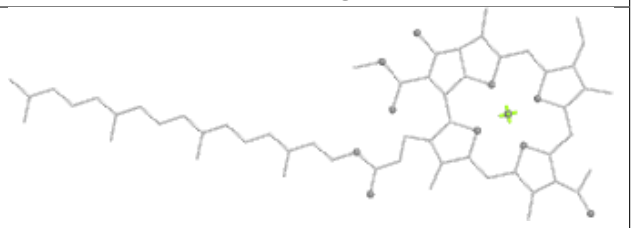
Ligand LMT A 704

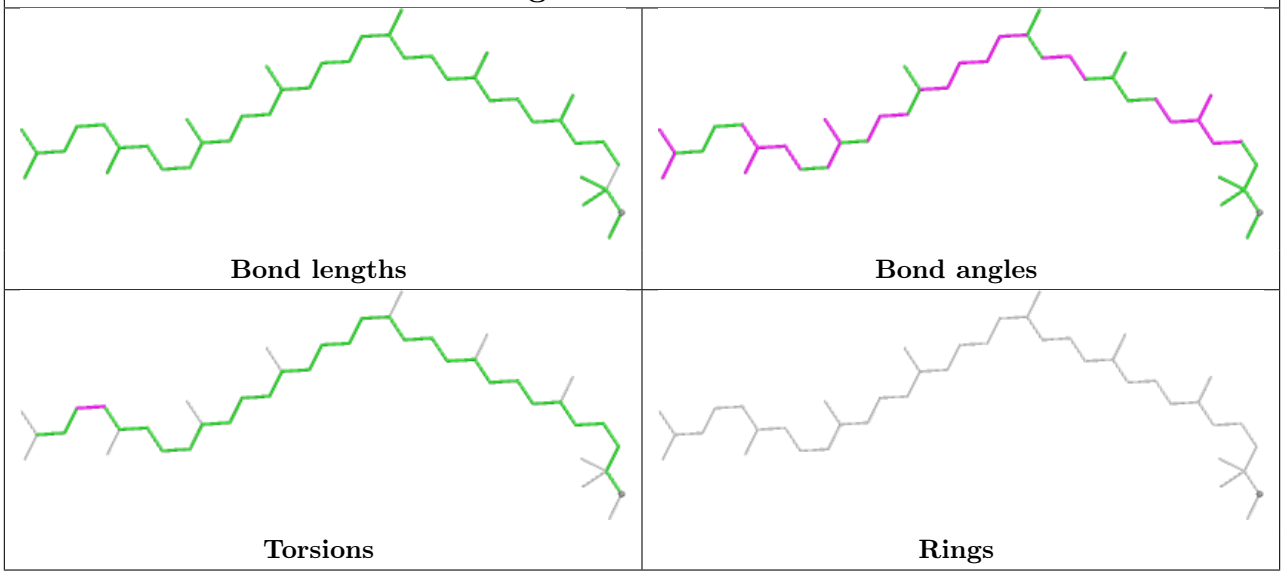


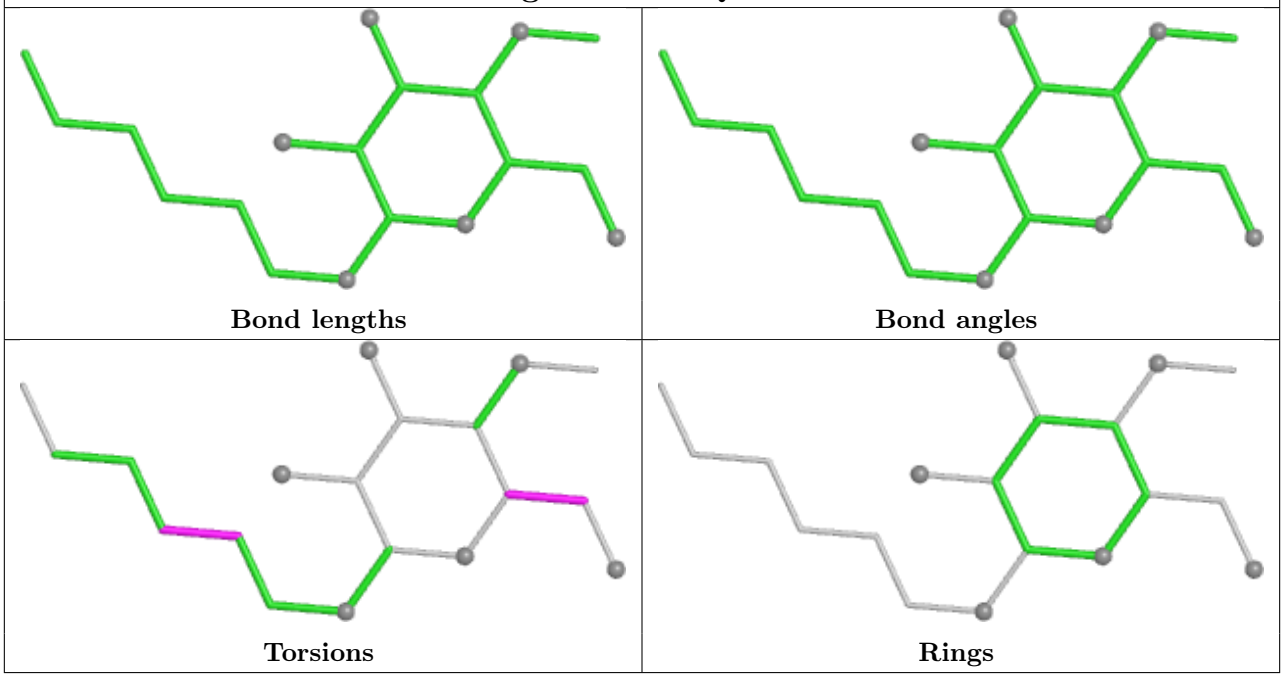
Ligand BCL E 102



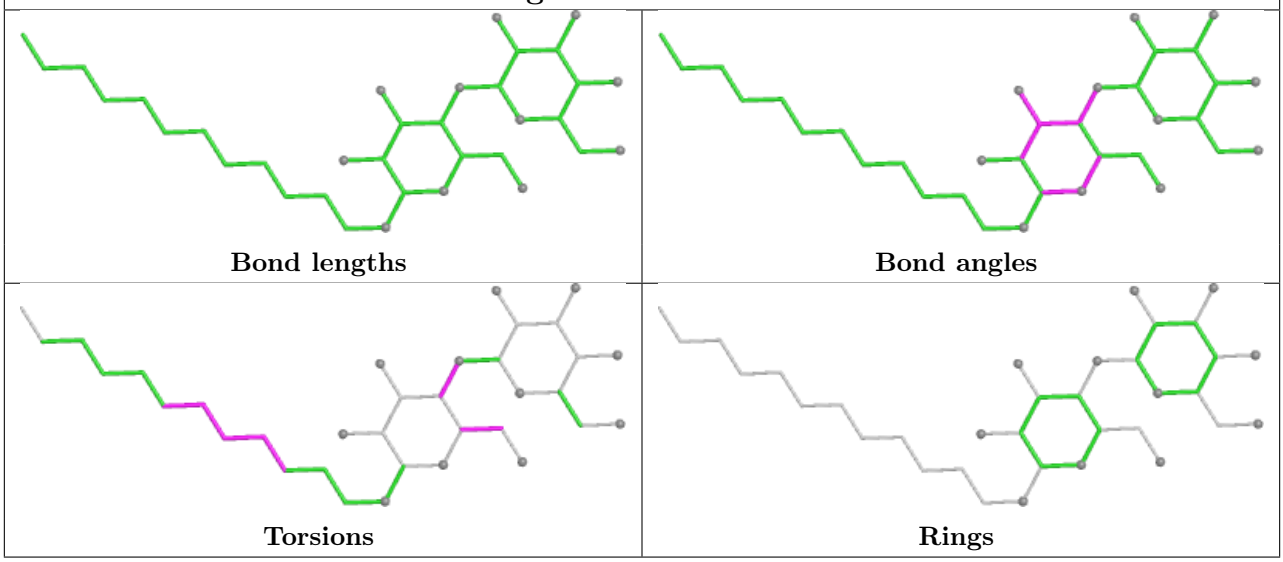
Ligand SPO G 102	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCL Q 104	
 Bond lengths	 Bond angles
 Torsions	 Rings

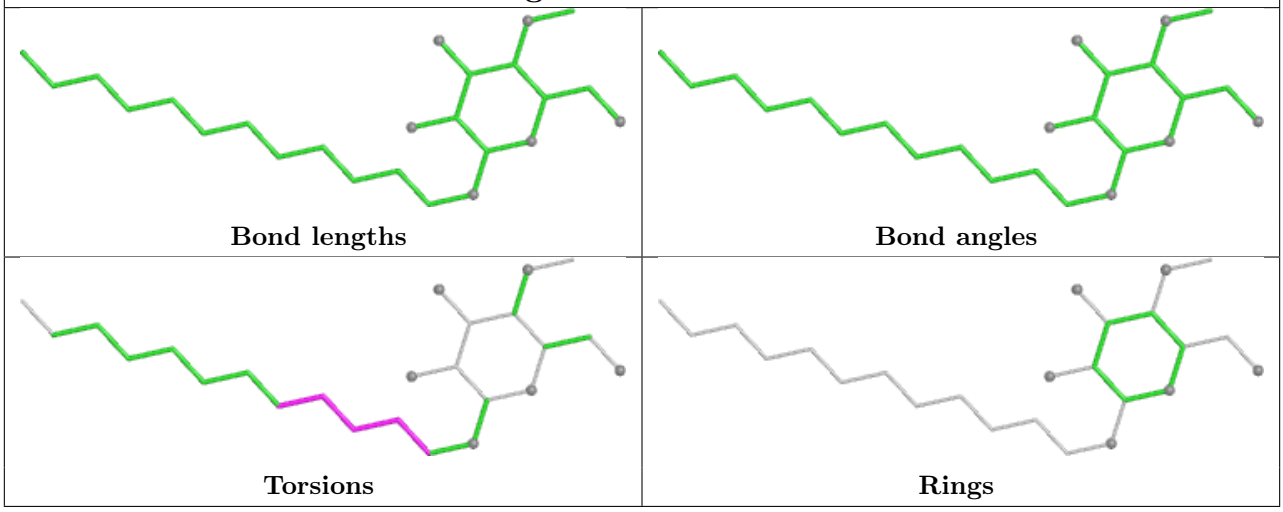
Ligand SPO F 104	
 Bond lengths	Bond angles
Torsions	Rings

Ligand LMT Q 102	
 Bond lengths	Bond angles
Torsions	Rings

Ligand LMT 3 101



Ligand LMT S 101



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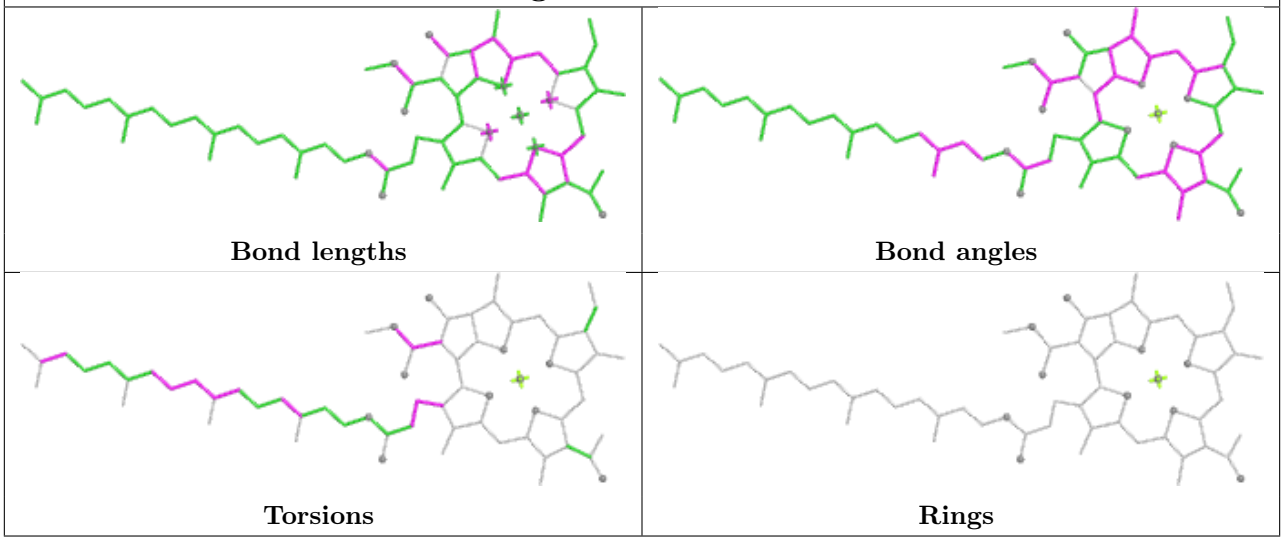

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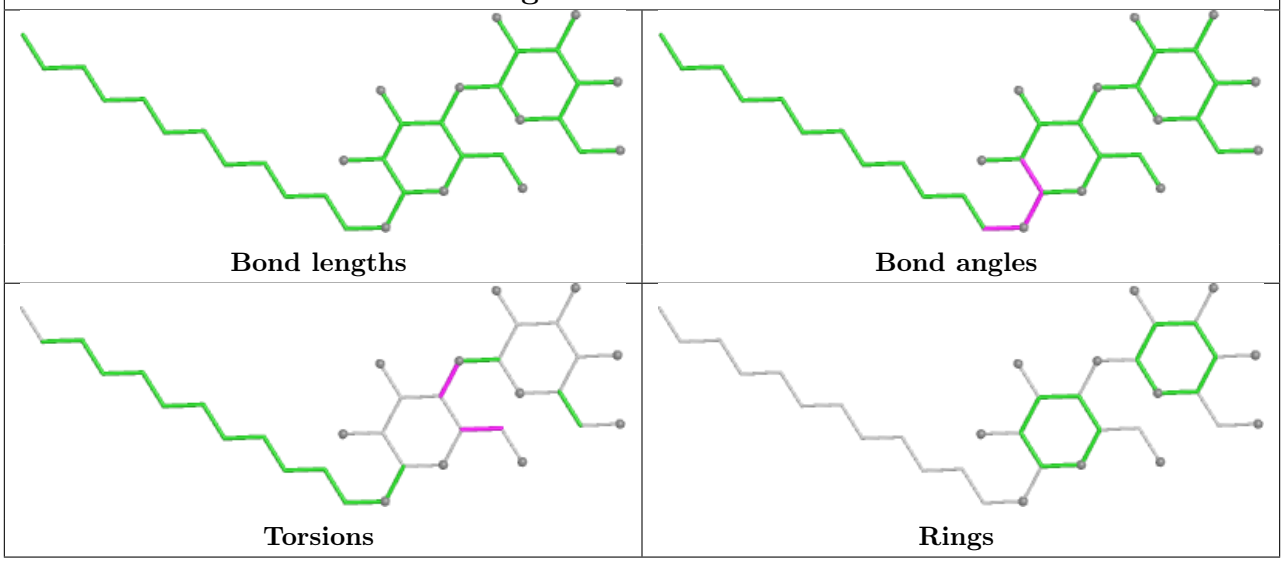

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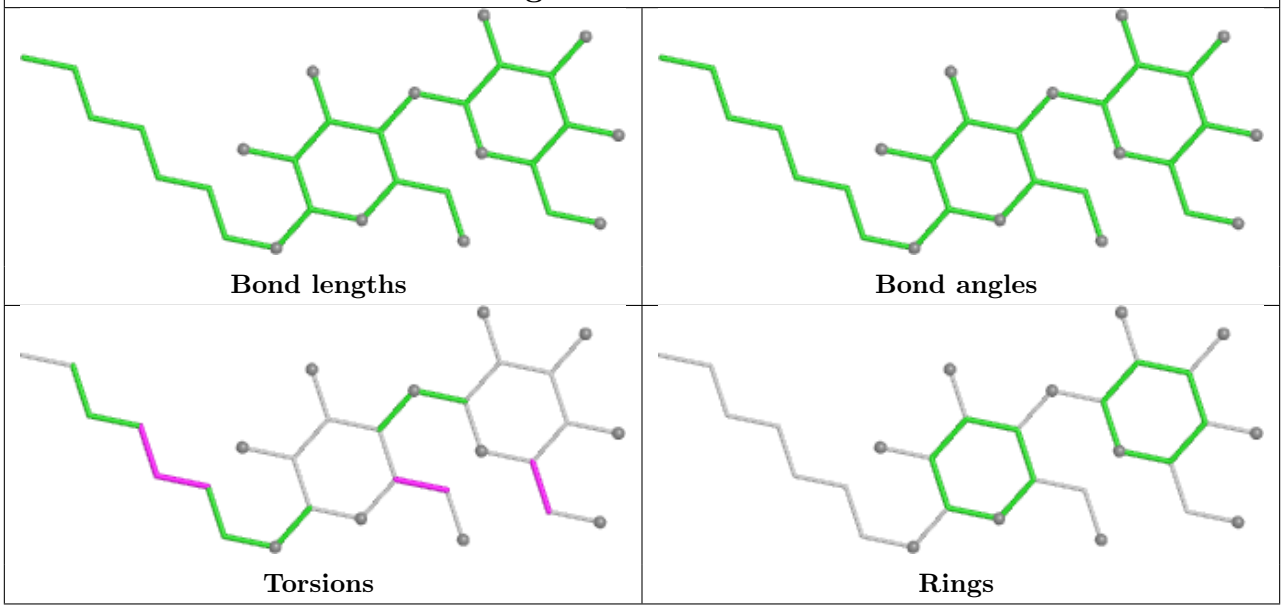

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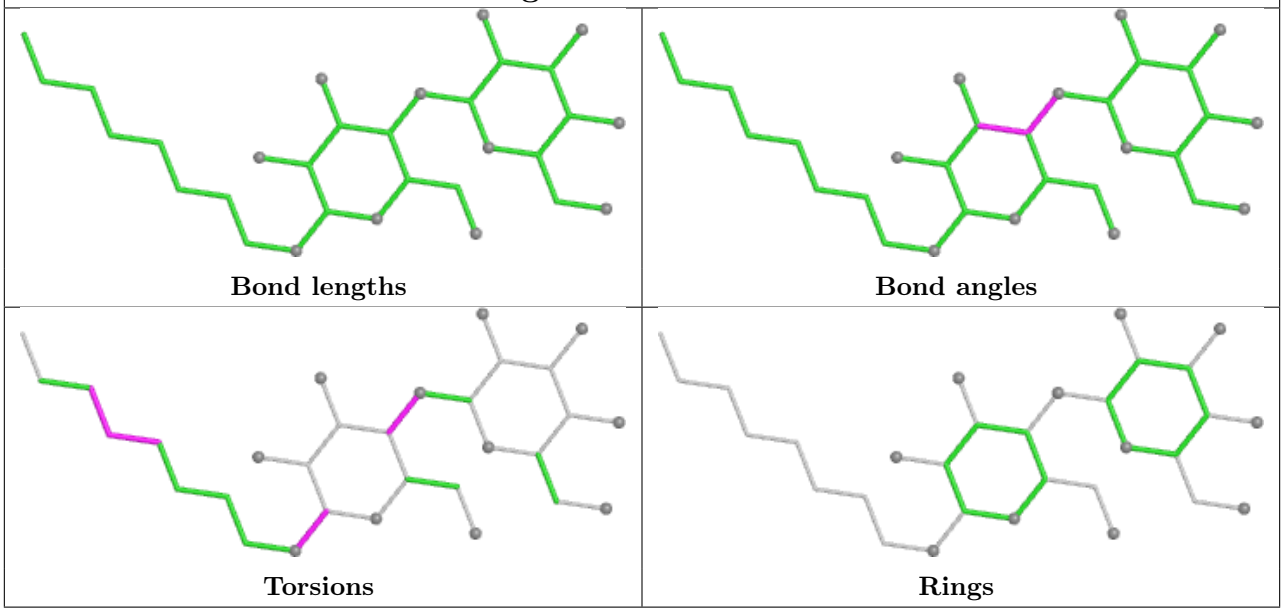

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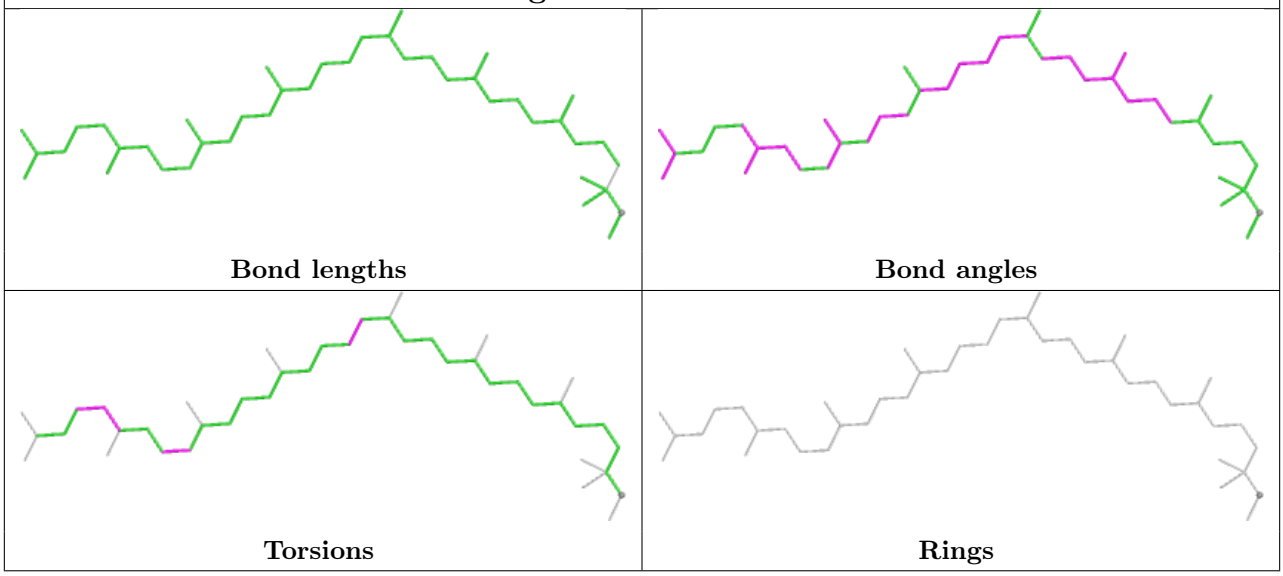
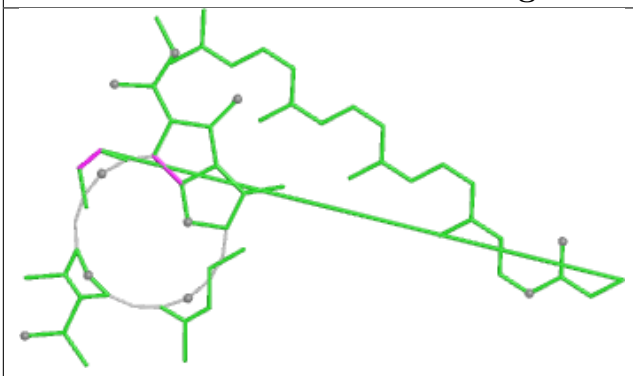
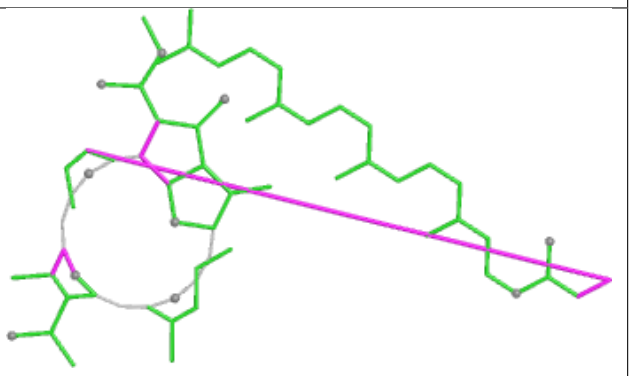


