wwPDB EM Validation Summary Report (i)

Aug 12, 2026 – 09:30 PM JST

PDB ID	:	8Z82 / pdb_00008z82
EMDB ID	:	EMD-39836
Title	:	Photosynthetic LH1-RC-HiPIP complex from the purple bacterium Halorhodospira halophila
Authors	:	Tani, K.; Kanno, R.; Nagashima, K.V.P.; Hiwatashi, N.; Kawakami, M.; Nakata, K.; Nagashima, S.; Inoue, K.; Takaichi, S.; Purba, E.R.; Hall, M.; Yu, L.-J.; Madigan, M.T.; Mizoguchi, A.; Humbel, B.M.; Kimura, Y.; Wang-Otomo, Z.-Y.
Deposited on	:	2024-04-21
Resolution	:	2.40 Å(reported)
Based on initial models	:	5Y5S, 5D8V

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:

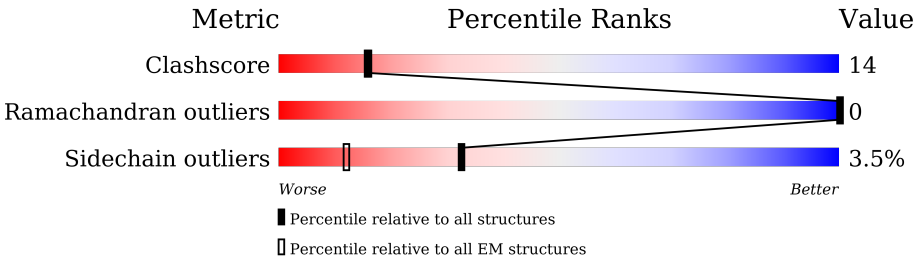
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using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

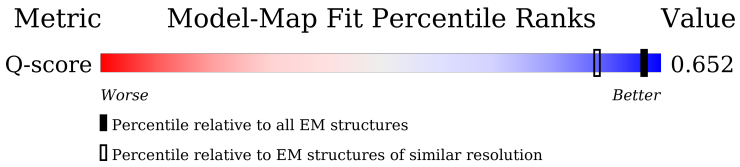
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.40 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	5628 (1.90 - 2.90)

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	C	362	75% 15% • 7%
2	L	276	75% 24% ••
3	M	323	77% 21% ••

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Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

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Mol	Chain	Length	Quality of chain
4	H	278	77% 23%
5	3	64	52% 20% 28%
5	7	64	48% 22% 28%
5	A	64	56% 14% 28%
5	F	64	56% 12% 28%
5	K	64	53% 17% 28%
5	Q	64	47% 25% 28%
5	U	64	52% 19% 28%
5	Y	64	58% 14% 28%
6	4	75	49% 13% 37%
6	8	75	49% 13% 37%
6	B	75	47% 16% 36%
6	G	75	49% 12% 37%
6	N	75	44% 19% 37%
6	R	75	52% 9% 37%
6	V	75	55% 8% 37%
6	Z	75	49% 15% 36%
7	1	67	42% 27% 31%
7	5	67	45% 24% 31%
7	9	67	46% 22% 31%
7	D	67	43% 25% 31%
7	I	67	42% 24% 31%
7	O	67	52% 15% 31%
7	S	67	45% 22% 31%
7	W	67	46% 22% 31%

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Mol	Chain	Length	Quality of chain
8	0	74	39% 19% • 39%
8	2	74	47% 14% 39%
8	6	74	54% 5% • 39%
8	E	74	53% 8% 39%
8	J	74	45% 16% 39%
8	P	74	50% 11% 39%
8	T	74	51% 9% 39%
8	X	74	• 50% 11% 39%
9	a	142	5% 49% 18% • 32%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	HEC	C	401	X	-	-	-
10	HEC	C	402	X	-	-	-
10	HEC	C	403	X	-	-	-
10	HEC	C	404	X	-	-	-

2 Entry composition (i)

There are 24 unique types of molecules in this entry. The entry contains 29045 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 cytochrome c subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	C	336	2642	1616	453	549	24	0	0

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	33	THR	SER	conflict	UNP A1WXF5
C	47	ASN	THR	conflict	UNP A1WXF5
C	72	ARG	LYS	conflict	UNP A1WXF5
C	84	ASP	THR	conflict	UNP A1WXF5
C	103	SER	ALA	conflict	UNP A1WXF5
C	143	ASP	GLU	conflict	UNP A1WXF5
C	172	THR	GLU	conflict	UNP A1WXF5
C	173	PRO	LEU	conflict	UNP A1WXF5
C	175	VAL	PHE	conflict	UNP A1WXF5
C	177	MET	VAL	conflict	UNP A1WXF5
C	178	ALA	HIS	conflict	UNP A1WXF5
C	183	THR	ASP	conflict	UNP A1WXF5
C	184	MET	GLN	conflict	UNP A1WXF5
C	193	THR	VAL	conflict	UNP A1WXF5
C	194	GLU	GLY	conflict	UNP A1WXF5
C	195	TYR	PHE	conflict	UNP A1WXF5
C	202	ALA	VAL	conflict	UNP A1WXF5
C	223	HIS	ASN	conflict	UNP A1WXF5
C	239	SER	GLY	conflict	UNP A1WXF5
C	246	ALA	ASP	conflict	UNP A1WXF5
C	269	GLU	VAL	conflict	UNP A1WXF5
C	289	ILE	MET	conflict	UNP A1WXF5
C	298	GLU	ASP	conflict	UNP A1WXF5
C	341	ALA	GLU	conflict	UNP A1WXF5
C	354	ASP	GLU	conflict	UNP A1WXF5
C	360	ASN	ASP	conflict	UNP A1WXF5

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	L	274	2170	1461	348	353	8	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	99	THR	ALA	conflict	UNP A0A2L1K3P0
L	205	PRO	SER	conflict	UNP A0A2L1K3P0
L	220	ILE	VAL	conflict	UNP A0A2L1K3P0
L	241	GLY	ALA	conflict	UNP A0A2L1K3P0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	M	318	2518	1679	410	420	9	0	0

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	34	ALA	SER	conflict	UNP A0A2L1K3T5
M	65	ILE	LEU	conflict	UNP A0A2L1K3T5
M	66	VAL	LEU	conflict	UNP A0A2L1K3T5
M	84	LEU	ILE	conflict	UNP A0A2L1K3T5
M	86	PHE	TRP	conflict	UNP A0A2L1K3T5
M	126	VAL	ILE	conflict	UNP A0A2L1K3T5
M	130	PHE	TRP	conflict	UNP A0A2L1K3T5
M	131	ALA	VAL	conflict	UNP A0A2L1K3T5
M	236	GLU	ASP	conflict	UNP A0A2L1K3T5

- Molecule 4 is a protein called Photosynthetic reaction centre, H-chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	H	278	2174	1379	374	410	11	0	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	69	VAL	THR	conflict	UNP A1WXI3
H	97	GLU	ALA	conflict	UNP A1WXI3
H	118	LEU	VAL	conflict	UNP A1WXI3

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Chain	Residue	Modelled	Actual	Comment	Reference
H	135	GLY	ALA	conflict	UNP A1WXI3
H	137	LYS	ASN	conflict	UNP A1WXI3
H	141	CYS	ALA	conflict	UNP A1WXI3
H	158	ALA	ARG	conflict	UNP A1WXI3
H	163	GLU	GLN	conflict	UNP A1WXI3
H	164	ILE	LEU	conflict	UNP A1WXI3
H	171	TYR	ASP	conflict	UNP A1WXI3
H	179	LYS	THR	conflict	UNP A1WXI3
H	210	GLY	SER	conflict	UNP A1WXI3
H	226	SER	GLY	conflict	UNP A1WXI3
H	236	GLN	LYS	conflict	UNP A1WXI3
H	247	ALA	SER	conflict	UNP A1WXI3
H	262	PHE	TYR	conflict	UNP A1WXI3

- Molecule 5 is a protein called Antenna complex, alpha/beta subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	A	46	385	263	66	55	1	0	0
5	F	46	385	263	66	55	1	0	0
5	K	46	385	263	66	55	1	0	0
5	Q	46	385	263	66	55	1	0	0
5	U	46	385	263	66	55	1	0	0
5	Y	46	385	263	66	55	1	0	0
5	3	46	385	263	66	55	1	0	0
5	7	46	385	263	66	55	1	0	0

- Molecule 6 is a protein called Antenna complex, alpha/beta subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	B	48	386	259	60	66	1	0	0
6	G	47	380	256	59	64	1	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	N	47	380	256	59	64	1	0	0
6	R	47	380	256	59	64	1	0	0
6	V	47	380	256	59	64	1	0	0
6	Z	48	386	259	60	66	1	0	0
6	4	47	380	256	59	64	1	0	0
6	8	47	380	256	59	64	1	0	0

- Molecule 7 is a protein called Antenna complex, alpha/beta subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	D	46	390	261	67	59	3	0	0
7	I	46	390	261	67	59	3	0	0
7	O	46	390	261	67	59	3	0	0
7	S	46	390	261	67	59	3	0	0
7	W	46	390	261	67	59	3	0	0
7	1	46	390	261	67	59	3	0	0
7	5	46	390	261	67	59	3	0	0
7	9	46	390	261	67	59	3	0	0

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	37	ASN	SER	conflict	UNP A1WXF8
D	42	GLN	GLU	conflict	UNP A1WXF8
D	48	ASP	ASN	conflict	UNP A1WXF8
D	57	ASP	GLU	conflict	UNP A1WXF8
I	37	ASN	SER	conflict	UNP A1WXF8
I	42	GLN	GLU	conflict	UNP A1WXF8

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Chain	Residue	Modelled	Actual	Comment	Reference
I	48	ASP	ASN	conflict	UNP A1WXF8
I	57	ASP	GLU	conflict	UNP A1WXF8
O	37	ASN	SER	conflict	UNP A1WXF8
O	42	GLN	GLU	conflict	UNP A1WXF8
O	48	ASP	ASN	conflict	UNP A1WXF8
O	57	ASP	GLU	conflict	UNP A1WXF8
S	37	ASN	SER	conflict	UNP A1WXF8
S	42	GLN	GLU	conflict	UNP A1WXF8
S	48	ASP	ASN	conflict	UNP A1WXF8
S	57	ASP	GLU	conflict	UNP A1WXF8
W	37	ASN	SER	conflict	UNP A1WXF8
W	42	GLN	GLU	conflict	UNP A1WXF8
W	48	ASP	ASN	conflict	UNP A1WXF8
W	57	ASP	GLU	conflict	UNP A1WXF8
1	37	ASN	SER	conflict	UNP A1WXF8
1	42	GLN	GLU	conflict	UNP A1WXF8
1	48	ASP	ASN	conflict	UNP A1WXF8
1	57	ASP	GLU	conflict	UNP A1WXF8
5	37	ASN	SER	conflict	UNP A1WXF8
5	42	GLN	GLU	conflict	UNP A1WXF8
5	48	ASP	ASN	conflict	UNP A1WXF8
5	57	ASP	GLU	conflict	UNP A1WXF8
9	37	ASN	SER	conflict	UNP A1WXF8
9	42	GLN	GLU	conflict	UNP A1WXF8
9	48	ASP	ASN	conflict	UNP A1WXF8
9	57	ASP	GLU	conflict	UNP A1WXF8

- Molecule 8 is a protein called Antenna complex, alpha/beta subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	E	45	362	240	58	63	1	0	0
			Total	C	N	O	S		
8	J	45	362	240	58	63	1	0	0
			Total	C	N	O	S		
8	P	45	362	240	58	63	1	0	0
			Total	C	N	O	S		
8	T	45	362	240	58	63	1	0	0
			Total	C	N	O	S		
8	X	45	362	240	58	63	1	0	0
			Total	C	N	O	S		
8	2	45	362	240	58	63	1	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	6	45	362	240	58	63	1	0	0
8	0	45	362	240	58	63	1	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	30	ILE	VAL	conflict	UNP A1WXF9
J	30	ILE	VAL	conflict	UNP A1WXF9
P	30	ILE	VAL	conflict	UNP A1WXF9
T	30	ILE	VAL	conflict	UNP A1WXF9
X	30	ILE	VAL	conflict	UNP A1WXF9
2	30	ILE	VAL	conflict	UNP A1WXF9
6	30	ILE	VAL	conflict	UNP A1WXF9
0	30	ILE	VAL	conflict	UNP A1WXF9

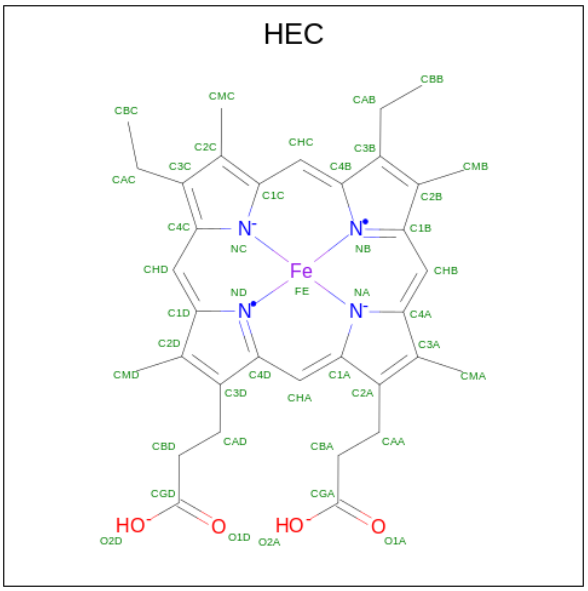
- Molecule 9 is a protein called High-potential iron-sulfur protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	a	97	763	471	135	151	6	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	3	LYS	ASN	conflict	UNP A1WXH6
a	38	ASP	ASN	conflict	UNP A1WXH6
a	?	-	GLY	deletion	UNP A1WXH6
a	?	-	ASN	deletion	UNP A1WXH6
a	45	ARG	GLN	conflict	UNP A1WXH6
a	114	ASN	SER	conflict	UNP A1WXH6
a	129	VAL	ILE	conflict	UNP A1WXH6
a	136	ALA	GLU	conflict	UNP A1WXH6

- Molecule 10 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{36}FeN_4O_4$).

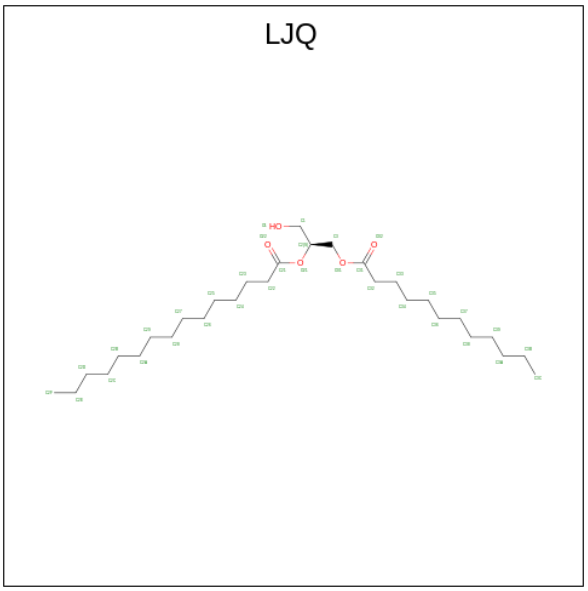


Mol	Chain	Residues	Atoms					AltConf
10	C	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
10	C	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
10	C	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
10	C	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 11 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

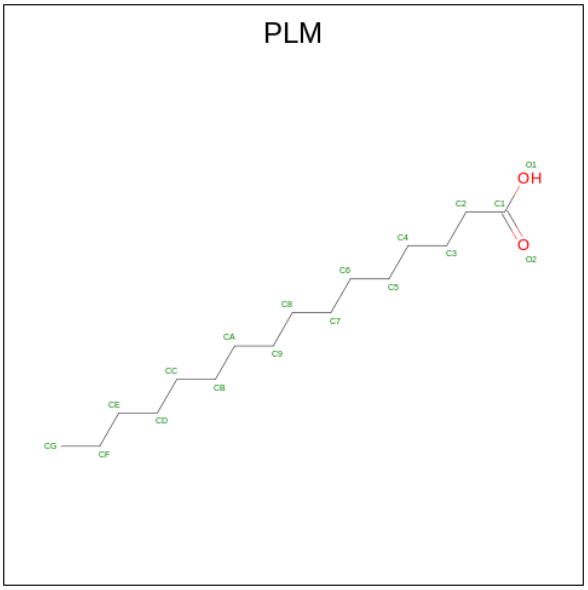
Mol	Chain	Residues	Atoms		AltConf
11	C	1	Total	Mg	0
			1	1	

- Molecule 12 is [(2 {S})-1-dodecanoyloxy-3-oxidanyl-propan-2-yl] pentadecanoate (CCD ID: LJQ) (formula: $C_{30}H_{58}O_5$).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
12	C	1	31	27	4	0

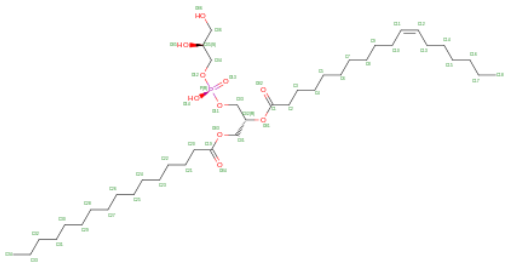
- Molecule 13 is PALMITIC ACID (CCD ID: PLM) (formula: $C_{16}H_{32}O_2$).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
13	C	1	12	11	1	0

- Molecule 14 is (1R)-2-{[{[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (CCD ID: PGV) (formula: $C_{40}H_{77}O_{10}P$).

PGV



Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
14	C	1	32	21	10	1	0
			Total	C	O	P	
14	L	1	43	32	10	1	0
			Total	C	O	P	
14	L	1	36	27	8	1	0
			Total	C	O	P	
14	L	1	41	30	10	1	0
			Total	C	O	P	
14	M	1	51	40	10	1	0
			Total	C	O	P	
14	H	1	36	25	10	1	0
			Total	C	O	P	
14	H	1	42	31	10	1	0
			Total	C	O	P	
14	B	1	44	33	10	1	0
			Total	C	O	P	
14	B	1	41	32	8	1	0
			Total	C	O	P	
14	E	1	38	27	10	1	0
			Total	C	O	P	
14	F	1	50	39	10	1	0
			Total	C	O	P	
14	G	1	49	38	10	1	0
			Total	C	O	P	
14	G	1	50	39	10	1	0
			Total	C	O	P	
14	G	1	42	33	8	1	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
14	J	1	33	24	8	1	0
			Total	C	O	P	
14	N	1	50	39	10	1	0
			Total	C	O	P	
14	N	1	47	36	10	1	0
			Total	C	O	P	
14	N	1	37	26	10	1	0
			Total	C	O	P	
14	P	1	47	36	10	1	0
			Total	C	O	P	
14	P	1	40	31	8	1	0
			Total	C	O	P	
14	R	1	43	32	10	1	0
			Total	C	O	P	
14	R	1	41	32	8	1	0
			Total	C	O	P	
14	T	1	46	35	10	1	0
			Total	C	O	P	
14	T	1	47	36	10	1	0
			Total	C	O	P	
14	V	1	44	33	10	1	0
			Total	C	O	P	
14	X	1	43	32	10	1	0
			Total	C	O	P	
14	X	1	45	34	10	1	0
			Total	C	O	P	
14	Z	1	46	35	10	1	0
			Total	C	O	P	
14	Z	1	44	33	10	1	0
			Total	C	O	P	
14	Z	1	43	34	8	1	0
			Total	C	O	P	
14	1	1	45	34	10	1	0
			Total	C	O	P	
14	2	1	46	36	9	1	0
			Total	C	O	P	
14	2	1	37	27	9	1	0
			Total	C	O	P	
14	3	1	30	21	8	1	0
			Total	C	O	P	
14	4	1	44	34	9	1	0

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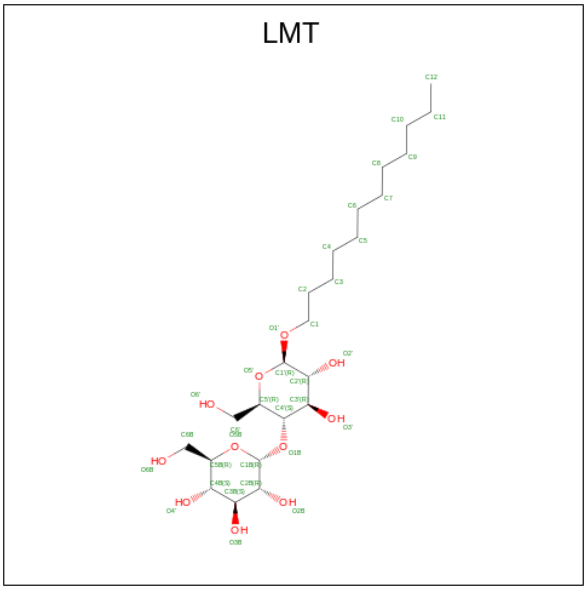
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
14	6	1	46	35	10	1	0
			Total	C	O	P	
14	6	1	44	34	9	1	0
			Total	C	O	P	
14	6	1	43	32	10	1	0
			Total	C	O	P	
14	8	1	43	32	10	1	0
			Total	C	O	P	
14	0	1	41	30	10	1	0
			Total	C	O	P	
14	0	1	44	33	10	1	0
			Total	C	O	P	
14	0	1	43	32	10	1	0

- Molecule 15 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: $C_{24}H_{46}O_{11}$).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
15	L	1	25	14	11	0
			Total	C	O	
15	L	1	35	24	11	0
			Total	C	O	
15	M	1	35	24	11	0
			Total	C	O	
15	H	1	30	19	11	0

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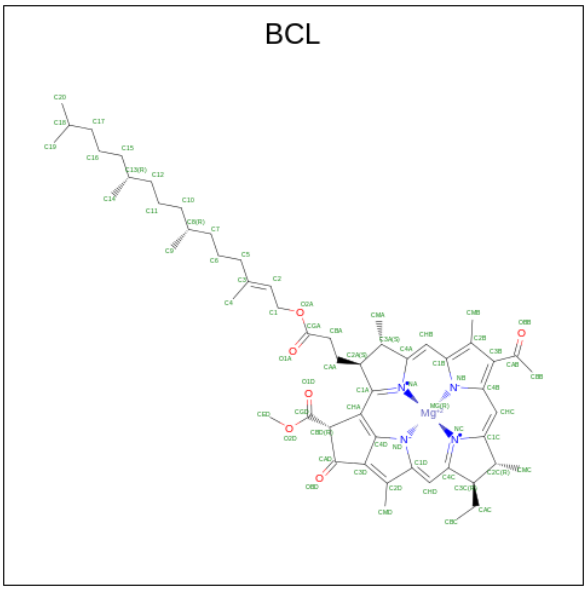
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
15	H	1	35	24	11	0
			Total	C	O	
15	H	1	26	15	11	0
			Total	C	O	
15	F	1	33	22	11	0
			Total	C	O	
15	I	1	25	14	11	0
			Total	C	O	
15	O	1	29	18	11	0
			Total	C	O	
15	Q	1	32	21	11	0
			Total	C	O	
15	5	1	35	24	11	0
			Total	C	O	
15	5	1	24	13	11	0
			Total	C	O	
15	7	1	25	14	11	0

- Molecule 16 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	
16	L	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
16	L	1	66	55	1	4	6	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
16	L	1	66	55	1	4	6	0
16	M	1	66	55	1	4	6	0
16	A	1	66	55	1	4	6	0
16	B	1	66	55	1	4	6	0
16	D	1	66	55	1	4	6	0
16	D	1	66	55	1	4	6	0
16	E	1	66	55	1	4	6	0
16	F	1	66	55	1	4	6	0
16	G	1	66	55	1	4	6	0
16	I	1	66	55	1	4	6	0
16	I	1	66	55	1	4	6	0
16	J	1	66	55	1	4	6	0
16	K	1	66	55	1	4	6	0
16	N	1	66	55	1	4	6	0
16	O	1	66	55	1	4	6	0
16	O	1	66	55	1	4	6	0
16	P	1	66	55	1	4	6	0
16	Q	1	66	55	1	4	6	0
16	R	1	66	55	1	4	6	0
16	S	1	66	55	1	4	6	0
16	S	1	66	55	1	4	6	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
16	T	1	66	55	1	4	6	0
16	U	1	66	55	1	4	6	0
16	V	1	66	55	1	4	6	0
16	W	1	66	55	1	4	6	0
16	W	1	66	55	1	4	6	0
16	X	1	66	55	1	4	6	0
16	Y	1	66	55	1	4	6	0
16	Y	1	66	55	1	4	6	0
16	Z	1	66	55	1	4	6	0
16	1	1	66	55	1	4	6	0
16	1	1	66	55	1	4	6	0
16	2	1	66	55	1	4	6	0
16	3	1	66	55	1	4	6	0
16	4	1	66	55	1	4	6	0
16	5	1	66	55	1	4	6	0
16	5	1	66	55	1	4	6	0
16	6	1	66	55	1	4	6	0
16	7	1	66	55	1	4	6	0
16	8	1	66	55	1	4	6	0
16	9	1	66	55	1	4	6	0
16	9	1	66	55	1	4	6	0

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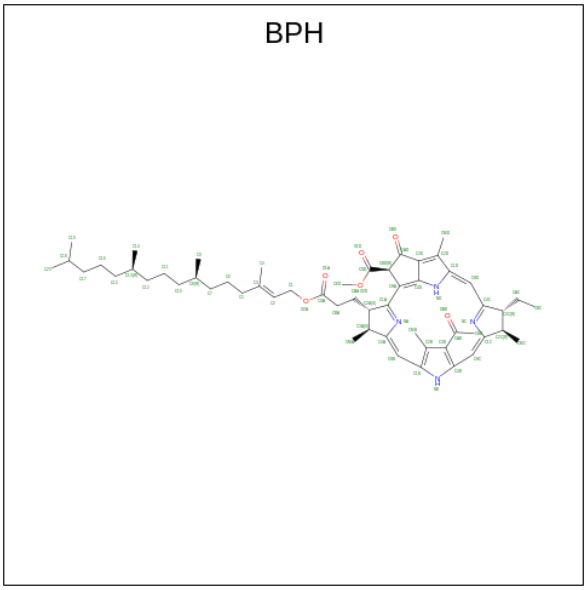
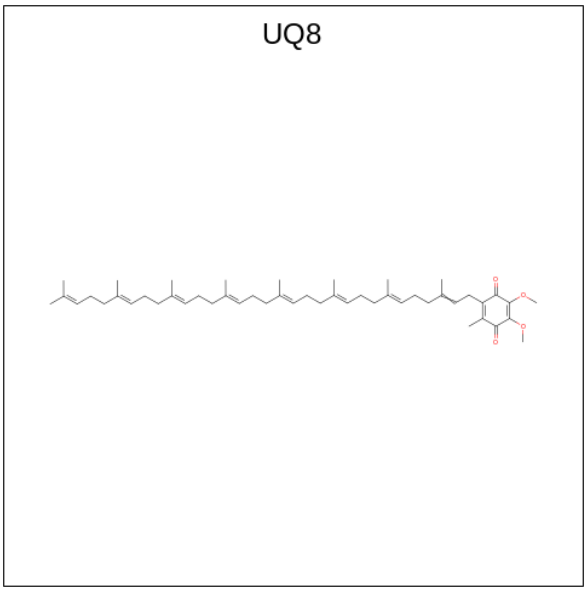
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
16	0	1	66	55	1	4	6	0

- Molecule 17 is BACTERIOPHEOPHYTIN A (CCD ID: BPH) (formula: $C_{55}H_{76}N_4O_6$).



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

- Molecule 18 is Ubiquinone-8 (CCD ID: UQ8) (formula: $C_{49}H_{74}O_4$).

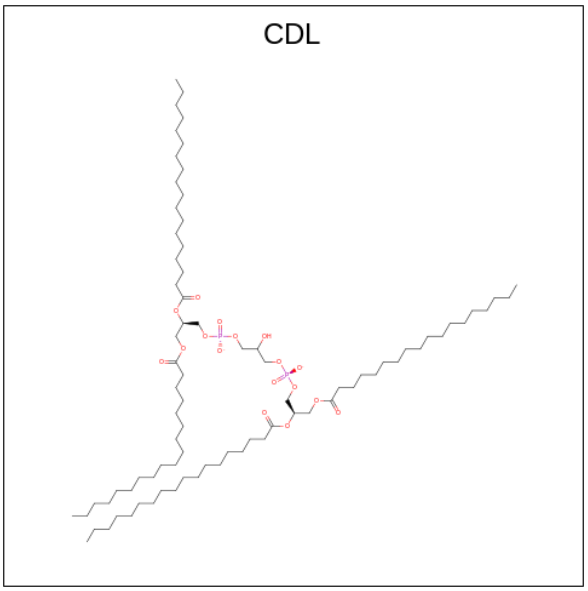


Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
18	L	1	33	29	4	0
			Total	C	O	
18	L	1	38	34	4	0
			Total	C	O	
18	L	1	17	13	4	0

- Molecule 19 is FE (III) ION (CCD ID: FE) (formula: Fe).

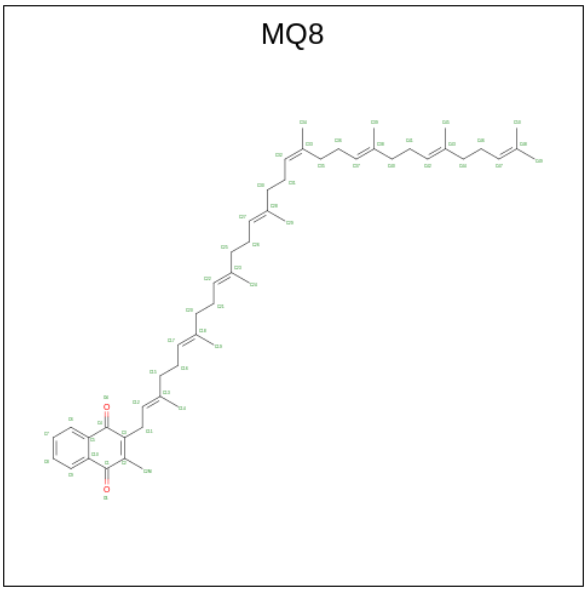
Mol	Chain	Residues	Atoms		AltConf
			Total	Fe	
19	M	1	1	1	0

- Molecule 20 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



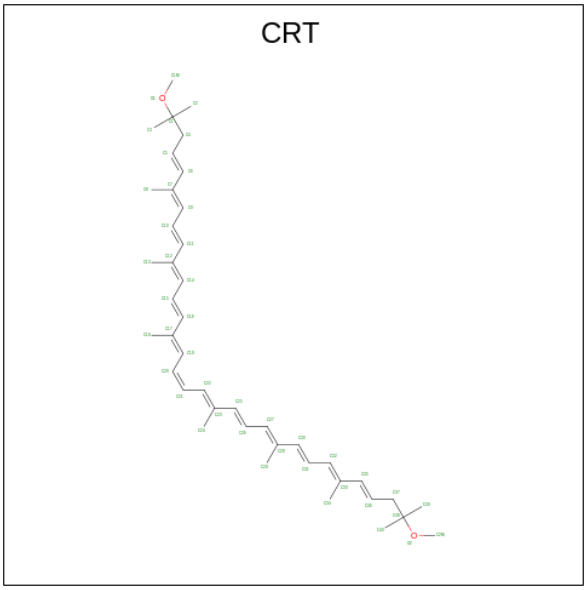
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
20	M	1	82	63	17	2	0
20	M	1	80	61	17	2	0
20	M	1	56	37	17	2	0
20	M	1	50	31	17	2	0
20	H	1	64	45	17	2	0
20	H	1	75	56	17	2	0
20	O	1	73	54	17	2	0
20	U	1	51	32	17	2	0
20	U	1	46	27	17	2	0

- Molecule 21 is MENAQUINONE 8 (CCD ID: MQ8) (formula: $C_{51}H_{72}O_2$).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
21	M	1	53	51	2	0

- Molecule 22 is SPIRILLOXANTHIN (CCD ID: CRT) (formula: $C_{42}H_{60}O_2$).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
22	M	1	44	42	2	0
22	B	1	44	42	2	0
22	G	1	44	42	2	0

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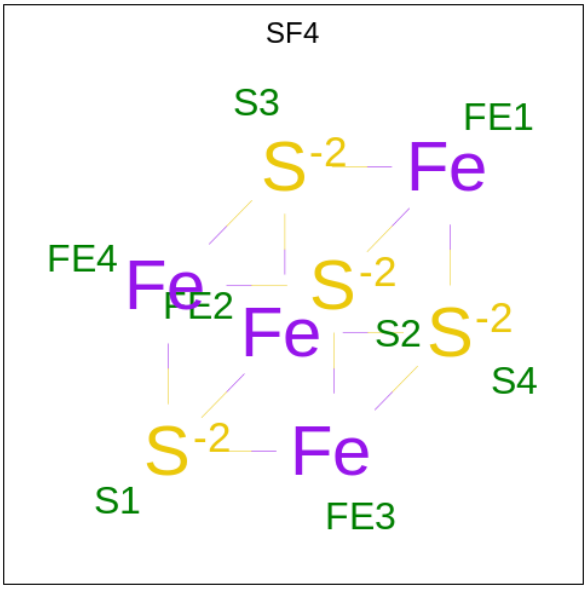
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
22	N	1	44	42	2	0
22	R	1	44	42	2	0
22	V	1	44	42	2	0
22	Y	1	44	42	2	0
22	4	1	44	42	2	0
22	8	1	44	42	2	0

- Molecule 23 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
23	a	1	8	4	4	0

- Molecule 24 is water.

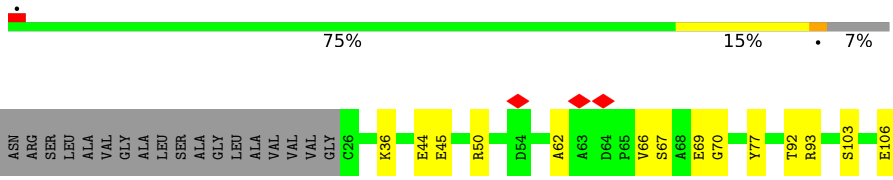
Mol	Chain	Residues	Atoms		AltConf
			Total	O	
24	C	4	4	4	0
24	M	1	1	1	0

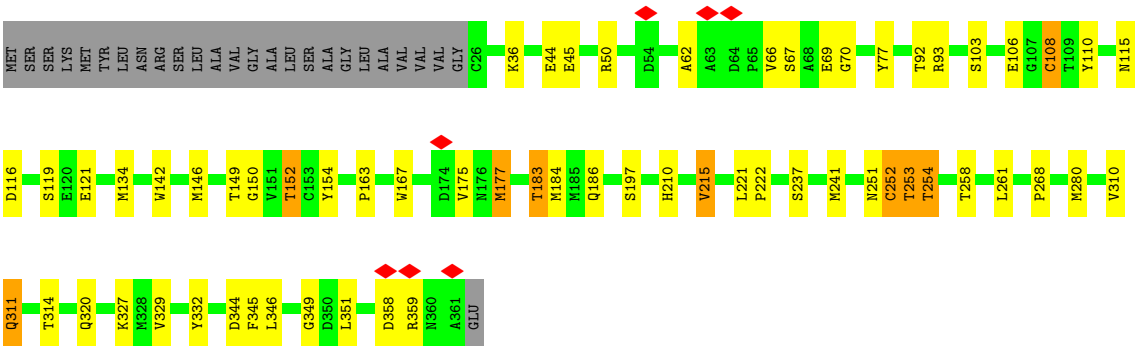
3 Residue-property plots (i)

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 cytochrome c subunit

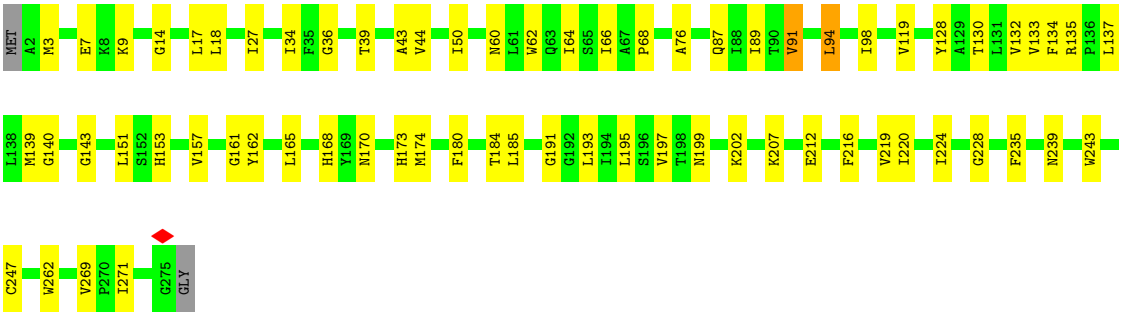
Chain C:





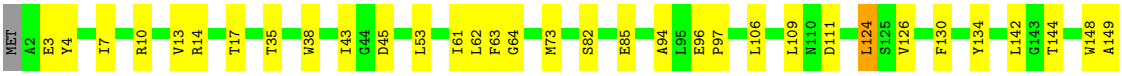
- Molecule 2: Reaction center protein L chain

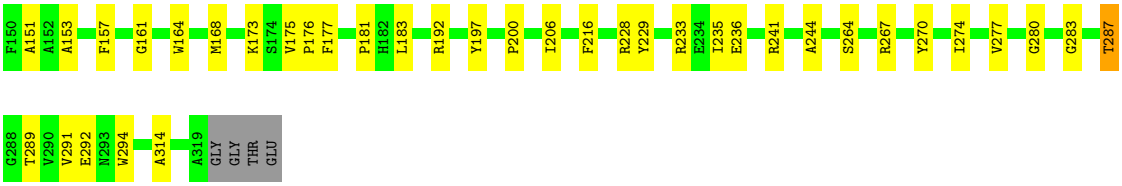
Chain L:



- Molecule 3: Reaction center protein M chain

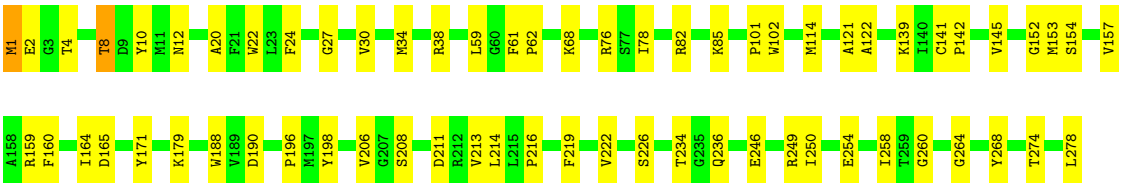
Chain M:





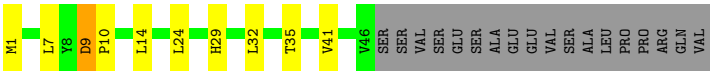
• Molecule 4: Photosynthetic reaction centre, H-chain

Chain H:



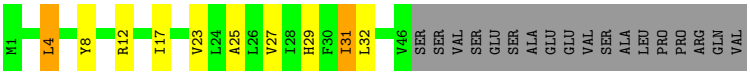
• Molecule 5: Antenna complex, alpha/beta subunit

Chain A:



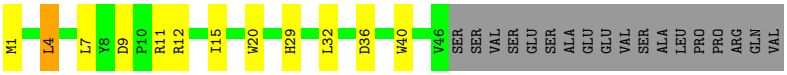
• Molecule 5: Antenna complex, alpha/beta subunit

Chain F:



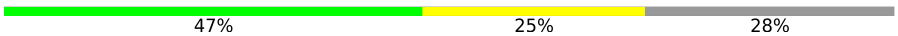
• Molecule 5: Antenna complex, alpha/beta subunit

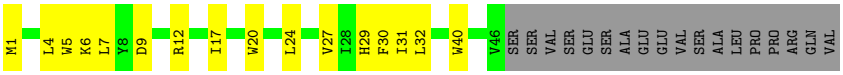
Chain K:



• Molecule 5: Antenna complex, alpha/beta subunit

Chain Q:





• Molecule 5: Antenna complex, alpha/beta subunit

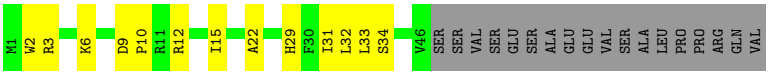
Chain U:

• Molecule 5: Antenna complex, alpha/beta subunit

Chain Y:

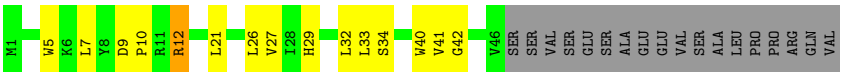
• Molecule 5: Antenna complex, alpha/beta subunit

Chain 3:



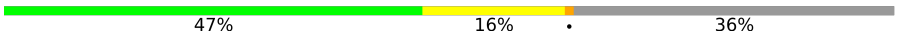
• Molecule 5: Antenna complex, alpha/beta subunit

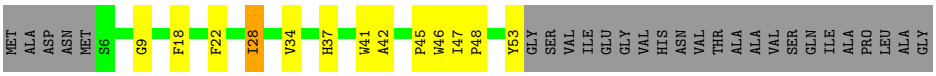
Chain 7:



• Molecule 6: Antenna complex, alpha/beta subunit

Chain B:



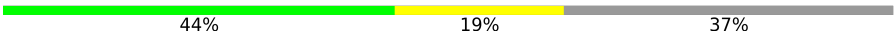


• Molecule 6: Antenna complex, alpha/beta subunit

Chain G:

• Molecule 6: Antenna complex, alpha/beta subunit

Chain N:

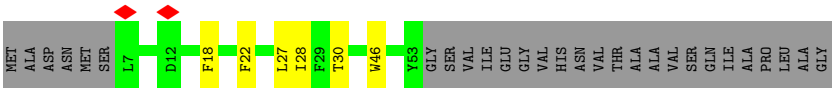


• Molecule 6: Antenna complex, alpha/beta subunit

Chain R:

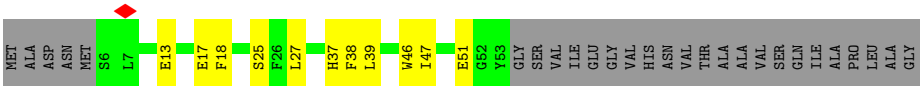
• Molecule 6: Antenna complex, alpha/beta subunit

Chain V:



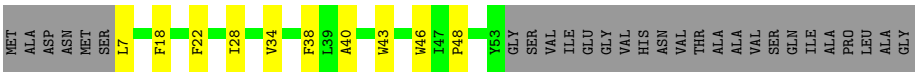
• Molecule 6: Antenna complex, alpha/beta subunit

Chain Z:



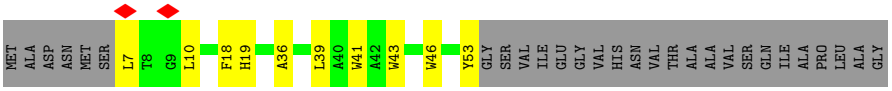
• Molecule 6: Antenna complex, alpha/beta subunit

Chain 4:



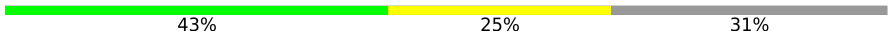
• Molecule 6: Antenna complex, alpha/beta subunit

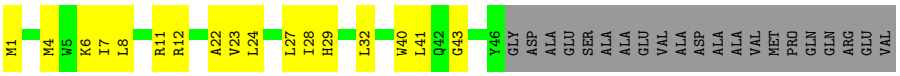
Chain 8:



• Molecule 7: Antenna complex, alpha/beta subunit

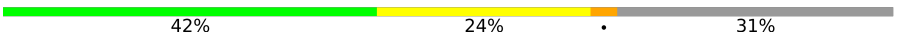
Chain D:

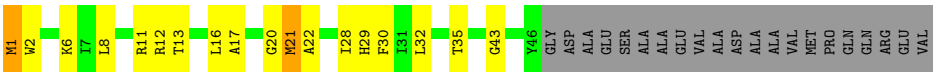




• Molecule 7: Antenna complex, alpha/beta subunit

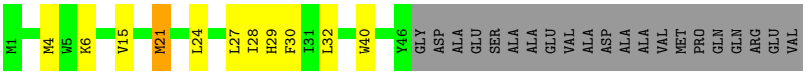
Chain I:





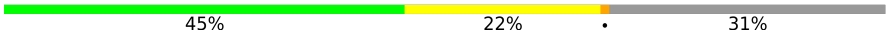
• Molecule 7: Antenna complex, alpha/beta subunit

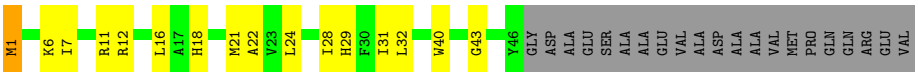
Chain O:



• Molecule 7: Antenna complex, alpha/beta subunit

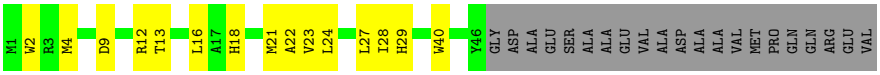
Chain S:





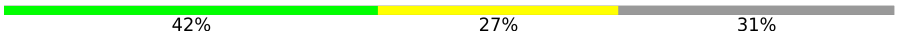
• Molecule 7: Antenna complex, alpha/beta subunit

Chain W:



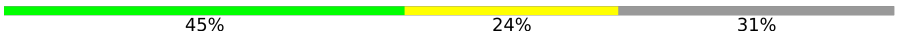
• Molecule 7: Antenna complex, alpha/beta subunit

Chain 1:



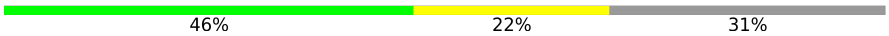
• Molecule 7: Antenna complex, alpha/beta subunit

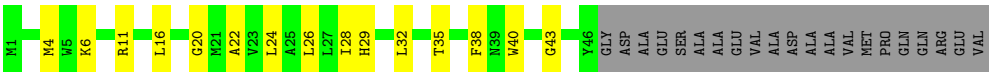
Chain 5:



• Molecule 7: Antenna complex, alpha/beta subunit

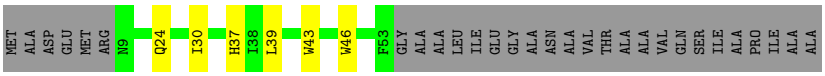
Chain 9:





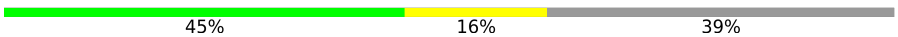
• Molecule 8: Antenna complex, alpha/beta subunit

Chain E:



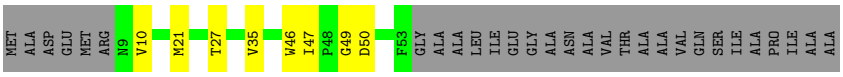
• Molecule 8: Antenna complex, alpha/beta subunit

Chain J:



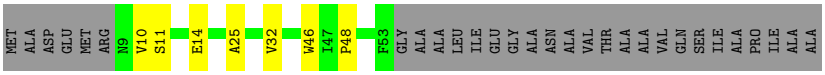
• Molecule 8: Antenna complex, alpha/beta subunit

Chain P:



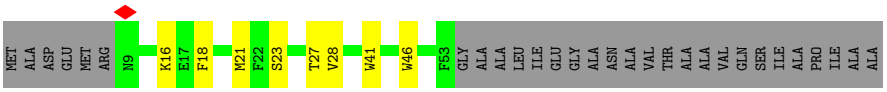
• Molecule 8: Antenna complex, alpha/beta subunit

Chain T:



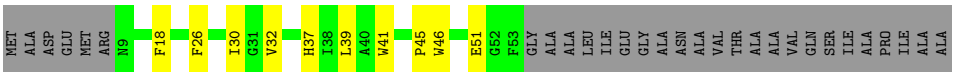
• Molecule 8: Antenna complex, alpha/beta subunit

Chain X:



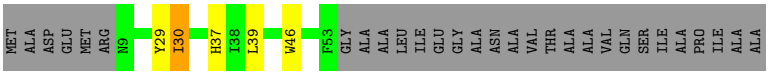
• Molecule 8: Antenna complex, alpha/beta subunit

Chain 2:



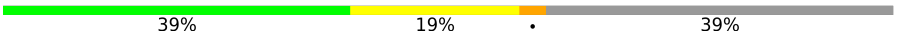
• Molecule 8: Antenna complex, alpha/beta subunit

Chain 6:



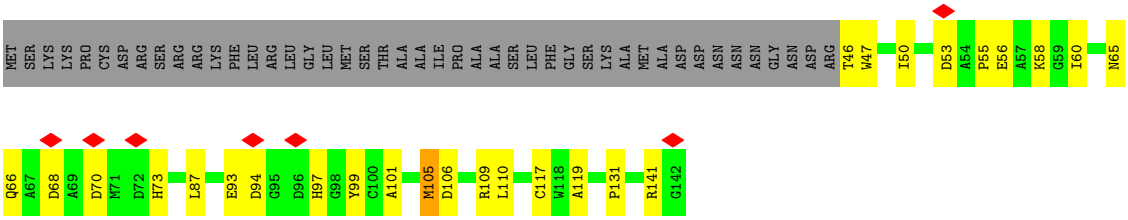
• Molecule 8: Antenna complex, alpha/beta subunit

Chain 0:



• Molecule 9: High-potential iron-sulfur protein

Chain a:


MET SER LYS LYS PRO CYS ASP ARG SER ARG ARG LYS PHE LEU ARG LEU GLY LEU MET SER THR ALA ALA ILE PRO ALA ALA SER LEU PHE GLY SER LYS ALA MET ALA ASP ASP ASN ASN ASN GLY ASN ASP ARG T46 W47 I50 D53 A54 P55 E56 A57 K58 G59 I60 N65
Q66 A67 D68 A69 D70 N71 D72 H73 L87 E93 D94 G95 D96 H97 G98 Y99 C100 A101 M105 D106 R109 L110 C117 W118 A119 P131 R141 G142

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	90126	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	1100	Depositor
Maximum defocus (nm)	2700	Depositor
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.213	Depositor
Minimum map value	-0.098	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.03	Depositor
Map size (Å)	328.0, 328.0, 328.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.82, 0.82, 0.82	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: FE, CDL, PGV, LJQ, LMT, MQ8, MG, BPH, HEC, PLM, SF4, CRT, BCL, UQ8

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	C	0.25	0/2702	0.40	0/3674
2	L	0.25	0/2252	0.36	0/3082
3	M	0.25	0/2613	0.35	0/3582
4	H	0.21	0/2229	0.33	0/3027
5	3	0.21	0/398	0.30	0/543
5	7	0.22	0/398	0.28	0/543
5	A	0.24	0/398	0.31	0/543
5	F	0.22	0/398	0.31	0/543
5	K	0.20	0/398	0.28	0/543
5	Q	0.20	0/398	0.29	0/543
5	U	0.22	0/398	0.29	0/543
5	Y	0.21	0/398	0.34	0/543
6	4	0.18	0/395	0.25	0/539
6	8	0.19	0/395	0.29	0/539
6	B	0.22	0/401	0.33	0/547
6	G	0.21	0/395	0.25	0/539
6	N	0.19	0/395	0.28	0/539
6	R	0.21	0/395	0.32	0/539
6	V	0.19	0/395	0.27	0/539
6	Z	0.18	0/401	0.29	0/547
7	1	0.21	0/402	0.29	0/547
7	5	0.21	0/402	0.30	0/547
7	9	0.23	0/402	0.31	0/547
7	D	0.25	0/402	0.33	0/547
7	I	0.23	0/402	0.31	0/547
7	O	0.21	0/402	0.31	0/547
7	S	0.23	0/402	0.36	0/547
7	W	0.22	0/402	0.33	0/547
8	0	0.20	0/376	0.24	0/514
8	2	0.19	0/376	0.24	0/514
8	6	0.20	0/376	0.25	0/514
8	E	0.21	0/376	0.26	0/514

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
8	J	0.19	0/376	0.25	0/514
8	P	0.22	0/376	0.25	0/514
8	T	0.20	0/376	0.29	0/514
8	X	0.20	0/376	0.25	0/514
9	a	0.18	0/786	0.46	0/1068
All	All	0.22	0/23162	0.33	0/31593

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	C	2642	0	2401	52	0
2	L	2170	0	2145	59	0
3	M	2518	0	2465	63	0
4	H	2174	0	2131	49	0
5	3	385	0	403	15	0
5	7	385	0	403	18	0
5	A	385	0	403	10	0
5	F	385	0	403	12	0
5	K	385	0	403	12	0
5	Q	385	0	403	18	0
5	U	385	0	403	16	0
5	Y	385	0	403	8	0
6	4	380	0	359	12	0
6	8	380	0	359	14	0
6	B	386	0	364	16	0
6	G	380	0	359	11	0
6	N	380	0	359	11	0
6	R	380	0	359	11	0
6	V	380	0	359	4	0
6	Z	386	0	364	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	1	390	0	401	23	0
7	5	390	0	401	17	0
7	9	390	0	401	17	0
7	D	390	0	401	21	0
7	I	390	0	401	20	0
7	O	390	0	401	12	0
7	S	390	0	401	19	0
7	W	390	0	401	15	0
8	0	362	0	333	16	0
8	2	362	0	333	12	0
8	6	362	0	333	5	0
8	E	362	0	333	6	0
8	J	362	0	333	15	0
8	P	362	0	333	8	0
8	T	362	0	333	5	0
8	X	362	0	333	9	0
9	a	763	0	666	14	0
10	C	172	0	121	14	0
11	C	1	0	0	0	0
12	C	31	0	0	0	0
13	C	12	0	18	5	0
14	0	128	0	161	16	0
14	1	45	0	58	12	0
14	2	83	0	106	6	0
14	3	30	0	31	4	0
14	4	44	0	59	4	0
14	6	133	0	173	9	0
14	8	43	0	54	8	0
14	B	85	0	107	12	0
14	C	32	0	34	3	0
14	E	38	0	44	2	0
14	F	50	0	71	6	0
14	G	141	0	193	16	0
14	H	78	0	99	8	0
14	J	33	0	37	4	0
14	L	120	0	150	15	0
14	M	51	0	76	5	0
14	N	134	0	178	10	0
14	P	87	0	116	9	0
14	R	84	0	107	8	0
14	T	93	0	128	9	0
14	V	44	0	56	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	X	88	0	116	8	0
14	Z	133	0	177	14	0
15	5	59	0	67	7	0
15	7	25	0	23	4	0
15	F	33	0	39	4	0
15	H	91	0	104	9	0
15	I	25	0	23	5	0
15	L	60	0	69	5	0
15	M	35	0	46	4	0
15	O	29	0	31	1	0
15	Q	32	0	37	3	0
16	0	66	0	74	9	0
16	1	132	0	148	17	0
16	2	66	0	74	10	0
16	3	66	0	74	8	0
16	4	66	0	74	5	0
16	5	132	0	148	20	0
16	6	66	0	74	7	0
16	7	66	0	74	3	0
16	8	66	0	74	11	0
16	9	132	0	148	11	0
16	A	66	0	74	4	0
16	B	66	0	74	11	0
16	D	132	0	148	10	0
16	E	66	0	74	6	0
16	F	66	0	74	2	0
16	G	66	0	74	10	0
16	I	132	0	148	20	0
16	J	66	0	74	8	0
16	K	66	0	74	7	0
16	L	198	0	221	13	0
16	M	66	0	74	7	0
16	N	66	0	74	8	0
16	O	132	0	148	11	0
16	P	66	0	74	9	0
16	Q	66	0	74	7	0
16	R	66	0	74	10	0
16	S	132	0	148	21	0
16	T	66	0	74	6	0
16	U	66	0	74	5	0
16	V	66	0	74	9	0
16	W	132	0	148	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	X	66	0	74	5	0
16	Y	132	0	148	8	0
16	Z	66	0	74	8	0
17	L	65	0	76	6	0
17	M	65	0	76	8	0
18	L	88	0	98	10	0
19	M	1	0	0	0	0
20	H	139	0	169	12	0
20	M	268	0	318	20	0
20	O	73	0	90	3	0
20	U	97	0	82	6	0
21	M	53	0	72	3	0
22	4	44	0	60	12	0
22	8	44	0	60	6	0
22	B	44	0	60	4	0
22	G	44	0	60	6	0
22	M	44	0	60	11	0
22	N	44	0	60	11	0
22	R	44	0	60	9	0
22	V	44	0	60	9	0
22	Y	44	0	60	9	0
23	a	8	0	0	0	0
24	C	4	0	0	0	0
24	M	1	0	0	0	0
All	All	29045	0	29545	844	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 14.

