



wwPDB EM Validation Summary Report ⓘ

Mar 5, 2026 – 07:50 AM UTC

PDB ID : 8WB4 / pdb_00008wb4
EMDB ID : EMD-37414
Title : Structure of PSII-ACPII supercomplex from cryptophyte algae
Authors : Li, X.Y.; Mao, Z.Y.; Shen, J.R.; Han, G.Y.
Deposited on : 2023-09-08
Resolution : 2.47 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ 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 ⓘ](#)) were used in the production of this report:

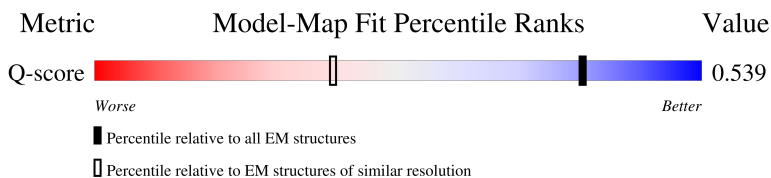
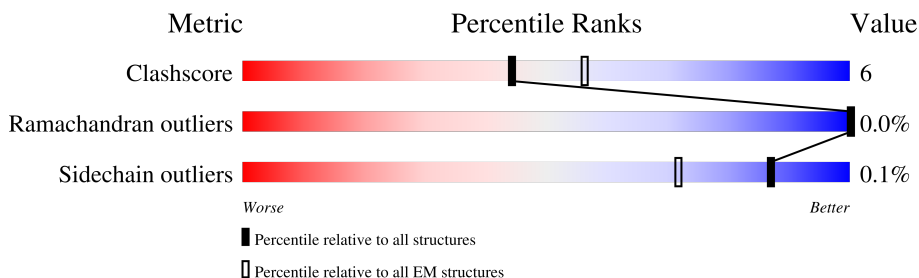
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 2.47 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	6086 (1.98 - 2.97)

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 $\leq 5\%$. 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	M	115	
1	m	115	
2	1	235	
2	7	235	

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Mol	Chain	Length	Quality of chain
3	2	217	
3	8	217	
4	3	222	
4	9	222	
5	0	226	
5	4	226	
6	5	218	
6	p	218	
7	6	220	
7	P	220	
8	A	360	
8	a	360	
9	D	351	
9	d	351	
10	E	84	
10	e	84	
11	F	42	
11	f	42	
12	H	67	
12	h	67	
13	I	38	
13	i	38	
14	J	39	
14	j	39	
15	K	45	

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Mol	Chain	Length	Quality of chain
15	k	45	
16	O	330	
16	o	330	
17	Q	21	
17	q	21	
18	R	26	
18	r	26	
19	S	285	
19	s	285	
20	T	32	
20	t	32	
21	U	150	
21	u	150	
22	V	163	
22	v	163	
23	X	39	
23	x	39	
24	Y	34	
24	y	34	
25	Z	62	
25	z	62	
26	B	509	
26	b	509	
27	C	461	
27	c	461	

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Mol	Chain	Length	Quality of chain
28	G	64	
28	g	64	
29	L	38	
29	l	38	
30	W	114	
30	w	114	

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
32	CLA	0	601	X	-	-	-
32	CLA	0	602	X	-	-	-
32	CLA	0	603	X	-	-	-
32	CLA	0	604	X	-	-	-
32	CLA	0	605	X	-	-	-
32	CLA	0	606	X	-	-	-
32	CLA	0	607	X	-	-	-
32	CLA	0	608	X	-	-	-
32	CLA	0	609	X	-	-	-
32	CLA	0	611	X	-	-	-
32	CLA	0	612	X	-	-	-
32	CLA	0	613	X	-	-	-
32	CLA	1	601	X	-	-	-
32	CLA	1	602	X	-	-	-
32	CLA	1	603	X	-	-	-
32	CLA	1	604	X	-	-	-
32	CLA	1	605	X	-	-	-
32	CLA	1	606	X	-	-	-
32	CLA	1	607	X	-	-	-
32	CLA	1	608	X	-	-	-
32	CLA	1	609	X	-	-	-
32	CLA	1	611	X	-	-	-
32	CLA	1	612	X	-	-	-
32	CLA	1	613	X	-	-	-
32	CLA	2	601	X	-	-	-
32	CLA	2	602	X	-	-	-
32	CLA	2	603	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
32	CLA	2	604	X	-	-	-
32	CLA	2	605	X	-	-	-
32	CLA	2	606	X	-	-	-
32	CLA	2	607	X	-	-	-
32	CLA	2	608	X	-	-	-
32	CLA	2	609	X	-	-	-
32	CLA	2	611	X	-	-	-
32	CLA	2	612	X	-	-	-
32	CLA	3	601	X	-	-	-
32	CLA	3	602	X	-	-	-
32	CLA	3	603	X	-	-	-
32	CLA	3	604	X	-	-	-
32	CLA	3	605	X	-	-	-
32	CLA	3	606	X	-	-	-
32	CLA	3	607	X	-	-	-
32	CLA	3	608	X	-	-	-
32	CLA	3	609	X	-	-	-
32	CLA	3	610	X	-	-	-
32	CLA	3	611	X	-	-	-
32	CLA	4	601	X	-	-	-
32	CLA	4	602	X	-	-	-
32	CLA	4	603	X	-	-	-
32	CLA	4	604	X	-	-	-
32	CLA	4	605	X	-	-	-
32	CLA	4	606	X	-	-	-
32	CLA	4	607	X	-	-	-
32	CLA	4	608	X	-	-	-
32	CLA	4	609	X	-	-	-
32	CLA	4	611	X	-	-	-
32	CLA	4	612	X	-	-	-
32	CLA	4	613	X	-	-	-
32	CLA	5	302	X	-	-	-
32	CLA	5	303	X	-	-	-
32	CLA	5	304	X	-	-	-
32	CLA	5	305	X	-	-	-
32	CLA	5	306	X	-	-	-
32	CLA	5	307	X	-	-	-
32	CLA	5	308	X	-	-	-
32	CLA	5	309	X	-	-	-
32	CLA	5	310	X	-	-	-
32	CLA	5	312	X	-	-	-
32	CLA	5	313	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
32	CLA	6	601	X	-	-	-
32	CLA	6	602	X	-	-	-
32	CLA	6	603	X	-	-	-
32	CLA	6	604	X	-	-	-
32	CLA	6	606	X	-	-	-
32	CLA	6	607	X	-	-	-
32	CLA	6	608	X	-	-	-
32	CLA	6	610	X	-	-	-
32	CLA	6	611	X	-	-	-
32	CLA	7	601	X	-	-	-
32	CLA	7	602	X	-	-	-
32	CLA	7	603	X	-	-	-
32	CLA	7	604	X	-	-	-
32	CLA	7	605	X	-	-	-
32	CLA	7	606	X	-	-	-
32	CLA	7	607	X	-	-	-
32	CLA	7	608	X	-	-	-
32	CLA	7	609	X	-	-	-
32	CLA	7	611	X	-	-	-
32	CLA	7	612	X	-	-	-
32	CLA	7	613	X	-	-	-
32	CLA	8	601	X	-	-	-
32	CLA	8	602	X	-	-	-
32	CLA	8	603	X	-	-	-
32	CLA	8	604	X	-	-	-
32	CLA	8	605	X	-	-	-
32	CLA	8	606	X	-	-	-
32	CLA	8	607	X	-	-	-
32	CLA	8	608	X	-	-	-
32	CLA	8	609	X	-	-	-
32	CLA	8	611	X	-	-	-
32	CLA	8	612	X	-	-	-
32	CLA	9	601	X	-	-	-
32	CLA	9	602	X	-	-	-
32	CLA	9	603	X	-	-	-
32	CLA	9	604	X	-	-	-
32	CLA	9	605	X	-	-	-
32	CLA	9	606	X	-	-	-
32	CLA	9	607	X	-	-	-
32	CLA	9	608	X	-	-	-
32	CLA	9	609	X	-	-	-
32	CLA	9	610	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
32	CLA	9	611	X	-	-	-
32	CLA	A	602	X	-	-	-
32	CLA	A	603	X	-	-	-
32	CLA	A	605	X	-	-	-
32	CLA	B	602	X	-	-	-
32	CLA	B	603	X	-	-	-
32	CLA	B	604	X	-	-	-
32	CLA	B	605	X	-	-	-
32	CLA	B	606	X	-	-	-
32	CLA	B	607	X	-	-	-
32	CLA	B	608	X	-	-	-
32	CLA	B	609	X	-	-	-
32	CLA	B	610	X	-	-	-
32	CLA	B	611	X	-	-	-
32	CLA	B	612	X	-	-	-
32	CLA	B	613	X	-	-	-
32	CLA	B	614	X	-	-	-
32	CLA	B	615	X	-	-	-
32	CLA	B	616	X	-	-	-
32	CLA	B	617	X	-	-	-
32	CLA	C	501	X	-	-	-
32	CLA	C	502	X	-	-	-
32	CLA	C	503	X	-	-	-
32	CLA	C	504	X	-	-	-
32	CLA	C	505	X	-	-	-
32	CLA	C	506	X	-	-	-
32	CLA	C	507	X	-	-	-
32	CLA	C	508	X	-	-	-
32	CLA	C	509	X	-	-	-
32	CLA	C	510	X	-	-	-
32	CLA	C	511	X	-	-	-
32	CLA	C	512	X	-	-	-
32	CLA	C	513	X	-	-	-
32	CLA	D	401	X	-	-	-
32	CLA	D	403	X	-	-	-
32	CLA	D	404	X	-	-	-
32	CLA	G	101	X	-	-	-
32	CLA	P	601	X	-	-	-
32	CLA	P	602	X	-	-	-
32	CLA	P	603	X	-	-	-
32	CLA	P	604	X	-	-	-
32	CLA	P	606	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
32	CLA	P	607	X	-	-	-
32	CLA	P	608	X	-	-	-
32	CLA	P	610	X	-	-	-
32	CLA	P	611	X	-	-	-
32	CLA	S	302	X	-	-	-
32	CLA	S	303	X	-	-	-
32	CLA	a	405	X	-	-	-
32	CLA	a	406	X	-	-	-
32	CLA	a	408	X	-	-	-
32	CLA	b	602	X	-	-	-
32	CLA	b	603	X	-	-	-
32	CLA	b	604	X	-	-	-
32	CLA	b	605	X	-	-	-
32	CLA	b	606	X	-	-	-
32	CLA	b	607	X	-	-	-
32	CLA	b	608	X	-	-	-
32	CLA	b	609	X	-	-	-
32	CLA	b	610	X	-	-	-
32	CLA	b	611	X	-	-	-
32	CLA	b	612	X	-	-	-
32	CLA	b	613	X	-	-	-
32	CLA	b	614	X	-	-	-
32	CLA	b	615	X	-	-	-
32	CLA	b	616	X	-	-	-
32	CLA	b	617	X	-	-	-
32	CLA	c	501	X	-	-	-
32	CLA	c	502	X	-	-	-
32	CLA	c	503	X	-	-	-
32	CLA	c	504	X	-	-	-
32	CLA	c	505	X	-	-	-
32	CLA	c	506	X	-	-	-
32	CLA	c	507	X	-	-	-
32	CLA	c	508	X	-	-	-
32	CLA	c	509	X	-	-	-
32	CLA	c	510	X	-	-	-
32	CLA	c	511	X	-	-	-
32	CLA	c	512	X	-	-	-
32	CLA	c	513	X	-	-	-
32	CLA	d	402	X	-	-	-
32	CLA	d	403	X	-	-	-
32	CLA	d	409	X	-	-	-
32	CLA	g	102	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
32	CLA	p	302	X	-	-	-
32	CLA	p	303	X	-	-	-
32	CLA	p	304	X	-	-	-
32	CLA	p	305	X	-	-	-
32	CLA	p	306	X	-	-	-
32	CLA	p	307	X	-	-	-
32	CLA	p	308	X	-	-	-
32	CLA	p	309	X	-	-	-
32	CLA	p	310	X	-	-	-
32	CLA	p	312	X	-	-	-
32	CLA	p	313	X	-	-	-
32	CLA	s	302	X	-	-	-
32	CLA	s	303	X	-	-	-

2 Entry composition

There are 47 unique types of molecules in this entry. The entry contains 80246 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Photosystem II reaction center M.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	m	36	Total	C	N	O	0	0
			265	175	42	48		
1	M	36	Total	C	N	O	0	0
			265	175	42	48		

- Molecule 2 is a protein called ACPII-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	194	Total	C	N	O	S	0	0
			1472	946	256	262	8		
2	7	194	Total	C	N	O	S	0	0
			1472	946	256	262	8		

- Molecule 3 is a protein called ACPII-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2	173	Total	C	N	O	S	0	0
			1362	899	222	238	3		
3	8	173	Total	C	N	O	S	0	0
			1362	899	222	238	3		

- Molecule 4 is a protein called ACPII-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	3	178	Total	C	N	O	S	0	0
			1371	885	230	247	9		
4	9	178	Total	C	N	O	S	0	0
			1371	885	230	247	9		

- Molecule 5 is a protein called ACPII-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	4	172	Total	C	N	O	S	0	0
			1308	845	225	229	9		
5	0	172	Total	C	N	O	S	0	0
			1308	845	225	229	9		

- Molecule 6 is a protein called ACPII-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	5	187	Total	C	N	O	S	0	0
			1471	956	243	267	5		
6	p	187	Total	C	N	O	S	0	0
			1471	956	243	267	5		

- Molecule 7 is a protein called ACPII-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	6	173	Total	C	N	O	S	0	0
			1344	878	221	237	8		
7	P	173	Total	C	N	O	S	0	0
			1344	878	221	237	8		

- Molecule 8 is a protein called Photosystem II protein D1.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	A	334	Total	C	N	O	S	0	0
			2618	1712	430	464	12		
8	a	334	Total	C	N	O	S	0	0
			2618	1712	430	464	12		

- Molecule 9 is a protein called Photosystem II D2 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	D	342	Total	C	N	O	S	0	0
			2713	1794	444	463	12		
9	d	342	Total	C	N	O	S	0	0
			2713	1794	444	463	12		

- Molecule 10 is a protein called Cytochrome b559 subunit alpha.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	E	77	Total	C	N	O	0	0
			629	409	104	116		

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Mol	Chain	Residues	Atoms				AltConf	Trace
10	e	77	Total	C	N	O	0	0
			629	409	104	116		

- Molecule 11 is a protein called Cytochrome b559 subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	F	30	Total	C	N	O	S	0	0
			247	168	41	37	1		
11	f	30	Total	C	N	O	S	0	0
			247	168	41	37	1		

- Molecule 12 is a protein called Photosystem II reaction center protein H.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	H	65	Total	C	N	O	S	0	0
			515	344	81	88	2		
12	h	65	Total	C	N	O	S	0	0
			515	344	81	88	2		

- Molecule 13 is a protein called Photosystem II reaction center protein I.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	I	35	Total	C	N	O	S	0	0
			287	191	46	49	1		
13	i	35	Total	C	N	O	S	0	0
			287	191	46	49	1		

- Molecule 14 is a protein called Photosystem II reaction center protein J.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	J	28	Total	C	N	O	0	0
			214	147	32	35		
14	j	28	Total	C	N	O	0	0
			214	147	32	35		

- Molecule 15 is a protein called Photosystem II reaction center protein K.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	K	37	Total	C	N	O	0	0
			297	209	44	44		
15	k	37	Total	C	N	O	0	0
			297	209	44	44		

- Molecule 16 is a protein called Photosystem II reaction center protein O.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	O	231	Total	C	N	O	S	0	0
			1749	1103	282	358	6		
16	o	231	Total	C	N	O	S	0	0
			1749	1103	282	358	6		

- Molecule 17 is a protein called Photosystem II reaction center protein Q.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	Q	21	Total	C	N	O	0	0
			105	63	21	21		
17	q	21	Total	C	N	O	0	0
			105	63	21	21		

- Molecule 18 is a protein called Photosystem II reaction center protein R.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	R	26	Total	C	N	O	0	0
			130	78	26	26		
18	r	26	Total	C	N	O	0	0
			130	78	26	26		

- Molecule 19 is a protein called CCPH-S.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	203	Total	C	N	O	S	0	0
			1563	1005	255	299	4		
19	s	203	Total	C	N	O	S	0	0
			1563	1005	255	299	4		

- Molecule 20 is a protein called Photosystem II reaction center protein T.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	32	Total	C	N	O	S	0	0
			260	179	40	40	1		
20	t	32	Total	C	N	O	S	0	0
			260	179	40	40	1		

- Molecule 21 is a protein called Photosystem II reaction center protein U.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	U	93	Total	C	N	O	S	0	0
			742	476	122	142	2		
21	u	93	Total	C	N	O	S	0	0
			742	476	122	142	2		

- Molecule 22 is a protein called Photosystem II cytochrome c550.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	V	131	Total	C	N	O	S	0	0
			996	626	170	196	4		
22	v	131	Total	C	N	O	S	0	0
			996	626	170	196	4		

- Molecule 23 is a protein called Photosystem II reaction center X protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	X	39	Total	C	N	O	S	0	0
			292	192	47	52	1		
23	x	39	Total	C	N	O	S	0	0
			292	192	47	52	1		

- Molecule 24 is a protein called Photosystem II reaction center protein Ycf12.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Y	34	Total	C	N	O	S	0	0
			266	180	43	42	1		
24	y	34	Total	C	N	O	S	0	0
			266	180	43	42	1		

- Molecule 25 is a protein called Photosystem II reaction center protein Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Z	61	Total	C	N	O	S	0	0
			457	315	67	74	1		
25	z	61	Total	C	N	O	S	0	0
			457	315	67	74	1		

- Molecule 26 is a protein called Photosystem II CP47 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	b	504	Total	C	N	O	S	0	0
			3962	2587	676	688	11		

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Mol	Chain	Residues	Atoms					AltConf	Trace
26	B	504	Total	C	N	O	S	0	0
			3962	2587	676	688	11		

- Molecule 27 is a protein called Photosystem II CP43 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	c	451	Total	C	N	O	S	0	0
			3504	2290	589	615	10		
27	C	451	Total	C	N	O	S	0	0
			3504	2290	589	615	10		

- Molecule 28 is a protein called Photosystem II reaction center protein G.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	g	64	Total	C	N	O	0	0
			320	192	64	64		
28	G	64	Total	C	N	O	0	0
			320	192	64	64		

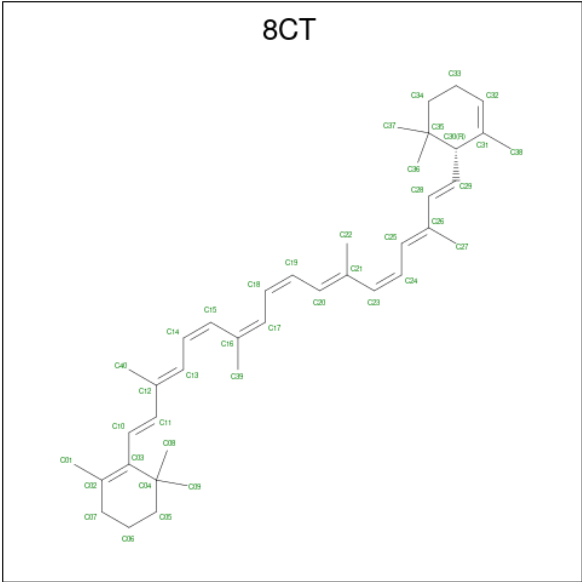
- Molecule 29 is a protein called Photosystem II reaction center protein L.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	l	38	Total	C	N	O	S	0	0
			310	209	48	52	1		
29	L	38	Total	C	N	O	S	0	0
			310	209	48	52	1		

- Molecule 30 is a protein called Photosystem II reaction center protein W.

Mol	Chain	Residues	Atoms				AltConf	Trace
30	w	45	Total	C	N	O	0	0
			367	238	57	72		
30	W	45	Total	C	N	O	0	0
			367	238	57	72		

- Molecule 31 is (6'R,11cis,11'cis,13cis,15cis)-4',5'-didehydro-5',6'-dihydro-beta,beta-carotene (CCD ID: 8CT) (formula: C₄₀H₅₆) (labeled as "Ligand of Interest" by depositor).



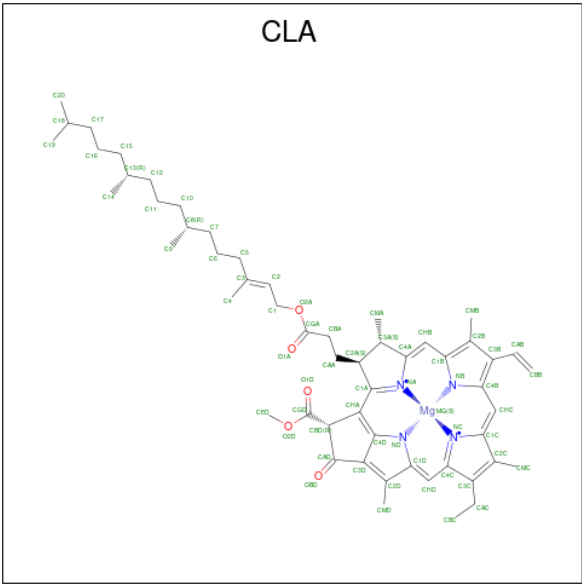
Mol	Chain	Residues	Atoms	AltConf
31	M	1	Total C 40 40	0
31	3	1	Total C 40 40	0
31	6	1	Total C 40 40	0
31	A	1	Total C 40 40	0
31	D	1	Total C 40 40	0
31	H	1	Total C 40 40	0
31	K	1	Total C 40 40	0
31	K	1	Total C 40 40	0
31	Z	1	Total C 40 40	0
31	b	1	Total C 40 40	0
31	b	1	Total C 40 40	0
31	c	1	Total C 40 40	0
31	d	1	Total C 40 40	0
31	k	1	Total C 40 40	0

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Mol	Chain	Residues	Atoms		AltConf
31	k	1	Total	C	0
			40	40	
31	z	1	Total	C	0
			40	40	
31	9	1	Total	C	0
			40	40	
31	C	1	Total	C	0
			40	40	
31	P	1	Total	C	0
			40	40	
31	a	1	Total	C	0
			40	40	
31	h	1	Total	C	0
			40	40	
31	B	1	Total	C	0
			40	40	
31	B	1	Total	C	0
			40	40	
31	B	1	Total	C	0
			40	40	

- Molecule 32 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
32	1	1	Total	C	Mg	N	O	0
			42	34	1	4	3	

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Mol	Chain	Residues	Atoms					AltConf
32	1	1	Total 59	C 49	Mg 1	N 4	O 5	0
32	1	1	Total 50	C 40	Mg 1	N 4	O 5	0
32	1	1	Total 55	C 45	Mg 1	N 4	O 5	0
32	1	1	Total 50	C 40	Mg 1	N 4	O 5	0
32	1	1	Total 45	C 35	Mg 1	N 4	O 5	0
32	1	1	Total 45	C 35	Mg 1	N 4	O 5	0
32	1	1	Total 60	C 50	Mg 1	N 4	O 5	0
32	1	1	Total 41	C 33	Mg 1	N 4	O 3	0
32	1	1	Total 45	C 35	Mg 1	N 4	O 5	0
32	1	1	Total 45	C 35	Mg 1	N 4	O 5	0
32	1	1	Total 45	C 35	Mg 1	N 4	O 5	0
32	2	1	Total 42	C 34	Mg 1	N 4	O 3	0
32	2	1	Total 59	C 49	Mg 1	N 4	O 5	0
32	2	1	Total 50	C 40	Mg 1	N 4	O 5	0
32	2	1	Total 55	C 45	Mg 1	N 4	O 5	0
32	2	1	Total 60	C 50	Mg 1	N 4	O 5	0
32	2	1	Total 45	C 35	Mg 1	N 4	O 5	0
32	2	1	Total 45	C 35	Mg 1	N 4	O 5	0
32	2	1	Total 60	C 50	Mg 1	N 4	O 5	0
32	2	1	Total 41	C 33	Mg 1	N 4	O 3	0
32	2	1	Total 45	C 35	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
32	2	1	Total 45	C 35	Mg 1	N 4	O 5	0
32	3	1	Total 42	C 34	Mg 1	N 4	O 3	0
32	3	1	Total 59	C 49	Mg 1	N 4	O 5	0
32	3	1	Total 50	C 40	Mg 1	N 4	O 5	0
32	3	1	Total 55	C 45	Mg 1	N 4	O 5	0
32	3	1	Total 46	C 36	Mg 1	N 4	O 5	0
32	3	1	Total 45	C 35	Mg 1	N 4	O 5	0
32	3	1	Total 60	C 50	Mg 1	N 4	O 5	0
32	3	1	Total 41	C 33	Mg 1	N 4	O 3	0
32	3	1	Total 60	C 50	Mg 1	N 4	O 5	0
32	3	1	Total 45	C 35	Mg 1	N 4	O 5	0
32	3	1	Total 45	C 35	Mg 1	N 4	O 5	0
32	4	1	Total 42	C 34	Mg 1	N 4	O 3	0
32	4	1	Total 59	C 49	Mg 1	N 4	O 5	0
32	4	1	Total 50	C 40	Mg 1	N 4	O 5	0
32	4	1	Total 55	C 45	Mg 1	N 4	O 5	0
32	4	1	Total 50	C 40	Mg 1	N 4	O 5	0
32	4	1	Total 45	C 35	Mg 1	N 4	O 5	0
32	4	1	Total 45	C 35	Mg 1	N 4	O 5	0
32	4	1	Total 60	C 50	Mg 1	N 4	O 5	0
32	4	1	Total 41	C 33	Mg 1	N 4	O 3	0