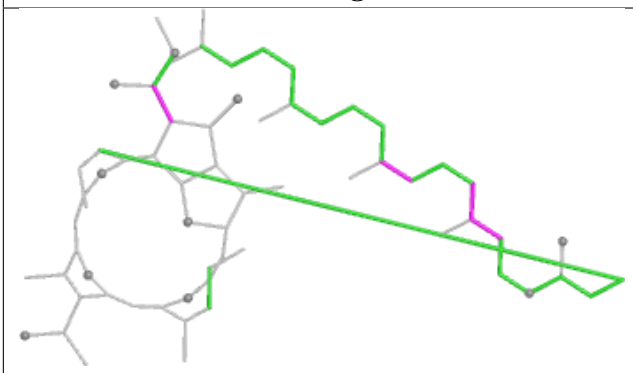
Ligand BPH M 804



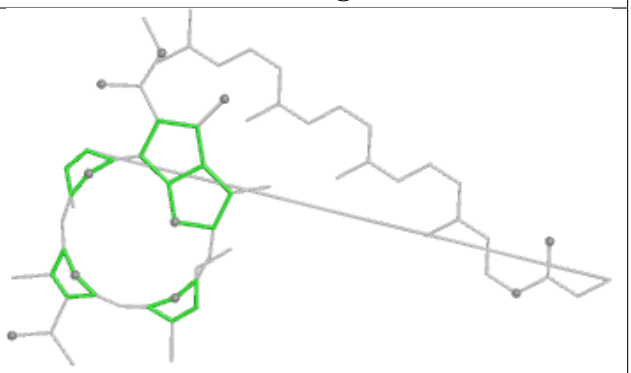
Bond lengths



Bond angles

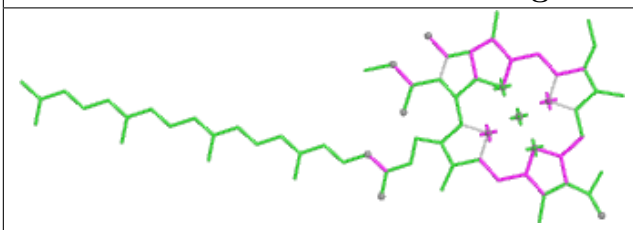


Torsions



Rings

Ligand BCL I 101



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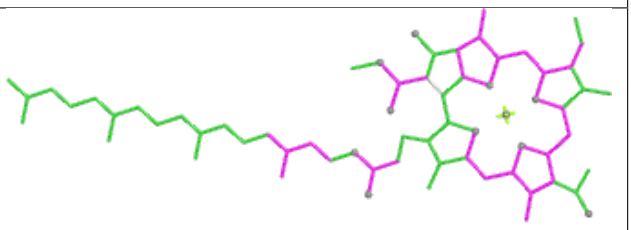
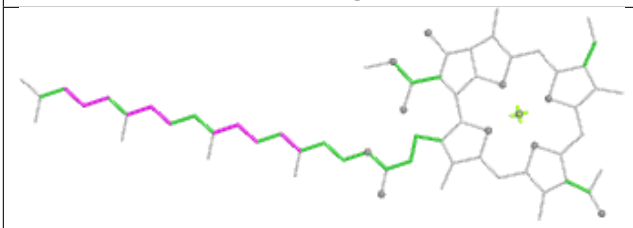
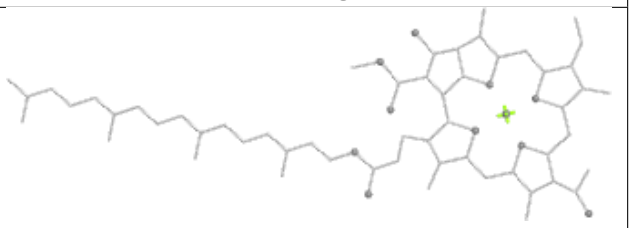


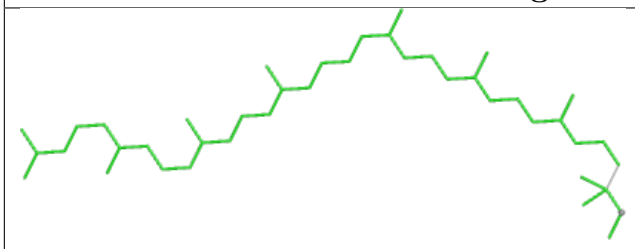
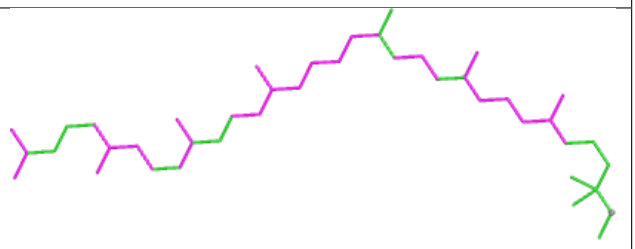
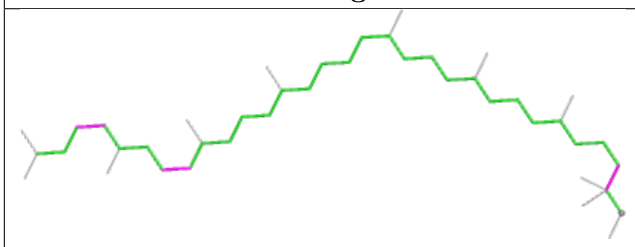
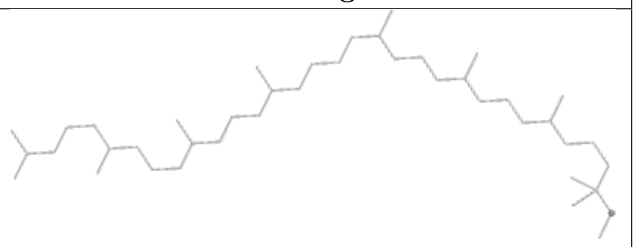
Bond angles

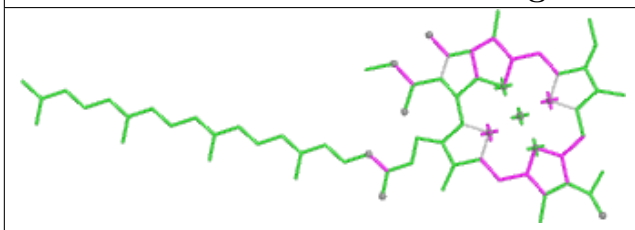
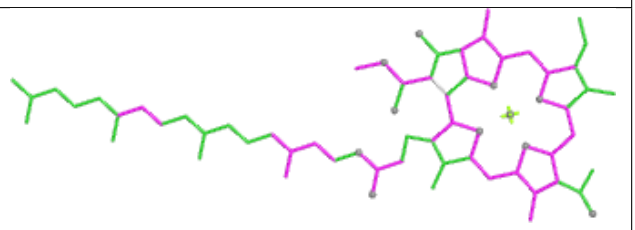
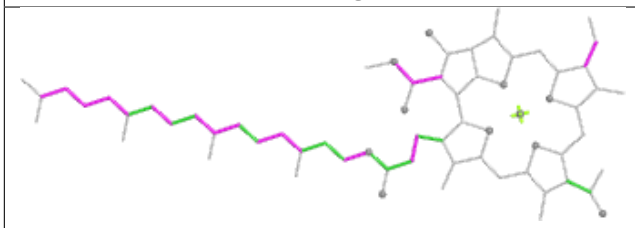
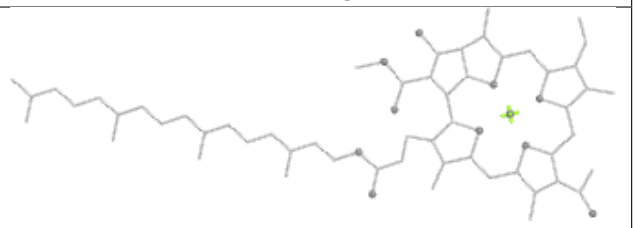


Torsions

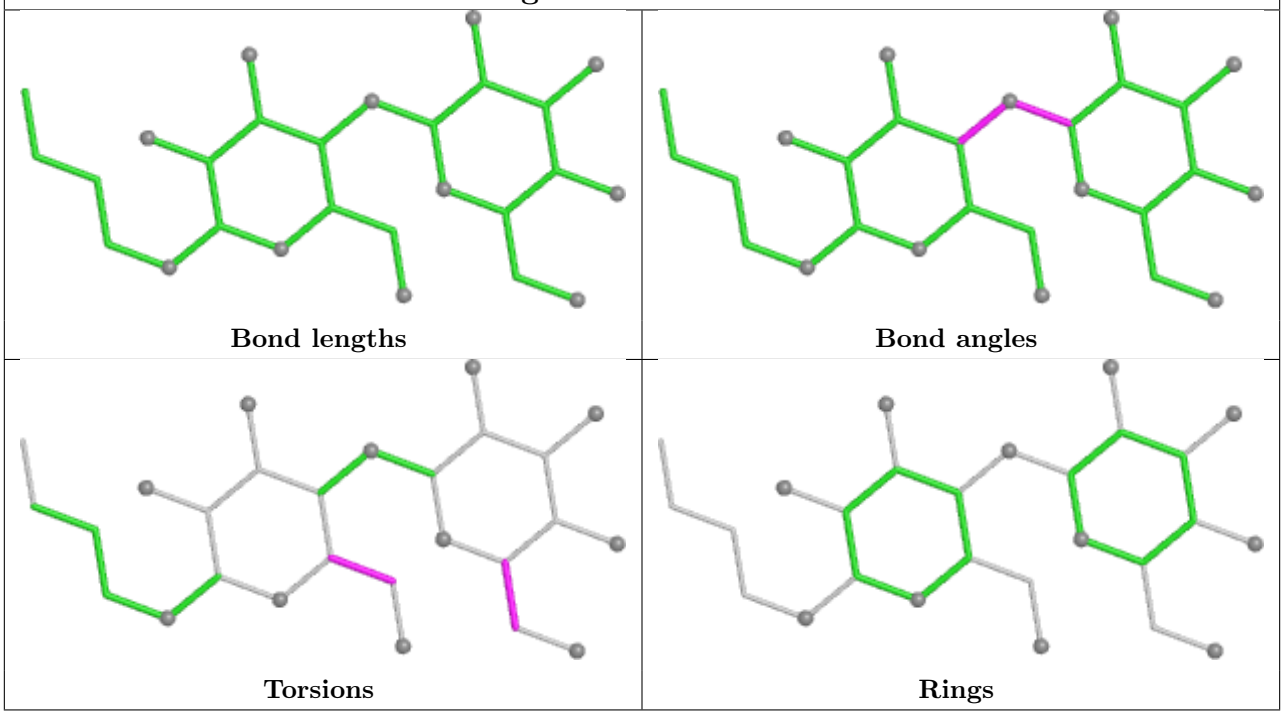


Rings

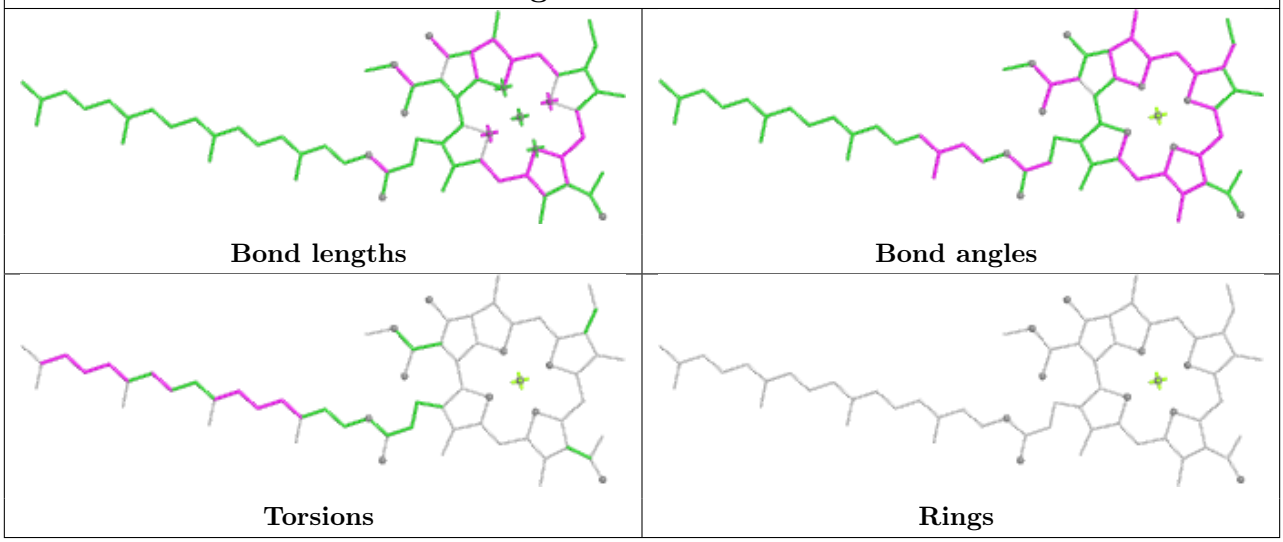
Ligand SPO 5 103	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCL L 301	
 Bond lengths	 Bond angles
 Torsions	 Rings

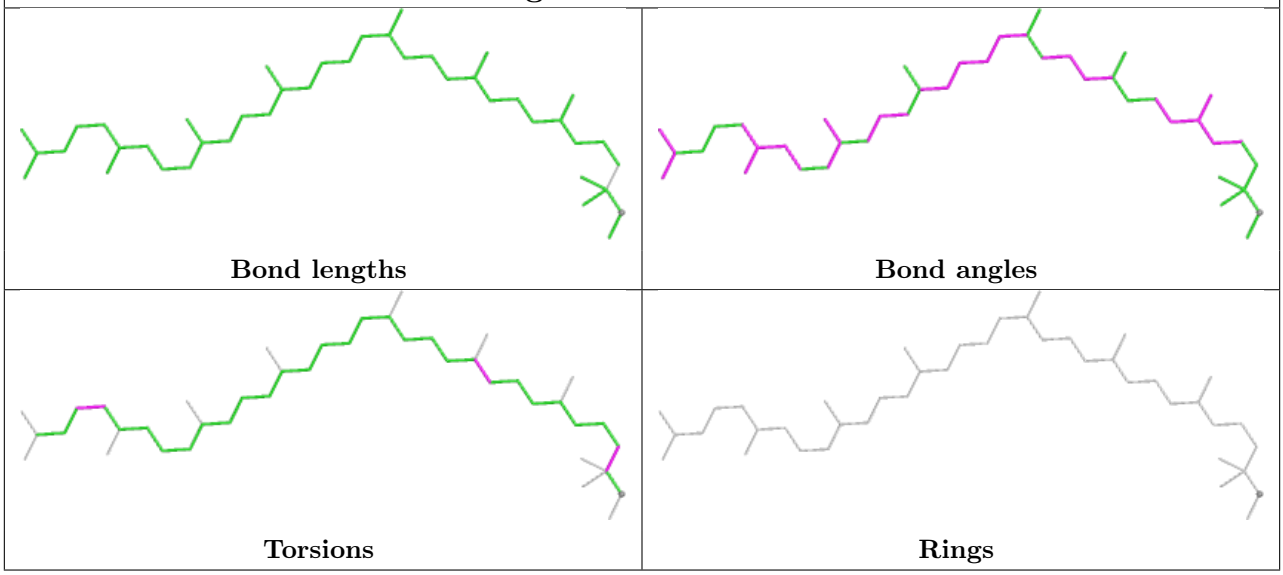
Ligand LMT D 103



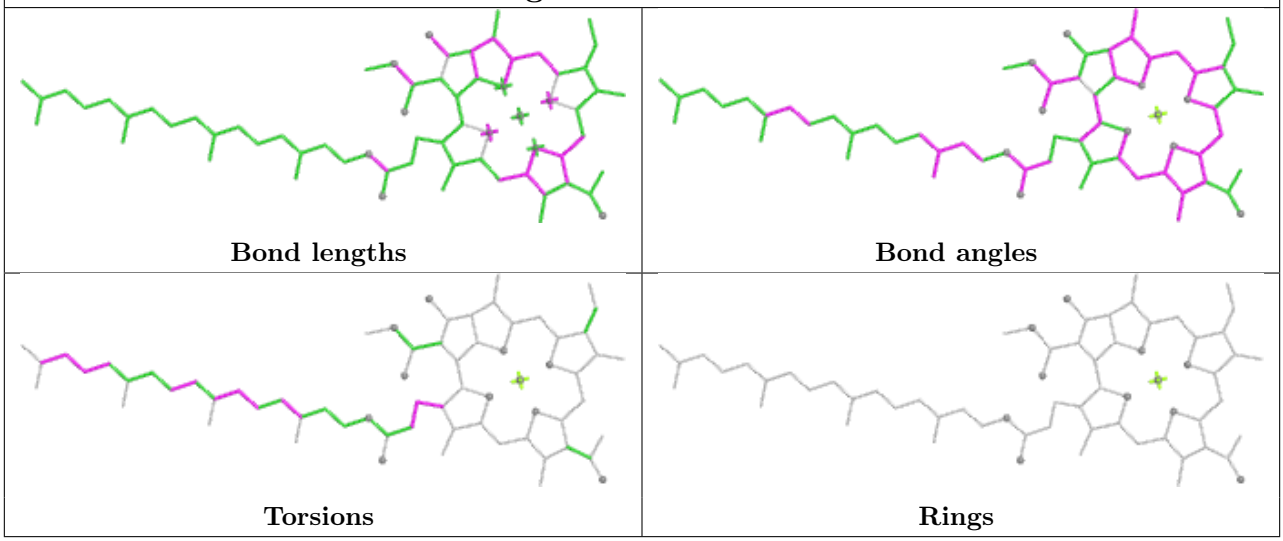
Ligand BCL 5 102



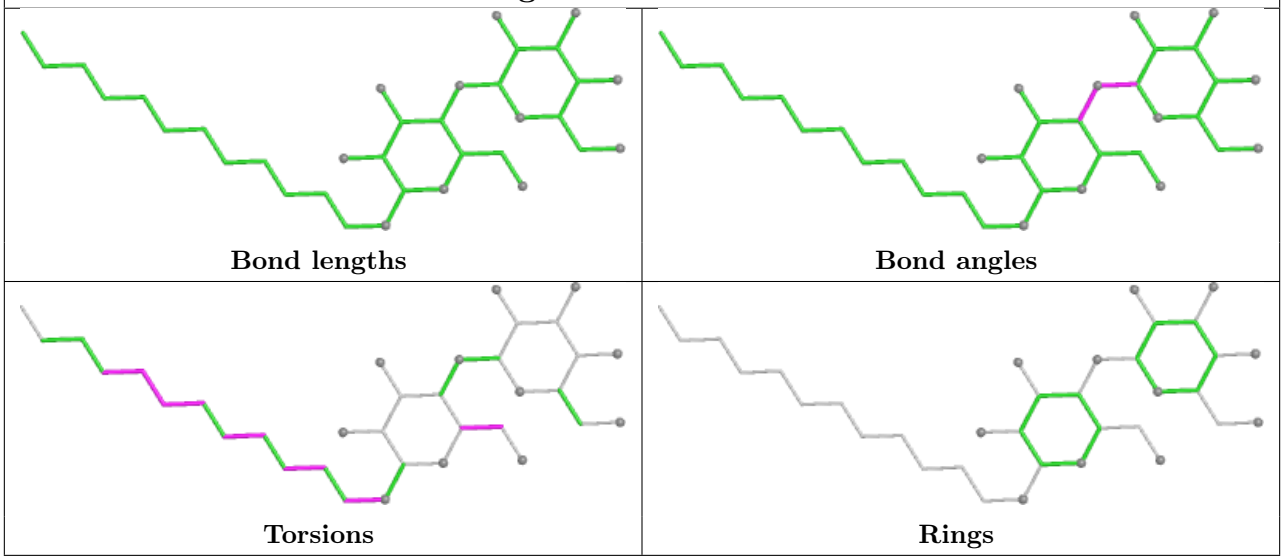
Ligand SPO G 103



Ligand BCL R 102



Ligand LMT M 809



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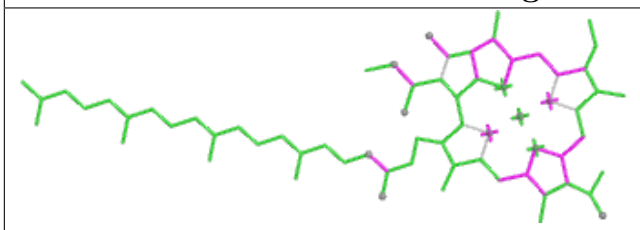
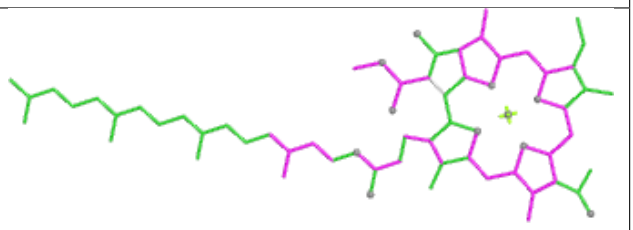
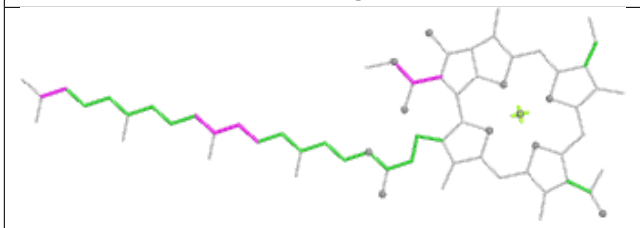
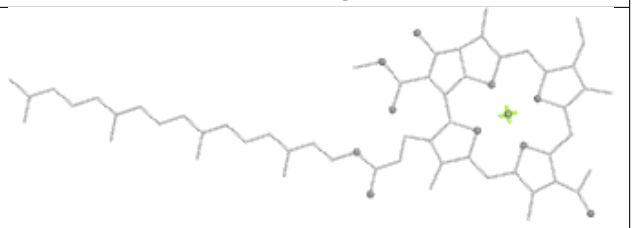
 Bond lengths	 Bond angles
 Torsions	 Rings

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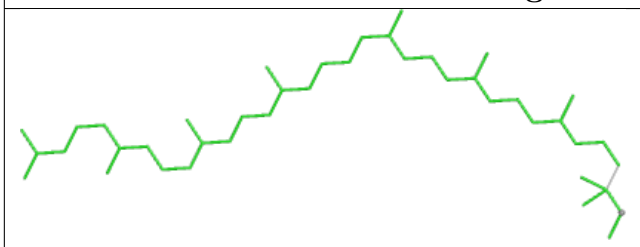
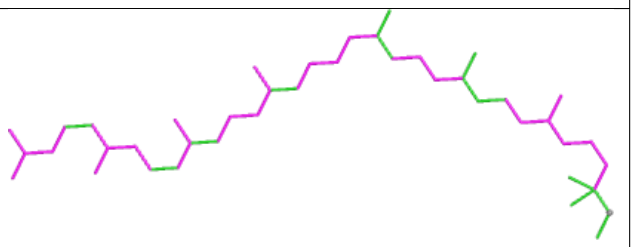
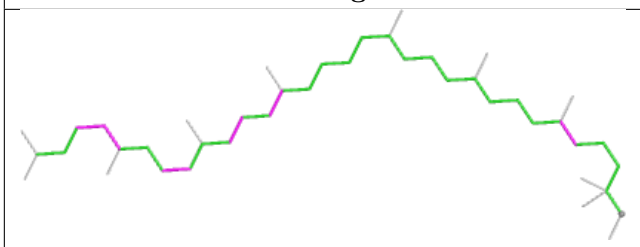
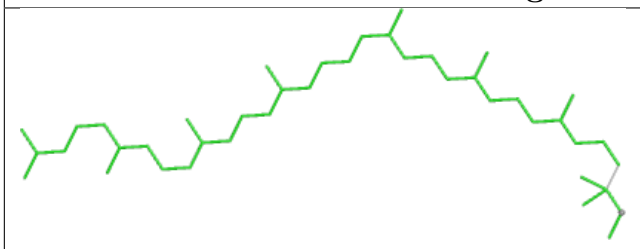
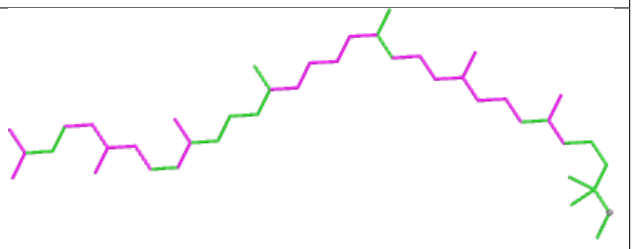
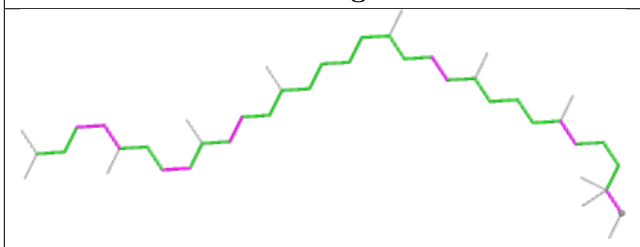
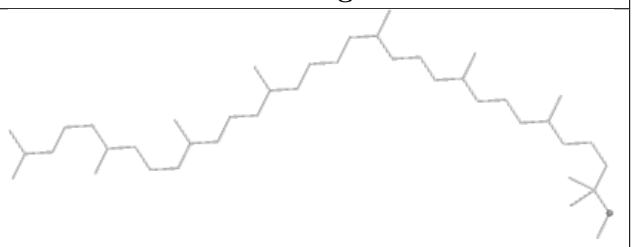
 Bond lengths	 Bond angles
 Torsions	Rings