The worst 5 of 844 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:C:108:CYS:SG	10:C:401:HEC:HAB	1.39	1.58
1:C:108:CYS:CB	10:C:401:HEC:HAB	1.51	1.40
1:C:108:CYS:SG	10:C:401:HEC:CAB	2.11	1.37
1:C:108:CYS:CB	10:C:401:HEC:CAB	2.27	1.11
1:C:108:CYS:HB3	10:C:401:HEC:CAB	1.86	1.05

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	C	334/362 (92%)	316 (95%)	18 (5%)	0	100	100
2	L	272/276 (99%)	261 (96%)	11 (4%)	0	100	100
3	M	316/323 (98%)	304 (96%)	12 (4%)	0	100	100
4	H	276/278 (99%)	272 (99%)	4 (1%)	0	100	100
5	3	44/64 (69%)	44 (100%)	0	0	100	100
5	7	44/64 (69%)	44 (100%)	0	0	100	100
5	A	44/64 (69%)	44 (100%)	0	0	100	100
5	F	44/64 (69%)	44 (100%)	0	0	100	100
5	K	44/64 (69%)	44 (100%)	0	0	100	100
5	Q	44/64 (69%)	44 (100%)	0	0	100	100
5	U	44/64 (69%)	44 (100%)	0	0	100	100
5	Y	44/64 (69%)	44 (100%)	0	0	100	100
6	4	45/75 (60%)	43 (96%)	2 (4%)	0	100	100
6	8	45/75 (60%)	43 (96%)	2 (4%)	0	100	100
6	B	46/75 (61%)	44 (96%)	2 (4%)	0	100	100
6	G	45/75 (60%)	44 (98%)	1 (2%)	0	100	100
6	N	45/75 (60%)	44 (98%)	1 (2%)	0	100	100
6	R	45/75 (60%)	44 (98%)	1 (2%)	0	100	100
6	V	45/75 (60%)	44 (98%)	1 (2%)	0	100	100
6	Z	46/75 (61%)	43 (94%)	3 (6%)	0	100	100
7	1	44/67 (66%)	44 (100%)	0	0	100	100
7	5	44/67 (66%)	44 (100%)	0	0	100	100
7	9	44/67 (66%)	43 (98%)	1 (2%)	0	100	100
7	D	44/67 (66%)	44 (100%)	0	0	100	100
7	I	44/67 (66%)	44 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	O	44/67 (66%)	44 (100%)	0	0	100	100
7	S	44/67 (66%)	43 (98%)	1 (2%)	0	100	100
7	W	44/67 (66%)	44 (100%)	0	0	100	100
8	0	43/74 (58%)	42 (98%)	1 (2%)	0	100	100
8	2	43/74 (58%)	42 (98%)	1 (2%)	0	100	100
8	6	43/74 (58%)	41 (95%)	2 (5%)	0	100	100
8	E	43/74 (58%)	42 (98%)	1 (2%)	0	100	100
8	J	43/74 (58%)	42 (98%)	1 (2%)	0	100	100
8	P	43/74 (58%)	42 (98%)	1 (2%)	0	100	100
8	T	43/74 (58%)	41 (95%)	2 (5%)	0	100	100
8	X	43/74 (58%)	42 (98%)	1 (2%)	0	100	100
9	a	95/142 (67%)	86 (90%)	9 (10%)	0	100	100
All	All	2703/3621 (75%)	2624 (97%)	79 (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	C	287/306 (94%)	271 (94%)	16 (6%)	19	33
2	L	218/219 (100%)	215 (99%)	3 (1%)	59	79
3	M	252/255 (99%)	244 (97%)	8 (3%)	34	56
4	H	228/228 (100%)	219 (96%)	9 (4%)	28	48
5	3	39/55 (71%)	39 (100%)	0	100	100
5	7	39/55 (71%)	38 (97%)	1 (3%)	40	63
5	A	39/55 (71%)	38 (97%)	1 (3%)	40	63
5	F	39/55 (71%)	37 (95%)	2 (5%)	21	37
5	K	39/55 (71%)	38 (97%)	1 (3%)	40	63

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	Q	39/55 (71%)	38 (97%)	1 (3%)	40	63
5	U	39/55 (71%)	38 (97%)	1 (3%)	40	63
5	Y	39/55 (71%)	38 (97%)	1 (3%)	40	63
6	4	37/57 (65%)	37 (100%)	0	100	100
6	8	37/57 (65%)	36 (97%)	1 (3%)	39	62
6	B	38/57 (67%)	37 (97%)	1 (3%)	40	63
6	G	37/57 (65%)	35 (95%)	2 (5%)	20	35
6	N	37/57 (65%)	36 (97%)	1 (3%)	39	62
6	R	37/57 (65%)	36 (97%)	1 (3%)	39	62
6	V	37/57 (65%)	35 (95%)	2 (5%)	20	35
6	Z	38/57 (67%)	35 (92%)	3 (8%)	11	19
7	1	41/55 (74%)	40 (98%)	1 (2%)	43	65
7	5	41/55 (74%)	41 (100%)	0	100	100
7	9	41/55 (74%)	40 (98%)	1 (2%)	43	65
7	D	41/55 (74%)	41 (100%)	0	100	100
7	I	41/55 (74%)	38 (93%)	3 (7%)	13	22
7	O	41/55 (74%)	38 (93%)	3 (7%)	13	22
7	S	41/55 (74%)	40 (98%)	1 (2%)	43	65
7	W	41/55 (74%)	39 (95%)	2 (5%)	22	39
8	0	35/52 (67%)	32 (91%)	3 (9%)	10	16
8	2	35/52 (67%)	35 (100%)	0	100	100
8	6	35/52 (67%)	34 (97%)	1 (3%)	37	60
8	E	35/52 (67%)	34 (97%)	1 (3%)	37	60
8	J	35/52 (67%)	34 (97%)	1 (3%)	37	60
8	P	35/52 (67%)	33 (94%)	2 (6%)	18	33
8	T	35/52 (67%)	34 (97%)	1 (3%)	37	60
8	X	35/52 (67%)	35 (100%)	0	100	100
9	a	75/111 (68%)	70 (93%)	5 (7%)	15	26
All	All	2278/2871 (79%)	2198 (96%)	80 (4%)	32	53

5 of 80 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	T	11	SER
7	9	16	LEU
6	V	27	LEU
6	Z	27	LEU
9	a	46	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
9	a	66	GLN
8	0	24	GLN
6	N	24	GLN
8	6	24	GLN
7	I	37	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 133 ligands modelled in this entry, 2 are monoatomic - leaving 131 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	$\#\|Z\| > 2$
18	UQ8	L	304	-	33,33,53	1.45	2 (6%)	40,43,67	1.72	8 (20%)
14	PGV	B	104	-	40,40,50	0.99	2 (5%)	42,45,56	1.15	4 (9%)
16	BCL	5	104	7	69,74,74	1.82	17 (24%)	83,115,115	2.39	25 (30%)
16	BCL	P	101	8	69,74,74	1.77	20 (28%)	83,115,115	2.46	23 (27%)
14	PGV	6	103	-	42,43,50	0.98	2 (4%)	45,49,56	0.99	3 (6%)
16	BCL	L	312	3	69,74,74	1.79	17 (24%)	83,115,115	2.62	27 (32%)
22	CRT	G	102	-	41,43,43	0.77	0	50,54,54	3.51	19 (38%)
15	LMT	H	305	-	31,31,36	0.42	0	42,42,47	1.05	2 (4%)
16	BCL	V	102	6	69,74,74	1.77	18 (26%)	83,115,115	2.36	26 (31%)
22	CRT	V	101	-	41,43,43	0.75	0	50,54,54	3.65	20 (40%)
18	UQ8	L	306	-	38,38,53	1.40	2 (5%)	46,49,67	1.57	11 (23%)
14	PGV	L	309	-	35,35,50	1.06	2 (5%)	38,40,56	1.10	1 (2%)
16	BCL	R	102	6	69,74,74	1.78	19 (27%)	83,115,115	2.50	23 (27%)
14	PGV	G	104	-	49,49,50	0.92	2 (4%)	52,55,56	0.93	3 (5%)
14	PGV	X	101	-	42,42,50	0.99	2 (4%)	44,48,56	1.09	3 (6%)
16	BCL	N	103	6	69,74,74	1.78	19 (27%)	83,115,115	2.41	23 (27%)
15	LMT	M	411	-	36,36,36	0.40	0	47,47,47	0.92	1 (2%)
17	BPH	L	303	-	59,70,70	0.81	4 (6%)	61,101,101	1.03	4 (6%)
20	CDL	O	101	-	72,72,99	1.07	4 (5%)	78,84,111	1.15	5 (6%)
14	PGV	N	105	-	36,36,50	1.05	2 (5%)	38,42,56	1.16	3 (7%)
14	PGV	J	102	-	32,32,50	1.20	2 (6%)	35,37,56	1.24	3 (8%)
14	PGV	M	410	-	50,50,50	0.92	2 (4%)	53,56,56	1.11	3 (5%)
16	BCL	M	403	3	69,74,74	1.79	17 (24%)	83,115,115	2.58	27 (32%)
14	PGV	Z	104	-	42,42,50	1.00	2 (4%)	45,47,56	1.11	4 (8%)
16	BCL	5	103	7	69,74,74	1.77	17 (24%)	83,115,115	2.51	30 (36%)
16	BCL	0	102	8	69,74,74	1.82	18 (26%)	83,115,115	2.47	24 (28%)
14	PGV	V	103	-	43,43,50	0.99	2 (4%)	45,49,56	1.08	2 (4%)
16	BCL	B	102	6	69,74,74	1.79	19 (27%)	83,115,115	2.42	24 (28%)
14	PGV	T	103	-	46,46,50	0.94	2 (4%)	48,52,56	0.93	3 (6%)
22	CRT	B	101	-	41,43,43	0.76	0	50,54,54	3.61	16 (32%)
16	BCL	O	104	7	69,74,74	1.80	17 (24%)	83,115,115	2.43	24 (28%)
15	LMT	L	308	-	36,36,36	0.42	0	47,47,47	0.80	1 (2%)
16	BCL	8	102	6	69,74,74	1.77	18 (26%)	83,115,115	2.50	26 (31%)
17	BPH	M	404	-	59,70,70	0.75	2 (3%)	61,101,101	0.90	2 (3%)
15	LMT	Q	101	-	33,33,36	0.45	0	44,44,47	1.04	4 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
16	BCL	W	101	7	69,74,74	1.79	17 (24%)	83,115,115	2.55	27 (32%)
16	BCL	Q	102	5	69,74,74	1.77	19 (27%)	83,115,115	2.56	26 (31%)
14	PGV	0	103	-	43,43,50	0.97	2 (4%)	46,49,56	0.95	3 (6%)
16	BCL	A	101	5	69,74,74	1.80	17 (24%)	83,115,115	2.46	23 (27%)
14	PGV	2	103	-	36,36,50	1.07	2 (5%)	39,41,56	1.10	2 (5%)
22	CRT	Y	403	-	41,43,43	0.73	0	50,54,54	3.52	16 (32%)
16	BCL	L	311	2	69,74,74	1.77	18 (26%)	83,115,115	2.49	26 (31%)
14	PGV	6	104	-	42,42,50	1.01	2 (4%)	45,48,56	1.01	2 (4%)
14	PGV	3	101	-	29,29,50	1.20	2 (6%)	32,34,56	1.15	2 (6%)
16	BCL	S	101	7	69,74,74	1.80	18 (26%)	83,115,115	2.52	29 (34%)
16	BCL	O	103	7	69,74,74	1.79	18 (26%)	83,115,115	2.57	24 (28%)
16	BCL	1	103	7	69,74,74	1.82	19 (27%)	83,115,115	2.62	29 (34%)
16	BCL	2	101	8	69,74,74	1.78	18 (26%)	83,115,115	2.45	24 (28%)
14	PGV	4	103	-	43,43,50	1.00	2 (4%)	46,48,56	1.09	3 (6%)
14	PGV	B	103	-	43,43,50	0.97	2 (4%)	46,49,56	1.14	3 (6%)
15	LMT	L	301	-	26,26,36	0.43	0	37,37,47	0.90	1 (2%)
14	PGV	E	102	-	37,37,50	1.07	2 (5%)	39,43,56	1.07	4 (10%)
16	BCL	D	102	7	69,74,74	1.81	18 (26%)	83,115,115	2.37	26 (31%)
15	LMT	I	101	-	26,26,36	0.51	0	37,37,47	1.29	4 (10%)
16	BCL	U	103	5	69,74,74	1.82	18 (26%)	83,115,115	2.59	24 (28%)
14	PGV	6	101	-	45,45,50	0.95	2 (4%)	48,51,56	1.10	3 (6%)
16	BCL	1	102	7	69,74,74	1.82	18 (26%)	83,115,115	2.57	28 (33%)
14	PGV	R	103	-	42,42,50	1.00	2 (4%)	45,48,56	1.13	3 (6%)
16	BCL	9	102	7	69,74,74	1.81	18 (26%)	83,115,115	2.42	26 (31%)
16	BCL	J	101	8	69,74,74	1.78	20 (28%)	83,115,115	2.52	28 (33%)
20	CDL	M	408	-	55,55,99	1.24	4 (7%)	61,67,111	1.30	6 (9%)
14	PGV	N	101	-	49,49,50	0.91	2 (4%)	52,55,56	1.01	2 (3%)
14	PGV	L	310	-	40,40,50	1.02	2 (5%)	42,46,56	1.08	2 (4%)
23	SF4	a	201	9	0,12,12	-	-	-		
15	LMT	O	102	-	30,30,36	0.43	0	41,41,47	0.98	3 (7%)
20	CDL	H	303	-	74,74,99	1.05	4 (5%)	80,86,111	1.14	8 (10%)
14	PGV	2	102	-	45,45,50	0.98	2 (4%)	48,50,56	1.03	2 (4%)
14	PGV	1	101	-	44,44,50	0.99	2 (4%)	47,50,56	1.03	3 (6%)
20	CDL	H	301	-	63,63,99	1.07	4 (6%)	69,75,111	1.21	5 (7%)
15	LMT	5	102	-	25,25,36	0.49	0	36,36,47	0.66	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
16	BCL	E	101	8	69,74,74	1.78	18 (26%)	83,115,115	2.46	26 (31%)
10	HEC	C	403	1	50,50,50	1.81	11 (22%)	68,82,82	1.81	17 (25%)
21	MQ8	M	405	-	54,54,54	1.25	2 (3%)	66,69,69	1.61	15 (22%)
14	PGV	Z	103	-	43,43,50	0.98	2 (4%)	46,49,56	1.05	3 (6%)
16	BCL	3	102	5	69,74,74	1.80	17 (24%)	83,115,115	2.52	26 (31%)
16	BCL	D	101	7	69,74,74	1.80	19 (27%)	83,115,115	2.59	30 (36%)
14	PGV	8	103	-	42,42,50	0.99	2 (4%)	45,48,56	1.03	3 (6%)
16	BCL	7	102	5	69,74,74	1.79	17 (24%)	83,115,115	2.52	27 (32%)
14	PGV	P	103	-	39,39,50	1.08	2 (5%)	43,44,56	1.17	4 (9%)
16	BCL	I	102	7	69,74,74	1.80	18 (26%)	83,115,115	2.51	27 (32%)
15	LMT	H	307	-	27,27,36	0.47	0	37,38,47	0.85	1 (2%)
16	BCL	X	102	8	69,74,74	1.76	18 (26%)	83,115,115	2.48	25 (30%)
14	PGV	C	408	-	31,31,50	1.13	2 (6%)	34,37,56	1.24	3 (8%)
15	LMT	H	306	-	36,36,36	0.41	0	47,47,47	0.98	3 (6%)
10	HEC	C	404	1	50,50,50	1.79	10 (20%)	68,82,82	1.79	20 (29%)
14	PGV	G	105	-	41,41,50	1.01	2 (4%)	44,46,56	1.12	4 (9%)
16	BCL	K	101	5	69,74,74	1.80	18 (26%)	83,115,115	2.51	22 (26%)
18	UQ8	L	307	-	17,17,53	2.08	2 (11%)	19,23,67	1.14	1 (5%)
16	BCL	4	102	6	69,74,74	1.80	20 (28%)	83,115,115	2.48	23 (27%)
15	LMT	5	101	-	36,36,36	0.34	0	47,47,47	0.91	2 (4%)
22	CRT	8	101	-	41,43,43	0.76	0	50,54,54	3.47	18 (36%)
16	BCL	G	103	6	69,74,74	1.81	18 (26%)	83,115,115	2.42	24 (28%)
16	BCL	Z	102	6	69,74,74	1.78	17 (24%)	83,115,115	2.42	25 (30%)
14	PGV	F	101	-	49,49,50	0.93	2 (4%)	52,55,56	1.02	2 (3%)
14	PGV	H	302	-	35,35,50	1.09	2 (5%)	38,41,56	1.17	3 (7%)
14	PGV	0	104	-	42,42,50	1.00	2 (4%)	44,48,56	1.12	3 (6%)
16	BCL	6	102	8	69,74,74	1.78	17 (24%)	83,115,115	2.43	25 (30%)
22	CRT	4	101	-	41,43,43	0.74	0	50,54,54	3.43	12 (24%)
12	LJQ	C	406	1	30,30,34	0.31	0	32,32,36	0.42	0
14	PGV	R	104	-	40,40,50	1.04	2 (5%)	43,45,56	1.12	3 (6%)
13	PLM	C	407	-	11,11,17	0.41	0	10,10,17	0.47	0
16	BCL	T	101	8	69,74,74	1.81	18 (26%)	83,115,115	2.41	24 (28%)
14	PGV	L	305	-	42,42,50	0.99	2 (4%)	45,48,56	1.07	3 (6%)
16	BCL	S	102	7	69,74,74	1.80	17 (24%)	83,115,115	2.44	24 (28%)
22	CRT	R	101	-	41,43,43	0.71	0	50,54,54	3.55	18 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
22	CRT	M	406	-	41,43,43	0.76	0	50,54,54	2.00	15 (30%)
20	CDL	M	407	-	79,79,99	1.00	4 (5%)	85,91,111	1.06	6 (7%)
14	PGV	H	304	-	41,41,50	0.99	2 (4%)	44,47,56	1.14	4 (9%)
10	HEC	C	402	1	50,50,50	1.78	11 (22%)	68,82,82	1.77	19 (27%)
14	PGV	X	103	-	44,44,50	0.96	2 (4%)	47,50,56	1.13	4 (8%)
14	PGV	0	101	-	40,40,50	1.02	2 (5%)	43,46,56	1.13	3 (6%)
20	CDL	M	402	-	81,81,99	1.03	4 (4%)	87,93,111	0.97	4 (4%)
16	BCL	W	102	7	69,74,74	1.82	17 (24%)	83,115,115	2.49	27 (32%)
22	CRT	N	102	-	41,43,43	0.72	0	50,54,54	3.40	14 (28%)
14	PGV	N	104	-	46,46,50	0.94	2 (4%)	49,52,56	0.93	2 (4%)
16	BCL	I	103	7	69,74,74	1.81	18 (26%)	83,115,115	2.43	25 (30%)
15	LMT	F	102	-	34,34,36	0.49	0	45,45,47	1.14	3 (6%)
14	PGV	Z	101	-	45,45,50	0.99	2 (4%)	48,51,56	1.07	3 (6%)
14	PGV	G	101	-	48,48,50	0.92	2 (4%)	51,54,56	0.94	3 (5%)
16	BCL	L	302	2	69,74,74	1.76	17 (24%)	83,115,115	2.54	27 (32%)
16	BCL	Y	402	5	69,74,74	1.79	17 (24%)	83,115,115	2.44	24 (28%)
20	CDL	M	409	16	49,49,99	1.30	4 (8%)	55,61,111	1.24	5 (9%)
20	CDL	U	102	-	45,45,99	1.41	4 (8%)	51,57,111	1.42	6 (11%)
16	BCL	F	103	5	69,74,74	1.76	17 (24%)	83,115,115	2.59	24 (28%)
20	CDL	U	101	-	50,50,99	1.29	4 (8%)	56,62,111	1.30	6 (10%)
14	PGV	T	102	-	45,45,50	0.94	2 (4%)	48,51,56	0.99	2 (4%)
16	BCL	9	101	7	69,74,74	1.79	18 (26%)	83,115,115	2.48	25 (30%)
14	PGV	P	102	-	46,46,50	0.95	2 (4%)	49,52,56	1.14	4 (8%)
16	BCL	Y	401	20	69,74,74	1.76	18 (26%)	83,115,115	2.50	23 (27%)
10	HEC	C	401	1	50,50,50	1.79	10 (20%)	68,82,82	1.75	16 (23%)
15	LMT	7	101	-	26,26,36	0.51	0	37,37,47	1.02	1 (2%)

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
18	UQ8	L	304	-	-	6/27/51/75	0/1/1/1
14	PGV	B	104	-	-	15/44/44/55	-
16	BCL	5	104	7	-	22/41/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	BCL	P	101	8	-	14/41/137/137	-
14	PGV	6	103	-	-	17/47/47/55	-
16	BCL	L	312	3	-	18/41/137/137	-
22	CRT	G	102	-	-	5/51/51/51	-
15	LMT	H	305	-	-	7/16/56/61	0/2/2/2
16	BCL	V	102	6	-	16/41/137/137	-
22	CRT	V	101	-	-	9/51/51/51	-
18	UQ8	L	306	-	-	7/33/57/75	0/1/1/1
14	PGV	L	309	-	-	12/39/39/55	-
16	BCL	R	102	6	-	18/41/137/137	-
14	PGV	G	104	-	-	21/54/54/55	-
14	PGV	X	101	-	-	19/47/47/55	-
16	BCL	N	103	6	-	15/41/137/137	-
15	LMT	M	411	-	-	7/21/61/61	0/2/2/2
17	BPH	L	303	-	-	8/37/105/105	0/5/6/6
20	CDL	O	101	-	-	25/83/83/110	-
14	PGV	N	105	-	-	14/41/41/55	-
14	PGV	J	102	-	-	6/34/34/55	-
14	PGV	M	410	-	-	24/55/55/55	-
16	BCL	M	403	3	-	13/41/137/137	-
14	PGV	Z	104	-	-	21/46/46/55	-
16	BCL	5	103	7	-	12/41/137/137	-
16	BCL	0	102	8	-	5/41/137/137	-
14	PGV	V	103	-	-	17/48/48/55	-
16	BCL	B	102	6	-	13/41/137/137	-
14	PGV	T	103	-	-	19/51/51/55	-
22	CRT	B	101	-	-	7/51/51/51	-
16	BCL	O	104	7	-	16/41/137/137	-
15	LMT	L	308	-	-	6/21/61/61	0/2/2/2
16	BCL	8	102	6	-	9/41/137/137	-
17	BPH	M	404	-	-	7/37/105/105	0/5/6/6
15	LMT	Q	101	-	-	10/18/58/61	0/2/2/2
16	BCL	W	101	7	-	15/41/137/137	-
16	BCL	Q	102	5	-	12/41/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	PGV	0	103	-	-	16/48/48/55	-
16	BCL	A	101	5	-	18/41/137/137	-
14	PGV	2	103	-	-	16/40/40/55	-
22	CRT	Y	403	-	-	2/51/51/51	-
16	BCL	L	311	2	-	11/41/137/137	-
14	PGV	6	104	-	-	10/47/47/55	-
14	PGV	3	101	-	-	10/33/33/55	-
16	BCL	S	101	7	-	20/41/137/137	-
16	BCL	O	103	7	-	15/41/137/137	-
16	BCL	1	103	7	-	17/41/137/137	-
16	BCL	2	101	8	-	11/41/137/137	-
14	PGV	4	103	-	-	13/47/47/55	-
14	PGV	B	103	-	-	21/48/48/55	-
15	LMT	L	301	-	-	3/11/51/61	0/2/2/2
14	PGV	E	102	-	-	9/42/42/55	-
16	BCL	D	102	7	-	17/41/137/137	-
15	LMT	I	101	-	-	8/11/51/61	0/2/2/2
16	BCL	U	103	5	-	15/41/137/137	-
14	PGV	6	101	-	-	15/50/50/55	-
16	BCL	1	102	7	-	14/41/137/137	-
14	PGV	R	103	-	-	14/47/47/55	-
16	BCL	9	102	7	-	9/41/137/137	-
16	BCL	J	101	8	-	12/41/137/137	-
20	CDL	M	408	-	-	28/66/66/110	-
14	PGV	N	101	-	-	22/54/54/55	-
14	PGV	L	310	-	-	20/45/45/55	-
23	SF4	a	201	9	-	-	0/6/5/5
15	LMT	O	102	-	-	6/15/55/61	0/2/2/2
20	CDL	H	303	-	-	43/85/85/110	-
14	PGV	2	102	-	-	15/49/49/55	-
14	PGV	1	101	-	-	17/49/49/55	-
20	CDL	H	301	-	-	23/73/73/110	-
15	LMT	5	102	-	-	4/10/50/61	0/2/2/2
16	BCL	E	101	8	-	10/41/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	HEC	C	403	1	1/1/3/7	6/14/54/54	-
21	MQ8	M	405	-	-	4/47/67/67	0/2/2/2
14	PGV	Z	103	-	-	22/48/48/55	-
16	BCL	3	102	5	-	14/41/137/137	-
16	BCL	D	101	7	-	14/41/137/137	-
14	PGV	8	103	-	-	17/47/47/55	-
16	BCL	7	102	5	-	17/41/137/137	-
14	PGV	P	103	-	-	9/41/41/55	-
16	BCL	I	102	7	-	15/41/137/137	-
15	LMT	H	307	-	-	3/12/52/61	0/2/2/2
16	BCL	X	102	8	-	15/41/137/137	-
14	PGV	C	408	-	-	10/36/36/55	-
15	LMT	H	306	-	-	6/21/61/61	0/2/2/2
10	HEC	C	404	1	1/1/3/7	2/14/54/54	-
14	PGV	G	105	-	-	19/45/45/55	-
16	BCL	K	101	5	-	20/41/137/137	-
18	UQ8	L	307	-	-	1/8/32/75	0/1/1/1
16	BCL	4	102	6	-	11/41/137/137	-
15	LMT	5	101	-	-	11/21/61/61	0/2/2/2
22	CRT	8	101	-	-	5/51/51/51	-
16	BCL	G	103	6	-	20/41/137/137	-
16	BCL	Z	102	6	-	18/41/137/137	-
14	PGV	F	101	-	-	15/54/54/55	-
14	PGV	H	302	-	-	19/40/40/55	-
14	PGV	0	104	-	-	13/47/47/55	-
16	BCL	6	102	8	-	9/41/137/137	-
22	CRT	4	101	-	-	8/51/51/51	-
12	LJQ	C	406	1	-	2/31/31/36	-
14	PGV	R	104	-	-	17/42/42/55	-
13	PLM	C	407	-	-	0/8/9/15	-
16	BCL	T	101	8	-	16/41/137/137	-
14	PGV	L	305	-	-	19/47/47/55	-
16	BCL	S	102	7	-	13/41/137/137	-
22	CRT	R	101	-	-	8/51/51/51	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CRT	M	406	-	-	11/51/51/51	-
20	CDL	M	407	-	-	41/90/90/110	-
14	PGV	H	304	-	-	18/46/46/55	-
10	HEC	C	402	1	1/1/3/7	4/14/54/54	-
14	PGV	X	103	-	-	14/49/49/55	-
14	PGV	0	101	-	-	20/45/45/55	-
20	CDL	M	402	-	-	41/92/92/110	-
16	BCL	W	102	7	-	17/41/137/137	-
22	CRT	N	102	-	-	5/51/51/51	-
14	PGV	N	104	-	-	14/51/51/55	-
16	BCL	I	103	7	-	18/41/137/137	-
15	LMT	F	102	-	-	8/19/59/61	0/2/2/2
14	PGV	Z	101	-	-	22/50/50/55	-
14	PGV	G	101	-	-	24/53/53/55	-
16	BCL	L	302	2	-	9/41/137/137	-
16	BCL	Y	402	5	-	15/41/137/137	-
20	CDL	M	409	16	-	22/60/60/110	-
20	CDL	U	102	-	-	17/55/55/110	-
16	BCL	F	103	5	-	16/41/137/137	-
20	CDL	U	101	-	-	26/61/61/110	-
14	PGV	T	102	-	-	18/50/50/55	-
16	BCL	9	101	7	-	11/41/137/137	-
14	PGV	P	102	-	-	23/51/51/55	-
16	BCL	Y	401	20	-	14/41/137/137	-
10	HEC	C	401	1	1/1/3/7	5/14/54/54	-
15	LMT	7	101	-	-	4/11/51/61	0/2/2/2

The worst 5 of 982 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	L	307	UQ8	C6-C1	7.65	1.49	1.35
18	L	306	UQ8	C6-C1	7.46	1.48	1.35
21	M	405	MQ8	C3-C2	7.46	1.48	1.35
18	L	304	UQ8	C6-C1	7.40	1.48	1.35
10	C	404	HEC	FE-NB	5.24	2.11	1.94

The worst 5 of 1606 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	R	101	CRT	C2-C1-C4	-17.36	84.21	110.86
22	B	101	CRT	C2-C1-C4	-16.59	85.38	110.86
22	V	101	CRT	C3-C1-C4	-16.16	86.04	110.86
22	G	102	CRT	C3-C1-C4	-16.10	86.13	110.86
22	N	102	CRT	C2-C1-C4	-16.04	86.23	110.86

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
10	C	401	HEC	NA
10	C	402	HEC	NA
10	C	403	HEC	NA
10	C	404	HEC	NA

5 of 1806 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	L	305	PGV	C03-O11-P-O13
14	L	309	PGV	C04-O12-P-O11
14	L	309	PGV	C04-O12-P-O13
14	L	310	PGV	C03-O11-P-O13
14	L	310	PGV	C03-O11-P-O14

There are no ring outliers.

126 monomers are involved in 630 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	L	304	UQ8	5	0
14	B	104	PGV	8	0
16	5	104	BCL	7	0
16	P	101	BCL	9	0
14	6	103	PGV	3	0
16	L	312	BCL	6	0
22	G	102	CRT	6	0
15	H	305	LMT	8	0
16	V	102	BCL	9	0
22	V	101	CRT	9	0
18	L	306	UQ8	4	0
14	L	309	PGV	5	0
16	R	102	BCL	10	0
14	G	104	PGV	7	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	X	101	PGV	2	0
16	N	103	BCL	8	0
15	M	411	LMT	4	0
17	L	303	BPH	6	0
20	O	101	CDL	3	0
14	J	102	PGV	4	0
14	M	410	PGV	5	0
16	M	403	BCL	7	0
14	Z	104	PGV	8	0
16	5	103	BCL	14	0
16	0	102	BCL	9	0
14	V	103	PGV	2	0
16	B	102	BCL	11	0
14	T	103	PGV	7	0
22	B	101	CRT	4	0
16	O	104	BCL	5	0
15	L	308	LMT	3	0
16	8	102	BCL	11	0
17	M	404	BPH	8	0
15	Q	101	LMT	3	0
16	W	101	BCL	11	0
16	Q	102	BCL	7	0
14	0	103	PGV	5	0
16	A	101	BCL	4	0
14	2	103	PGV	1	0
22	Y	403	CRT	9	0
16	L	311	BCL	4	0
14	6	104	PGV	3	0
14	3	101	PGV	4	0
16	S	101	BCL	12	0
16	O	103	BCL	6	0
16	1	103	BCL	7	0
16	2	101	BCL	10	0
14	4	103	PGV	4	0
14	B	103	PGV	5	0
15	L	301	LMT	2	0
14	E	102	PGV	2	0
16	D	102	BCL	5	0
15	I	101	LMT	5	0
16	U	103	BCL	5	0
14	6	101	PGV	3	0
16	1	102	BCL	10	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	R	103	PGV	3	0
16	9	102	BCL	6	0
16	J	101	BCL	8	0
20	M	408	CDL	3	0
14	N	101	PGV	8	0
14	L	310	PGV	8	0
15	O	102	LMT	1	0
20	H	303	CDL	9	0
14	2	102	PGV	6	0
14	1	101	PGV	12	0
20	H	301	CDL	5	0
15	5	102	LMT	3	0
16	E	101	BCL	6	0
10	C	403	HEC	2	0
21	M	405	MQ8	3	0
14	Z	103	PGV	3	0
16	3	102	BCL	8	0
16	D	101	BCL	5	0
14	8	103	PGV	8	0
16	7	102	BCL	3	0
14	P	103	PGV	2	0
16	I	102	BCL	6	0
16	X	102	BCL	5	0
14	C	408	PGV	3	0
15	H	306	LMT	1	0
14	G	105	PGV	6	0
16	K	101	BCL	7	0
18	L	307	UQ8	1	0
16	4	102	BCL	5	0
15	5	101	LMT	4	0
22	8	101	CRT	6	0
16	G	103	BCL	10	0
16	Z	102	BCL	8	0
14	F	101	PGV	6	0
14	H	302	PGV	5	0
14	0	104	PGV	7	0
16	6	102	BCL	7	0
22	4	101	CRT	12	0
14	R	104	PGV	6	0
13	C	407	PLM	5	0
16	T	101	BCL	6	0
14	L	305	PGV	4	0

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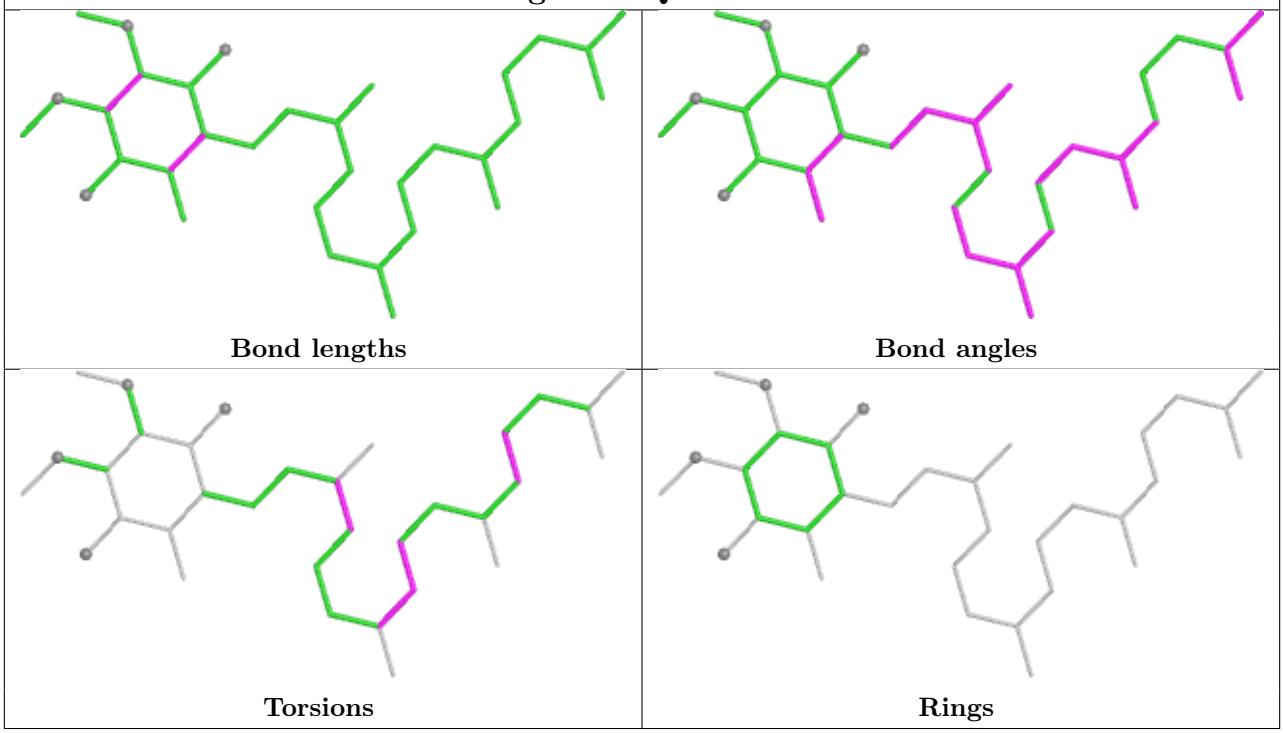
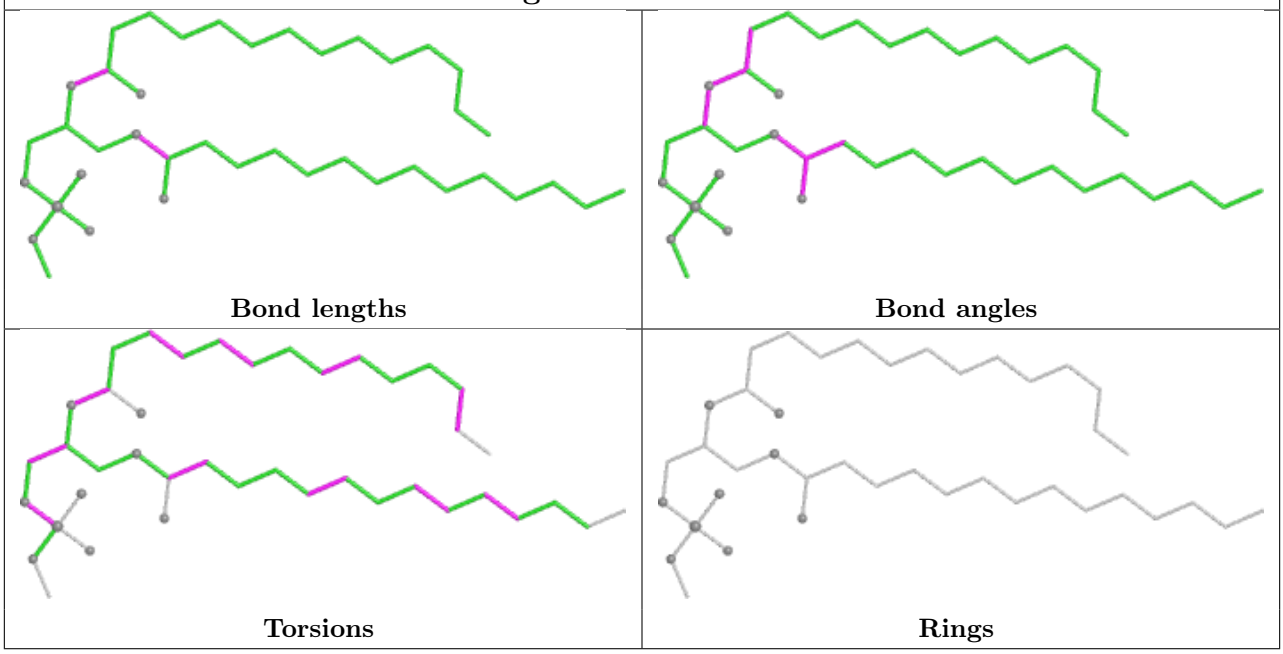
Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	S	102	BCL	9	0
22	R	101	CRT	9	0
22	M	406	CRT	11	0
20	M	407	CDL	4	0
14	H	304	PGV	3	0
10	C	402	HEC	1	0
14	X	103	PGV	6	0
14	0	101	PGV	6	0
20	M	402	CDL	9	0
16	W	102	BCL	3	0
22	N	102	CRT	11	0
14	N	104	PGV	2	0
16	I	103	BCL	14	0
15	F	102	LMT	4	0
14	Z	101	PGV	4	0
14	G	101	PGV	6	0
16	L	302	BCL	3	0
16	Y	402	BCL	3	0
20	M	409	CDL	4	0
20	U	102	CDL	1	0
16	F	103	BCL	2	0
20	U	101	CDL	5	0
14	T	102	PGV	6	0
16	9	101	BCL	5	0
14	P	102	PGV	9	0
16	Y	401	BCL	5	0
10	C	401	HEC	11	0
15	7	101	LMT	4	0

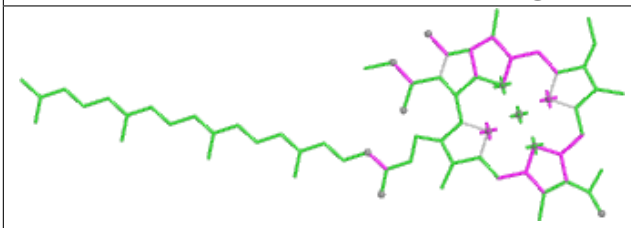
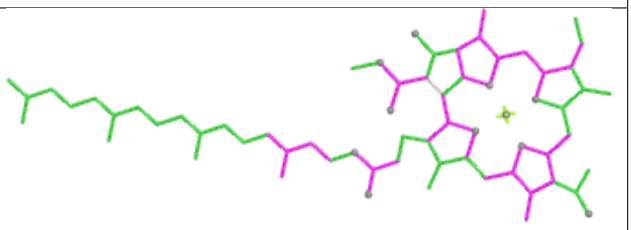
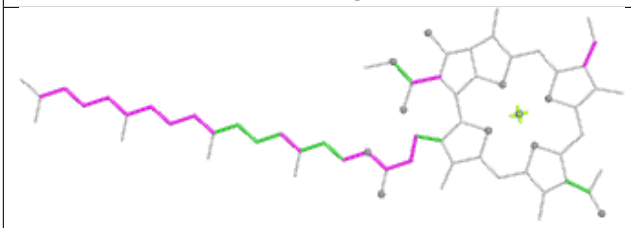
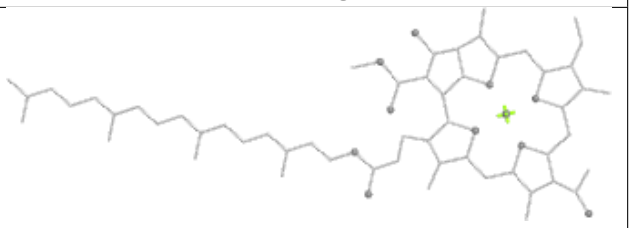
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

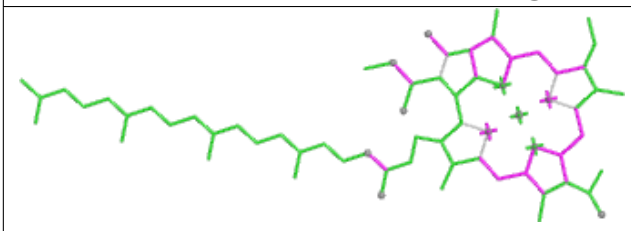
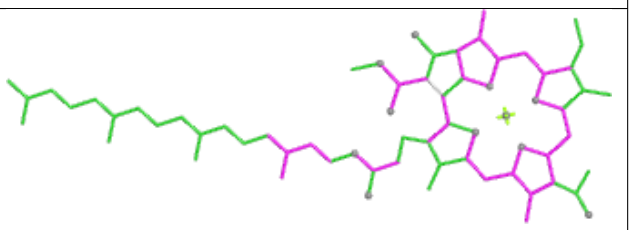
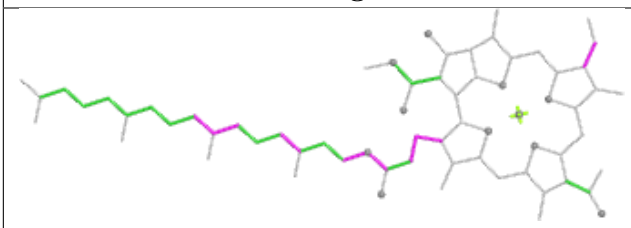
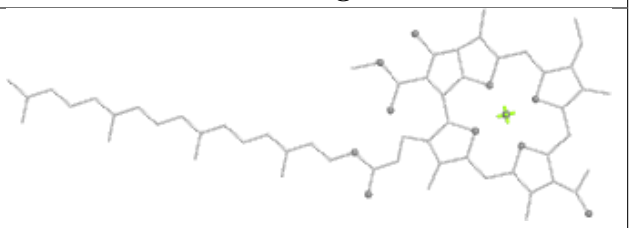
Ligand UQ8 L 304



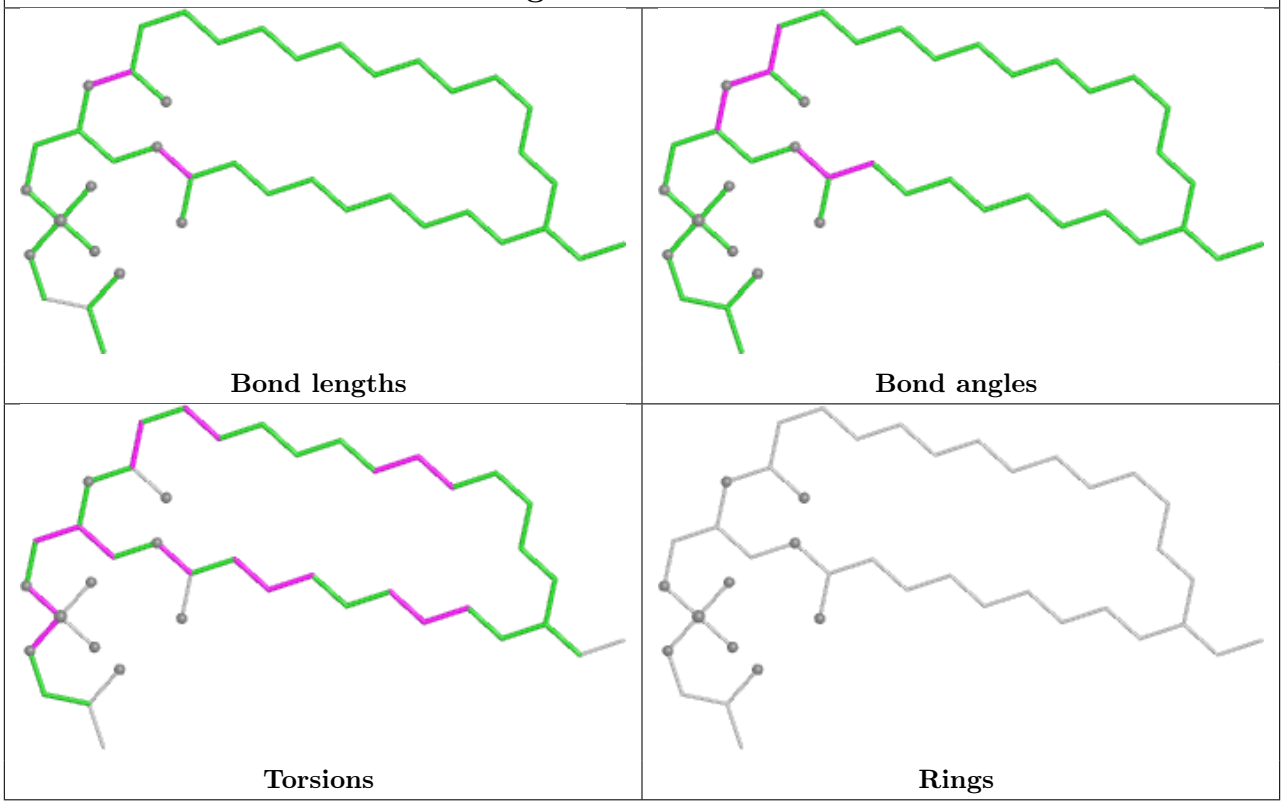
Ligand PGV B 104



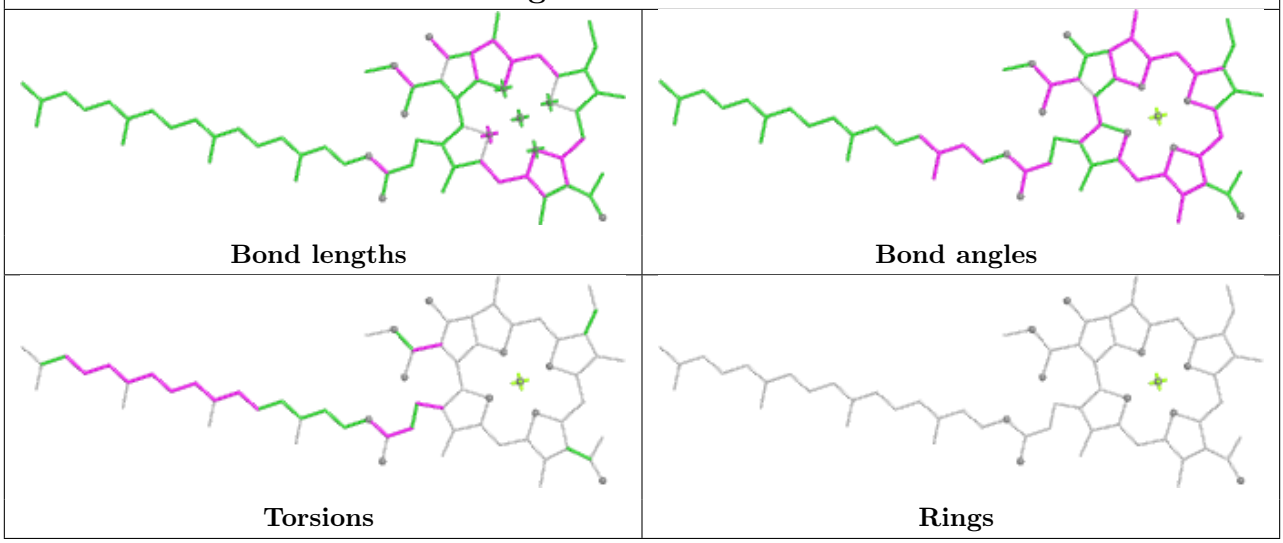
Ligand BCL 5 104	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCL P 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

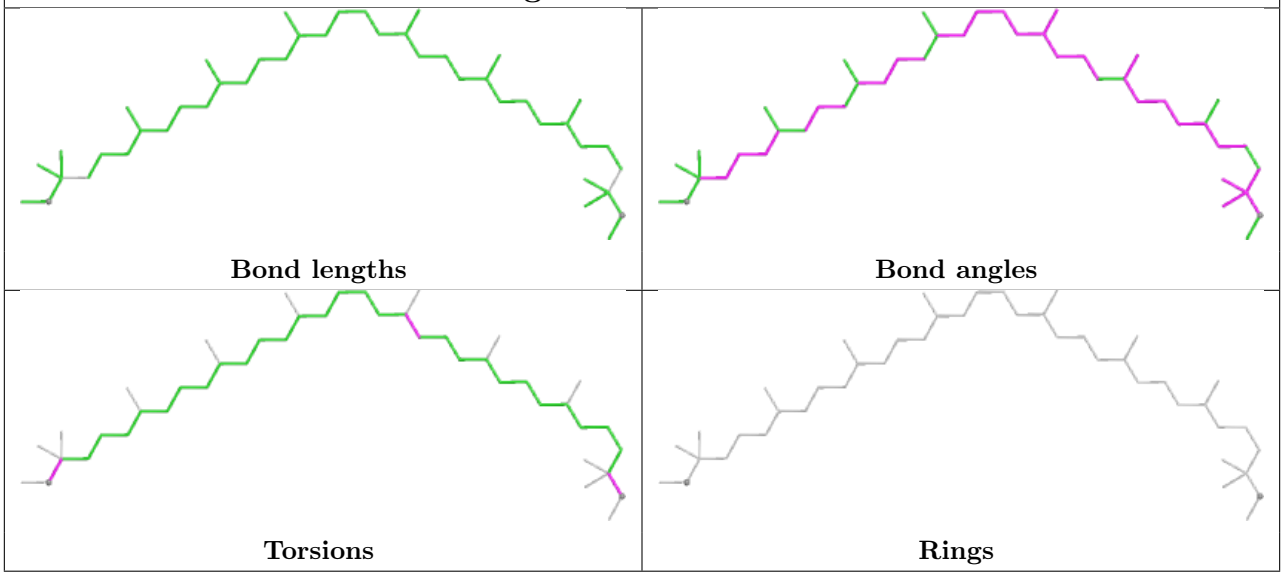
Ligand PGV 6 103



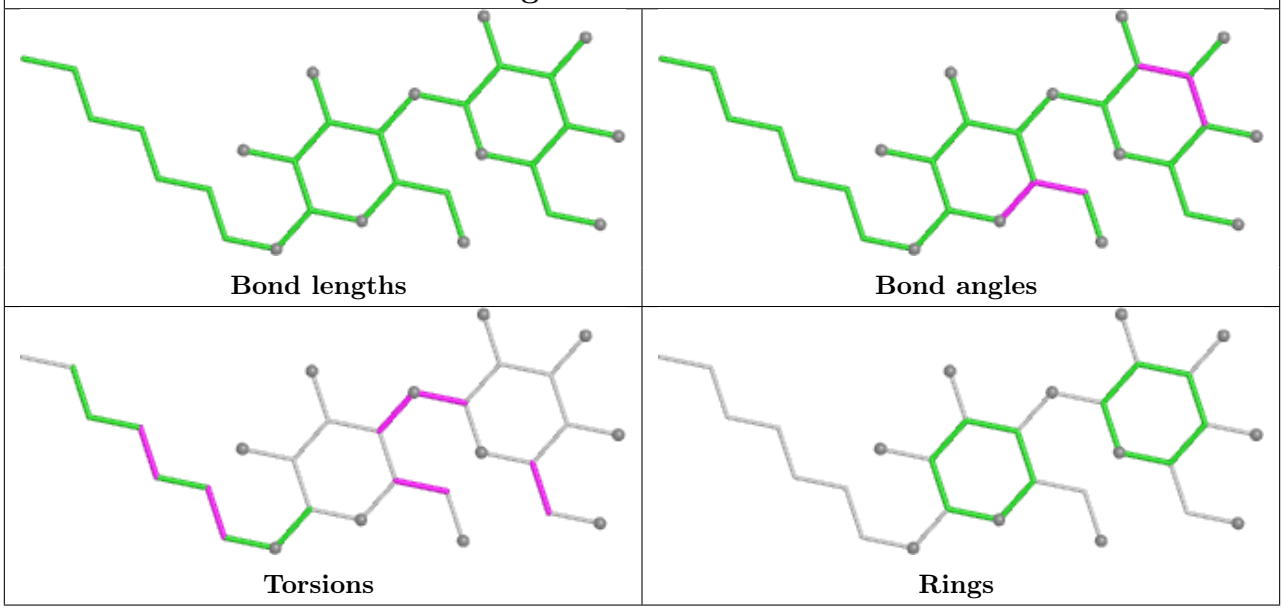
Ligand BCL L 312



Ligand CRT G 102



Ligand LMT H 305



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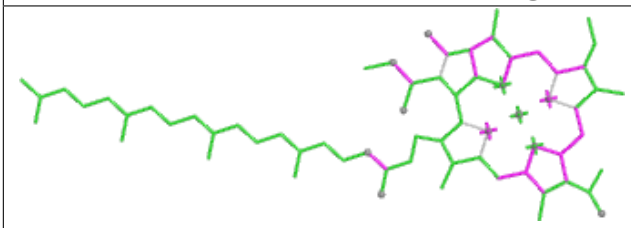
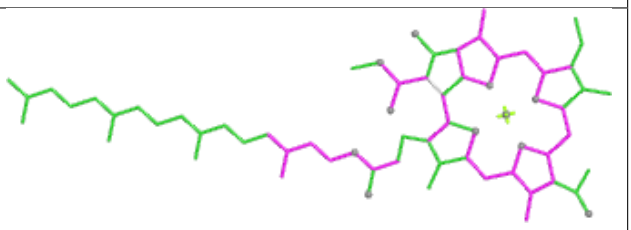
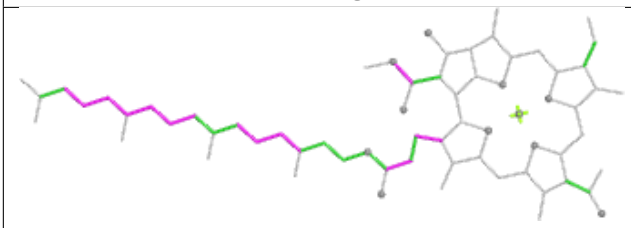
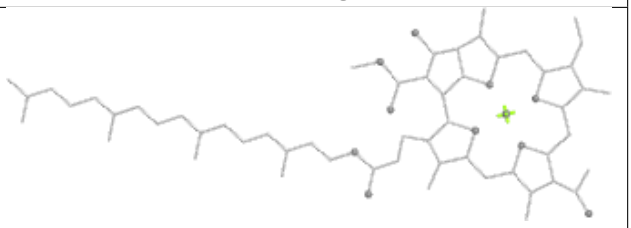
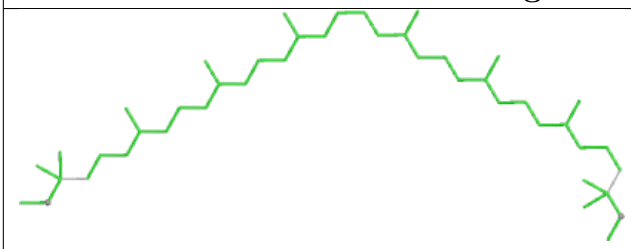
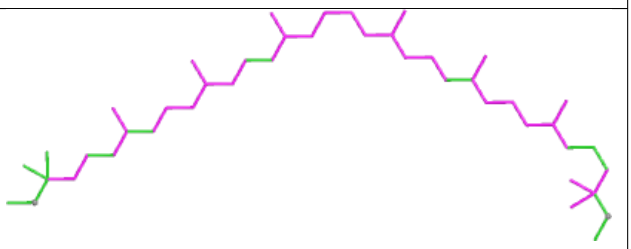
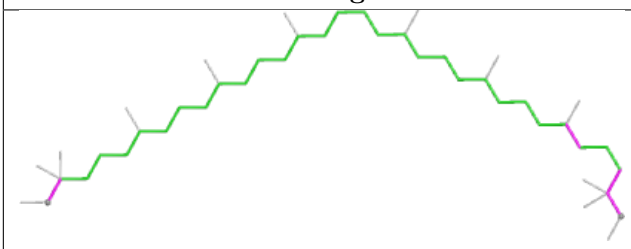
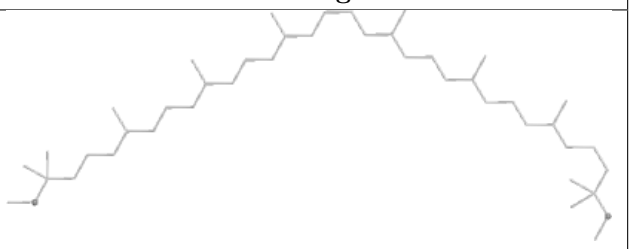
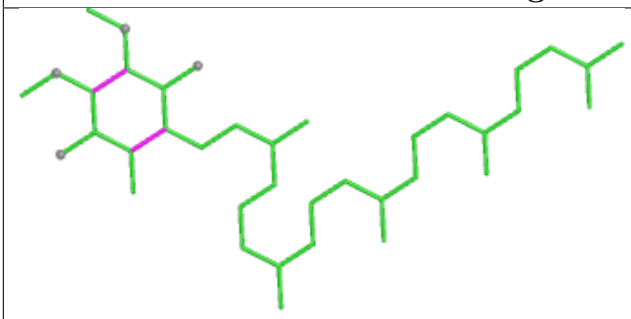
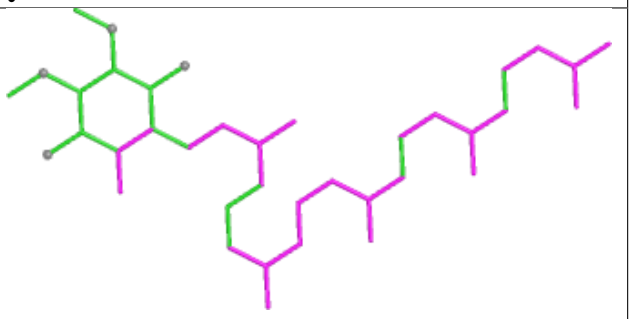
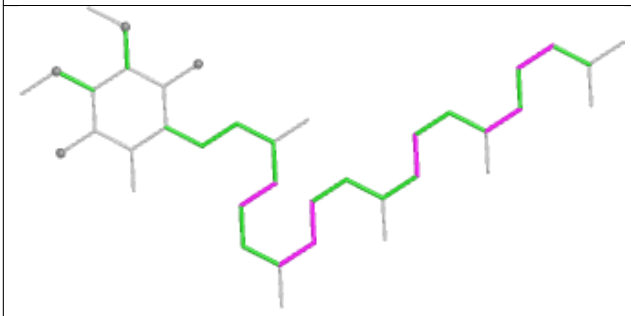
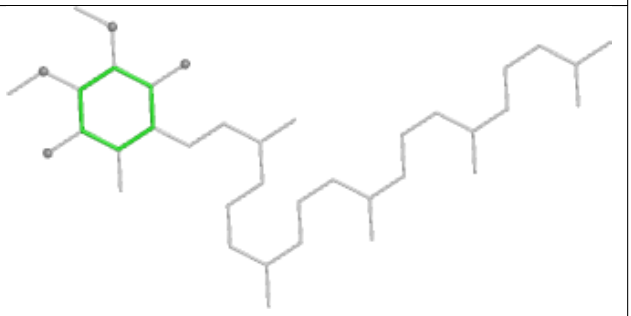
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CRT V 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand UQ8 L 306	
 Bond lengths	 Bond angles
 Torsions	 Rings