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Mol	Chain	Residues	Atoms					AltConf
32	4	1	Total 45	C 35	Mg 1	N 4	O 5	0
32	4	1	Total 45	C 35	Mg 1	N 4	O 5	0
32	4	1	Total 45	C 35	Mg 1	N 4	O 5	0
32	5	1	Total 42	C 34	Mg 1	N 4	O 3	0
32	5	1	Total 59	C 49	Mg 1	N 4	O 5	0
32	5	1	Total 50	C 40	Mg 1	N 4	O 5	0
32	5	1	Total 55	C 45	Mg 1	N 4	O 5	0
32	5	1	Total 60	C 50	Mg 1	N 4	O 5	0
32	5	1	Total 45	C 35	Mg 1	N 4	O 5	0
32	5	1	Total 45	C 35	Mg 1	N 4	O 5	0
32	5	1	Total 60	C 50	Mg 1	N 4	O 5	0
32	5	1	Total 41	C 33	Mg 1	N 4	O 3	0
32	5	1	Total 45	C 35	Mg 1	N 4	O 5	0
32	5	1	Total 45	C 35	Mg 1	N 4	O 5	0
32	6	1	Total 42	C 34	Mg 1	N 4	O 3	0
32	6	1	Total 59	C 49	Mg 1	N 4	O 5	0
32	6	1	Total 50	C 40	Mg 1	N 4	O 5	0
32	6	1	Total 55	C 45	Mg 1	N 4	O 5	0
32	6	1	Total 45	C 35	Mg 1	N 4	O 5	0
32	6	1	Total 60	C 50	Mg 1	N 4	O 5	0
32	6	1	Total 41	C 33	Mg 1	N 4	O 3	0

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Mol	Chain	Residues	Atoms					AltConf
32	6	1	Total 45	C 35	Mg 1	N 4	O 5	0
32	6	1	Total 45	C 35	Mg 1	N 4	O 5	0
32	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	A	1	Total 49	C 39	Mg 1	N 4	O 5	0
32	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
32	D	1	Total 59	C 49	Mg 1	N 4	O 5	0
32	D	1	Total 57	C 47	Mg 1	N 4	O 5	0
32	D	1	Total 60	C 50	Mg 1	N 4	O 5	0
32	S	1	Total 45	C 35	Mg 1	N 4	O 5	0
32	S	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	b	1	Total 47	C 37	Mg 1	N 4	O 5	0
32	b	1	Total 61	C 52	Mg 1	N 4	O 4	0
32	b	1	Total 64	C 54	Mg 1	N 4	O 5	0
32	b	1	Total 61	C 51	Mg 1	N 4	O 5	0
32	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	b	1	Total 41	C 33	Mg 1	N 4	O 3	0
32	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	b	1	Total 64	C 54	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
32	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	b	1	Total 64	C 54	Mg 1	N 4	O 5	0
32	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	c	1	Total 64	C 54	Mg 1	N 4	O 5	0
32	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	c	1	Total 64	C 54	Mg 1	N 4	O 5	0
32	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	c	1	Total 45	C 35	Mg 1	N 4	O 5	0
32	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	c	1	Total 57	C 47	Mg 1	N 4	O 5	0
32	c	1	Total 49	C 39	Mg 1	N 4	O 5	0
32	d	1	Total 57	C 47	Mg 1	N 4	O 5	0
32	d	1	Total 60	C 50	Mg 1	N 4	O 5	0
32	d	1	Total 59	C 49	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
32	g	1	Total 45	C 35	Mg 1	N 4	O 5	0
32	0	1	Total 42	C 34	Mg 1	N 4	O 3	0
32	0	1	Total 59	C 49	Mg 1	N 4	O 5	0
32	0	1	Total 50	C 40	Mg 1	N 4	O 5	0
32	0	1	Total 55	C 45	Mg 1	N 4	O 5	0
32	0	1	Total 50	C 40	Mg 1	N 4	O 5	0
32	0	1	Total 45	C 35	Mg 1	N 4	O 5	0
32	0	1	Total 45	C 35	Mg 1	N 4	O 5	0
32	0	1	Total 60	C 50	Mg 1	N 4	O 5	0
32	0	1	Total 41	C 33	Mg 1	N 4	O 3	0
32	0	1	Total 45	C 35	Mg 1	N 4	O 5	0
32	0	1	Total 45	C 35	Mg 1	N 4	O 5	0
32	0	1	Total 45	C 35	Mg 1	N 4	O 5	0
32	7	1	Total 42	C 34	Mg 1	N 4	O 3	0
32	7	1	Total 59	C 49	Mg 1	N 4	O 5	0
32	7	1	Total 50	C 40	Mg 1	N 4	O 5	0
32	7	1	Total 55	C 45	Mg 1	N 4	O 5	0
32	7	1	Total 50	C 40	Mg 1	N 4	O 5	0
32	7	1	Total 45	C 35	Mg 1	N 4	O 5	0
32	7	1	Total 45	C 35	Mg 1	N 4	O 5	0
32	7	1	Total 60	C 50	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
32	7	1	Total 41	C 33	Mg 1	N 4	O 3	0
32	7	1	Total 45	C 35	Mg 1	N 4	O 5	0
32	7	1	Total 45	C 35	Mg 1	N 4	O 5	0
32	7	1	Total 45	C 35	Mg 1	N 4	O 5	0
32	8	1	Total 42	C 34	Mg 1	N 4	O 3	0
32	8	1	Total 59	C 49	Mg 1	N 4	O 5	0
32	8	1	Total 50	C 40	Mg 1	N 4	O 5	0
32	8	1	Total 55	C 45	Mg 1	N 4	O 5	0
32	8	1	Total 60	C 50	Mg 1	N 4	O 5	0
32	8	1	Total 45	C 35	Mg 1	N 4	O 5	0
32	8	1	Total 45	C 35	Mg 1	N 4	O 5	0
32	8	1	Total 60	C 50	Mg 1	N 4	O 5	0
32	8	1	Total 41	C 33	Mg 1	N 4	O 3	0
32	8	1	Total 45	C 35	Mg 1	N 4	O 5	0
32	8	1	Total 45	C 35	Mg 1	N 4	O 5	0
32	9	1	Total 42	C 34	Mg 1	N 4	O 3	0
32	9	1	Total 59	C 49	Mg 1	N 4	O 5	0
32	9	1	Total 50	C 40	Mg 1	N 4	O 5	0
32	9	1	Total 55	C 45	Mg 1	N 4	O 5	0
32	9	1	Total 46	C 36	Mg 1	N 4	O 5	0
32	9	1	Total 45	C 35	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
32	9	1	Total 60	C 50	Mg 1	N 4	O 5	0
32	9	1	Total 41	C 33	Mg 1	N 4	O 3	0
32	9	1	Total 60	C 50	Mg 1	N 4	O 5	0
32	9	1	Total 45	C 35	Mg 1	N 4	O 5	0
32	9	1	Total 45	C 35	Mg 1	N 4	O 5	0
32	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	C	1	Total 64	C 54	Mg 1	N 4	O 5	0
32	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	C	1	Total 64	C 54	Mg 1	N 4	O 5	0
32	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	C	1	Total 45	C 35	Mg 1	N 4	O 5	0
32	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	C	1	Total 57	C 47	Mg 1	N 4	O 5	0
32	C	1	Total 49	C 39	Mg 1	N 4	O 5	0
32	G	1	Total 45	C 35	Mg 1	N 4	O 5	0
32	P	1	Total 42	C 34	Mg 1	N 4	O 3	0
32	P	1	Total 59	C 49	Mg 1	N 4	O 5	0

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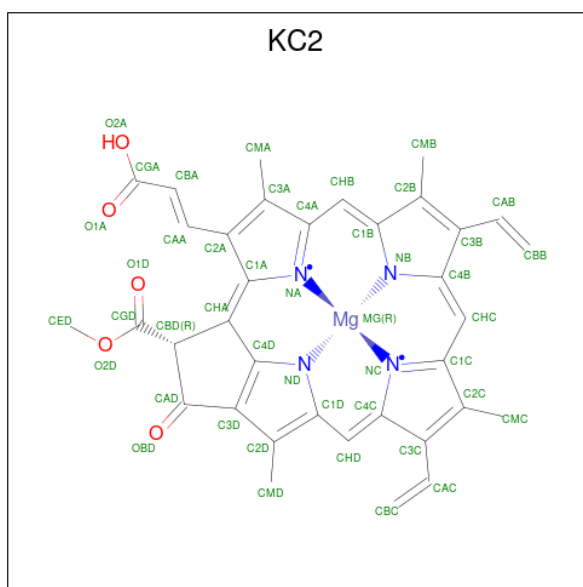
Mol	Chain	Residues	Atoms					AltConf
32	P	1	Total 50	C 40	Mg 1	N 4	O 5	0
32	P	1	Total 55	C 45	Mg 1	N 4	O 5	0
32	P	1	Total 45	C 35	Mg 1	N 4	O 5	0
32	P	1	Total 60	C 50	Mg 1	N 4	O 5	0
32	P	1	Total 41	C 33	Mg 1	N 4	O 3	0
32	P	1	Total 45	C 35	Mg 1	N 4	O 5	0
32	P	1	Total 45	C 35	Mg 1	N 4	O 5	0
32	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	a	1	Total 49	C 39	Mg 1	N 4	O 5	0
32	a	1	Total 60	C 50	Mg 1	N 4	O 5	0
32	p	1	Total 42	C 34	Mg 1	N 4	O 3	0
32	p	1	Total 59	C 49	Mg 1	N 4	O 5	0
32	p	1	Total 50	C 40	Mg 1	N 4	O 5	0
32	p	1	Total 55	C 45	Mg 1	N 4	O 5	0
32	p	1	Total 60	C 50	Mg 1	N 4	O 5	0
32	p	1	Total 45	C 35	Mg 1	N 4	O 5	0
32	p	1	Total 45	C 35	Mg 1	N 4	O 5	0
32	p	1	Total 60	C 50	Mg 1	N 4	O 5	0
32	p	1	Total 41	C 33	Mg 1	N 4	O 3	0
32	p	1	Total 45	C 35	Mg 1	N 4	O 5	0
32	p	1	Total 45	C 35	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
32	s	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
32	s	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
32	B	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
32	B	1	Total	C	Mg	N	O	0
			61	52	1	4	4	
32	B	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
32	B	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
32	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
32	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
32	B	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
32	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
32	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
32	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
32	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
32	B	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
32	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
32	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
32	B	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
32	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
32	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

- Molecule 33 is Chlorophyll c2 (CCD ID: KC2) (formula: $C_{35}H_{28}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
33	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
33	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
33	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
33	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
33	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
33	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
33	0	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
33	7	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
33	8	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
33	P	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
33	P	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
33	p	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

- Molecule 34 is (1 {R})-3,5,5-trimethyl-4-[(3 {E},5 {E},7 {E},9 {E},11 {E},13 {E},15 {E})-3,7,12,16-tetramethyl-18-[(4 {R})-2,6,6-trimethyl-4-oxidanyl-cyclohexen-1-yl]octadeca-3,5,7,9,11,13,15-heptaen-1,17-diynyl]cyclohex-3-en-1-ol (CCD ID: II0) (formula: C₄₀H₅₂O₂)

The chemical structure of IIO is a long-chain polyene. It features a central chain of alternating double and single bonds. At the left end, there is a hydroxyl group (OH) attached to carbon C08. The chain continues through several conjugated double bonds, including C11=C12, C15=C16, C19=C20, C23=C24, C27=C28, C31=C32, C35=C36, C39=C40, C43=C44, C47=C48, C51=C52, C55=C56, and C59=C60. The chain terminates at the right end with a hydroxyl group (OH) attached to carbon C61. The structure is labeled with carbon atoms from C01 to C61, with the two hydroxyl groups highlighted in red.

Mol	Chain	Residues	Atoms			AltConf
34	1	1	Total 42	C 40	O 2	0
34	1	1	Total 42	C 40	O 2	0
34	1	1	Total 42	C 40	O 2	0
34	1	1	Total 42	C 40	O 2	0
34	2	1	Total 42	C 40	O 2	0
34	2	1	Total 42	C 40	O 2	0
34	2	1	Total 42	C 40	O 2	0
34	2	1	Total 42	C 40	O 2	0
34	3	1	Total 42	C 40	O 2	0
34	3	1	Total 42	C 40	O 2	0
34	3	1	Total 42	C 40	O 2	0
34	4	1	Total 42	C 40	O 2	0
34	4	1	Total 42	C 40	O 2	0



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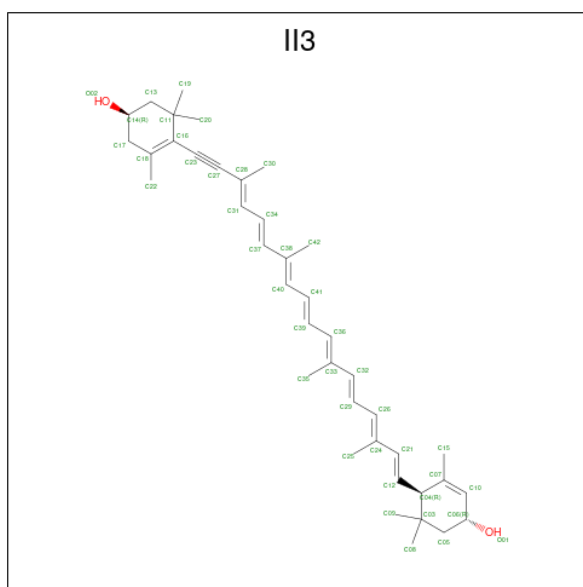
Mol	Chain	Residues	Atoms			AltConf
34	4	1	Total 42	C 40	O 2	0
34	5	1	Total 42	C 40	O 2	0
34	5	1	Total 42	C 40	O 2	0
34	5	1	Total 42	C 40	O 2	0
34	5	1	Total 42	C 40	O 2	0
34	5	1	Total 42	C 40	O 2	0
34	6	1	Total 42	C 40	O 2	0
34	6	1	Total 42	C 40	O 2	0
34	0	1	Total 42	C 40	O 2	0
34	0	1	Total 42	C 40	O 2	0
34	0	1	Total 42	C 40	O 2	0
34	0	1	Total 42	C 40	O 2	0
34	0	1	Total 42	C 40	O 2	0
34	7	1	Total 42	C 40	O 2	0
34	7	1	Total 42	C 40	O 2	0
34	7	1	Total 42	C 40	O 2	0
34	7	1	Total 42	C 40	O 2	0
34	8	1	Total 42	C 40	O 2	0
34	8	1	Total 42	C 40	O 2	0
34	8	1	Total 42	C 40	O 2	0
34	8	1	Total 42	C 40	O 2	0
34	9	1	Total 42	C 40	O 2	0

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Mol	Chain	Residues	Atoms			AltConf
34	9	1	Total	C	O	0
			42	40	2	
34	9	1	Total	C	O	0
			42	40	2	
34	P	1	Total	C	O	0
			42	40	2	
34	P	1	Total	C	O	0
			42	40	2	
34	p	1	Total	C	O	0
			42	40	2	
34	p	1	Total	C	O	0
			42	40	2	
34	p	1	Total	C	O	0
			42	40	2	
34	p	1	Total	C	O	0
			42	40	2	

- Molecule 35 is (1 {R})-3,5,5-trimethyl-4-[(3 {E},5 {E},7 {E},9 {E},11 {E},13 {E},15 {E},17 {E})-3,7,12,16-tetramethyl-18-[(1 {R},4 {R})-2,6,6-trimethyl-4-oxidanyl-cyclohex-2-en-1-yl]octadeca-3,5,7,9,11,13,15,17-octaen-1-ynyl]cyclohex-3-en-1-ol (CCD ID: II3) (formula: $C_{40}H_{54}O_2$) (labeled as "Ligand of Interest" by depositor).



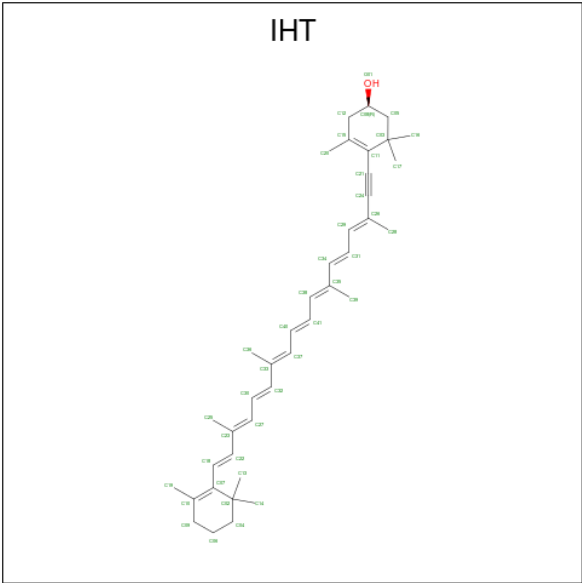
Mol	Chain	Residues	Atoms			AltConf
35	1	1	Total	C	O	0
			42	40	2	
35	6	1	Total	C	O	0
			42	40	2	

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Mol	Chain	Residues	Atoms			AltConf
35	7	1	Total	C	O	0
			42	40	2	
35	P	1	Total	C	O	0
			42	40	2	

- Molecule 36 is (1 {R})-3,5,5-trimethyl-4-[(3 {E},5 {E},7 {E},9 {E},11 {E},13 {E},15 {E},17 {E})-3,7,12,16-tetramethyl-18-(2,6,6-trimethylcyclohexen-1-yl)octadeca-3,5,7,9,11,13,15,17-octaen-1-ynyl]cyclohex-3-en-1-ol (CCD ID: IHT) (formula: C₄₀H₅₄O) (labeled as "Ligand of Interest" by depositor).



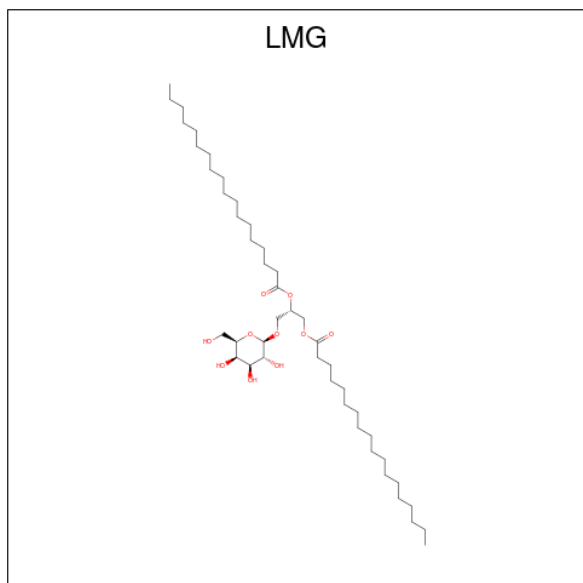
Mol	Chain	Residues	Atoms			AltConf
36	1	1	Total	C	O	0
			41	40	1	
36	2	1	Total	C	O	0
			41	40	1	
36	4	1	Total	C	O	0
			41	40	1	
36	4	1	Total	C	O	0
			41	40	1	
36	5	1	Total	C	O	0
			41	40	1	
36	0	1	Total	C	O	0
			41	40	1	
36	0	1	Total	C	O	0
			41	40	1	
36	7	1	Total	C	O	0
			41	40	1	

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Mol	Chain	Residues	Atoms			AltConf
36	8	1	Total	C	O	0
			41	40	1	
36	p	1	Total	C	O	0
			41	40	1	

- Molecule 37 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: C₄₅H₈₆O₁₀) (labeled as "Ligand of Interest" by depositor).



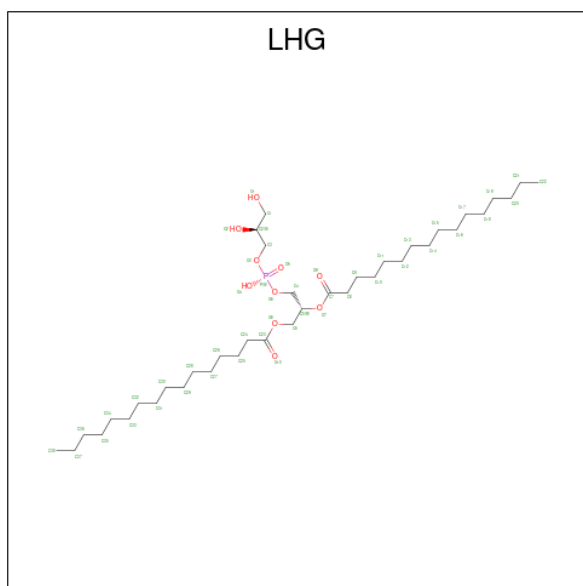
Mol	Chain	Residues	Atoms			AltConf
37	2	1	Total	C	O	0
			36	26	10	
37	4	1	Total	C	O	0
			36	26	10	
37	6	1	Total	C	O	0
			28	18	10	
37	A	1	Total	C	O	0
			48	38	10	
37	D	1	Total	C	O	0
			46	36	10	
37	D	1	Total	C	O	0
			40	30	10	
37	b	1	Total	C	O	0
			51	41	10	
37	c	1	Total	C	O	0
			46	36	10	
37	d	1	Total	C	O	0
			40	30	10	

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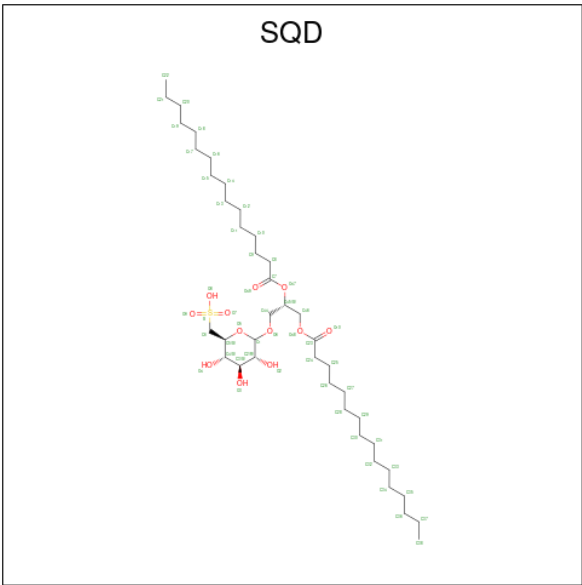
Mol	Chain	Residues	Atoms			AltConf
37	d	1	Total	C	O	0
			46	36	10	
37	g	1	Total	C	O	0
			28	18	10	
37	l	1	Total	C	O	0
			40	30	10	
37	o	1	Total	C	O	0
			36	26	10	
37	8	1	Total	C	O	0
			36	26	10	
37	C	1	Total	C	O	0
			46	36	10	
37	G	1	Total	C	O	0
			28	18	10	
37	L	1	Total	C	O	0
			40	30	10	
37	P	1	Total	C	O	0
			28	18	10	
37	a	1	Total	C	O	0
			48	38	10	
37	B	1	Total	C	O	0
			51	41	10	

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



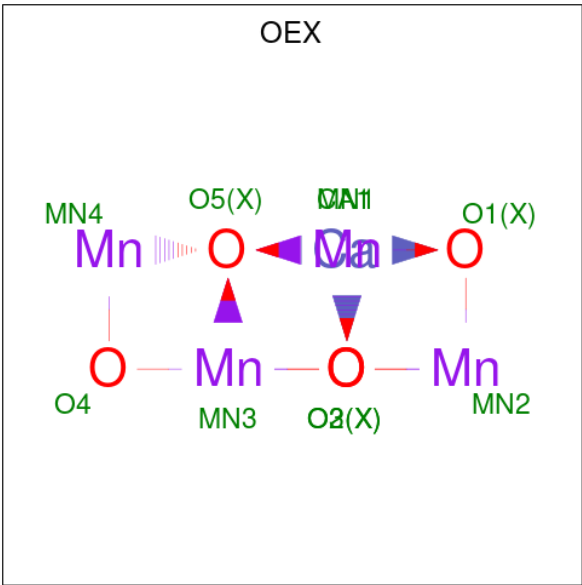
Mol	Chain	Residues	Atoms				AltConf
38	2	1	Total	C	O	P	0
			22	12	9	1	
38	A	1	Total	C	O	P	0
			43	32	10	1	
38	A	1	Total	C	O	P	0
			49	38	10	1	
38	D	1	Total	C	O	P	0
			48	38	9	1	
38	D	1	Total	C	O	P	0
			32	21	10	1	
38	S	1	Total	C	O	P	0
			37	26	10	1	
38	b	1	Total	C	O	P	0
			39	28	10	1	
38	b	1	Total	C	O	P	0
			39	28	10	1	
38	d	1	Total	C	O	P	0
			48	38	9	1	
38	d	1	Total	C	O	P	0
			32	21	10	1	
38	l	1	Total	C	O	P	0
			49	38	10	1	
38	8	1	Total	C	O	P	0
			22	12	9	1	
38	L	1	Total	C	O	P	0
			49	38	10	1	
38	a	1	Total	C	O	P	0
			43	32	10	1	
38	a	1	Total	C	O	P	0
			49	38	10	1	
38	s	1	Total	C	O	P	0
			37	26	10	1	
38	B	1	Total	C	O	P	0
			39	28	10	1	
38	B	1	Total	C	O	P	0
			39	28	10	1	

- Molecule 39 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: C₄₁H₇₈O₁₂S) (labeled as "Ligand of Interest" by depositor).