Ligand SPO O 103	
 Bond lengths	 Bond angles
 Torsions	 Rings

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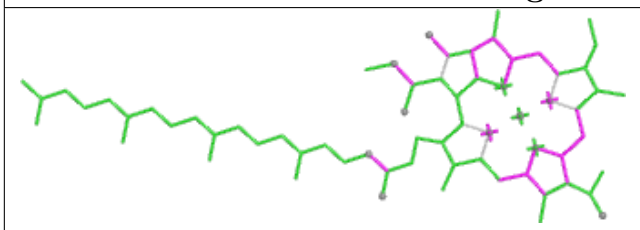
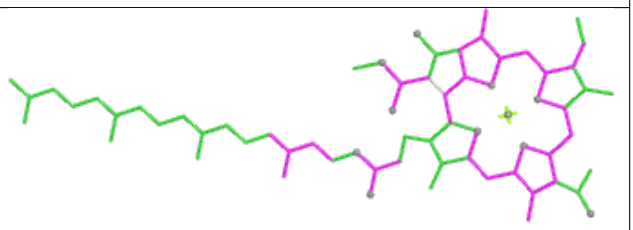
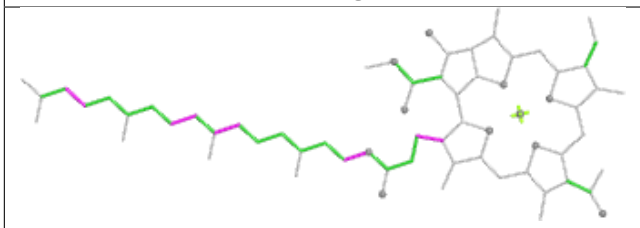
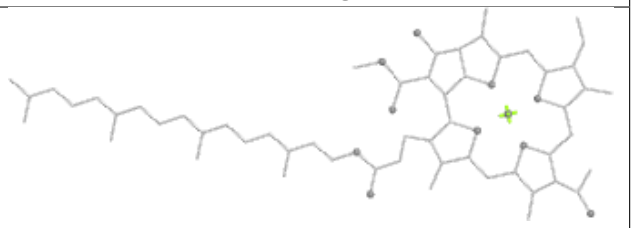
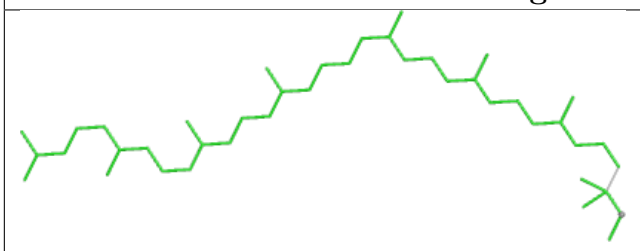
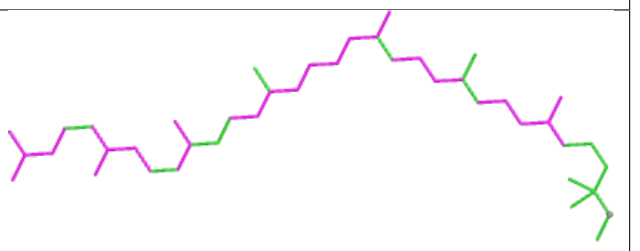
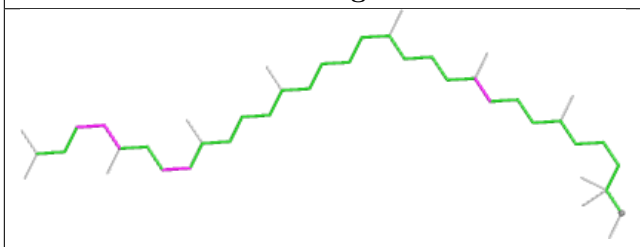
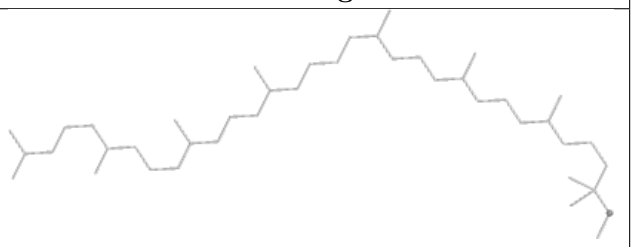
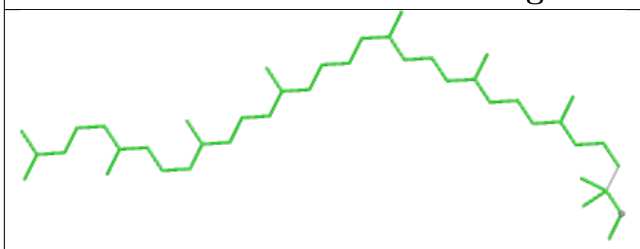
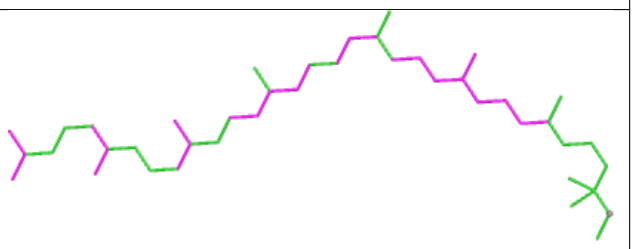
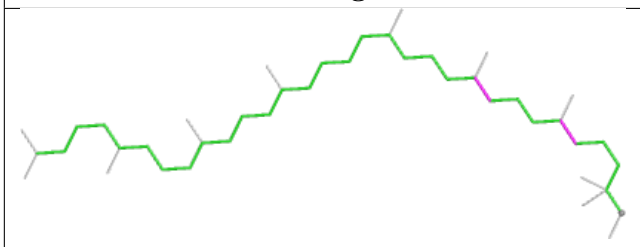
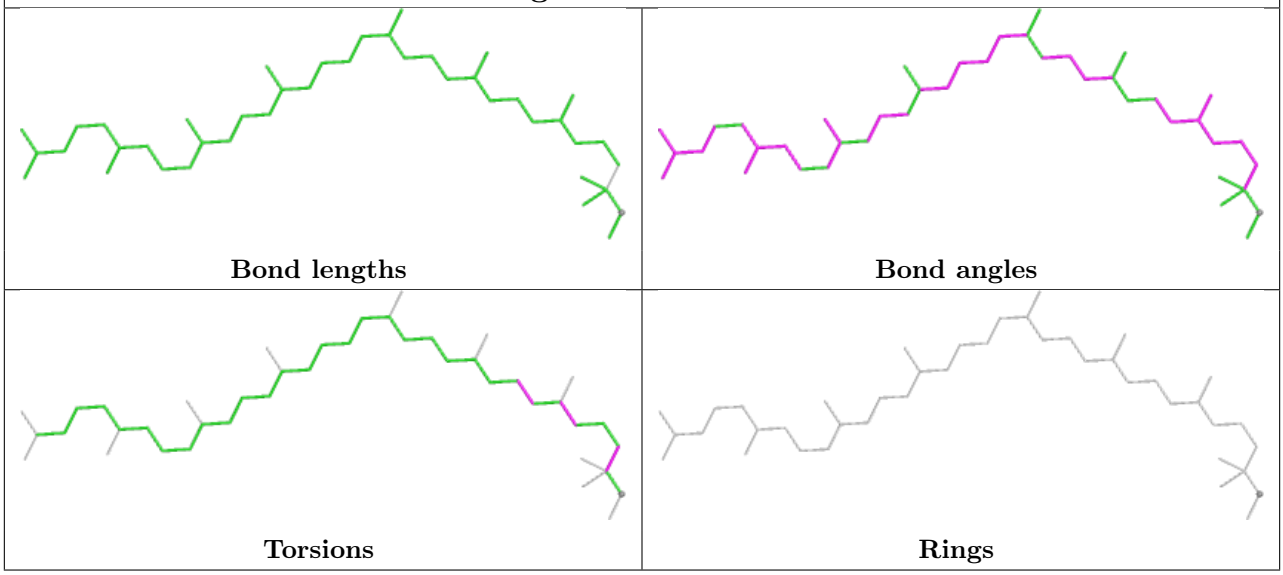
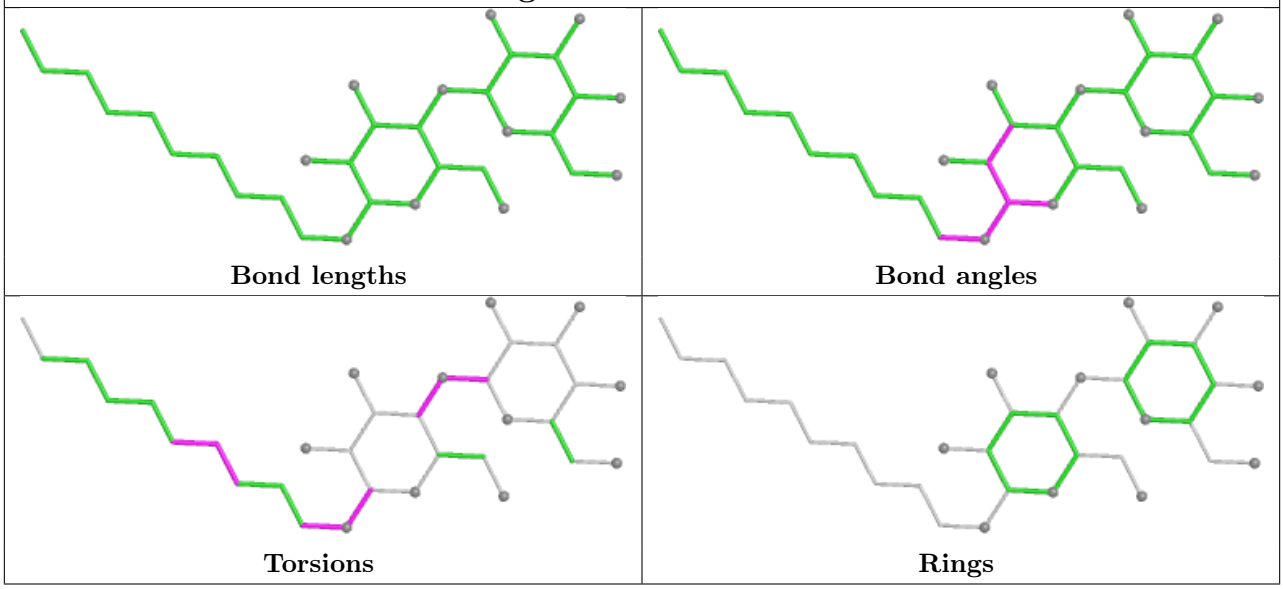
 Bond lengths	 Bond angles
 Torsions	 Rings

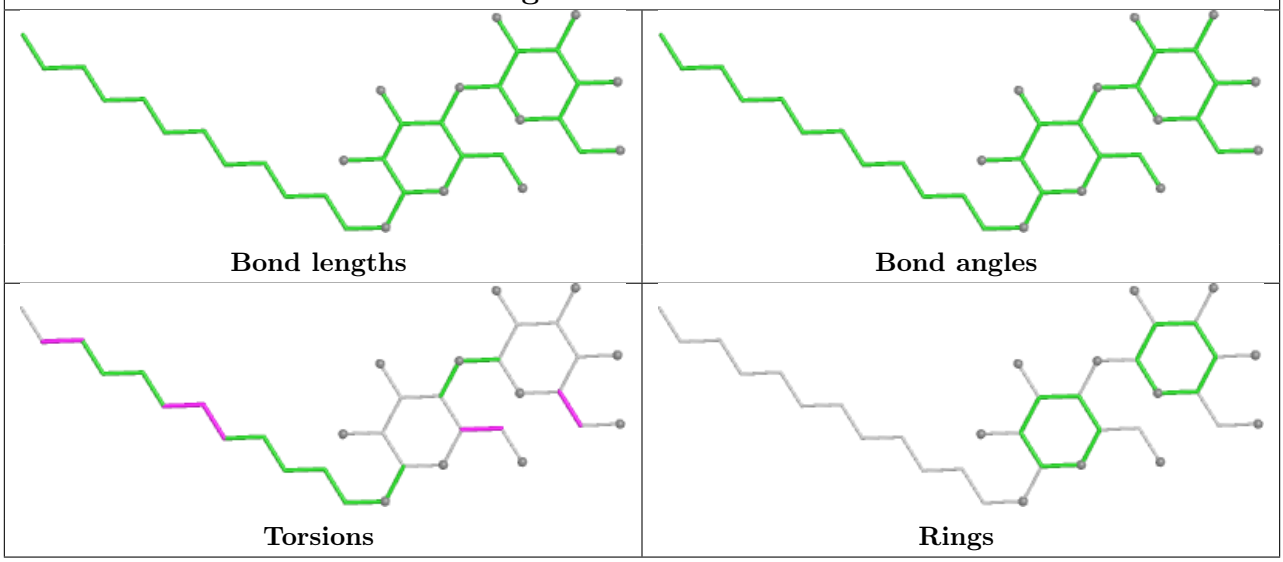
Ligand SPO S 103	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand SPO X 102	
 Bond lengths	 Bond angles
 Torsions	Rings

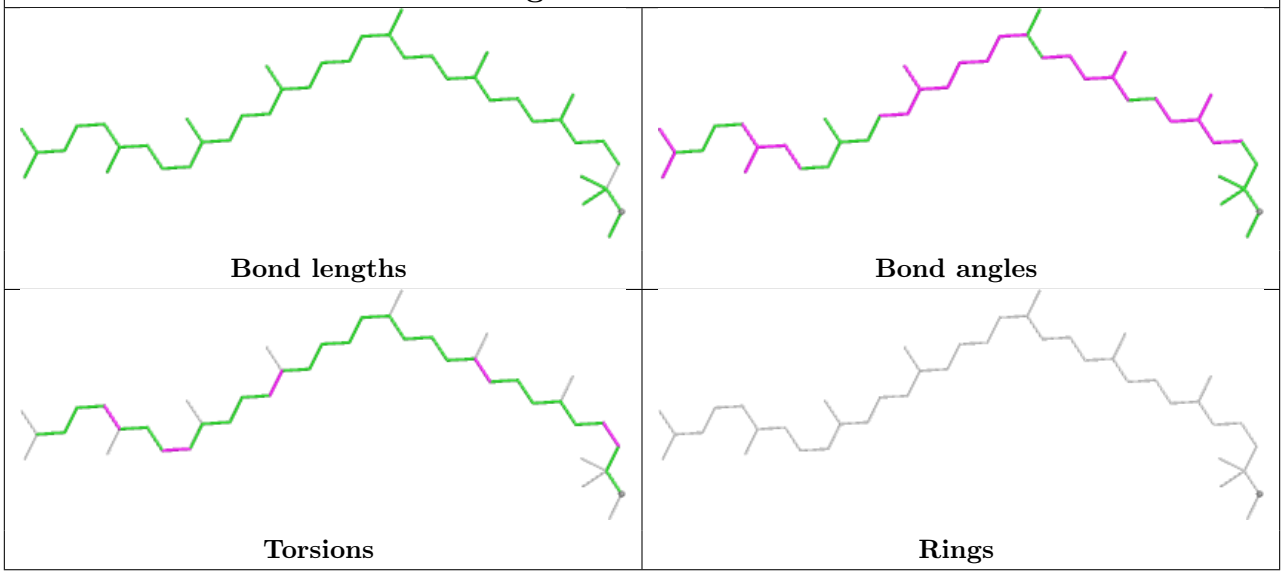
Ligand SPO 3 104	
 Bond lengths	Bond angles
Torsions	Rings

Ligand LMT M 810	
 Bond lengths	Bond angles
Torsions	Rings

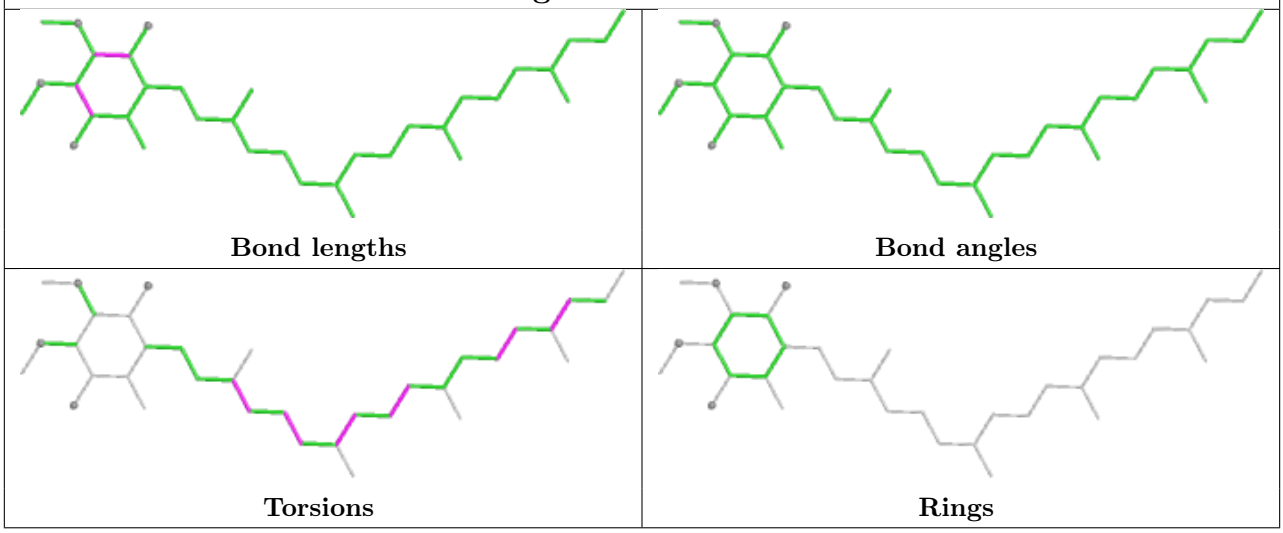
Ligand LMT A 701



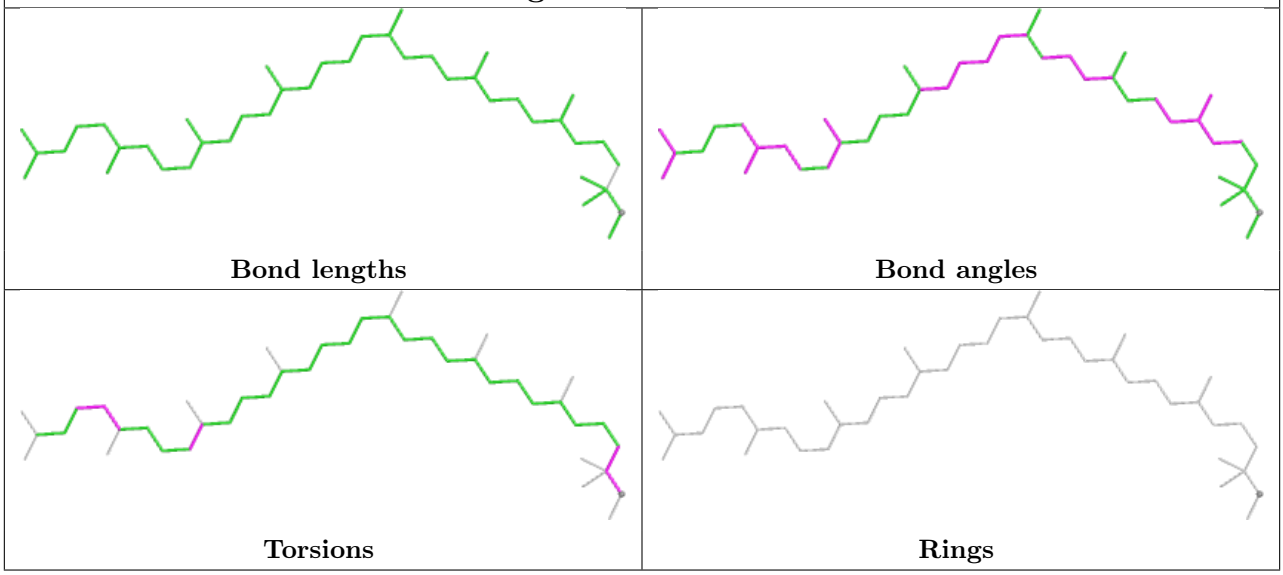
Ligand SPO R 101



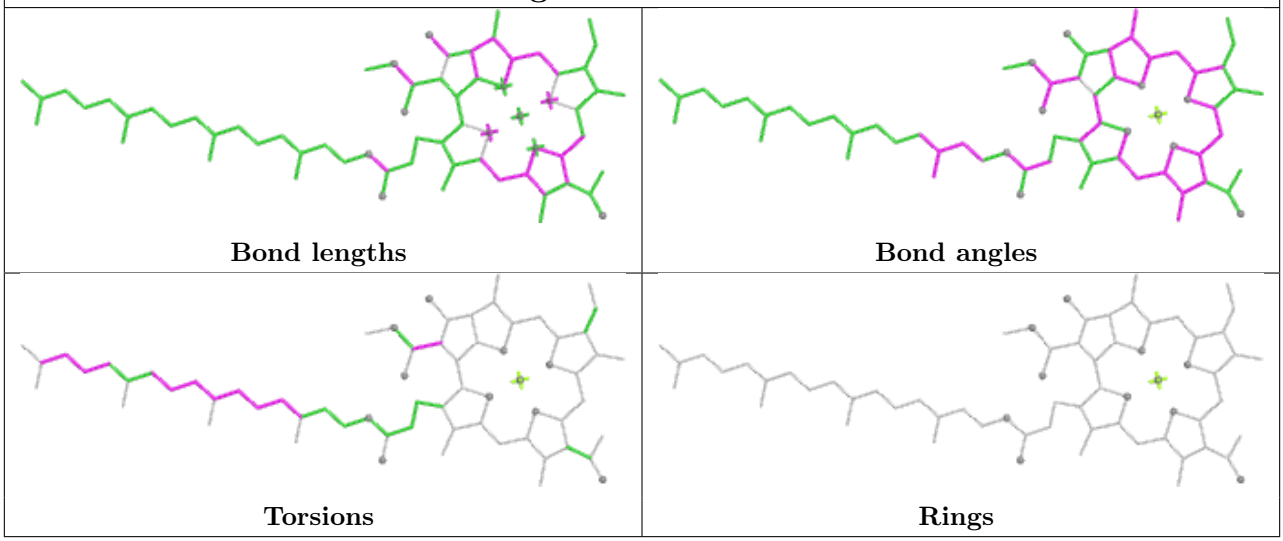
Ligand U10 L 303



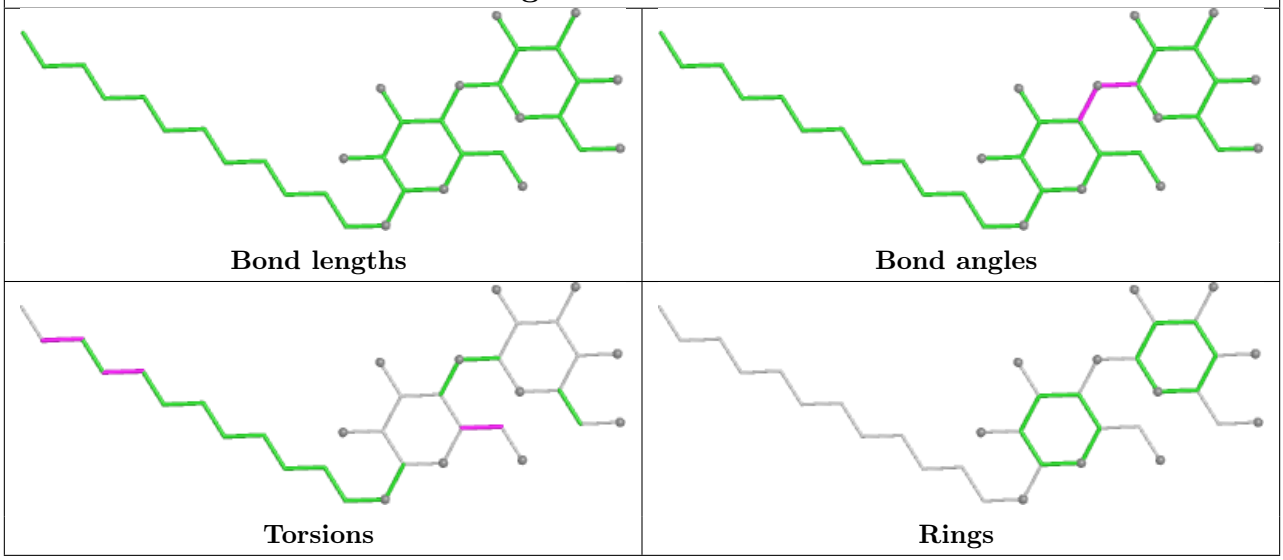
Ligand SPO T 102



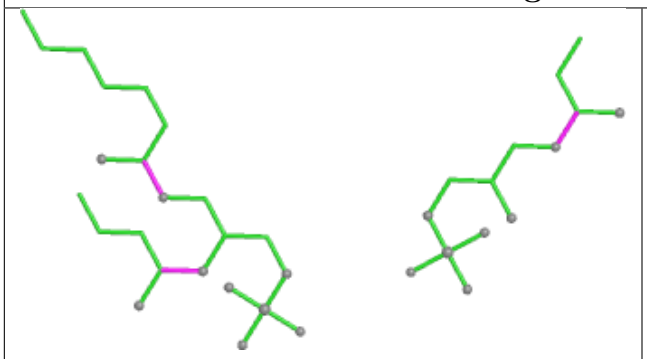
Ligand BCL 7 101



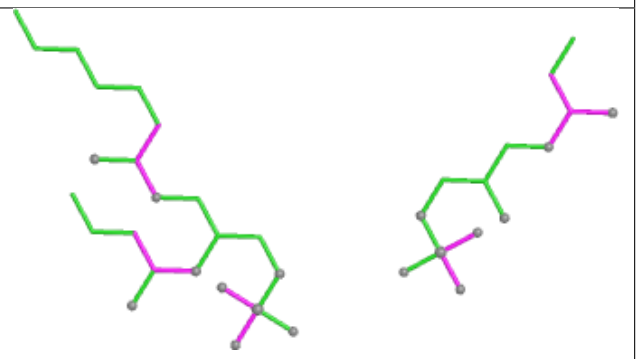
Ligand LMT U 102



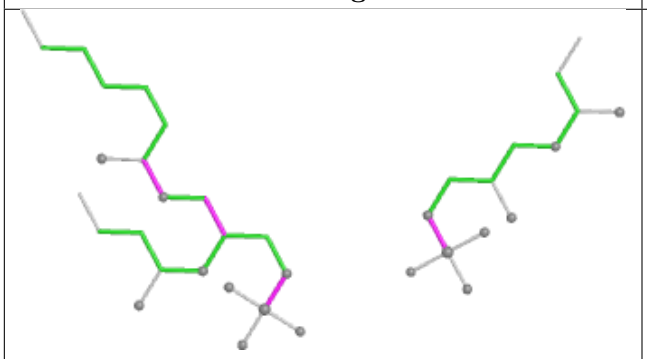
Ligand CDL H 305



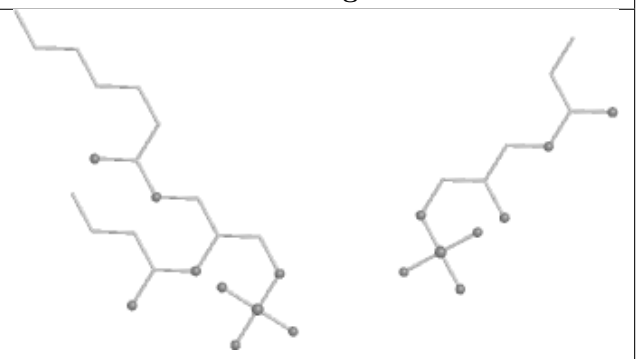
Bond lengths



Bond angles

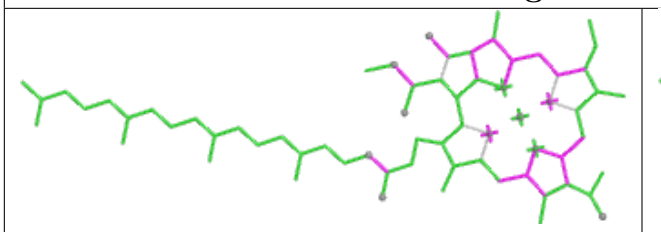


Torsions



Rings

Ligand BCL N 102



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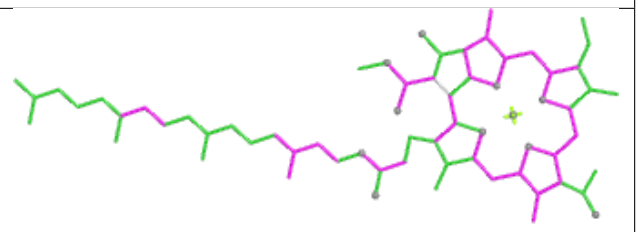
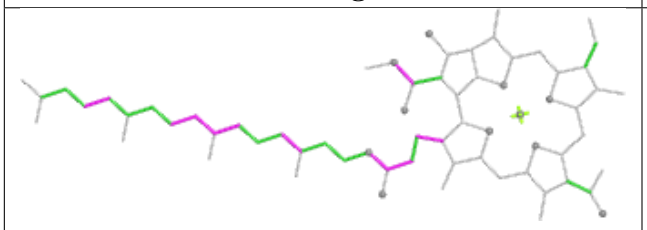
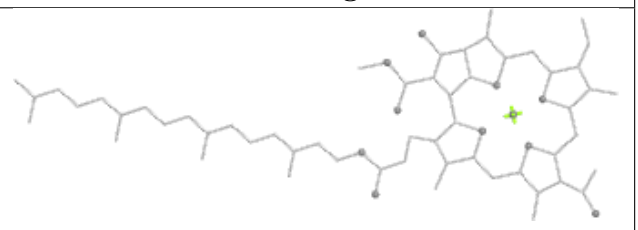