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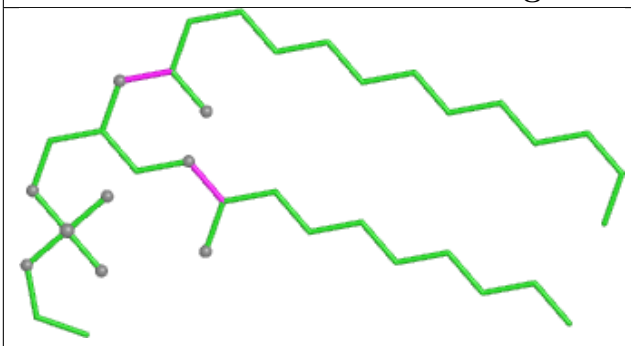
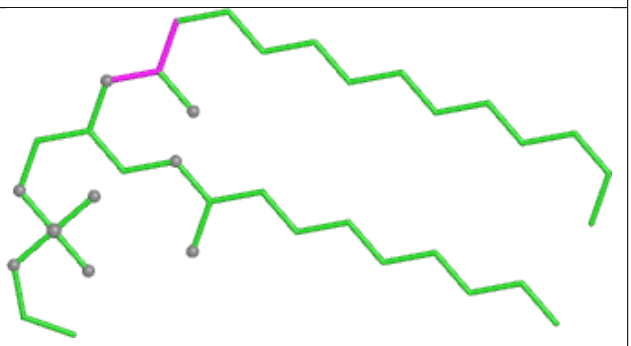
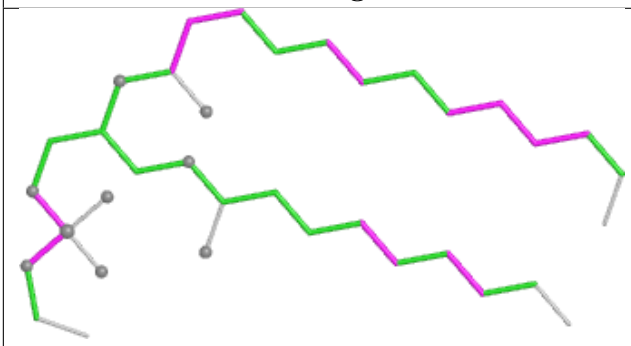
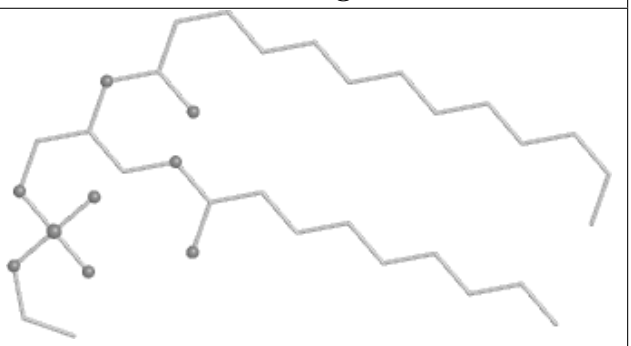
 Bond lengths	 Bond angles
 Torsions	 Rings

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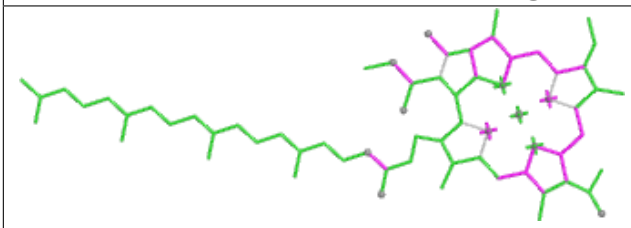
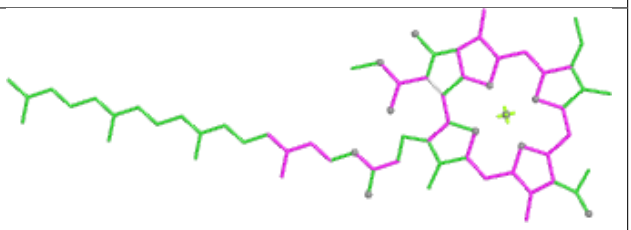
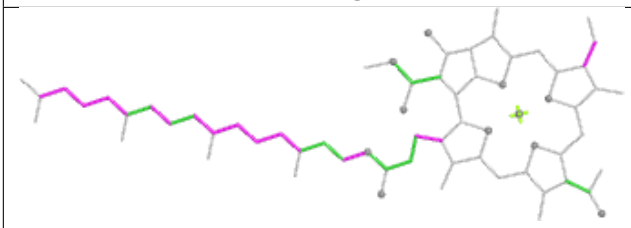
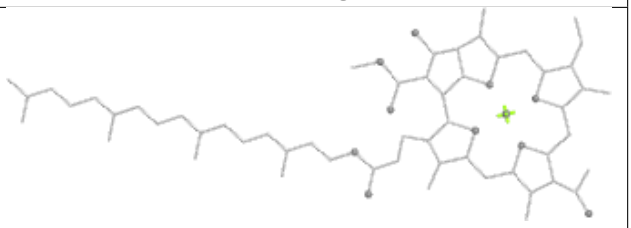
 Bond lengths	 Bond angles
 Torsions	 Rings

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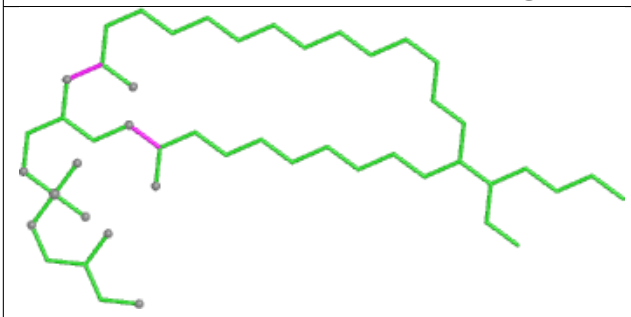
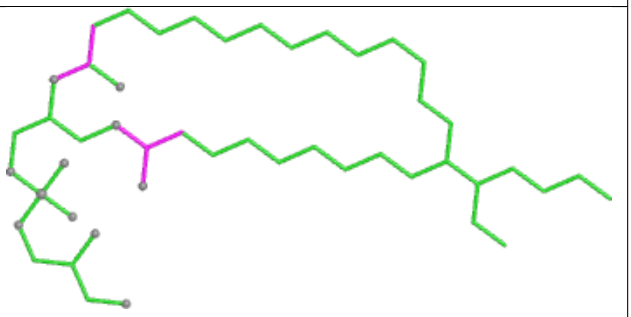
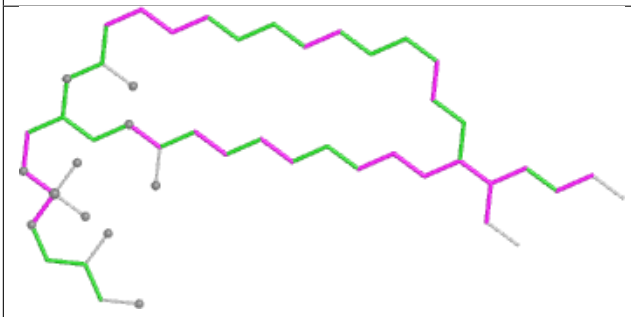
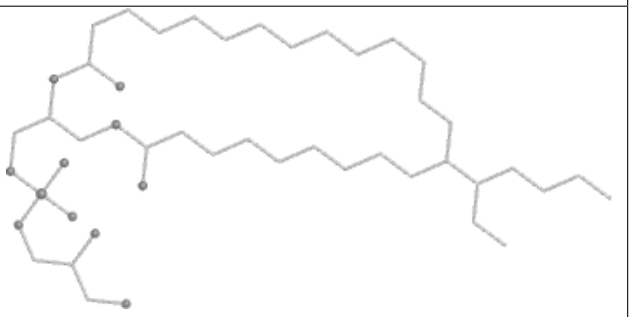
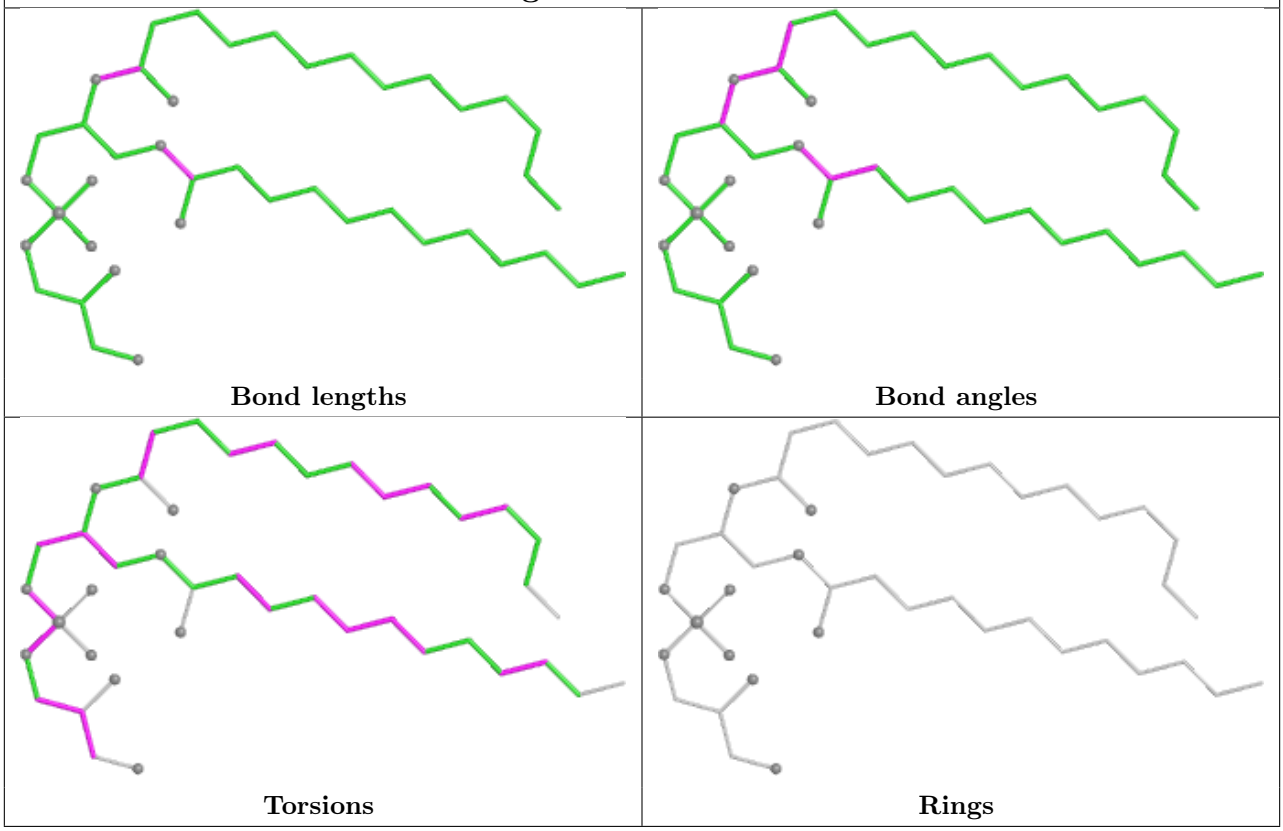
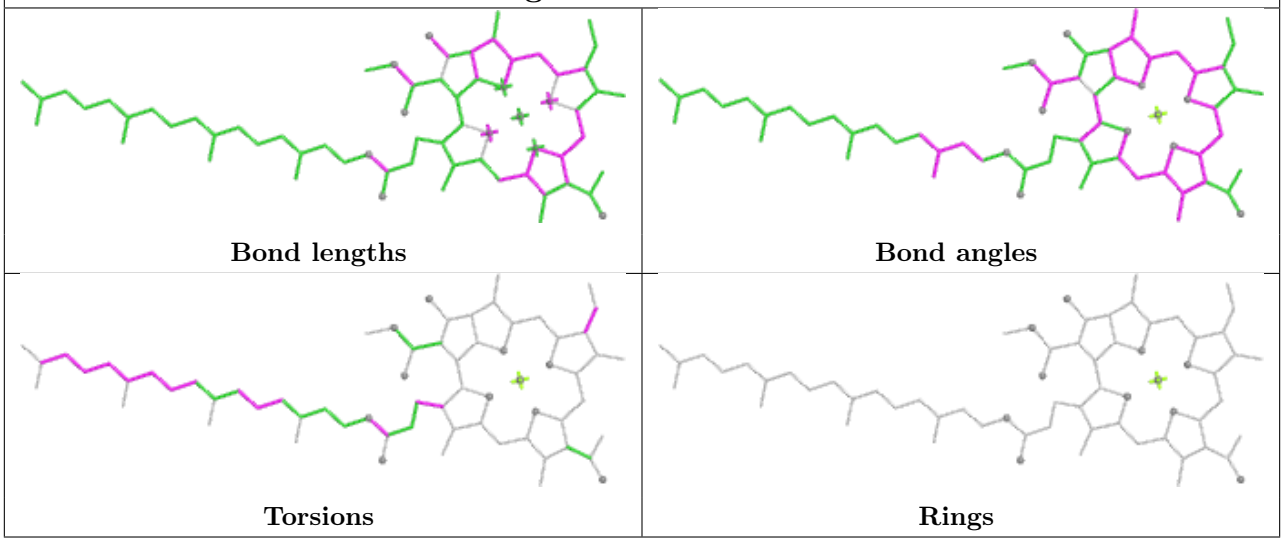
 Bond lengths	 Bond angles
 Torsions	 Rings

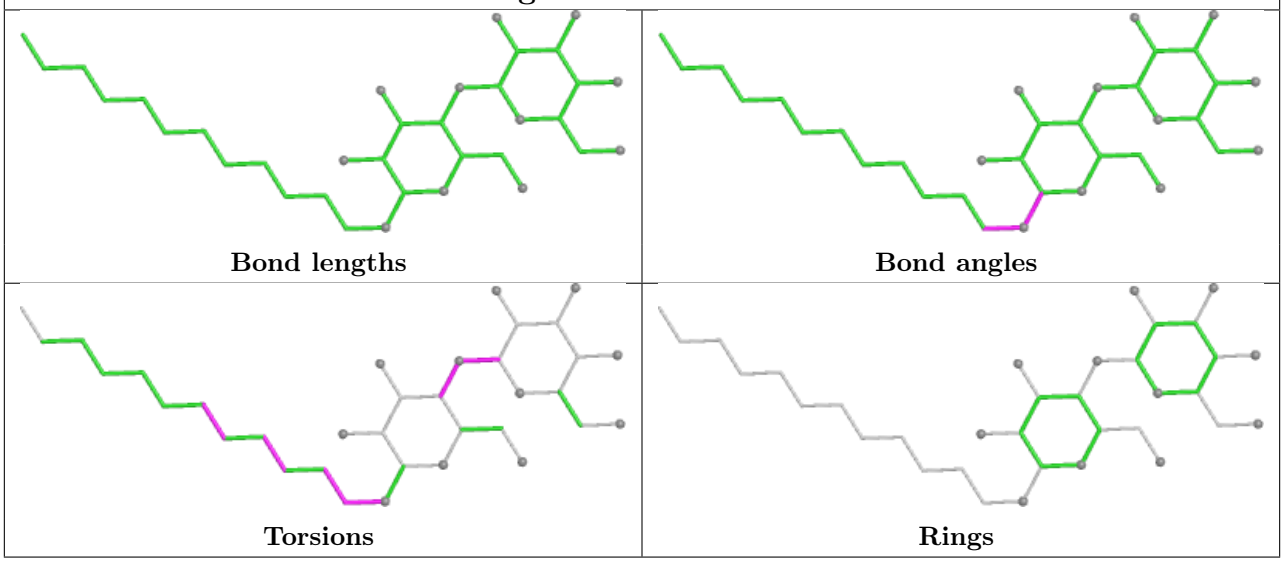
Ligand PGV X 101



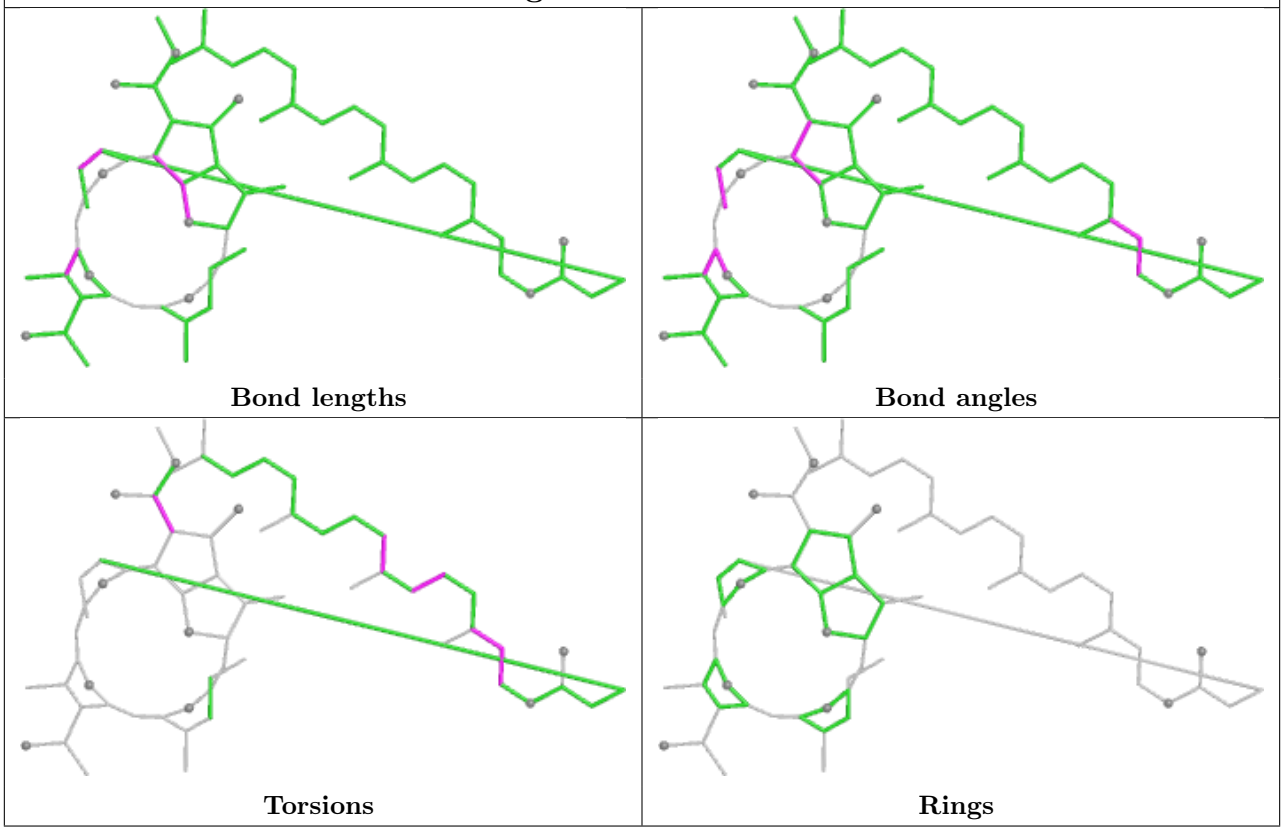
Ligand BCL N 103



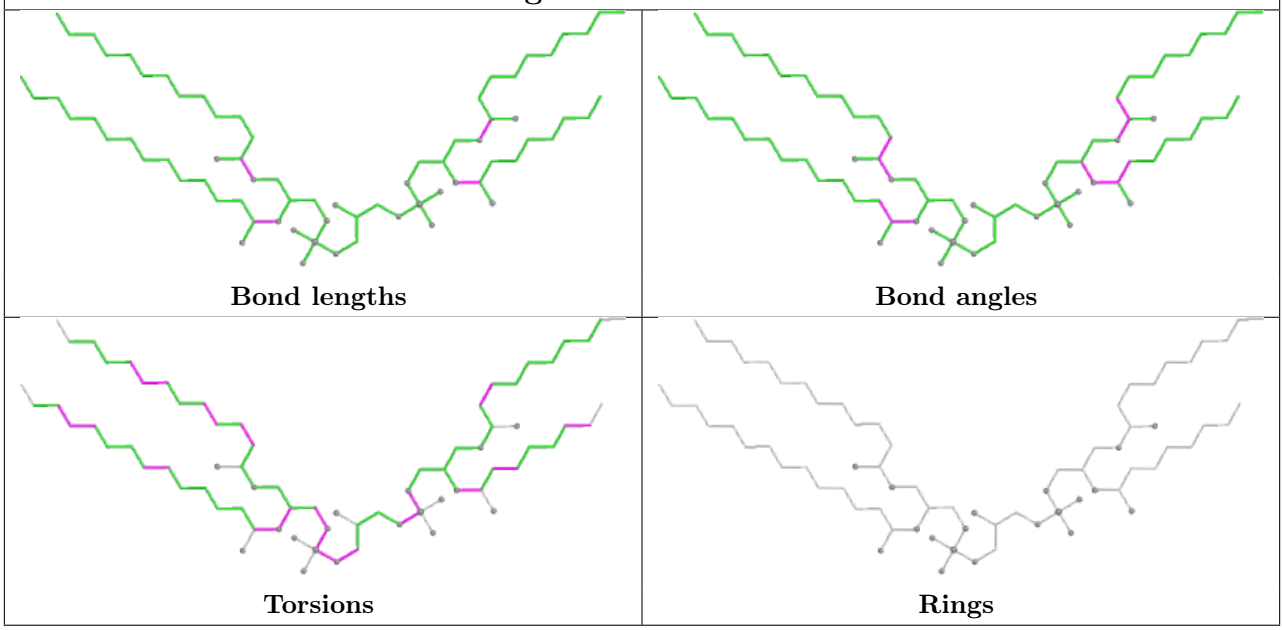
Ligand LMT M 411



Ligand BPH L 303



Ligand CDL O 101



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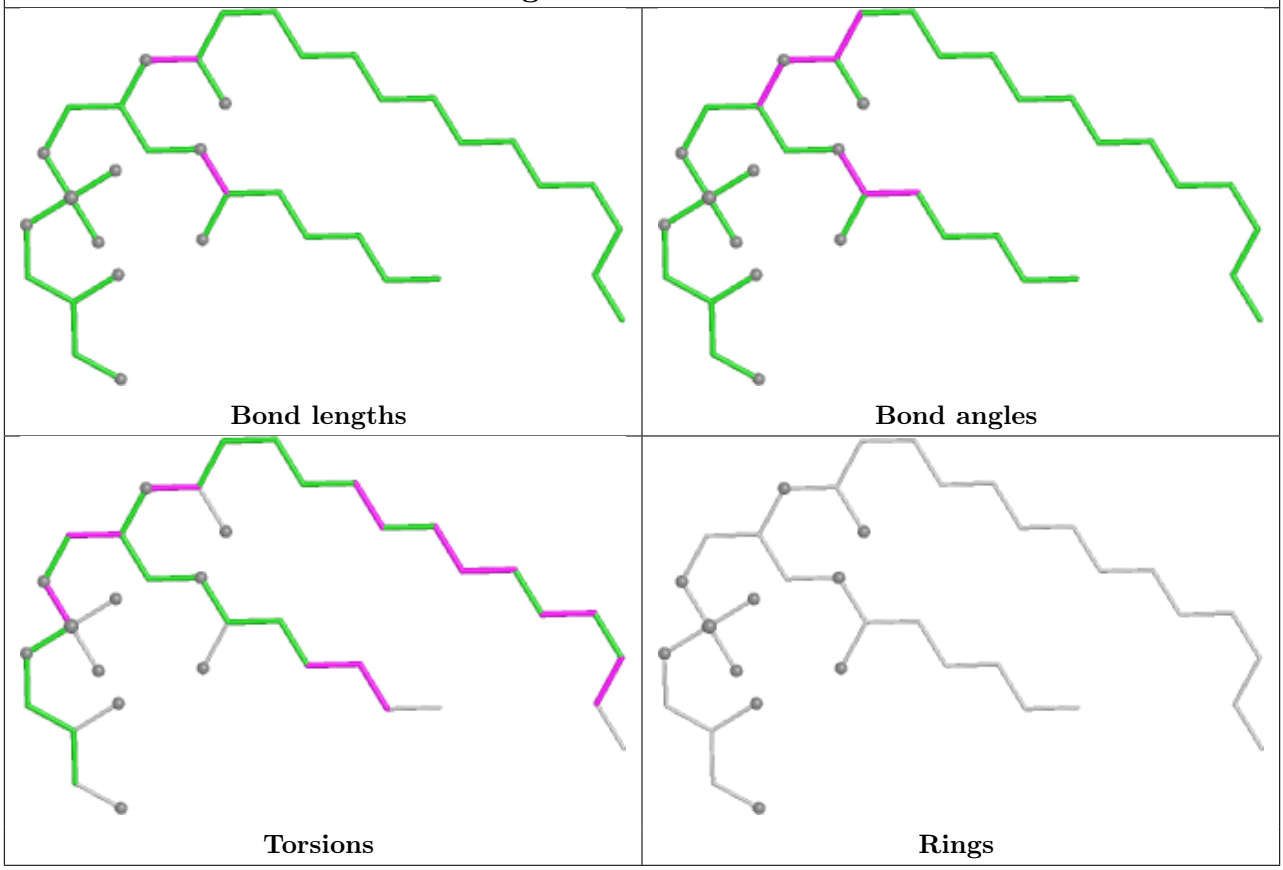

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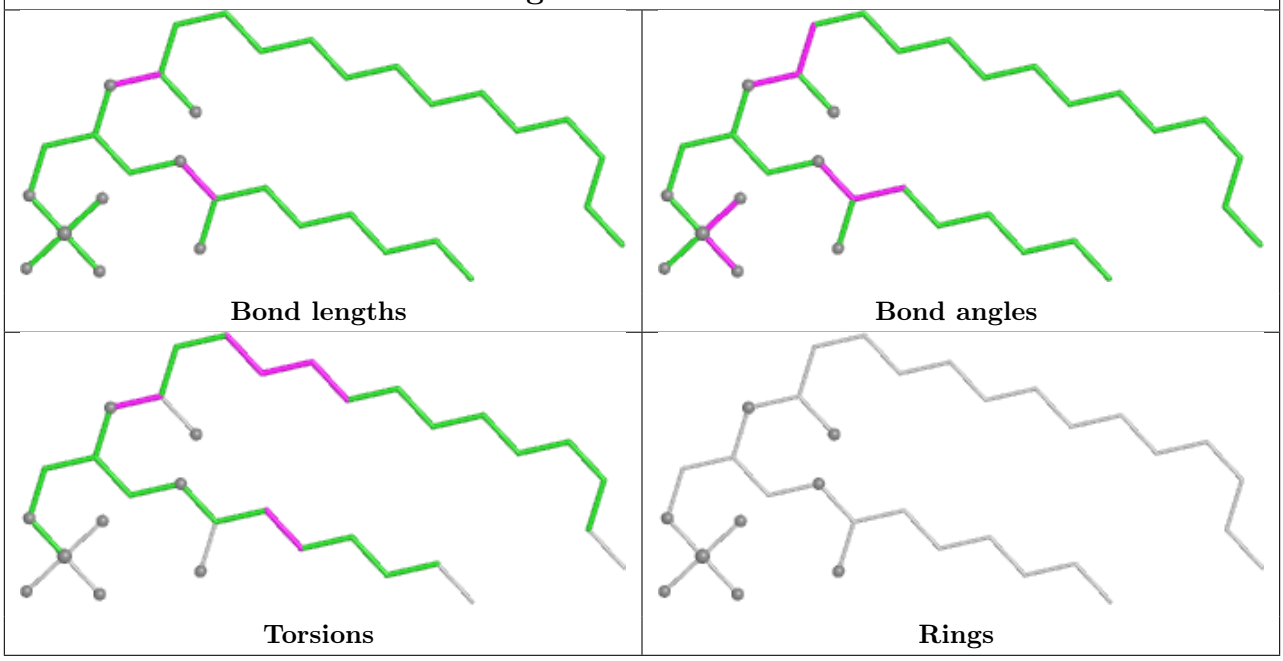
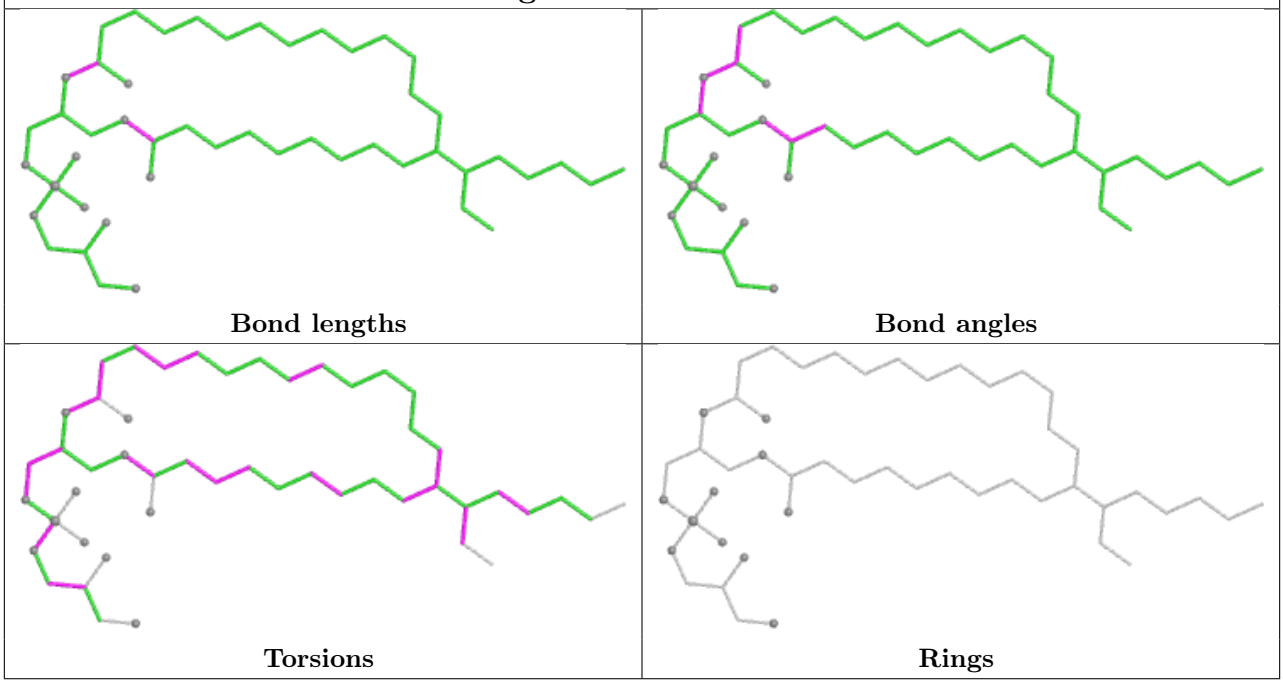


Ligand PGV M 410



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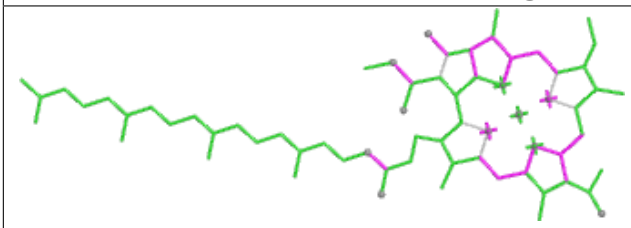
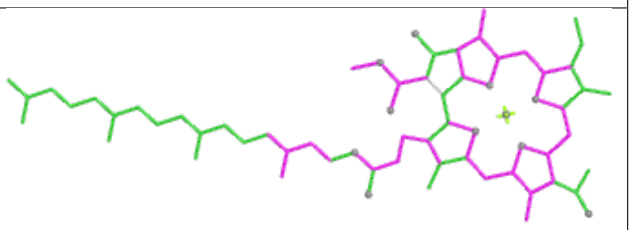
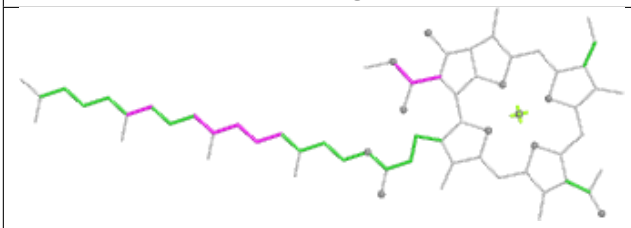
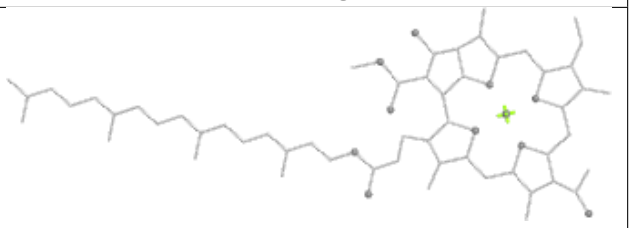
 Bond lengths	 Bond angles
 Torsions	 Rings

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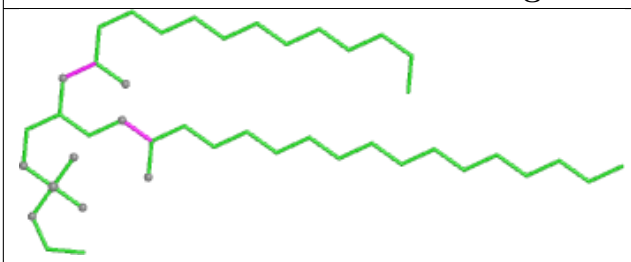
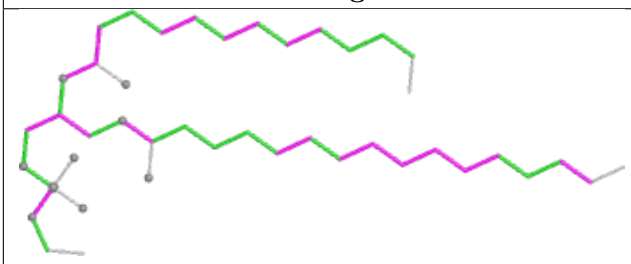
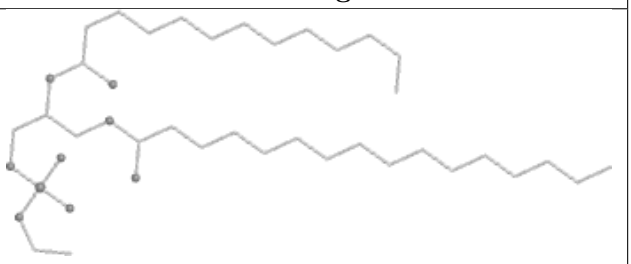
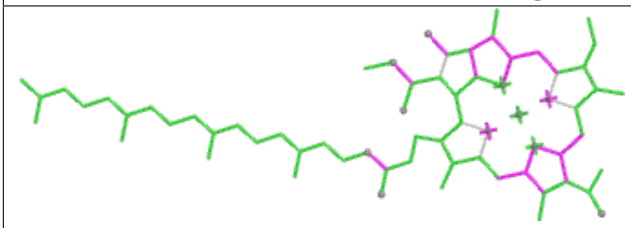
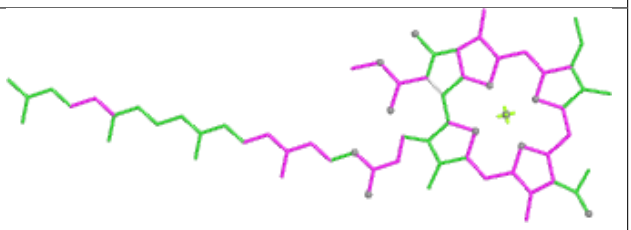
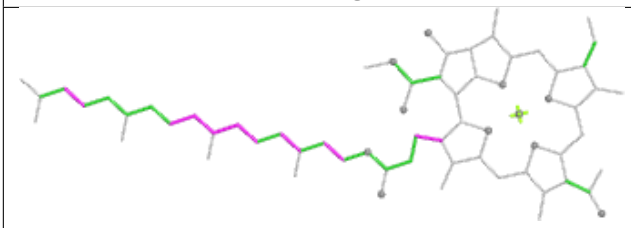
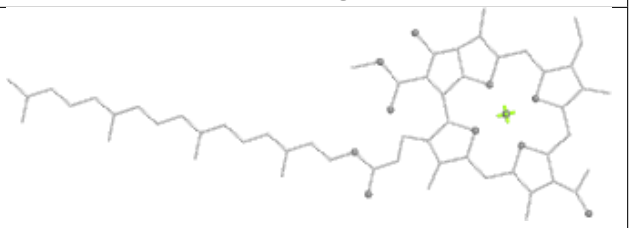
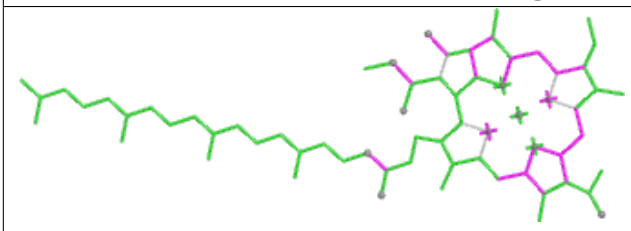
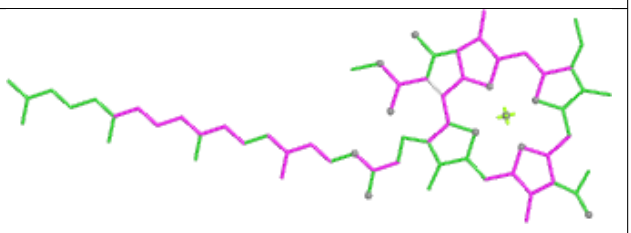
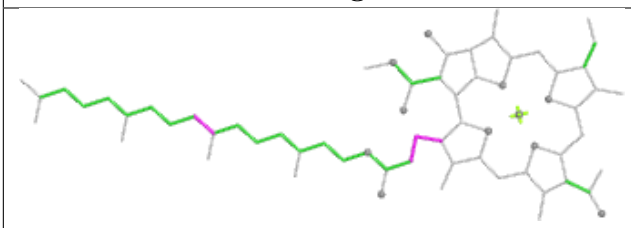
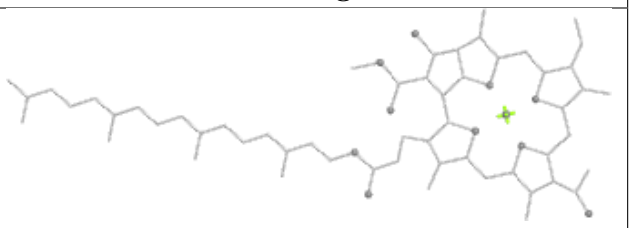
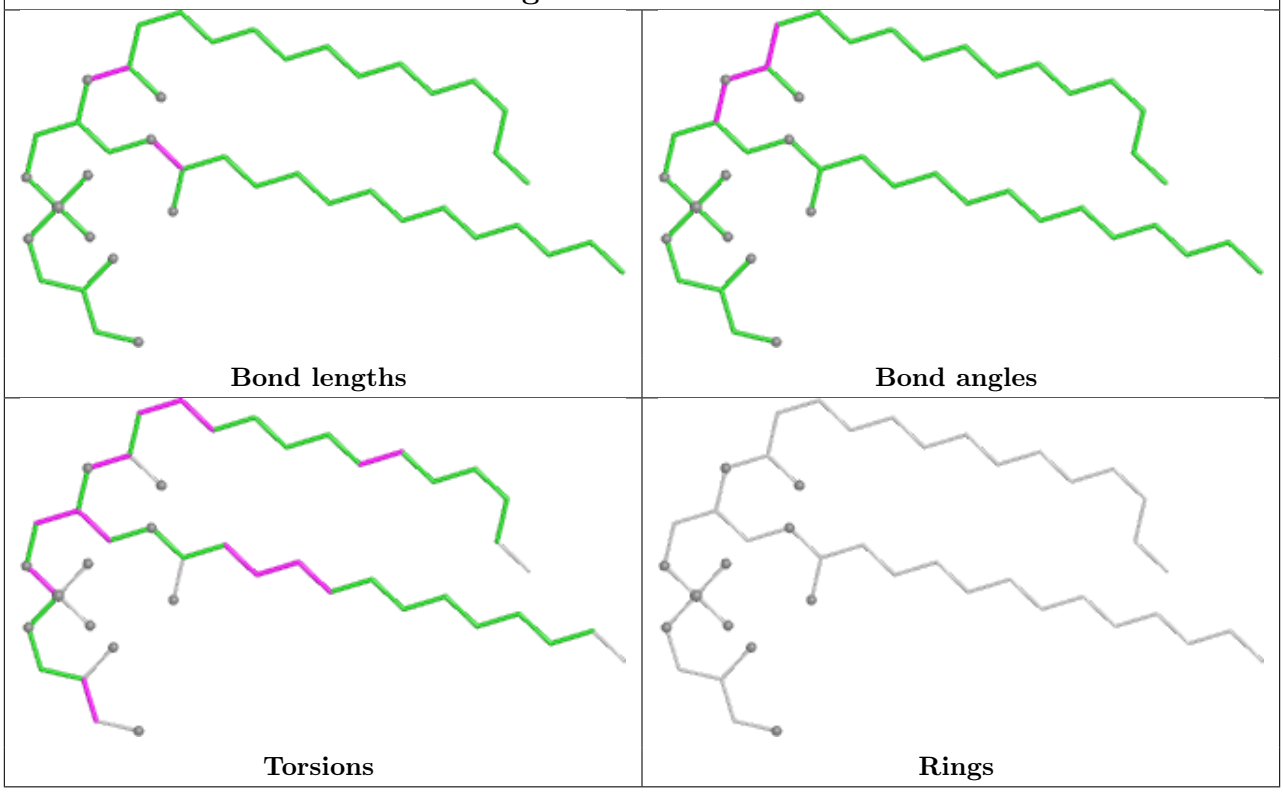
 Bond lengths	Bond angles
 Torsions	 Rings

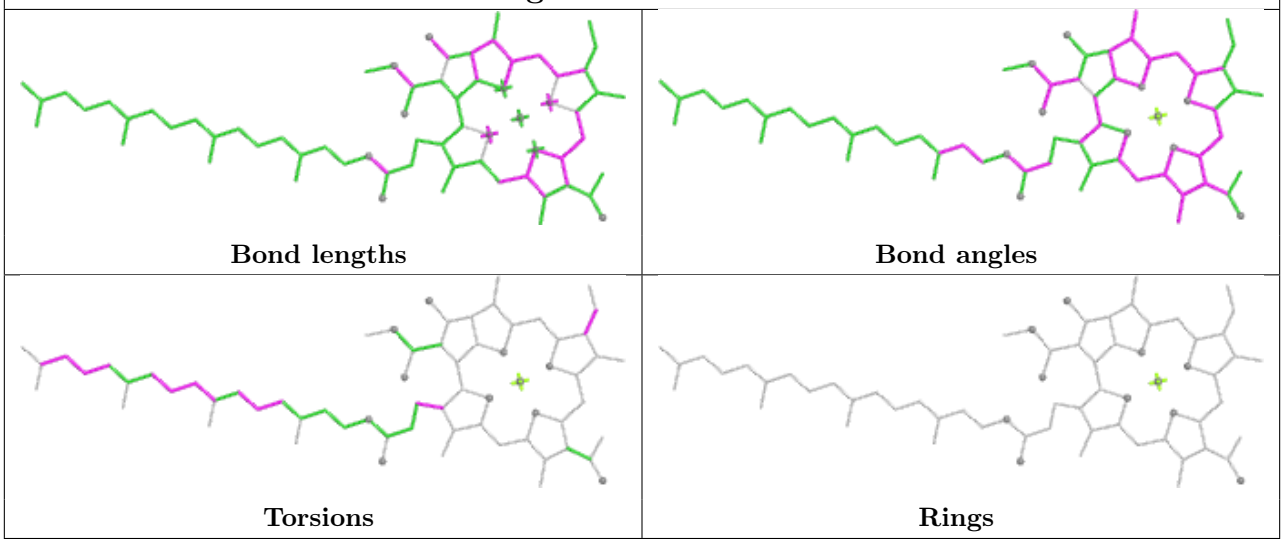
Ligand BCL 5 103	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCL 0 102	
 Bond lengths	 Bond angles
 Torsions	 Rings

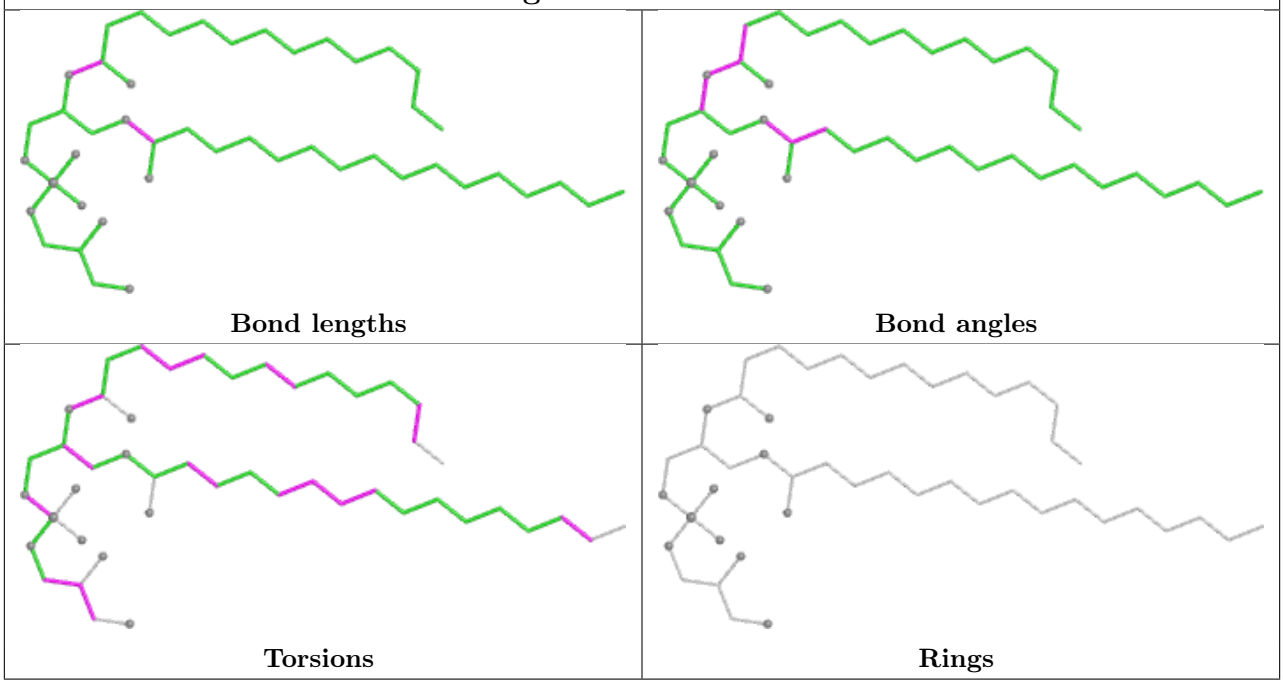
Ligand PGV V 103



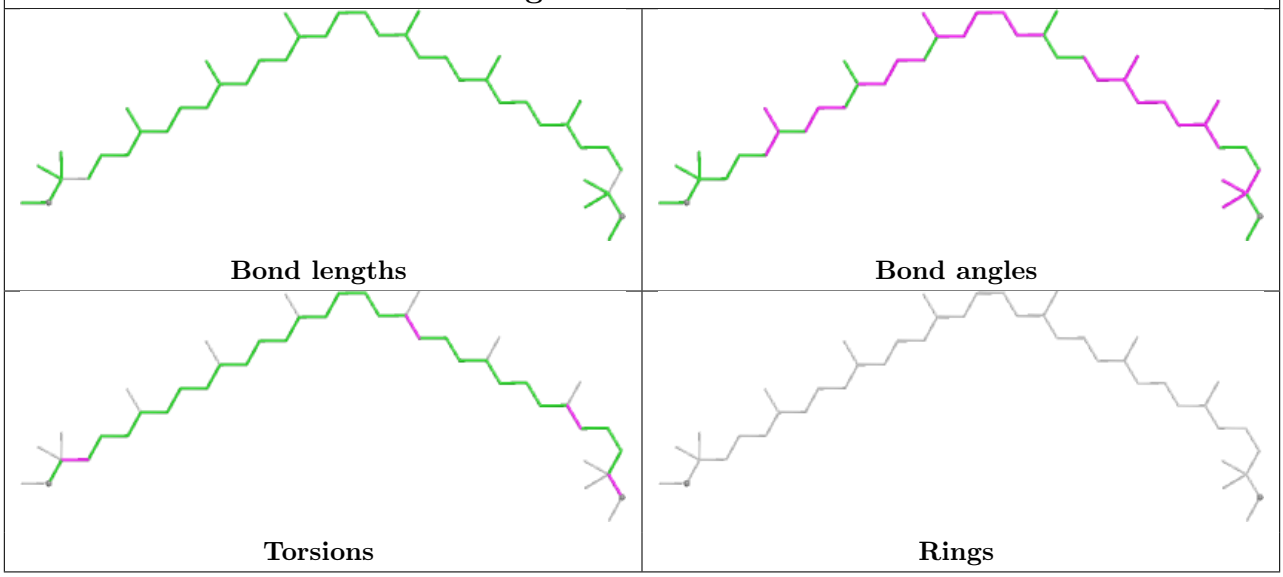
Ligand BCL B 102



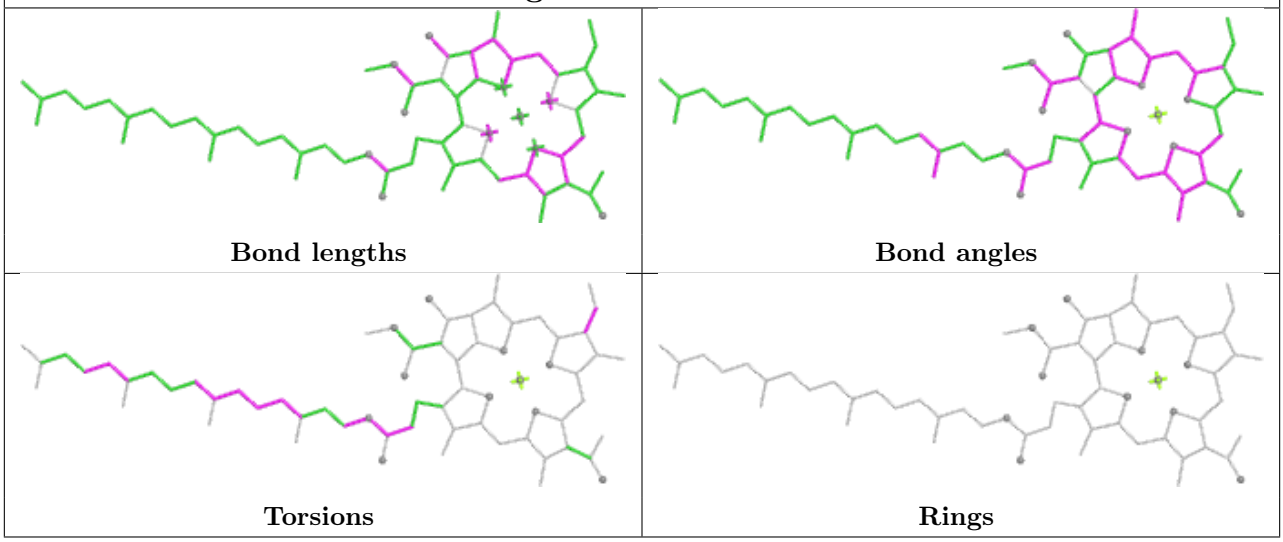
Ligand PGV T 103



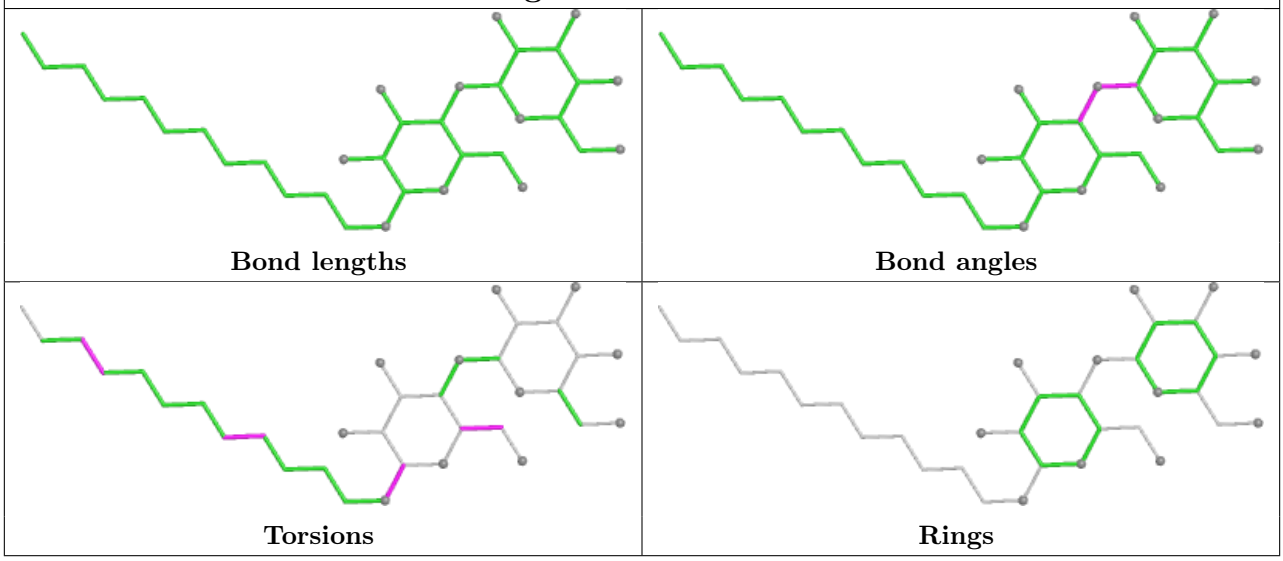
Ligand CRT B 101



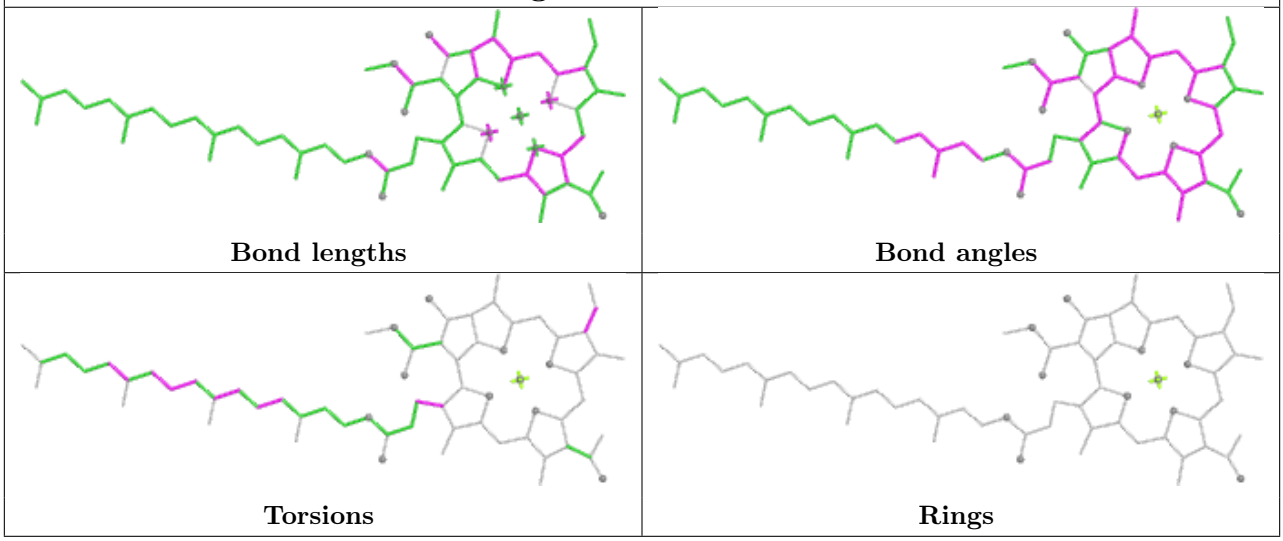
Ligand BCL O 104



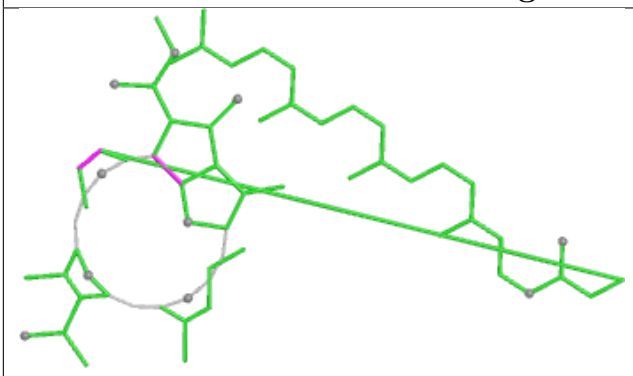
Ligand LMT L 308



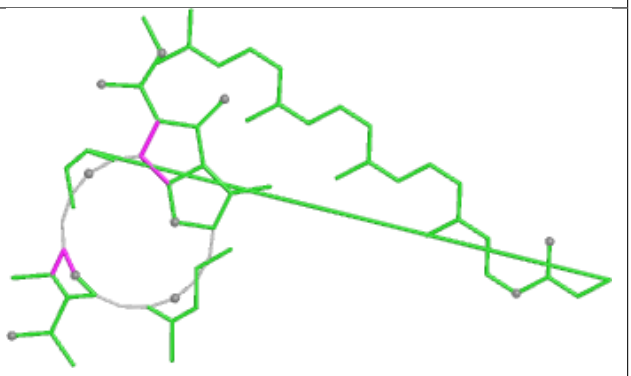
Ligand BCL 8 102



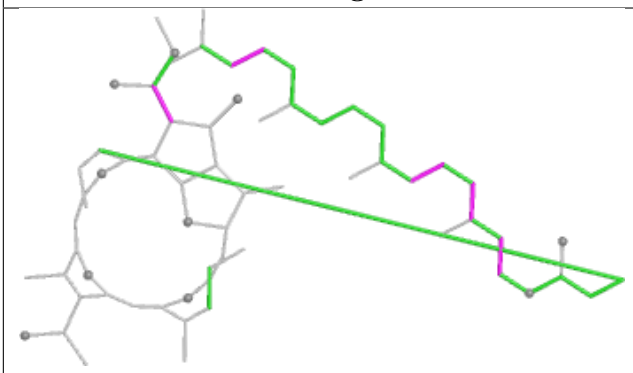
Ligand BPH M 404



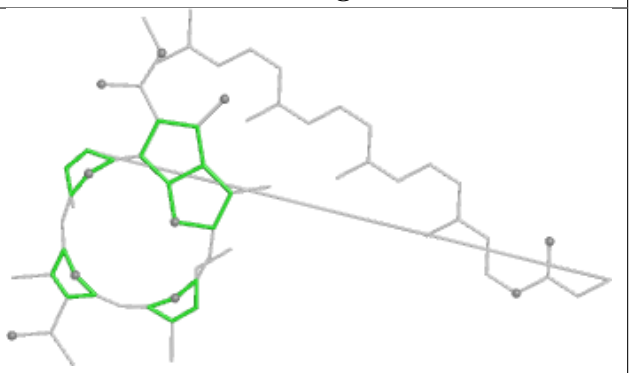
Bond lengths



Bond angles

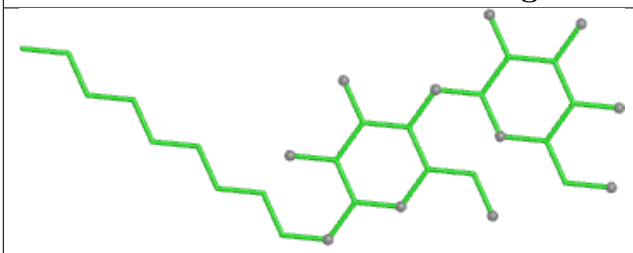


Torsions

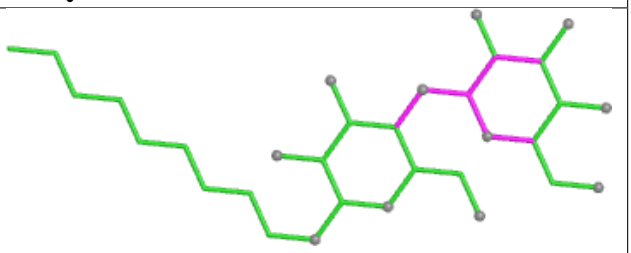


Rings

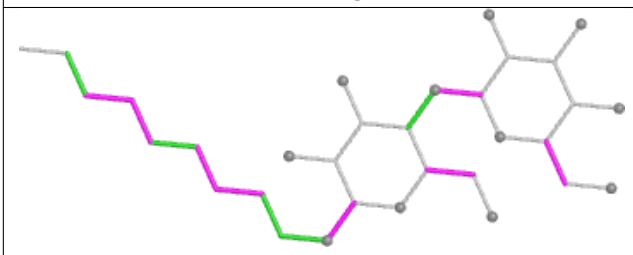
Ligand LMT Q 101



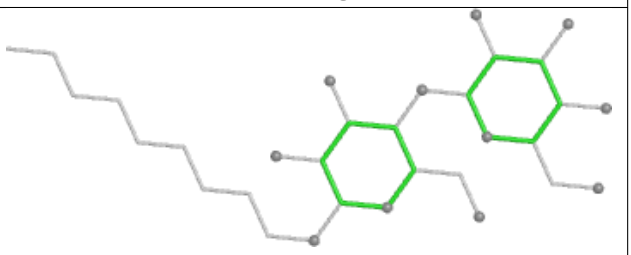
Bond lengths



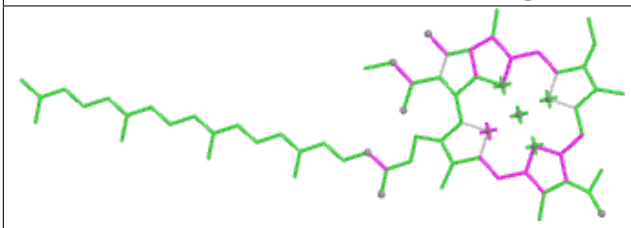
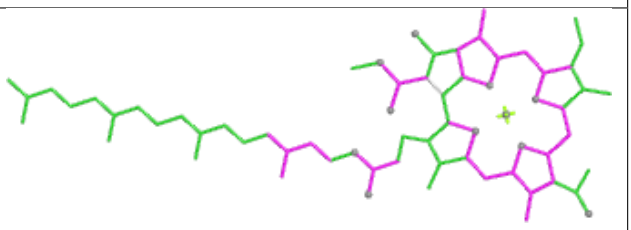
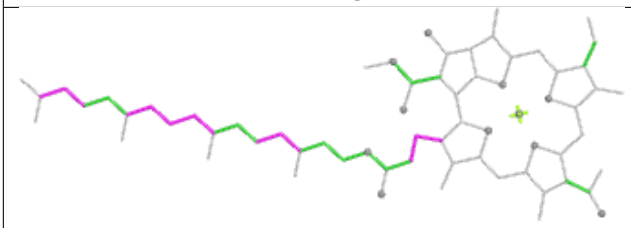
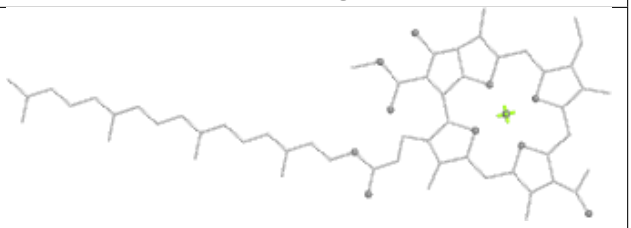
Bond angles