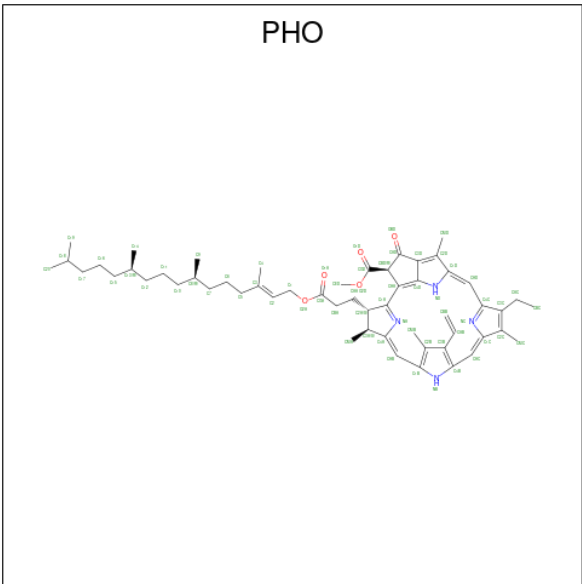
Mol	Chain	Residues	Atoms				AltConf
39	5	1	Total	C	O	S	0
			35	22	12	1	
39	A	1	Total	C	O	S	0
			54	41	12	1	
39	b	1	Total	C	O	S	0
			48	35	12	1	
39	b	1	Total	C	O	S	0
			54	41	12	1	
39	a	1	Total	C	O	S	0
			54	41	12	1	
39	p	1	Total	C	O	S	0
			35	22	12	1	
39	B	1	Total	C	O	S	0
			48	35	12	1	
39	B	1	Total	C	O	S	0
			54	41	12	1	

- Molecule 40 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula: CaMn_4O_5) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
40	A	1	Total	Ca	Mn	O	0
			10	1	4	5	
40	a	1	Total	Ca	Mn	O	0
			10	1	4	5	

- Molecule 41 is PHEOPHYTIN A (CCD ID: PHO) (formula: C₅₅H₇₄N₄O₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
41	A	1	Total	C	N	O	0
			64	55	4	5	

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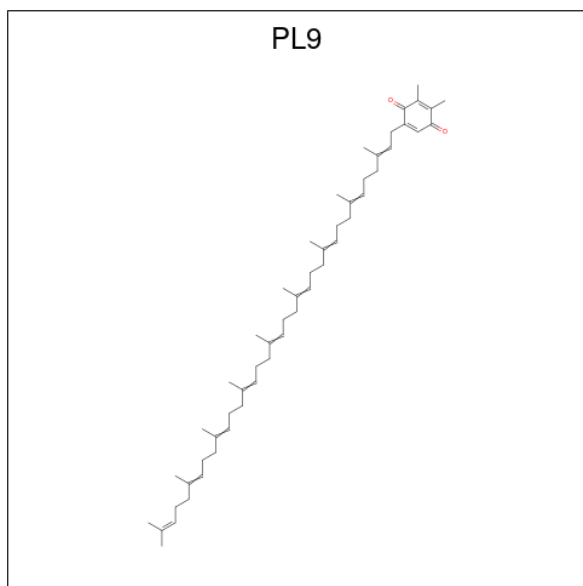
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Mol	Chain	Residues	Atoms				AltConf
41	D	1	Total	C	N	O	0
			64	55	4	5	
41	d	1	Total	C	N	O	0
			64	55	4	5	
41	a	1	Total	C	N	O	0
			64	55	4	5	

- Molecule 42 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		AltConf
42	A	1	Total	Cl	0
			1	1	
42	a	1	Total	Cl	0
			1	1	

- Molecule 43 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (CCD ID: PL9) (formula: C₅₃H₈₀O₂) (labeled as "Ligand of Interest" by depositor).



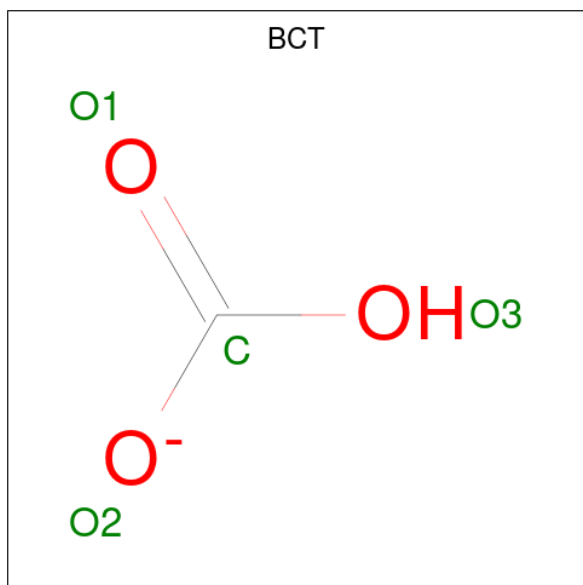
Mol	Chain	Residues	Atoms			AltConf
43	A	1	Total	C	O	0
			13	11	2	
43	D	1	Total	C	O	0
			55	53	2	
43	d	1	Total	C	O	0
			55	53	2	

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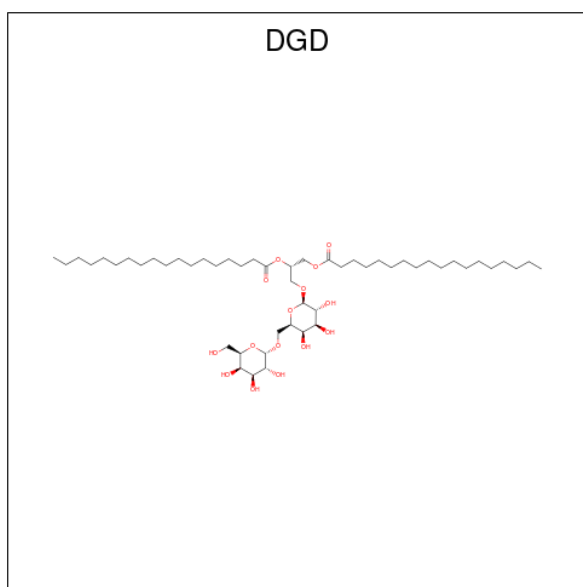
Mol	Chain	Residues	Atoms			AltConf
43	a	1	Total	C	O	0
			13	11	2	

- Molecule 44 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3^-) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
44	A	1	Total	C	O	0
			4	1	3	
44	a	1	Total	C	O	0
			4	1	3	

- Molecule 45 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $\text{C}_{51}\text{H}_{96}\text{O}_{15}$) (labeled as "Ligand of Interest" by depositor).

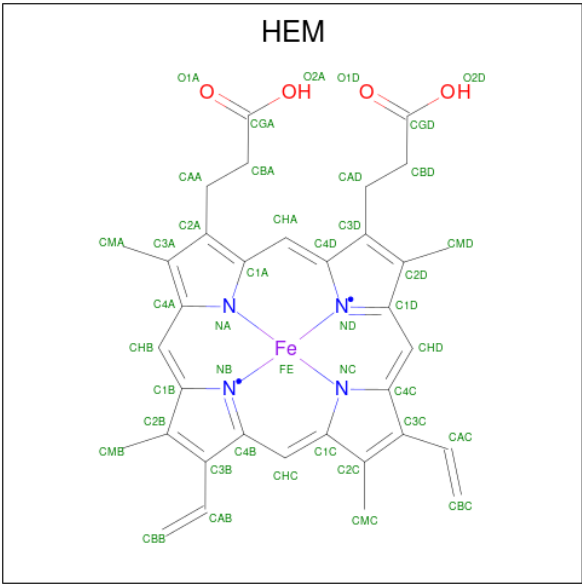


Mol	Chain	Residues	Atoms			AltConf
45	A	1	Total	C	O	0
			53	39	14	
45	H	1	Total	C	O	0
			62	47	15	
45	c	1	Total	C	O	0
			55	40	15	
45	c	1	Total	C	O	0
			56	41	15	
45	c	1	Total	C	O	0
			55	40	15	
45	C	1	Total	C	O	0
			55	40	15	
45	C	1	Total	C	O	0
			56	41	15	
45	C	1	Total	C	O	0
			55	40	15	
45	a	1	Total	C	O	0
			53	39	14	
45	h	1	Total	C	O	0
			62	47	15	

- Molecule 46 is FE (II) ION (CCD ID: FE2) (formula: Fe).

Mol	Chain	Residues	Atoms		AltConf
46	D	1	Total	Fe	0
			1	1	
46	d	1	Total	Fe	0
			1	1	

- Molecule 47 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).

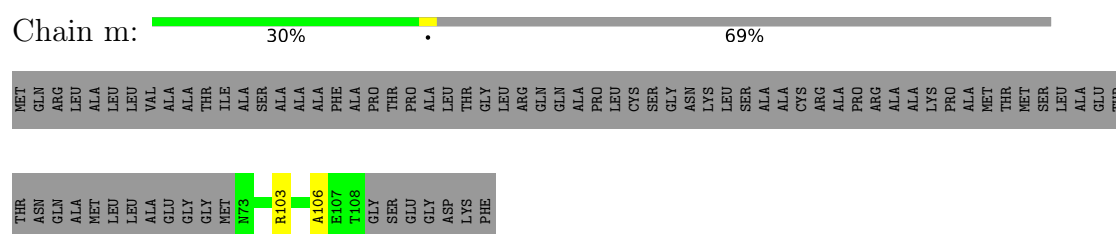


Mol	Chain	Residues	Atoms					AltConf
47	E	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
47	V	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
47	f	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
47	v	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

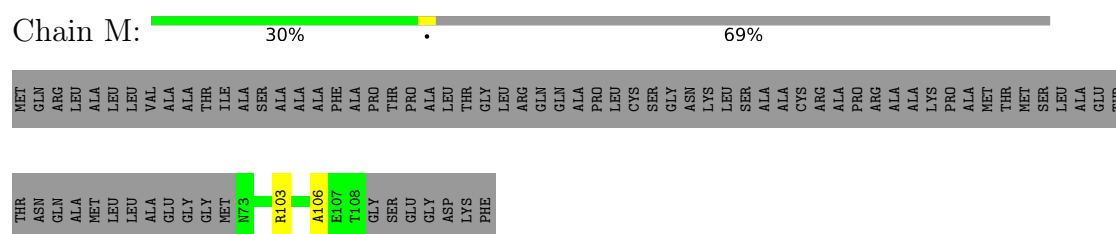
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

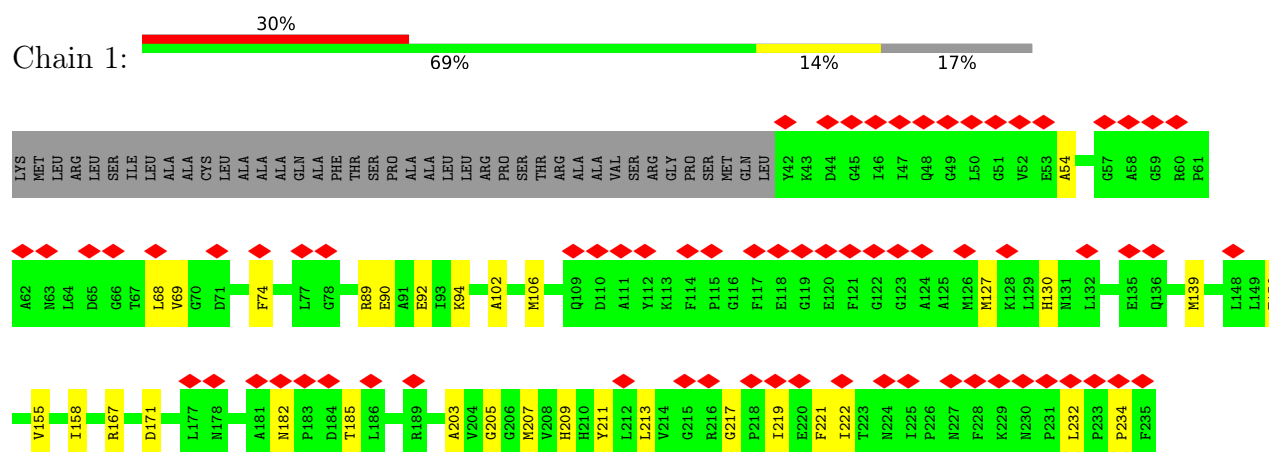
- Molecule 1: Photosystem II reaction center M