Bond angles

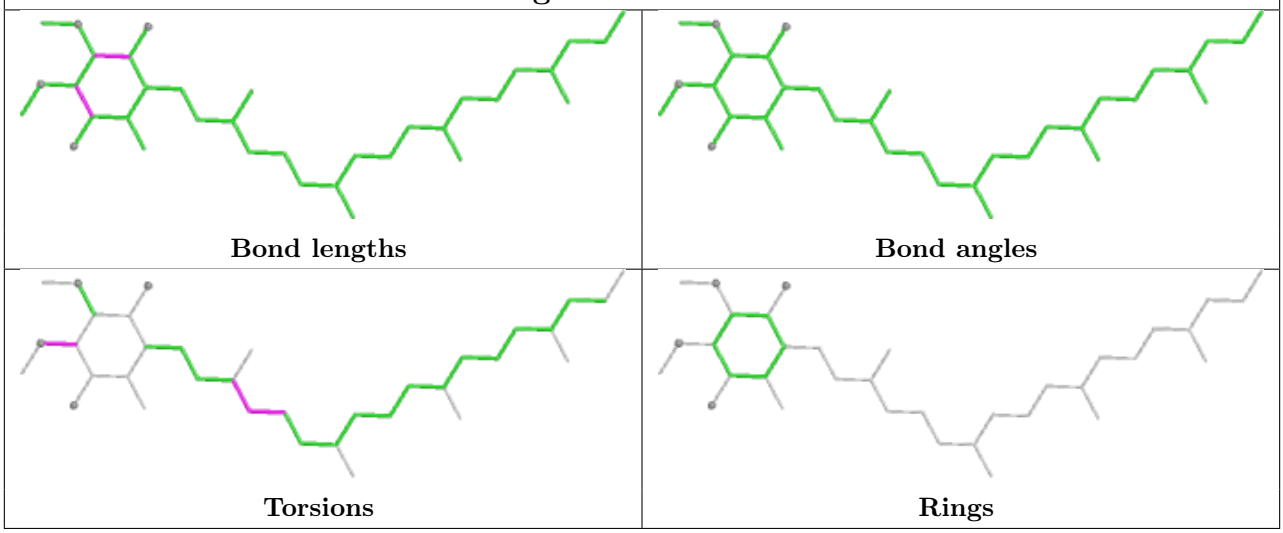


Torsions

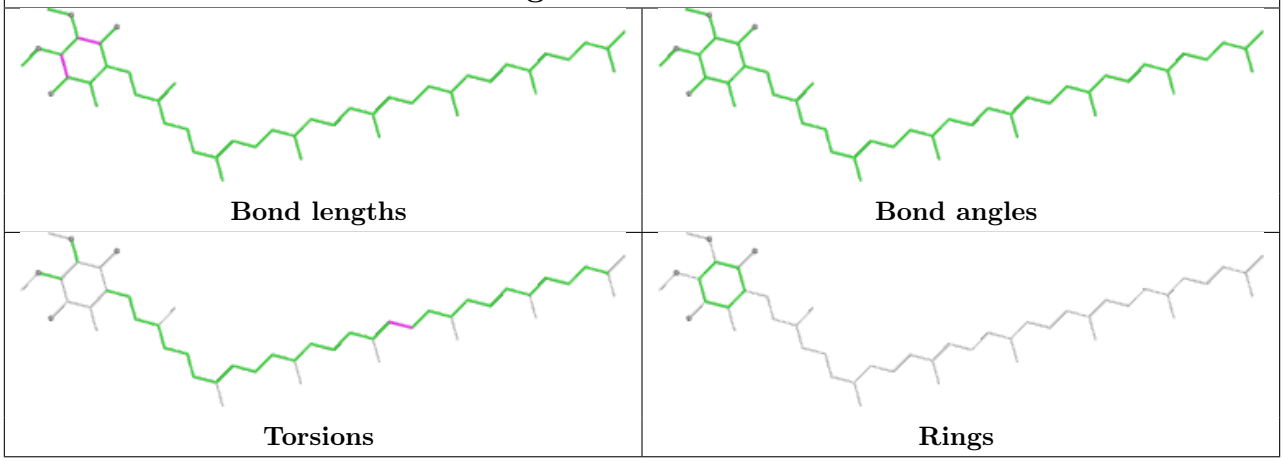


Rings

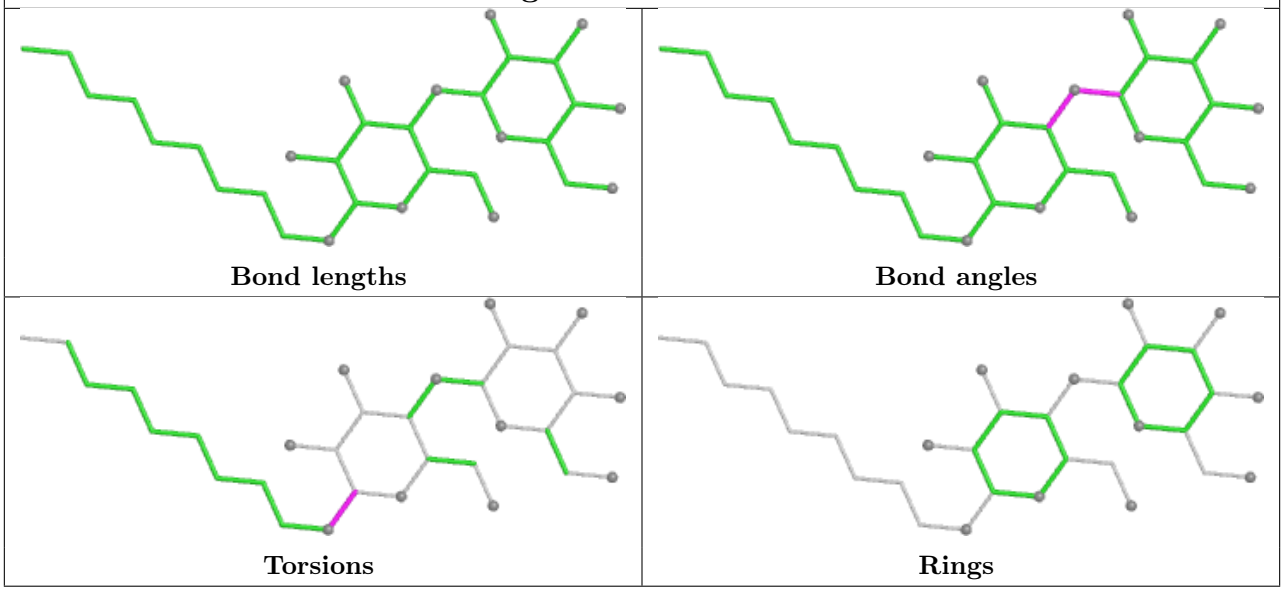
Ligand U10 L 304



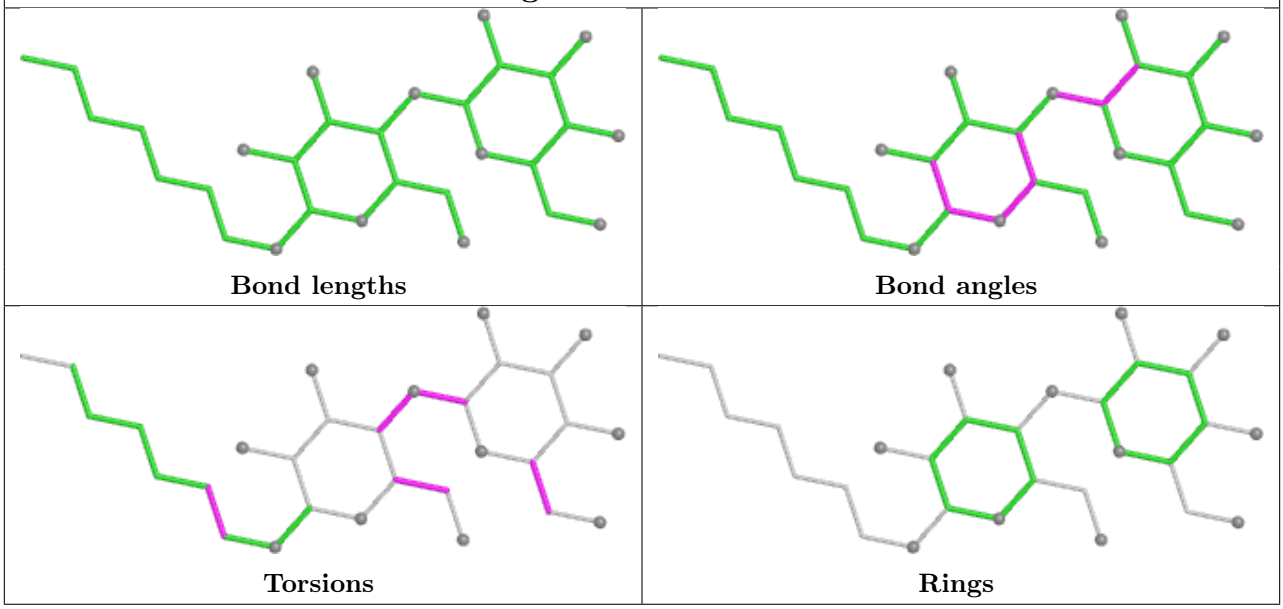
Ligand U10 M 806



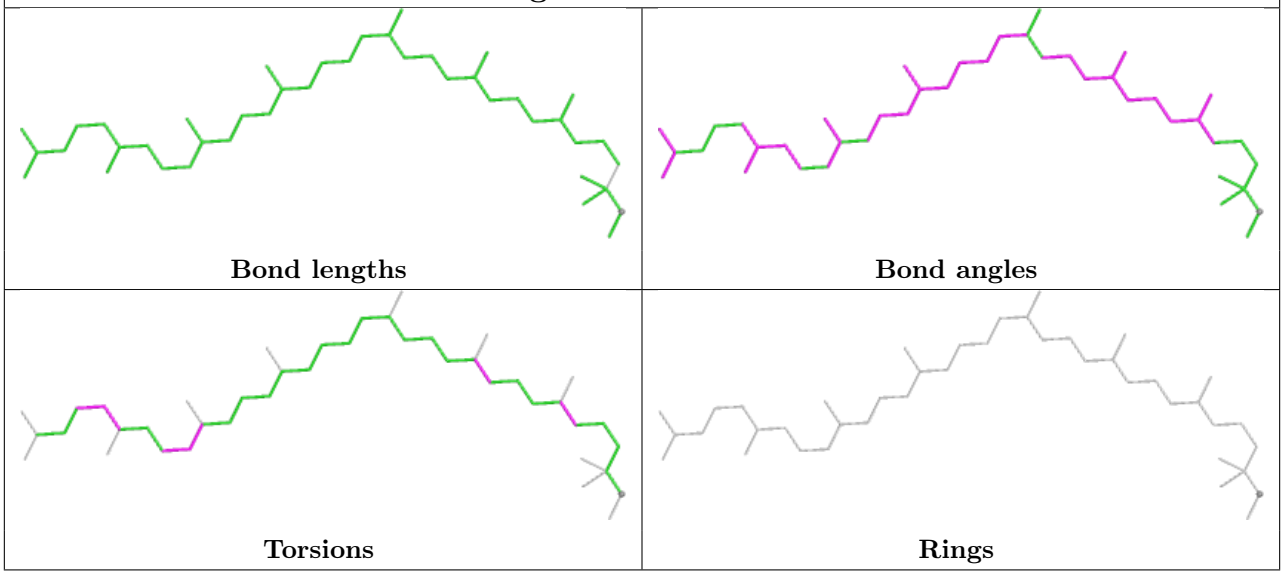
Ligand LMT U 101



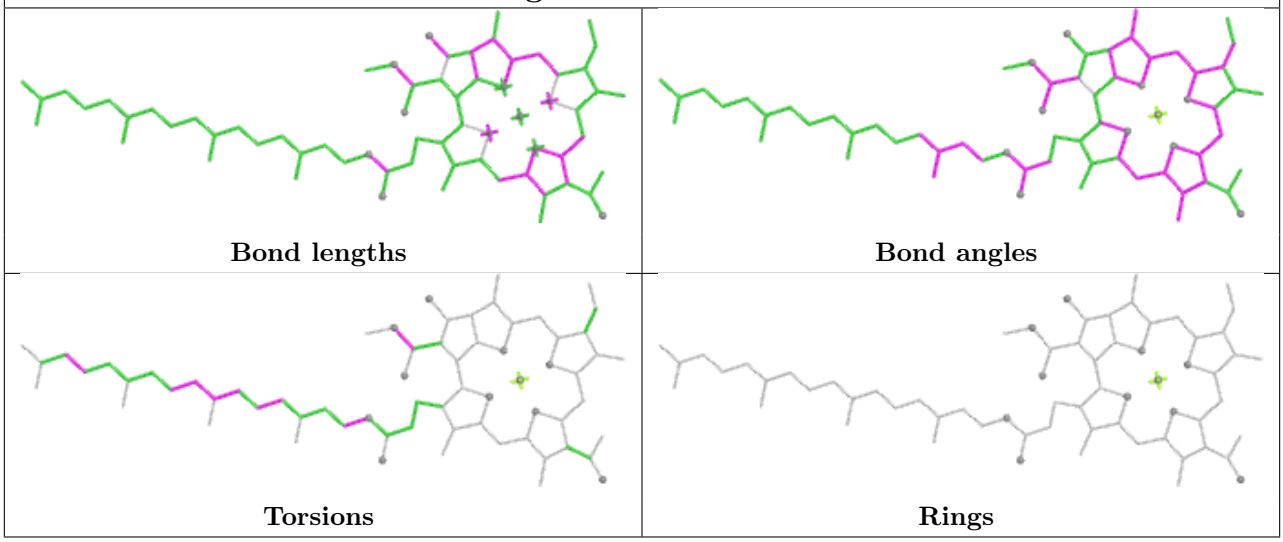
Ligand LMT H 302



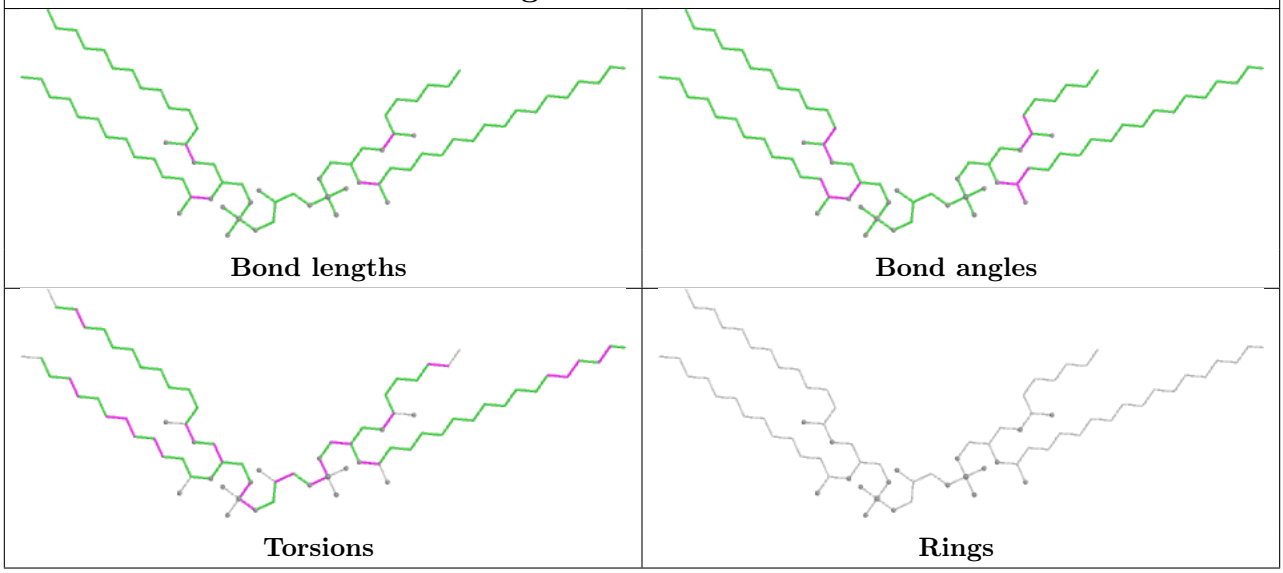
Ligand SPO S 104



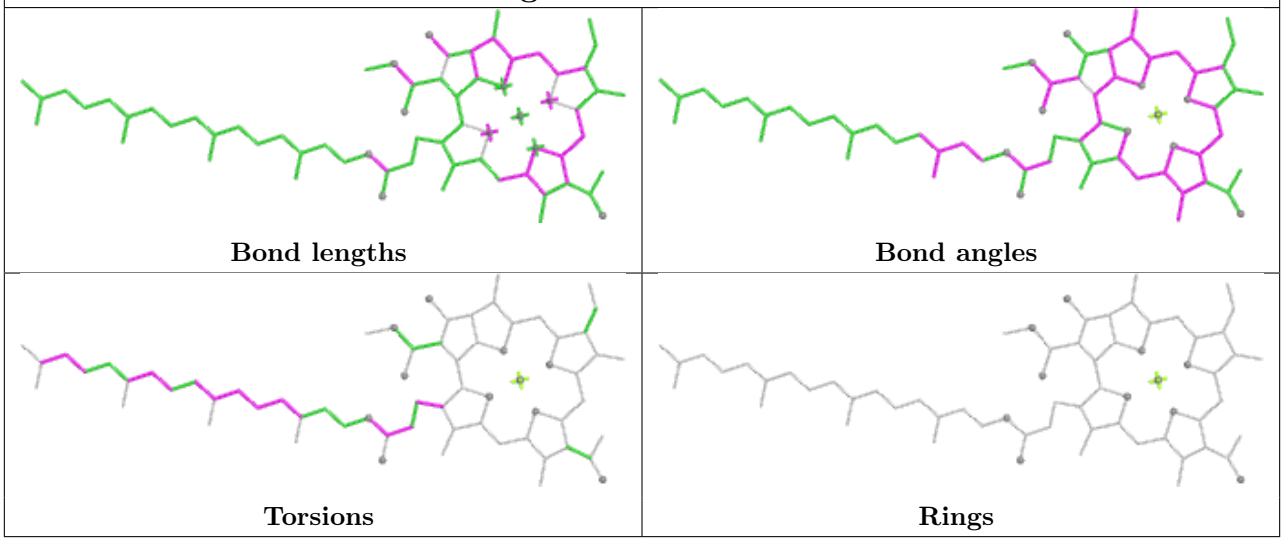
Ligand BCL D 101



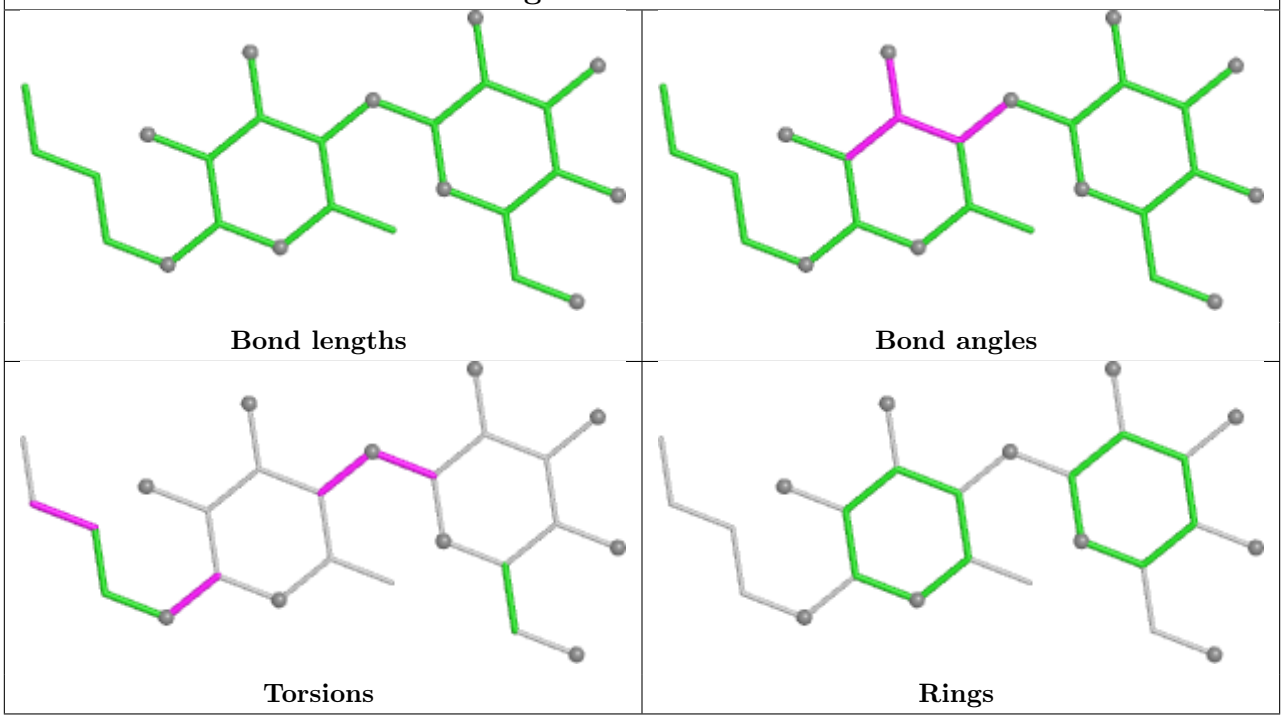
Ligand CDL M 811



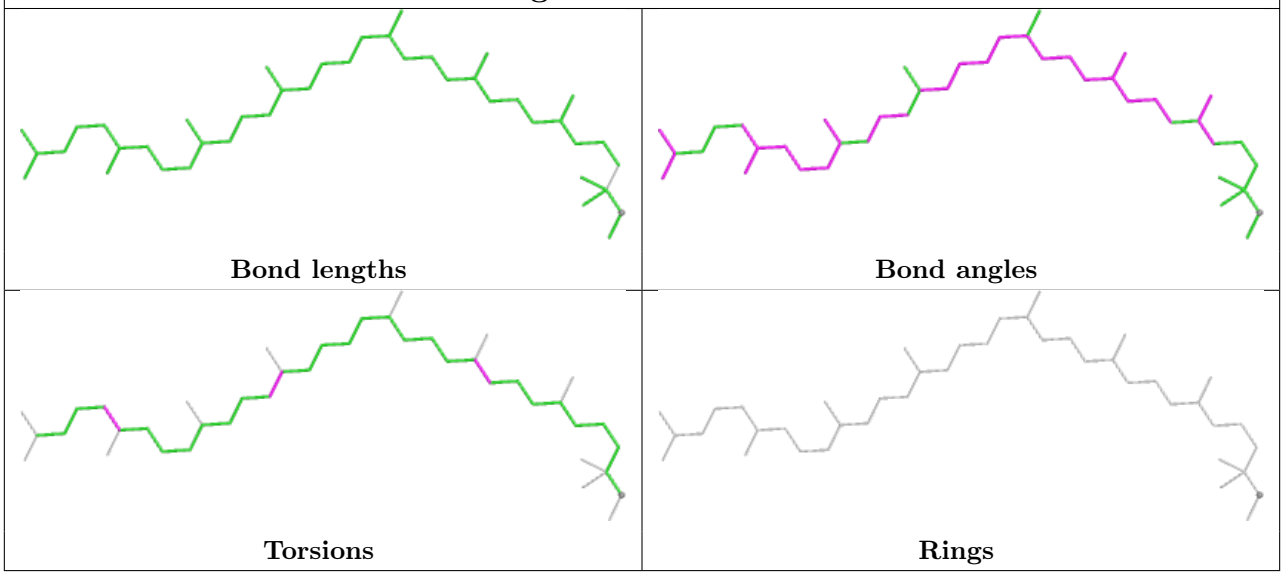
Ligand BCL W 101



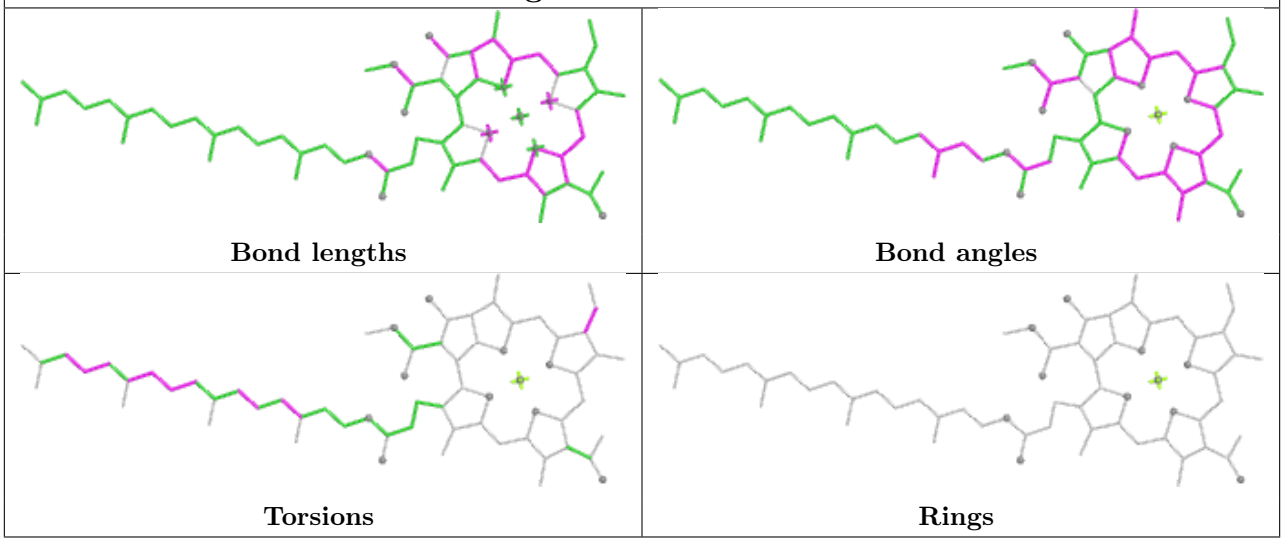