Torsions



Rings

Ligand BCL W 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

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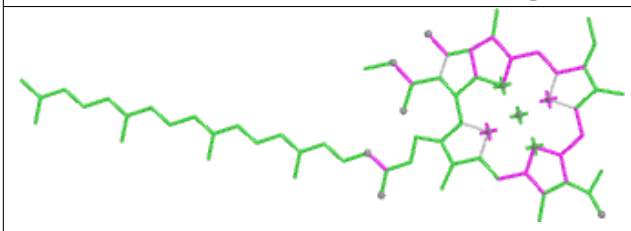
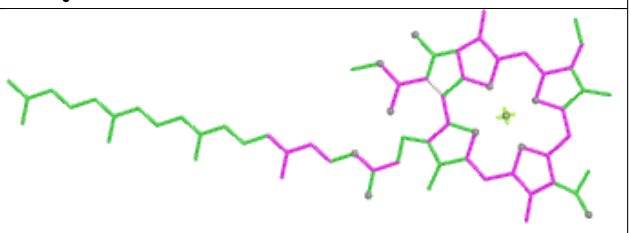
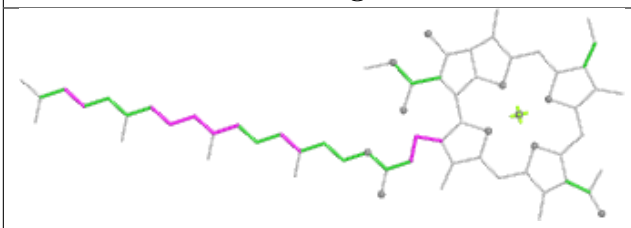
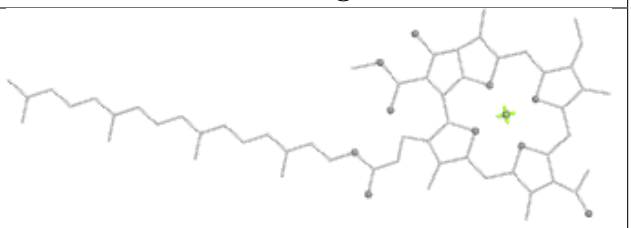
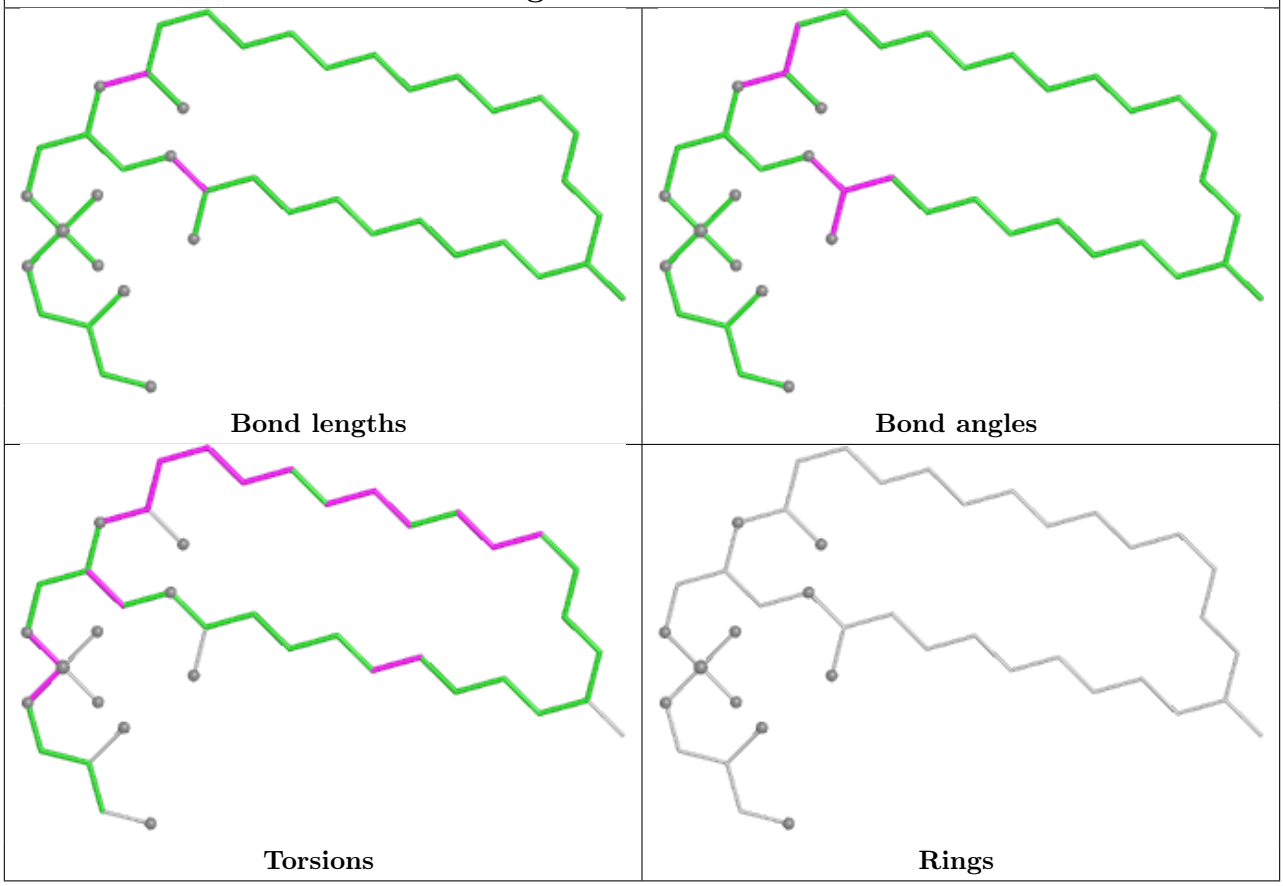
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PGV 0 103



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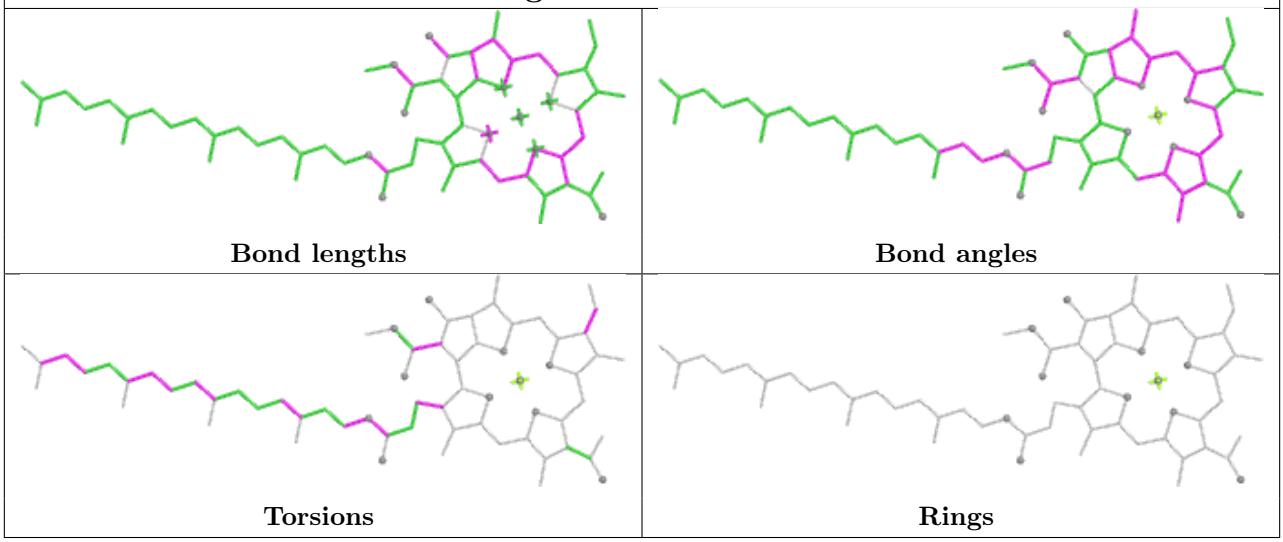

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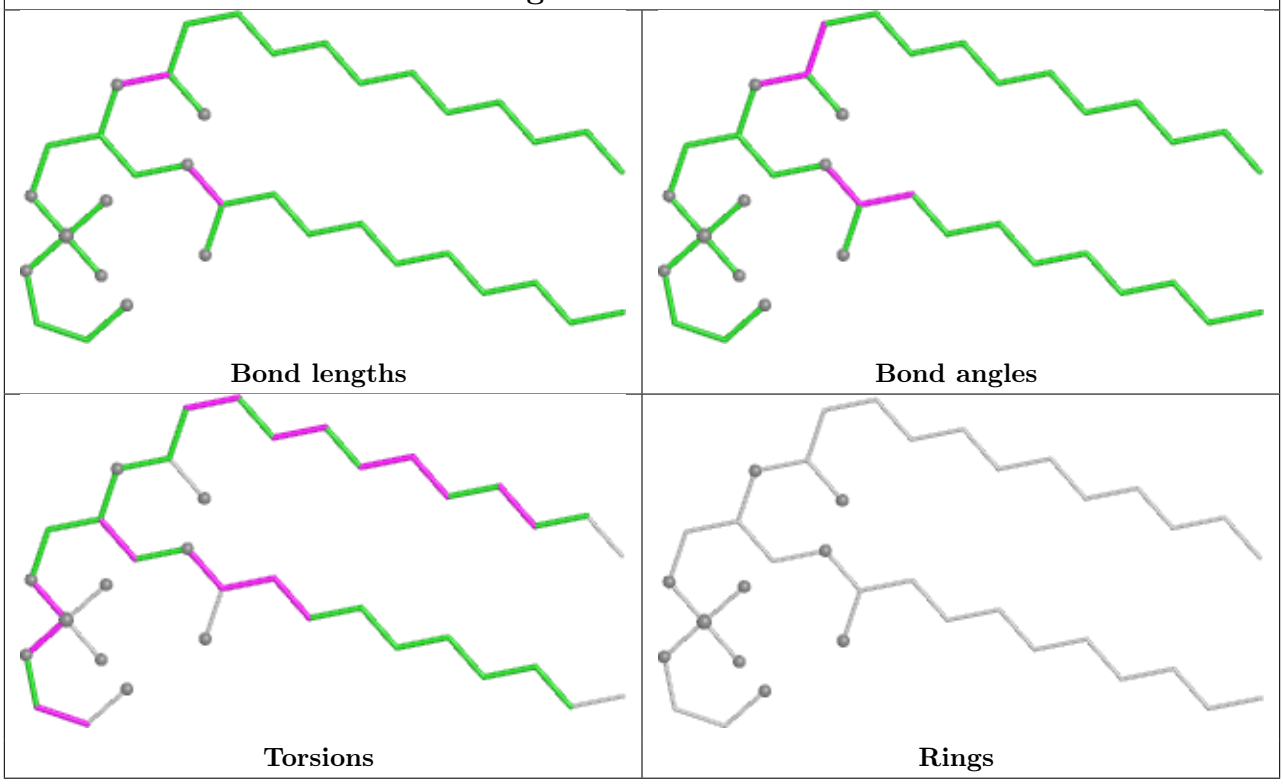
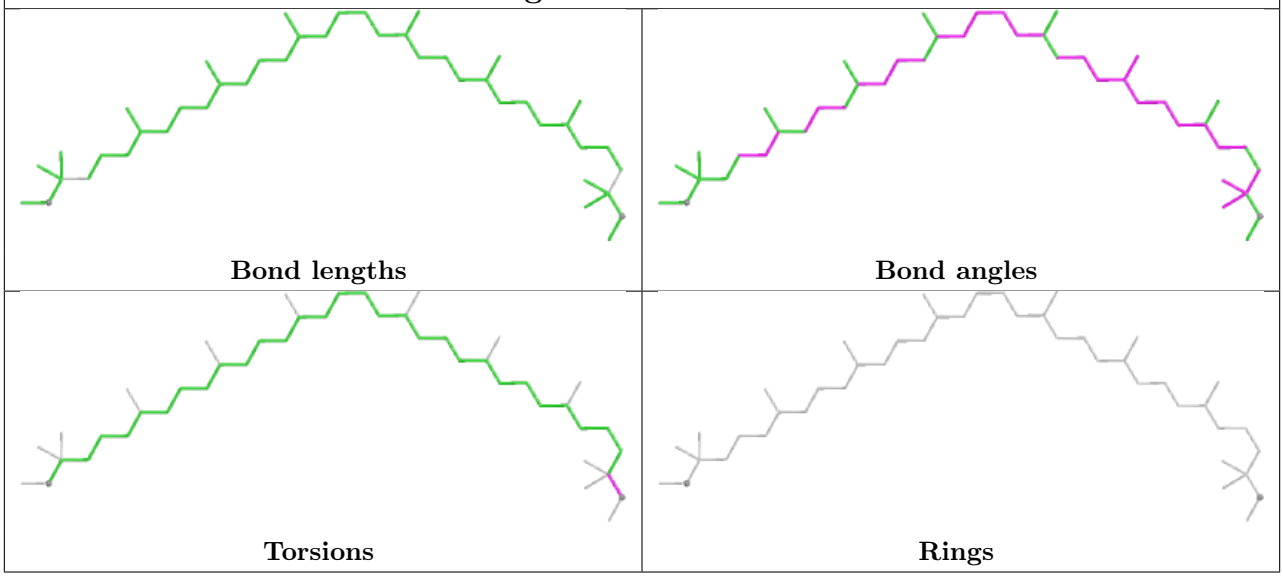


Ligand CRT Y 403



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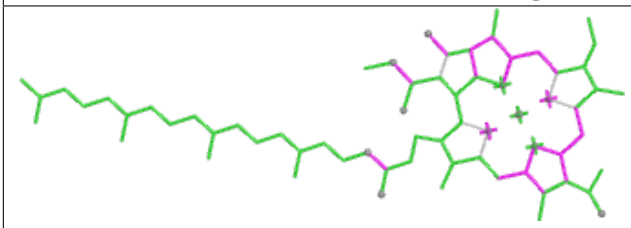
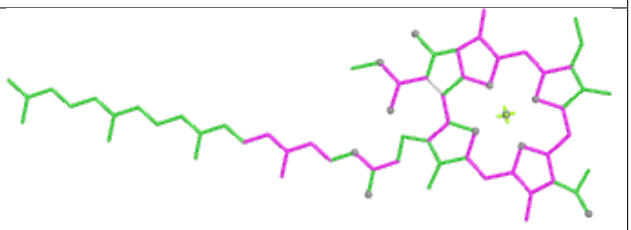
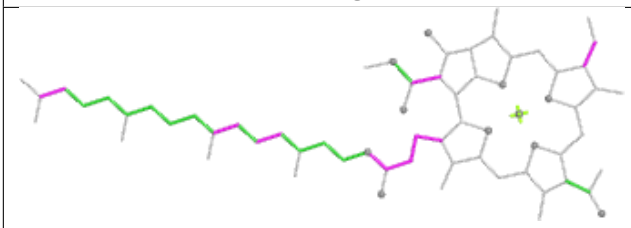
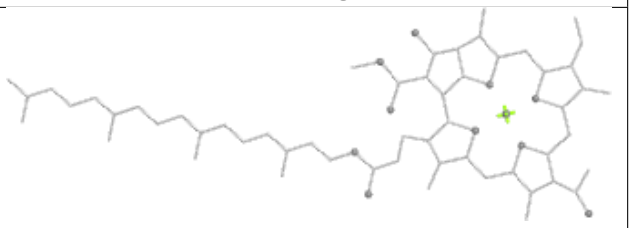
 Bond lengths	 Bond angles
 Torsions	 Rings

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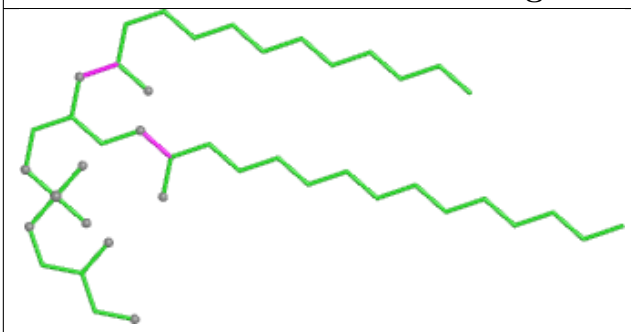
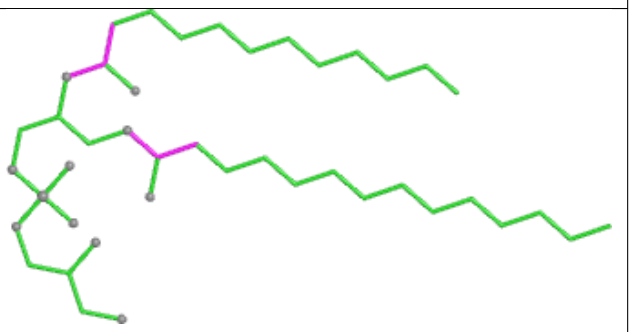
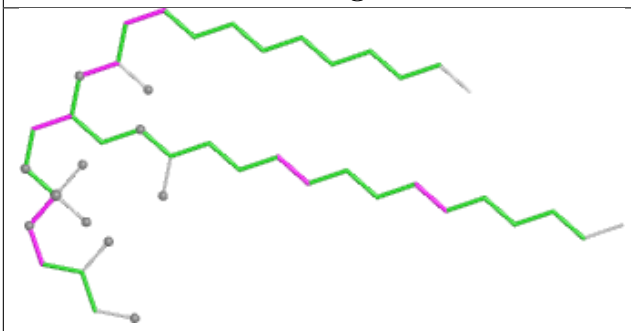
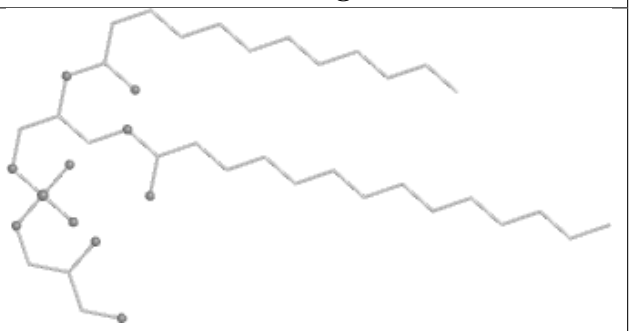
 Bond lengths	 Bond angles
 Torsions	 Rings

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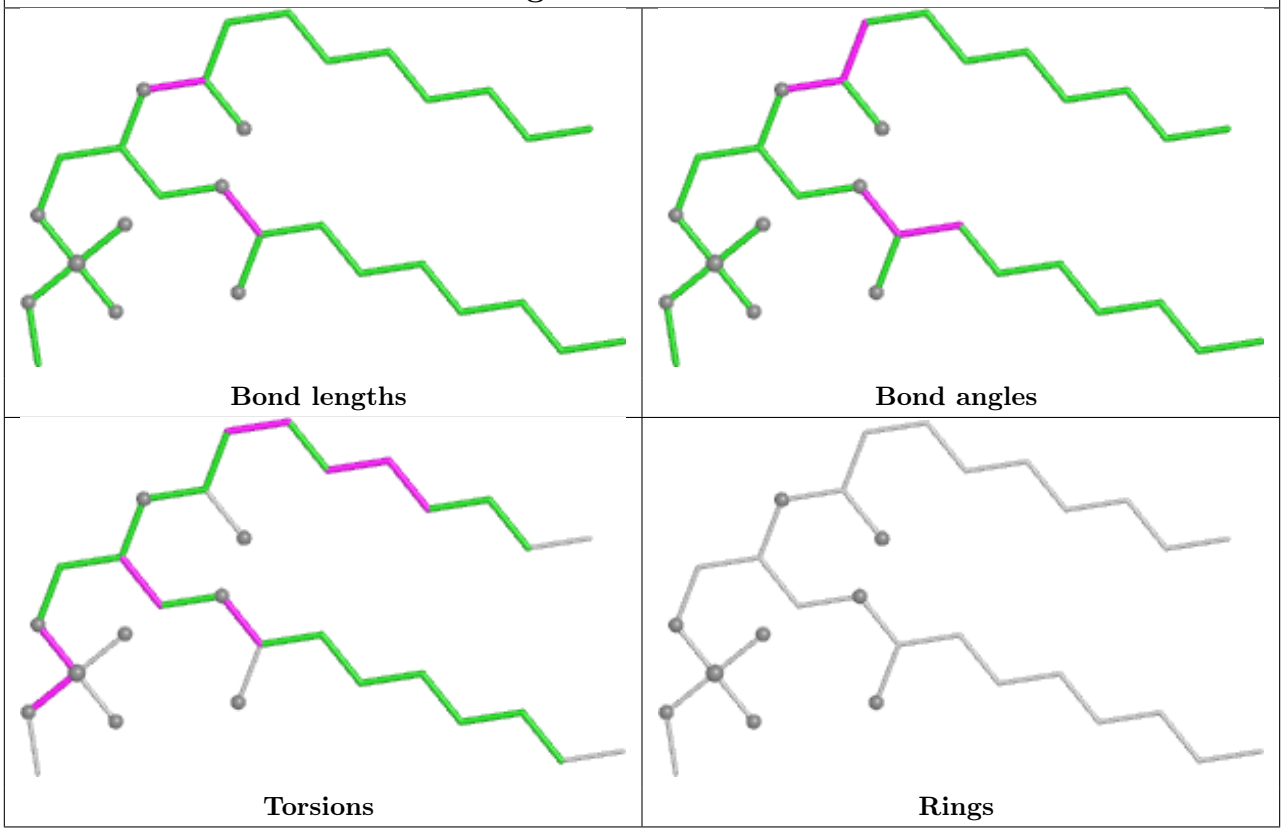

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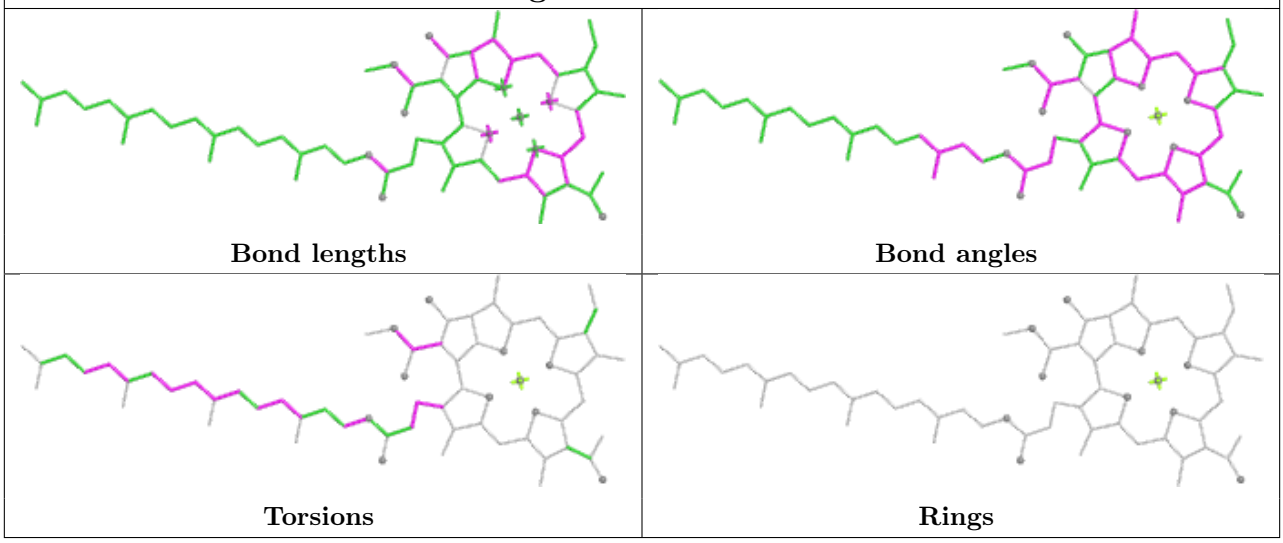

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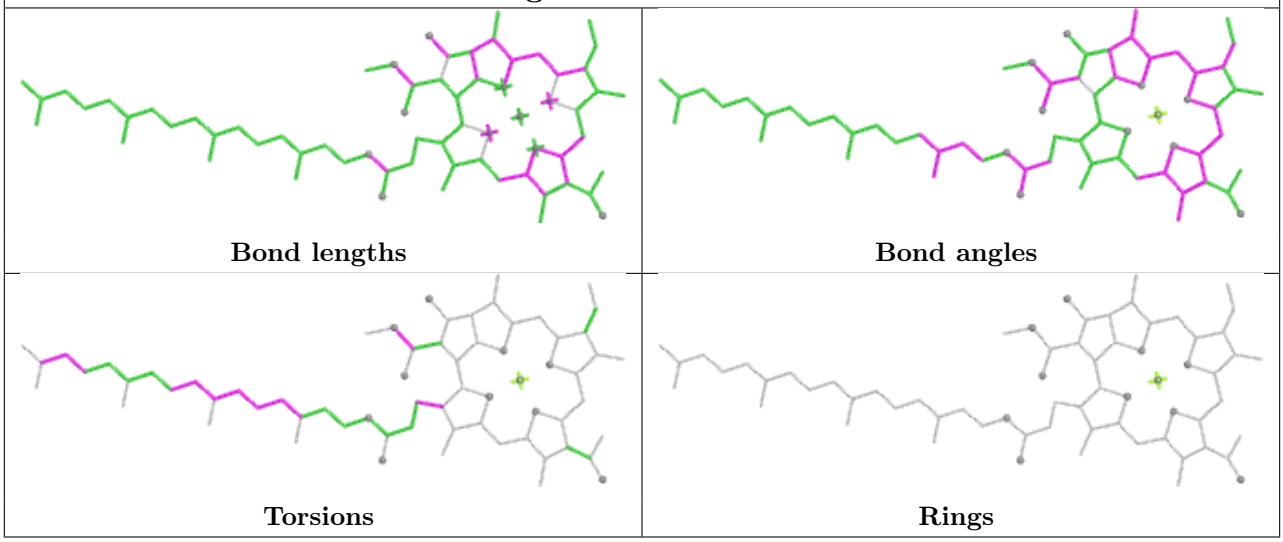

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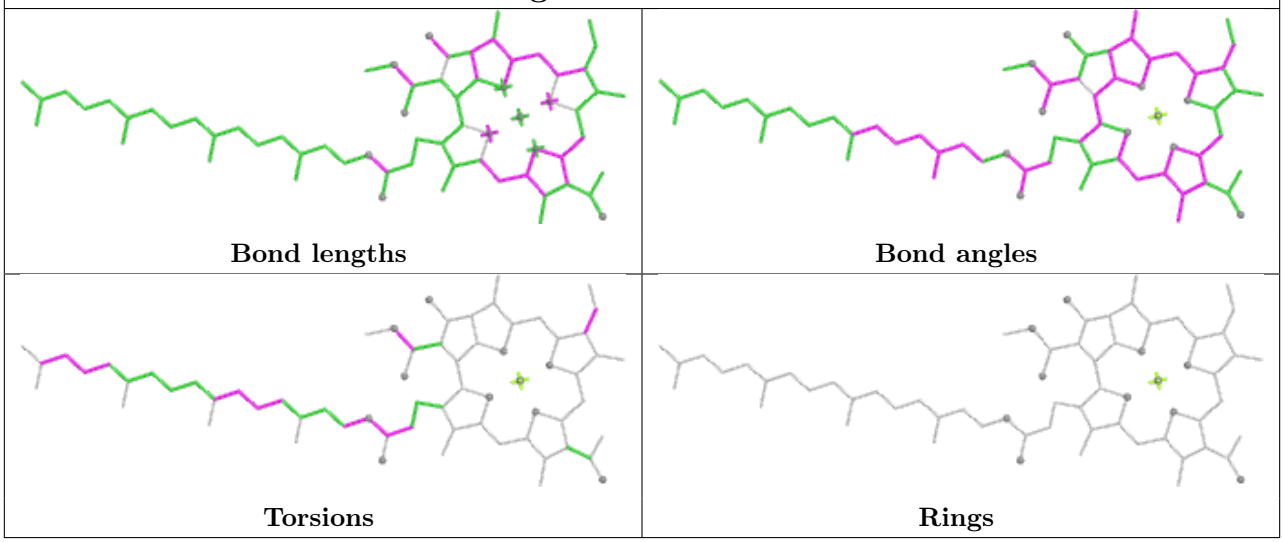

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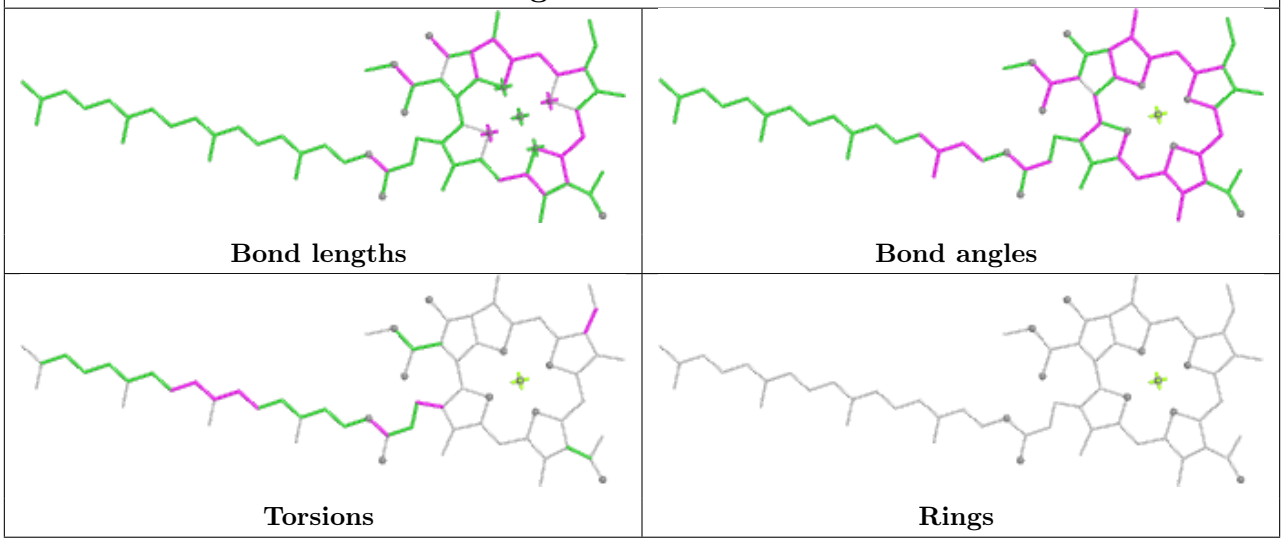

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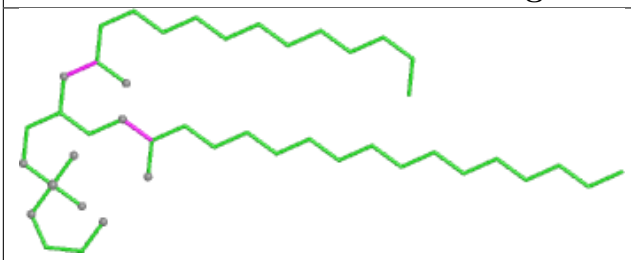
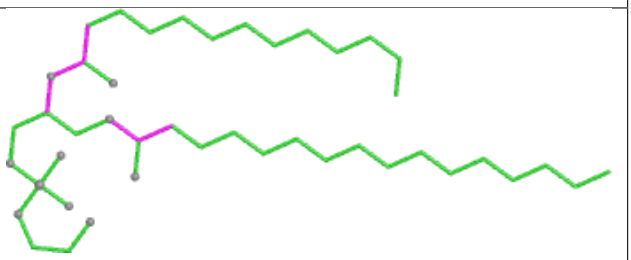
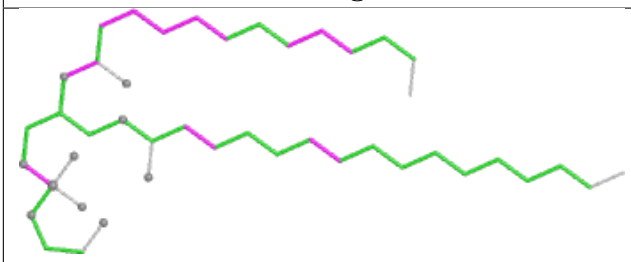
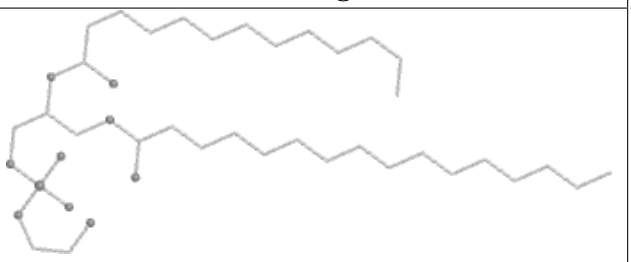
 Bond lengths	 Bond angles
 Torsions	 Rings

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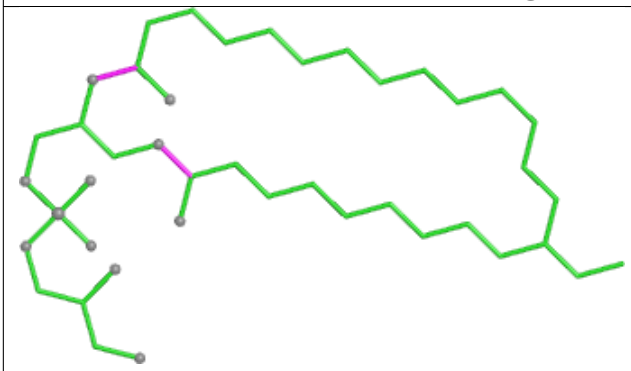
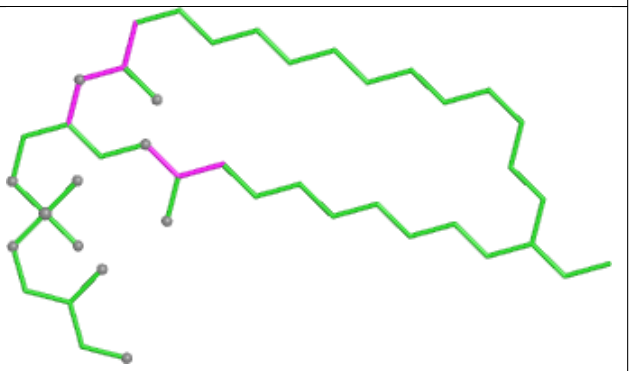
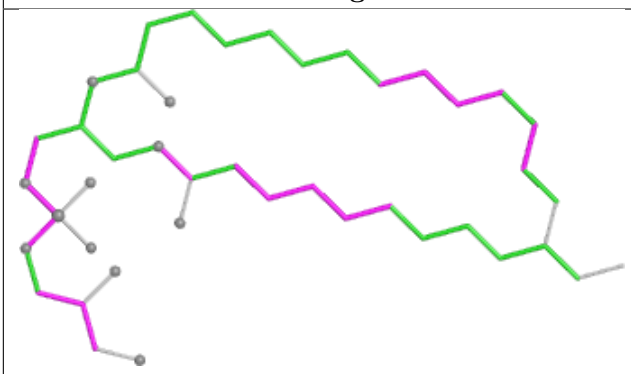
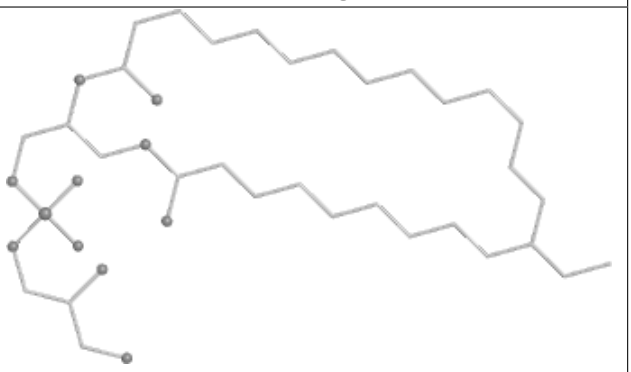
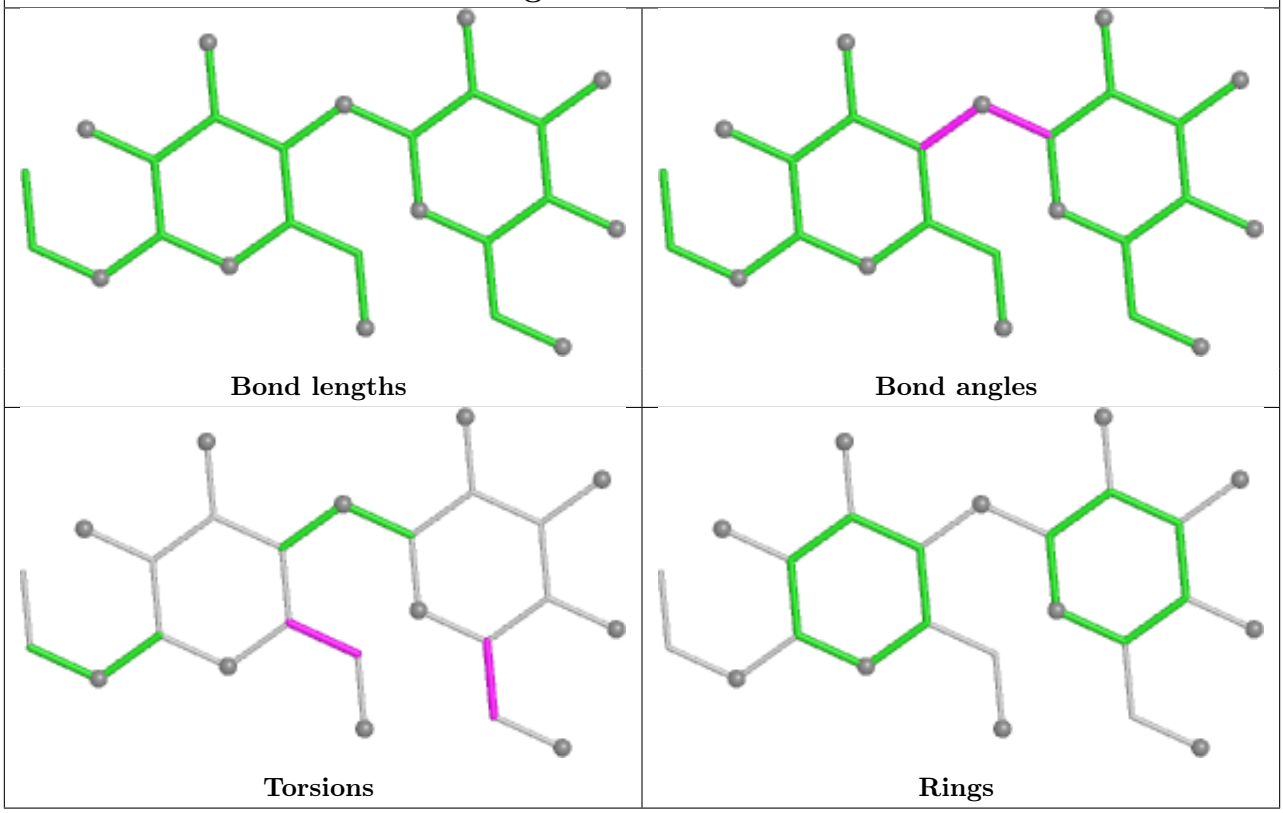
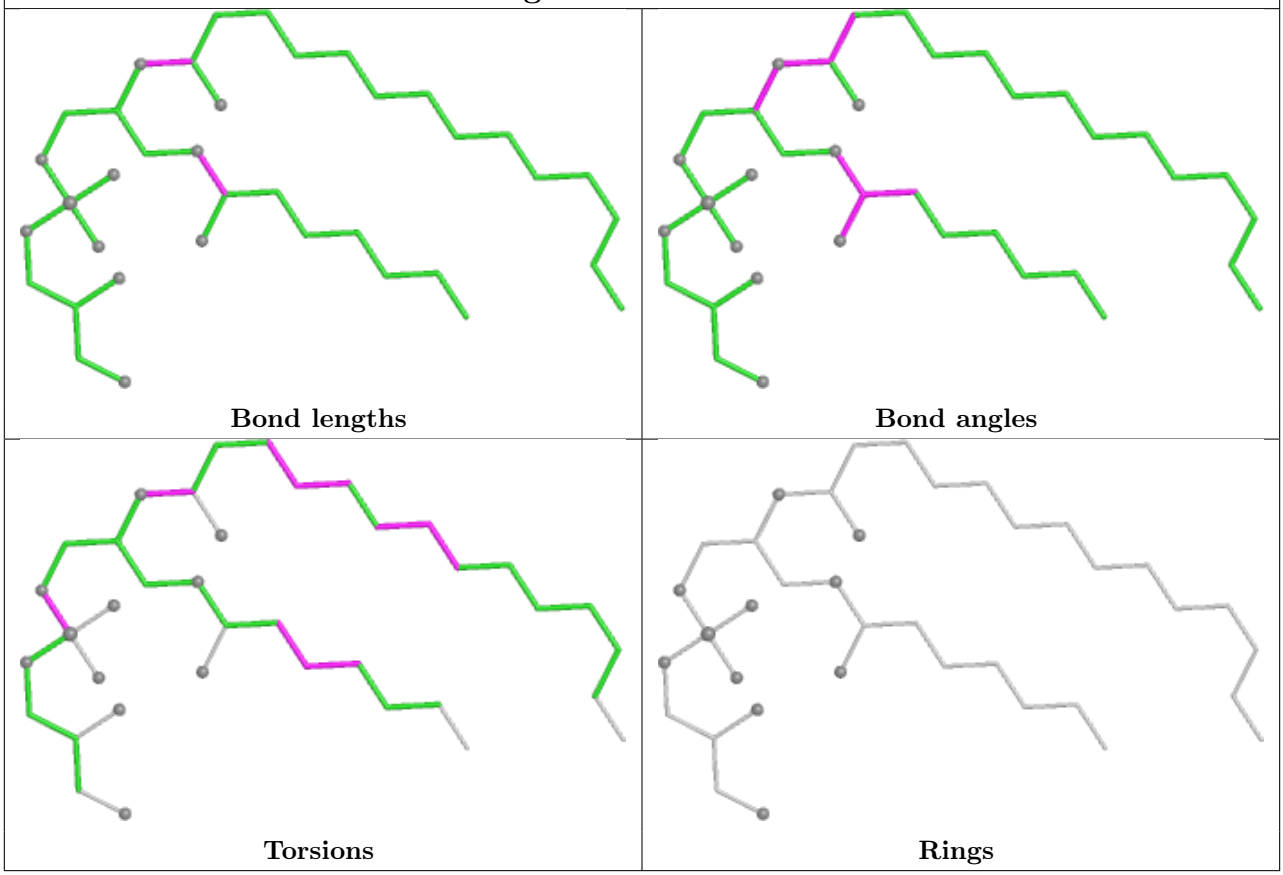
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LMT L 301



Ligand PGV E 102



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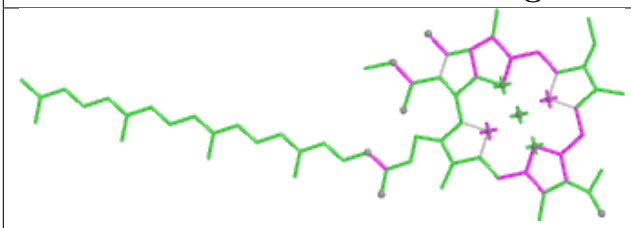
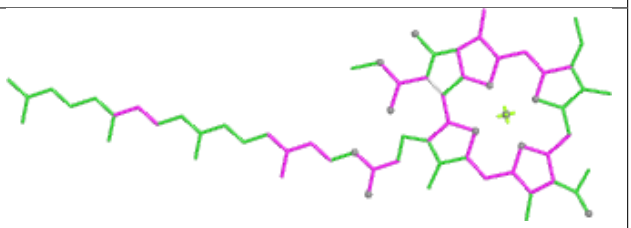
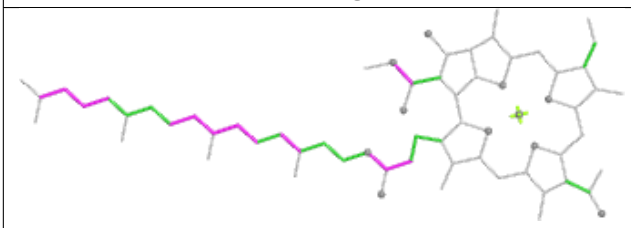
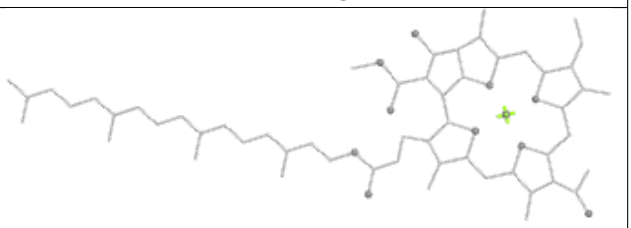
 Bond lengths	 Bond angles
 Torsions	 Rings

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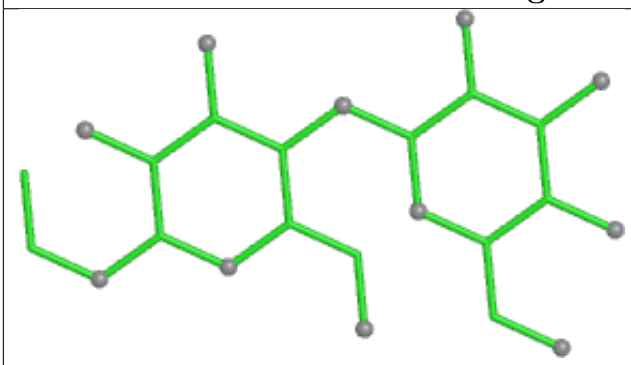
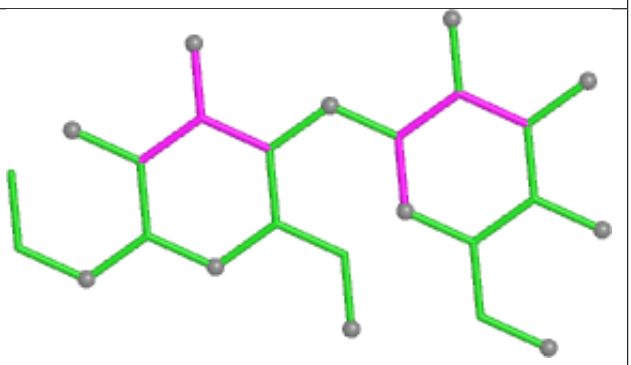
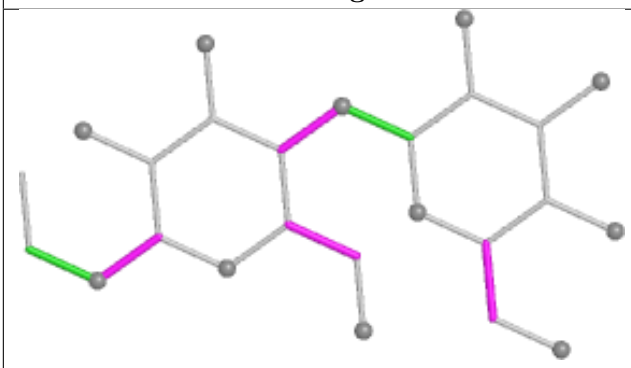
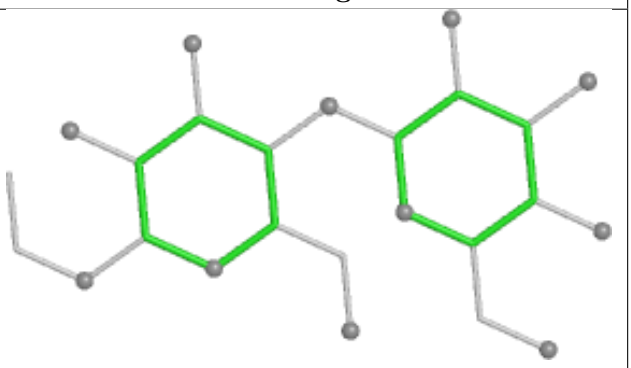
 Bond lengths	 Bond angles
 Torsions	 Rings