- Molecule 1: Photosystem II reaction center M

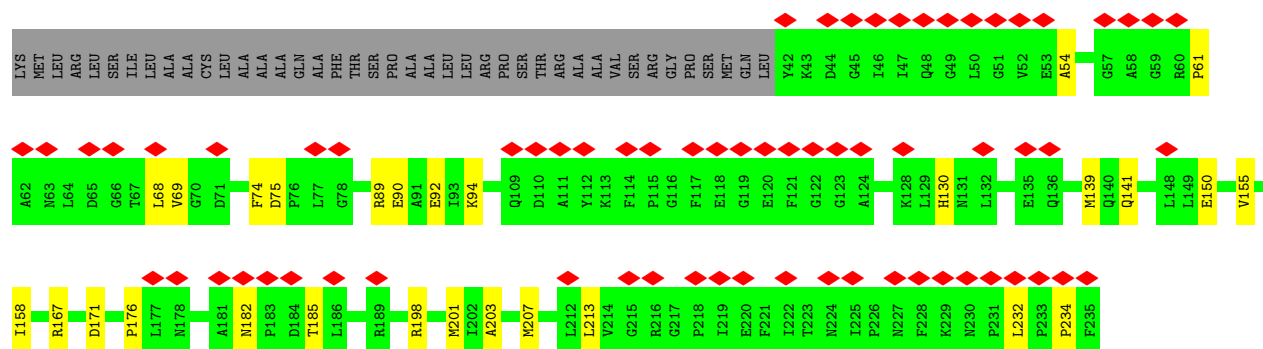


- Molecule 2: ACPII-1

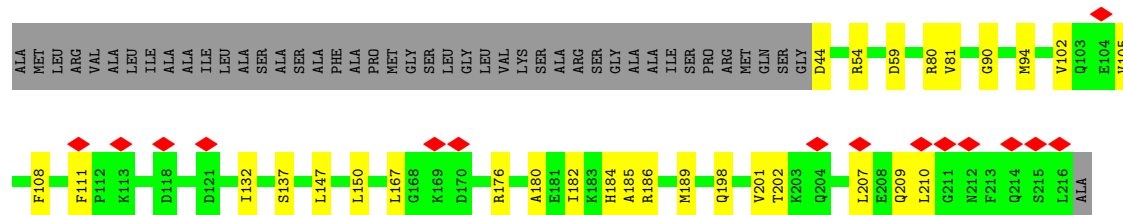


- Molecule 2: ACPII-1

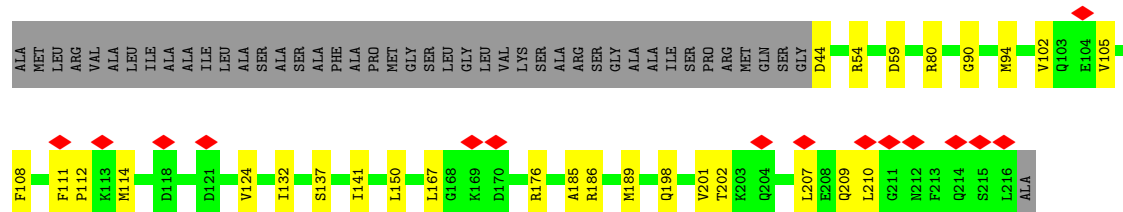




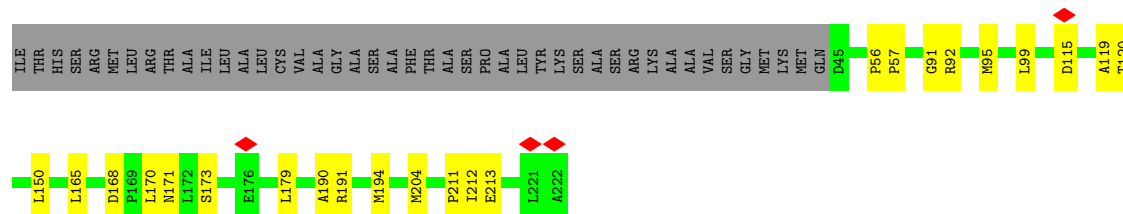
• Molecule 3: ACPII-2



• Molecule 3: ACPII-2

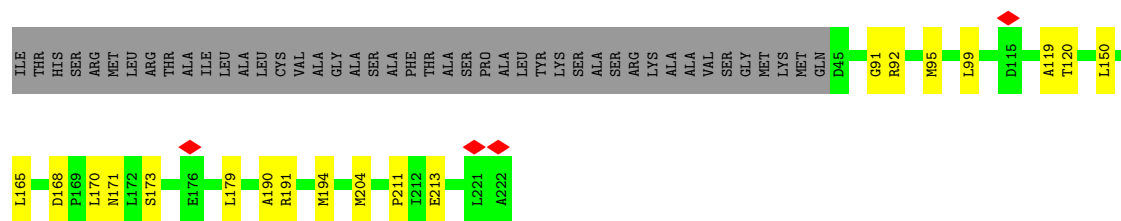


• Molecule 4: ACPII-3

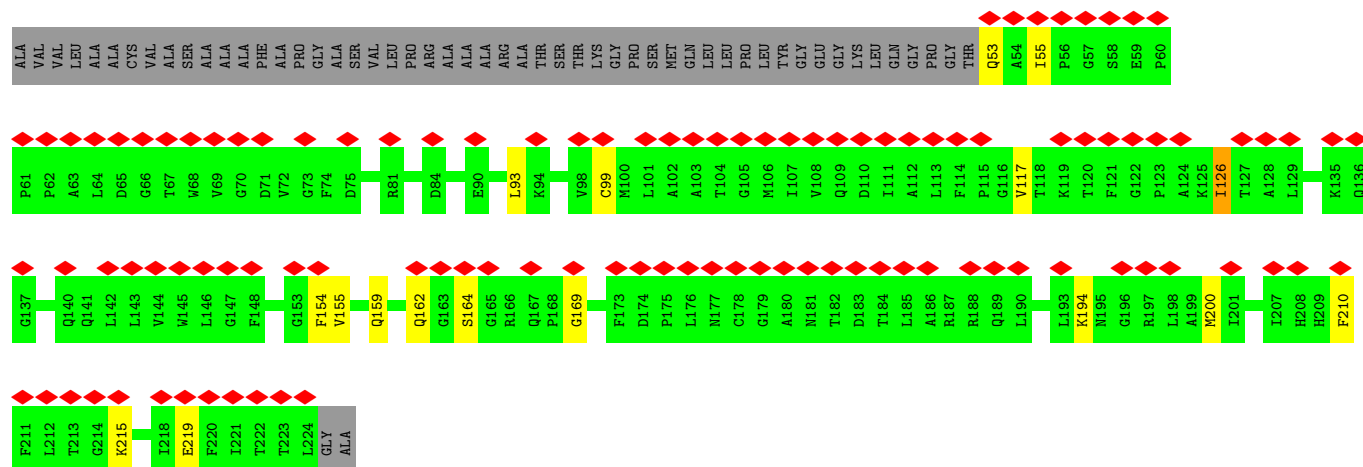


• Molecule 4: ACPII-3

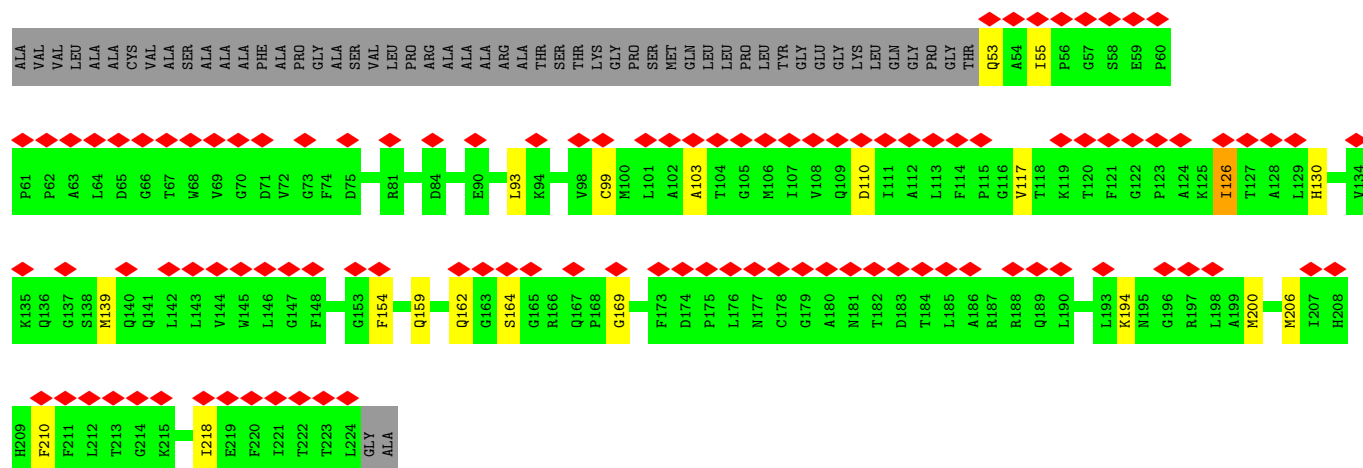




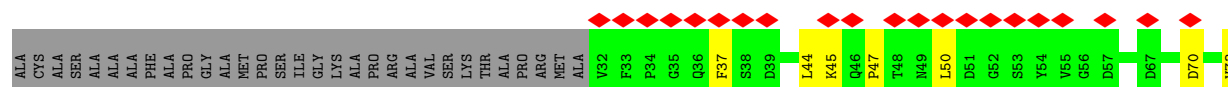
• Molecule 5: ACPII-4

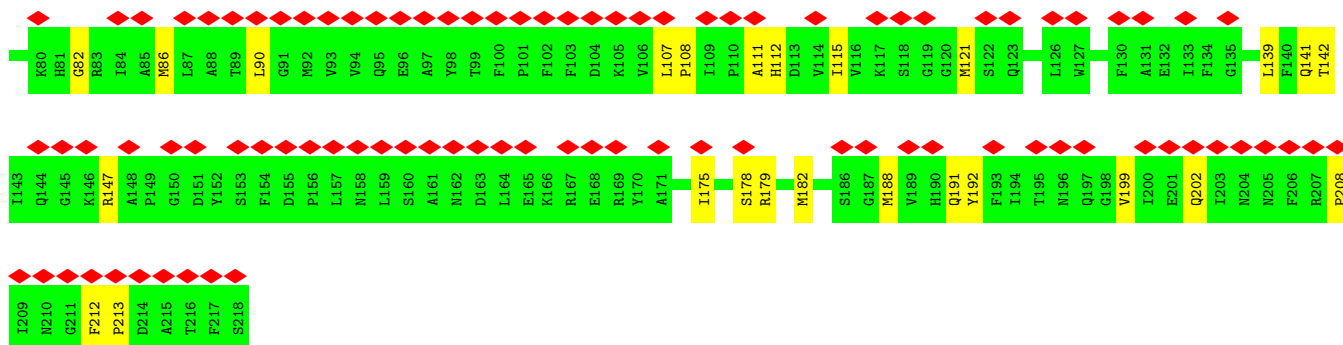


• Molecule 5: ACPII-4

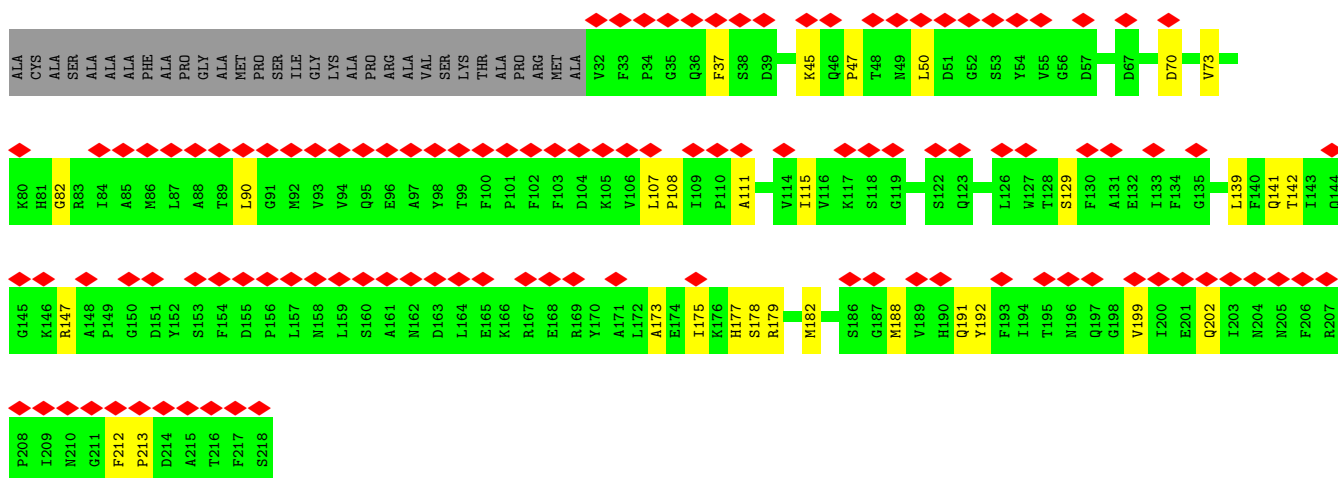


• Molecule 6: ACPII-5

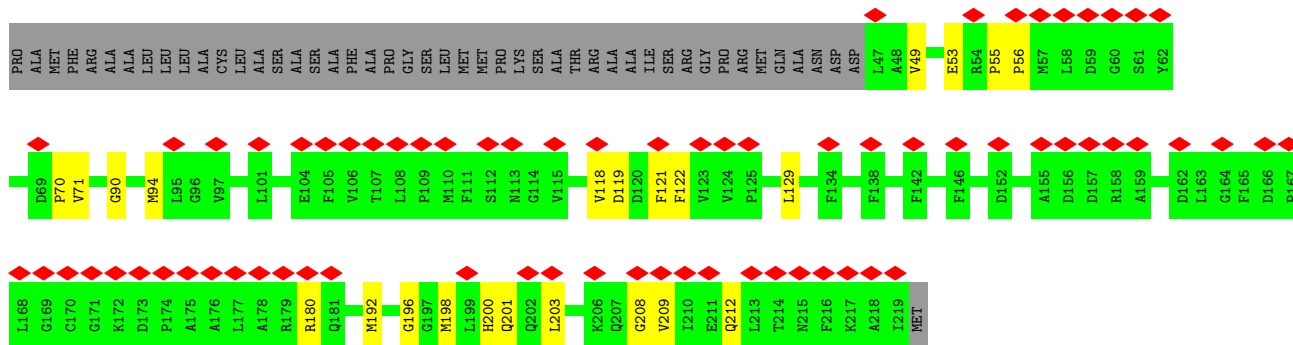




• Molecule 6: ACPII-5

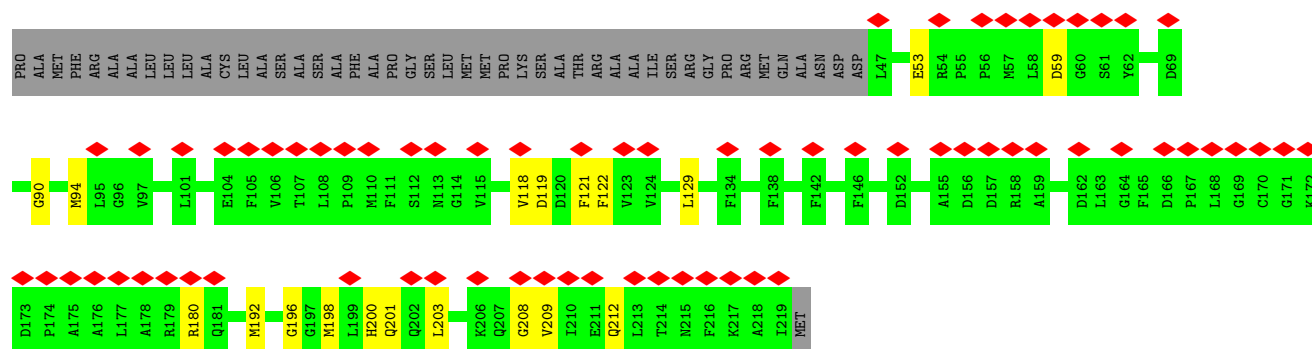


• Molecule 7: ACPII-6



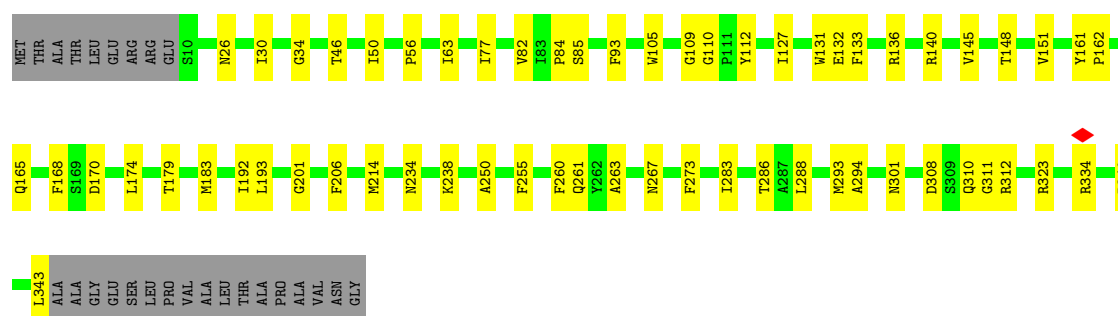
• Molecule 7: ACPII-6





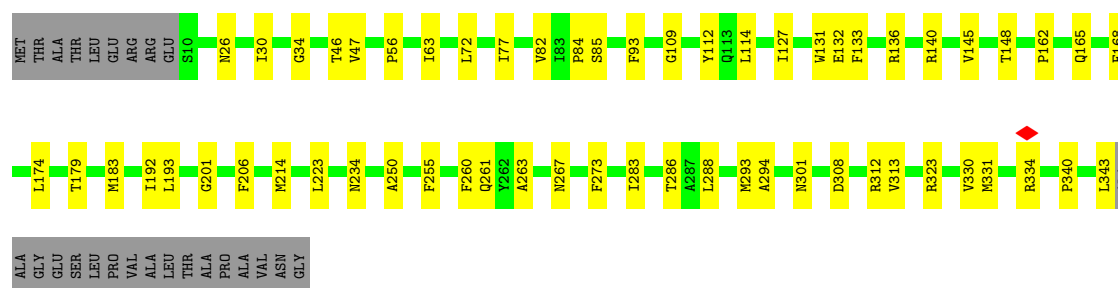
• Molecule 8: Photosystem II protein D1

Chain A: 76% 17% 7%



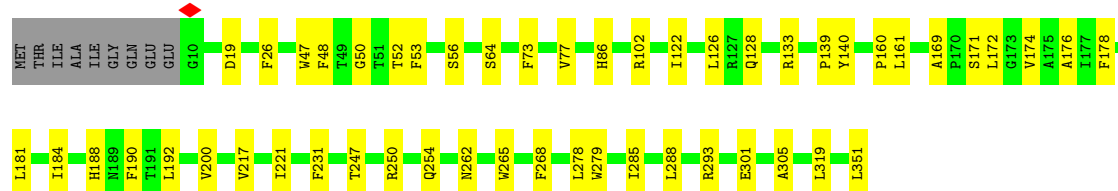
• Molecule 8: Photosystem II protein D1

Chain a: 76% 16% 7%



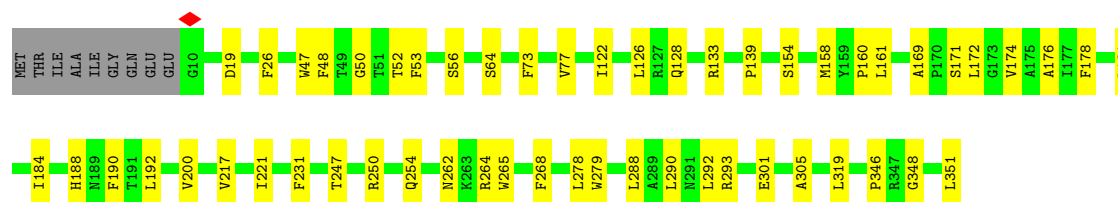
• Molecule 9: Photosystem II D2 protein

Chain D: 83% 15%



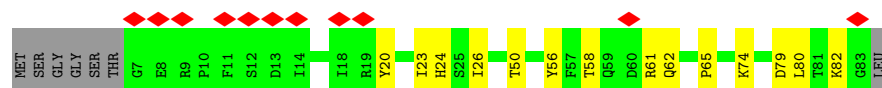
• Molecule 9: Photosystem II D2 protein

Chain d:  82% 15% .



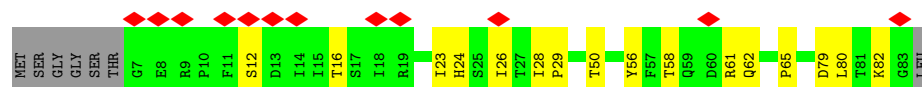
- Molecule 10: Cytochrome b559 subunit alpha

Chain E:  13% 75% 17% 8%



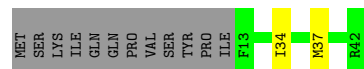
- Molecule 10: Cytochrome b559 subunit alpha

Chain e:  14% 73% 19% 8%



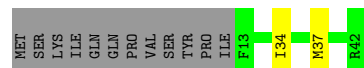
- Molecule 11: Cytochrome b559 subunit beta

Chain F:  67% 5% 29%



- Molecule 11: Cytochrome b559 subunit beta

Chain f:  67% 5% 29%



- Molecule 12: Photosystem II reaction center protein H

Chain H:  85% 12% .



- Molecule 12: Photosystem II reaction center protein H

Chain h:  85% 12% .



- Molecule 13: Photosystem II reaction center protein I

Chain I: 82% 11% 8%



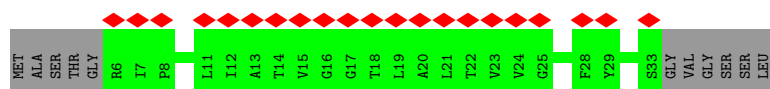
- Molecule 13: Photosystem II reaction center protein I

Chain i: 82% 11% 8%



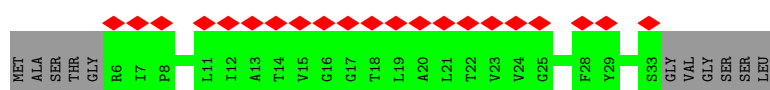
- Molecule 14: Photosystem II reaction center protein J

Chain J: 54% 72% 28%



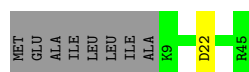
- Molecule 14: Photosystem II reaction center protein J

Chain j: 54% 72% 28%



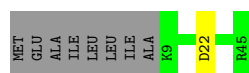
- Molecule 15: Photosystem II reaction center protein K

Chain K: 80% 18% 2%



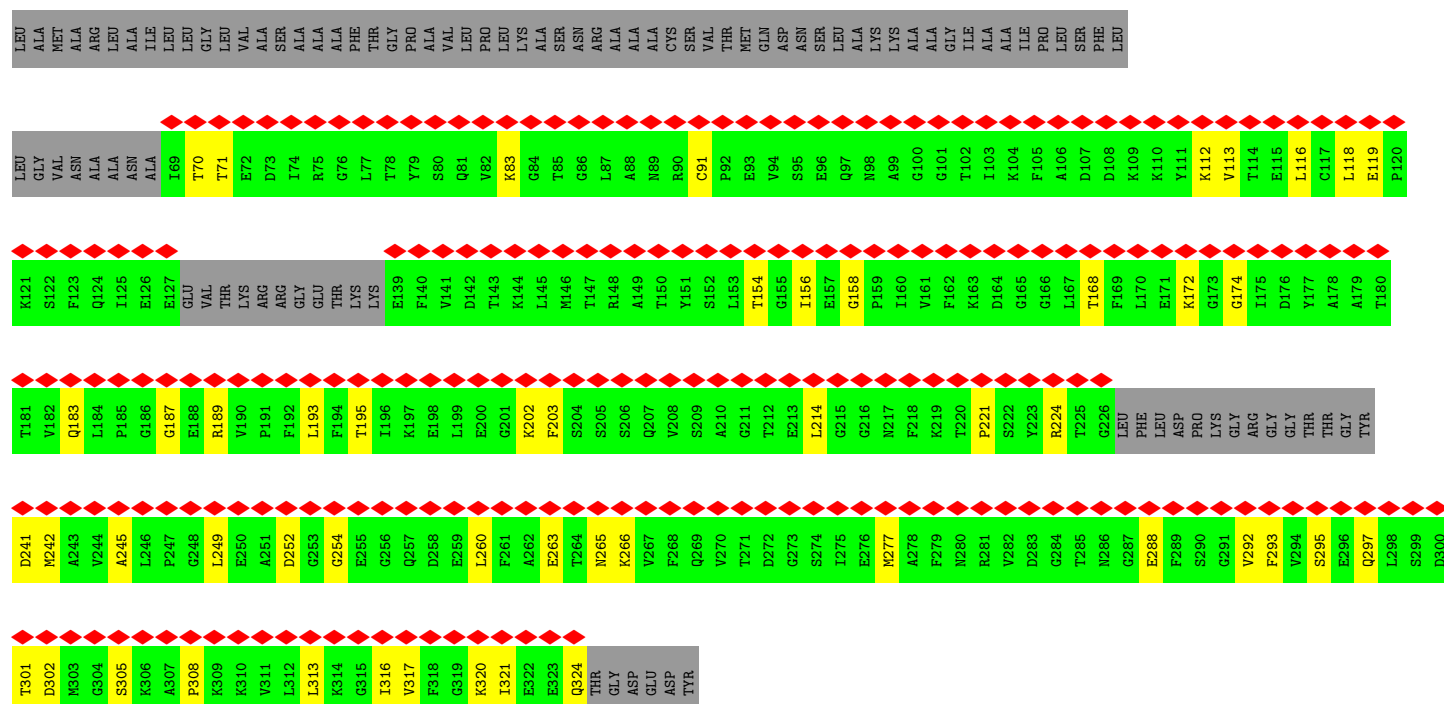
- Molecule 15: Photosystem II reaction center protein K

Chain k: 80% 18% 2%

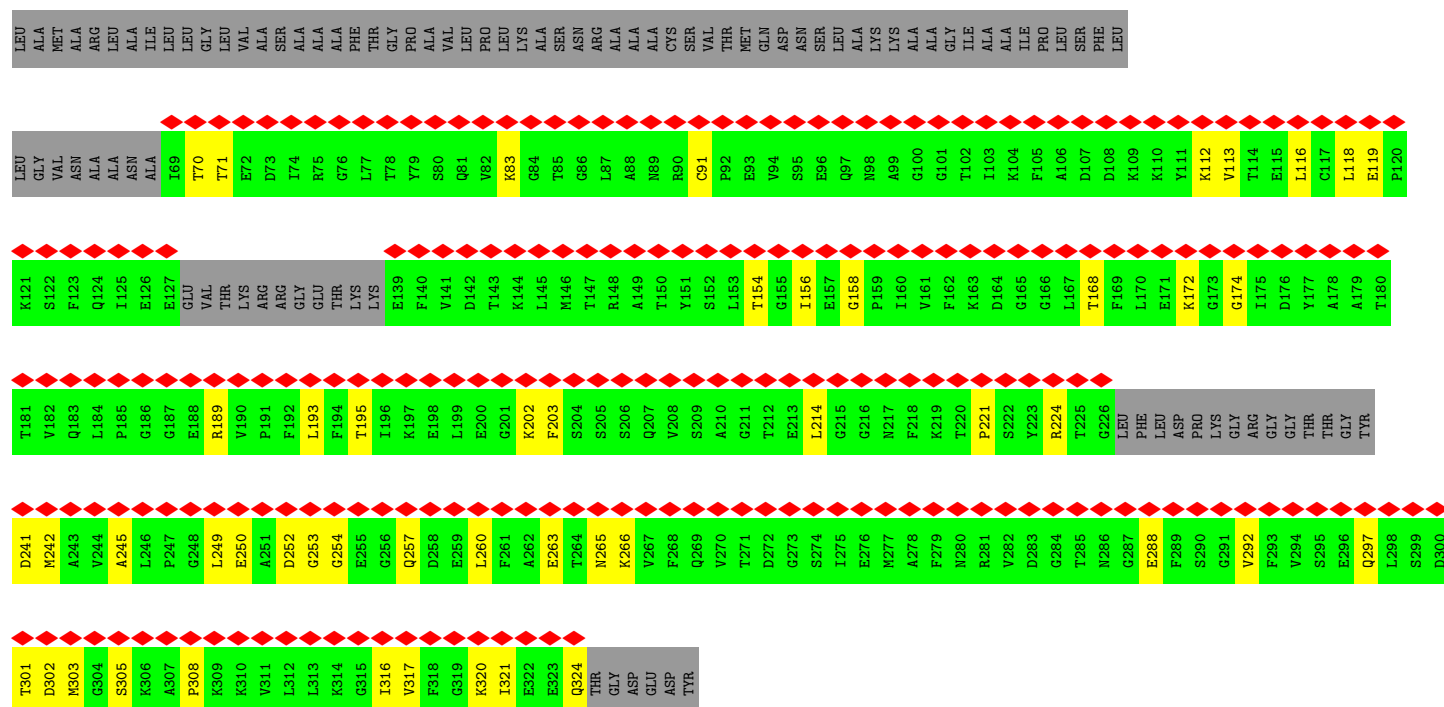


- Molecule 16: Photosystem II reaction center protein O

Chain O: 70% 55% 15% 30%

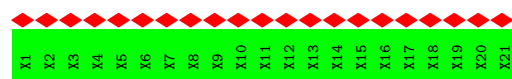


• Molecule 16: Photosystem II reaction center protein O

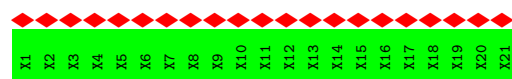


• Molecule 17: Photosystem II reaction center protein Q

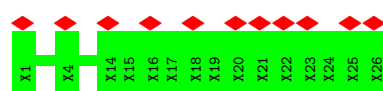
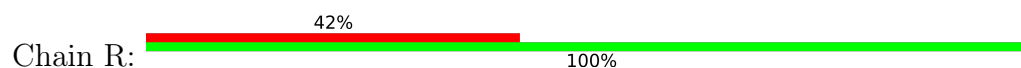




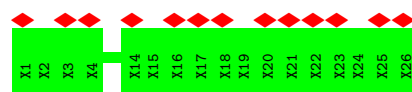
- Molecule 17: Photosystem II reaction center protein Q



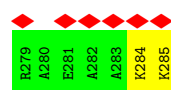
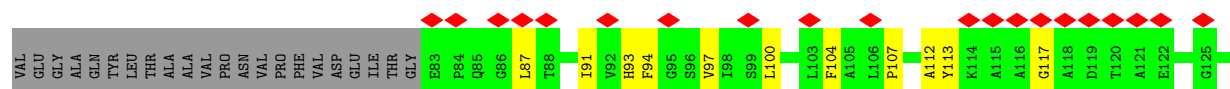
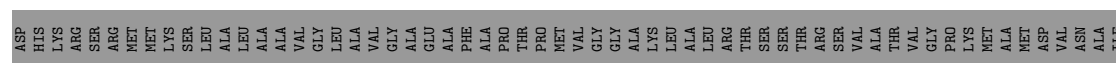
- Molecule 18: Photosystem II reaction center protein R



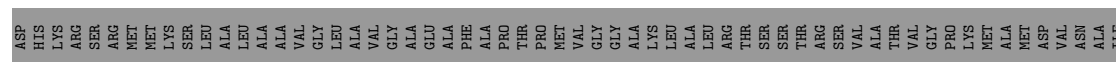
- Molecule 18: Photosystem II reaction center protein R

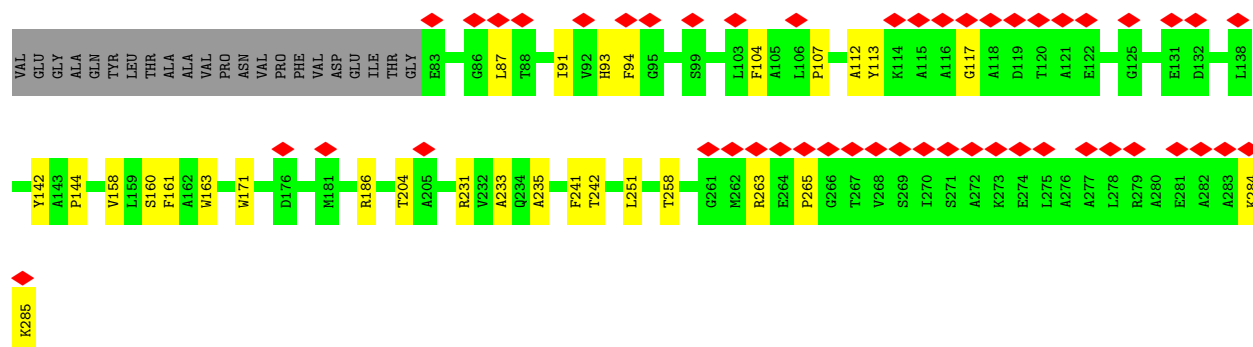


- Molecule 19: CCPH-S



- Molecule 19: CCPH-S





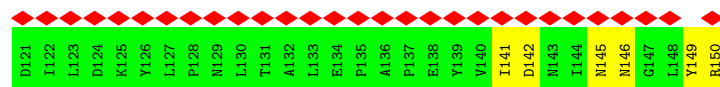
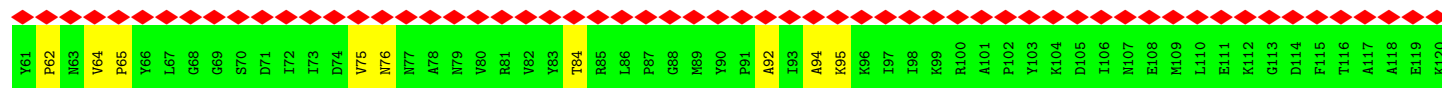
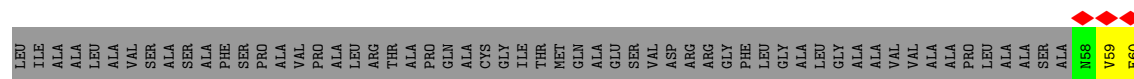
- Molecule 20: Photosystem II reaction center protein T



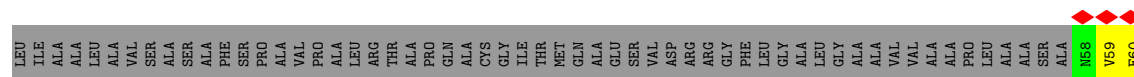
- Molecule 20: Photosystem II reaction center protein T