Ligand LMT F 101



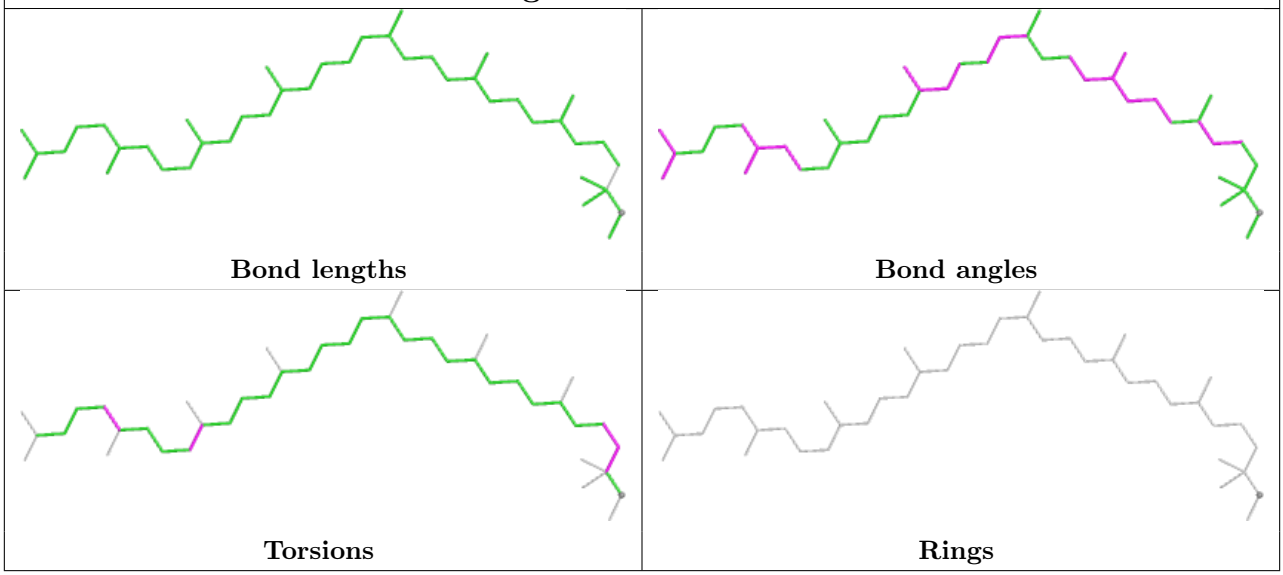
Ligand SPO 1 102

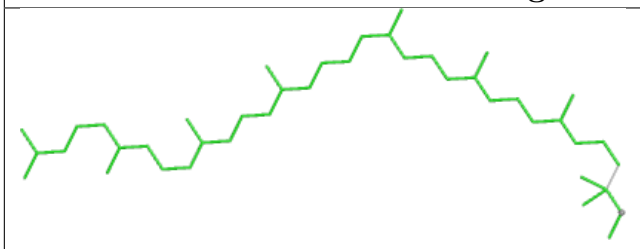
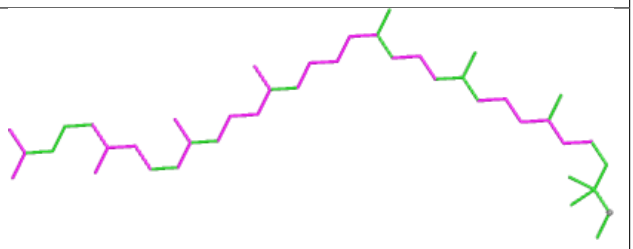
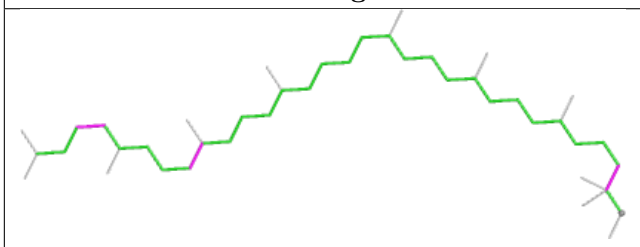
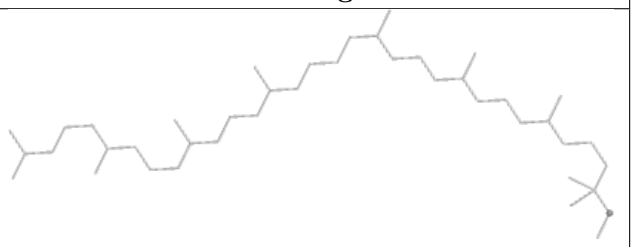


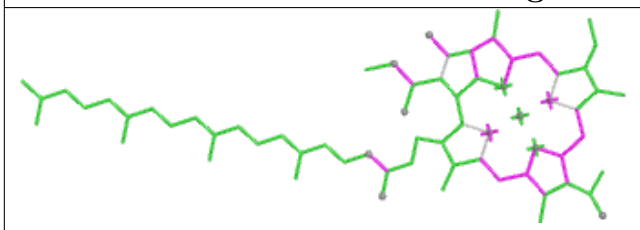
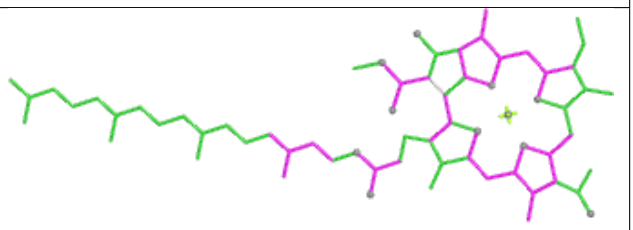
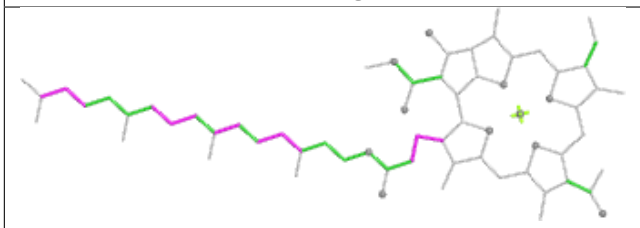
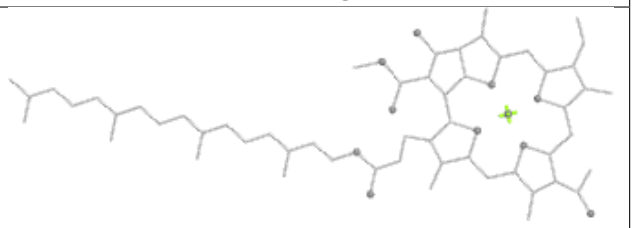
Ligand BCL K 102



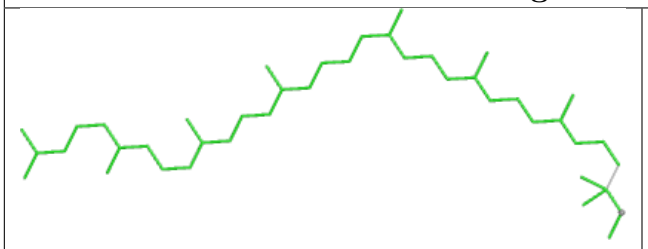
Ligand SPO M 807



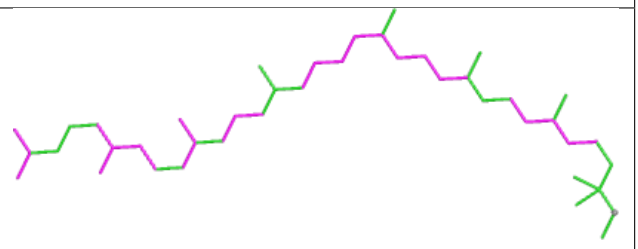
Ligand SPO E 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCL T 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