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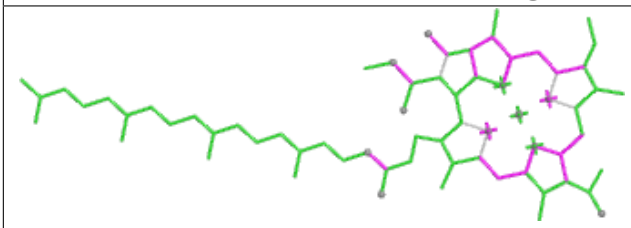
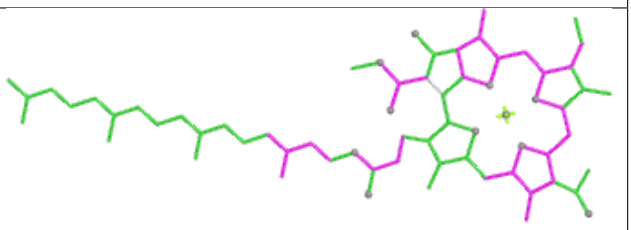
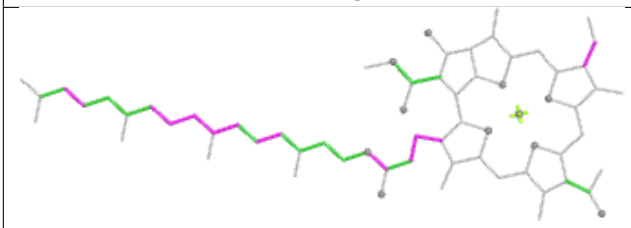
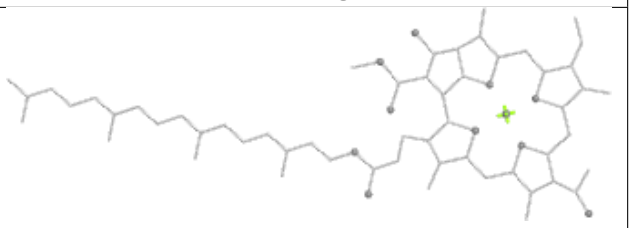
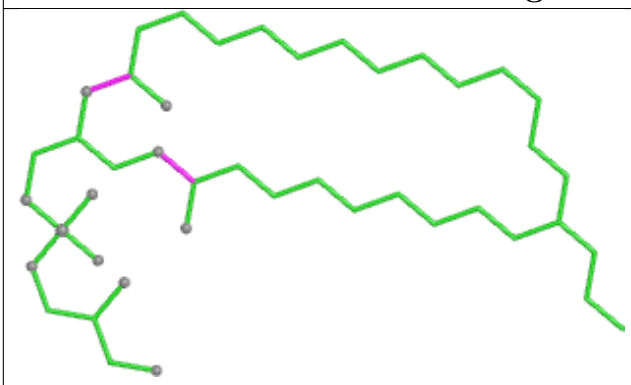
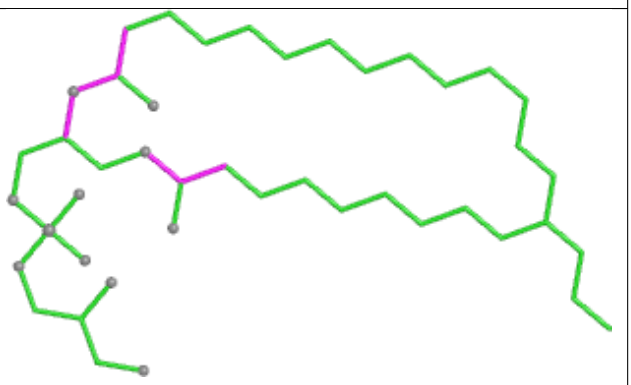
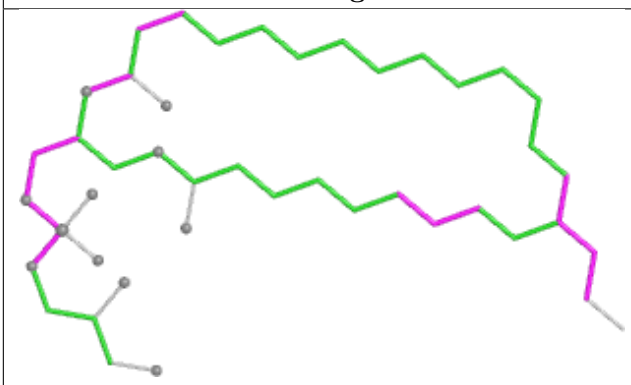
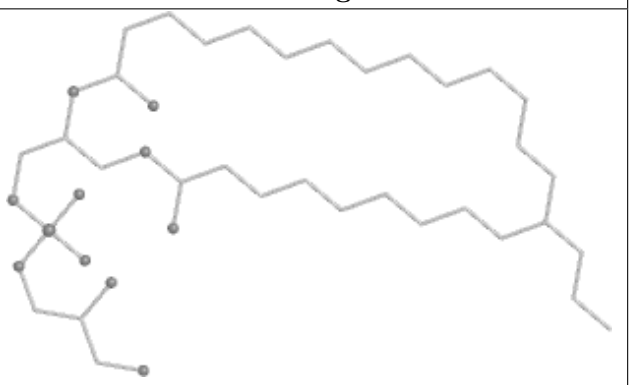
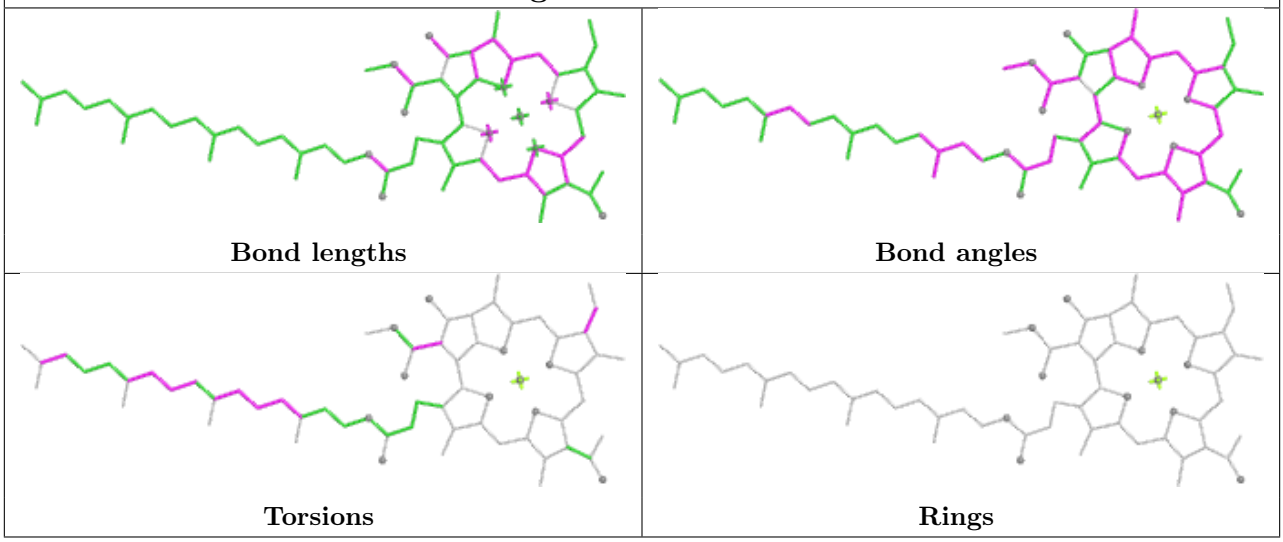
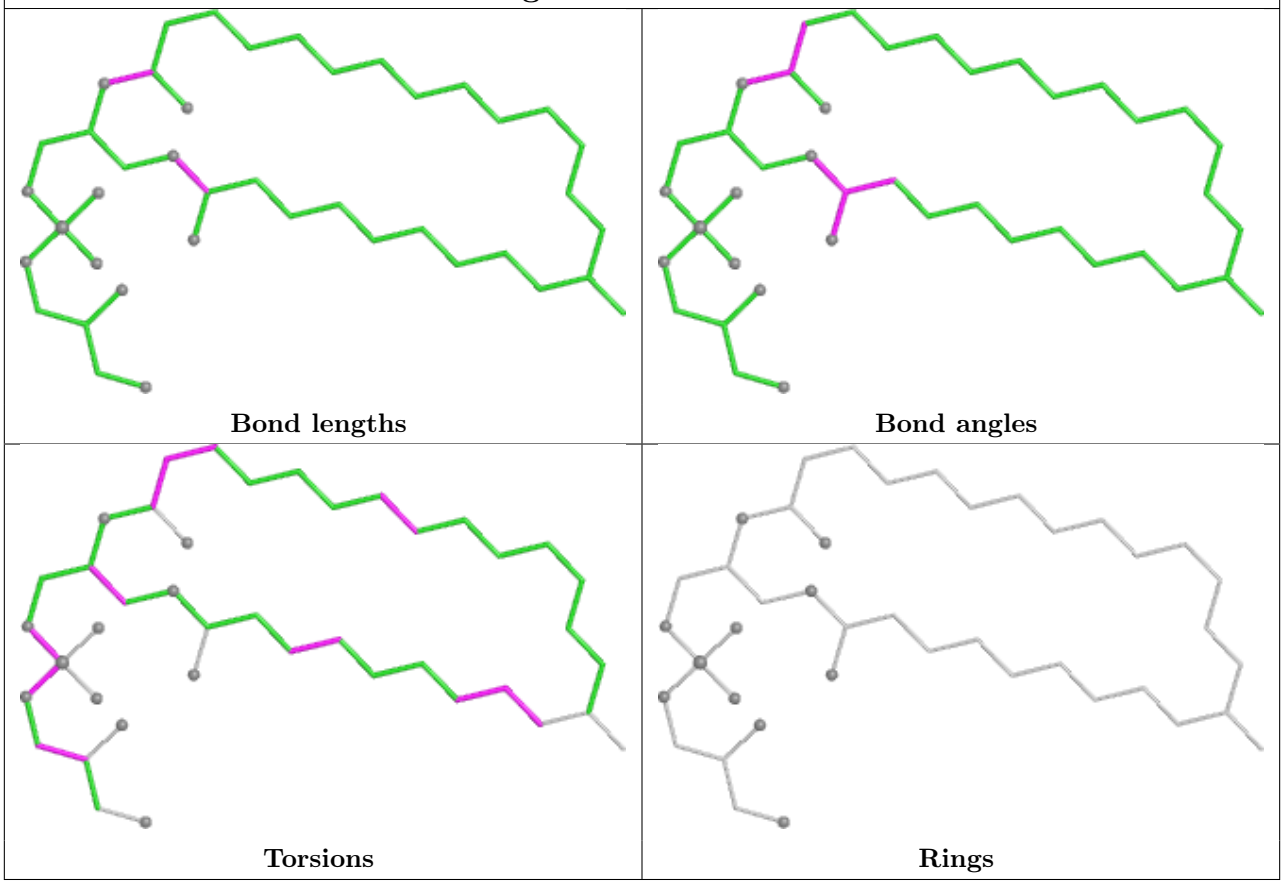
 Bond lengths	 Bond angles
 Torsions	 Rings

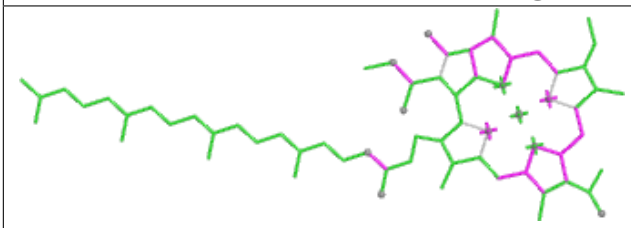
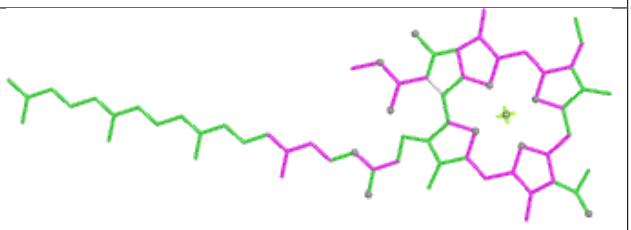
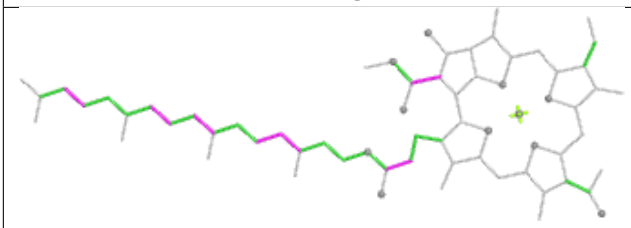
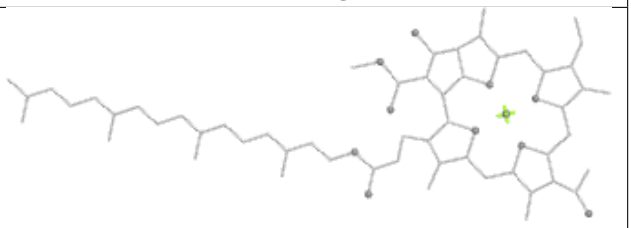
Ligand PGV 6 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

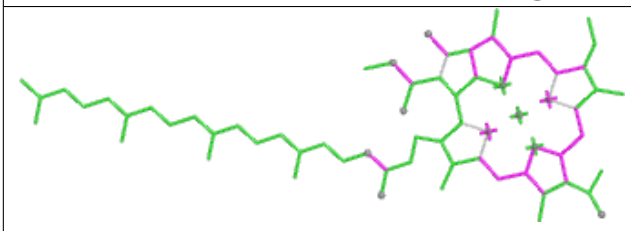
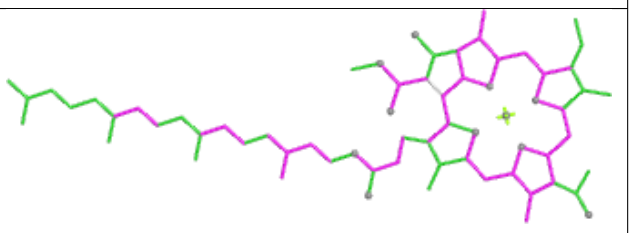
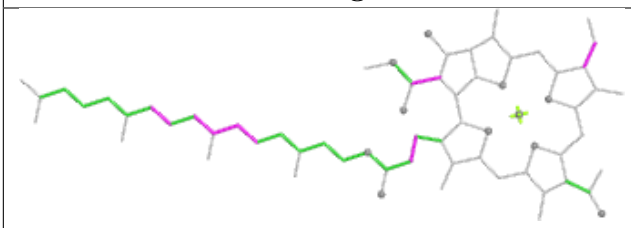
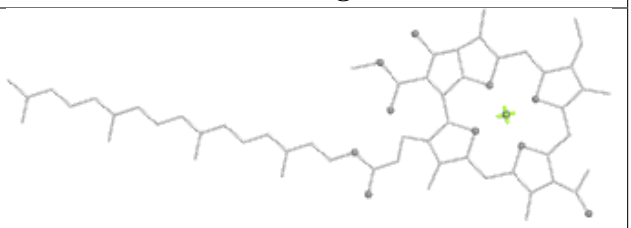
Ligand BCL 1 102



Ligand PGV R 103



Ligand BCL 9 102	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCL J 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

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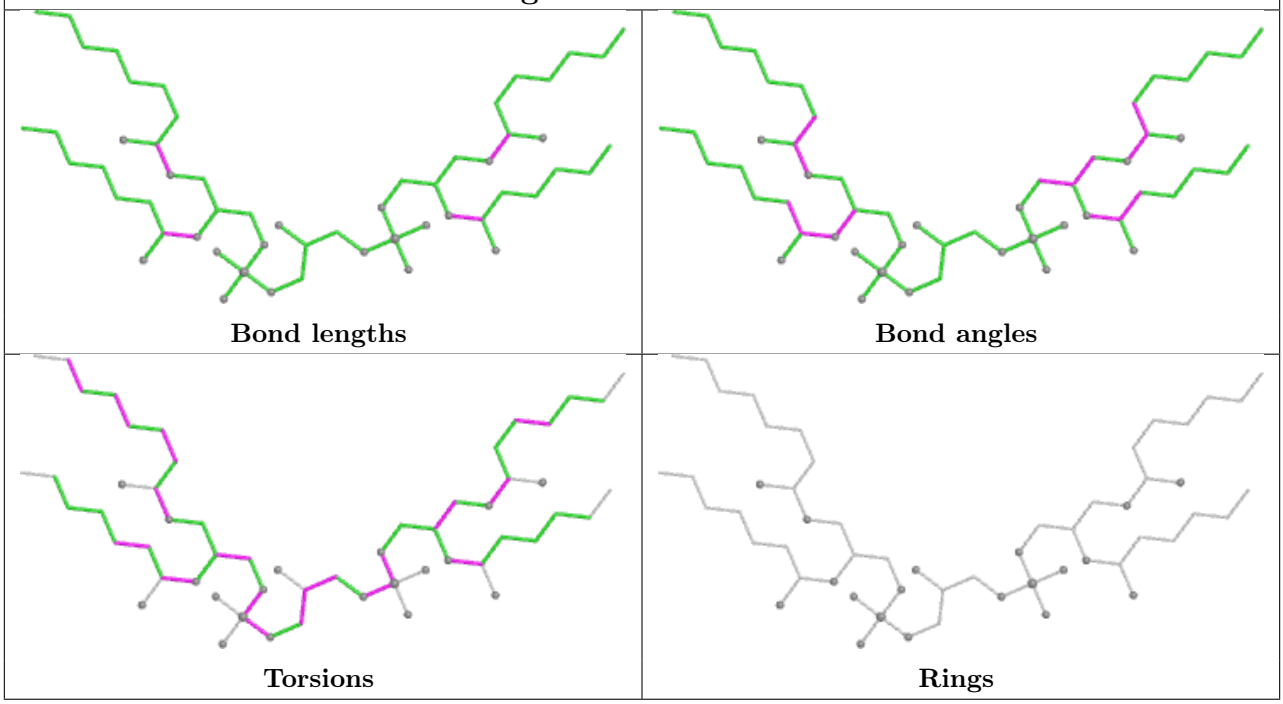

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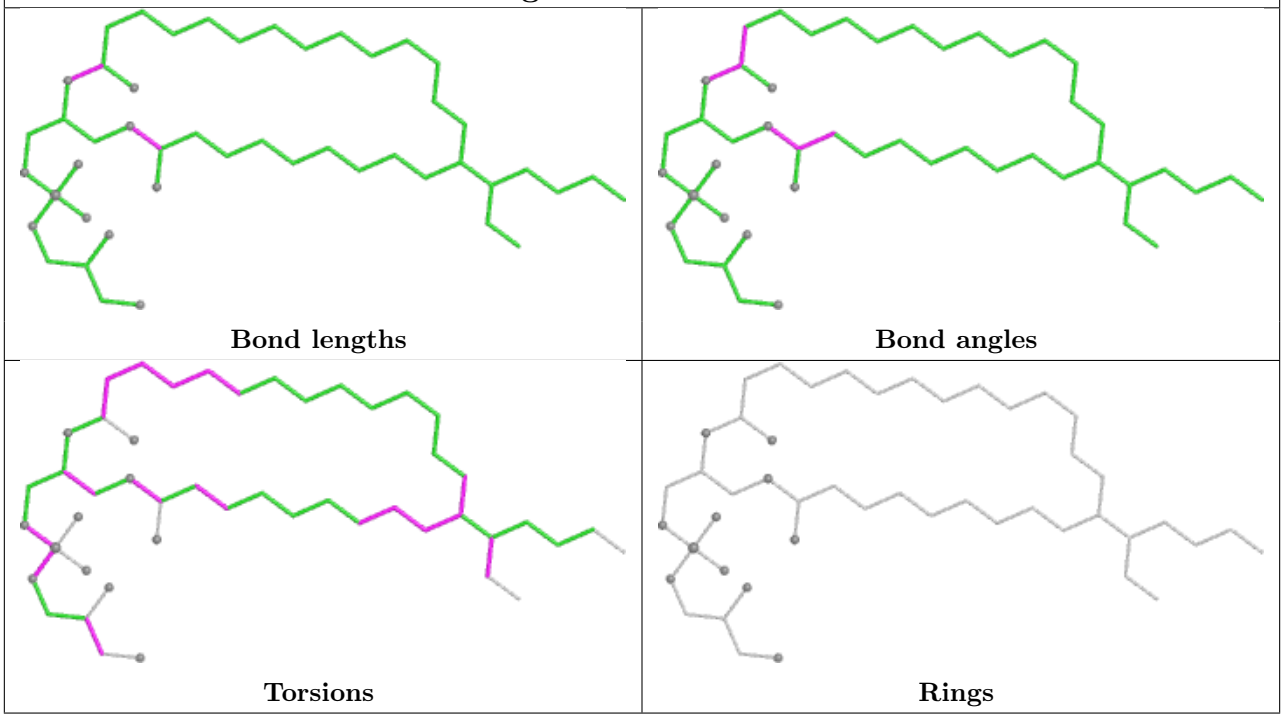

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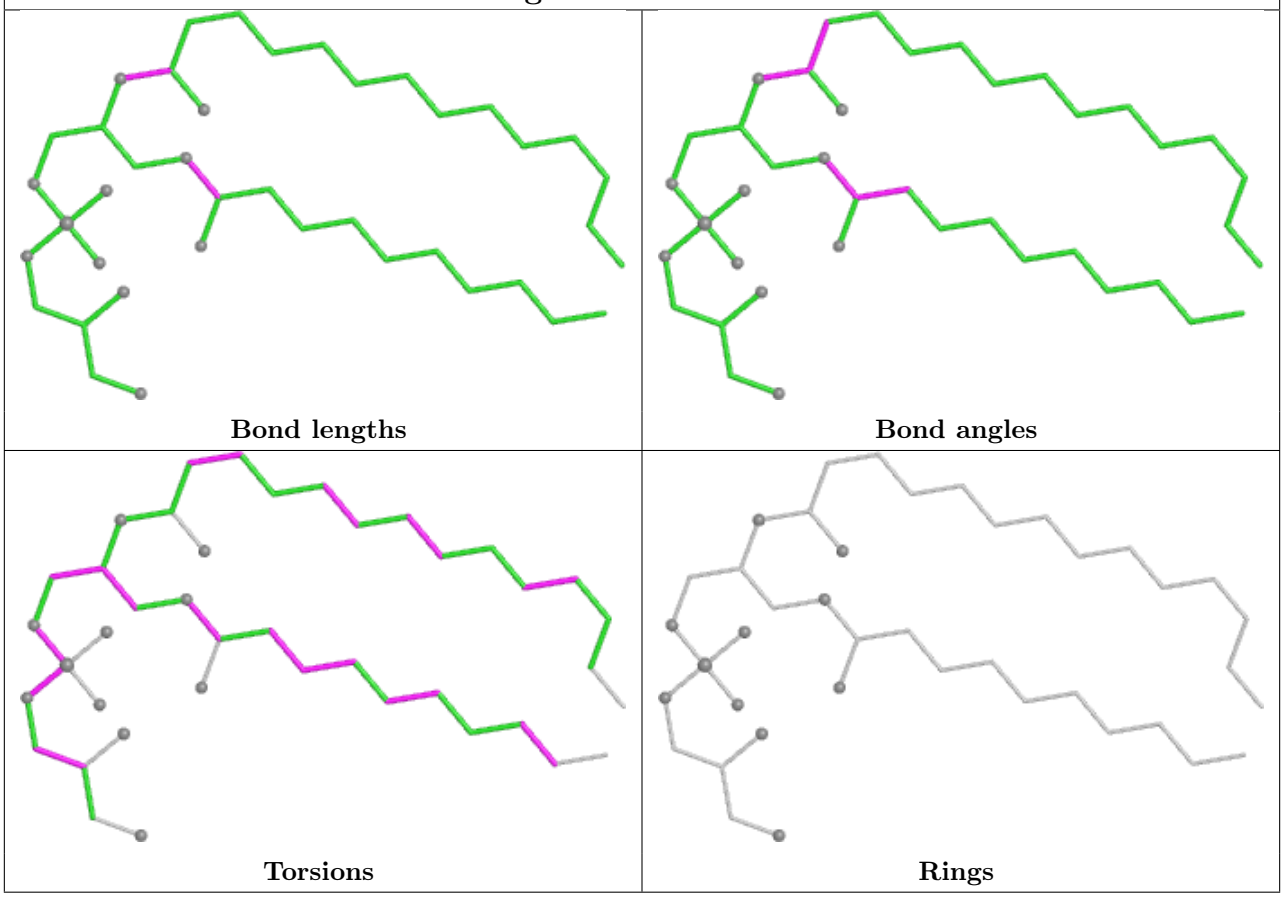

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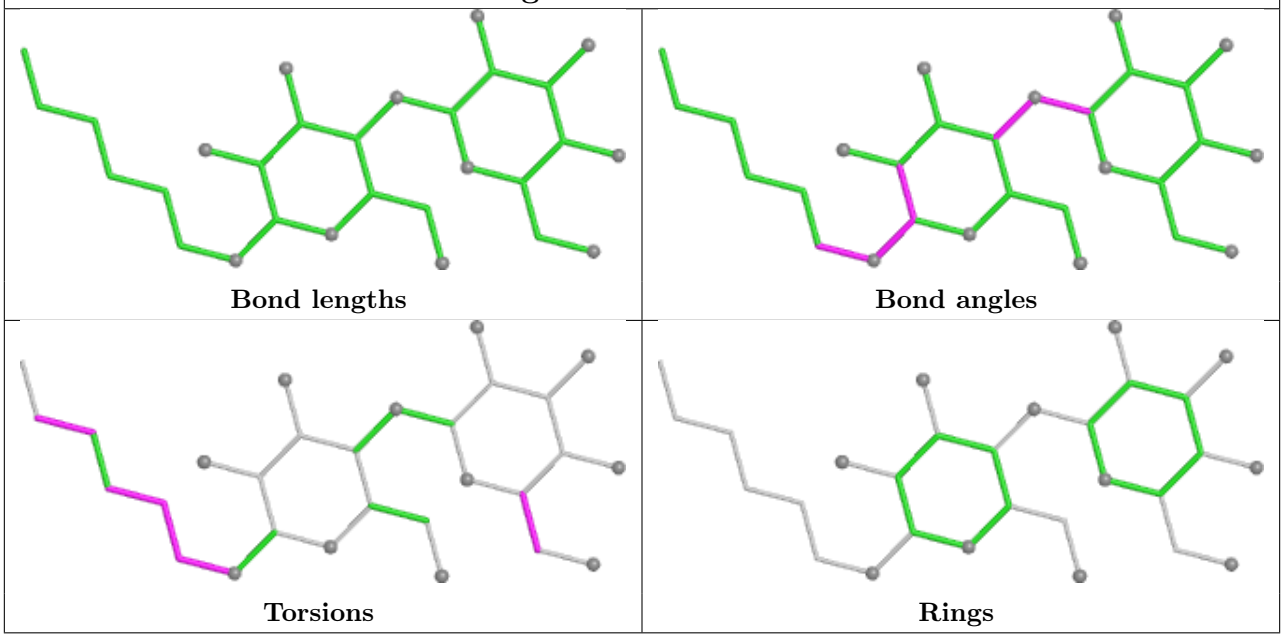

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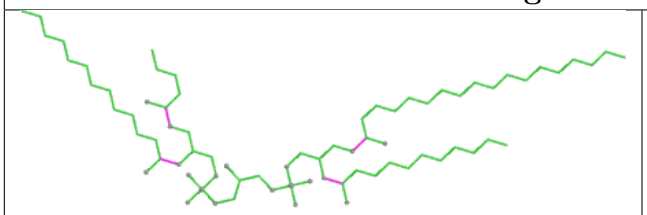
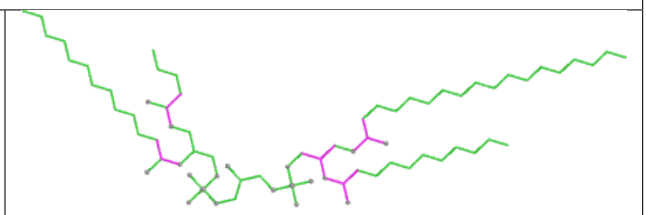
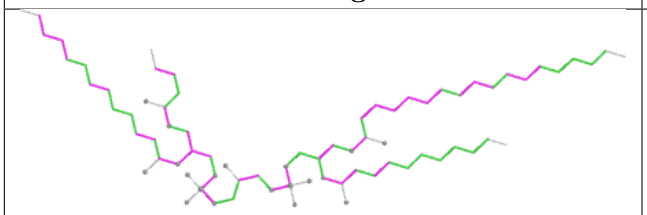


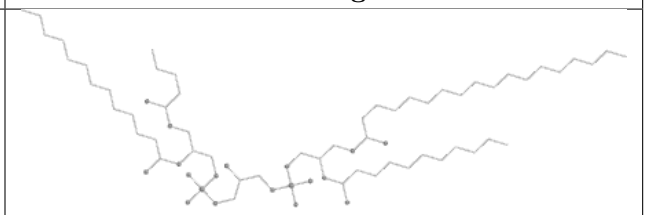
Bond lengths



Bond angles

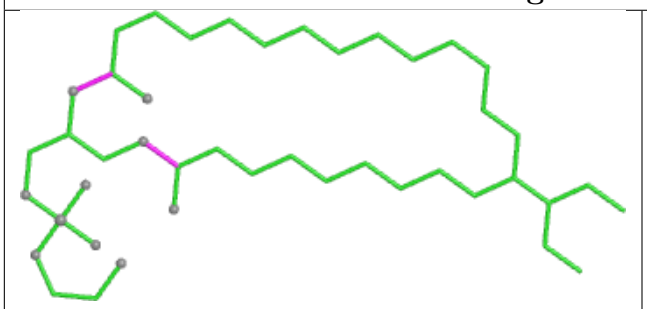


Torsions



Rings

Ligand PGV 2 102



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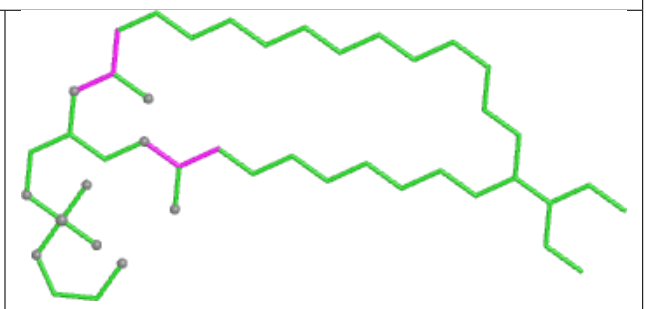

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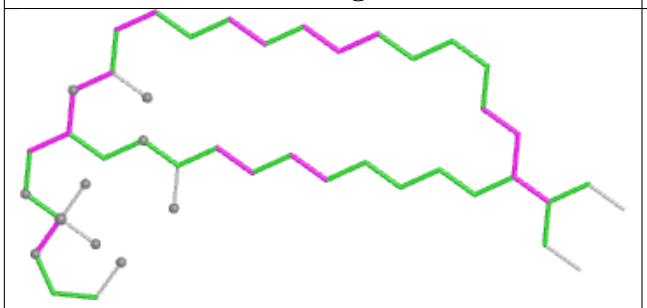

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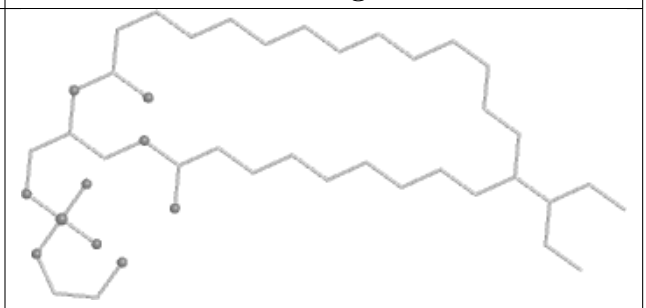

Rings

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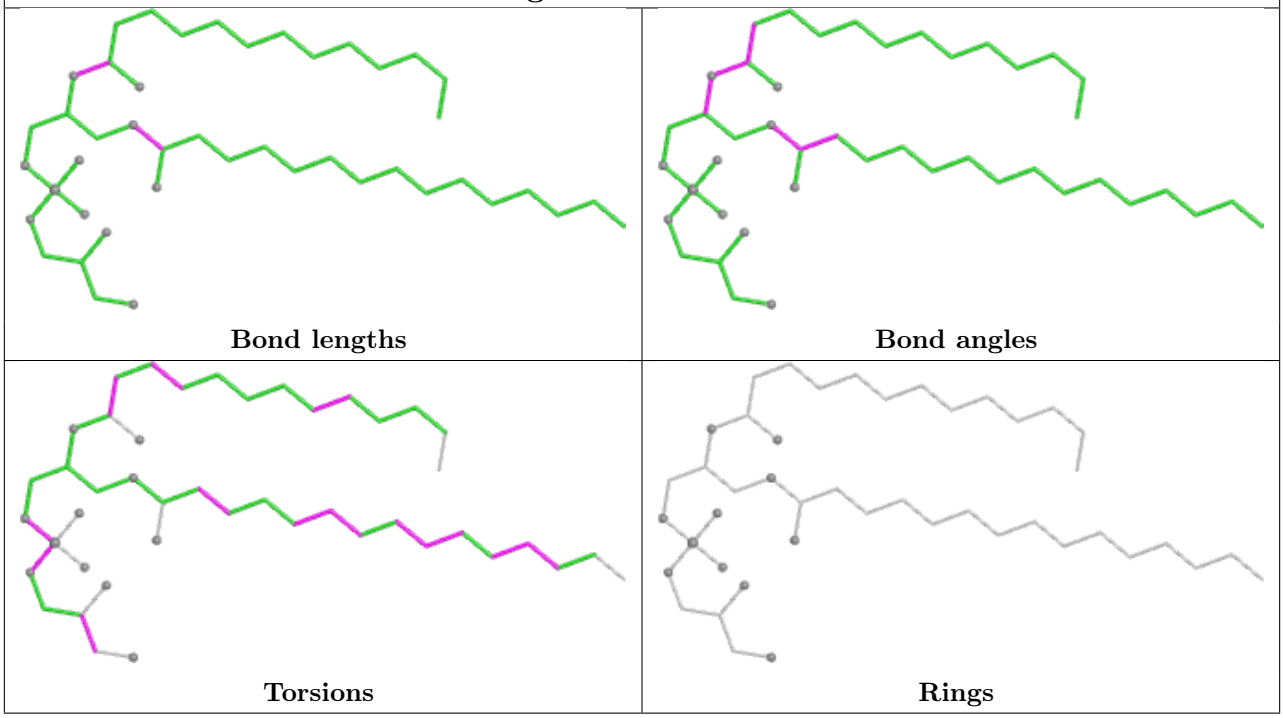
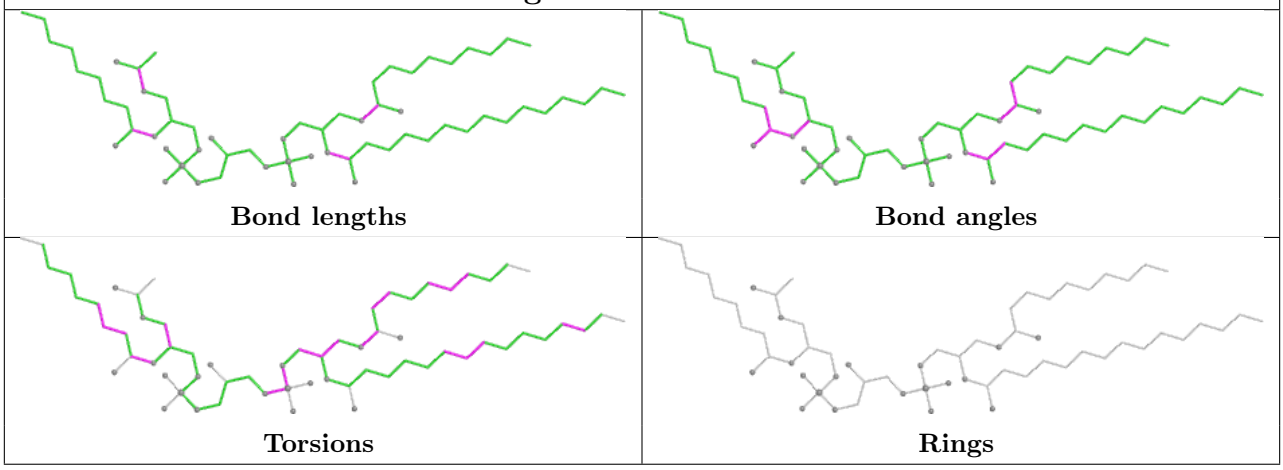
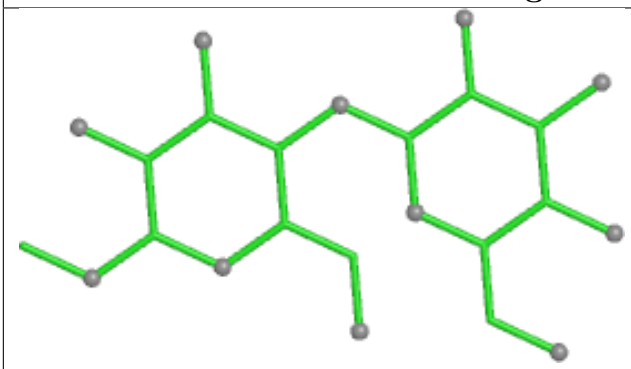
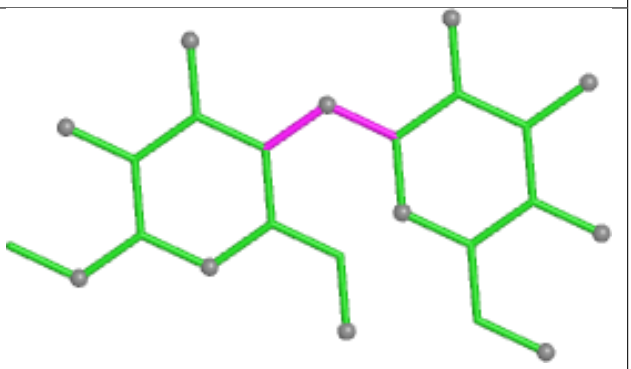
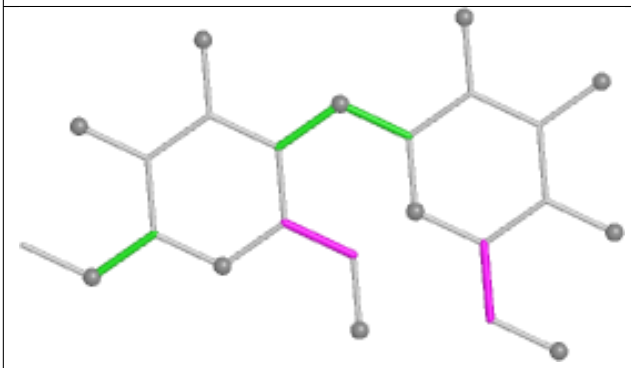
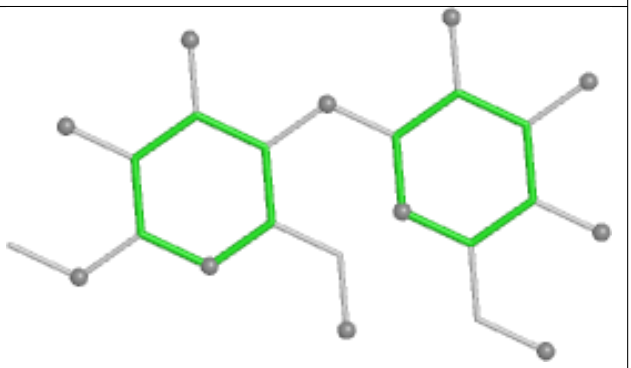


Ligand CDL H 301



Ligand LMT 5 102	
 Bond lengths	 Bond angles
 Torsions	 Rings

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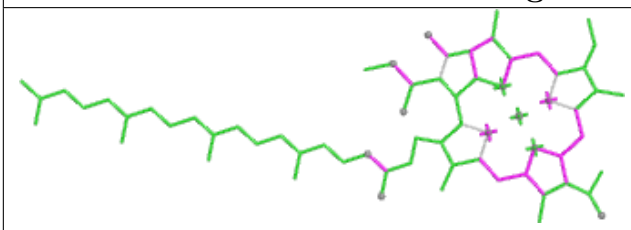
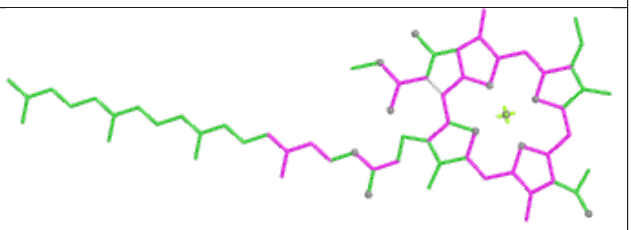
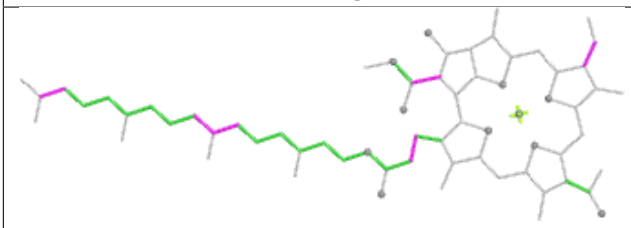
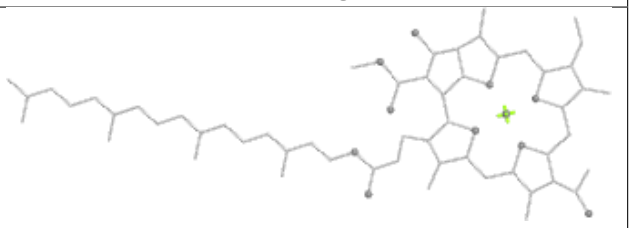
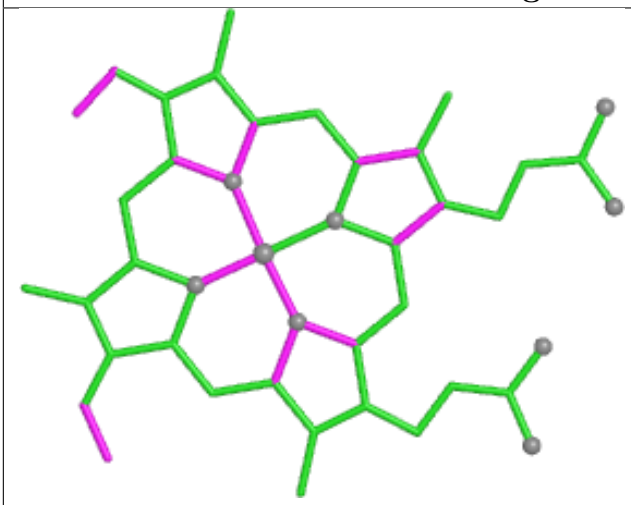
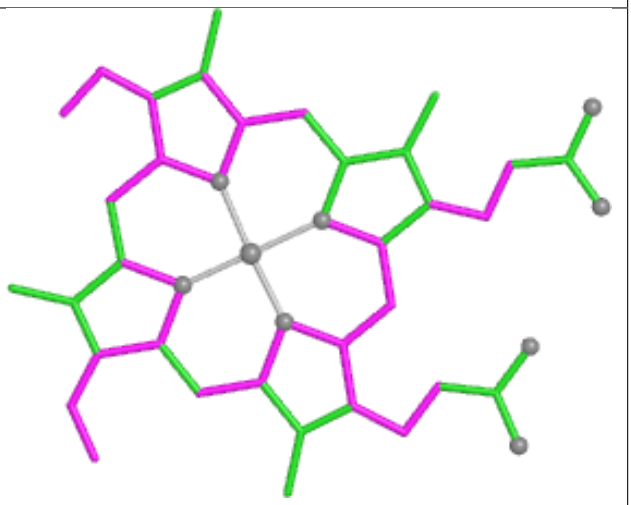
 Bond lengths	 Bond angles
 Torsions	 Rings

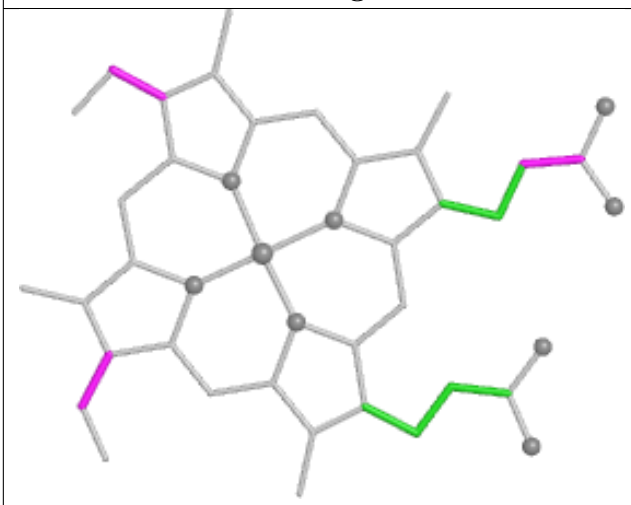
Ligand HEC C 403



Bond lengths



Bond angles



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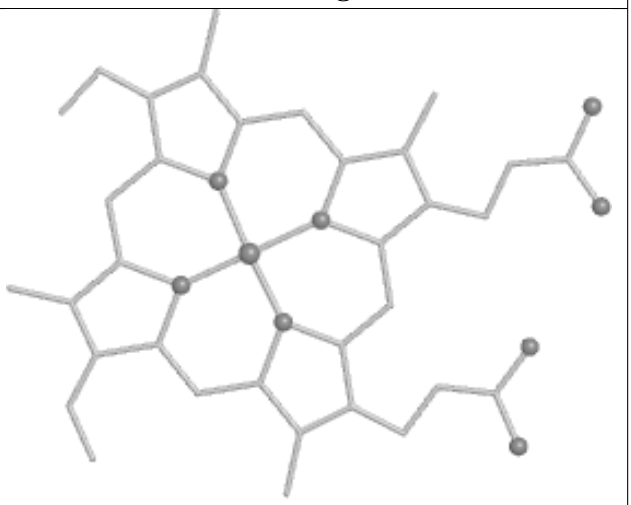
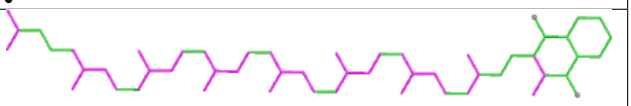


Rings

Ligand MQ8 M 405

Bond lengths



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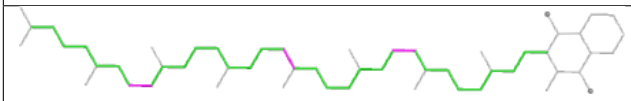

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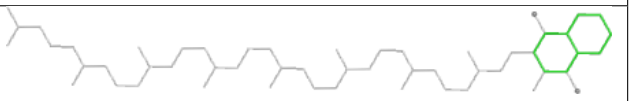
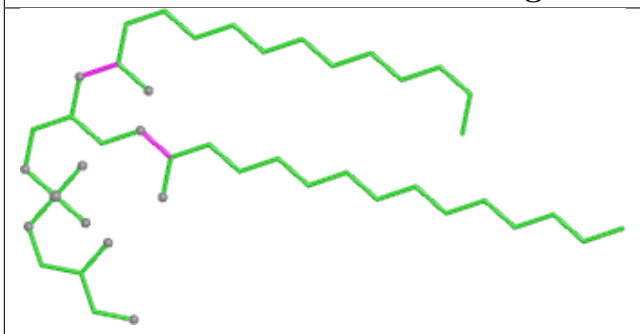
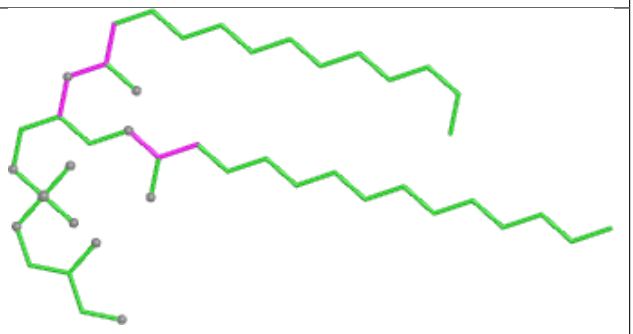
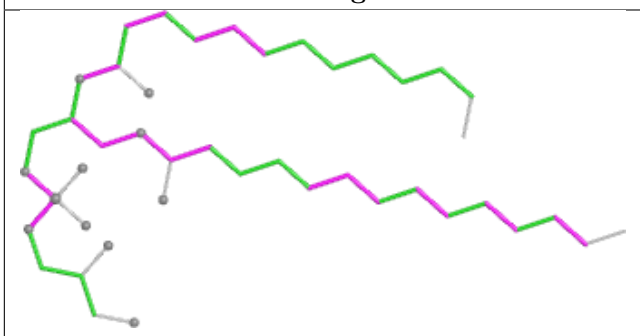
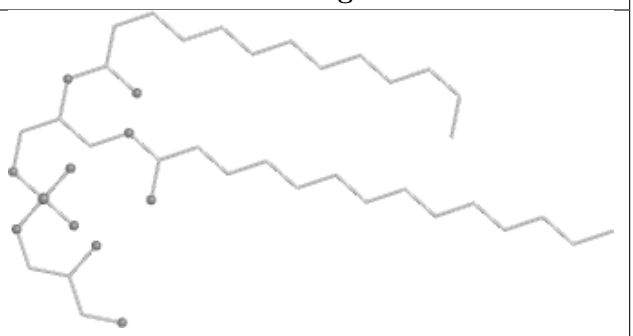


Rings

Ligand PGV Z 103	
 Bond lengths	 Bond angles
 Torsions	 Rings

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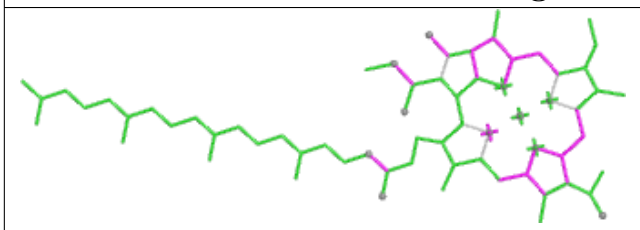
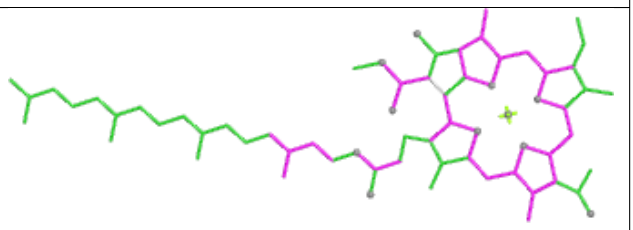
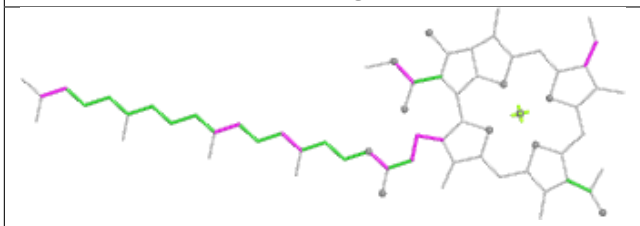
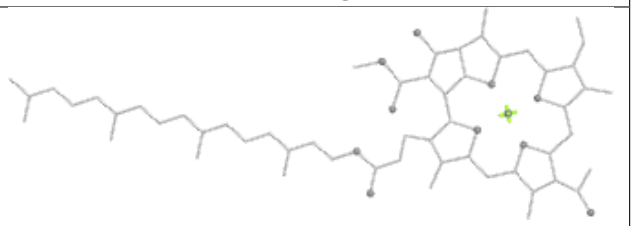
 Bond lengths	 Bond angles
 Torsions	 Rings

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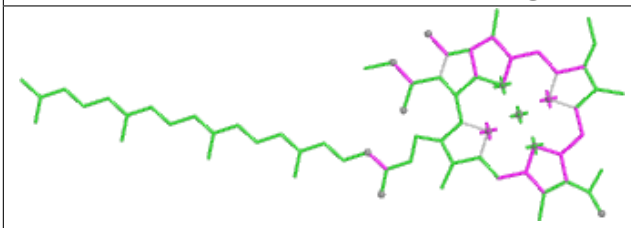
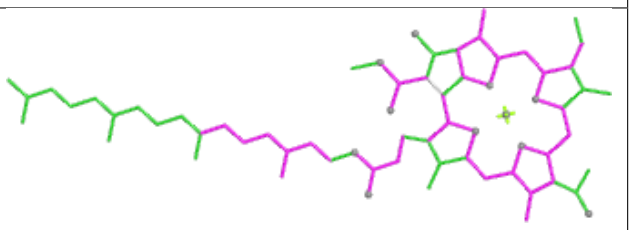
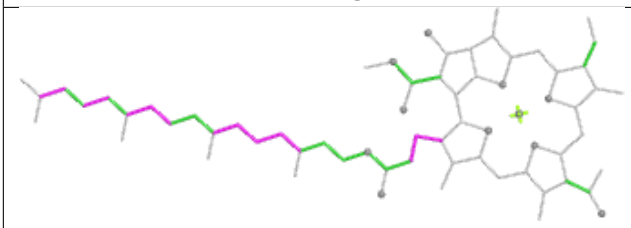
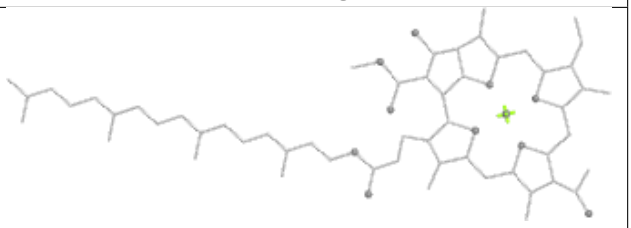
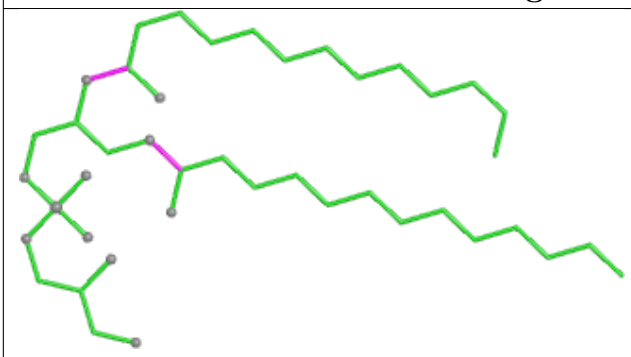
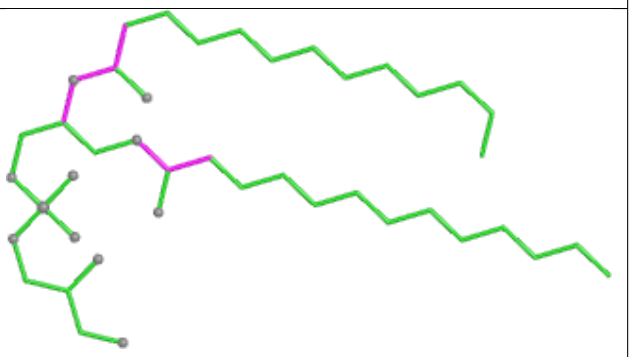
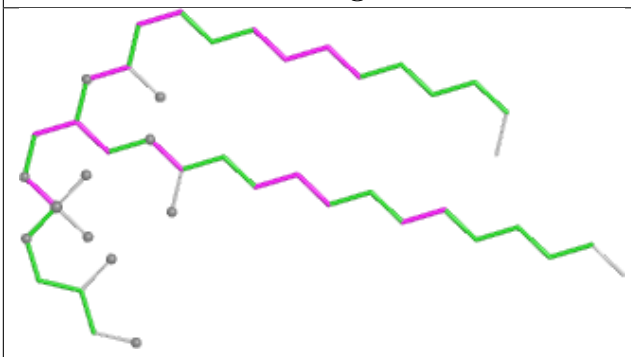
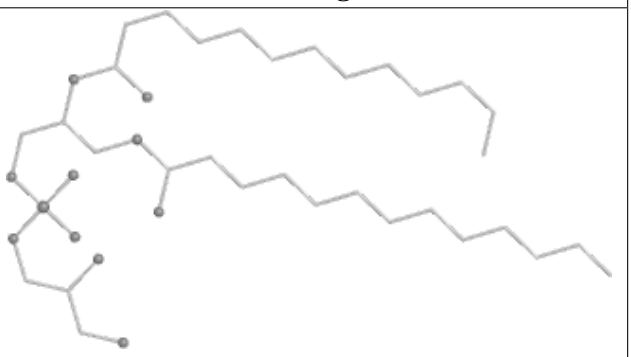
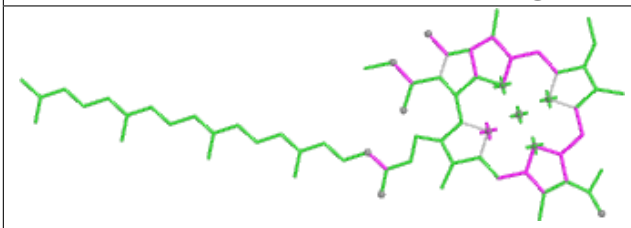
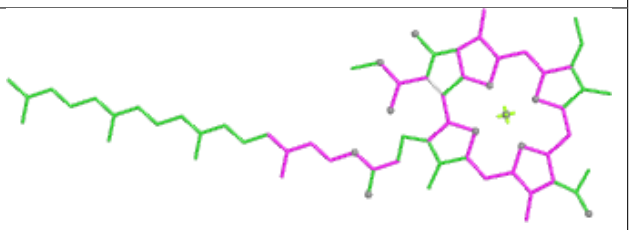
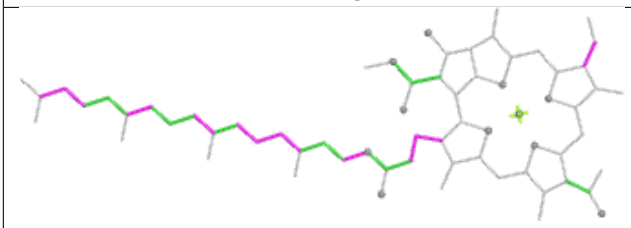
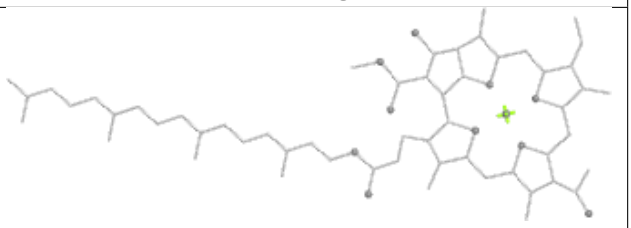
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PGV 8 103	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCL 7 102	
 Bond lengths	 Bond angles
 Torsions	 Rings