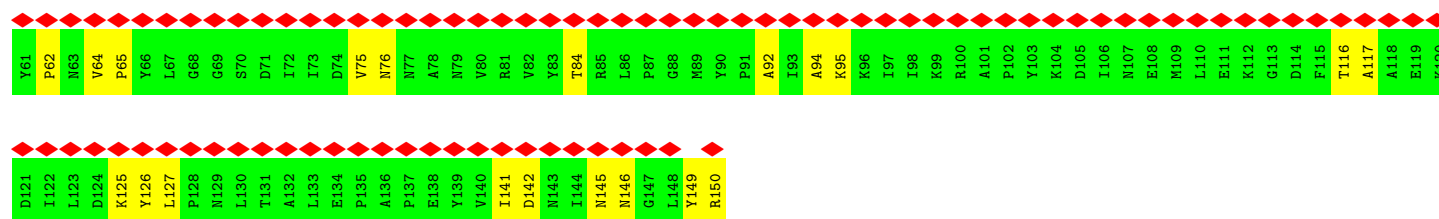


- Molecule 21: Photosystem II reaction center protein U

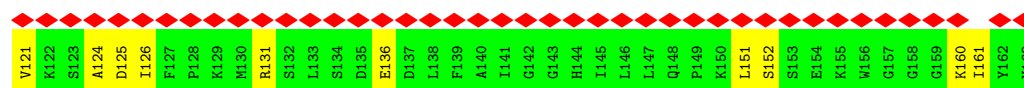
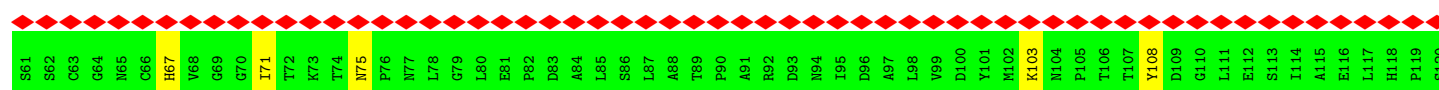
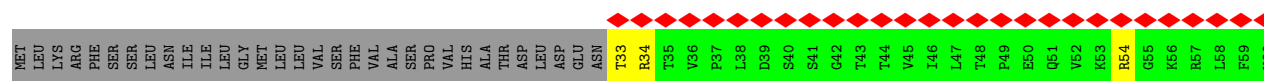
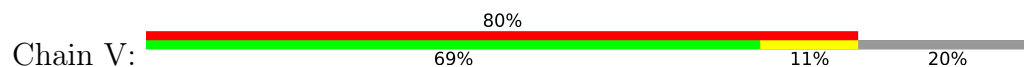


- Molecule 21: Photosystem II reaction center protein U

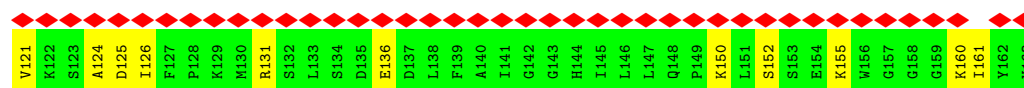
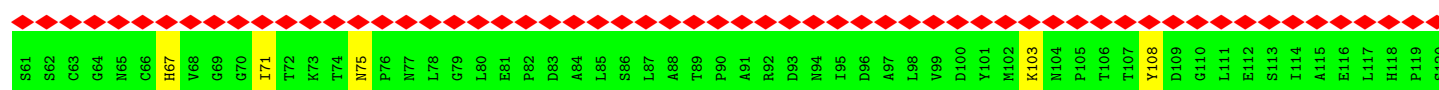
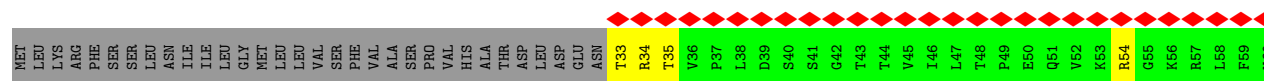
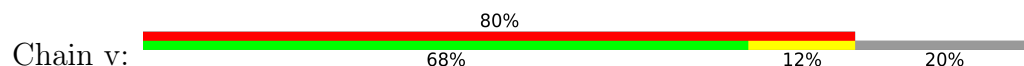




• Molecule 22: Photosystem II cytochrome c550



• Molecule 22: Photosystem II cytochrome c550



• Molecule 23: Photosystem II reaction center X protein

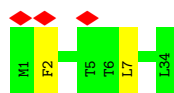


• Molecule 23: Photosystem II reaction center X protein

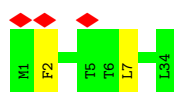




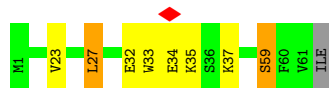
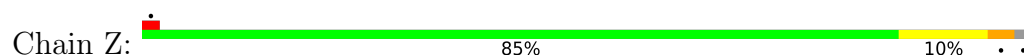
- Molecule 24: Photosystem II reaction center protein Ycf12



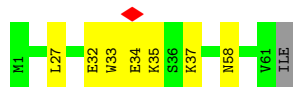
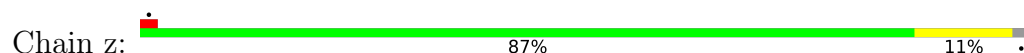
- Molecule 24: Photosystem II reaction center protein Ycf12



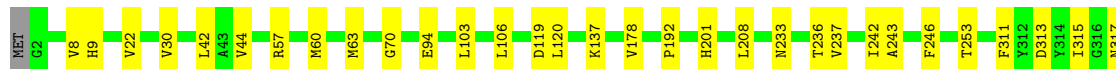
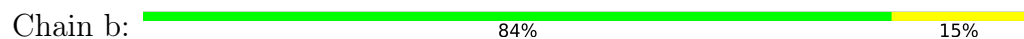
- Molecule 25: Photosystem II reaction center protein Z



- Molecule 25: Photosystem II reaction center protein Z

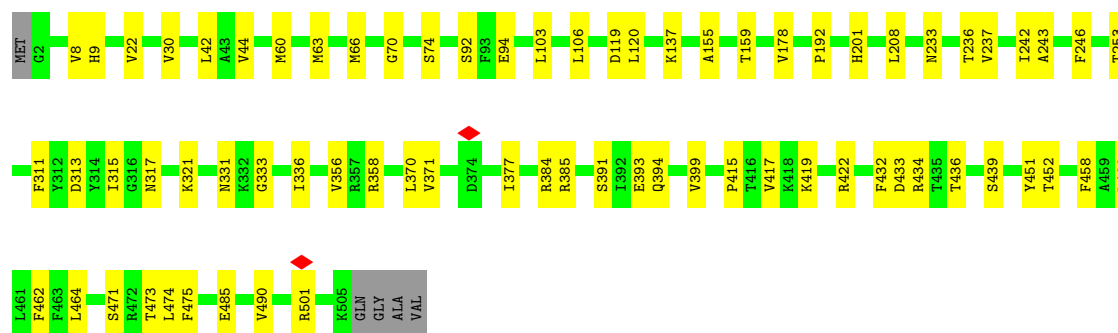


- Molecule 26: Photosystem II CP47 reaction center protein



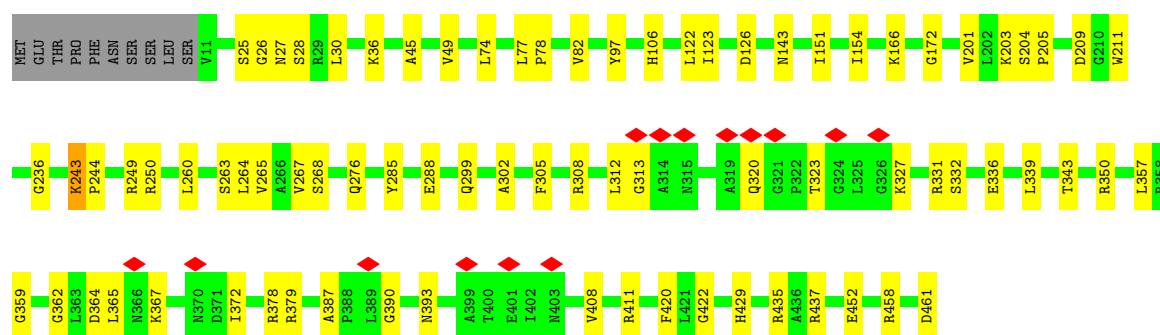
- Molecule 26: Photosystem II CP47 reaction center protein

Chain B:  85% 14%



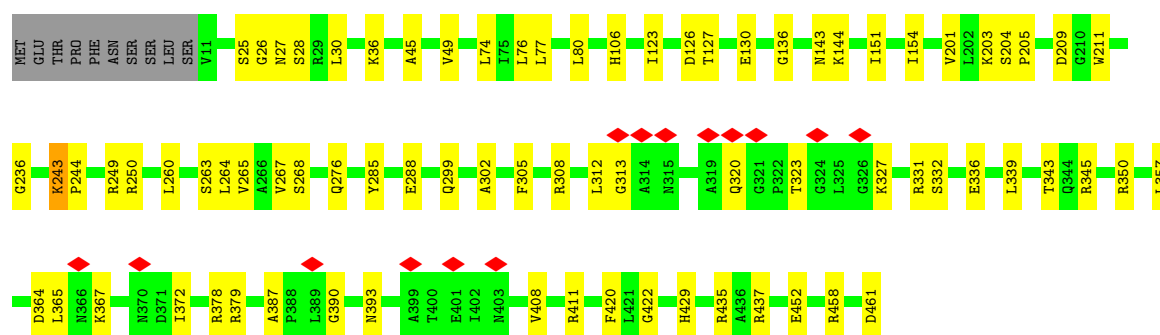
- Molecule 27: Photosystem II CP43 reaction center protein

Chain c:  81% 17%

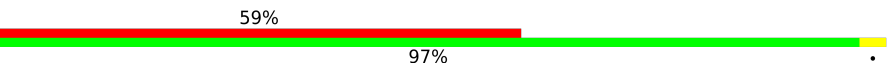


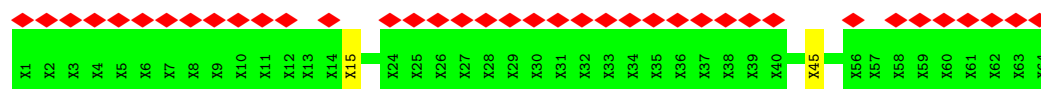
- Molecule 27: Photosystem II CP43 reaction center protein

Chain C:  81% 17%

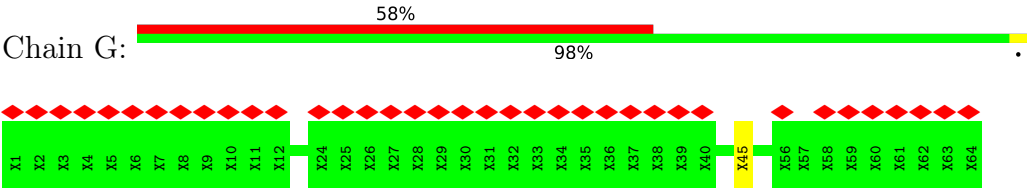


- Molecule 28: Photosystem II reaction center protein G

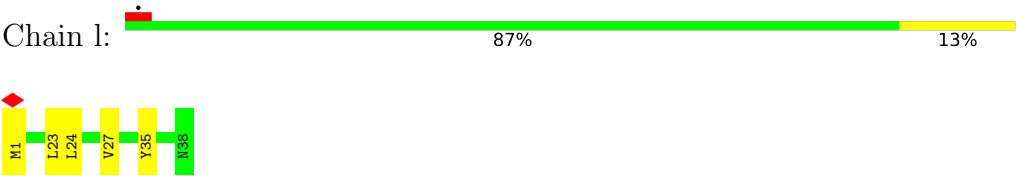
Chain g:  59% 97%



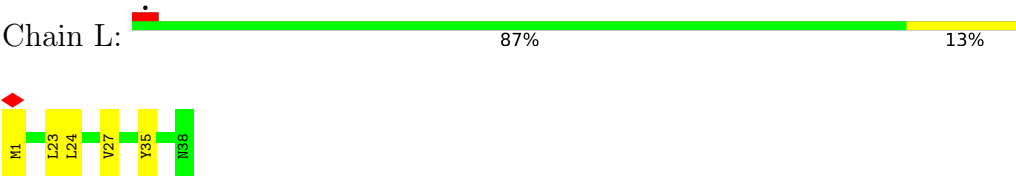
- Molecule 28: Photosystem II reaction center protein G



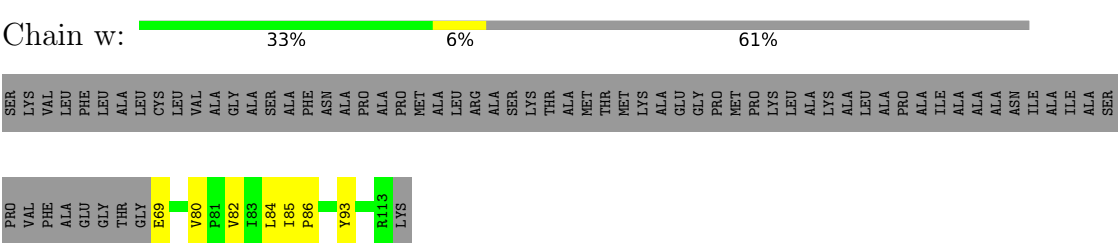
• Molecule 29: Photosystem II reaction center protein L



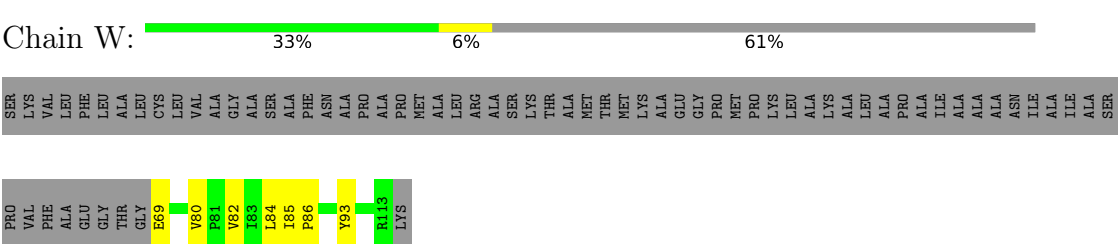
• Molecule 29: Photosystem II reaction center protein L



• Molecule 30: Photosystem II reaction center protein W



• Molecule 30: Photosystem II reaction center protein W



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	305400	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.307	Depositor
Minimum map value	-0.333	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.030	Depositor
Recommended contour level	0.253	Depositor
Map size (Å)	532.48, 532.48, 532.48	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.04, 1.04, 1.04	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SQD, CLA, II3, PL9, FE2, DGD, OEX, CL, IHT, LHG, BCT, 8CT, PHO, HEM, II0, LMG, KC2

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	M	0.19	0/268	0.32	0/367
1	m	0.20	0/268	0.36	0/367
2	1	0.12	0/1507	0.34	0/2043
2	7	0.12	0/1507	0.34	0/2043
3	2	0.12	0/1399	0.28	0/1893
3	8	0.12	0/1399	0.28	0/1893
4	3	0.13	0/1404	0.27	0/1895
4	9	0.13	0/1404	0.25	0/1895
5	0	0.12	0/1339	0.29	0/1814
5	4	0.12	0/1339	0.30	0/1814
6	5	0.11	0/1510	0.30	0/2046
6	p	0.11	0/1510	0.31	0/2046
7	6	0.09	0/1380	0.27	0/1870
7	P	0.10	0/1380	0.27	0/1870
8	A	0.20	0/2702	0.31	0/3688
8	a	0.19	0/2702	0.31	0/3688
9	D	0.19	0/2806	0.29	0/3823
9	d	0.19	0/2806	0.29	0/3823
10	E	0.13	0/647	0.31	0/882
10	e	0.14	0/647	0.36	0/882
11	F	0.15	0/255	0.31	0/344
11	f	0.15	0/255	0.31	0/344
12	H	0.17	0/527	0.29	0/717
12	h	0.17	0/527	0.29	0/717
13	I	0.18	0/294	0.32	0/397
13	i	0.18	0/294	0.31	0/397
14	J	0.11	0/220	0.26	0/301
14	j	0.10	0/220	0.25	0/301
15	K	0.20	0/308	0.34	0/421
15	k	0.20	0/308	0.34	0/421
16	O	0.08	0/1774	0.26	0/2385
16	o	0.08	0/1774	0.26	0/2385

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
19	S	0.13	0/1603	0.31	0/2180
19	s	0.13	0/1603	0.31	0/2180
20	T	0.17	0/267	0.23	0/359
20	t	0.17	0/267	0.22	0/359
21	U	0.11	0/758	0.32	0/1031
21	u	0.12	0/758	0.33	0/1031
22	V	0.08	0/1016	0.25	0/1377
22	v	0.08	0/1016	0.25	0/1377
23	X	0.17	0/296	0.31	0/402
23	x	0.16	0/296	0.26	0/402
24	Y	0.11	0/271	0.26	0/367
24	y	0.11	0/271	0.25	0/367
25	Z	0.21	0/467	0.39	0/638
25	z	0.13	0/467	0.31	0/638
26	B	0.17	0/4093	0.28	0/5569
26	b	0.17	0/4093	0.28	0/5569
27	C	0.19	0/3619	0.32	0/4937
27	c	0.19	0/3619	0.32	0/4937
29	L	0.18	0/320	0.23	0/434
29	l	0.18	0/320	0.23	0/434
30	W	0.19	0/374	0.38	0/509
30	w	0.19	0/374	0.38	0/509
All	All	0.16	0/62848	0.30	0/85378

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

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	M	265	0	280	5	0
1	m	265	0	280	4	0
2	1	1472	0	1473	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	7	1472	0	1473	20	0
3	2	1362	0	1348	20	0
3	8	1362	0	1348	20	0
4	3	1371	0	1370	16	0
4	9	1371	0	1370	13	0
5	0	1308	0	1323	13	0
5	4	1308	0	1323	12	0
6	5	1471	0	1445	21	0
6	p	1471	0	1445	18	0
7	6	1344	0	1329	17	0
7	P	1344	0	1329	13	0
8	A	2618	0	2514	55	0
8	a	2618	0	2514	54	0
9	D	2713	0	2613	50	0
9	d	2713	0	2613	52	0
10	E	629	0	613	8	0
10	e	629	0	613	10	0
11	F	247	0	250	1	0
11	f	247	0	250	1	0
12	H	515	0	535	7	0
12	h	515	0	535	7	0
13	I	287	0	293	3	0
13	i	287	0	293	3	0
14	J	214	0	222	0	0
14	j	214	0	222	0	0
15	K	297	0	312	1	0
15	k	297	0	312	1	0
16	O	1749	0	1721	36	0
16	o	1749	0	1721	35	0
17	Q	105	0	23	0	0
17	q	105	0	23	0	0
18	R	130	0	29	0	0
18	r	130	0	29	0	0
19	S	1563	0	1540	25	0
19	s	1563	0	1540	23	0
20	T	260	0	278	4	0
20	t	260	0	278	4	0
21	U	742	0	743	15	0
21	u	742	0	743	18	0
22	V	996	0	998	15	0
22	v	996	0	998	16	0
23	X	292	0	318	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	x	292	0	318	1	0
24	Y	266	0	293	1	0
24	y	266	0	293	1	0
25	Z	457	0	501	9	0
25	z	457	0	501	5	0
26	B	3962	0	3858	63	0
26	b	3962	0	3858	63	0
27	C	3504	0	3421	61	0
27	c	3504	0	3421	62	0
28	G	320	0	70	1	0
28	g	320	0	71	2	0
29	L	310	0	313	5	0
29	l	310	0	313	5	0
30	W	367	0	354	5	0
30	w	367	0	354	5	0
31	3	40	0	0	0	0
31	6	40	0	0	0	0
31	9	40	0	0	0	0
31	A	40	0	0	0	0
31	B	120	0	0	0	0
31	C	40	0	0	0	0
31	D	40	0	0	0	0
31	H	40	0	0	0	0
31	K	80	0	0	0	0
31	M	40	0	0	0	0
31	P	40	0	0	0	0
31	Z	40	0	0	1	0
31	a	40	0	0	0	0
31	b	80	0	0	0	0
31	c	40	0	0	0	0
31	d	40	0	0	0	0
31	h	40	0	0	0	0
31	k	80	0	0	0	0
31	z	40	0	0	1	0
32	0	582	0	469	14	0
32	1	582	0	469	15	0
32	2	547	0	456	14	0
32	3	548	0	456	11	0
32	4	582	0	469	15	0
32	5	547	0	456	8	0
32	6	442	0	364	6	0
32	7	582	0	469	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	8	547	0	456	13	0
32	9	548	0	456	12	0
32	A	174	0	170	11	0
32	B	987	0	1039	35	0
32	C	799	0	836	26	0
32	D	176	0	164	5	0
32	G	45	0	33	1	0
32	P	442	0	364	7	0
32	S	110	0	105	5	0
32	a	174	0	170	9	0
32	b	987	0	1039	29	0
32	c	799	0	836	21	0
32	d	176	0	164	2	0
32	g	45	0	33	2	0
32	p	547	0	456	8	0
32	s	110	0	105	4	0
33	0	45	0	0	0	0
33	1	45	0	0	0	0
33	2	45	0	0	0	0
33	4	45	0	0	0	0
33	5	45	0	0	0	0
33	6	90	0	0	0	0
33	7	45	0	0	0	0
33	8	45	0	0	0	0
33	P	90	0	0	3	0
33	p	45	0	0	0	0
34	0	168	0	0	1	0
34	1	168	0	0	1	0
34	2	168	0	0	0	0
34	3	126	0	0	0	0
34	4	126	0	0	1	0
34	5	210	0	0	0	0
34	6	84	0	0	0	0
34	7	168	0	0	1	0
34	8	168	0	0	0	0
34	9	126	0	0	0	0
34	P	84	0	0	0	0
34	p	168	0	0	0	0
35	1	42	0	0	0	0
35	6	42	0	0	0	0
35	7	42	0	0	0	0
35	P	42	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	0	82	0	0	0	0
36	1	41	0	0	1	0
36	2	41	0	0	0	0
36	4	82	0	0	0	0
36	5	41	0	0	0	0
36	7	41	0	0	0	0
36	8	41	0	0	0	0
36	p	41	0	0	0	0
37	0	36	0	42	0	0
37	2	36	0	42	1	0
37	4	36	0	42	0	0
37	6	28	0	26	0	0
37	8	36	0	42	2	0
37	A	48	0	66	2	0
37	B	51	0	72	0	0
37	C	46	0	62	3	0
37	D	86	0	112	1	0
37	G	28	0	26	0	0
37	L	40	0	50	1	0
37	P	28	0	26	0	0
37	a	48	0	66	3	0
37	b	51	0	72	1	0
37	c	46	0	62	3	0
37	d	86	0	112	1	0
37	g	28	0	26	0	0
37	l	40	0	50	0	0
38	2	22	0	20	0	0
38	8	22	0	20	0	0
38	A	92	0	133	10	0
38	B	78	0	96	3	0
38	D	80	0	108	1	0
38	L	49	0	74	2	0
38	S	37	0	44	1	0
38	a	92	0	133	10	0
38	b	78	0	96	3	0
38	d	80	0	108	1	0
38	l	49	0	74	2	0
38	s	37	0	44	1	0
39	5	35	0	34	4	0
39	A	54	0	78	5	0
39	B	102	0	141	3	0
39	a	54	0	78	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
39	b	102	0	141	2	0
39	p	35	0	34	3	0
40	A	10	0	0	0	0
40	a	10	0	0	0	0
41	A	64	0	74	1	0
41	D	64	0	74	3	0
41	a	64	0	74	1	0
41	d	64	0	74	3	0
42	A	1	0	0	0	0
42	a	1	0	0	0	0
43	A	13	0	7	0	0
43	D	55	0	80	0	0
43	a	13	0	7	0	0
43	d	55	0	80	0	0
44	A	4	0	1	0	0
44	a	4	0	1	0	0
45	A	53	0	64	1	0
45	C	166	0	206	11	0
45	H	62	0	82	6	0
45	a	53	0	64	1	0
45	c	166	0	206	8	0
45	h	62	0	82	5	0
46	D	1	0	0	0	0
46	d	1	0	0	0	0
47	E	43	0	30	2	0
47	V	43	0	30	3	0
47	f	43	0	30	3	0
47	v	43	0	30	3	0
All	All	80246	0	74543	987	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 6.