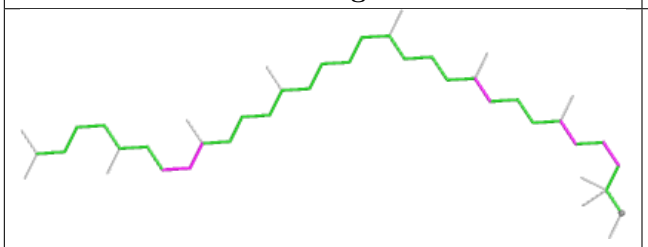
Ligand SPO 5 104



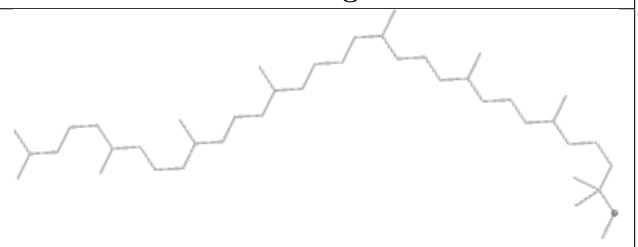
Bond lengths



Bond angles

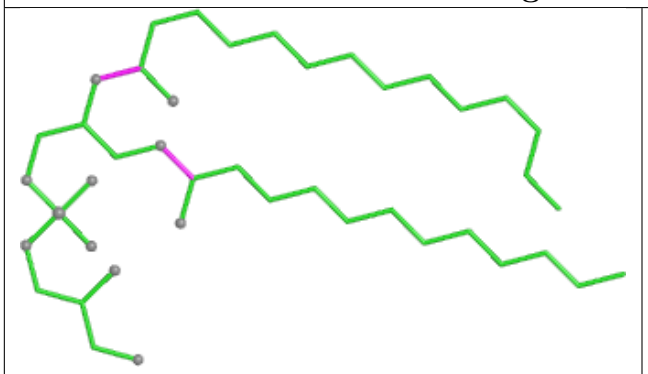


Torsions

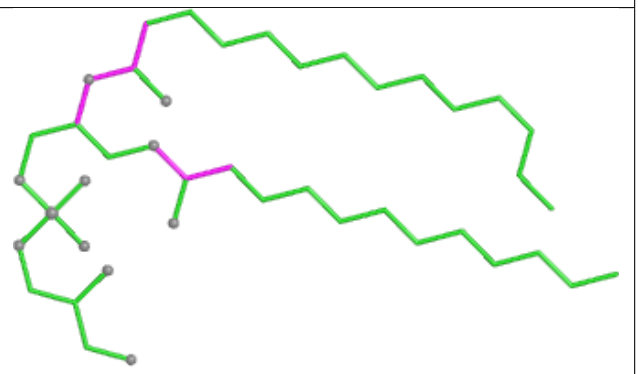


Rings

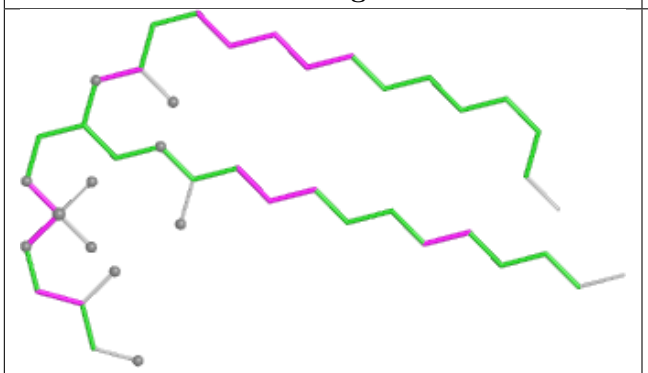
Ligand PGV Y 104



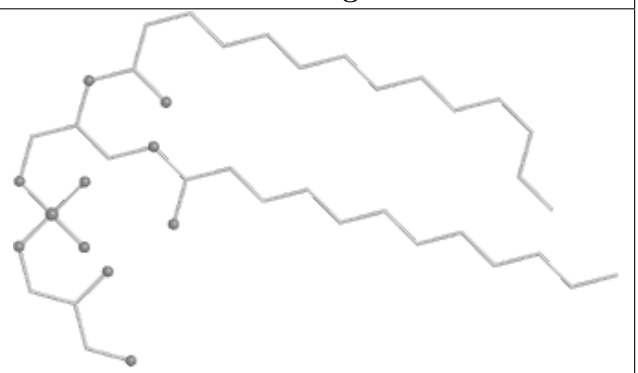
Bond lengths



Bond angles

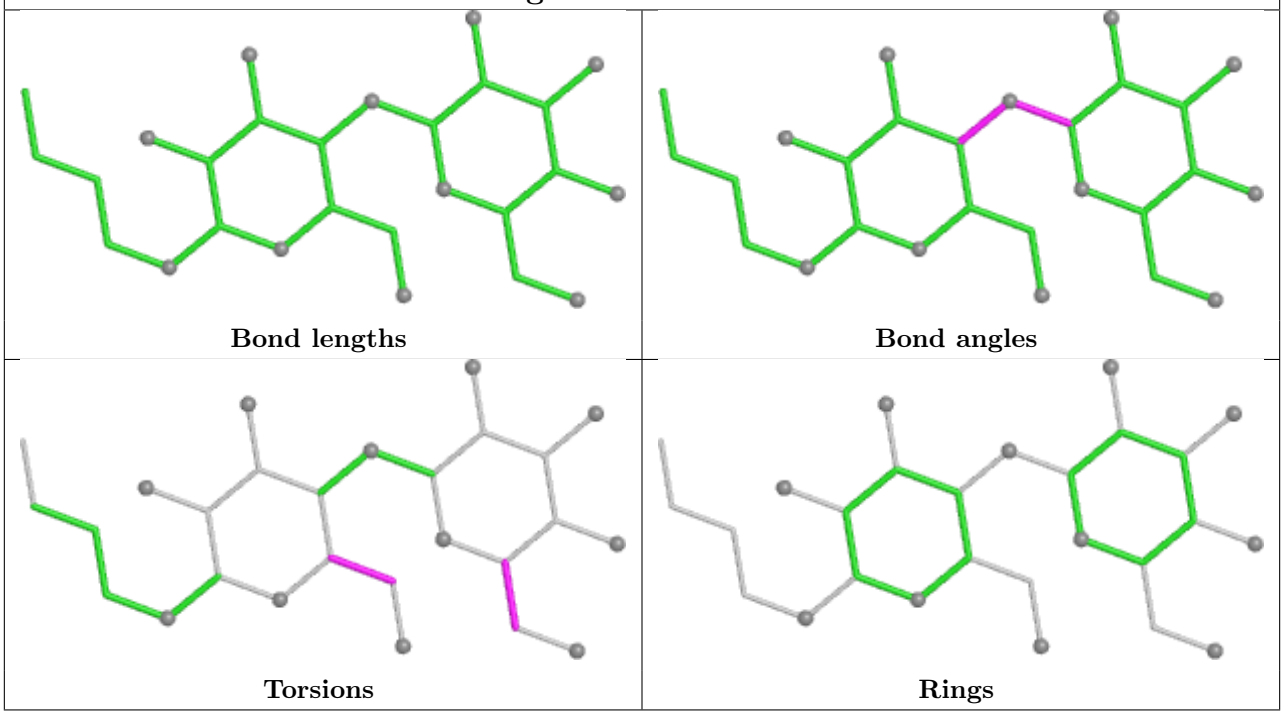


Torsions

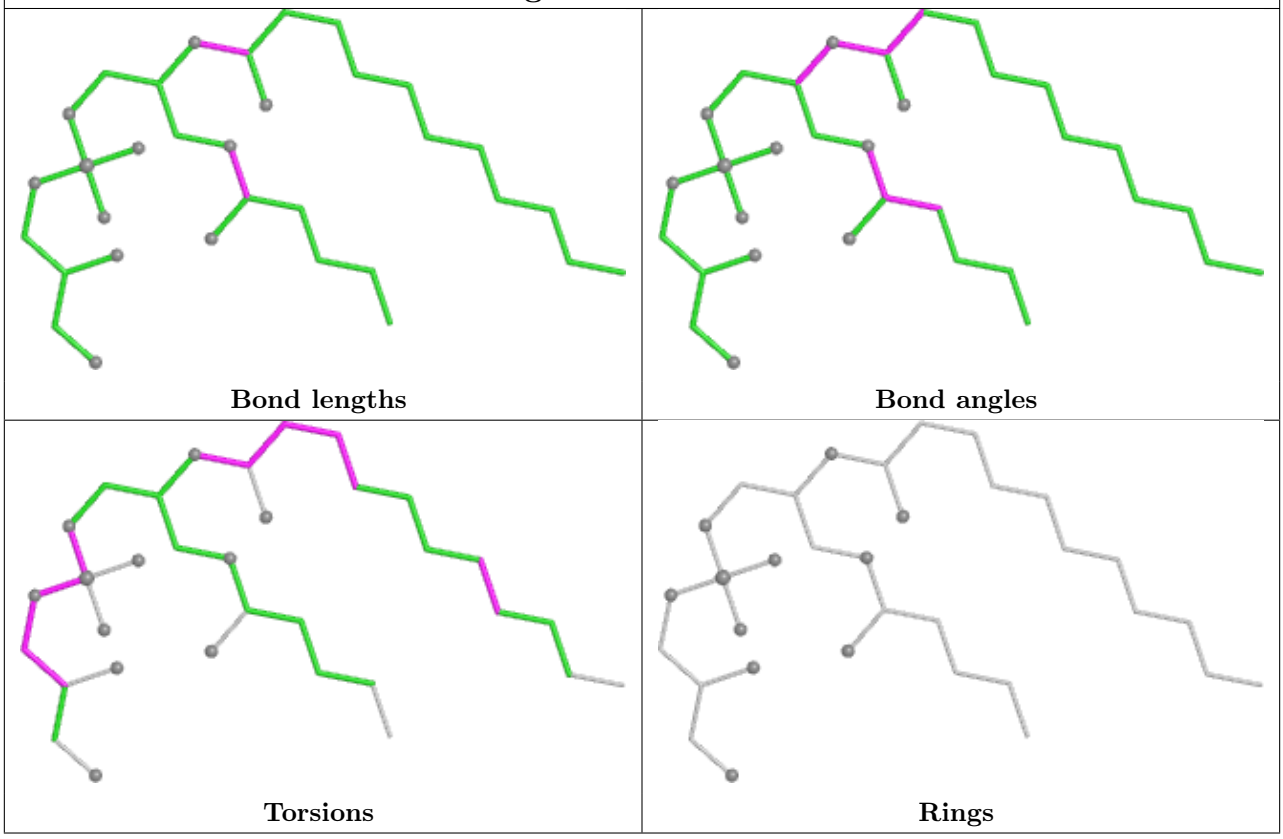


Rings

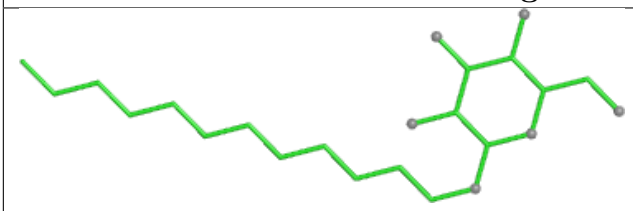
Ligand LMT 4 102



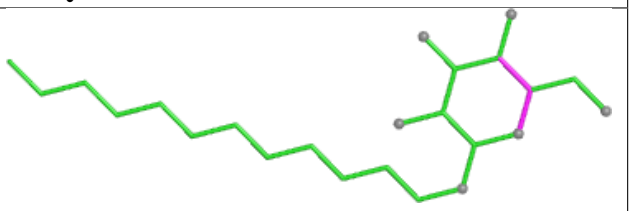
Ligand PGV L 306



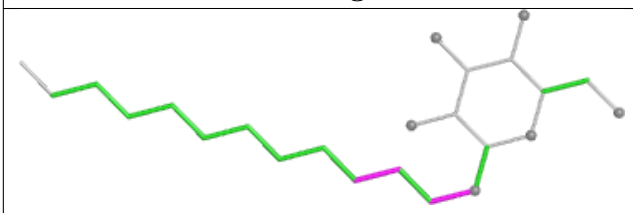
Ligand LMT Q 101



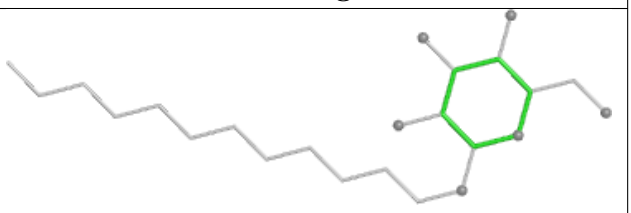
Bond lengths



Bond angles

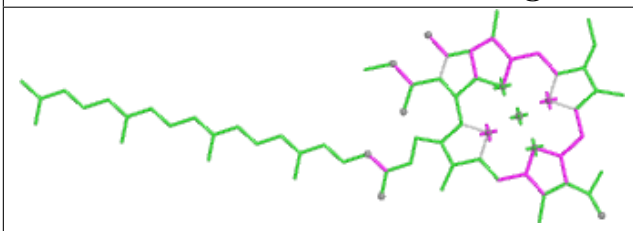


Torsions

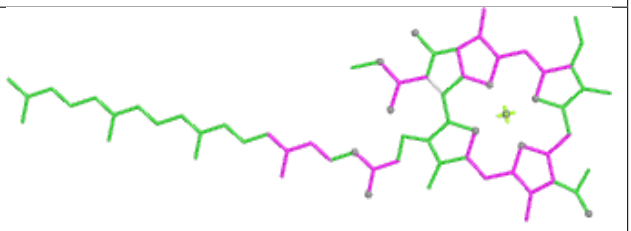


Rings

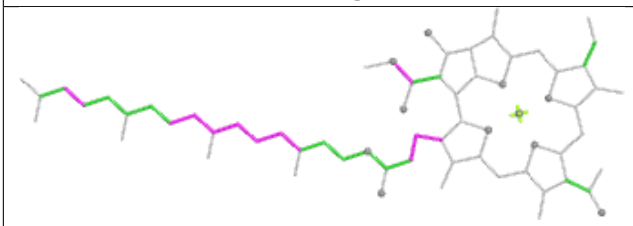
Ligand BCL G 101



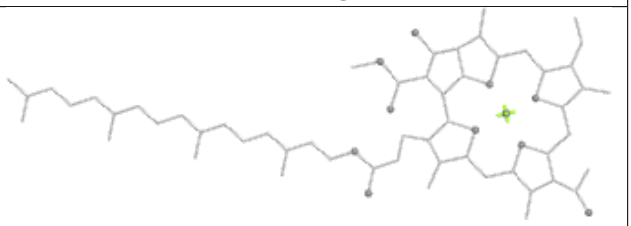
Bond lengths



Bond angles

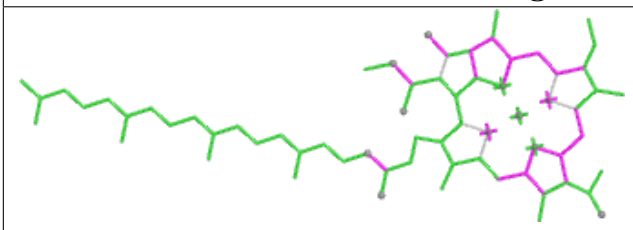


Torsions

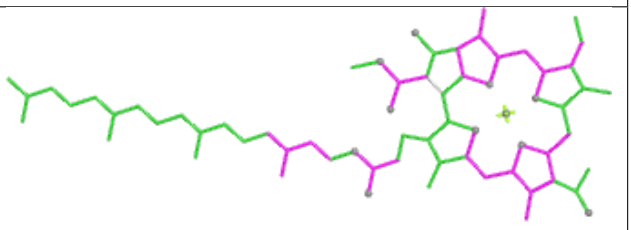


Rings

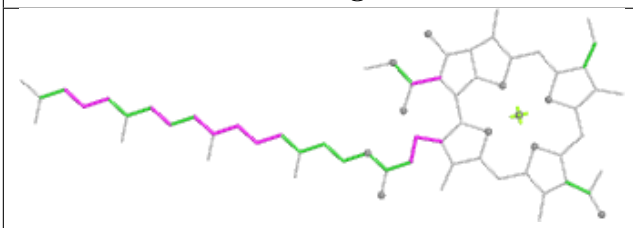
Ligand BCL J 101



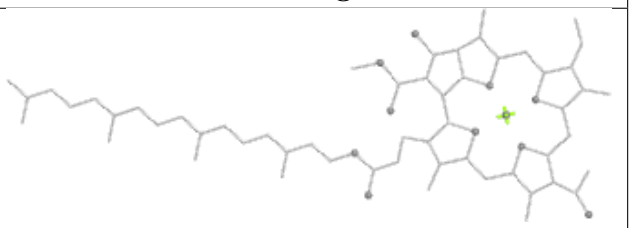
Bond lengths



Bond angles

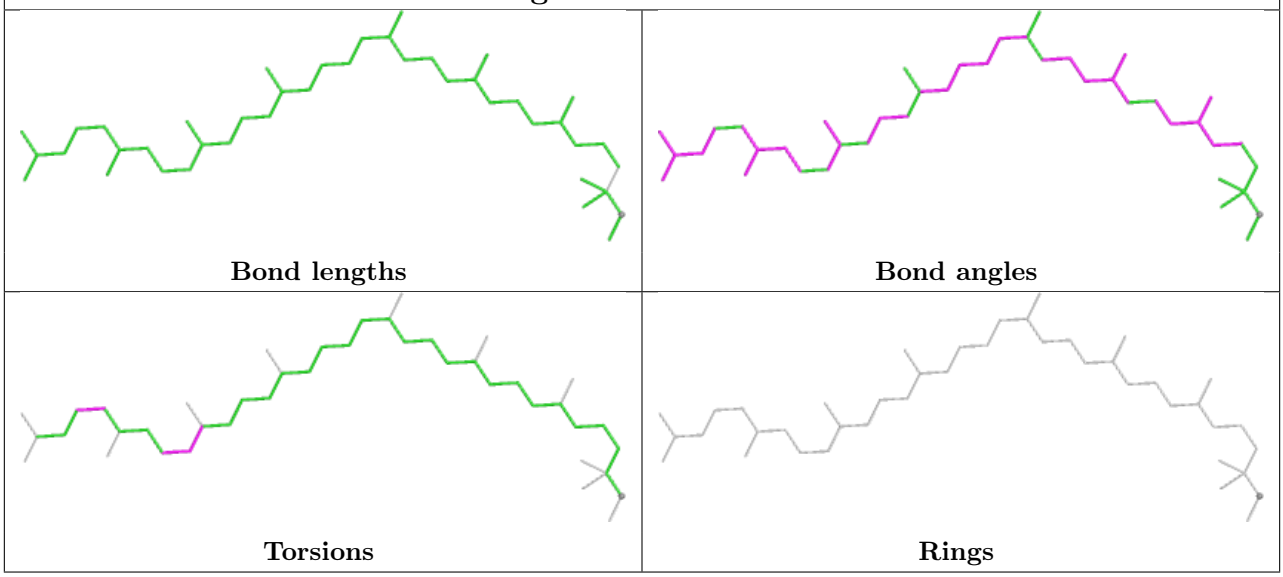


Torsions

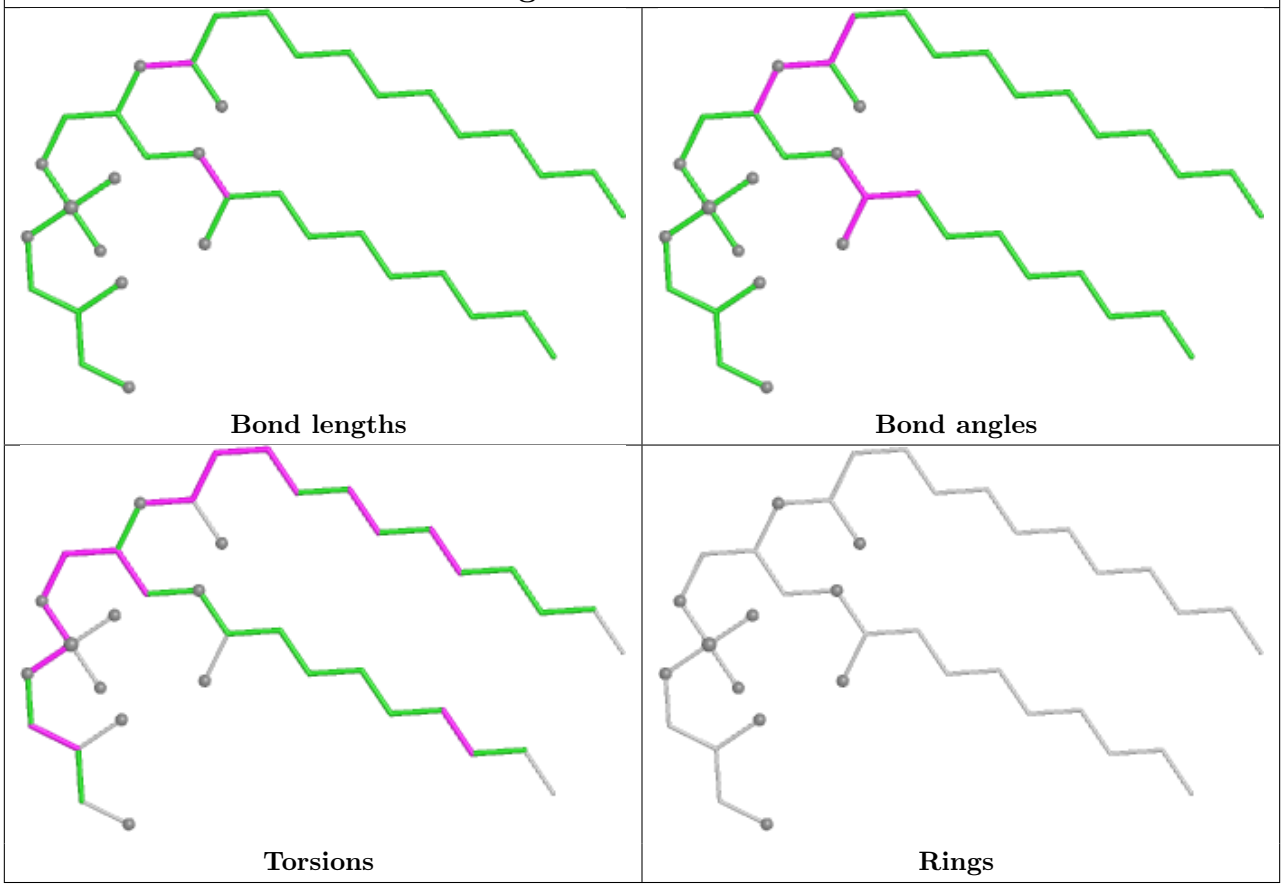


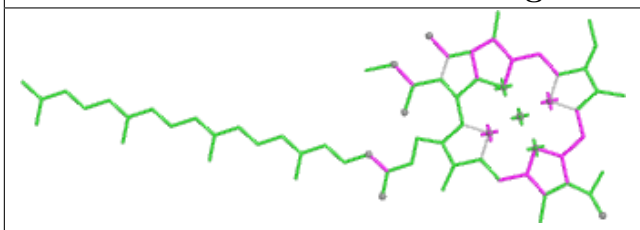
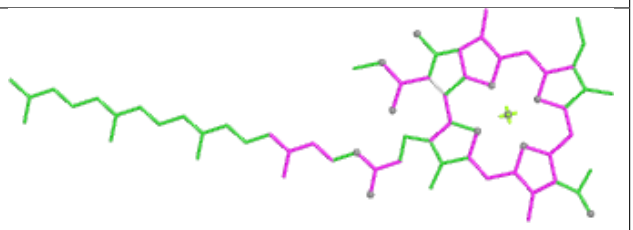
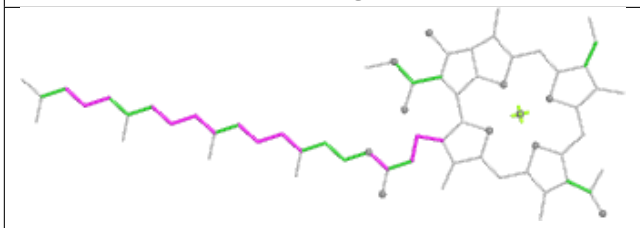
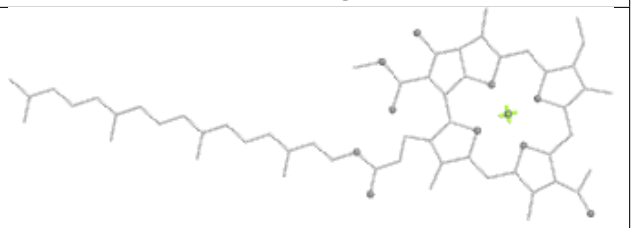
Rings

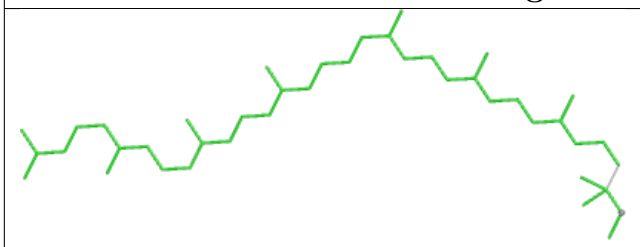
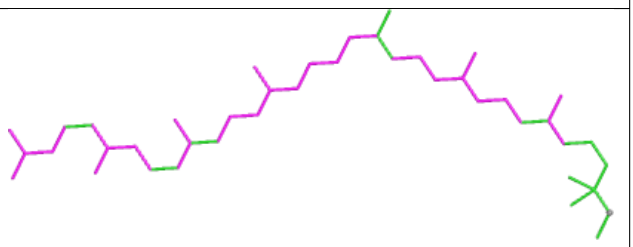
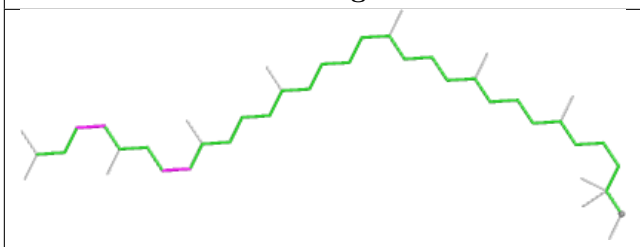
Ligand SPO 1 103



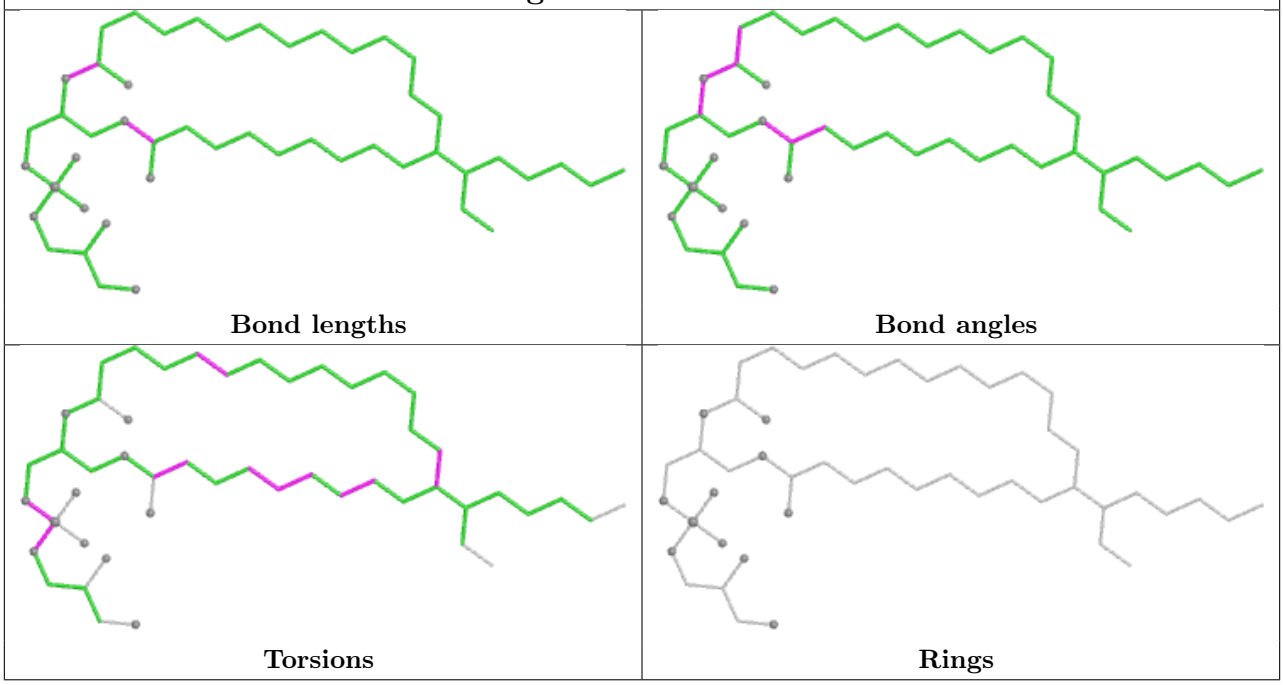
Ligand PGV M 812



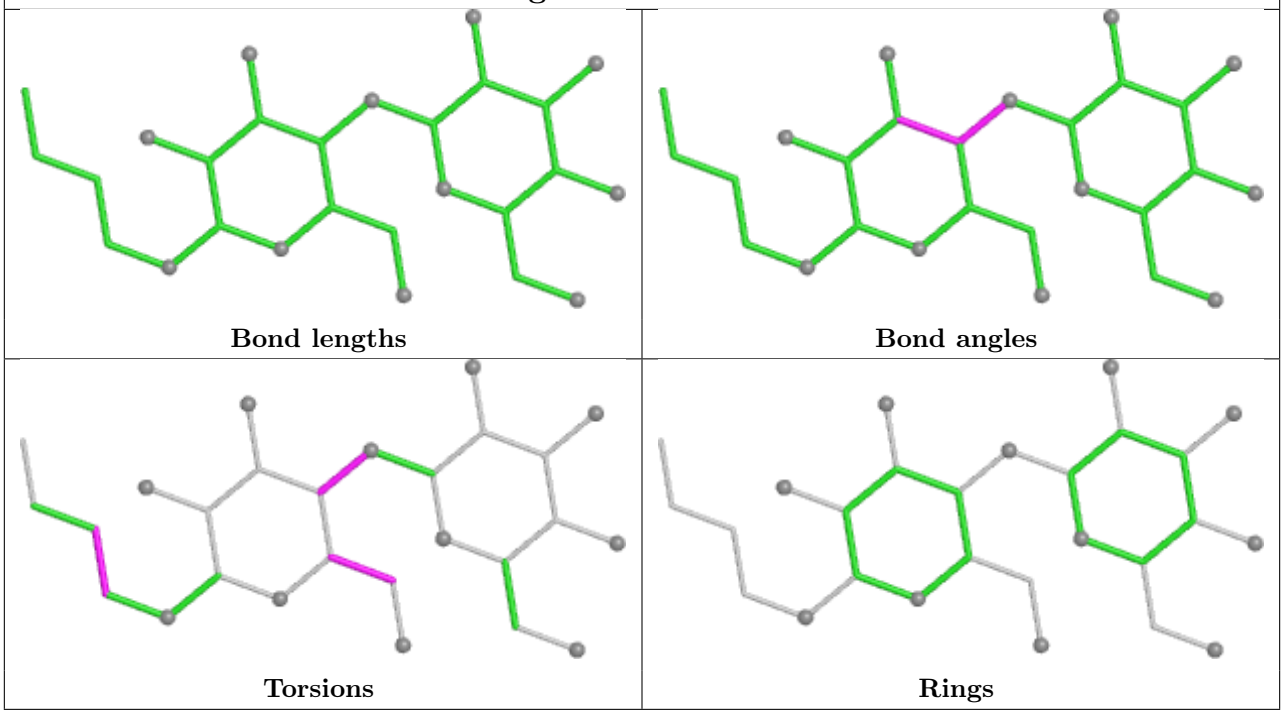
Ligand BCL Y 103	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand SPO D 102	
 Bond lengths	 Bond angles
 Torsions	Rings