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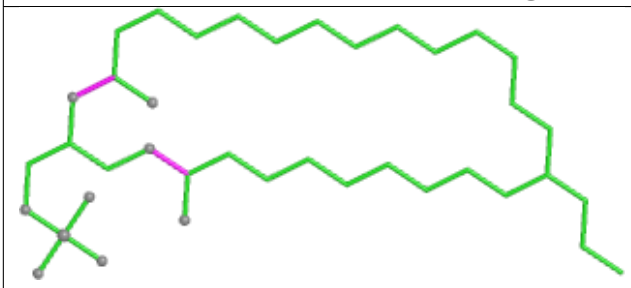
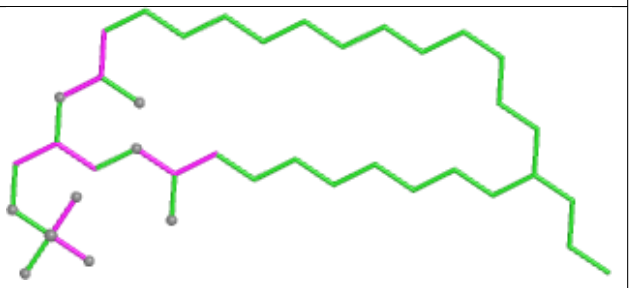
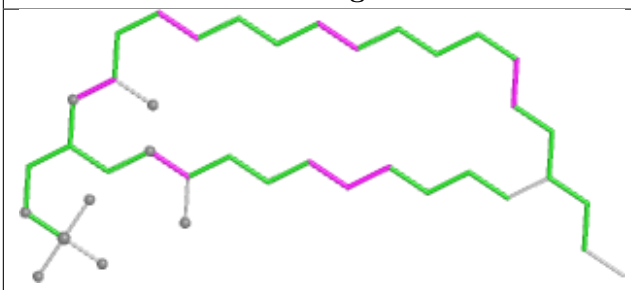
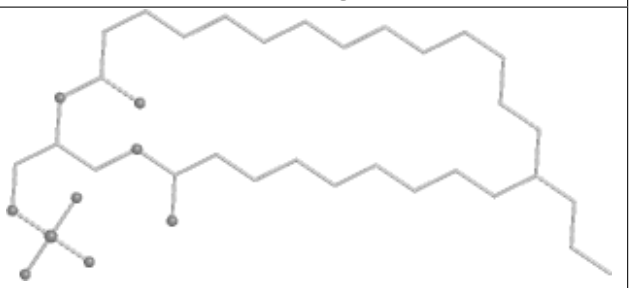
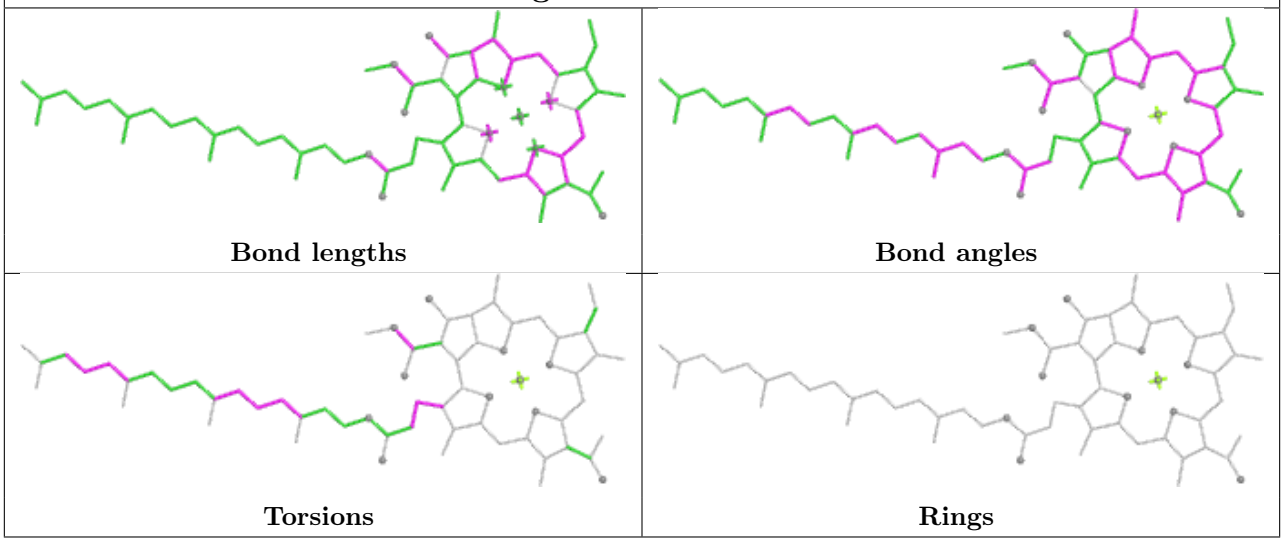
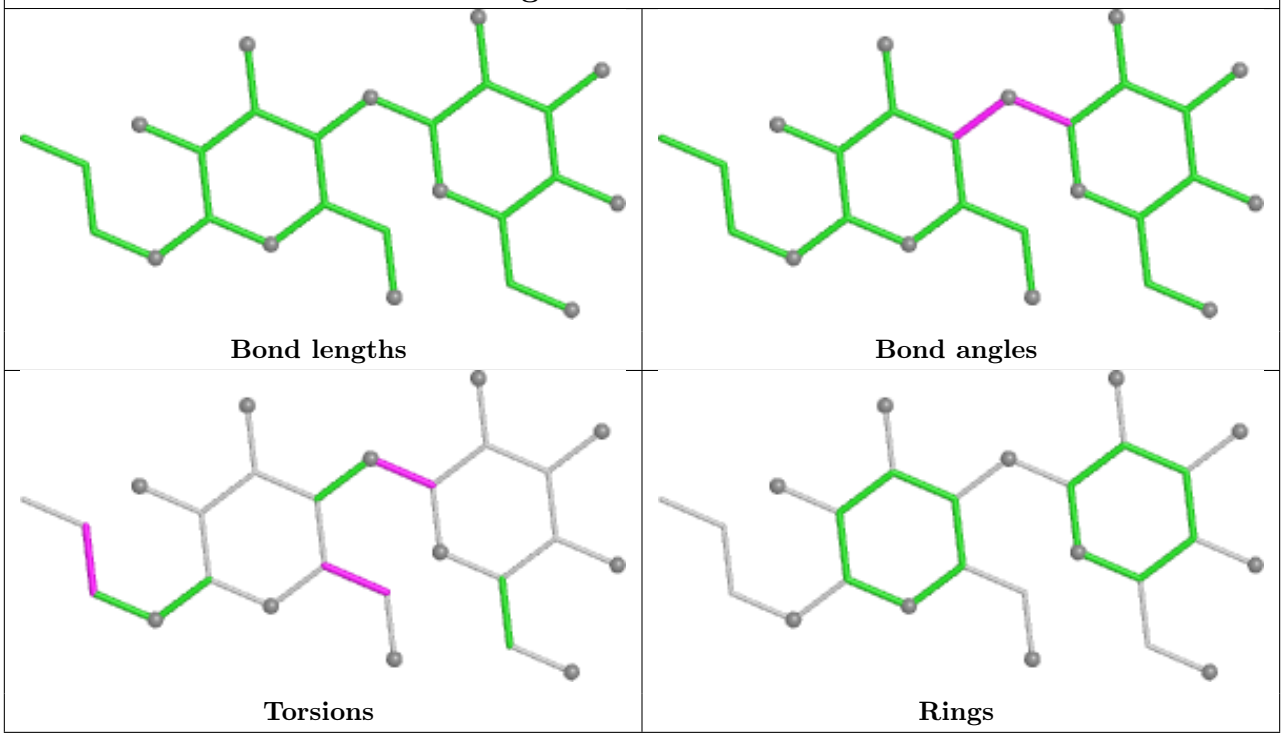
 Bond lengths	 Bond angles
 Torsions	 Rings

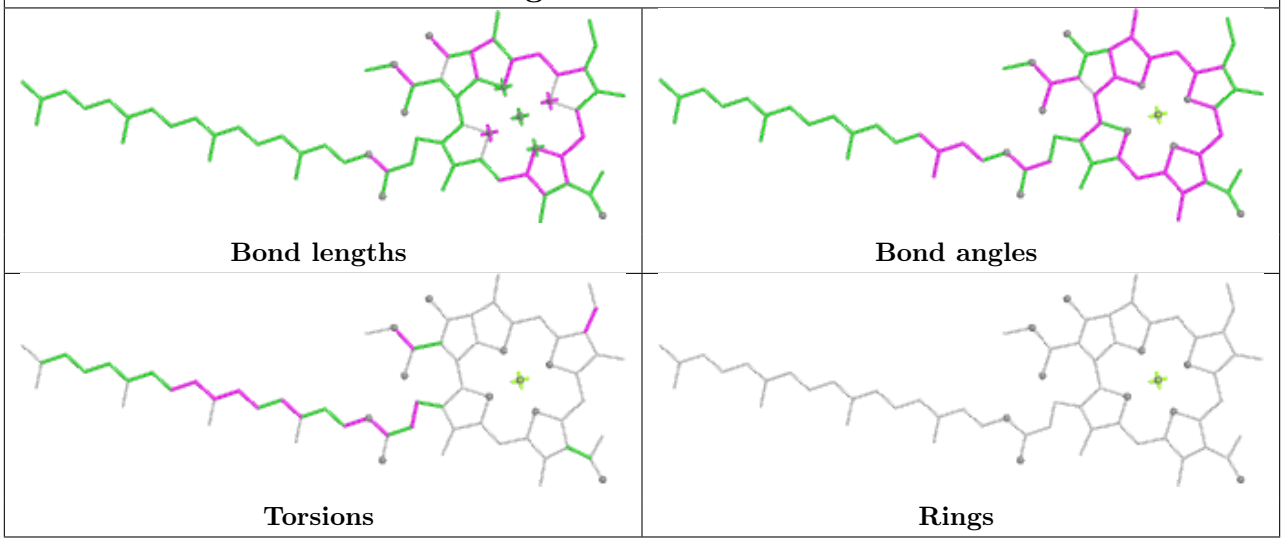
Ligand BCL I 102



Ligand LMT H 307



Ligand BCL X 102



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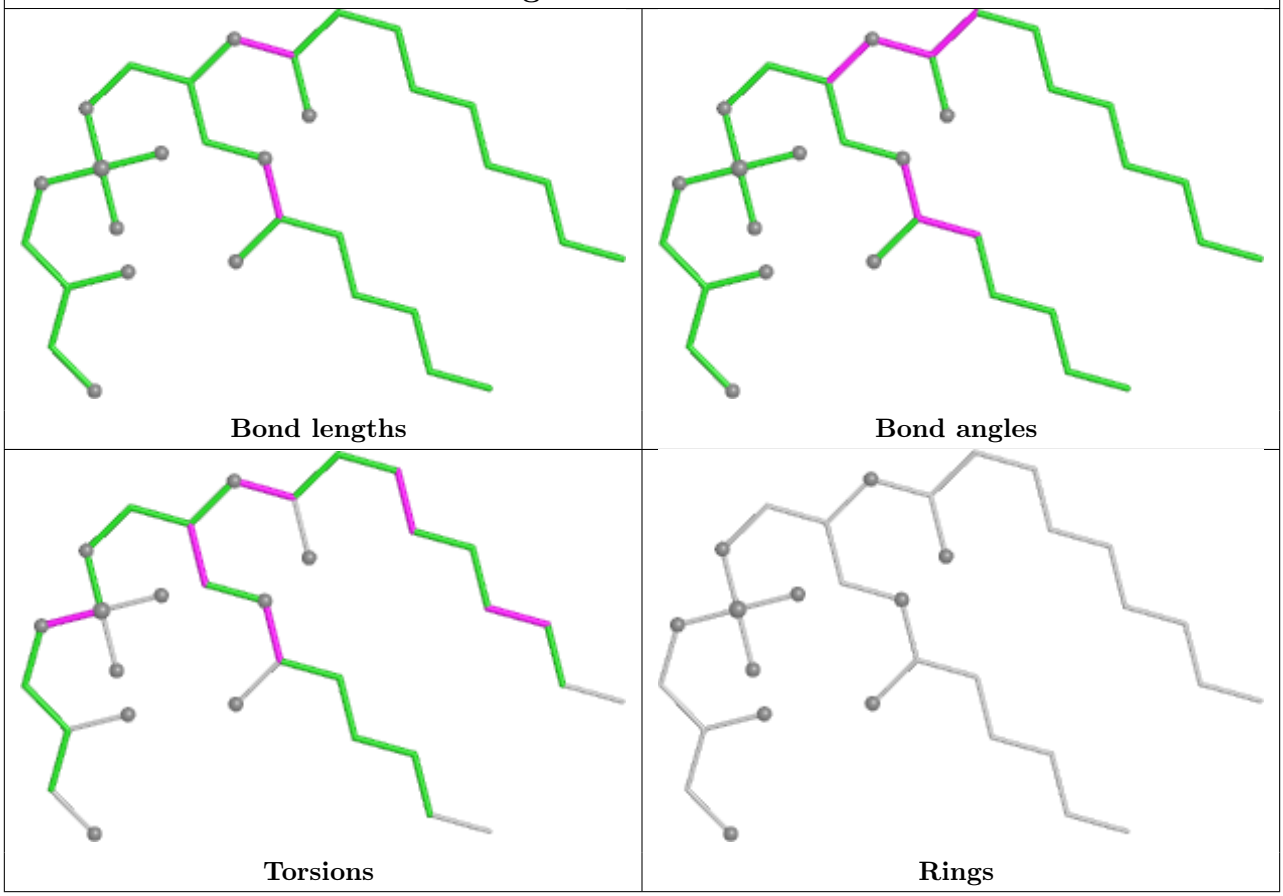

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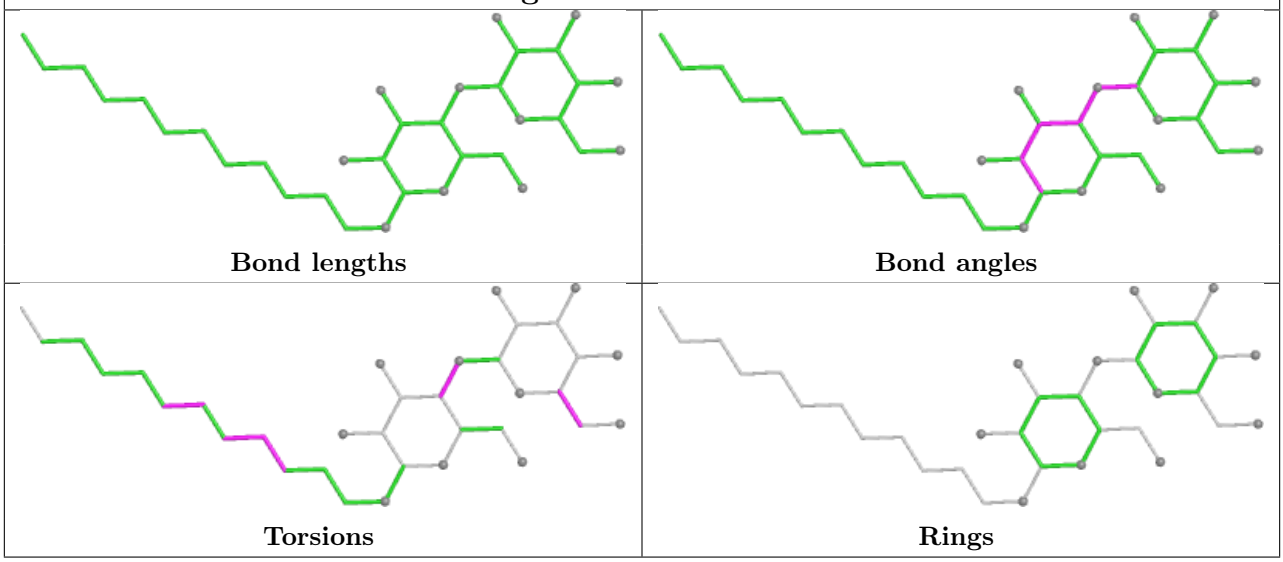
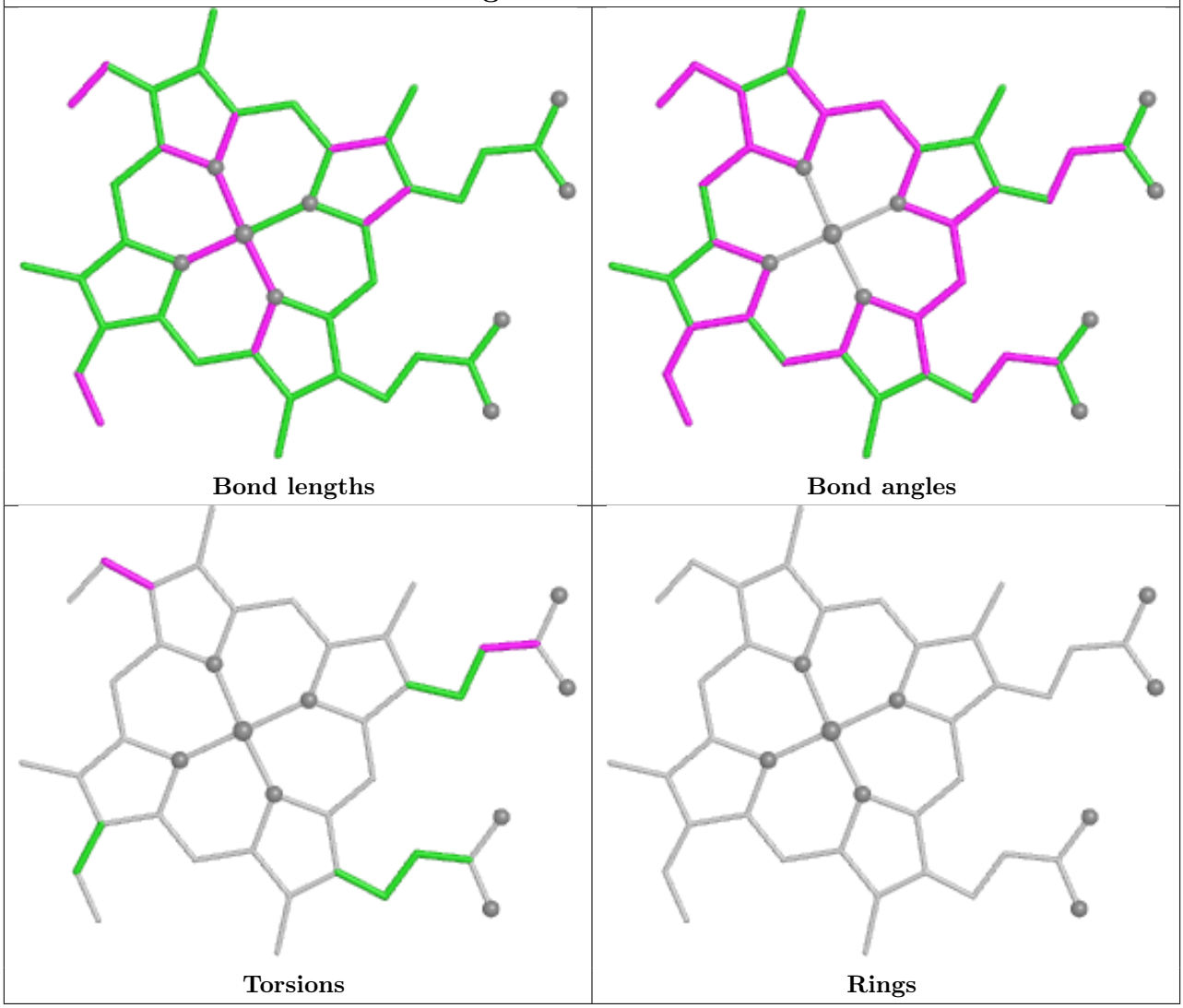
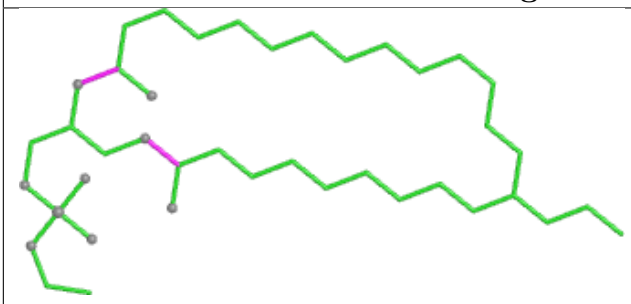
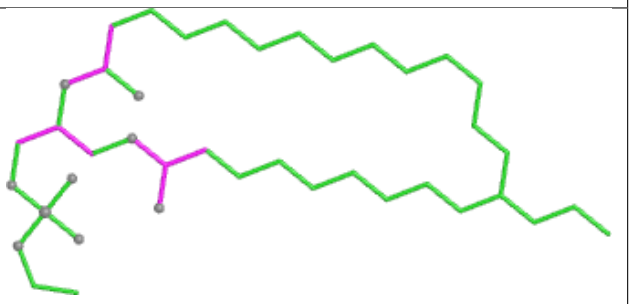
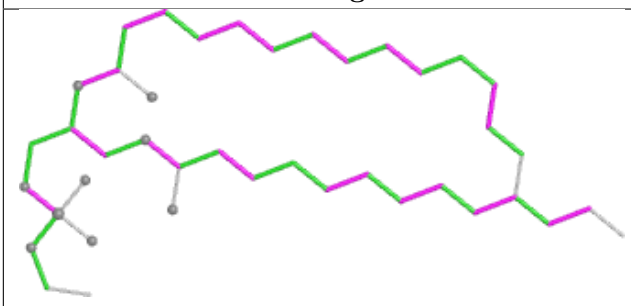
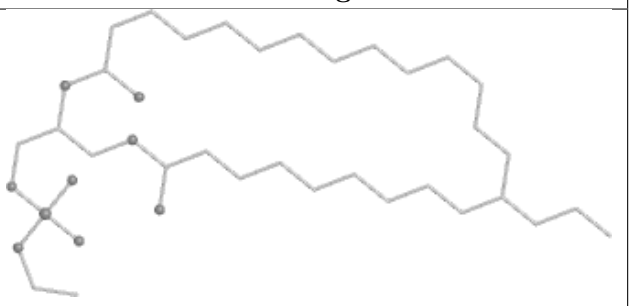


Ligand HEC C 404



Ligand PGV G 105	
 Bond lengths	 Bond angles
 Torsions	 Rings

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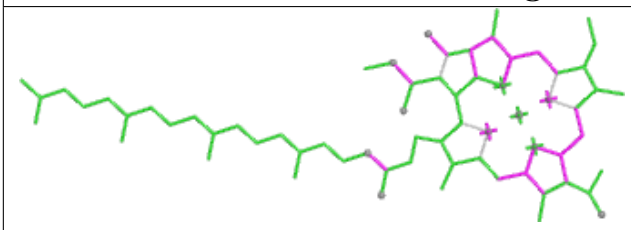
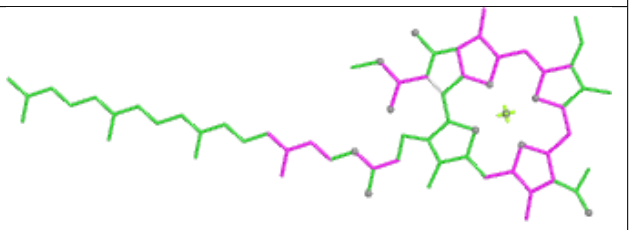
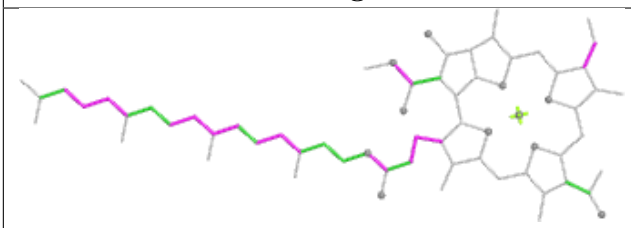
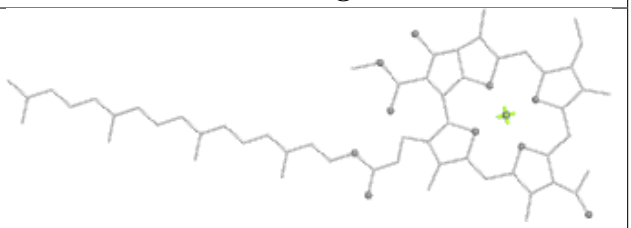
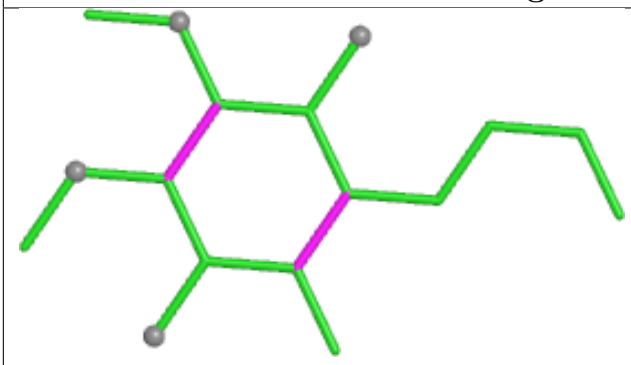
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand UQ8 L 307



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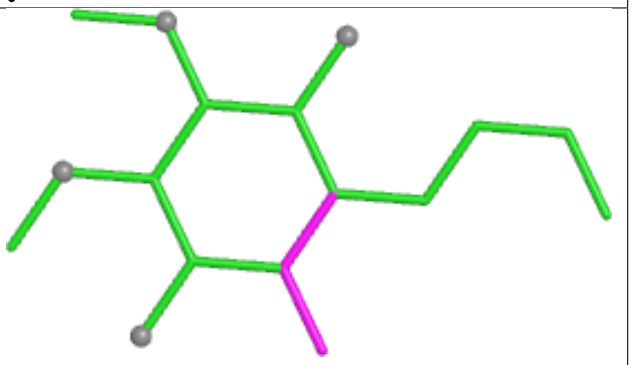
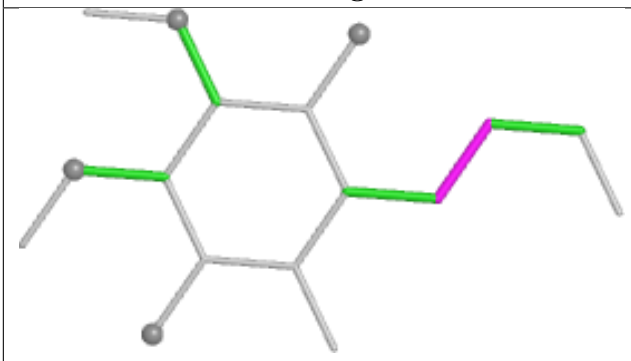


Bond angles



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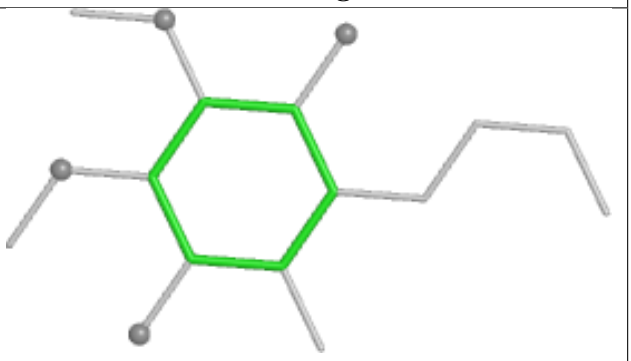
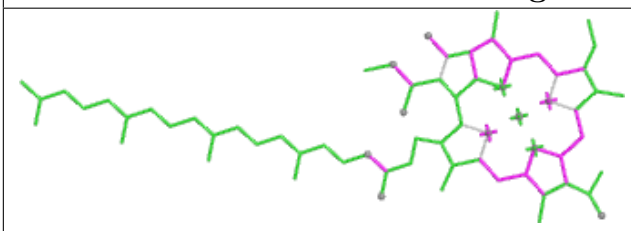


Rings

Ligand BCL 4 102



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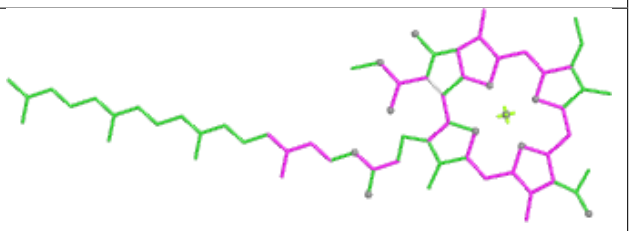

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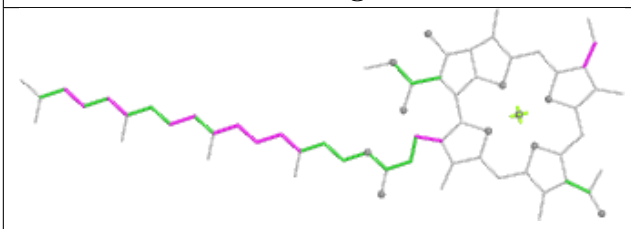

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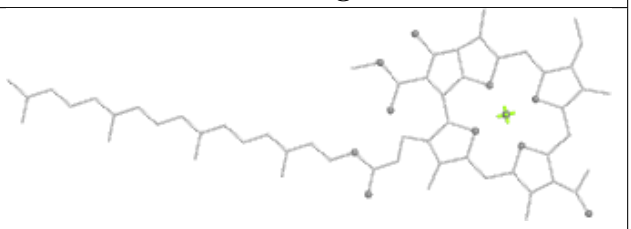
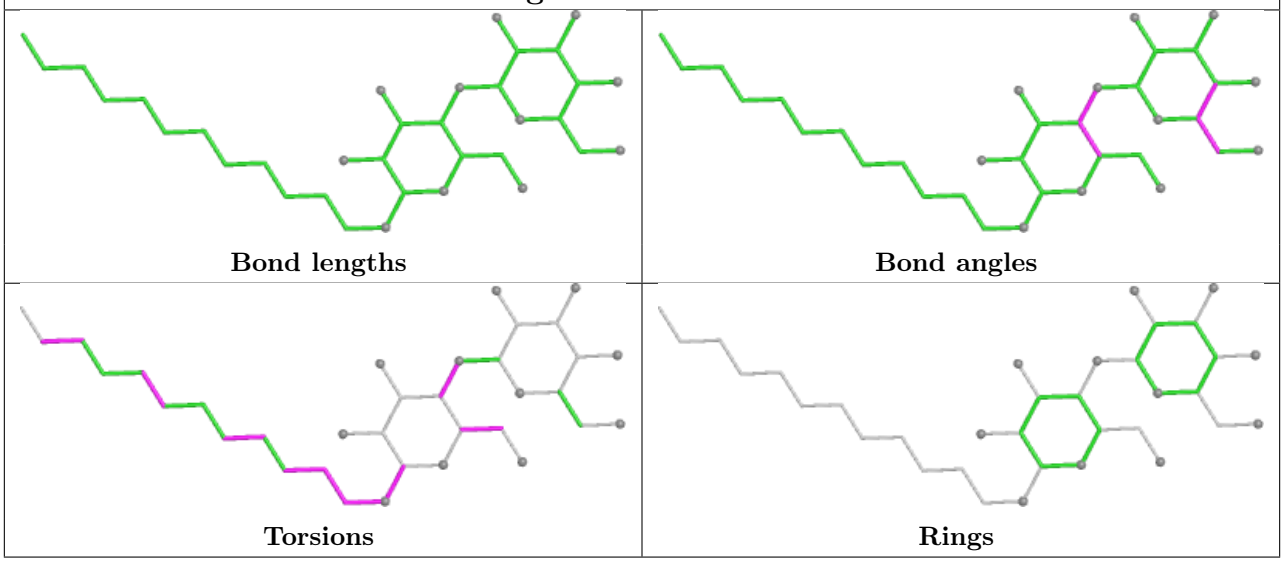
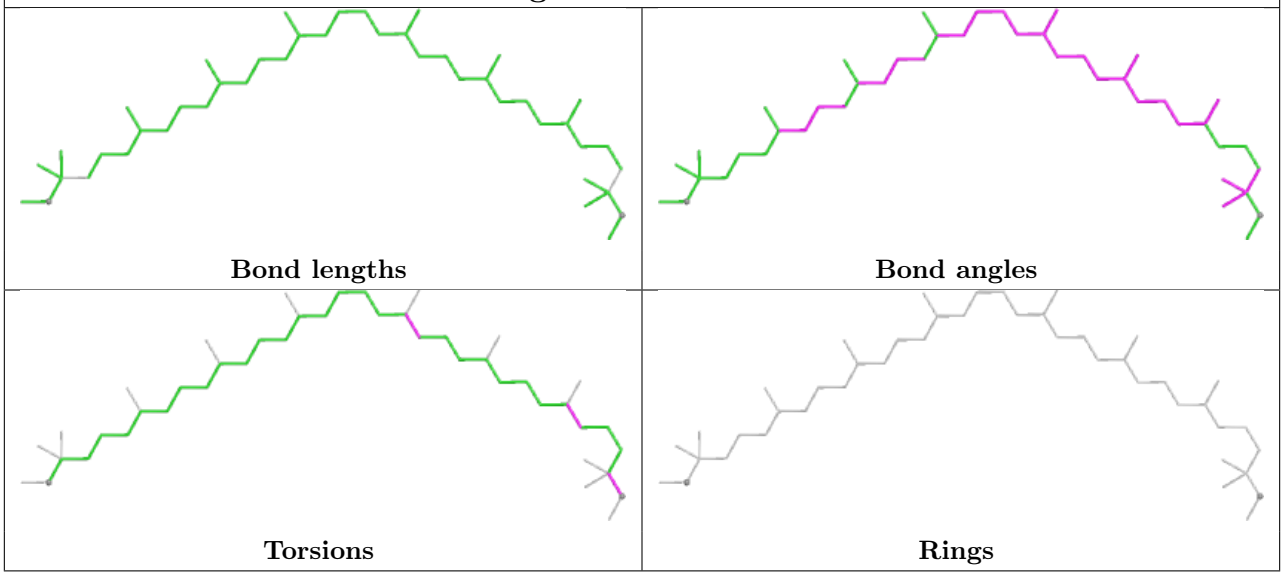


Rings

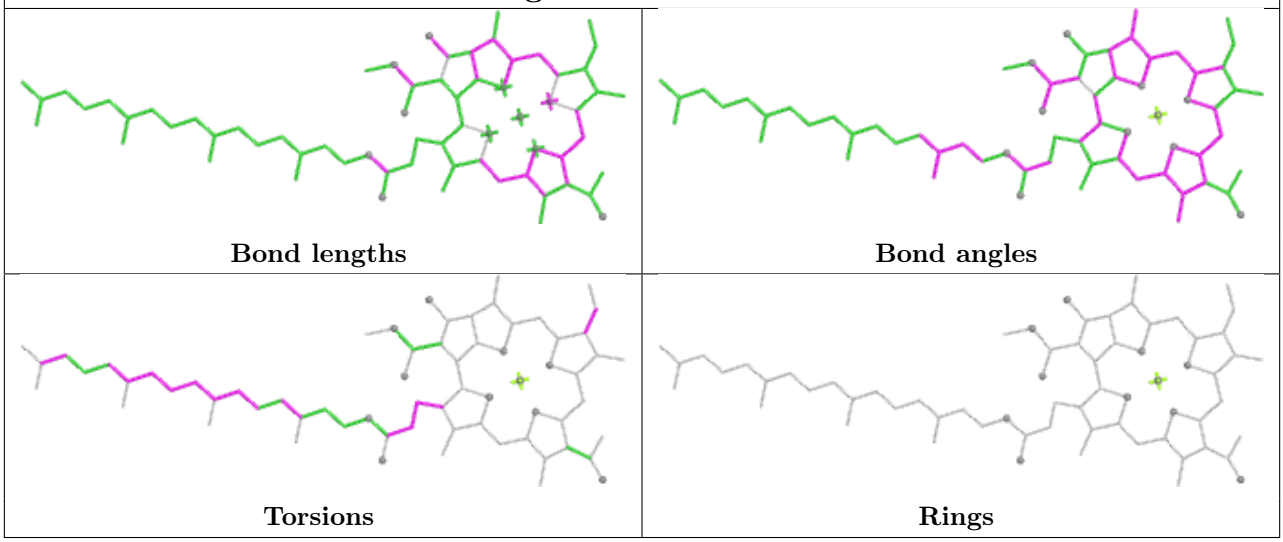
Ligand LMT 5 101

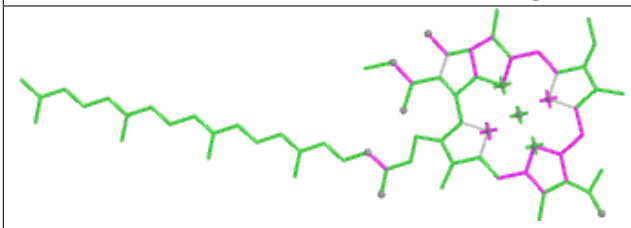
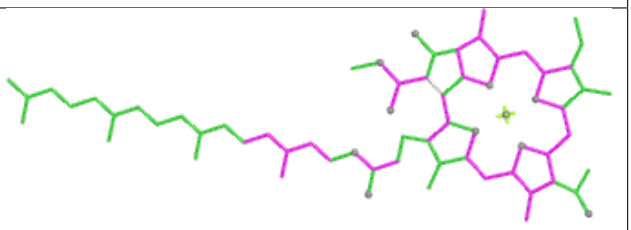
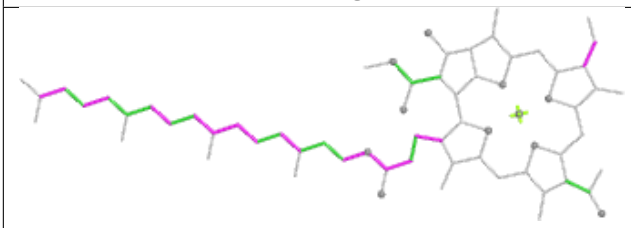
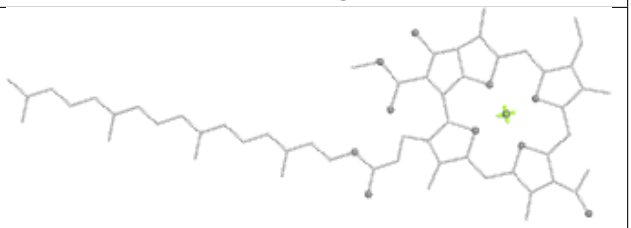


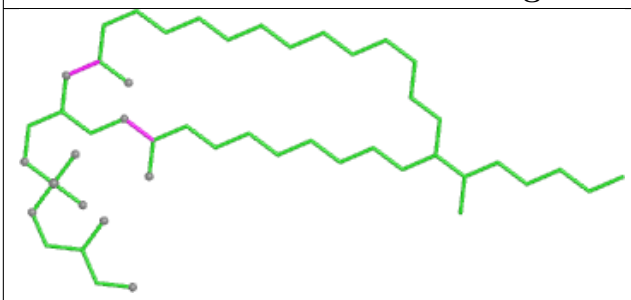
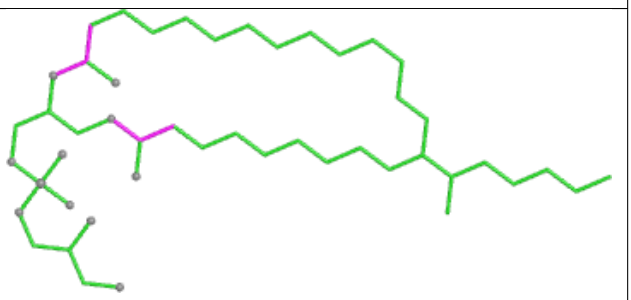
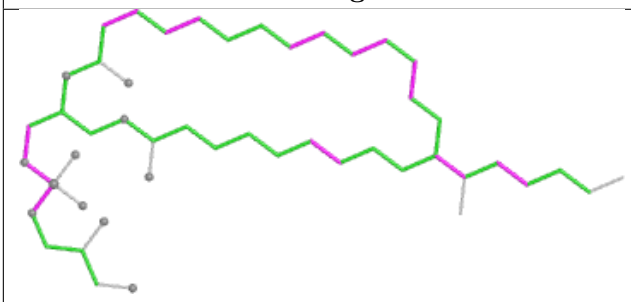
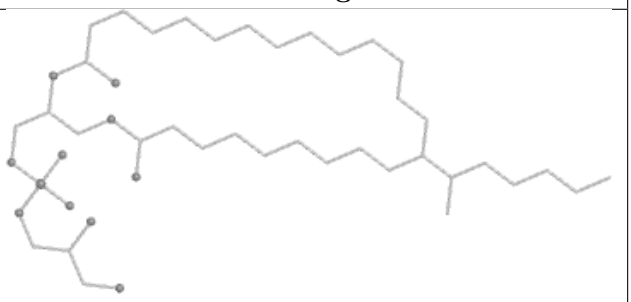
Ligand CRT 8 101



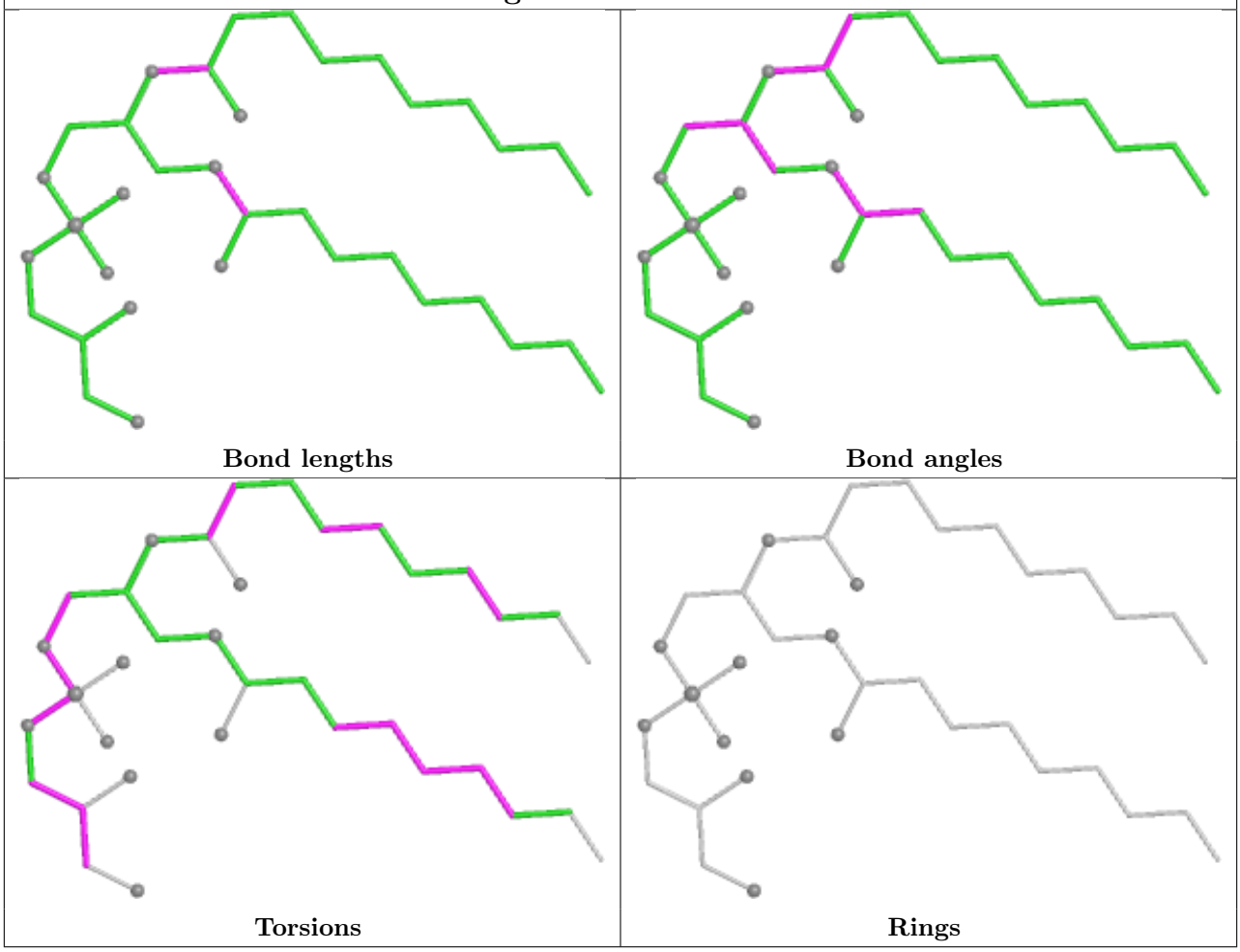
Ligand BCL G 103



Ligand BCL Z 102	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PGV F 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PGV H 302



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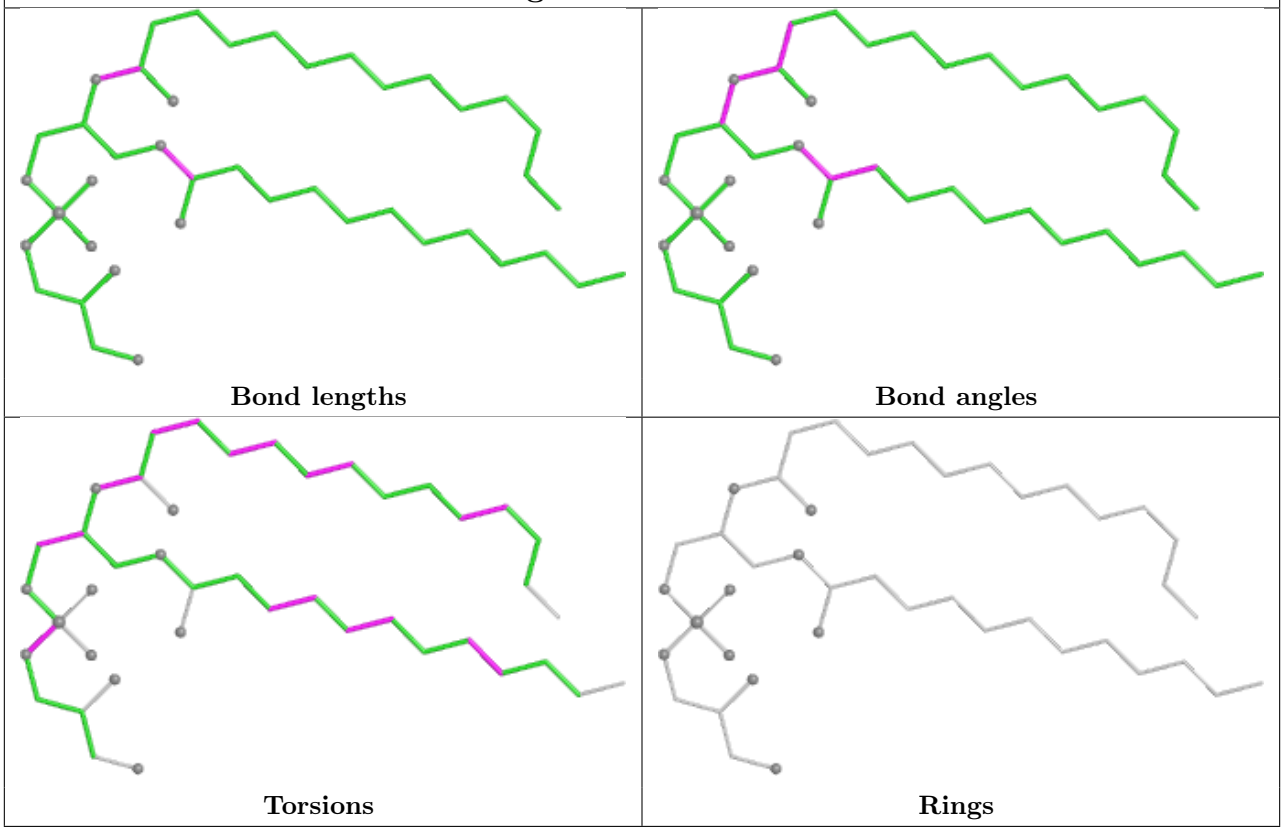
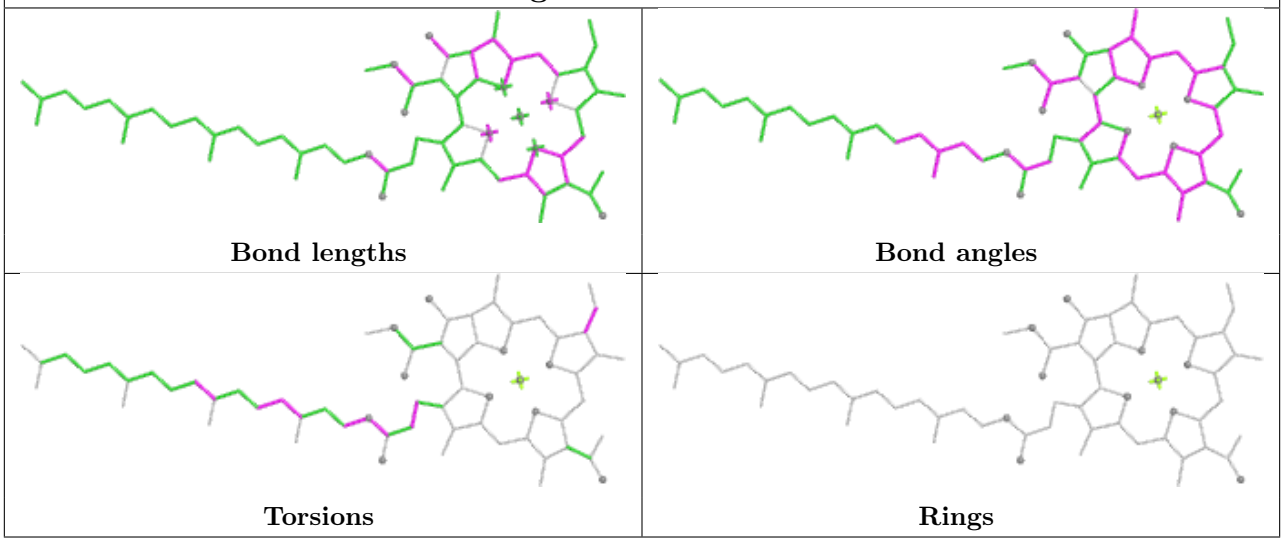
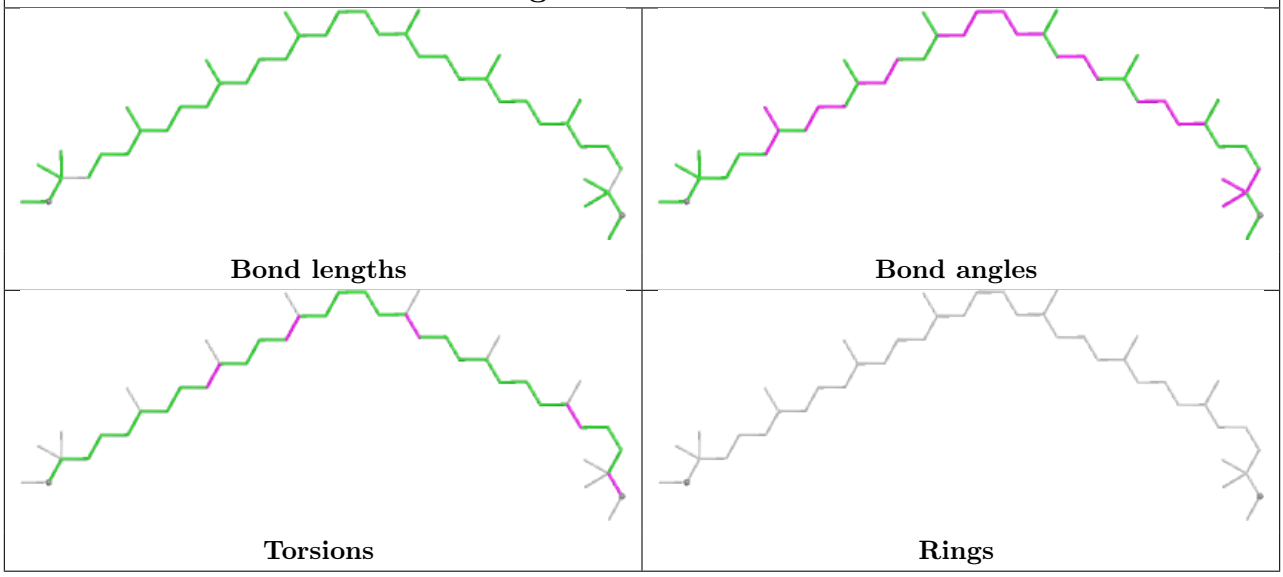


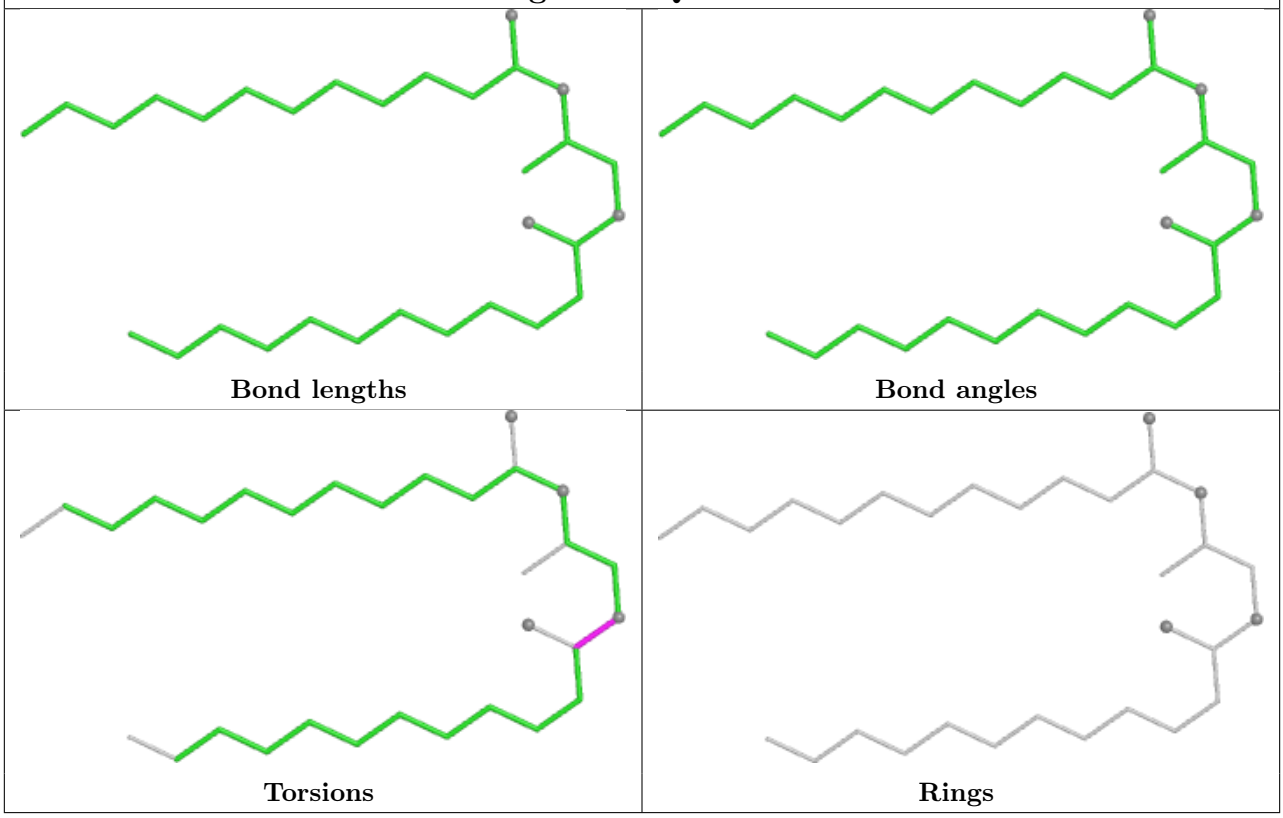
Ligand BCL 6 102



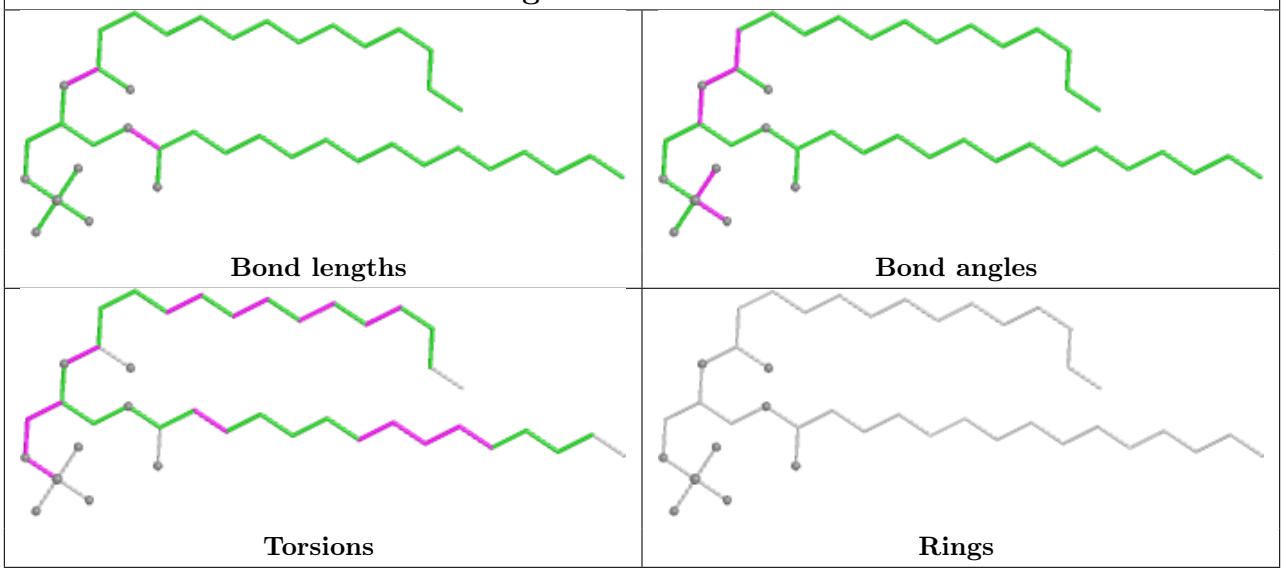
Ligand CRT 4 101



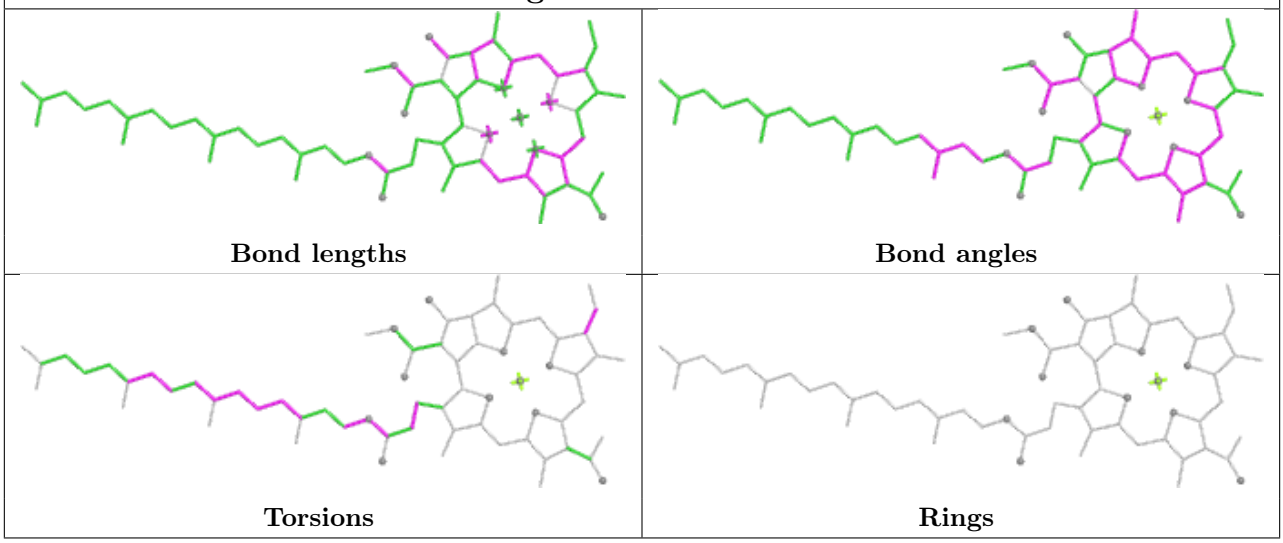
Ligand LJQ C 406

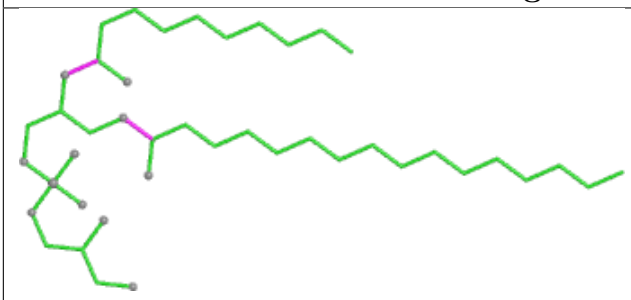
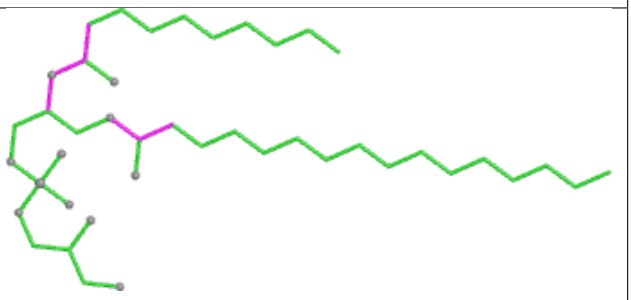
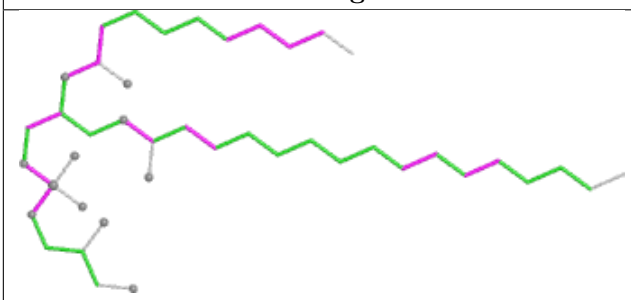
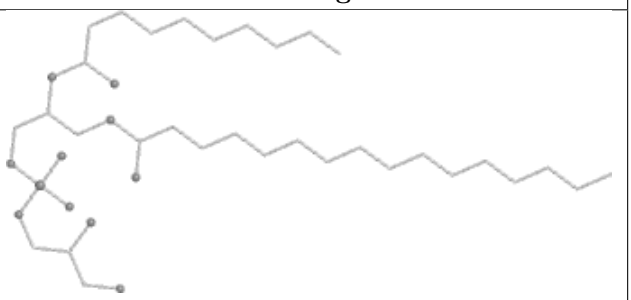