The worst 5 of 987 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:m:103:ARG:HG3	1:M:106:ALA:HB2	1.64	0.80
26:b:434:ARG:HH12	16:o:249:LEU:HA	1.48	0.79
25:Z:59:SER:HB2	33:P:605:KC2:O1A	1.83	0.77
1:m:106:ALA:HB2	1:M:103:ARG:HG3	1.65	0.76
9:d:351:LEU:HD21	8:a:334:ARG:HE	1.50	0.76

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	M	34/115 (30%)	32 (94%)	2 (6%)	0	100	100
1	m	34/115 (30%)	32 (94%)	2 (6%)	0	100	100
2	1	192/235 (82%)	183 (95%)	9 (5%)	0	100	100
2	7	192/235 (82%)	186 (97%)	6 (3%)	0	100	100
3	2	171/217 (79%)	168 (98%)	3 (2%)	0	100	100
3	8	171/217 (79%)	169 (99%)	2 (1%)	0	100	100
4	3	176/222 (79%)	173 (98%)	2 (1%)	1 (1%)	21	35
4	9	176/222 (79%)	173 (98%)	3 (2%)	0	100	100
5	0	170/226 (75%)	167 (98%)	2 (1%)	1 (1%)	21	35
5	4	170/226 (75%)	167 (98%)	2 (1%)	1 (1%)	21	35
6	5	185/218 (85%)	182 (98%)	3 (2%)	0	100	100
6	p	185/218 (85%)	181 (98%)	4 (2%)	0	100	100
7	6	171/220 (78%)	171 (100%)	0	0	100	100
7	P	171/220 (78%)	171 (100%)	0	0	100	100
8	A	332/360 (92%)	326 (98%)	6 (2%)	0	100	100
8	a	332/360 (92%)	328 (99%)	4 (1%)	0	100	100
9	D	340/351 (97%)	335 (98%)	5 (2%)	0	100	100
9	d	340/351 (97%)	337 (99%)	3 (1%)	0	100	100
10	E	75/84 (89%)	75 (100%)	0	0	100	100
10	e	75/84 (89%)	75 (100%)	0	0	100	100
11	F	28/42 (67%)	28 (100%)	0	0	100	100
11	f	28/42 (67%)	28 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	H	63/67 (94%)	60 (95%)	3 (5%)	0	100	100
12	h	63/67 (94%)	60 (95%)	3 (5%)	0	100	100
13	I	33/38 (87%)	33 (100%)	0	0	100	100
13	i	33/38 (87%)	33 (100%)	0	0	100	100
14	J	26/39 (67%)	26 (100%)	0	0	100	100
14	j	26/39 (67%)	26 (100%)	0	0	100	100
15	K	35/45 (78%)	34 (97%)	1 (3%)	0	100	100
15	k	35/45 (78%)	34 (97%)	1 (3%)	0	100	100
16	O	225/330 (68%)	212 (94%)	13 (6%)	0	100	100
16	o	225/330 (68%)	213 (95%)	12 (5%)	0	100	100
19	S	201/285 (70%)	183 (91%)	18 (9%)	0	100	100
19	s	201/285 (70%)	183 (91%)	18 (9%)	0	100	100
20	T	30/32 (94%)	29 (97%)	1 (3%)	0	100	100
20	t	30/32 (94%)	29 (97%)	1 (3%)	0	100	100
21	U	91/150 (61%)	84 (92%)	7 (8%)	0	100	100
21	u	91/150 (61%)	82 (90%)	9 (10%)	0	100	100
22	V	129/163 (79%)	125 (97%)	4 (3%)	0	100	100
22	v	129/163 (79%)	125 (97%)	4 (3%)	0	100	100
23	X	37/39 (95%)	36 (97%)	1 (3%)	0	100	100
23	x	37/39 (95%)	36 (97%)	1 (3%)	0	100	100
24	Y	32/34 (94%)	32 (100%)	0	0	100	100
24	y	32/34 (94%)	32 (100%)	0	0	100	100
25	Z	59/62 (95%)	56 (95%)	3 (5%)	0	100	100
25	z	59/62 (95%)	57 (97%)	2 (3%)	0	100	100
26	B	502/509 (99%)	496 (99%)	6 (1%)	0	100	100
26	b	502/509 (99%)	497 (99%)	5 (1%)	0	100	100
27	C	449/461 (97%)	443 (99%)	6 (1%)	0	100	100
27	c	449/461 (97%)	442 (98%)	7 (2%)	0	100	100
29	L	36/38 (95%)	34 (94%)	2 (6%)	0	100	100
29	l	36/38 (95%)	34 (94%)	2 (6%)	0	100	100
30	W	43/114 (38%)	43 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
30	w	43/114 (38%)	43 (100%)	0	0	100	100
All	All	7730/9392 (82%)	7539 (98%)	188 (2%)	3 (0%)	100	100

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	3	212	ILE
5	4	126	ILE
5	0	126	ILE

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	M	28/84 (33%)	28 (100%)	0	100	100
1	m	28/84 (33%)	28 (100%)	0	100	100
2	1	149/179 (83%)	149 (100%)	0	100	100
2	7	149/179 (83%)	149 (100%)	0	100	100
3	2	139/167 (83%)	139 (100%)	0	100	100
3	8	139/167 (83%)	139 (100%)	0	100	100
4	3	143/175 (82%)	143 (100%)	0	100	100
4	9	143/175 (82%)	143 (100%)	0	100	100
5	0	136/169 (80%)	136 (100%)	0	100	100
5	4	136/169 (80%)	136 (100%)	0	100	100
6	5	157/175 (90%)	157 (100%)	0	100	100
6	p	157/175 (90%)	157 (100%)	0	100	100
7	6	141/174 (81%)	141 (100%)	0	100	100
7	P	141/174 (81%)	141 (100%)	0	100	100
8	A	271/289 (94%)	271 (100%)	0	100	100
8	a	271/289 (94%)	271 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	D	274/281 (98%)	274 (100%)	0	100	100
9	d	274/281 (98%)	274 (100%)	0	100	100
10	E	68/73 (93%)	68 (100%)	0	100	100
10	e	68/73 (93%)	68 (100%)	0	100	100
11	F	25/37 (68%)	25 (100%)	0	100	100
11	f	25/37 (68%)	25 (100%)	0	100	100
12	H	56/58 (97%)	56 (100%)	0	100	100
12	h	56/58 (97%)	56 (100%)	0	100	100
13	I	33/36 (92%)	33 (100%)	0	100	100
13	i	33/36 (92%)	33 (100%)	0	100	100
14	J	22/29 (76%)	22 (100%)	0	100	100
14	j	22/29 (76%)	22 (100%)	0	100	100
15	K	30/36 (83%)	30 (100%)	0	100	100
15	k	30/36 (83%)	30 (100%)	0	100	100
16	O	189/258 (73%)	189 (100%)	0	100	100
16	o	189/258 (73%)	189 (100%)	0	100	100
19	S	159/219 (73%)	159 (100%)	0	100	100
19	s	159/219 (73%)	159 (100%)	0	100	100
20	T	27/27 (100%)	27 (100%)	0	100	100
20	t	27/27 (100%)	27 (100%)	0	100	100
21	U	80/115 (70%)	80 (100%)	0	100	100
21	u	80/115 (70%)	79 (99%)	1 (1%)	61	80
22	V	112/141 (79%)	112 (100%)	0	100	100
22	v	112/141 (79%)	112 (100%)	0	100	100
23	X	34/34 (100%)	34 (100%)	0	100	100
23	x	34/34 (100%)	34 (100%)	0	100	100
24	Y	29/29 (100%)	29 (100%)	0	100	100
24	y	29/29 (100%)	29 (100%)	0	100	100
25	Z	50/51 (98%)	48 (96%)	2 (4%)	28	51
25	z	50/51 (98%)	50 (100%)	0	100	100
26	B	401/404 (99%)	401 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
26	b	401/404 (99%)	401 (100%)	0	100	100
27	C	356/366 (97%)	355 (100%)	1 (0%)	86	93
27	c	356/366 (97%)	355 (100%)	1 (0%)	86	93
29	L	35/35 (100%)	35 (100%)	0	100	100
29	l	35/35 (100%)	35 (100%)	0	100	100
30	W	40/85 (47%)	40 (100%)	0	100	100
30	w	40/85 (47%)	40 (100%)	0	100	100
All	All	6368/7452 (86%)	6363 (100%)	5 (0%)	87	95

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
25	Z	27	LEU
25	Z	59	SER
27	c	243	LYS
21	u	127	LEU
27	C	243	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 95 such sidechains are listed below:

Mol	Chain	Res	Type
5	0	208	HIS
27	C	299	GLN
2	7	182	ASN
27	C	41	HIS
7	P	103	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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 376 ligands modelled in this entry, 4 are monoatomic - leaving 372 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
38	LHG	L	101	-	48,48,48	0.65	1 (2%)	51,54,54	1.30	7 (13%)
32	CLA	5	312	-	49,53,73	1.39	8 (16%)	58,89,113	1.43	4 (6%)
43	PL9	d	404	-	55,55,55	1.27	5 (9%)	68,69,69	1.51	13 (19%)
37	LMG	c	517	-	46,46,55	0.77	1 (2%)	54,54,63	1.32	6 (11%)
32	CLA	p	313	-	49,53,73	1.39	8 (16%)	58,89,113	1.37	4 (6%)
33	KC2	P	609	-	49,53,53	1.74	8 (16%)	60,89,89	1.87	15 (25%)
32	CLA	3	610	4	49,53,73	1.39	9 (18%)	58,89,113	1.43	4 (6%)
32	CLA	1	609	-	45,49,73	1.42	8 (17%)	54,84,113	1.47	5 (9%)
32	CLA	c	502	-	68,72,73	1.17	8 (11%)	80,111,113	1.29	5 (6%)
33	KC2	6	605	7	49,53,53	1.78	8 (16%)	60,89,89	1.83	14 (23%)
32	CLA	B	610	-	69,73,73	1.16	9 (13%)	82,113,113	1.27	6 (7%)
34	II0	5	314	-	39,43,43	2.02	2 (5%)	48,60,60	1.71	13 (27%)
32	CLA	1	601	-	46,50,73	1.41	8 (17%)	53,85,113	1.40	4 (7%)
33	KC2	8	610	-	49,53,53	1.76	9 (18%)	60,89,89	1.87	14 (23%)
32	CLA	7	607	-	49,53,73	1.39	8 (16%)	58,89,113	1.35	4 (6%)
32	CLA	d	403	-	64,68,73	1.19	9 (14%)	76,107,113	1.35	9 (11%)
32	CLA	1	612	-	49,53,73	1.39	7 (14%)	58,89,113	1.36	4 (6%)
32	CLA	P	611	-	49,53,73	1.39	8 (16%)	58,89,113	1.43	4 (6%)
31	8CT	k	101	-	40,41,41	4.79	23 (57%)	51,56,56	2.72	20 (39%)
32	CLA	c	505	-	69,73,73	1.15	8 (11%)	82,113,113	1.28	7 (8%)
38	LHG	d	405	-	44,47,48	0.56	1 (2%)	44,51,54	1.20	6 (13%)
34	II0	7	619	-	39,43,43	2.00	2 (5%)	48,60,60	1.57	9 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
34	II0	p	315	-	39,43,43	2.05	2 (5%)	48,60,60	1.62	10 (20%)
31	8CT	B	624	-	40,41,41	4.81	23 (57%)	51,56,56	2.84	17 (33%)
32	CLA	4	613	5	49,53,73	1.40	8 (16%)	58,89,113	1.40	4 (6%)
47	HEM	v	201	-	50,50,50	1.45	9 (18%)	67,82,82	1.05	5 (7%)
31	8CT	M	201	-	40,41,41	4.78	23 (57%)	51,56,56	3.01	19 (37%)
45	DGD	H	101	-	63,63,67	0.88	2 (3%)	77,77,81	1.37	8 (10%)
32	CLA	5	310	-	45,49,73	1.42	8 (17%)	54,84,113	1.46	5 (9%)
33	KC2	0	610	5	49,53,53	1.74	8 (16%)	60,89,89	1.89	15 (25%)
37	LMG	B	618	-	51,51,55	0.74	1 (1%)	59,59,63	1.35	6 (10%)
32	CLA	9	610	4	49,53,73	1.39	8 (16%)	58,89,113	1.44	4 (6%)
32	CLA	0	608	5	64,68,73	1.21	8 (12%)	76,107,113	1.28	5 (6%)
34	II0	2	613	-	39,43,43	2.02	2 (5%)	48,60,60	1.62	9 (18%)
38	LHG	a	402	-	42,42,48	0.68	1 (2%)	45,48,54	1.25	4 (8%)
32	CLA	p	304	-	54,58,73	1.32	8 (14%)	64,95,113	1.38	6 (9%)
32	CLA	B	603	-	64,69,73	1.17	9 (14%)	73,106,113	1.21	4 (5%)
32	CLA	c	501	-	69,73,73	1.14	9 (13%)	82,113,113	1.30	6 (7%)
32	CLA	g	102	-	49,53,73	1.40	8 (16%)	58,89,113	1.37	4 (6%)
32	CLA	4	607	5	49,53,73	1.39	8 (16%)	58,89,113	1.34	4 (6%)
32	CLA	5	304	-	54,58,73	1.33	8 (14%)	64,95,113	1.39	6 (9%)
32	CLA	c	506	-	49,53,73	1.37	9 (18%)	58,89,113	1.44	5 (8%)
32	CLA	7	601	-	46,50,73	1.41	8 (17%)	53,85,113	1.40	4 (7%)
32	CLA	0	603	-	54,58,73	1.32	8 (14%)	64,95,113	1.38	6 (9%)
32	CLA	1	603	-	54,58,73	1.32	8 (14%)	64,95,113	1.38	6 (9%)
34	II0	1	616	-	39,43,43	2.05	2 (5%)	48,60,60	1.63	11 (22%)
34	II0	7	617	-	39,43,43	2.05	2 (5%)	48,60,60	1.63	9 (18%)
33	KC2	7	610	-	49,53,53	1.74	8 (16%)	60,89,89	1.88	15 (25%)
32	CLA	0	609	-	45,49,73	1.43	8 (17%)	54,84,113	1.46	5 (9%)
45	DGD	c	514	-	56,56,67	0.98	2 (3%)	70,70,81	1.47	10 (14%)
32	CLA	2	605	3	64,68,73	1.23	8 (12%)	76,107,113	1.29	5 (6%)
32	CLA	c	507	-	69,73,73	1.15	9 (13%)	82,113,113	1.28	5 (6%)
32	CLA	B	609	-	69,73,73	1.15	9 (13%)	82,113,113	1.28	6 (7%)
38	LHG	l	102	-	48,48,48	0.65	1 (2%)	51,54,54	1.30	6 (11%)
31	8CT	B	623	-	40,41,41	4.81	23 (57%)	51,56,56	2.52	17 (33%)
34	II0	2	615	-	39,43,43	2.04	3 (7%)	48,60,60	1.67	11 (22%)
32	CLA	4	604	-	59,63,73	1.27	8 (13%)	70,101,113	1.35	8 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	CLA	8	603	-	54,58,73	1.31	8 (14%)	64,95,113	1.40	6 (9%)
31	8CT	k	102	-	40,41,41	4.81	23 (57%)	51,56,56	2.81	18 (35%)
32	CLA	7	603	-	54,58,73	1.32	7 (12%)	64,95,113	1.40	8 (12%)
32	CLA	8	607	3	49,53,73	1.37	8 (16%)	58,89,113	1.40	4 (6%)
39	SQD	A	606	-	52,54,54	1.54	7 (13%)	62,65,65	1.35	8 (12%)
32	CLA	b	611	-	69,73,73	1.16	8 (11%)	82,113,113	1.27	6 (7%)
32	CLA	3	601	4	46,50,73	1.40	8 (17%)	53,85,113	1.44	4 (7%)
32	CLA	8	608	3	64,68,73	1.21	9 (14%)	76,107,113	1.29	5 (6%)
34	II0	9	612	-	39,43,43	2.02	2 (5%)	48,60,60	1.57	11 (22%)
32	CLA	p	312	-	49,53,73	1.39	8 (16%)	58,89,113	1.43	4 (6%)
32	CLA	p	302	6	46,50,73	1.41	8 (17%)	53,85,113	1.42	4 (7%)
32	CLA	b	614	-	69,73,73	1.15	9 (13%)	82,113,113	1.25	6 (7%)
32	CLA	b	608	-	45,49,73	1.38	9 (20%)	54,84,113	1.48	5 (9%)
32	CLA	9	601	4	46,50,73	1.40	8 (17%)	53,85,113	1.46	5 (9%)
32	CLA	s	303	19	69,73,73	1.17	8 (11%)	82,113,113	1.26	5 (6%)
38	LHG	D	406	-	44,47,48	0.56	1 (2%)	44,51,54	1.21	6 (13%)
32	CLA	5	302	6	46,50,73	1.41	8 (17%)	53,85,113	1.42	4 (7%)
32	CLA	P	608	-	45,49,73	1.41	8 (17%)	54,84,113	1.44	5 (9%)
32	CLA	0	601	5	46,50,73	1.41	8 (17%)	53,85,113	1.42	4 (7%)
47	HEM	E	101	-	50,50,50	1.44	7 (14%)	67,82,82	1.13	4 (5%)
32	CLA	B	613	-	69,73,73	1.14	9 (13%)	82,113,113	1.31	8 (9%)
32	CLA	4	606	-	49,53,73	1.40	8 (16%)	58,89,113	1.33	4 (6%)
32	CLA	8	609	38	45,49,73	1.41	8 (17%)	54,84,113	1.46	5 (9%)
32	CLA	C	501	-	69,73,73	1.15	9 (13%)	82,113,113	1.30	6 (7%)
38	LHG	a	403	-	48,48,48	0.66	1 (2%)	51,54,54	1.28	6 (11%)
32	CLA	C	502	-	68,72,73	1.17	9 (13%)	80,111,113	1.29	5 (6%)
34	II0	P	614	-	39,43,43	2.02	2 (5%)	48,60,60	1.60	10 (20%)
32	CLA	C	504	-	68,72,73	1.15	9 (13%)	80,111,113	1.30	6 (7%)
33	KC2	6	609	-	49,53,53	1.74	8 (16%)	60,89,89	1.86	15 (25%)
36	IHT	2	616	-	40,42,42	1.53	2 (5%)	52,58,58	1.93	13 (25%)
32	CLA	8	601	3	46,50,73	1.40	8 (17%)	53,85,113	1.41	4 (7%)
32	CLA	P	607	7	64,68,73	1.22	9 (14%)	76,107,113	1.29	5 (6%)
32	CLA	5	308	6	49,53,73	1.39	9 (18%)	58,89,113	1.40	4 (6%)
32	CLA	7	612	-	49,53,73	1.39	8 (16%)	58,89,113	1.37	4 (6%)
32	CLA	p	305	-	59,63,73	1.27	8 (13%)	70,101,113	1.35	6 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	CLA	p	308	6	49,53,73	1.40	9 (18%)	58,89,113	1.41	4 (6%)
34	II0	0	616	-	39,43,43	2.04	2 (5%)	48,60,60	1.63	11 (22%)
34	II0	9	613	-	39,43,43	2.03	2 (5%)	48,60,60	1.58	9 (18%)
32	CLA	6	601	7	46,50,73	1.41	8 (17%)	53,85,113	1.40	4 (7%)
32	CLA	3	611	-	49,53,73	1.37	9 (18%)	58,89,113	1.39	4 (6%)
32	CLA	b	615	-	68,72,73	1.15	9 (13%)	80,111,113	1.27	5 (6%)
39	SQD	p	318	-	33,35,54	1.77	7 (21%)	43,46,65	1.50	6 (13%)
34	II0	0	615	-	39,43,43	2.01	2 (5%)	48,60,60	1.62	12 (25%)
32	CLA	D	404	-	64,68,73	1.19	9 (14%)	76,107,113	1.35	9 (11%)
31	8CT	d	408	-	40,41,41	4.84	23 (57%)	51,56,56	2.49	16 (31%)
32	CLA	1	607	-	49,53,73	1.38	8 (16%)	58,89,113	1.36	4 (6%)
32	CLA	3	607	4	64,68,73	1.21	9 (14%)	76,107,113	1.31	4 (5%)
41	PHO	a	407	-	58,69,69	2.10	11 (18%)	55,99,99	1.44	7 (12%)
34	II0	p	314	-	39,43,43	2.02	2 (5%)	48,60,60	1.71	13 (27%)
32	CLA	b	602	-	51,55,73	1.33	9 (17%)	60,91,113	1.38	5 (8%)
32	CLA	S	303	19	69,73,73	1.17	8 (11%)	82,113,113	1.26	5 (6%)
32	CLA	C	505	-	69,73,73	1.15	8 (11%)	82,113,113	1.28	7 (8%)
45	DGD	c	515	-	57,57,67	0.95	2 (3%)	71,71,81	1.41	9 (12%)
34	II0	5	319	-	39,43,43	2.04	2 (5%)	48,60,60	1.71	12 (25%)
36	IHT	1	618	-	40,42,42	1.52	1 (2%)	52,58,58	1.90	12 (23%)
32	CLA	a	406	-	53,57,73	1.30	9 (16%)	61,93,113	1.46	5 (8%)
32	CLA	3	606	-	49,53,73	1.38	9 (18%)	58,89,113	1.33	4 (6%)
32	CLA	B	612	-	68,72,73	1.16	9 (13%)	80,111,113	1.29	6 (7%)
34	II0	6	614	-	39,43,43	2.04	3 (7%)	48,60,60	1.59	8 (16%)
34	II0	7	614	-	39,43,43	2.03	2 (5%)	48,60,60	1.61	6 (12%)
36	IHT	4	614	-	40,42,42	1.51	1 (2%)	52,58,58	1.79	10 (19%)
32	CLA	c	503	-	69,73,73	1.16	9 (13%)	82,113,113	1.35	7 (8%)
43	PL9	A	609	-	13,13,55	1.58	2 (15%)	17,17,69	1.79	4 (23%)
34	II0	6	612	-	39,43,43	2.01	2 (5%)	48,60,60	1.67	11 (22%)
44	BCT	a	401	46	3,3,3	1.10	0	2,3,3	4.56	2 (100%)
32	CLA	0	602	5	63,67,73	1.22	8 (12%)	74,105,113	1.31	6 (8%)
31	8CT	h	102	-	40,41,41	4.84	23 (57%)	51,56,56	2.79	13 (25%)
32	CLA	p	310	-	45,49,73	1.42	8 (17%)	54,84,113	1.46	5 (9%)
32	CLA	2	603	-	54,58,73	1.32	8 (14%)	64,95,113	1.40	6 (9%)
32	CLA	9	608	-	45,49,73	1.40	8 (17%)	54,84,113	1.47	6 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
35	II3	6	613	-	40,43,43	1.50	1 (2%)	47,60,60	1.68	11 (23%)
31	8CT	c	518	-	40,41,41	4.86	22 (55%)	51,56,56	2.89	17 (33%)
37	LMG	d	406	-	46,46,55	0.78	1 (2%)	54,54,63	1.34	5 (9%)
31	8CT	B	622	-	40,41,41	4.78	23 (57%)	51,56,56	3.00	19 (37%)
34	II0	8	615	-	39,43,43	2.04	2 (5%)	48,60,60	1.69	10 (20%)
37	LMG	A	607	-	48,48,55	0.78	1 (2%)	56,56,63	1.34	5 (8%)
32	CLA	2	609	38	45,49,73	1.41	8 (17%)	54,84,113	1.45	5 (9%)
32	CLA	C	506	-	49,53,73	1.36	9 (18%)	58,89,113	1.44	5 (8%)
32	CLA	P	603	-	54,58,73	1.31	8 (14%)	64,95,113	1.41	5 (7%)
31	8CT	D	409	-	40,41,41	4.84	23 (57%)	51,56,56	2.48	16 (31%)
32	CLA	5	307	-	49,53,73	1.39	8 (16%)	58,89,113	1.41	4 (6%)
32	CLA	6	604	-	59,63,73	1.27	7 (11%)	70,101,113	1.33	6 (8%)
32	CLA	P	610	-	49,53,73	1.40	9 (18%)	58,89,113	1.44	4 (6%)
32	CLA	4	612	-	49,53,73	1.40	7 (14%)	58,89,113	1.46	5 (8%)
32	CLA	4	602	5	63,67,73	1.22	8 (12%)	74,105,113	1.31	6 (8%)
32	CLA	3	609	-	64,68,73	1.21	8 (12%)	76,107,113	1.29	5 (6%)
32	CLA	D	401	-	63,67,73	1.19	9 (14%)	74,105,113	1.37	8 (10%)
31	8CT	P	615	-	40,41,41	4.87	23 (57%)	51,56,56	2.60	17 (33%)
34	II0	9	614	-	39,43,43	2.01	2 (5%)	48,60,60	1.57	12 (25%)
34	II0	8	619	-	39,43,43	2.07	2 (5%)	48,60,60	1.61	10 (20%)
34	II0	p	316	-	39,43,43	2.03	2 (5%)	48,60,60	1.58	9 (18%)
32	CLA	B	616	-	69,73,73	1.15	9 (13%)	82,113,113	1.29	5 (6%)
37	LMG	2	617	-	36,36,55	0.86	1 (2%)	44,44,63	1.25	5 (11%)
34	II0	2	614	-	39,43,43	2.02	2 (5%)	48,60,60	1.61	11 (22%)
32	CLA	8	612	-	49,53,73	1.38	8 (16%)	58,89,113	1.38	4 (6%)
32	CLA	8	605	3	64,68,73	1.22	9 (14%)	76,107,113	1.27	5 (6%)
32	CLA	B	617	-	69,73,73	1.15	9 (13%)	82,113,113	1.31	5 (6%)
32	CLA	B	602	-	51,55,73	1.33	9 (17%)	60,91,113	1.39	5 (8%)
32	CLA	P	604	-	59,63,73	1.27	7 (11%)	70,101,113	1.32	6 (8%)
47	HEM	f	101	11	50,50,50	1.47	7 (14%)	67,82,82	1.12	1 (1%)
32	CLA	p	303	6	63,67,73	1.23	8 (12%)	74,105,113	1.31	6 (8%)
32	CLA	C	503	-	69,73,73	1.15	9 (13%)	82,113,113	1.34	7 (8%)
34	II0	5	316	-	39,43,43	2.04	2 (5%)	48,60,60	1.60	9 (18%)
38	LHG	8	618	32	21,21,48	0.77	0	23,26,54	1.31	2 (8%)
37	LMG	l	101	-	40,40,55	0.88	2 (5%)	48,48,63	1.29	6 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
34	II0	5	315	-	39,43,43	2.03	2 (5%)	48,60,60	1.61	10 (20%)
37	LMG	D	411	-	40,40,55	0.81	0	48,48,63	1.25	6 (12%)
32	CLA	7	609	-	45,49,73	1.42	8 (17%)	54,84,113	1.48	5 (9%)
37	LMG	0	619	-	36,36,55	0.87	1 (2%)	44,44,63	1.26	5 (11%)
34	II0	0	620	-	39,43,43	2.04	2 (5%)	48,60,60	1.65	13 (27%)
34	II0	3	613	-	39,43,43	2.04	2 (5%)	48,60,60	1.60	9 (18%)
32	CLA	9	602	4	63,67,73	1.21	9 (14%)	74,105,113	1.32	6 (8%)
32	CLA	2	612	-	49,53,73	1.38	8 (16%)	58,89,113	1.38	4 (6%)
32	CLA	4	611	-	49,53,73	1.40	8 (16%)	58,89,113	1.40	4 (6%)
32	CLA	b	616	-	69,73,73	1.16	9 (13%)	82,113,113	1.29	5 (6%)
34	II0	3	612	-	39,43,43	2.02	2 (5%)	48,60,60	1.59	11 (22%)
32	CLA	c	508	-	69,73,73	1.14	9 (13%)	82,113,113	1.30	6 (7%)
32	CLA	7	604	2	59,63,73	1.27	8 (13%)	70,101,113	1.35	6 (8%)
37	LMG	6	616	-	28,28,55	0.98	1 (3%)	36,36,63	1.27	6 (16%)
31	8CT	Z	101	-	40,41,41	4.77	23 (57%)	51,56,56	2.63	21 (41%)
32	CLA	S	302	-	49,53,73	1.39	7 (14%)	58,89,113	1.40	4 (6%)
31	8CT	b	623	-	40,41,41	4.80	23 (57%)	51,56,56	2.85	16 (31%)
32	CLA	4	608	5	64,68,73	1.21	8 (12%)	76,107,113	1.28	5 (6%)
36	IHT	0	614	-	40,42,42	1.49	1 (2%)	52,58,58	1.77	10 (19%)
32	CLA	7	605	-	54,58,73	1.32	8 (14%)	64,95,113	1.35	6 (9%)
45	DGD	C	514	-	56,56,67	0.98	2 (3%)	70,70,81	1.47	10 (14%)
32	CLA	P	602	7	63,67,73	1.22	8 (12%)	74,105,113	1.32	6 (8%)
31	8CT	K	101	-	40,41,41	4.81	23 (57%)	51,56,56	2.81	18 (35%)
32	CLA	b	604	-	68,72,73	1.16	9 (13%)	80,111,113	1.27	6 (7%)
33	KC2	5	311	-	49,53,53	1.75	9 (18%)	60,89,89	1.91	15 (25%)
38	LHG	2	618	32	21,21,48	0.77	0	23,26,54	1.31	2 (8%)
32	CLA	6	606	7	49,53,73	1.38	6 (12%)	58,89,113	1.32	4 (6%)
32	CLA	9	606	-	49,53,73	1.39	9 (18%)	58,89,113	1.34	4 (6%)
41	PHO	d	410	-	58,69,69	2.10	9 (15%)	55,99,99	1.49	7 (12%)
32	CLA	4	605	-	54,58,73	1.32	8 (14%)	64,95,113	1.38	6 (9%)
32	CLA	C	507	-	69,73,73	1.15	9 (13%)	82,113,113	1.27	5 (6%)
31	8CT	A	610	-	40,41,41	4.77	23 (57%)	51,56,56	2.77	21 (41%)
45	DGD	C	516	-	56,56,67	0.93	2 (3%)	70,70,81	1.41	8 (11%)
32	CLA	1	604	2	59,63,73	1.27	8 (13%)	70,101,113	1.36	6 (8%)
34	II0	4	615	-	39,43,43	2.01	2 (5%)	48,60,60	1.63	10 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	CLA	b	607	-	69,73,73	1.15	9 (13%)	82,113,113	1.31	8 (9%)
45	DGD	C	515	-	57,57,67	0.95	2 (3%)	71,71,81	1.41	9 (12%)
32	CLA	b	605	-	65,69,73	1.20	8 (12%)	77,108,113	1.36	7 (9%)
32	CLA	4	609	-	45,49,73	1.42	8 (17%)	54,84,113	1.47	5 (9%)
36	IHT	8	616	-	40,42,42	1.53	2 (5%)	52,58,58	1.92	13 (25%)
36	IHT	4	617	-	40,42,42	1.56	2 (5%)	52,58,58	1.93	13 (25%)
32	CLA	b	606	-	69,73,73	1.15	9 (13%)	82,113,113	1.26	4 (4%)
32	CLA	C	512	-	61,65,73	1.22	9 (14%)	71,102,113	1.36	5 (7%)
32	CLA	G	101	-	49,53,73	1.40	8 (16%)	58,89,113	1.38	4 (6%)
32	CLA	6	610	-	49,53,73	1.40	8 (16%)	58,89,113	1.44	4 (6%)
34	II0	8	613	-	39,43,43	2.04	2 (5%)	48,60,60	1.60	9 (18%)
32	CLA	p	306	-	64,68,73	1.22	8 (12%)	76,107,113	1.27	4 (5%)
34	II0	1	617	-	39,43,43	2.06	2 (5%)	48,60,60	1.65	9 (18%)
39	SQD	B	620	-	52,54,54	1.55	7 (13%)	62,65,65	1.35	6 (9%)
38	LHG	D	410	-	31,31,48	0.77	1 (3%)	34,37,54	1.30	3 (8%)
32	CLA	P	601	7	46,50,73	1.40	8 (17%)	53,85,113	1.40	4 (7%)
32	CLA	0	605	-	54,58,73	1.32	8 (14%)	64,95,113	1.37	6 (9%)
32	CLA	c	510	-	69,73,73	1.15	9 (13%)	82,113,113	1.28	5 (6%)
32	CLA	C	509	-	69,73,73	1.15	9 (13%)	82,113,113	1.31	8 (9%)
34	II0	1	614	-	39,43,43	2.02	2 (5%)	48,60,60	1.57	8 (16%)
32	CLA	5	306	-	64,68,73	1.22	8 (12%)	76,107,113	1.29	4 (5%)
38	LHG	b	621	-	38,38,48	0.70	2 (5%)	41,44,54	1.29	4 (9%)
32	CLA	C	508	-	69,73,73	1.15	9 (13%)	82,113,113	1.30	6 (7%)
45	DGD	A	614	-	54,54,67	1.04	4 (7%)	67,67,81	1.47	10 (14%)
32	CLA	a	408	-	64,68,73	1.18	9 (14%)	76,107,113	1.31	6 (7%)
34	II0	7	616	-	39,43,43	2.05	2 (5%)	48,60,60	1.65	10 (20%)
32	CLA	9	609	-	64,68,73	1.21	9 (14%)	76,107,113	1.29	6 (7%)
32	CLA	b	610	-	69,73,73	1.16	9 (13%)	82,113,113	1.27	6 (7%)
37	LMG	D	407	-	46,46,55	0.78	1 (2%)	54,54,63	1.34	5 (9%)
38	LHG	d	411	-	31,31,48	0.77	1 (3%)	34,37,54	1.30	3 (8%)
34	II0	0	617	-	39,43,43	2.01	2 (5%)	48,60,60	1.67	10 (20%)
32	CLA	9	611	-	49,53,73	1.38	9 (18%)	58,89,113	1.40	4 (6%)
34	II0	4	616	-	39,43,43	2.04	2 (5%)	48,60,60	1.62	11 (22%)
31	8CT	K	102	-	40,41,41	4.78	23 (57%)	51,56,56	2.73	20 (39%)
33	KC2	p	311	-	49,53,53	1.75	9 (18%)	60,89,89	1.92	15 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
37	LMG	a	410	-	48,48,55	0.77	1 (2%)	56,56,63	1.34	5 (8%)
32	CLA	1	602	2	63,67,73	1.22	8 (12%)	74,105,113	1.31	6 (8%)
32	CLA	2	601	3	46,50,73	1.40	8 (17%)	53,85,113	1.40	4 (7%)
32	CLA	B	615	-	68,72,73	1.15	9 (13%)	80,111,113	1.27	5 (6%)
43	PL9	a	412	-	13,13,55	1.58	2 (15%)	17,17,69	1.78	4 (23%)
32	CLA	9	607	4	64,68,73	1.20	9 (14%)	76,107,113	1.32	4 (5%)
33	KC2	2	610	-	49,53,53	1.76	9 (18%)	60,89,89	1.88	14 (23%)
32	CLA	c	512	-	61,65,73	1.21	9 (14%)	71,102,113	1.36	5 (7%)
32	CLA	8	604	-	59,63,73	1.26	8 (13%)	70,101,113	1.36	6 (8%)
39	SQD	b	601	-	46,48,54	1.60	7 (15%)	56,59,65	1.44	5 (8%)
33	KC2	1	610	-	49,53,53	1.75	9 (18%)	60,89,89	1.88	14 (23%)
32	CLA	b	603	-	64,69,73	1.16	9 (14%)	73,106,113	1.21	4 (5%)
32	CLA	4	603	-	54,58,73	1.33	8 (14%)	64,95,113	1.38	6 (9%)
32	CLA	0	607	5	49,53,73	1.39	8 (16%)	58,89,113	1.33	4 (6%)
34	II0	8	614	-	39,43,43	2.03	2 (5%)	48,60,60	1.59	11 (22%)
32	CLA	D	403	-	61,65,73	1.33	10 (16%)	74,103,113	1.35	7 (9%)
37	LMG	G	102	-	28,28,55	0.98	1 (3%)	36,36,63	1.29	5 (13%)
32	CLA	3	604	4	59,63,73	1.26	9 (15%)	70,101,113	1.34	6 (8%)
32	CLA	c	509	-	69,73,73	1.15	9 (13%)	82,113,113	1.31	8 (9%)
32	CLA	3	608	-	45,49,73	1.39	8 (17%)	54,84,113	1.48	6 (11%)
32	CLA	0	613	5	49,53,73	1.40	8 (16%)	58,89,113	1.40	4 (6%)
32	CLA	7	611	-	49,53,73	1.40	8 (16%)	58,89,113	1.44	4 (6%)
32	CLA	9	604	4	59,63,73	1.26	9 (15%)	70,101,113	1.34	6 (8%)
32	CLA	6	602	7	63,67,73	1.22	9 (14%)	74,105,113	1.31	7 (9%)
31	8CT	H	102	-	40,41,41	4.84	23 (57%)	51,56,56	2.78	13 (25%)
38	LHG	A	612	-	42,42,48	0.68	1 (2%)	45,48,54	1.25	4 (8%)
40	OEX	A	601	8	0,15,15	-	-	-	-	-
32	CLA	1	606	-	49,53,73	1.38	8 (16%)	58,89,113	1.41	4 (6%)
32	CLA	0	604	-	59,63,73	1.27	7 (11%)	70,101,113	1.34	8 (11%)
32	CLA	a	405	-	69,73,73	1.16	9 (13%)	82,113,113	1.30	5 (6%)
32	CLA	A	602	-	69,73,73	1.15	9 (13%)	82,113,113	1.30	5 (6%)
41	PHO	D	402	-	58,69,69	2.10	9 (15%)	55,99,99	1.49	7 (12%)
32	CLA	B	604	-	68,72,73	1.16	9 (13%)	80,111,113	1.26	6 (7%)
43	PL9	D	405	-	55,55,55	1.27	5 (9%)	68,69,69	1.51	13 (19%)
31	8CT	a	413	-	40,41,41	4.77	23 (57%)	51,56,56	3.10	18 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
38	LHG	B	619	-	38,38,48	0.70	1 (2%)	41,44,54	1.31	4 (9%)
32	CLA	c	504	-	68,72,73	1.16	9 (13%)	80,111,113	1.30	6 (7%)
31	8CT	z	101	-	40,41,41	4.76	23 (57%)	51,56,56	2.67	22 (43%)
35	II3	7	615	-	40,43,43	1.50	1 (2%)	47,60,60	1.60	10 (21%)
32	CLA	0	606	-	49,53,73	1.40	8 (16%)	58,89,113	1.35	4 (6%)
36	IHT	7	618	-	40,42,42	1.53	1 (2%)	52,58,58	1.89	10 (19%)
45	DGD	a	414	-	54,54,67	1.04	5 (9%)	67,67,81	1.46	10 (14%)
32	CLA	B	607	-	69,73,73	1.15	9 (13%)	82,113,113	1.30	8 (9%)
32	CLA	5	305	-	59,63,73	1.28	8 (13%)	70,101,113	1.35	6 (8%)
32	CLA	c	513	-	53,57,73	1.30	9 (16%)	61,93,113	1.42	6 (9%)
32	CLA	7	606	-	49,53,73	1.38	7 (14%)	58,89,113	1.44	6 (10%)
32	CLA	b	612	-	68,72,73	1.16	9 (13%)	80,111,113	1.29	6 (7%)
44	BCT	A	611	46	3,3,3	1.11	0	2,3,3	4.58	2 (100%)
32	CLA	5	303	6	63,67,73	1.23	9 (14%)	74,105,113	1.32	6 (8%)
38	LHG	b	619	-	38,38,48	0.69	1 (2%)	41,44,54	1.30	4 (9%)
32	CLA	C	511	27	69,73,73	1.16	9 (13%)	82,113,113	1.29	4 (4%)
32	CLA	4	601	5	46,50,73	1.41	8 (17%)	53,85,113	1.41	4 (7%)
36	IHT	0	618	-	40,42,42	1.51	2 (5%)	52,58,58	1.92	13 (25%)
33	KC2	P	605	-	49,53,53	1.77	8 (16%)	60,89,89	1.80	15 (25%)
32	CLA	7	608	2	64,68,73	1.21	8 (12%)	76,107,113	1.27	4 (5%)
32	CLA	C	510	-	69,73,73	1.16	9 (13%)	82,113,113	1.27	5 (6%)
32	CLA	c	511	27	69,73,73	1.16	9 (13%)	82,113,113	1.28	4 (4%)
32	CLA	p	309	6	64,68,73	1.21	8 (12%)	76,107,113	1.28	5 (6%)
31	8CT	9	615	-	40,41,41	4.83	23 (57%)	51,56,56	2.79	18 (35%)
32	CLA	b	613	-	69,73,73	1.14	9 (13%)	82,113,113	1.31	8 (9%)
38	LHG	A	613	-	48,48,48	0.66	1 (2%)	51,54,54	1.28	6 (11%)
39	SQD	a	409	-	52,54,54	1.54	7 (13%)	62,65,65	1.34	8 (12%)
32	CLA	2	604	-	59,63,73	1.26	8 (13%)	70,101,113	1.36	6 (8%)
32	CLA	0	612	-	49,53,73	1.40	8 (16%)	58,89,113	1.46	5 (8%)
32	CLA	2	602	3	63,67,73	1.22	9 (14%)	74,105,113	1.31	6 (8%)
34	II0	5	301	-	39,43,43	2.00	2 (5%)	48,60,60	1.66	9 (18%)
32	CLA	1	611	-	49,53,73	1.40	7 (14%)	58,89,113	1.43	4 (6%)
32	CLA	8	611	-	49,53,73	1.39	8 (16%)	58,89,113	1.42	4 (6%)
47	HEM	V	201	-	50,50,50	1.46	8 (16%)	67,82,82	1.04	4 (5%)
36	IHT	5	317	-	40,42,42	1.50	1 (2%)	52,58,58	1.77	13 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	CLA	7	613	-	49,53,73	1.39	7 (14%)	58,89,113	1.42	4 (6%)
32	CLA	B	608	-	45,49,73	1.38	9 (20%)	54,84,113	1.48	5 (9%)
32	CLA	9	603	-	54,58,73	1.30	8 (14%)	64,95,113	1.41	6 (9%)
32	CLA	8	606	-	49,53,73	1.39	8 (16%)	58,89,113	1.36	4 (6%)
32	CLA	B	606	-	69,73,73	1.16	9 (13%)	82,113,113	1.26	4 (4%)
32	CLA	1	605	-	54,58,73	1.32	8 (14%)	64,95,113	1.35	6 (9%)
31	8CT	b	622	-	40,41,41	4.80	23 (57%)	51,56,56	2.52	17 (33%)
37	LMG	d	401	-	40,40,55	0.80	0	48,48,63	1.24	6 (12%)
32	CLA	3	603	-	54,58,73	1.30	9 (16%)	64,95,113	1.42	6 (9%)
34	II0	4	619	-	39,43,43	2.03	2 (5%)	48,60,60	1.64	13 (27%)
41	PHO	A	604	-	58,69,69	2.10	11 (18%)	55,99,99	1.46	7 (12%)
36	IHT	p	317	-	40,42,42	1.50	1 (2%)	52,58,58	1.81	13 (25%)
35	II3	P	613	-	40,43,43	1.49	1 (2%)	47,60,60	1.67	10 (21%)
32	CLA	2	611	-	49,53,73	1.39	7 (14%)	58,89,113	1.43	4 (6%)
37	LMG	4	618	-	36,36,55	0.87	1 (2%)	44,44,63	1.26	5 (11%)
32	CLA	1	613	-	49,53,73	1.40	8 (16%)	58,89,113	1.40	4 (6%)
32	CLA	b	617	-	69,73,73	1.15	9 (13%)	82,113,113	1.31	5 (6%)
32	CLA	B	614	-	69,73,73	1.15	9 (13%)	82,113,113	1.24	6 (7%)
32	CLA	6	611	-	49,53,73	1.39	8 (16%)	58,89,113	1.42	4 (6%)
38	LHG	B	621	-	38,38,48	0.70	2 (5%)	41,44,54	1.29	4 (9%)
40	OEX	a	404	8	0,15,15	-	-	-	-	-
32	CLA	d	409	-	63,67,73	1.18	9 (14%)	74,105,113	1.36	8 (10%)
37	LMG	P	616	-	28,28,55	0.98	1 (3%)	36,36,63	1.27	6 (16%)
32	CLA	6	603	-	54,58,73	1.31	8 (14%)	64,95,113	1.40	5 (7%)
37	LMG	b	618	-	51,51,55	0.73	1 (1%)	59,59,63	1.36	6 (10%)
32	CLA	6	607	7	64,68,73	1.21	8 (12%)	76,107,113	1.29	5 (6%)
37	LMG	8	617	-	36,36,55	0.85	1 (2%)	44,44,63	1.25	5 (11%)
32	CLA	7	602	2	63,67,73	1.22	8 (12%)	74,105,113	1.32	6 (8%)
32	CLA	6	608	-	45,49,73	1.42	8 (17%)	54,84,113	1.45	5 (9%)
32	CLA	C	513	-	53,57,73	1.30	9 (16%)	61,93,113	1.41	5 (8%)
32	CLA	d	402	-	61,65,73	1.32	10 (16%)	74,103,113	1.35	7 (9%)
32	CLA	2	607	3	49,53,73	1.38	8 (16%)	58,89,113	1.37	4 (6%)
32	CLA	9	605	-	50,54,73	1.35	9 (18%)	59,90,113	1.36	4 (6%)
32	CLA	0	611	-	49,53,73	1.40	8 (16%)	58,89,113	1.40	4 (6%)
39	SQD	5	318	-	33,35,54	1.77	8 (24%)	43,46,65	1.49	6 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
37	LMG	g	101	-	28,28,55	0.98	1 (3%)	36,36,63	1.28	5 (13%)
32	CLA	2	608	3	64,68,73	1.20	9 (14%)	76,107,113	1.30	5 (6%)
39	SQD	B	601	-	46,48,54	1.60	7 (15%)	56,59,65	1.44	5 (8%)
32	CLA	B	611	-	69,73,73	1.16	9 (13%)	82,113,113	1.27	6 (7%)
32	CLA	P	606	7	49,53,73	1.39	6 (12%)	58,89,113	1.31	4 (6%)
32	CLA	5	309	-	64,68,73	1.21	8 (12%)	76,107,113	1.29	5 (6%)
34	II0	2	619	-	39,43,43	2.05	2 (5%)	48,60,60	1.63	10 (20%)
31	8CT	C	518	-	40,41,41	4.85	22 (55%)	51,56,56	2.89	17 (33%)
32	CLA	A	605	-	64,68,73	1.18	9 (14%)	76,107,113	1.30	6 (7%)
37	LMG	L	102	-	40,40,55	0.88	2 (5%)	48,48,63	1.29	6 (12%)
39	SQD	b	620	-	52,54,54	1.55	7 (13%)	62,65,65	1.34	6 (9%)
32	CLA	p	307	-	49,53,73	1.40	8 (16%)	58,89,113	1.41	4 (6%)
32	CLA	2	606	-	49,53,73	1.39	8 (16%)	58,89,113	1.37	4 (6%)
37	LMG	C	517	-	46,46,55	0.77	1 (2%)	54,54,63	1.32	6 (11%)
34	II0	3	614	-	39,43,43	2.01	2 (5%)	48,60,60	1.57	10 (20%)
38	LHG	s	301	-	36,36,48	0.72	1 (2%)	39,42,54	1.27	4 (10%)
32	CLA	s	302	-	49,53,73	1.40	8 (16%)	58,89,113	1.40	4 (6%)
31	8CT	3	615	-	40,41,41	4.83	23 (57%)	51,56,56	2.79	17 (33%)
38	LHG	S	301	-	36,36,48	0.72	1 (2%)	39,42,54	1.27	4 (10%)
35	II3	1	615	-	40,43,43	1.50	1 (2%)	47,60,60	1.56	6 (12%)
45	DGD	c	516	-	56,56,67	0.93	2 (3%)	70,70,81	1.41	7 (10%)
32	CLA	3	605	-	50,54,73	1.35	8 (16%)	59,90,113	1.35	4 (6%)
32	CLA	b	609	-	69,73,73	1.14	9 (13%)	82,113,113	1.29	7 (8%)
34	II0	p	301	-	39,43,43	2.03	2 (5%)	48,60,60	1.67	12 (25%)
34	II0	P	612	-	39,43,43	1.99	2 (5%)	48,60,60	1.66	12 (25%)
32	CLA	B	605	-	65,69,73	1.20	8 (12%)	77,108,113	1.36	7 (9%)
32	CLA	8	602	3	63,67,73	1.22	9 (14%)	74,105,113	1.31	6 (8%)
32	CLA	A	603	-	53,57,73	1.28	8 (15%)	61,93,113	1.43	5 (8%)
32	CLA	3	602	4	63,67,73	1.21	9 (14%)	74,105,113	1.33	6 (8%)
32	CLA	1	608	2	64,68,73	1.21	9 (14%)	76,107,113	1.28	4 (5%)
32	CLA	5	313	-	49,53,73	1.39	7 (14%)	58,89,113	1.37	4 (6%)
31	8CT	6	615	-	40,41,41	4.87	23 (57%)	51,56,56	2.59	18 (35%)
33	KC2	4	610	5	49,53,53	1.74	8 (16%)	60,89,89	1.88	15 (25%)
45	DGD	h	101	-	63,63,67	0.88	2 (3%)	77,77,81	1.37	8 (10%)
34	II0	1	619	-	39,43,43	1.99	2 (5%)	48,60,60	1.59	9 (18%)