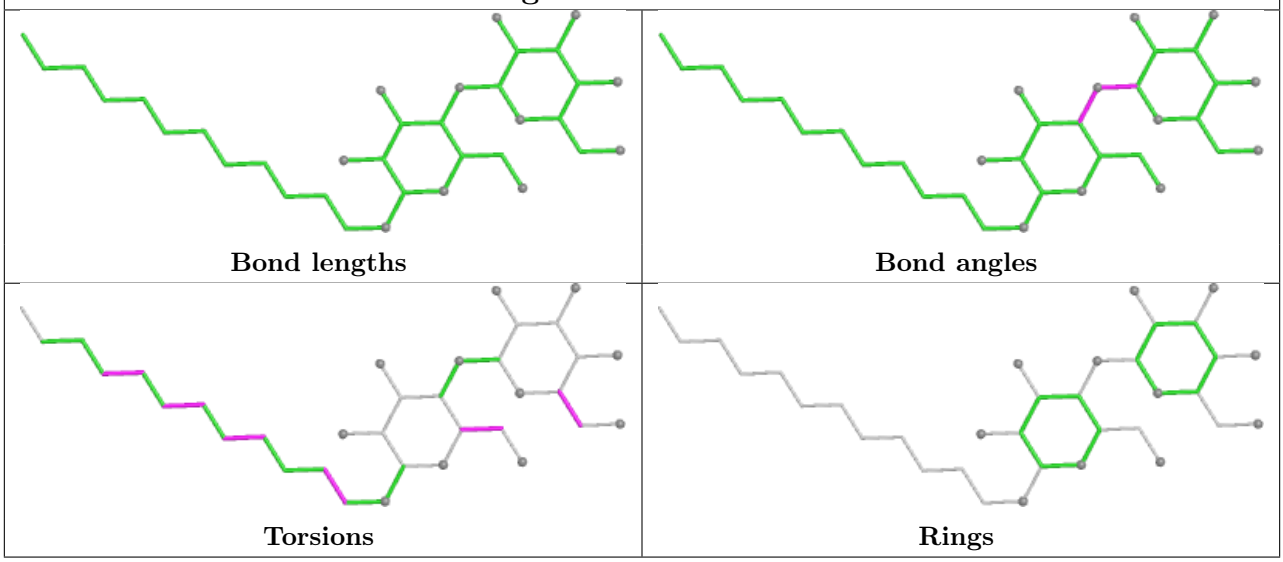
Ligand PGV 3 102



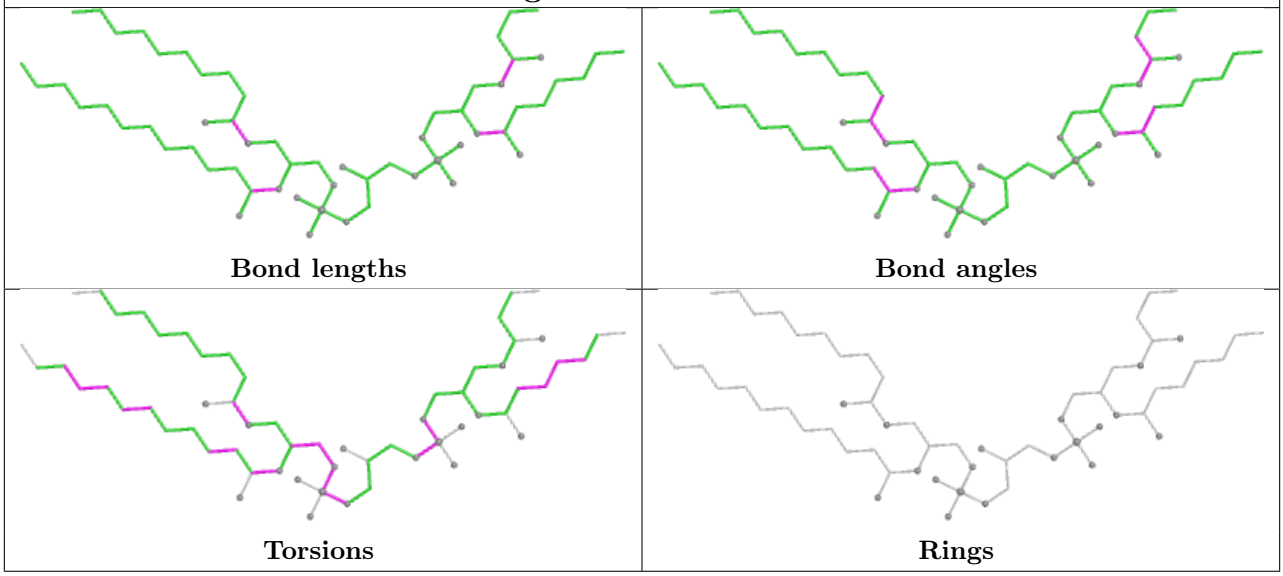
Ligand LMT I 102



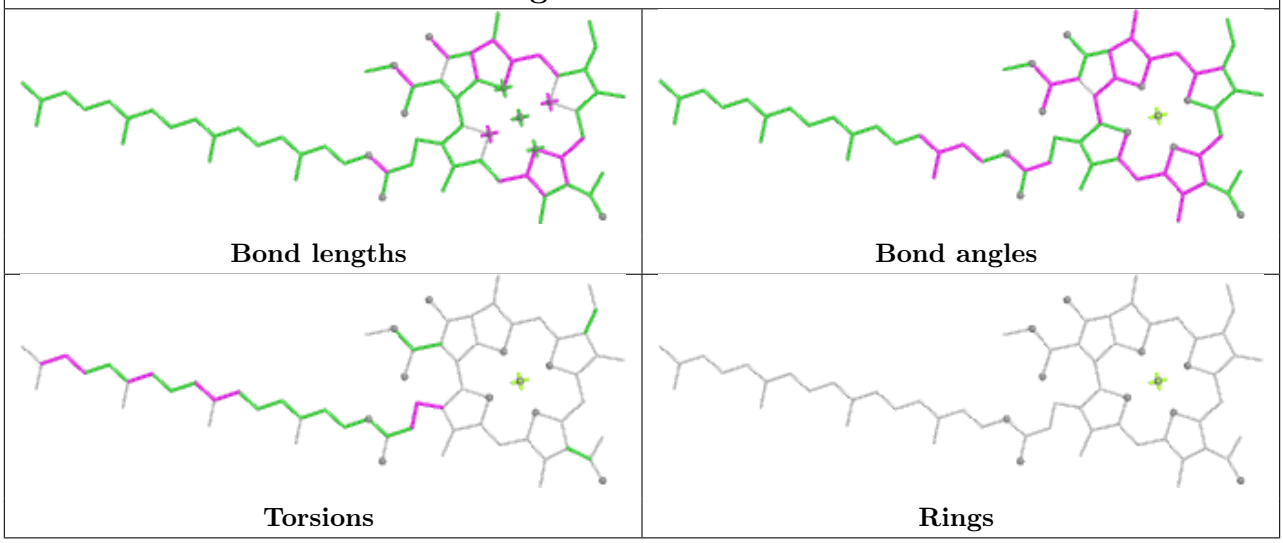
Ligand LMT A 702



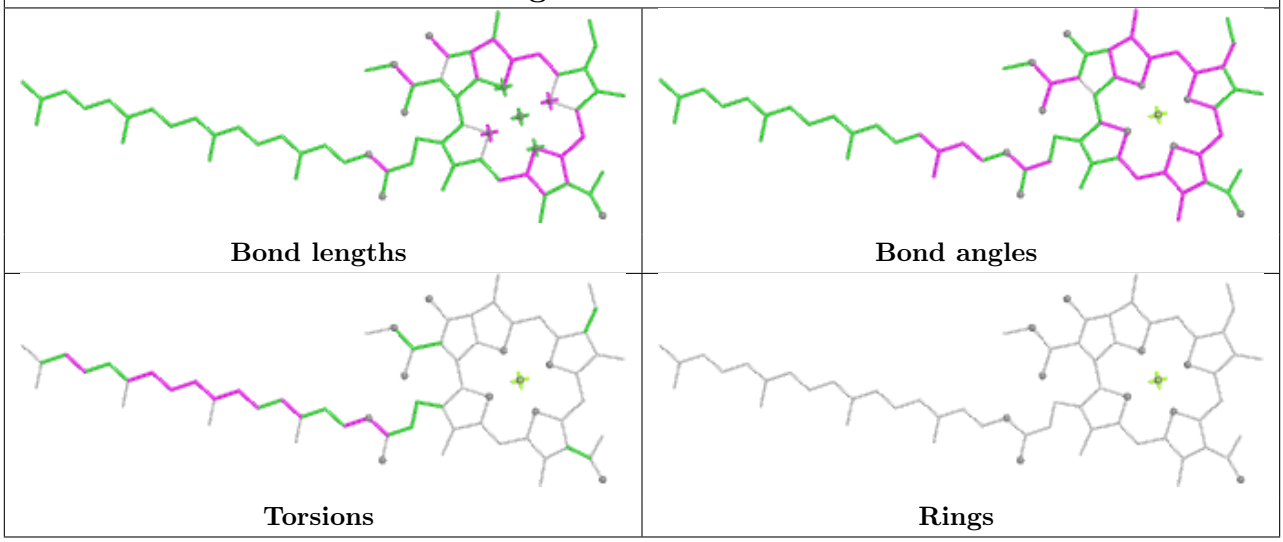
Ligand CDL H 304



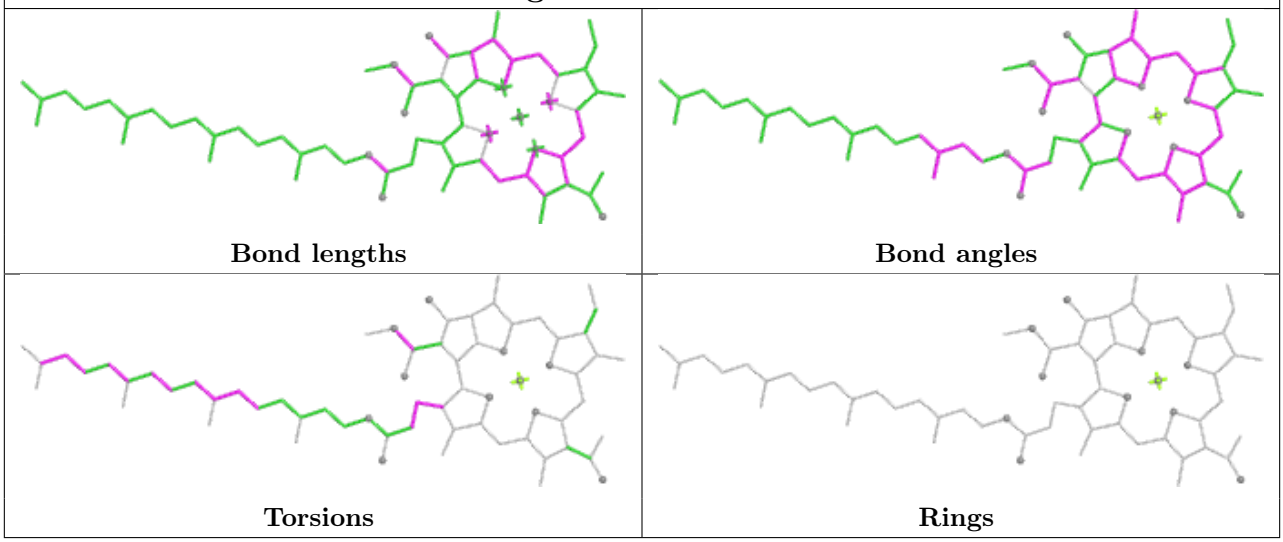
Ligand BCL 4 101



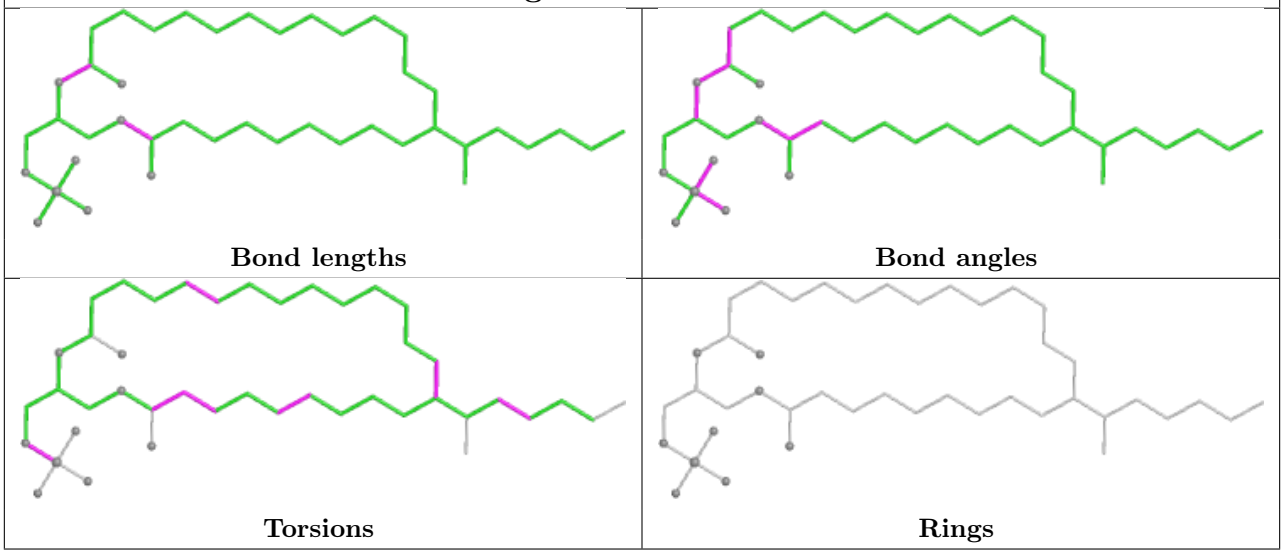
Ligand BCL S 102

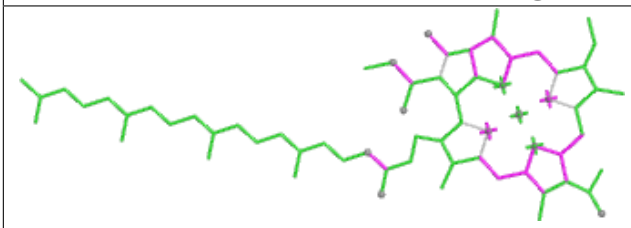
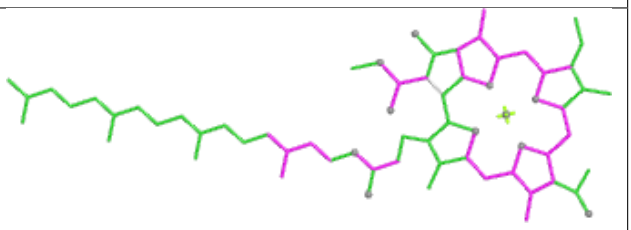
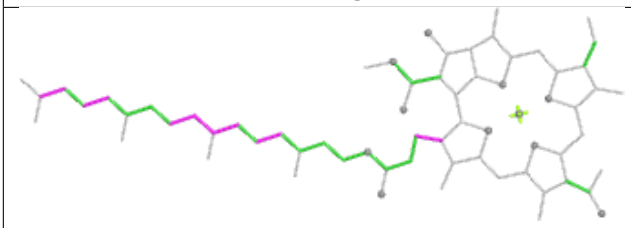
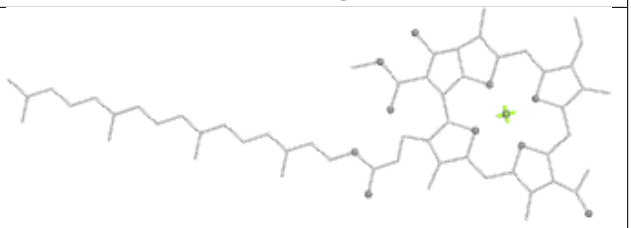


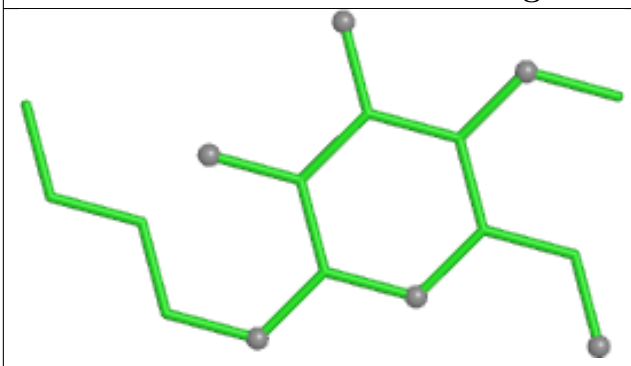
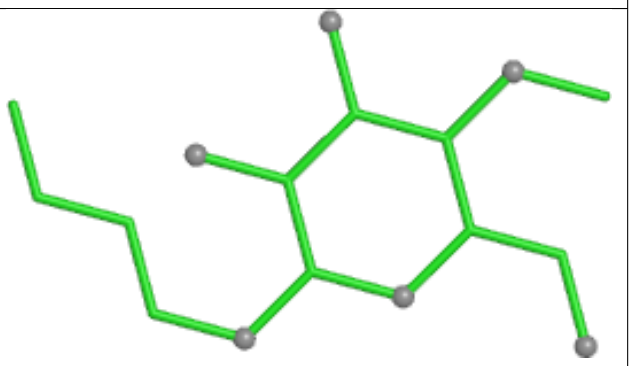
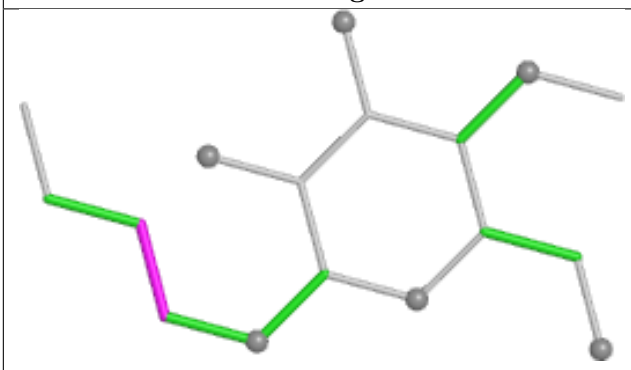
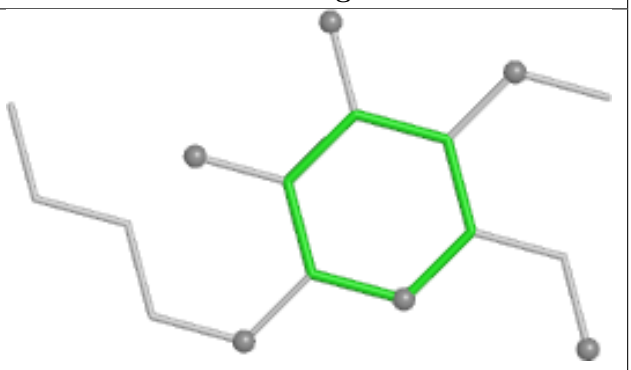
Ligand BCL P 102



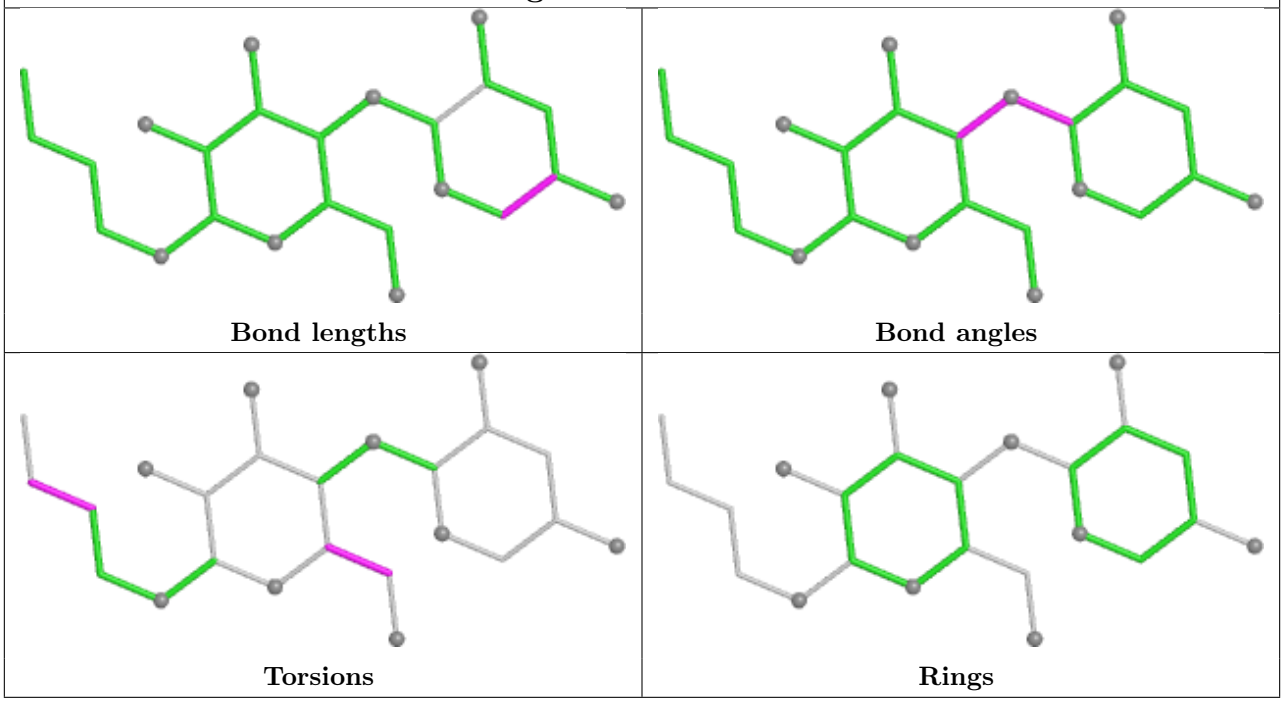
Ligand PGV L 310



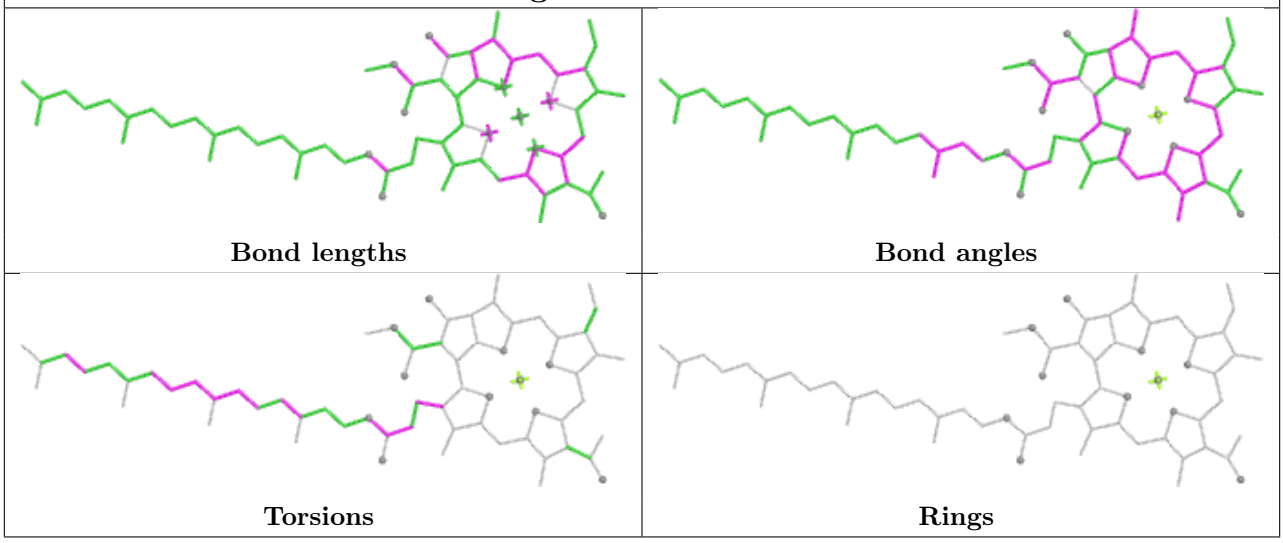
Ligand BCL 3 103	
 Bond lengths	 Bond angles
 Torsions	 Rings

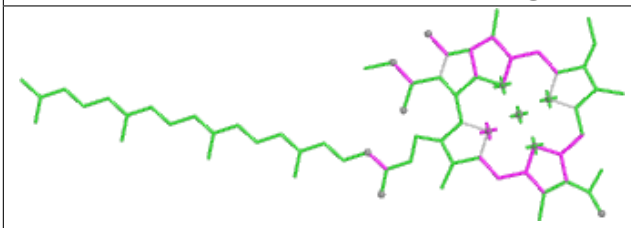
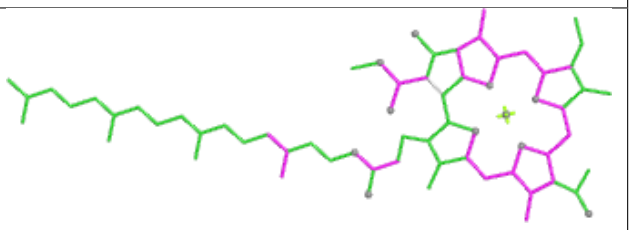
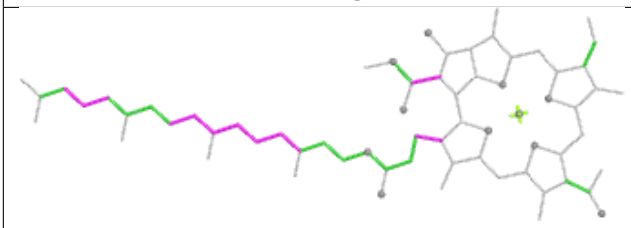
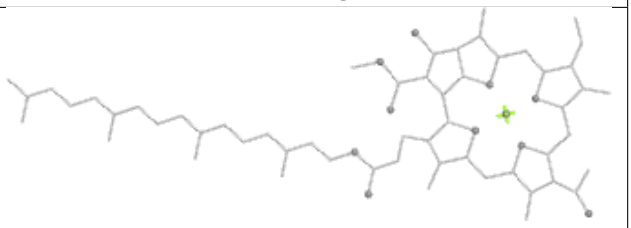
Ligand LMT F 105	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LMT 1 104



Ligand BCL 2 101



Ligand BCL O 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

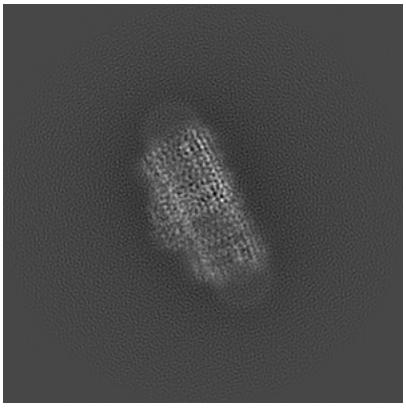
6 Map visualisation (i)

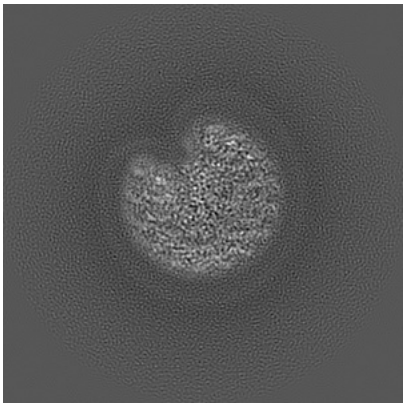
This section contains visualisations of the EMDB entry EMD-31400. These allow visual inspection of the internal detail of the map and identification of artifacts.

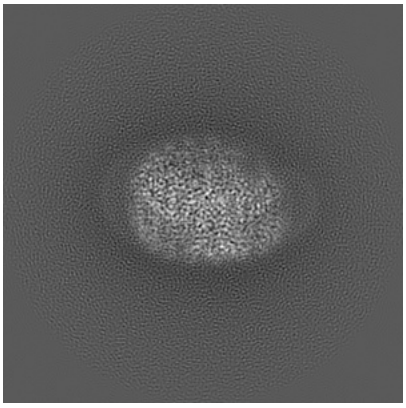
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

6.1.1 Primary map


X

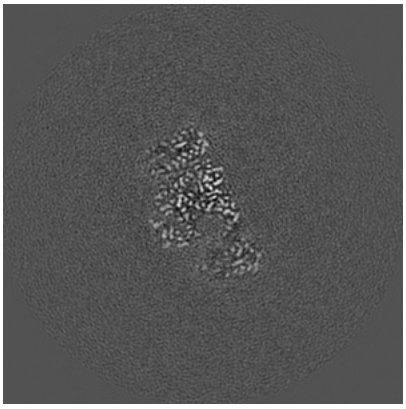

Y

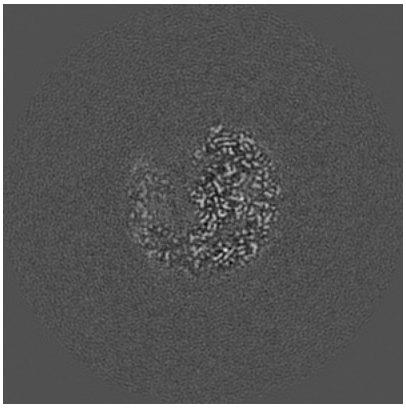

Z

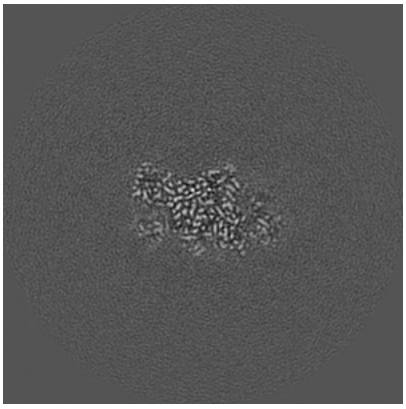
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

6.2.1 Primary map


X Index: 140

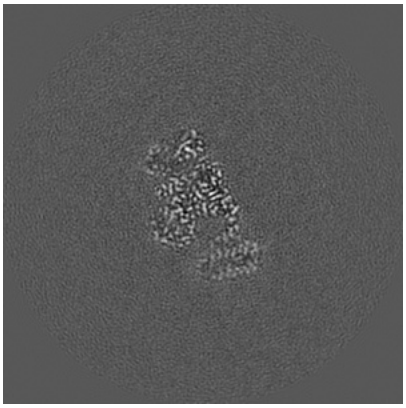

Y Index: 140

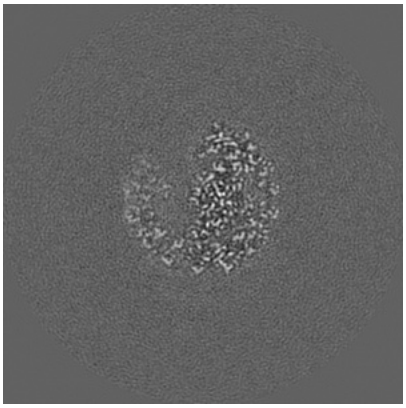

Z Index: 140

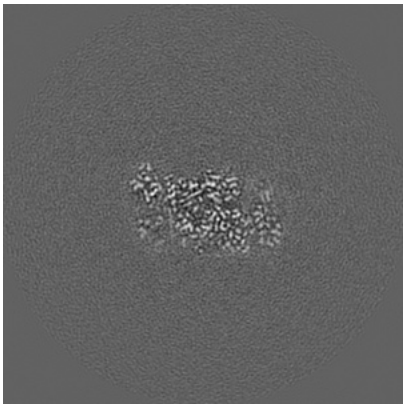
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map


X Index: 142

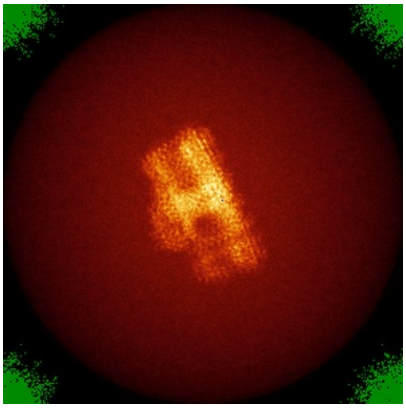

Y Index: 142

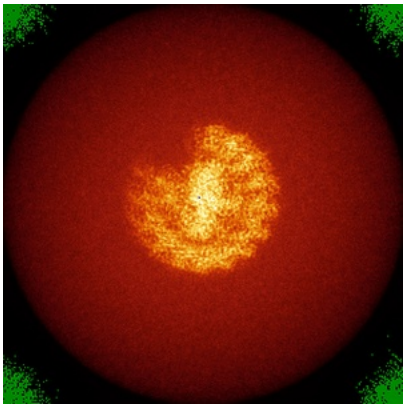

Z Index: 142

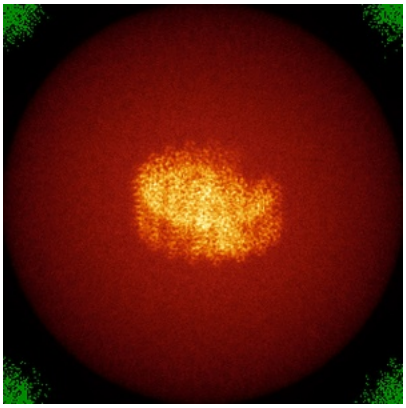
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map