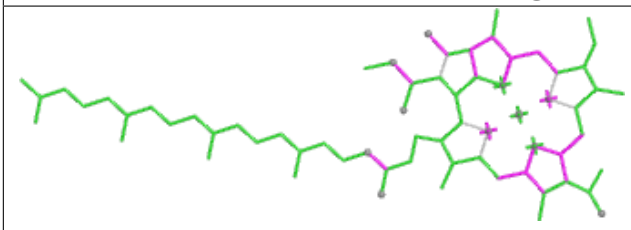
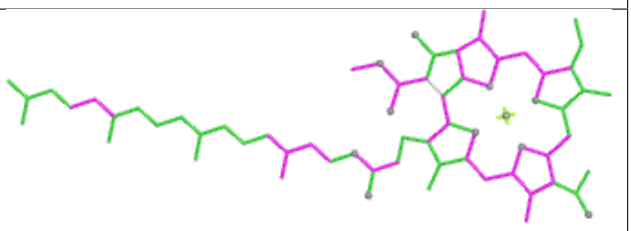
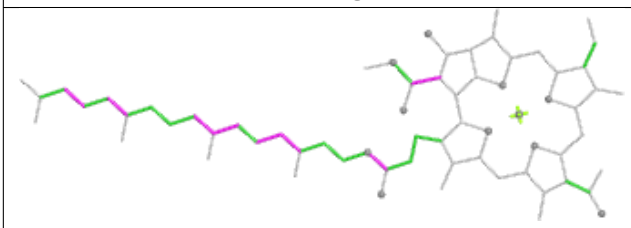
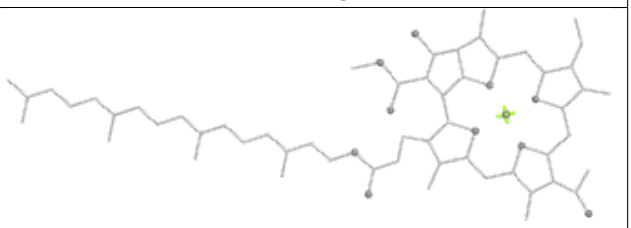
Ligand PGV R 104

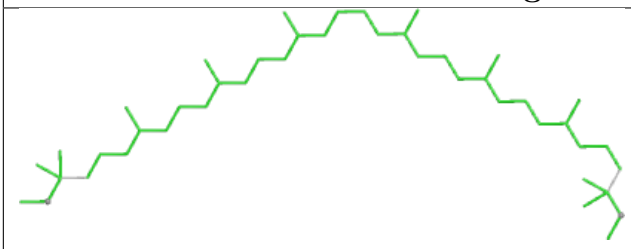
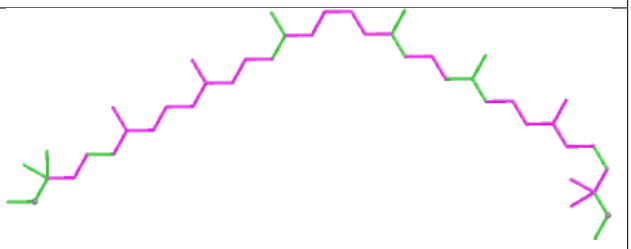
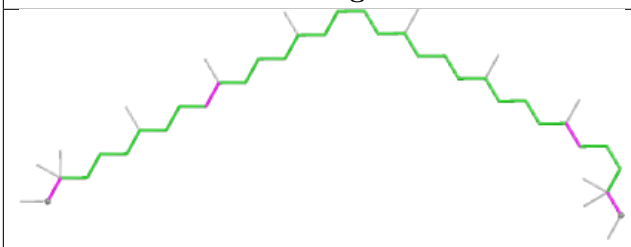


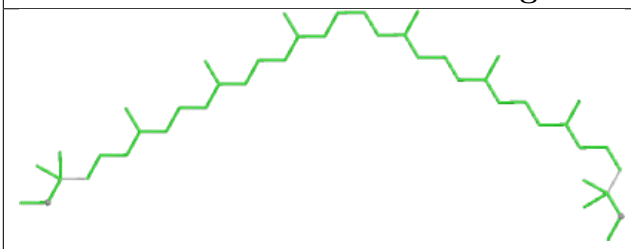
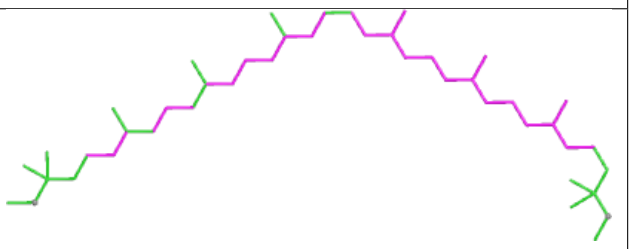
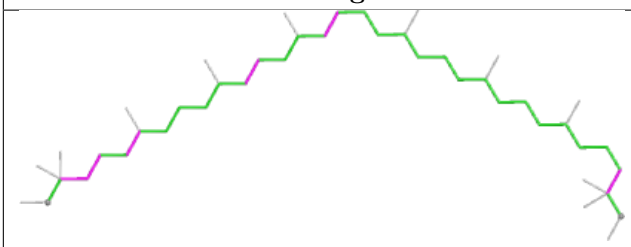
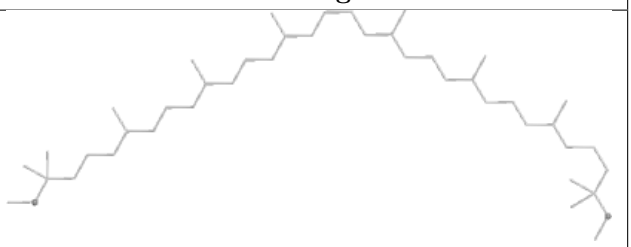
Ligand BCL T 101



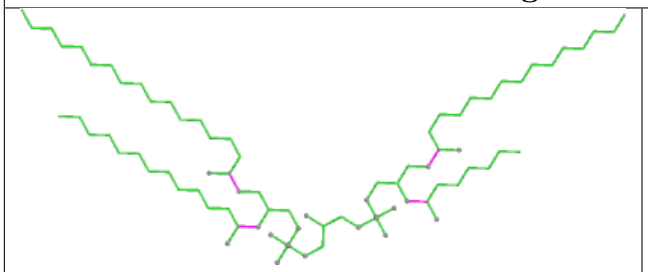
Ligand PGV L 305	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCL S 102	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CRT R 101	
 Bond lengths	 Bond angles
 Torsions	Rings

Ligand CRT M 406	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CDL M 407



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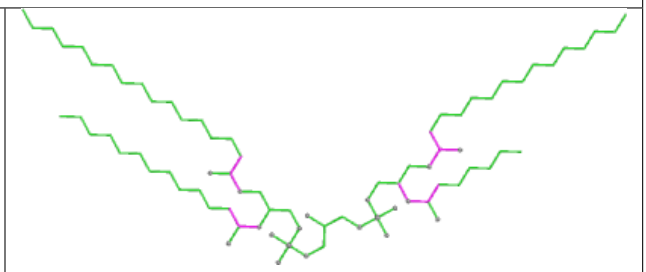
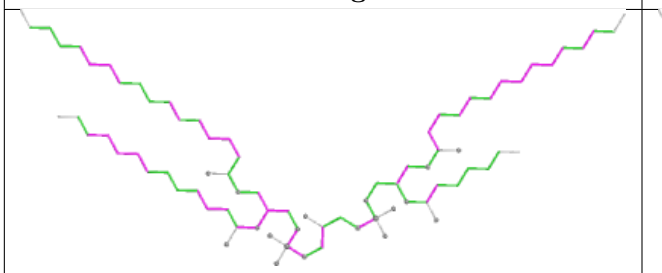


Bond angles



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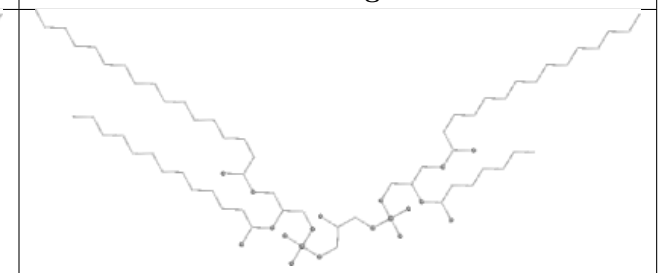
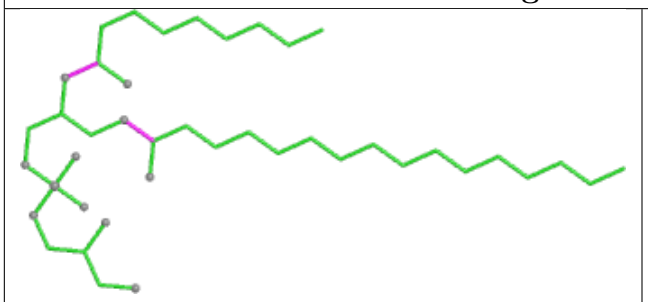


Rings

Ligand PGV H 304



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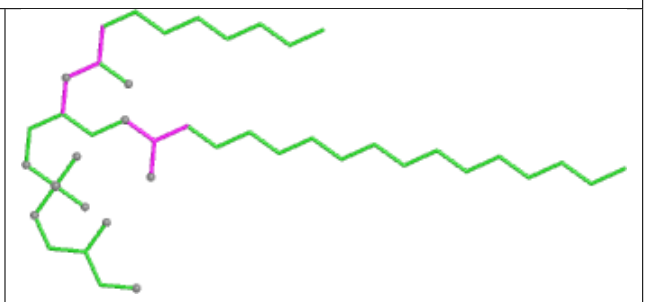

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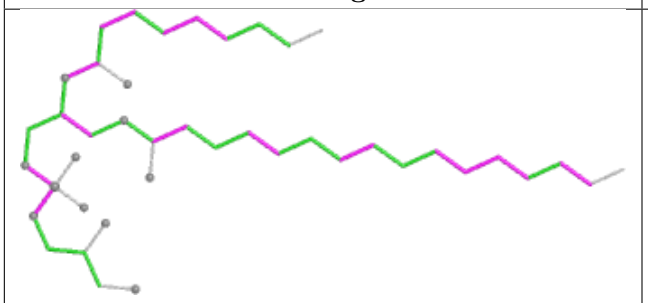

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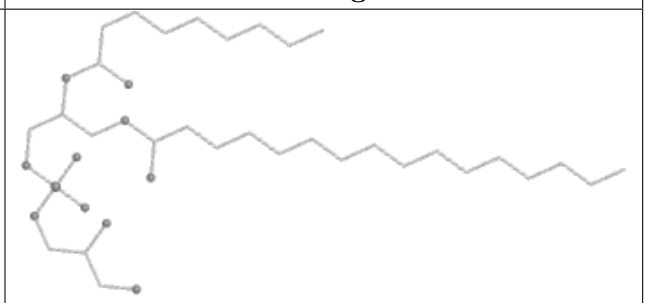
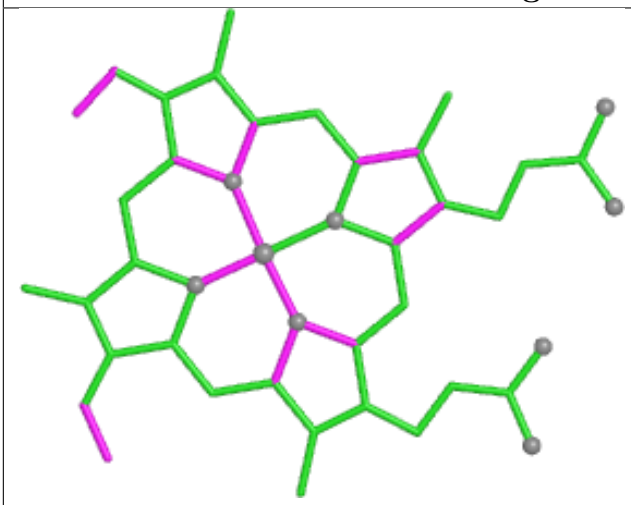


Rings

Ligand HEC C 402



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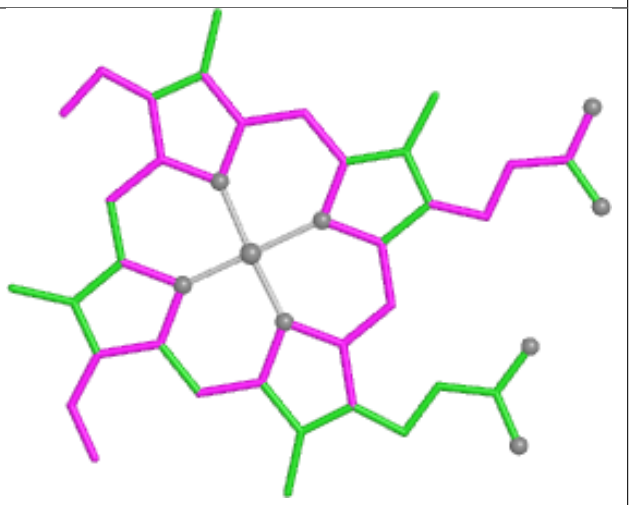

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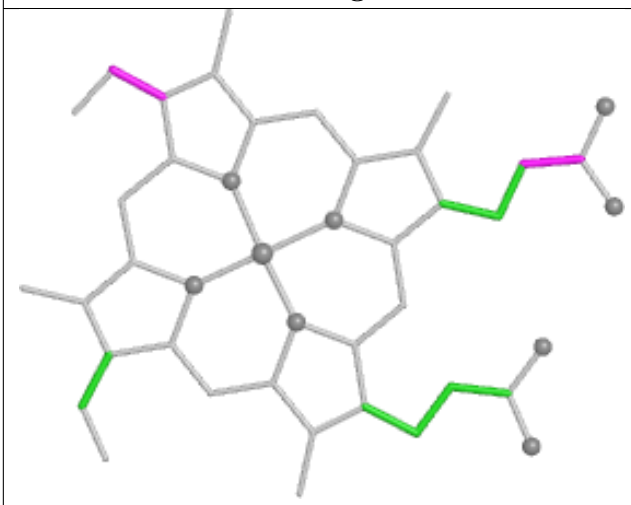

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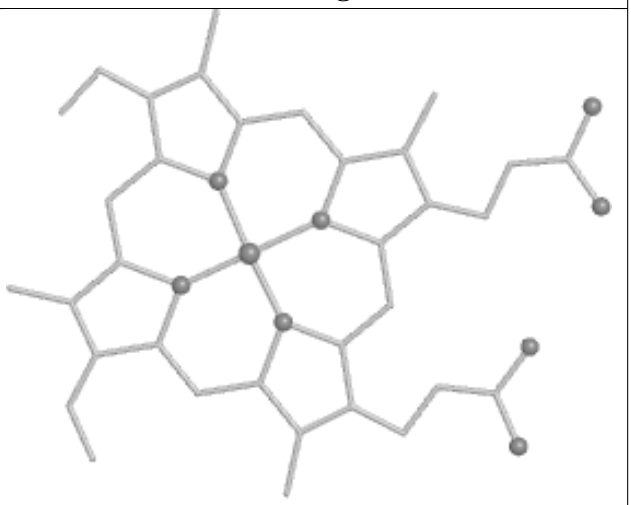
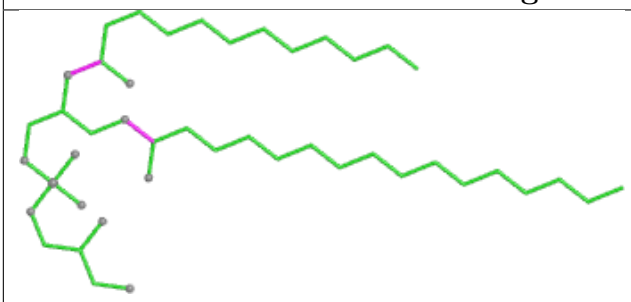
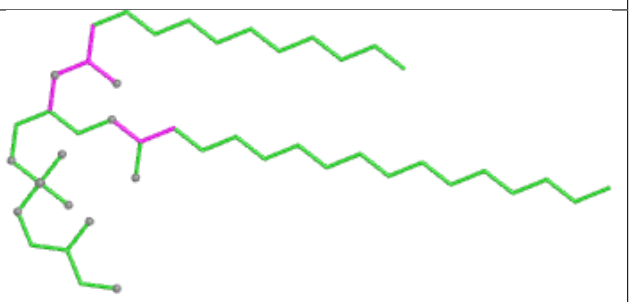
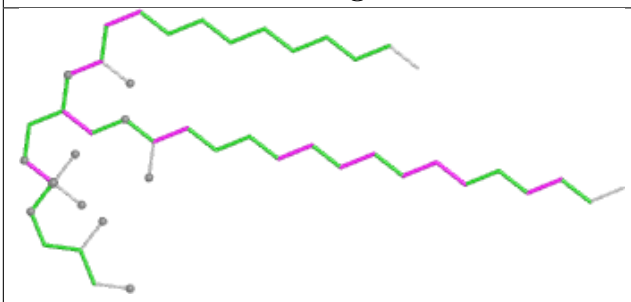
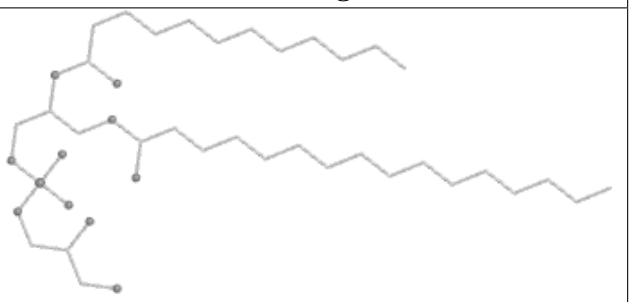
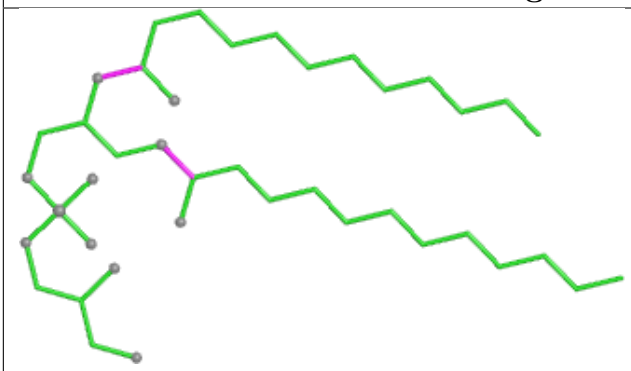
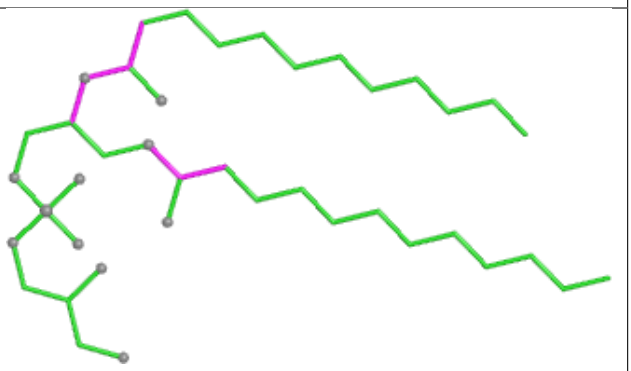
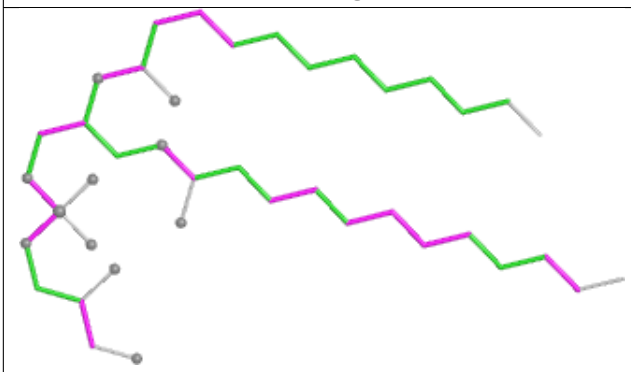
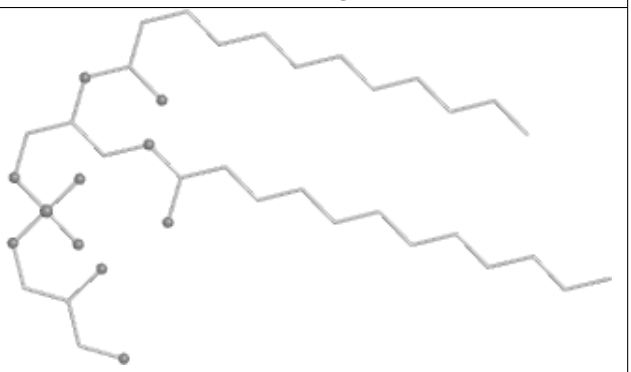
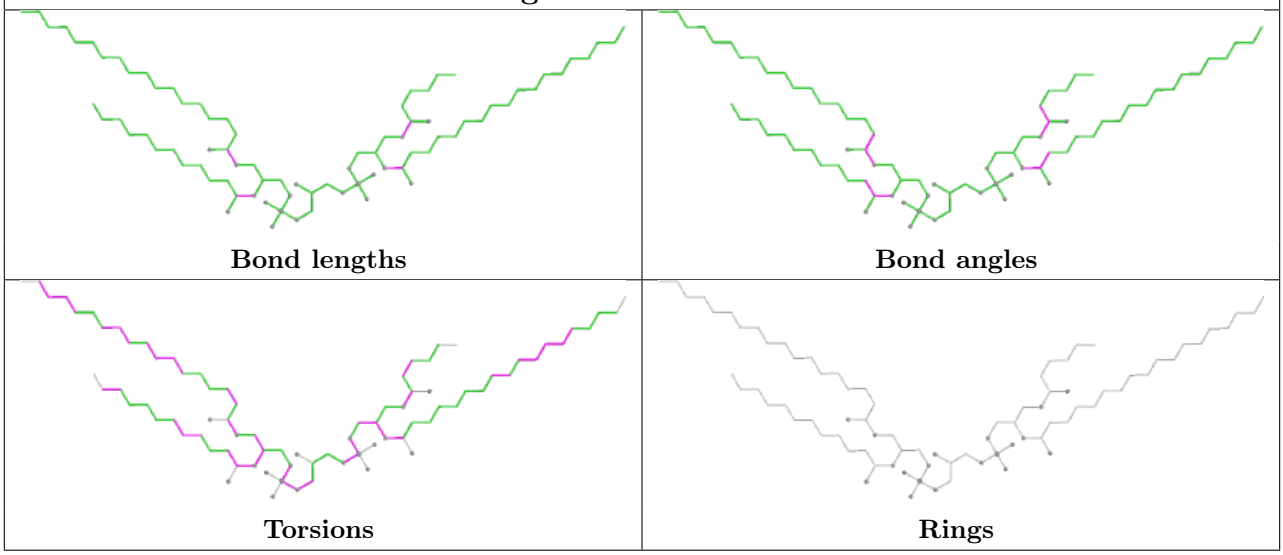


Rings

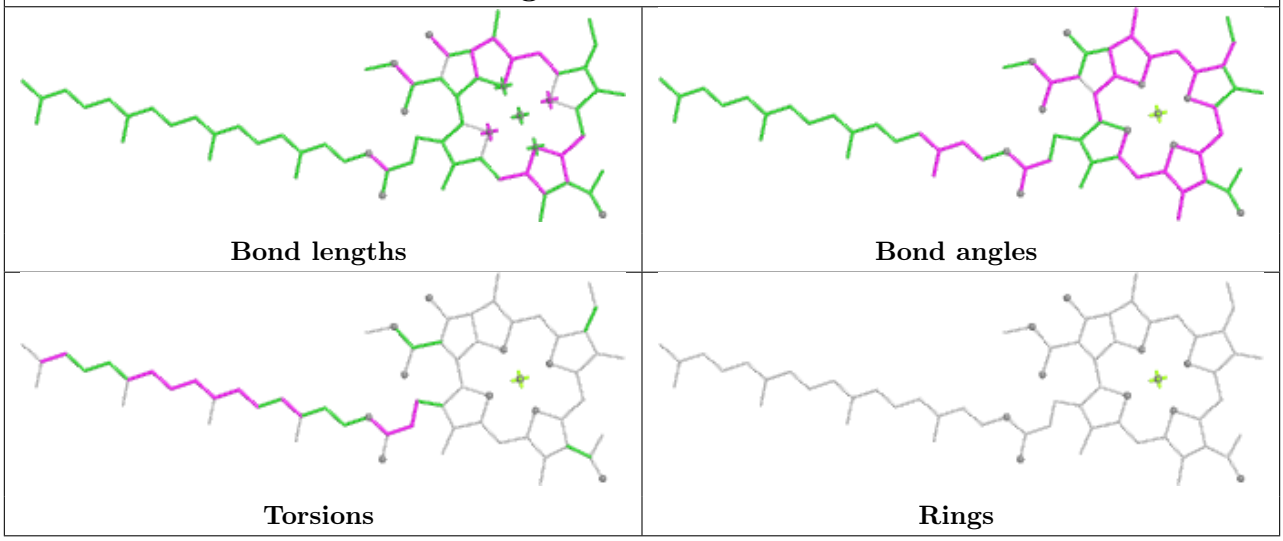
Ligand PGV X 103	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PGV 0 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

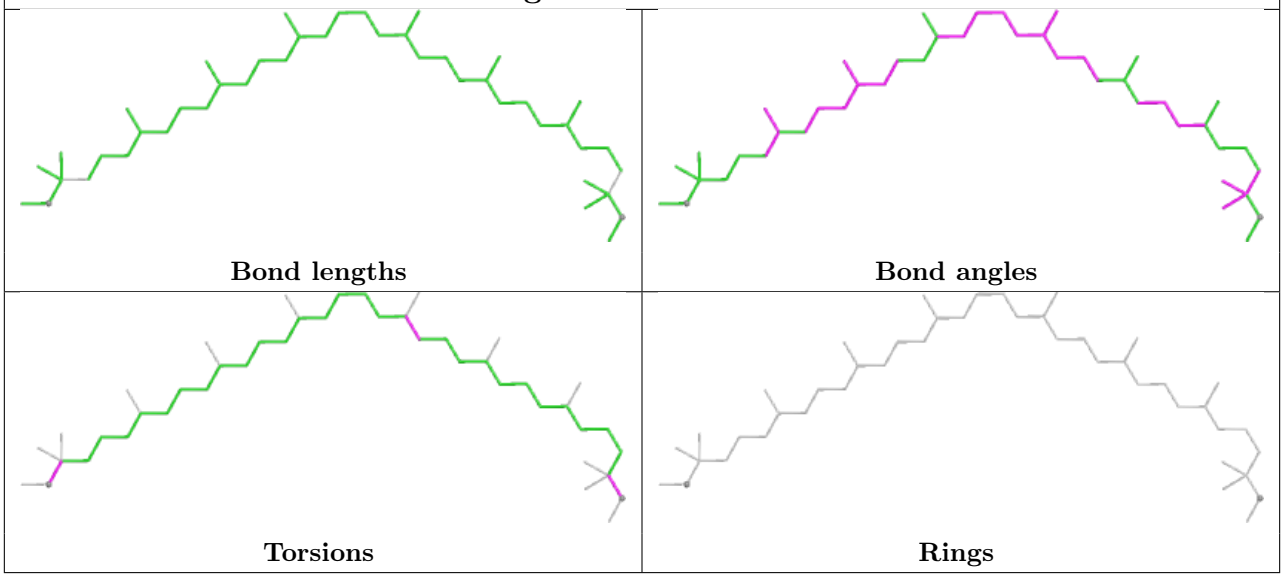
Ligand CDL M 402



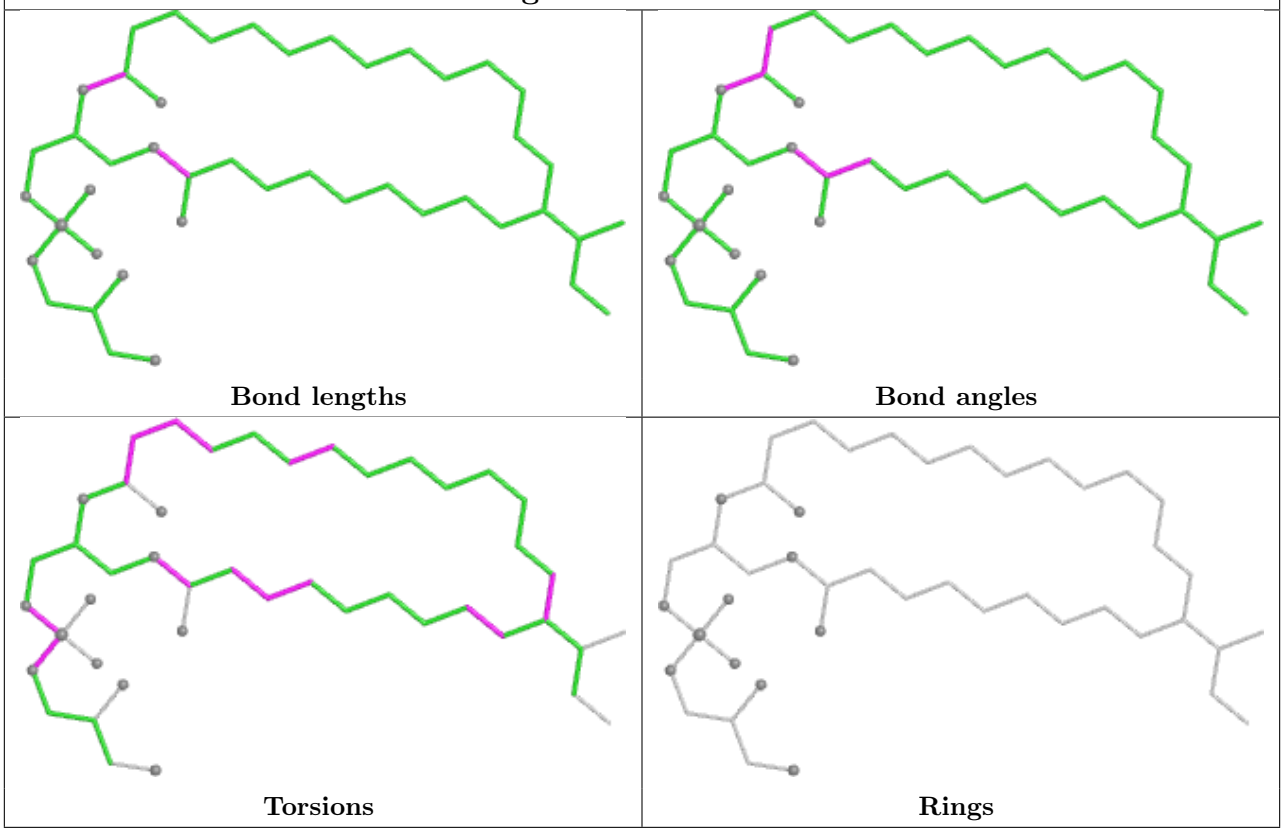
Ligand BCL W 102



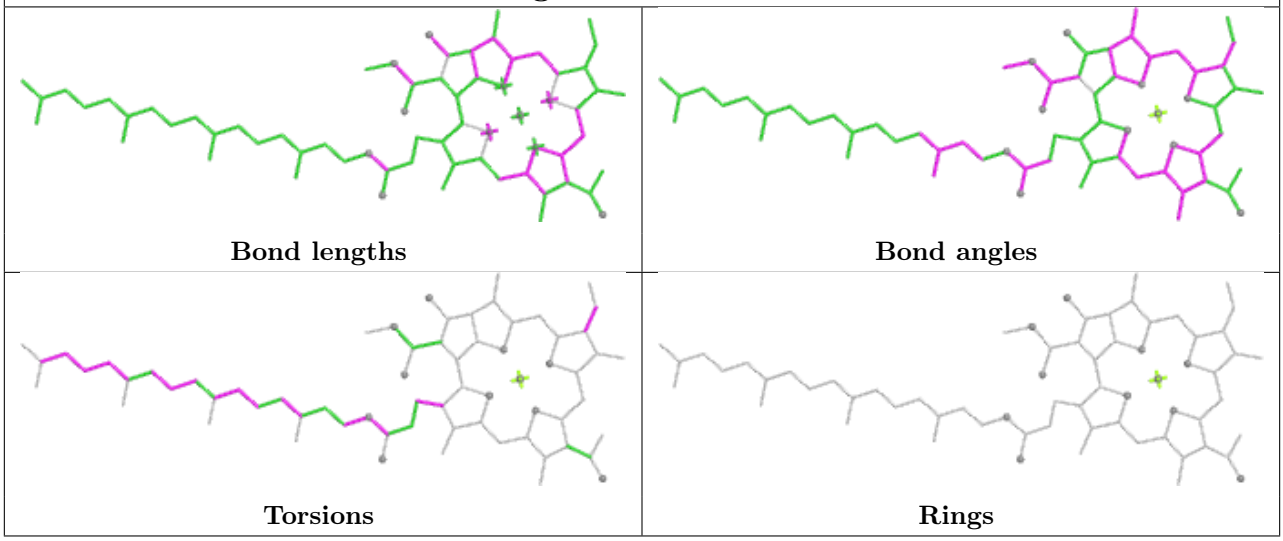
Ligand CRT N 102



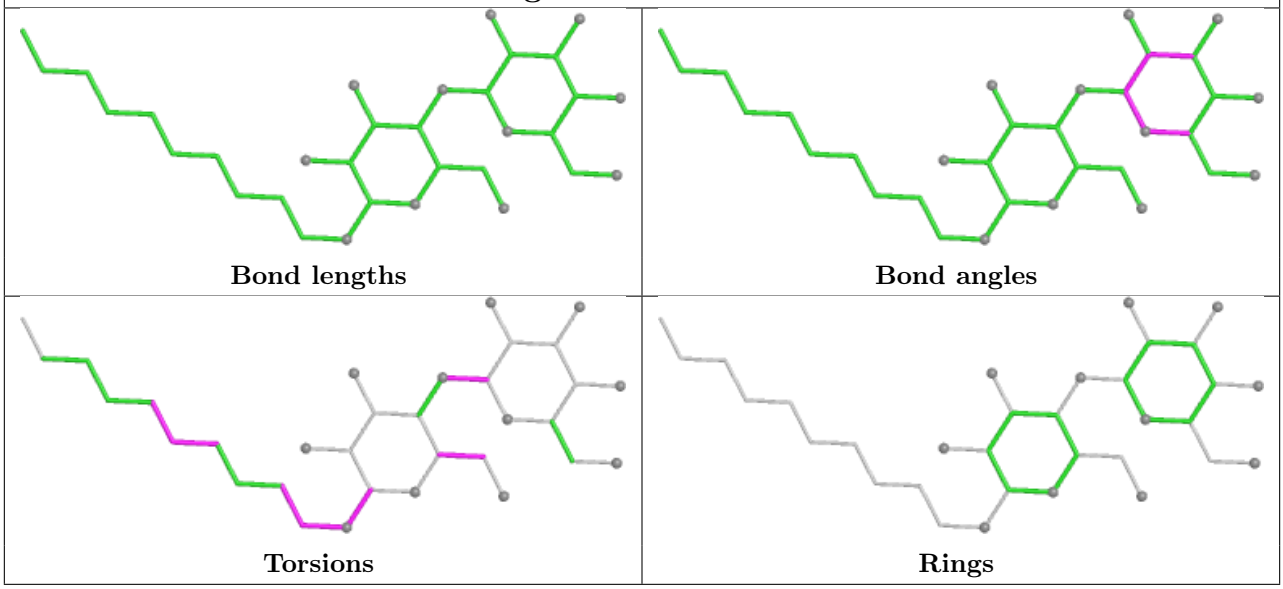
Ligand PGV N 104



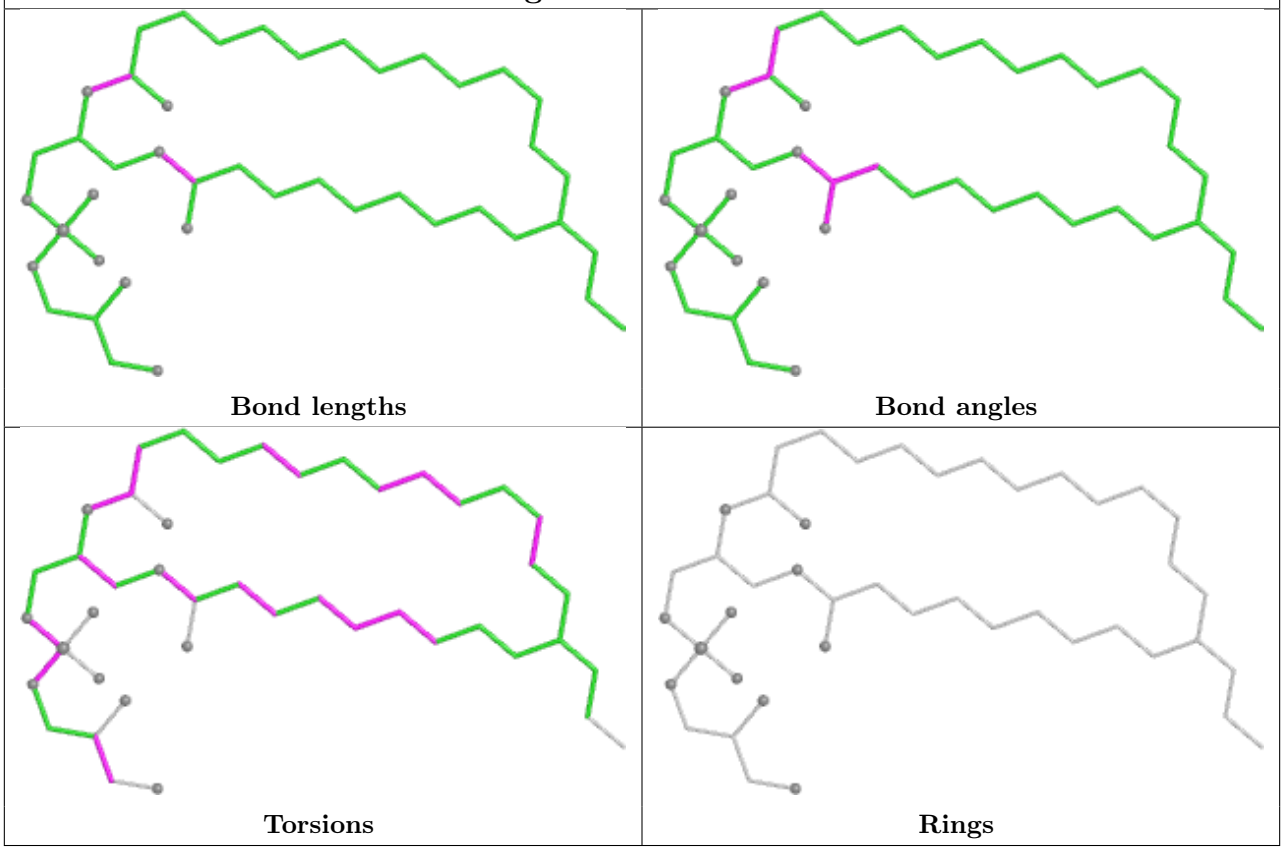
Ligand BCL I 103



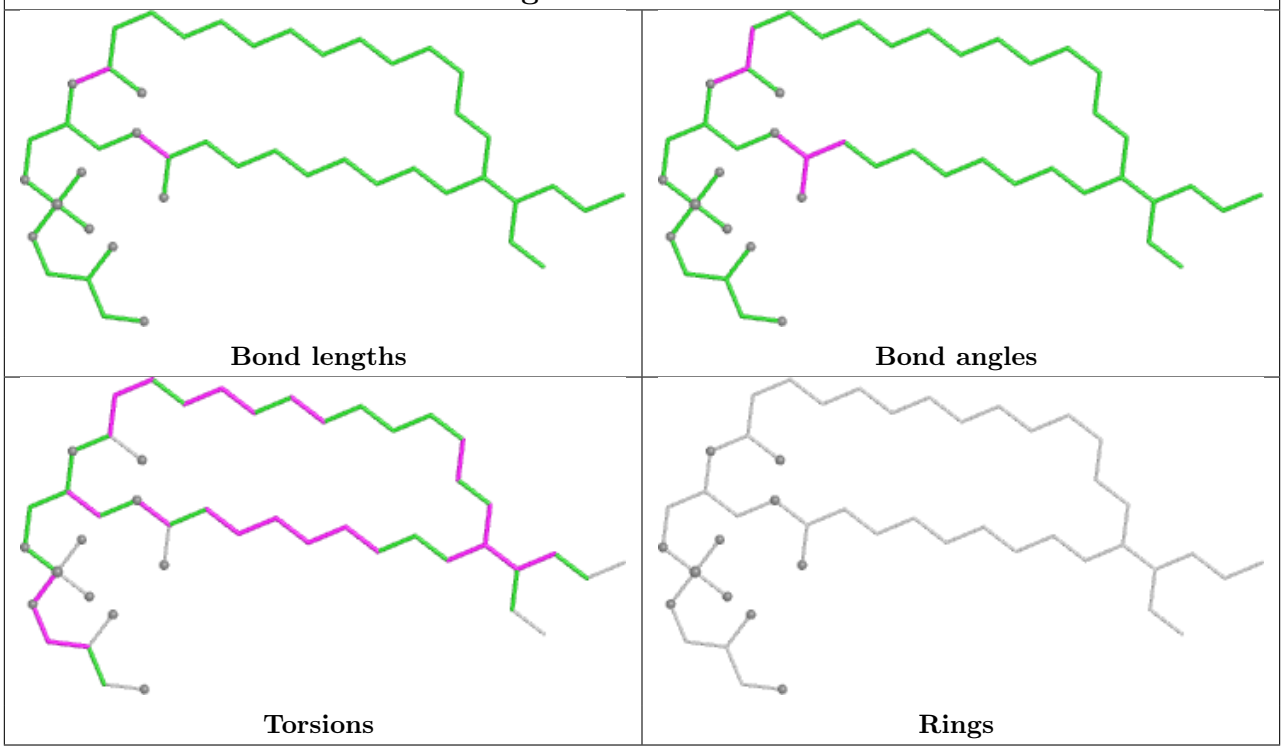
Ligand LMT F 102



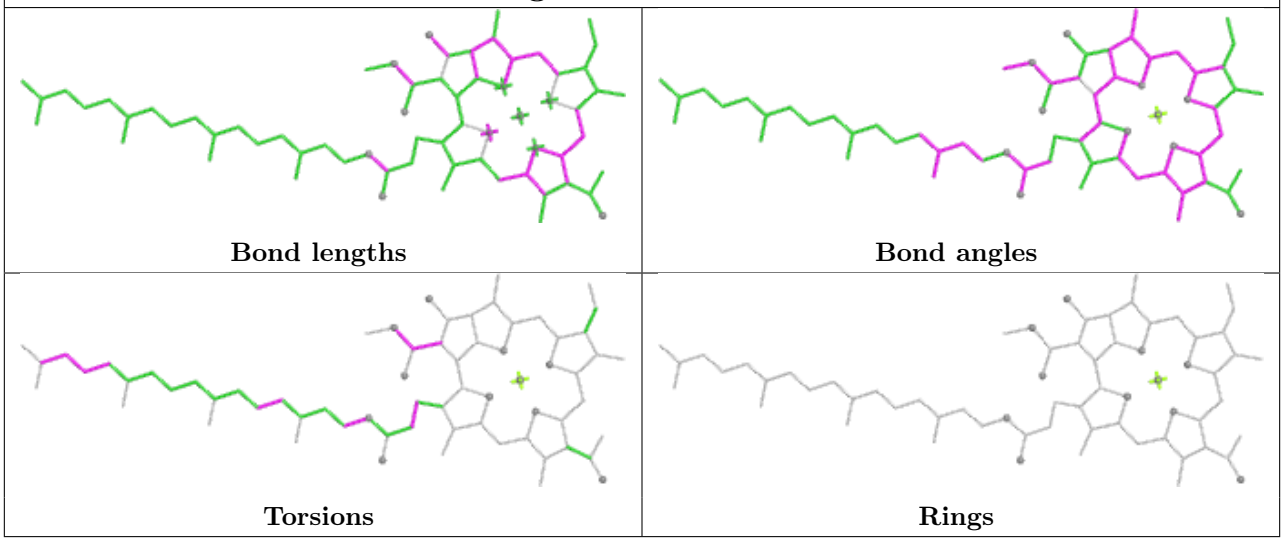
Ligand PGV Z 101

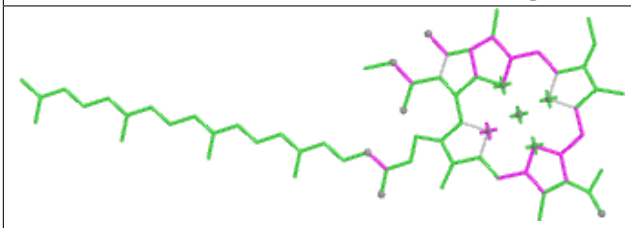
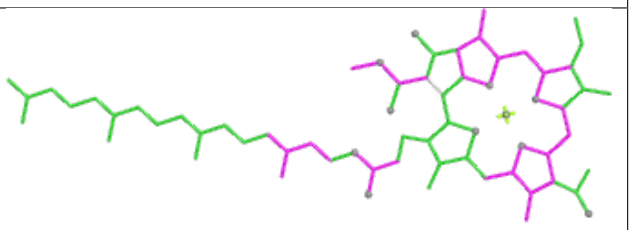
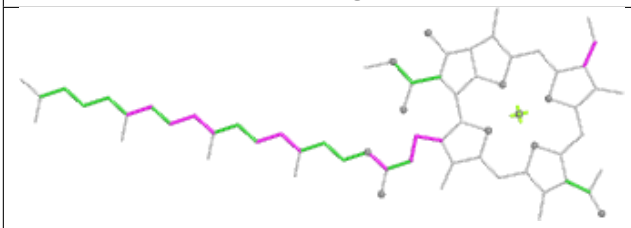
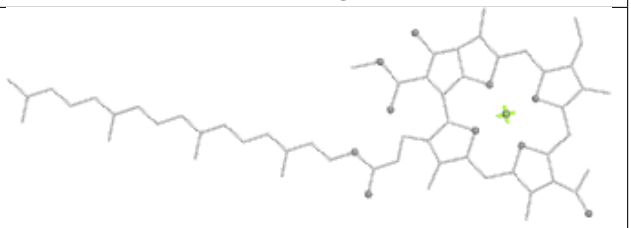


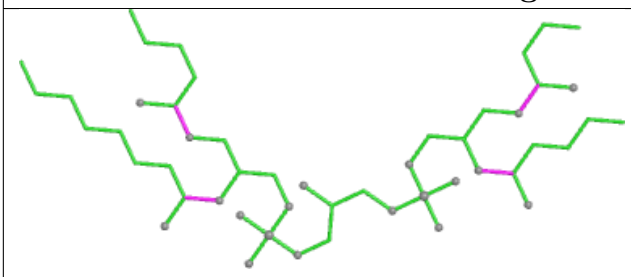
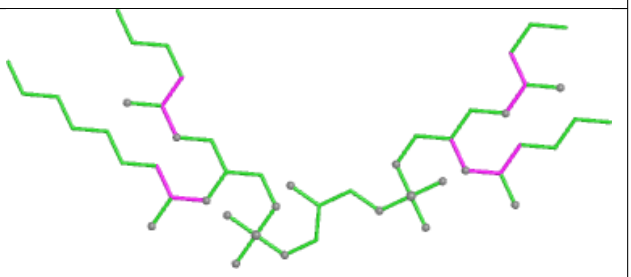
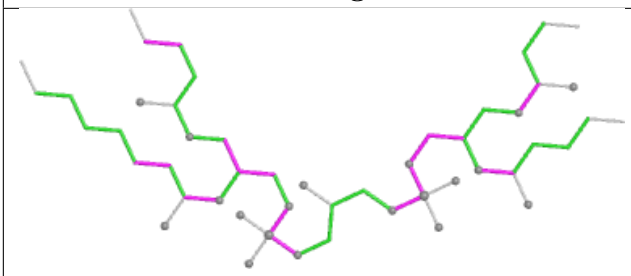
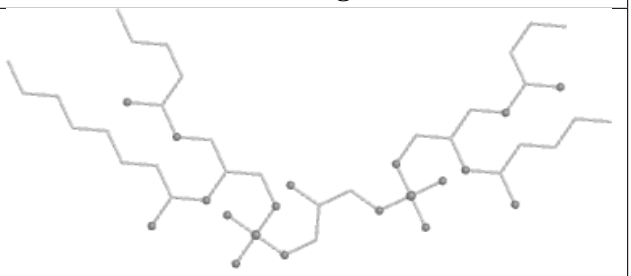
Ligand PGV G 101

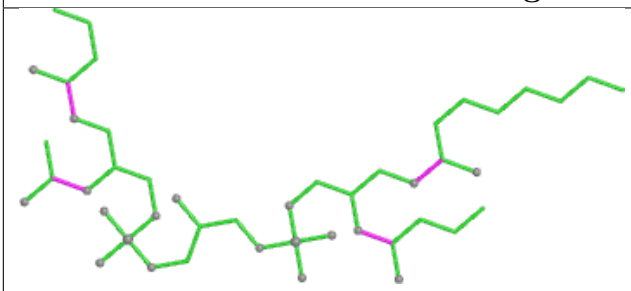
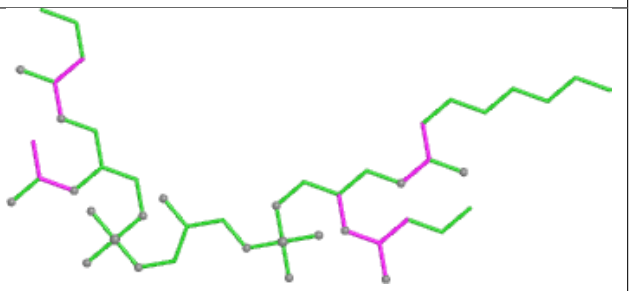
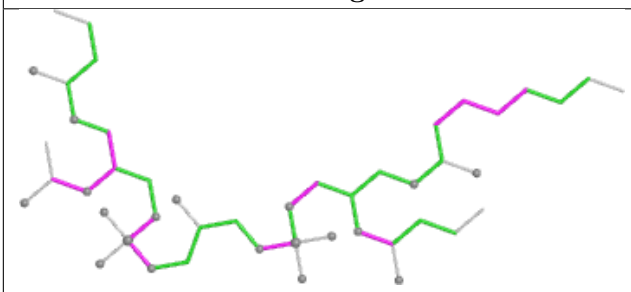
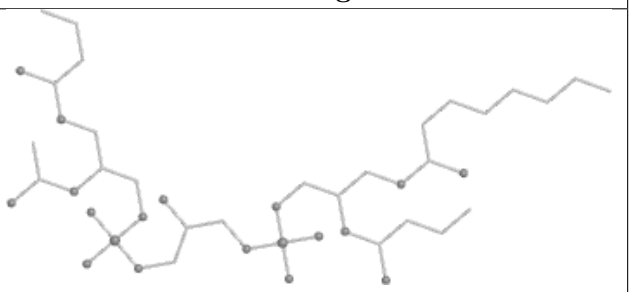


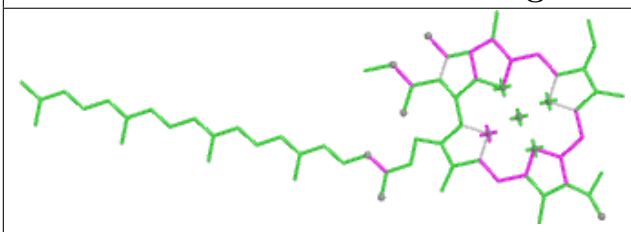
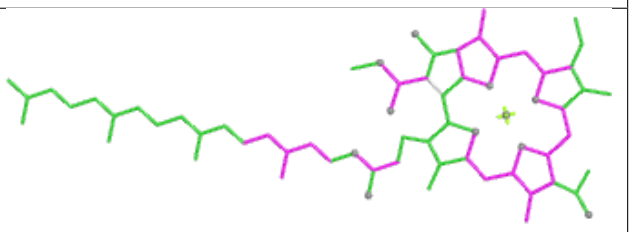
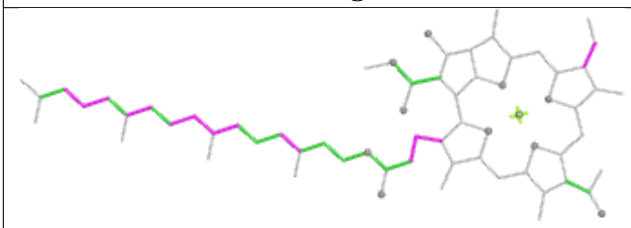
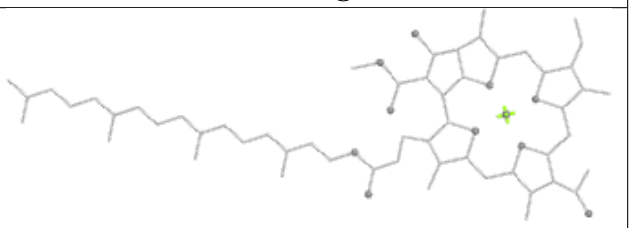
Ligand BCL L 302



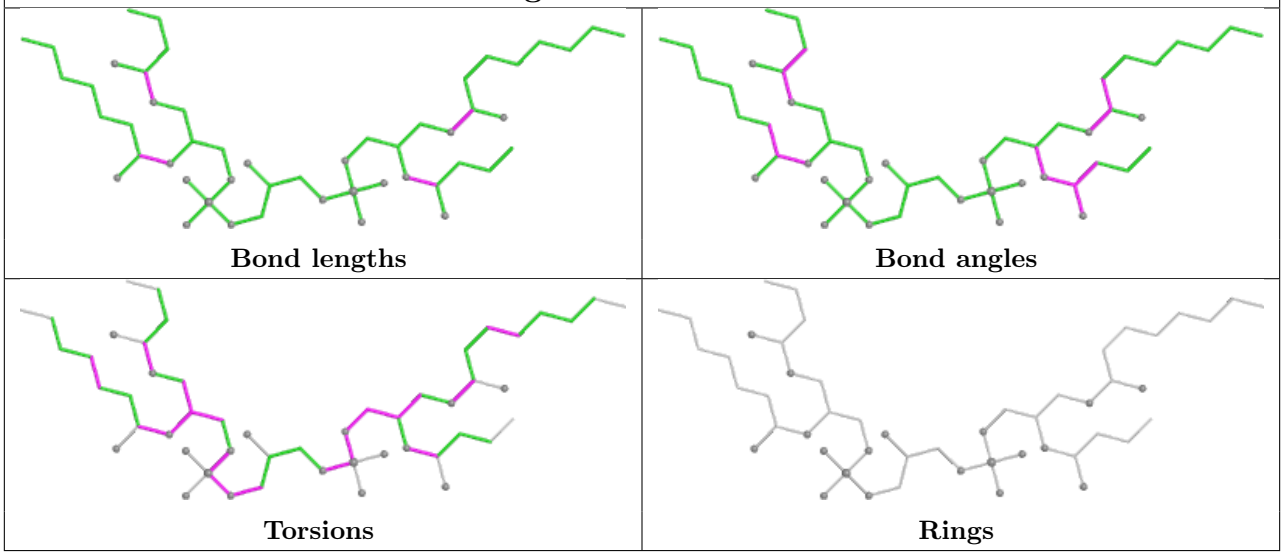
Ligand BCL Y 402	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CDL M 409	
 Bond lengths	 Bond angles
 Torsions	 Rings