X

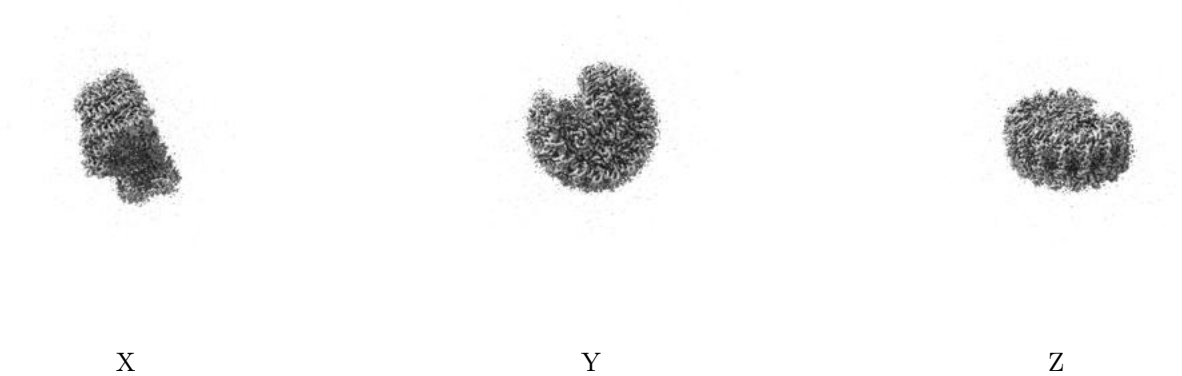

Y


Z

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

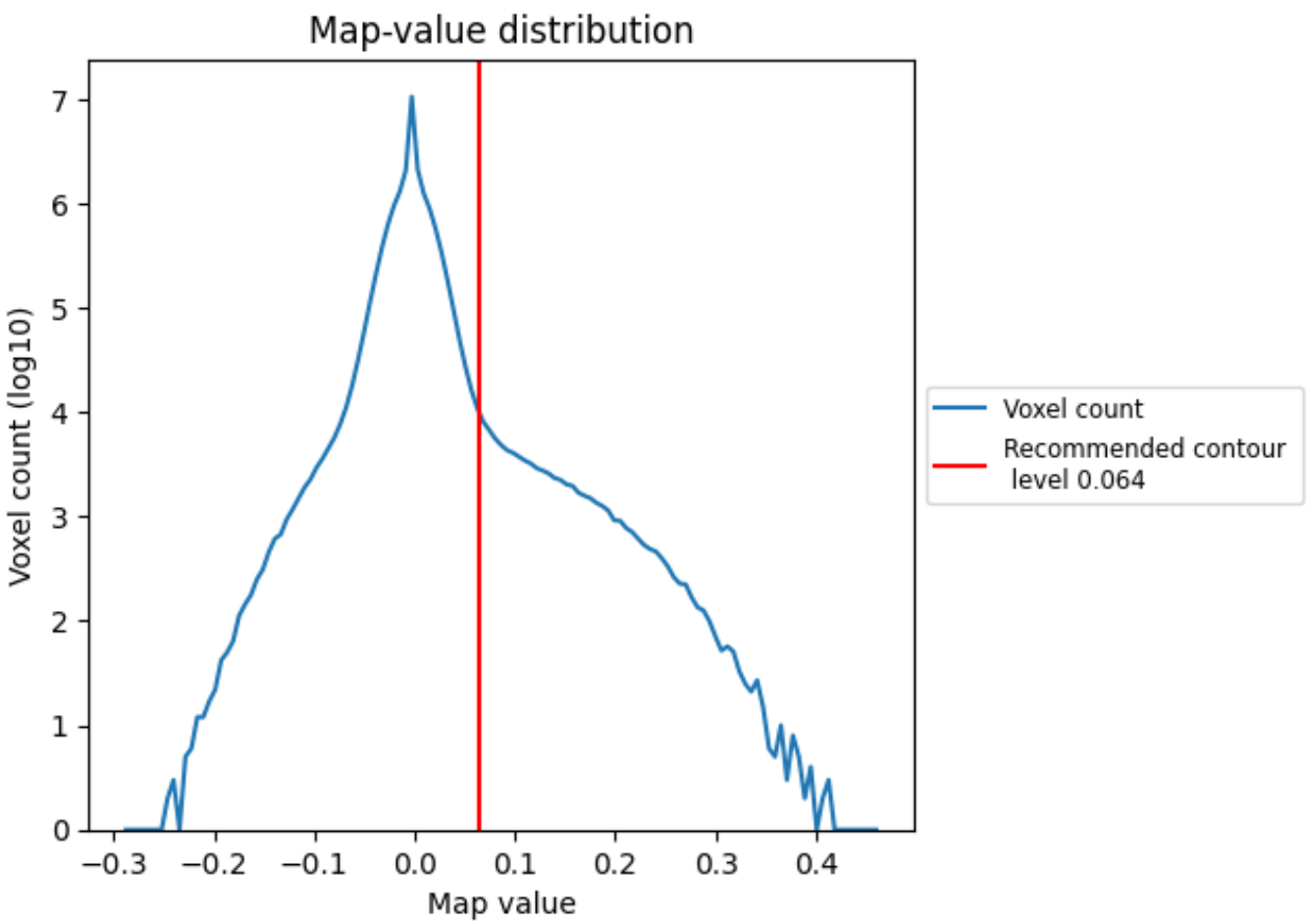
6.6 Mask visualisation (i)

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

7 Map analysis (i)

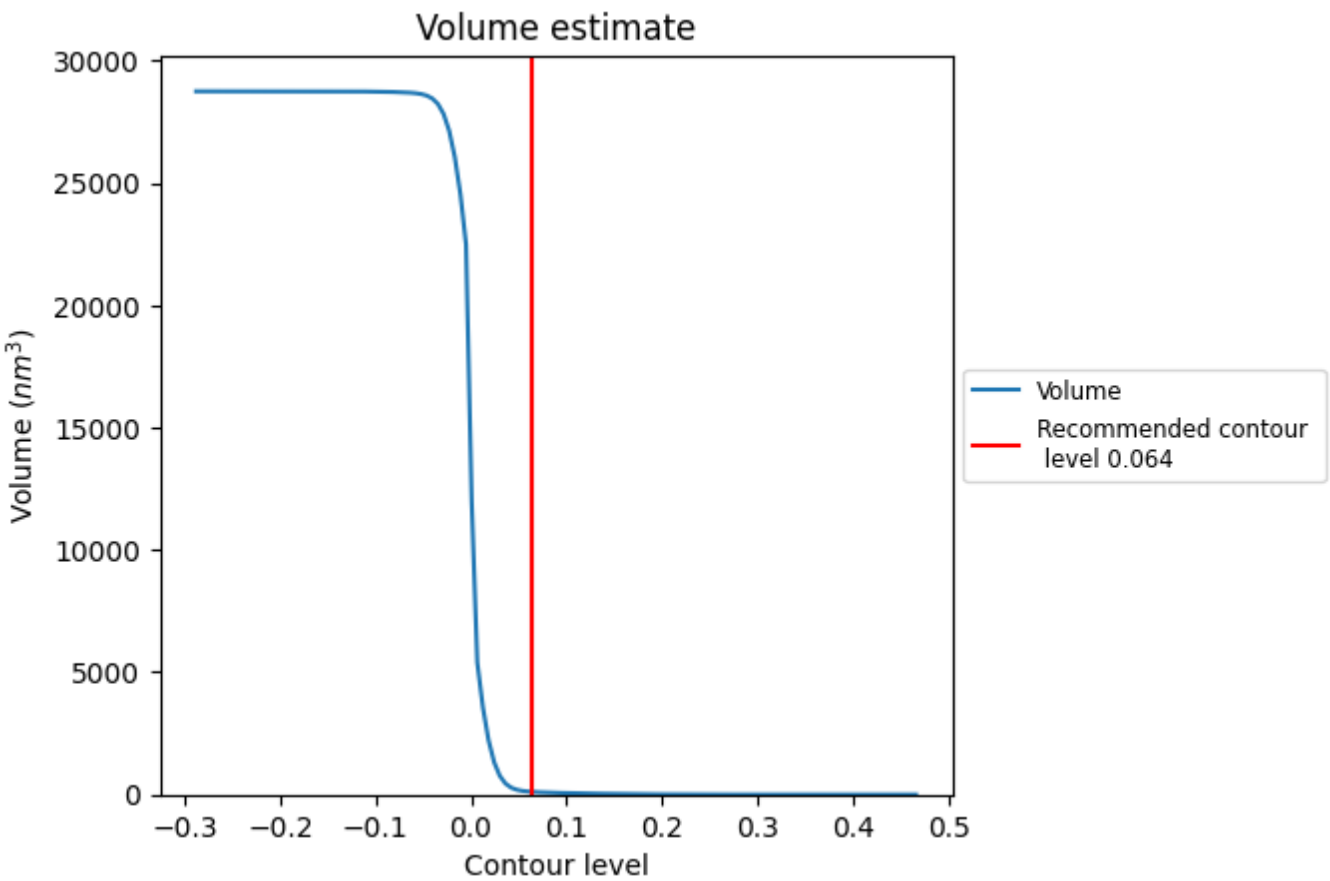
This section contains the results of statistical analysis of the map.

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.

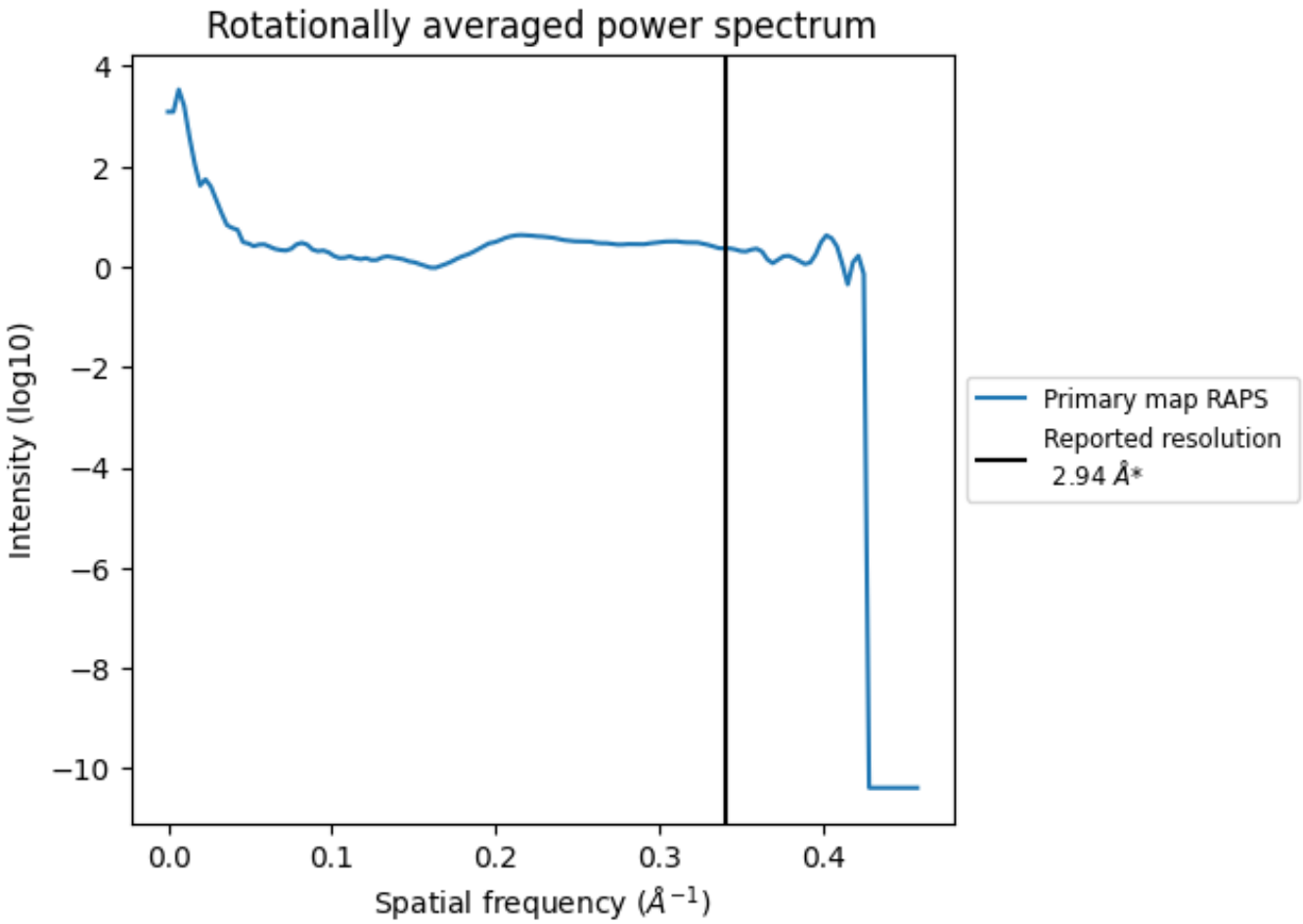
7.2 Volume estimate (i)



The volume at the recommended contour level is 112 nm^3; this corresponds to an approximate mass of 101 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)

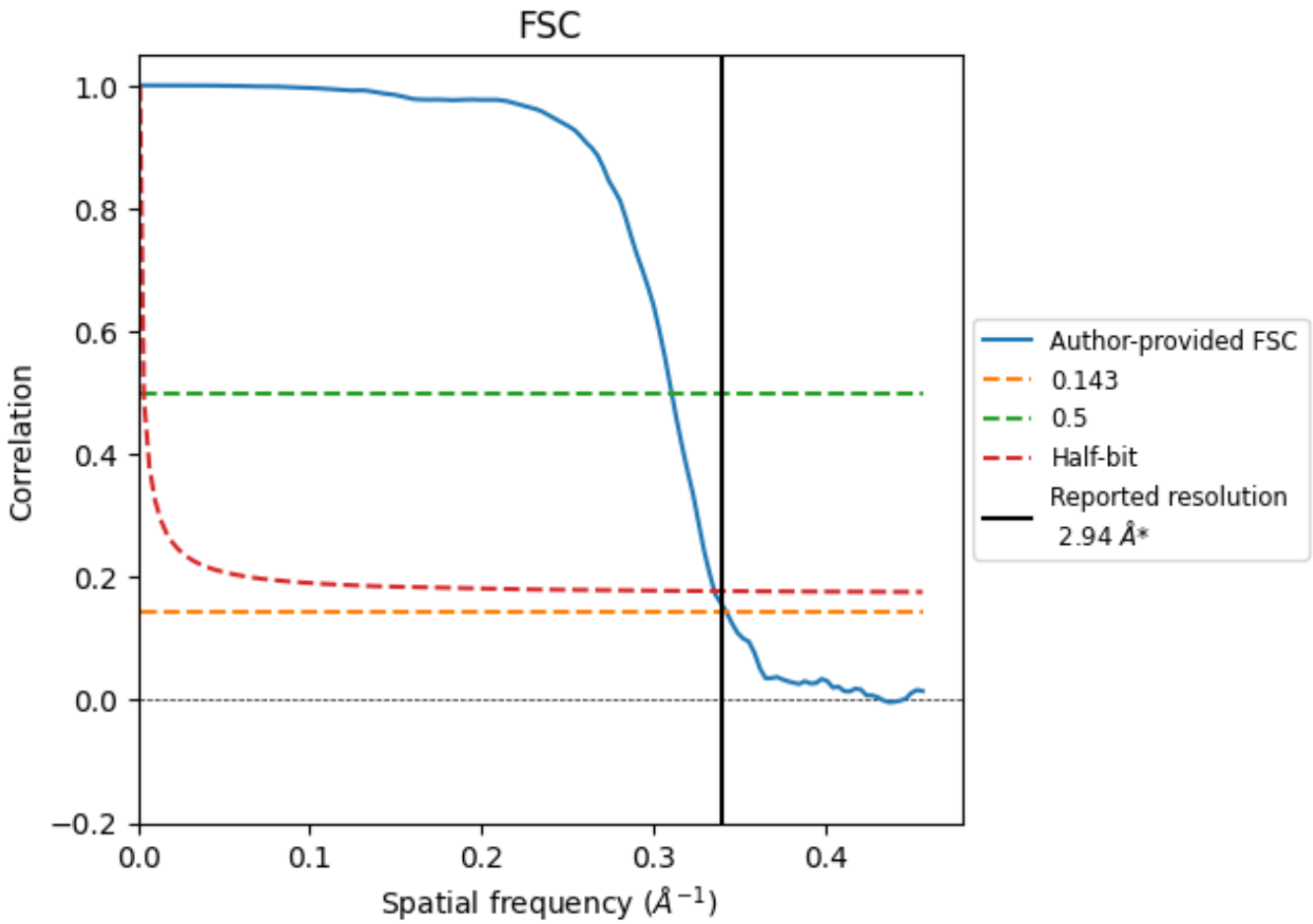


*Reported resolution corresponds to spatial frequency of 0.340 Å^{-1}

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 0.340 Å^{-1}

8.2 Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.94	-	-
Author-provided FSC curve	2.92	3.22	2.98
Unmasked-calculated*	-	-	-

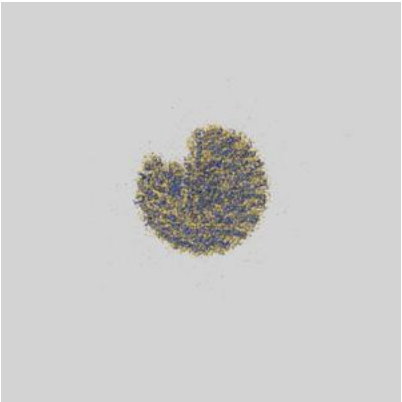
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit (i)

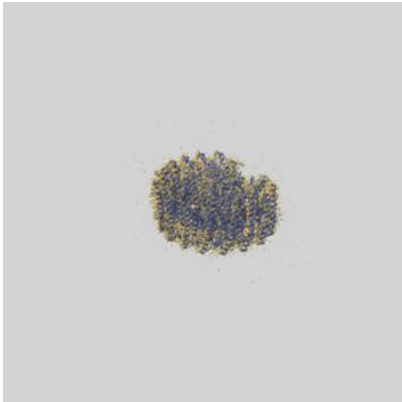
This section contains information regarding the fit between EMDB map EMD-31400 and PDB model 7F0L. Per-residue inclusion information can be found in section 3 on page 18.

9.1 Map-model overlay (i)

X



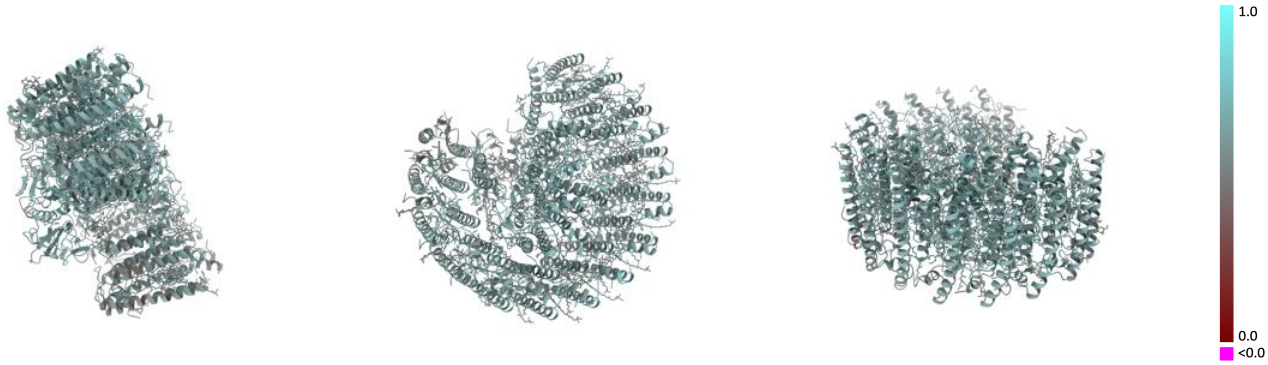
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.064 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.

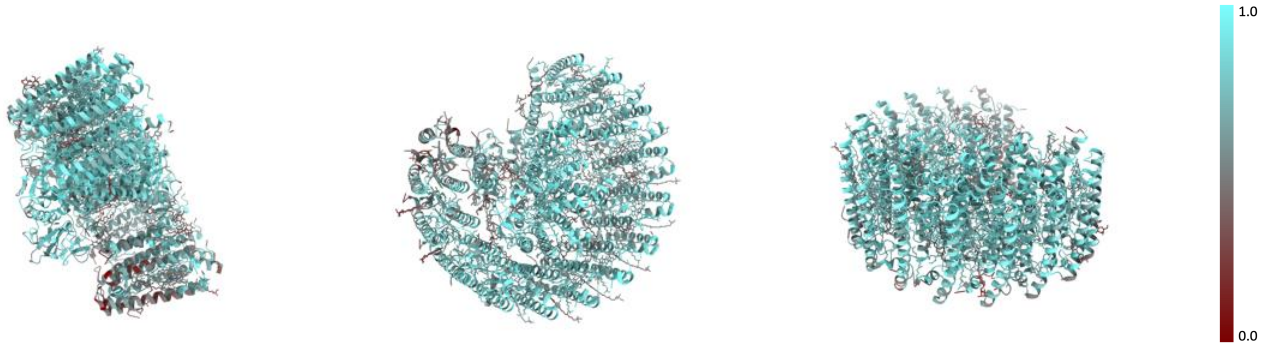
9.2 Q-score mapped to coordinate model (i)



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.

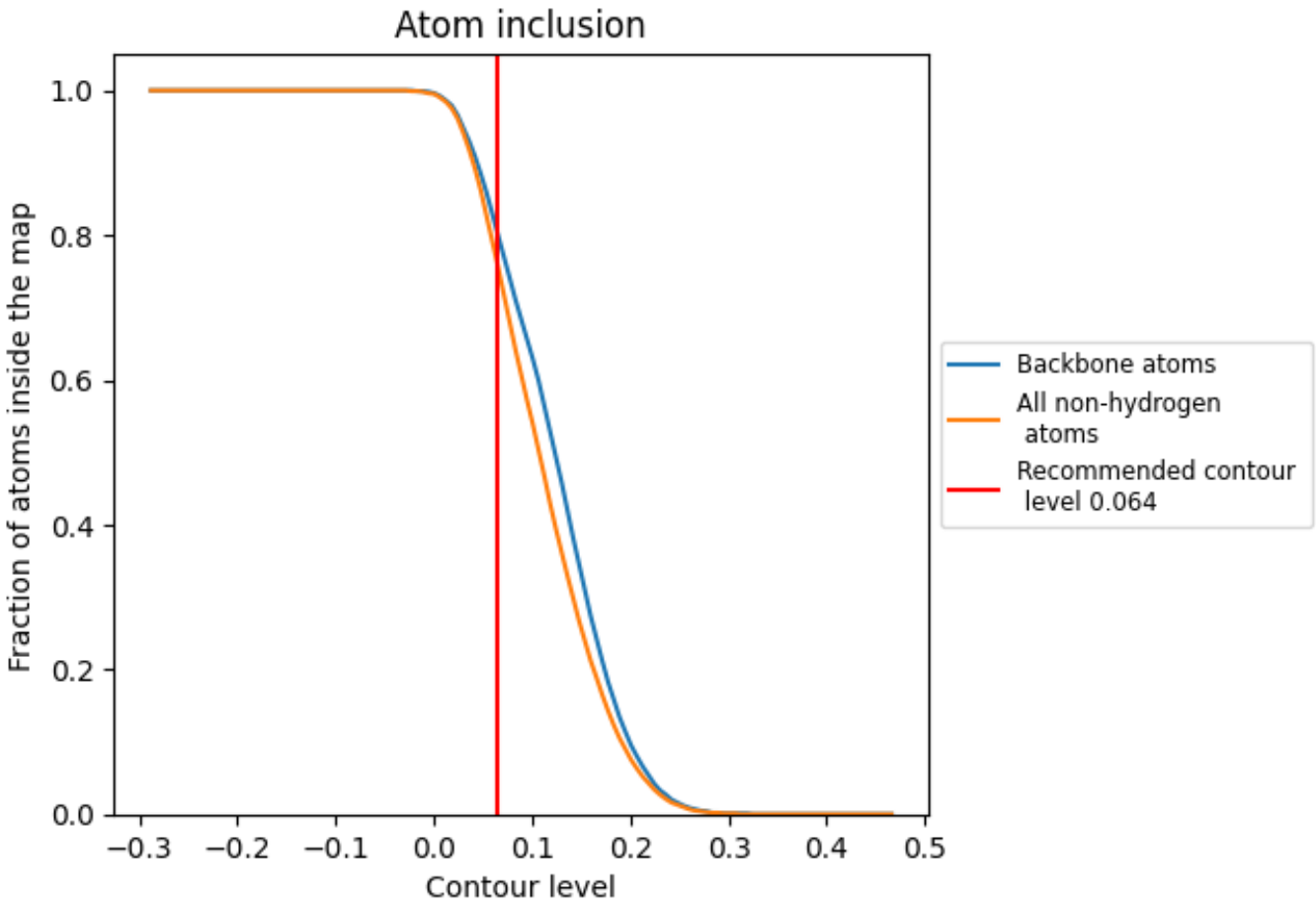
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.064).

9.4 Atom inclusion (i)



At the recommended contour level, 81% of all backbone atoms, 77% 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 (0.064) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7660	0.5970
1	0.7660	0.5980
2	0.7530	0.5810
3	0.6840	0.5720
4	0.6830	0.5670
5	0.6540	0.5810
6	0.6330	0.5530
7	0.5420	0.5360
8	0.4700	0.5080
A	0.7480	0.5780
B	0.7600	0.5800
D	0.8090	0.6140
E	0.8010	0.6060
F	0.7860	0.6070
G	0.7610	0.5920
H	0.7630	0.5980
I	0.8070	0.6070
J	0.8000	0.5950
K	0.7560	0.6060
L	0.8690	0.6310
M	0.8680	0.6330
N	0.7520	0.5950
O	0.7870	0.6020
P	0.7320	0.5920
Q	0.7220	0.5870
R	0.7520	0.5770
S	0.7760	0.5990
T	0.7320	0.5640
U	0.5910	0.5540
V	0.7620	0.5940
W	0.7540	0.5710
X	0.6690	0.5750
Y	0.7400	0.5960
Z	0.7530	0.5810