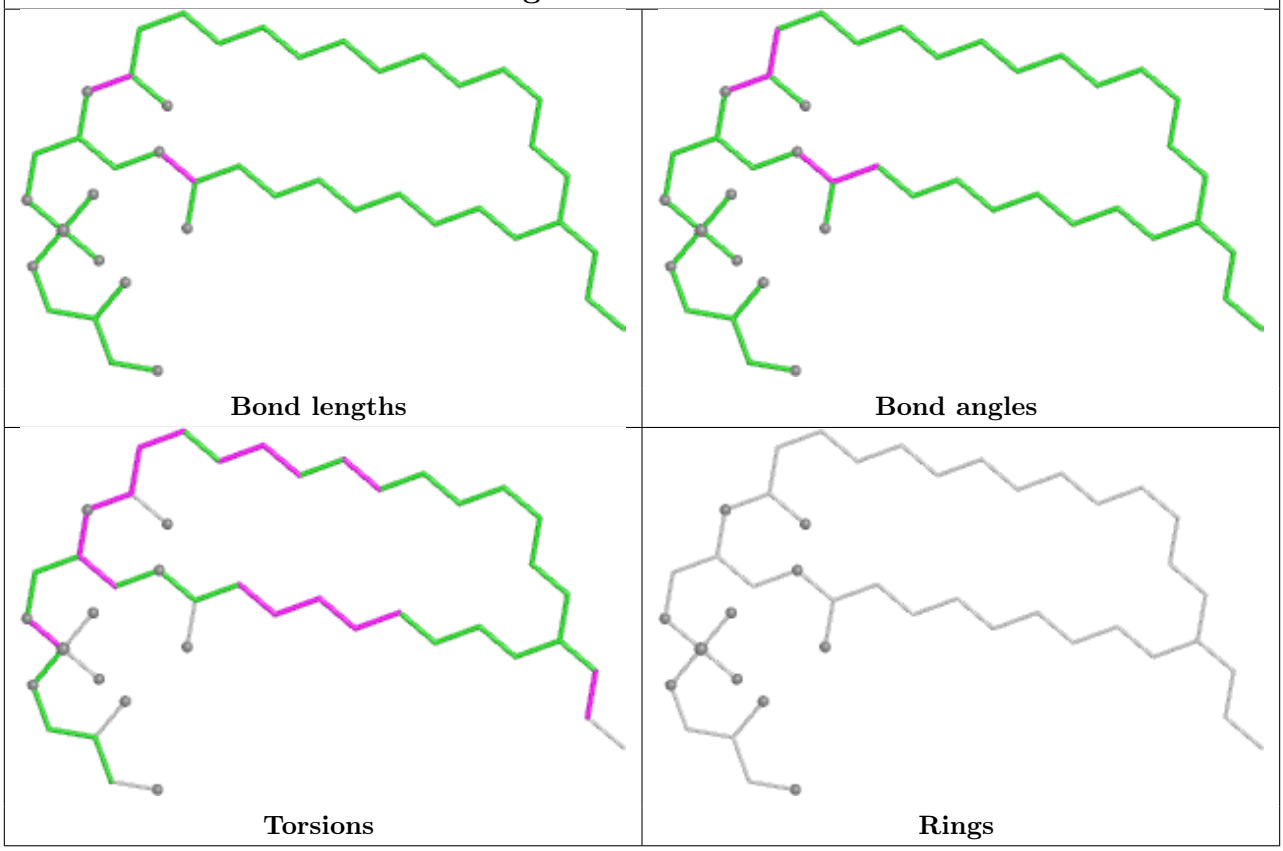
Ligand CDL U 102	
 Bond lengths	 Bond angles
 Torsions	 Rings

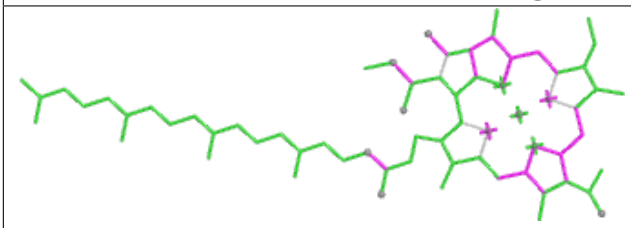
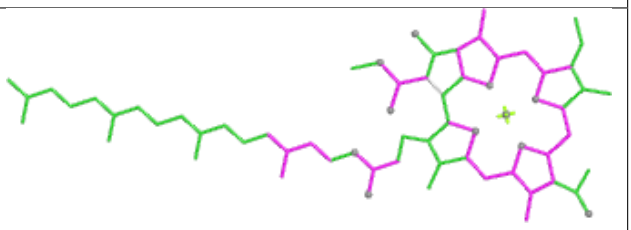
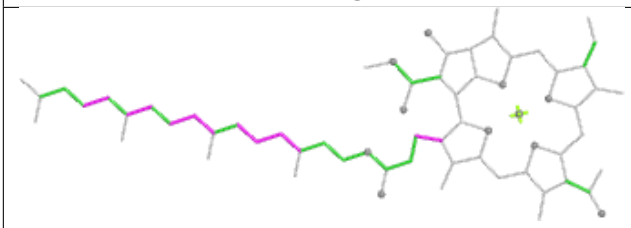
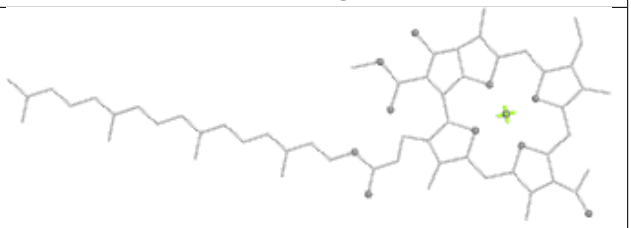
Ligand BCL F 103	
 Bond lengths	 Bond angles
 Torsions	 Rings

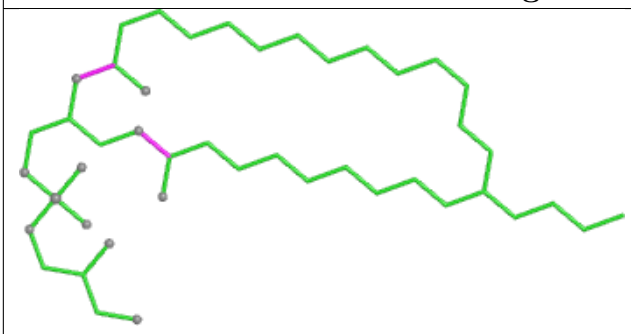
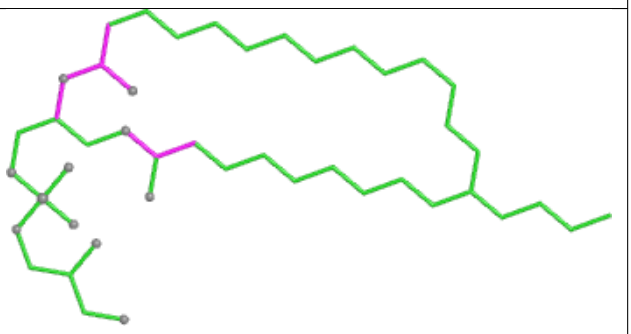
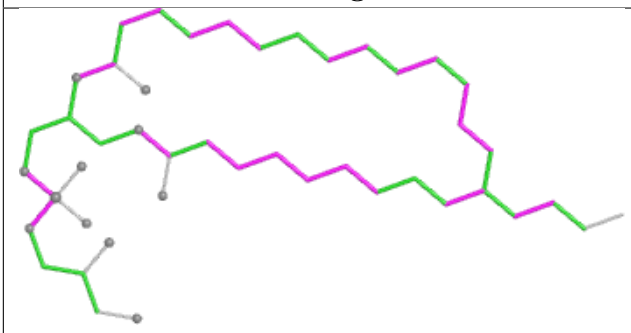
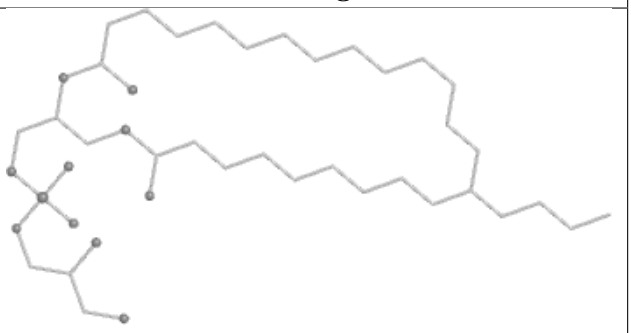
Ligand CDL U 101



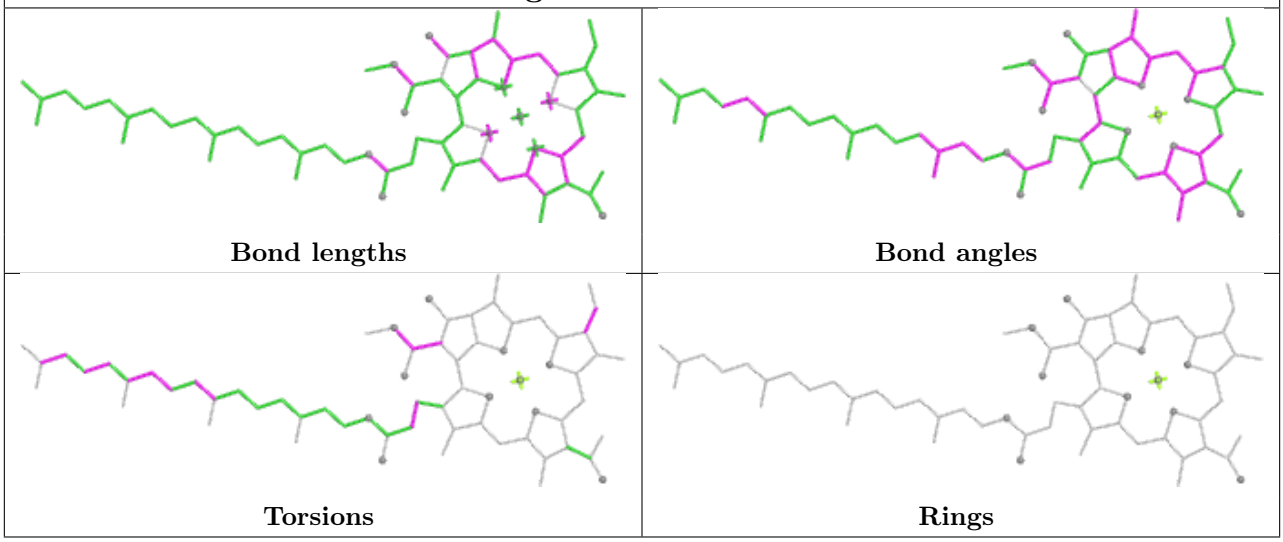
Ligand PGV T 102



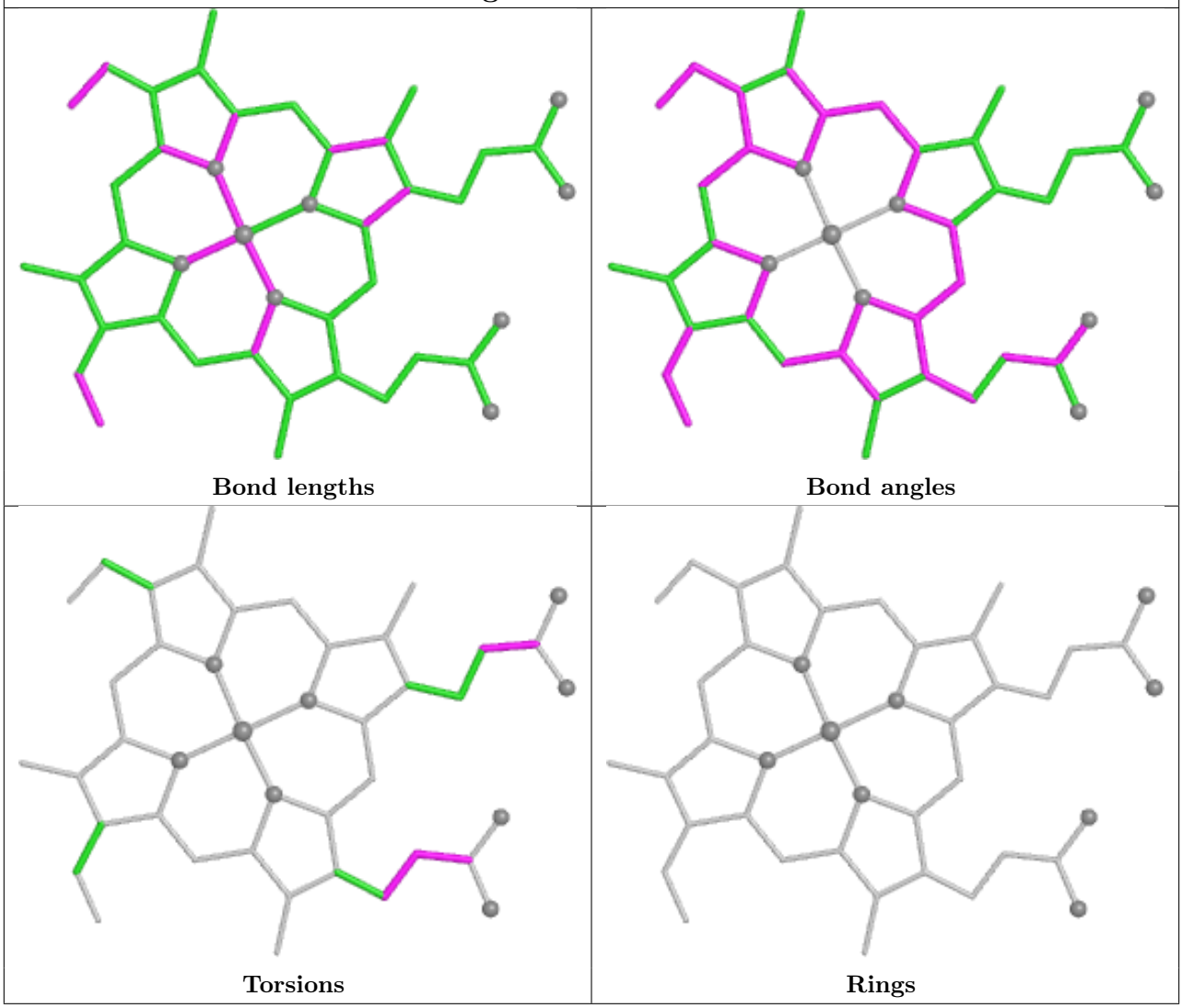
Ligand BCL 9 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

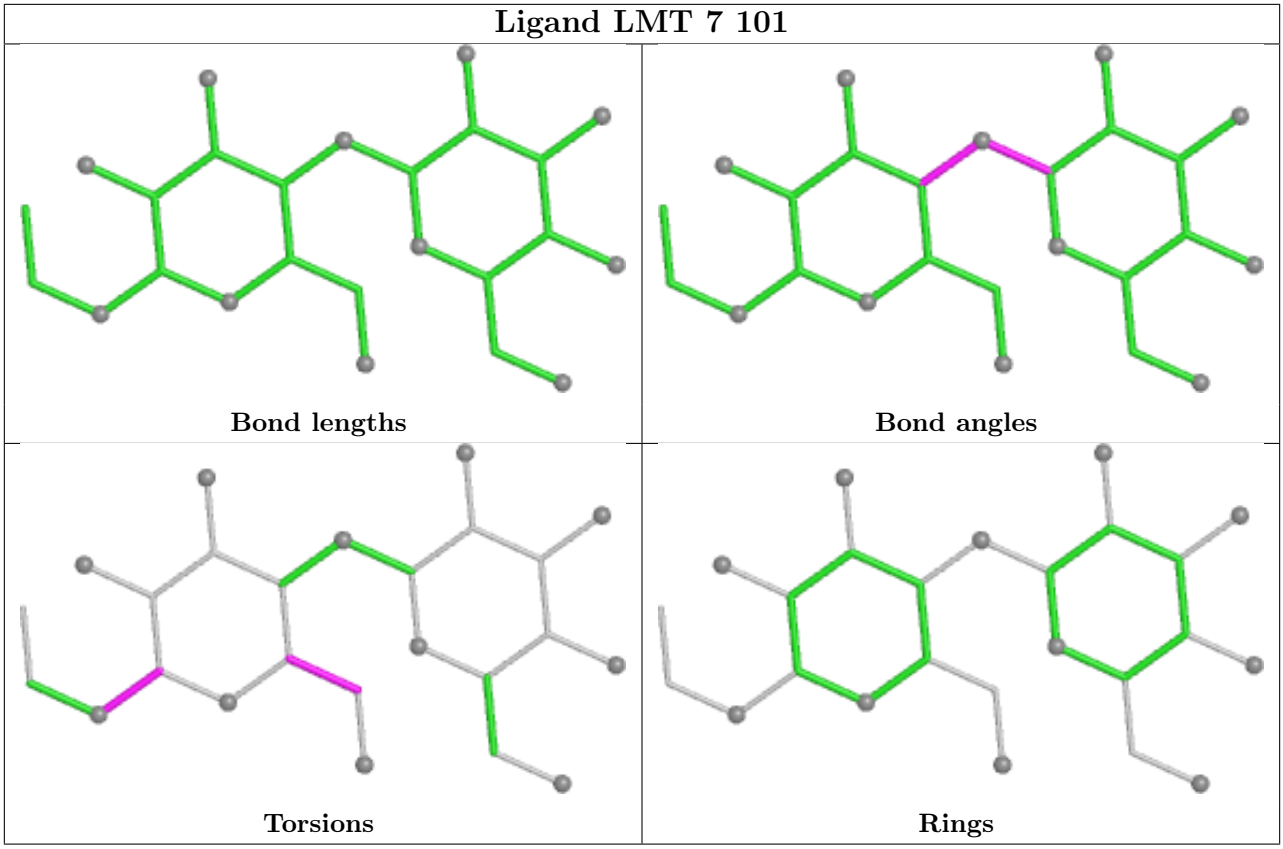
Ligand PGV P 102	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCL Y 401



Ligand HEC C 401





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.

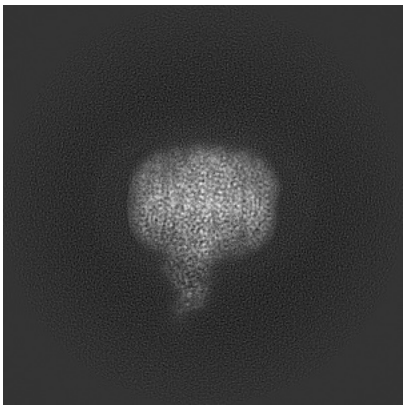
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-39836. These allow visual inspection of the internal detail of the map and identification of artifacts.

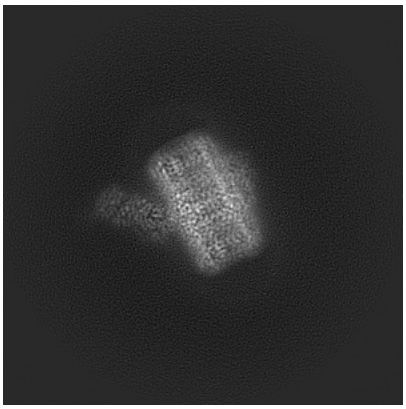
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

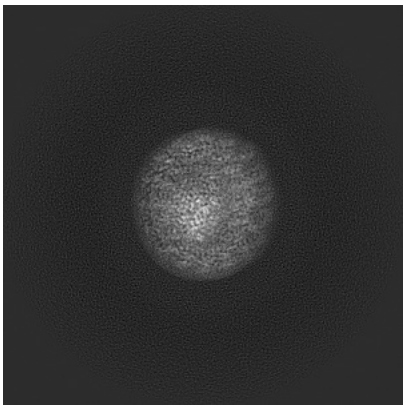
6.1.1 Primary map



X

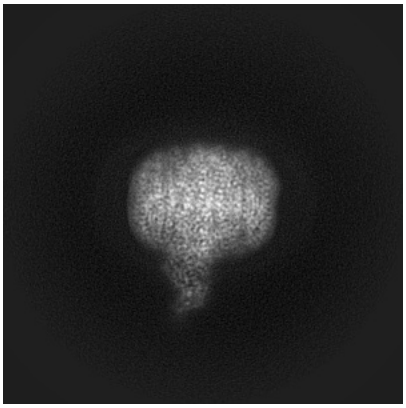


Y

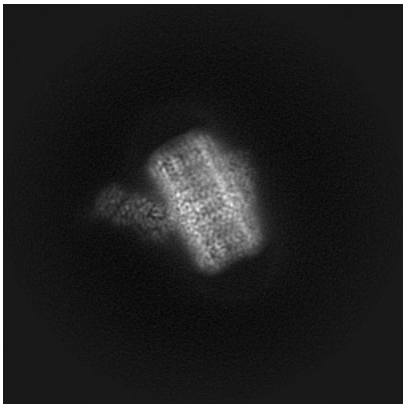


Z

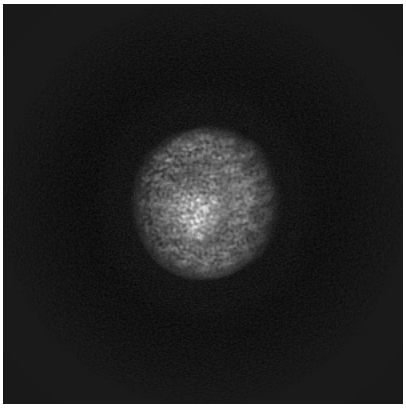
6.1.2 Raw map



X



Y

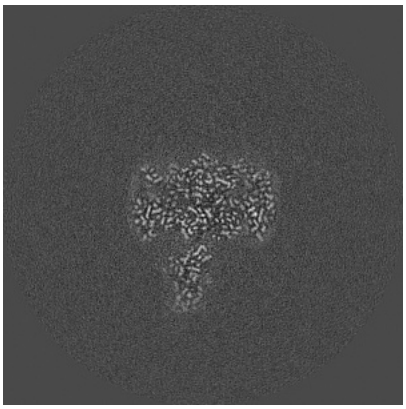


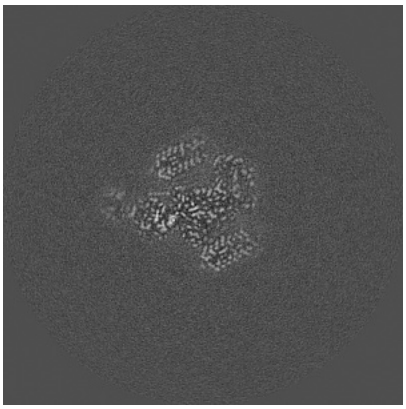
Z

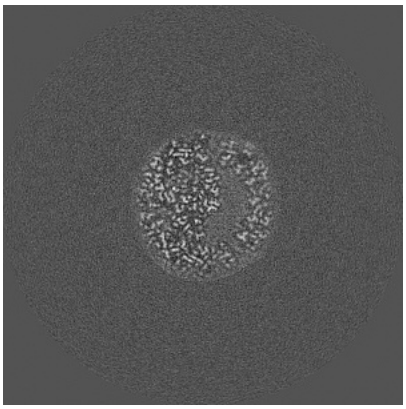
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

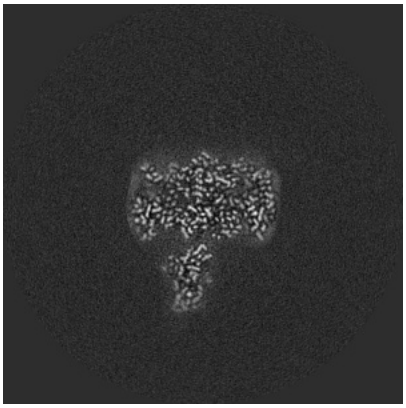
6.2.1 Primary map

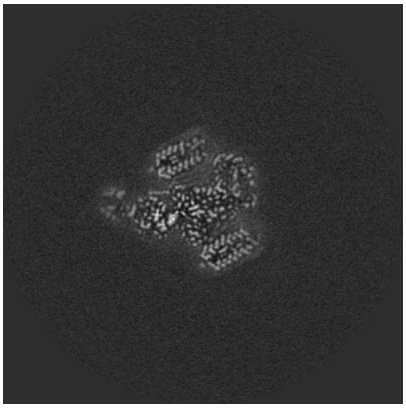

X Index: 200

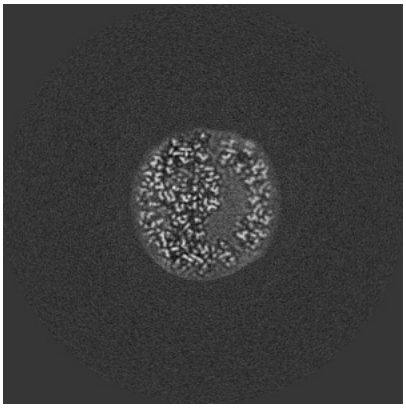

Y Index: 200


Z Index: 200

6.2.2 Raw map


X Index: 200

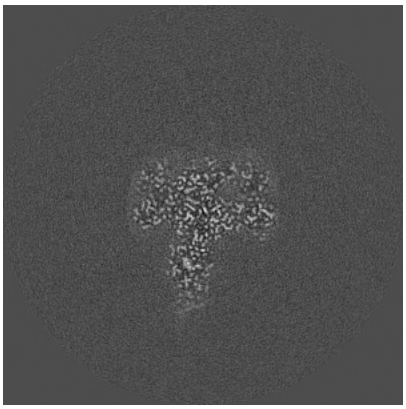

Y Index: 200

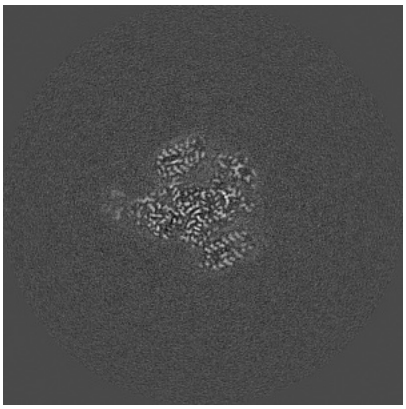

Z Index: 200

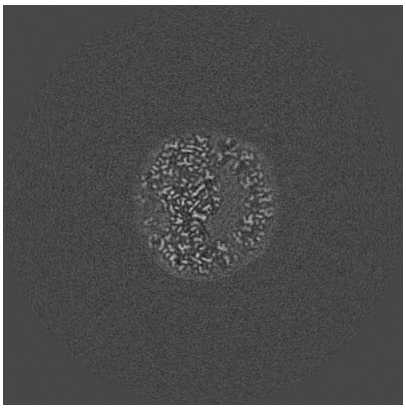
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

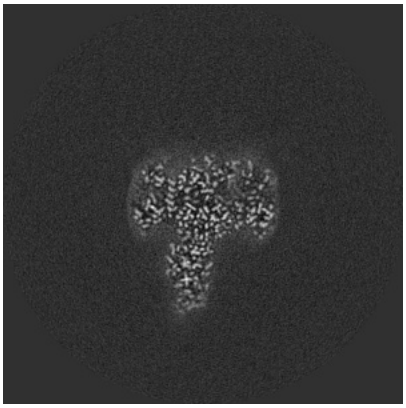
6.3.1 Primary map

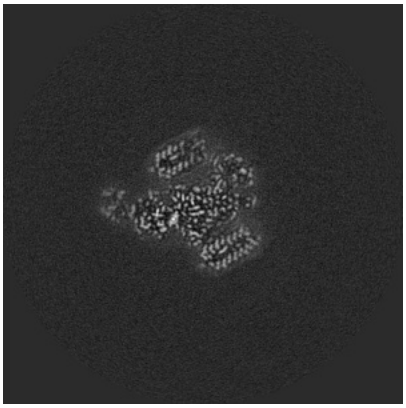

X Index: 193

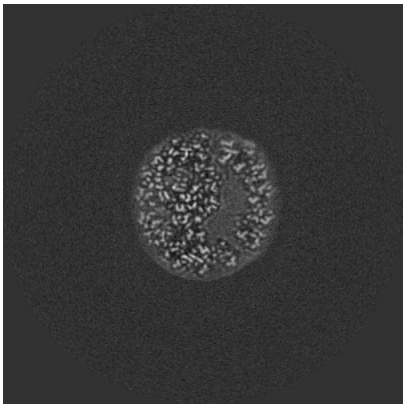

Y Index: 202


Z Index: 196

6.3.2 Raw map


X Index: 194

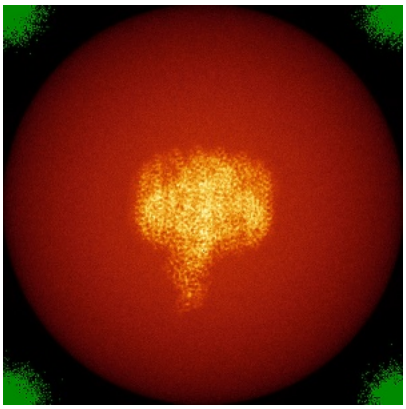

Y Index: 199

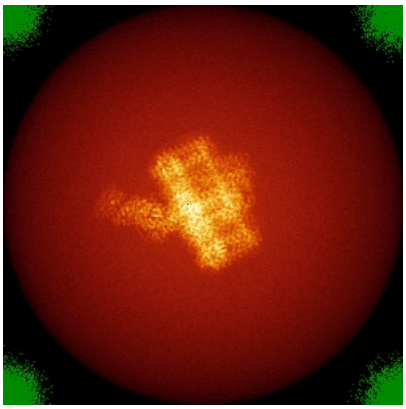

Z Index: 199

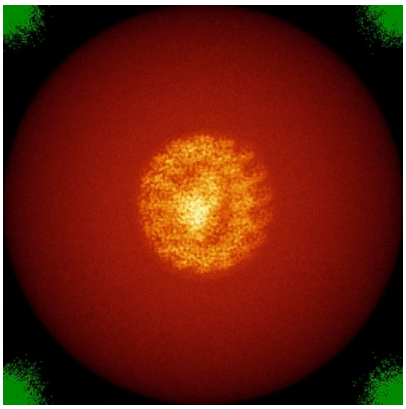
The images above show the largest variance slices of the map in three orthogonal directions.

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

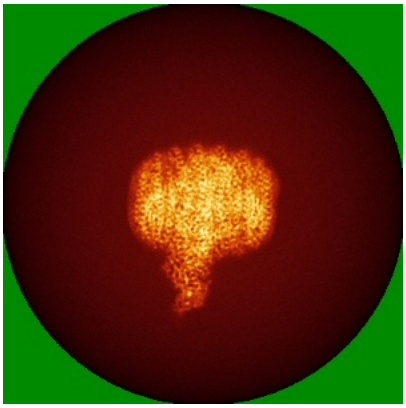
6.4.1 Primary map

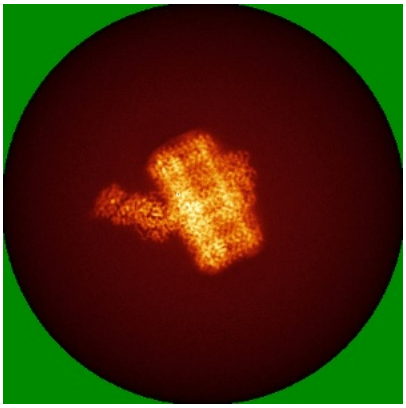

X

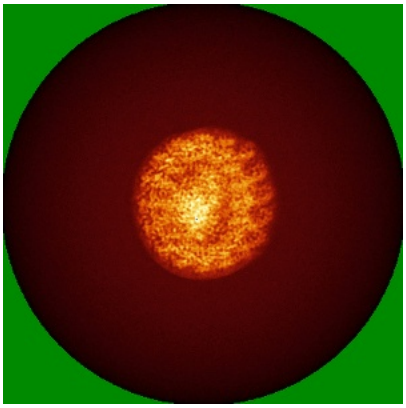

Y


Z

6.4.2 Raw map


X

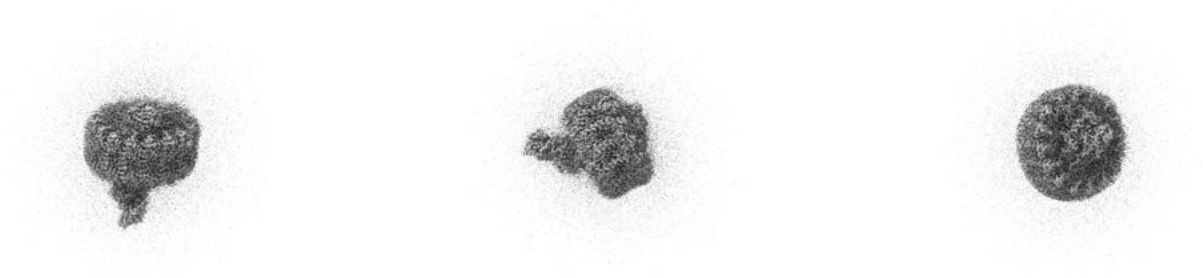

Y


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.03. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

X Y Z

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

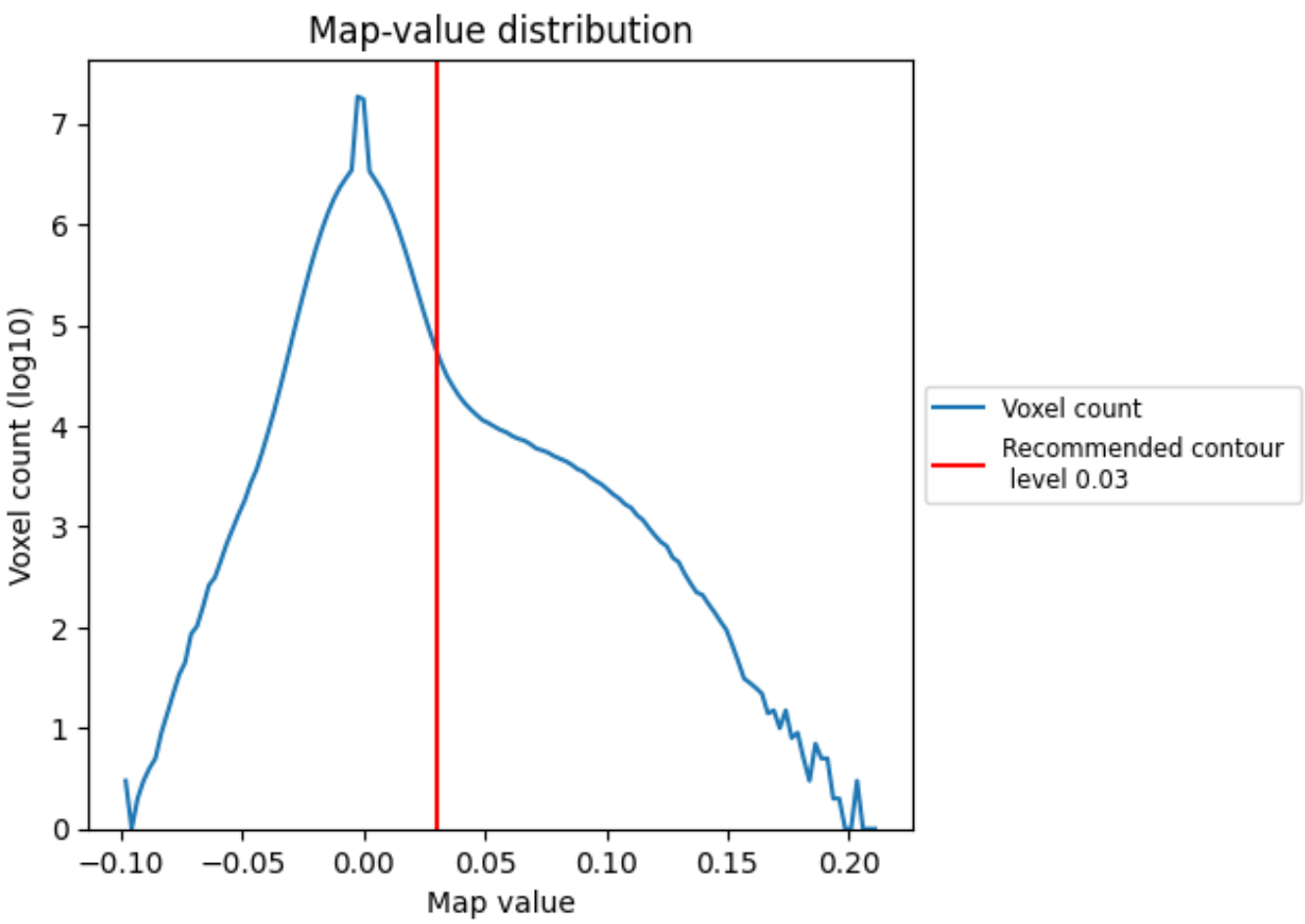
6.6 Mask visualisation (i)

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

7 Map analysis (i)

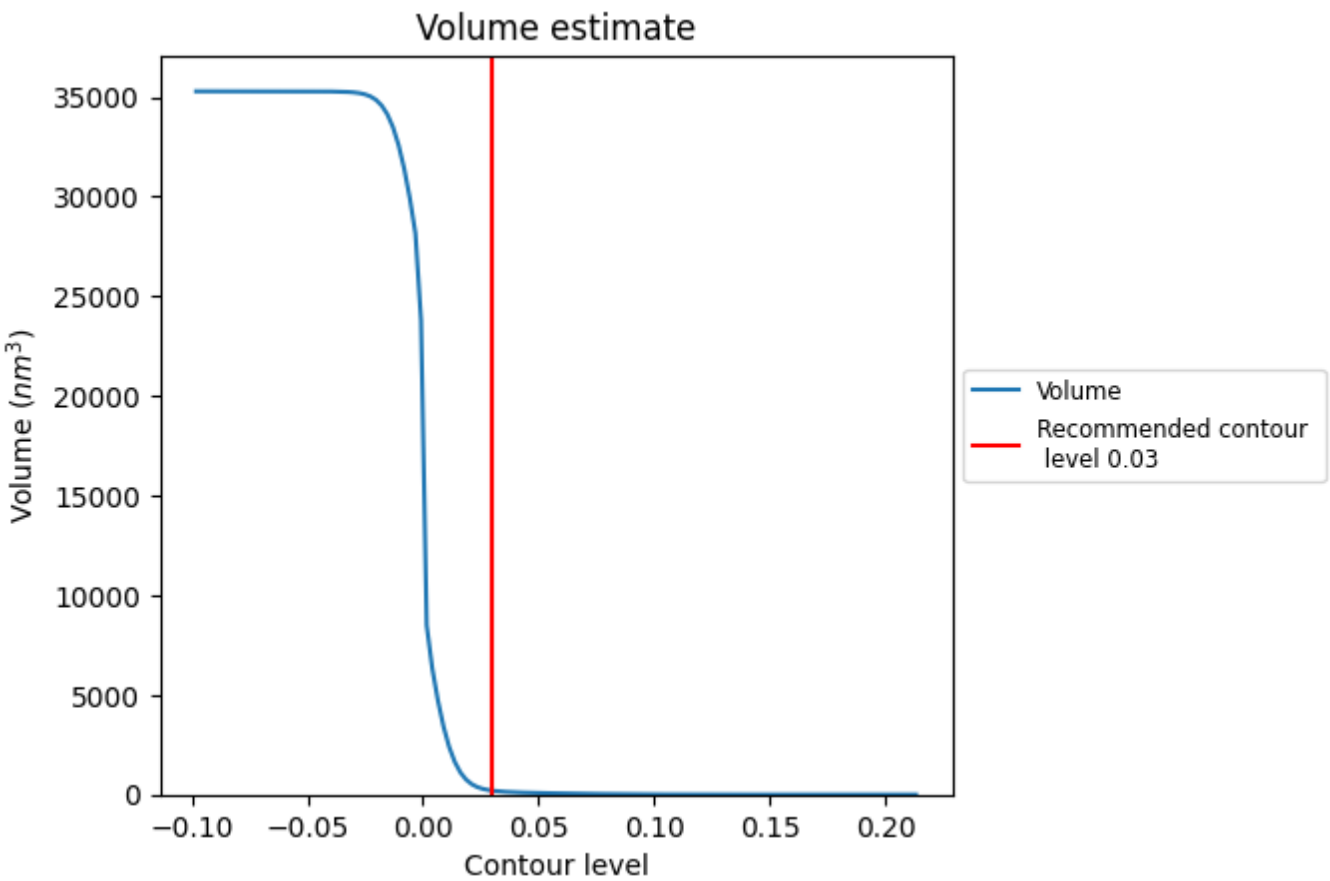
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

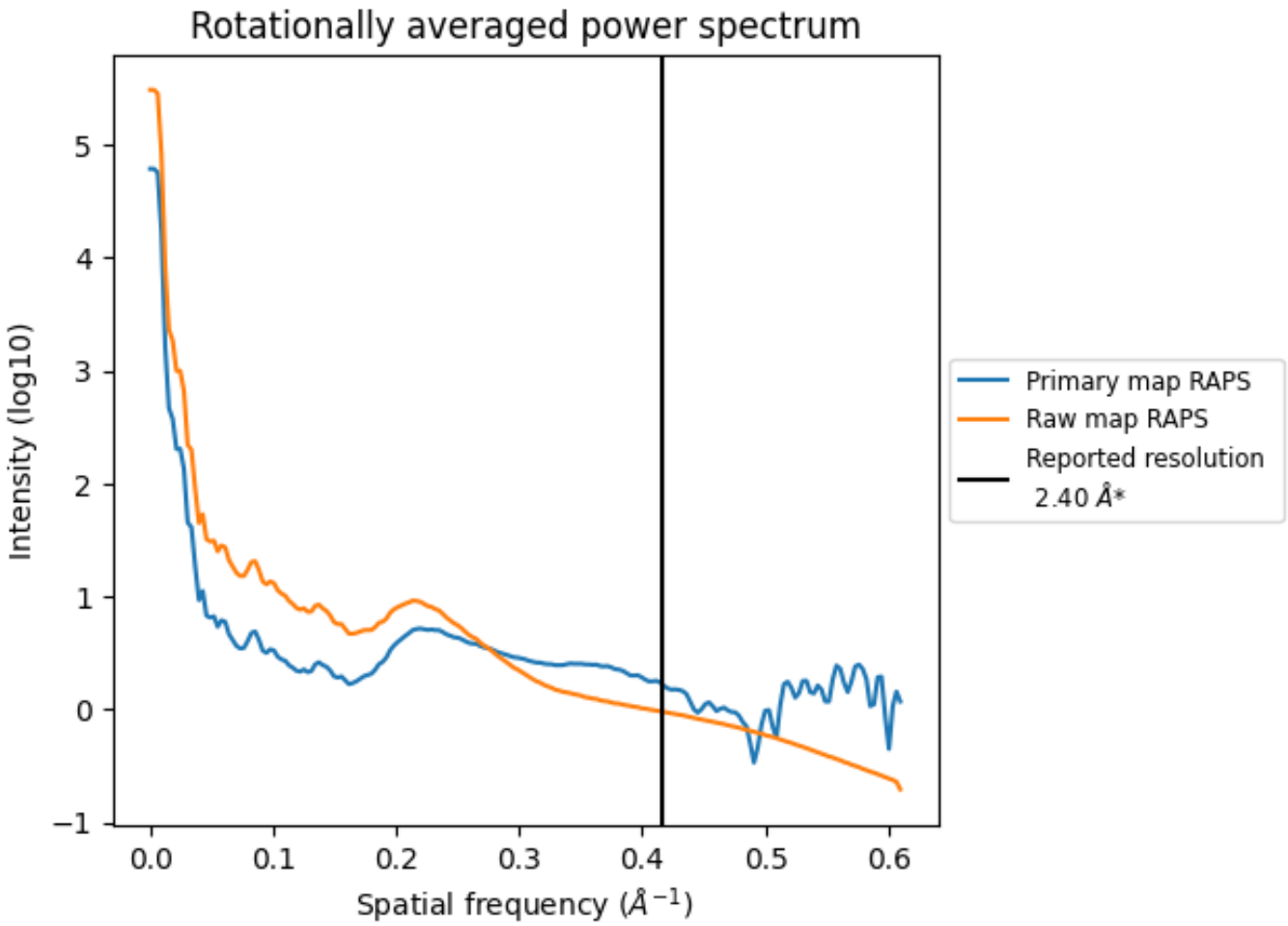
7.2 Volume estimate (i)



The volume at the recommended contour level is 197 nm^3; this corresponds to an approximate mass of 178 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)

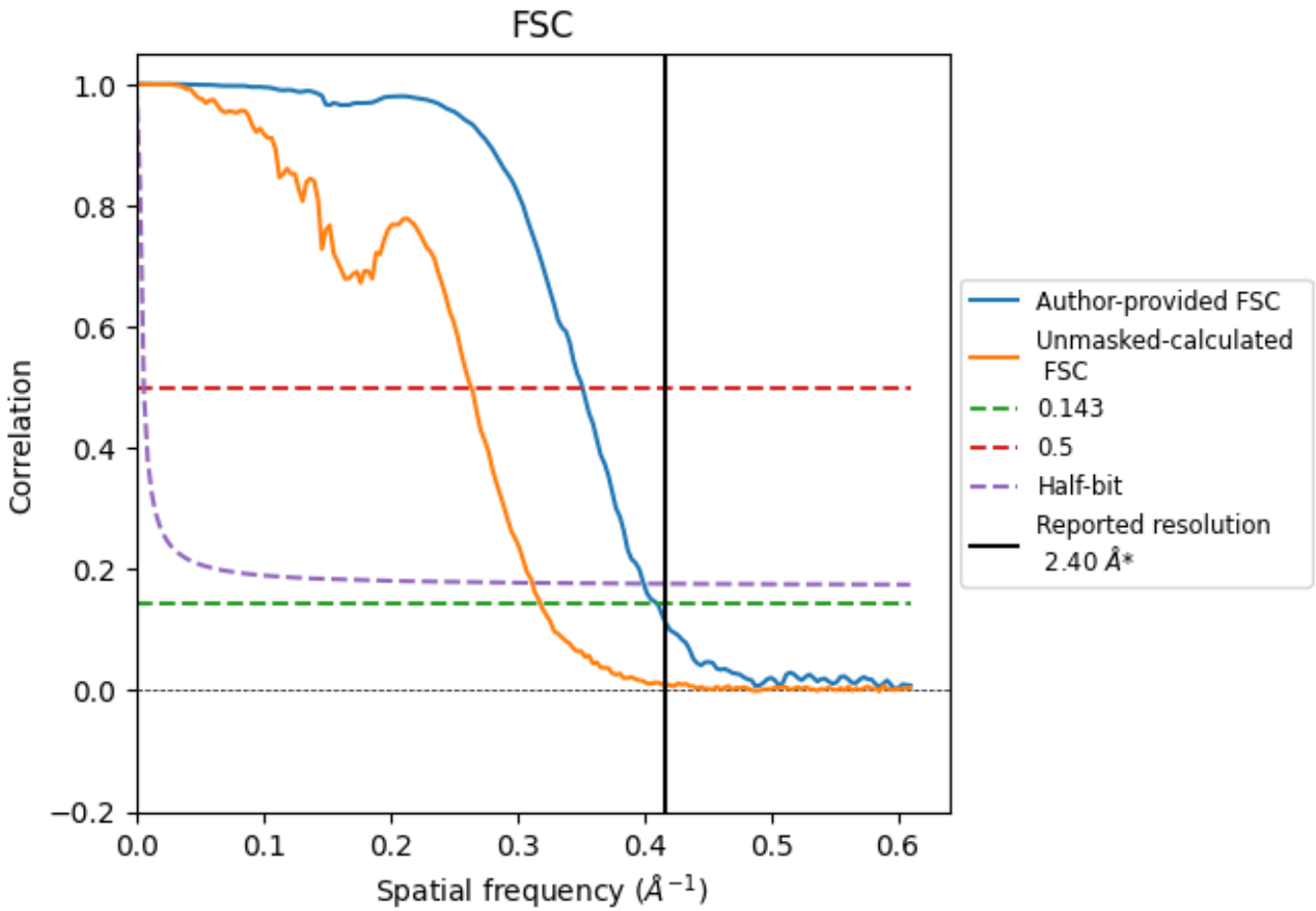


*Reported resolution corresponds to spatial frequency of 0.417 Å^{-1}

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 0.417 Å^{-1}

8.2 Resolution estimates (i)

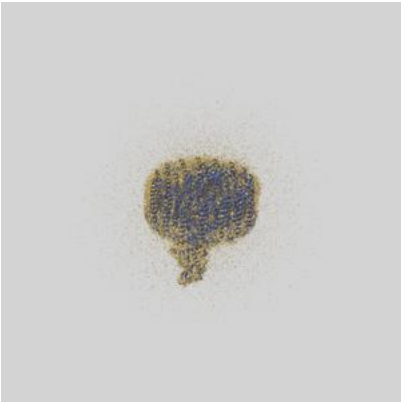
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.40	-	-
Author-provided FSC curve	2.44	2.84	2.50
Unmasked-calculated*	3.14	3.79	3.21

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.14 differs from the reported value 2.4 by more than 10 %

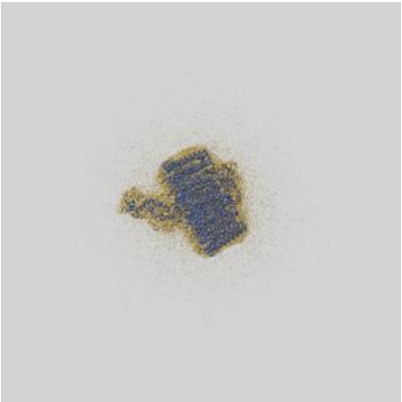
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-39836 and PDB model 8Z82. Per-residue inclusion information can be found in section 3 on page 24.

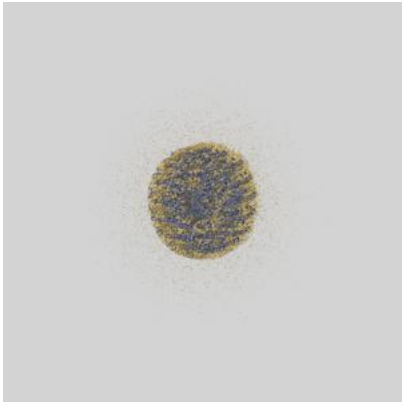
9.1 Map-model overlay (i)



X



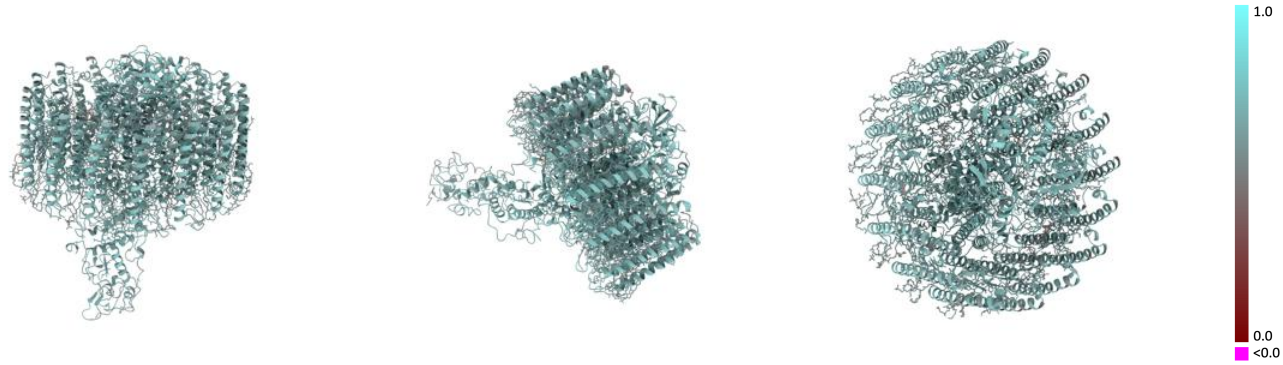
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.03 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.

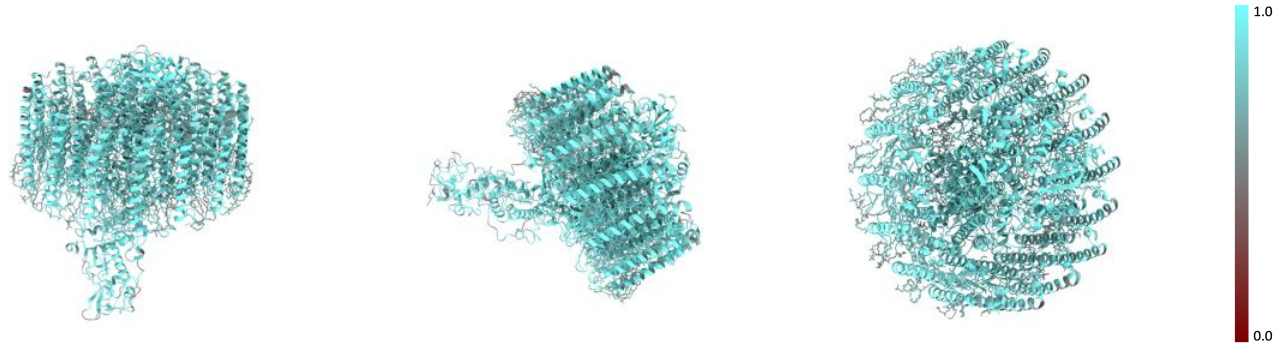
9.2 Q-score mapped to coordinate model (i)



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.

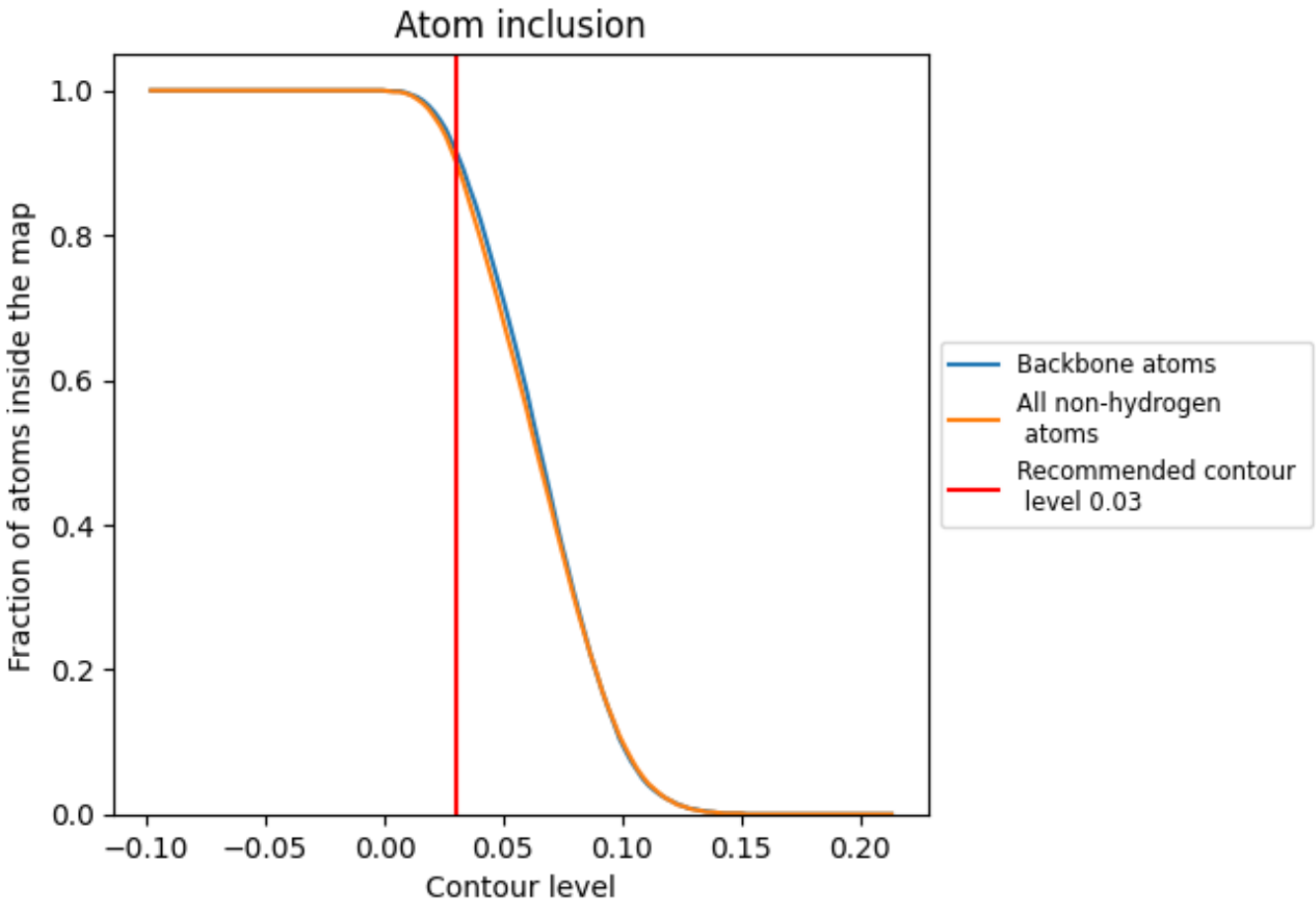
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.03).

9.4 Atom inclusion (i)



At the recommended contour level, 92% of all backbone atoms, 90% 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 (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9030	0.6520
0	0.8440	0.6300
1	0.9180	0.6560
2	0.8800	0.6360
3	0.9070	0.6430
4	0.8720	0.6330
5	0.8750	0.6290
6	0.8190	0.6160
7	0.9060	0.6340
8	0.8640	0.6330
9	0.9360	0.6570
A	0.9520	0.6650
B	0.9050	0.6510
C	0.9240	0.6680
D	0.9660	0.6790
E	0.9060	0.6520
F	0.9030	0.6540
G	0.8420	0.6310
H	0.9110	0.6530
I	0.9300	0.6530
J	0.8850	0.6540
K	0.9350	0.6540
L	0.9550	0.6810
M	0.9470	0.6800
N	0.8470	0.6270
O	0.8810	0.6370
P	0.8570	0.6330
Q	0.9250	0.6470
R	0.8920	0.6400
S	0.9480	0.6700
T	0.8590	0.6310
U	0.8830	0.6340
V	0.8440	0.6310
W	0.9400	0.6580
X	0.8540	0.6400

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Chain	Atom inclusion	Q-score
Y	0.9330	0.6570
Z	0.8400	0.6180
a	0.7760	0.5860