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
38	LHG	L	101	-	-	19/53/53/53	-
32	CLA	5	312	-	1/1/11/20	7/15/91/115	-
43	PL9	d	404	-	-	3/53/73/73	0/1/1/1
37	LMG	c	517	-	-	25/41/61/70	0/1/1/1
32	CLA	p	313	-	1/1/11/20	10/15/91/115	-
33	KC2	P	609	-	-	12/15/71/71	-
32	CLA	3	610	4	1/1/11/20	7/15/91/115	-
32	CLA	1	609	-	1/1/10/20	4/10/86/115	-
32	CLA	c	502	-	1/1/14/20	17/37/113/115	-
33	KC2	6	605	7	-	9/15/71/71	-
32	CLA	B	610	-	1/1/15/20	9/39/115/115	-
34	II0	5	314	-	-	2/21/67/67	0/2/2/2
32	CLA	1	601	-	1/1/10/20	4/12/88/115	-
33	KC2	8	610	-	-	11/15/71/71	-
32	CLA	7	607	-	1/1/11/20	8/15/91/115	-
32	CLA	d	403	-	1/1/14/20	10/33/109/115	-
32	CLA	1	612	-	1/1/11/20	7/15/91/115	-
32	CLA	P	611	-	1/1/11/20	9/15/91/115	-
31	8CT	k	101	-	-	6/29/63/63	0/2/2/2
32	CLA	c	505	-	1/1/15/20	13/39/115/115	-
38	LHG	d	405	-	-	17/47/51/53	-
34	II0	7	619	-	-	1/21/67/67	0/2/2/2
34	II0	p	315	-	-	4/21/67/67	0/2/2/2
31	8CT	B	624	-	-	7/29/63/63	0/2/2/2
32	CLA	4	613	5	1/1/11/20	8/15/91/115	-
47	HEM	v	201	-	-	1/14/54/54	-
31	8CT	M	201	-	-	16/29/63/63	0/2/2/2
45	DGD	H	101	-	-	19/51/91/95	0/2/2/2
32	CLA	5	310	-	1/1/10/20	4/10/86/115	-
33	KC2	0	610	5	-	12/15/71/71	-
37	LMG	B	618	-	-	19/46/66/70	0/1/1/1
32	CLA	9	610	4	1/1/11/20	7/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	CLA	0	608	5	1/1/14/20	9/33/109/115	-
34	II0	2	613	-	-	1/21/67/67	0/2/2/2
38	LHG	a	402	-	-	10/47/47/53	-
32	CLA	p	304	-	1/1/12/20	11/21/97/115	-
32	CLA	B	603	-	1/1/12/20	13/29/107/115	-
32	CLA	c	501	-	1/1/15/20	17/39/115/115	-
32	CLA	g	102	-	1/1/11/20	5/15/91/115	-
32	CLA	5	304	-	1/1/12/20	11/21/97/115	-
32	CLA	4	607	5	1/1/11/20	4/15/91/115	-
32	CLA	c	506	-	1/1/11/20	4/15/91/115	-
32	CLA	7	601	-	1/1/10/20	5/12/88/115	-
32	CLA	0	603	-	1/1/12/20	4/21/97/115	-
32	CLA	1	603	-	1/1/12/20	7/21/97/115	-
34	II0	1	616	-	-	4/21/67/67	0/2/2/2
34	II0	7	617	-	-	4/21/67/67	0/2/2/2
33	KC2	7	610	-	-	12/15/71/71	-
32	CLA	0	609	-	1/1/10/20	2/10/86/115	-
45	DGD	c	514	-	-	19/44/84/95	0/2/2/2
32	CLA	2	605	3	1/1/14/20	11/33/109/115	-
32	CLA	c	507	-	1/1/15/20	15/39/115/115	-
32	CLA	B	609	-	1/1/15/20	8/39/115/115	-
38	LHG	l	102	-	-	19/53/53/53	-
31	8CT	B	623	-	-	8/29/63/63	0/2/2/2
34	II0	2	615	-	-	2/21/67/67	0/2/2/2
32	CLA	4	604	-	1/1/13/20	11/27/103/115	-
32	CLA	8	603	-	1/1/12/20	6/21/97/115	-
31	8CT	k	102	-	-	13/29/63/63	0/2/2/2
32	CLA	7	603	-	1/1/12/20	7/21/97/115	-
32	CLA	8	607	3	1/1/11/20	4/15/91/115	-
39	SQD	A	606	-	-	27/49/69/69	0/1/1/1
32	CLA	b	611	-	1/1/15/20	7/39/115/115	-
32	CLA	3	601	4	1/1/10/20	5/12/88/115	-
32	CLA	8	608	3	1/1/14/20	10/33/109/115	-
34	II0	9	612	-	-	3/21/67/67	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	CLA	p	312	-	1/1/11/20	7/15/91/115	-
32	CLA	p	302	6	1/1/10/20	4/12/88/115	-
32	CLA	b	614	-	1/1/15/20	13/39/115/115	-
32	CLA	b	608	-	1/1/10/20	3/10/86/115	-
32	CLA	9	601	4	1/1/10/20	5/12/88/115	-
32	CLA	s	303	19	1/1/15/20	17/39/115/115	-
38	LHG	D	406	-	-	17/47/51/53	-
32	CLA	5	302	6	1/1/10/20	4/12/88/115	-
32	CLA	P	608	-	1/1/10/20	2/10/86/115	-
32	CLA	0	601	5	1/1/10/20	4/12/88/115	-
47	HEM	E	101	-	-	4/14/54/54	-
32	CLA	B	613	-	1/1/15/20	15/39/115/115	-
32	CLA	4	606	-	1/1/11/20	6/15/91/115	-
32	CLA	8	609	38	1/1/10/20	4/10/86/115	-
32	CLA	C	501	-	1/1/15/20	17/39/115/115	-
38	LHG	a	403	-	-	24/53/53/53	-
32	CLA	C	502	-	1/1/14/20	17/37/113/115	-
34	II0	P	614	-	-	2/21/67/67	0/2/2/2
32	CLA	C	504	-	1/1/14/20	12/37/113/115	-
33	KC2	6	609	-	-	12/15/71/71	-
36	IHT	2	616	-	-	1/25/65/65	0/2/2/2
32	CLA	8	601	3	1/1/10/20	4/12/88/115	-
32	CLA	P	607	7	1/1/14/20	7/33/109/115	-
32	CLA	5	308	6	1/1/11/20	5/15/91/115	-
32	CLA	7	612	-	1/1/11/20	7/15/91/115	-
32	CLA	p	305	-	1/1/13/20	8/27/103/115	-
32	CLA	p	308	6	1/1/11/20	5/15/91/115	-
34	II0	0	616	-	-	4/21/67/67	0/2/2/2
34	II0	9	613	-	-	1/21/67/67	0/2/2/2
32	CLA	6	601	7	1/1/10/20	2/12/88/115	-
32	CLA	3	611	-	1/1/11/20	7/15/91/115	-
32	CLA	b	615	-	1/1/14/20	13/37/113/115	-
39	SQD	p	318	-	-	19/30/50/69	0/1/1/1
34	II0	0	615	-	-	1/21/67/67	0/2/2/2
32	CLA	D	404	-	1/1/14/20	11/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	8CT	d	408	-	-	13/29/63/63	0/2/2/2
32	CLA	1	607	-	1/1/11/20	8/15/91/115	-
32	CLA	3	607	4	1/1/14/20	8/33/109/115	-
41	PHO	a	407	-	-	8/37/103/103	0/5/6/6
34	II0	p	314	-	-	0/21/67/67	0/2/2/2
32	CLA	b	602	-	1/1/11/20	6/18/94/115	-
32	CLA	S	303	19	1/1/15/20	17/39/115/115	-
32	CLA	C	505	-	1/1/15/20	13/39/115/115	-
45	DGD	c	515	-	-	18/45/85/95	0/2/2/2
34	II0	5	319	-	-	2/21/67/67	0/2/2/2
36	IHT	1	618	-	-	4/25/65/65	0/2/2/2
32	CLA	a	406	-	1/1/11/20	4/20/96/115	-
32	CLA	3	606	-	1/1/11/20	0/15/91/115	-
32	CLA	B	612	-	1/1/14/20	15/37/113/115	-
34	II0	6	614	-	-	3/21/67/67	0/2/2/2
34	II0	7	614	-	-	1/21/67/67	0/2/2/2
36	IHT	4	614	-	-	5/25/65/65	0/2/2/2
32	CLA	c	503	-	1/1/15/20	16/39/115/115	-
43	PL9	A	609	-	-	1/5/18/73	0/1/1/1
34	II0	6	612	-	-	1/21/67/67	0/2/2/2
32	CLA	0	602	5	1/1/13/20	11/32/108/115	-
31	8CT	h	102	-	-	9/29/63/63	0/2/2/2
32	CLA	p	310	-	1/1/10/20	4/10/86/115	-
32	CLA	2	603	-	1/1/12/20	6/21/97/115	-
32	CLA	9	608	-	1/1/10/20	2/10/86/115	-
35	II3	6	613	-	-	1/25/67/67	0/2/2/2
31	8CT	c	518	-	-	10/29/63/63	0/2/2/2
37	LMG	d	406	-	-	18/41/61/70	0/1/1/1
31	8CT	B	622	-	-	16/29/63/63	0/2/2/2
34	II0	8	615	-	-	2/21/67/67	0/2/2/2
37	LMG	A	607	-	-	16/43/63/70	0/1/1/1
32	CLA	2	609	38	1/1/10/20	4/10/86/115	-
32	CLA	C	506	-	1/1/11/20	4/15/91/115	-
32	CLA	P	603	-	1/1/12/20	2/21/97/115	-
31	8CT	D	409	-	-	13/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	CLA	5	307	-	1/1/11/20	5/15/91/115	-
32	CLA	6	604	-	1/1/13/20	6/27/103/115	-
32	CLA	P	610	-	1/1/11/20	6/15/91/115	-
32	CLA	4	612	-	1/1/11/20	9/15/91/115	-
32	CLA	4	602	5	1/1/13/20	11/32/108/115	-
32	CLA	3	609	-	1/1/14/20	7/33/109/115	-
32	CLA	D	401	-	1/1/13/20	3/32/108/115	-
31	8CT	P	615	-	-	4/29/63/63	0/2/2/2
34	II0	9	614	-	-	3/21/67/67	0/2/2/2
34	II0	8	619	-	-	1/21/67/67	0/2/2/2
34	II0	p	316	-	-	3/21/67/67	0/2/2/2
32	CLA	B	616	-	1/1/15/20	7/39/115/115	-
37	LMG	2	617	-	-	10/31/51/70	0/1/1/1
34	II0	2	614	-	-	0/21/67/67	0/2/2/2
32	CLA	8	612	-	1/1/11/20	7/15/91/115	-
32	CLA	8	605	3	1/1/14/20	11/33/109/115	-
32	CLA	B	617	-	1/1/15/20	13/39/115/115	-
32	CLA	B	602	-	1/1/11/20	6/18/94/115	-
32	CLA	P	604	-	1/1/13/20	6/27/103/115	-
47	HEM	f	101	11	-	4/14/54/54	-
32	CLA	p	303	6	1/1/13/20	12/32/108/115	-
32	CLA	C	503	-	1/1/15/20	14/39/115/115	-
34	II0	5	316	-	-	2/21/67/67	0/2/2/2
38	LHG	8	618	32	-	10/24/24/53	-
37	LMG	1	101	-	-	17/35/55/70	0/1/1/1
34	II0	5	315	-	-	3/21/67/67	0/2/2/2
37	LMG	D	411	-	-	26/35/55/70	0/1/1/1
32	CLA	7	609	-	1/1/10/20	4/10/86/115	-
37	LMG	0	619	-	-	10/31/51/70	0/1/1/1
34	II0	0	620	-	-	1/21/67/67	0/2/2/2
34	II0	3	613	-	-	0/21/67/67	0/2/2/2
32	CLA	9	602	4	1/1/13/20	9/32/108/115	-
32	CLA	2	612	-	1/1/11/20	7/15/91/115	-
32	CLA	4	611	-	1/1/11/20	7/15/91/115	-
32	CLA	b	616	-	1/1/15/20	7/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	II0	3	612	-	-	2/21/67/67	0/2/2/2
32	CLA	c	508	-	1/1/15/20	9/39/115/115	-
32	CLA	7	604	2	1/1/13/20	6/27/103/115	-
37	LMG	6	616	-	-	10/23/43/70	0/1/1/1
31	8CT	Z	101	-	-	12/29/63/63	0/2/2/2
32	CLA	S	302	-	1/1/11/20	7/15/91/115	-
31	8CT	b	623	-	-	7/29/63/63	0/2/2/2
32	CLA	4	608	5	1/1/14/20	9/33/109/115	-
36	IHT	0	614	-	-	5/25/65/65	0/2/2/2
32	CLA	7	605	-	1/1/12/20	8/21/97/115	-
45	DGD	C	514	-	-	19/44/84/95	0/2/2/2
32	CLA	P	602	7	1/1/13/20	14/32/108/115	-
31	8CT	K	101	-	-	12/29/63/63	0/2/2/2
32	CLA	b	604	-	1/1/14/20	8/37/113/115	-
33	KC2	5	311	-	-	10/15/71/71	-
38	LHG	2	618	32	-	11/24/24/53	-
32	CLA	6	606	7	1/1/11/20	4/15/91/115	-
32	CLA	9	606	-	1/1/11/20	0/15/91/115	-
41	PHO	d	410	-	-	8/37/103/103	0/5/6/6
32	CLA	4	605	-	1/1/12/20	7/21/97/115	-
32	CLA	C	507	-	1/1/15/20	15/39/115/115	-
31	8CT	A	610	-	-	5/29/63/63	0/2/2/2
45	DGD	C	516	-	-	18/44/84/95	0/2/2/2
32	CLA	1	604	2	1/1/13/20	6/27/103/115	-
34	II0	4	615	-	-	0/21/67/67	0/2/2/2
32	CLA	b	607	-	1/1/15/20	7/39/115/115	-
45	DGD	C	515	-	-	18/45/85/95	0/2/2/2
32	CLA	b	605	-	1/1/14/20	8/35/111/115	-
32	CLA	4	609	-	1/1/10/20	2/10/86/115	-
36	IHT	8	616	-	-	0/25/65/65	0/2/2/2
36	IHT	4	617	-	-	6/25/65/65	0/2/2/2
32	CLA	b	606	-	1/1/15/20	12/39/115/115	-
32	CLA	C	512	-	1/1/12/20	10/29/105/115	-
32	CLA	G	101	-	1/1/11/20	5/15/91/115	-
32	CLA	6	610	-	1/1/11/20	6/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	II0	8	613	-	-	0/21/67/67	0/2/2/2
32	CLA	p	306	-	1/1/14/20	14/33/109/115	-
34	II0	1	617	-	-	3/21/67/67	0/2/2/2
39	SQD	B	620	-	-	23/49/69/69	0/1/1/1
38	LHG	D	410	-	-	18/36/36/53	-
32	CLA	P	601	7	1/1/10/20	2/12/88/115	-
32	CLA	0	605	-	1/1/12/20	7/21/97/115	-
32	CLA	c	510	-	1/1/15/20	8/39/115/115	-
32	CLA	C	509	-	1/1/15/20	6/39/115/115	-
34	II0	1	614	-	-	0/21/67/67	0/2/2/2
32	CLA	5	306	-	1/1/14/20	15/33/109/115	-
38	LHG	b	621	-	-	14/43/43/53	-
32	CLA	C	508	-	1/1/15/20	9/39/115/115	-
45	DGD	A	614	-	-	15/43/79/95	0/2/2/2
32	CLA	a	408	-	1/1/14/20	3/33/109/115	-
34	II0	7	616	-	-	3/21/67/67	0/2/2/2
32	CLA	9	609	-	1/1/14/20	7/33/109/115	-
32	CLA	b	610	-	1/1/15/20	9/39/115/115	-
37	LMG	D	407	-	-	18/41/61/70	0/1/1/1
38	LHG	d	411	-	-	18/36/36/53	-
34	II0	0	617	-	-	2/21/67/67	0/2/2/2
32	CLA	9	611	-	1/1/11/20	7/15/91/115	-
34	II0	4	616	-	-	4/21/67/67	0/2/2/2
31	8CT	K	102	-	-	6/29/63/63	0/2/2/2
33	KC2	p	311	-	-	10/15/71/71	-
37	LMG	a	410	-	-	16/43/63/70	0/1/1/1
32	CLA	1	602	2	1/1/13/20	12/32/108/115	-
32	CLA	2	601	3	1/1/10/20	4/12/88/115	-
32	CLA	B	615	-	1/1/14/20	13/37/113/115	-
43	PL9	a	412	-	-	1/5/18/73	0/1/1/1
32	CLA	9	607	4	1/1/14/20	8/33/109/115	-
33	KC2	2	610	-	-	11/15/71/71	-
32	CLA	c	512	-	1/1/12/20	10/29/105/115	-
32	CLA	8	604	-	1/1/13/20	2/27/103/115	-
39	SQD	b	601	-	-	23/43/63/69	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	KC2	1	610	-	-	12/15/71/71	-
32	CLA	b	603	-	1/1/12/20	13/29/107/115	-
32	CLA	4	603	-	1/1/12/20	4/21/97/115	-
32	CLA	0	607	5	1/1/11/20	2/15/91/115	-
34	II0	8	614	-	-	0/21/67/67	0/2/2/2
32	CLA	D	403	-	1/1/13/20	8/28/104/115	-
37	LMG	G	102	-	-	9/23/43/70	0/1/1/1
32	CLA	3	604	4	1/1/13/20	5/27/103/115	-
32	CLA	c	509	-	1/1/15/20	6/39/115/115	-
32	CLA	3	608	-	1/1/10/20	2/10/86/115	-
32	CLA	0	613	5	1/1/11/20	8/15/91/115	-
32	CLA	7	611	-	1/1/11/20	6/15/91/115	-
32	CLA	9	604	4	1/1/13/20	5/27/103/115	-
32	CLA	6	602	7	1/1/13/20	14/32/108/115	-
31	8CT	H	102	-	-	9/29/63/63	0/2/2/2
38	LHG	A	612	-	-	10/47/47/53	-
32	CLA	1	606	-	1/1/11/20	12/15/91/115	-
32	CLA	0	604	-	1/1/13/20	11/27/103/115	-
32	CLA	a	405	-	1/1/15/20	7/39/115/115	-
32	CLA	A	602	-	1/1/15/20	7/39/115/115	-
41	PHO	D	402	-	-	8/37/103/103	0/5/6/6
32	CLA	B	604	-	1/1/14/20	8/37/113/115	-
43	PL9	D	405	-	-	3/53/73/73	0/1/1/1
31	8CT	a	413	-	-	6/29/63/63	0/2/2/2
38	LHG	B	619	-	-	19/43/43/53	-
32	CLA	c	504	-	1/1/14/20	12/37/113/115	-
31	8CT	z	101	-	-	12/29/63/63	0/2/2/2
35	II3	7	615	-	-	2/25/67/67	0/2/2/2
32	CLA	0	606	-	1/1/11/20	6/15/91/115	-
36	IHT	7	618	-	-	2/25/65/65	0/2/2/2
45	DGD	a	414	-	-	13/43/79/95	0/2/2/2
32	CLA	B	607	-	1/1/15/20	7/39/115/115	-
32	CLA	5	305	-	1/1/13/20	8/27/103/115	-
32	CLA	c	513	-	1/1/11/20	10/20/96/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	CLA	7	606	-	1/1/11/20	11/15/91/115	-
32	CLA	b	612	-	1/1/14/20	15/37/113/115	-
32	CLA	5	303	6	1/1/13/20	11/32/108/115	-
38	LHG	b	619	-	-	19/43/43/53	-
32	CLA	C	511	27	1/1/15/20	8/39/115/115	-
32	CLA	4	601	5	1/1/10/20	4/12/88/115	-
36	IHT	0	618	-	-	5/25/65/65	0/2/2/2
33	KC2	P	605	-	-	10/15/71/71	-
32	CLA	7	608	2	1/1/14/20	10/33/109/115	-
32	CLA	C	510	-	1/1/15/20	8/39/115/115	-
32	CLA	c	511	27	1/1/15/20	8/39/115/115	-
32	CLA	p	309	6	1/1/14/20	10/33/109/115	-
32	CLA	b	613	-	1/1/15/20	15/39/115/115	-
31	8CT	9	615	-	-	10/29/63/63	0/2/2/2
38	LHG	A	613	-	-	23/53/53/53	-
39	SQD	a	409	-	-	27/49/69/69	0/1/1/1
32	CLA	2	604	-	1/1/13/20	2/27/103/115	-
32	CLA	0	612	-	1/1/11/20	9/15/91/115	-
32	CLA	2	602	3	1/1/13/20	9/32/108/115	-
34	II0	5	301	-	-	3/21/67/67	0/2/2/2
32	CLA	1	611	-	1/1/11/20	6/15/91/115	-
32	CLA	8	611	-	1/1/11/20	5/15/91/115	-
47	HEM	V	201	-	-	1/14/54/54	-
36	IHT	5	317	-	-	1/25/65/65	0/2/2/2
32	CLA	7	613	-	1/1/11/20	6/15/91/115	-
32	CLA	B	608	-	1/1/10/20	2/10/86/115	-
32	CLA	9	603	-	1/1/12/20	8/21/97/115	-
32	CLA	8	606	-	1/1/11/20	4/15/91/115	-
32	CLA	B	606	-	1/1/15/20	12/39/115/115	-
32	CLA	1	605	-	1/1/12/20	9/21/97/115	-
31	8CT	b	622	-	-	8/29/63/63	0/2/2/2
37	LMG	d	401	-	-	26/35/55/70	0/1/1/1
32	CLA	3	603	-	1/1/12/20	8/21/97/115	-
34	II0	4	619	-	-	2/21/67/67	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
41	PHO	A	604	-	-	8/37/103/103	0/5/6/6
36	IHT	p	317	-	-	0/25/65/65	0/2/2/2
35	II3	P	613	-	-	3/25/67/67	0/2/2/2
32	CLA	2	611	-	1/1/11/20	5/15/91/115	-
37	LMG	4	618	-	-	11/31/51/70	0/1/1/1
32	CLA	1	613	-	1/1/11/20	6/15/91/115	-
32	CLA	b	617	-	1/1/15/20	13/39/115/115	-
32	CLA	B	614	-	1/1/15/20	13/39/115/115	-
32	CLA	6	611	-	1/1/11/20	9/15/91/115	-
38	LHG	B	621	-	-	14/43/43/53	-
32	CLA	d	409	-	1/1/13/20	3/32/108/115	-
37	LMG	P	616	-	-	10/23/43/70	0/1/1/1
32	CLA	6	603	-	1/1/12/20	2/21/97/115	-
37	LMG	b	618	-	-	17/46/66/70	0/1/1/1
32	CLA	6	607	7	1/1/14/20	7/33/109/115	-
37	LMG	8	617	-	-	10/31/51/70	0/1/1/1
32	CLA	7	602	2	1/1/13/20	12/32/108/115	-
32	CLA	6	608	-	1/1/10/20	2/10/86/115	-
32	CLA	C	513	-	1/1/11/20	10/20/96/115	-
32	CLA	d	402	-	1/1/13/20	8/28/104/115	-
32	CLA	2	607	3	1/1/11/20	4/15/91/115	-
32	CLA	9	605	-	1/1/11/20	8/17/93/115	-
32	CLA	0	611	-	1/1/11/20	7/15/91/115	-
39	SQD	5	318	-	-	19/30/50/69	0/1/1/1
37	LMG	g	101	-	-	10/23/43/70	0/1/1/1
32	CLA	2	608	3	1/1/14/20	10/33/109/115	-
39	SQD	B	601	-	-	23/43/63/69	0/1/1/1
32	CLA	B	611	-	1/1/15/20	7/39/115/115	-
32	CLA	P	606	7	1/1/11/20	4/15/91/115	-
32	CLA	5	309	-	1/1/14/20	10/33/109/115	-
34	II0	2	619	-	-	2/21/67/67	0/2/2/2
32	CLA	A	605	-	1/1/14/20	3/33/109/115	-
31	8CT	C	518	-	-	10/29/63/63	0/2/2/2
37	LMG	L	102	-	-	19/35/55/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
39	SQD	b	620	-	-	24/49/69/69	0/1/1/1
32	CLA	p	307	-	1/1/11/20	5/15/91/115	-
32	CLA	2	606	-	1/1/11/20	4/15/91/115	-
37	LMG	C	517	-	-	25/41/61/70	0/1/1/1
34	II0	3	614	-	-	4/21/67/67	0/2/2/2
38	LHG	s	301	-	-	19/41/41/53	-
32	CLA	s	302	-	1/1/11/20	6/15/91/115	-
31	8CT	3	615	-	-	10/29/63/63	0/2/2/2
38	LHG	S	301	-	-	20/41/41/53	-
35	II3	1	615	-	-	2/25/67/67	0/2/2/2
45	DGD	c	516	-	-	19/44/84/95	0/2/2/2
32	CLA	3	605	-	1/1/11/20	8/17/93/115	-
32	CLA	b	609	-	1/1/15/20	8/39/115/115	-
34	II0	p	301	-	-	2/21/67/67	0/2/2/2
34	II0	P	612	-	-	0/21/67/67	0/2/2/2
32	CLA	B	605	-	1/1/14/20	8/35/111/115	-
32	CLA	8	602	3	1/1/13/20	10/32/108/115	-
32	CLA	A	603	-	1/1/11/20	4/20/96/115	-
32	CLA	3	602	4	1/1/13/20	9/32/108/115	-
32	CLA	1	608	2	1/1/14/20	10/33/109/115	-
32	CLA	5	313	-	1/1/11/20	10/15/91/115	-
31	8CT	6	615	-	-	4/29/63/63	0/2/2/2
33	KC2	4	610	5	-	12/15/71/71	-
45	DGD	h	101	-	-	19/51/91/95	0/2/2/2
34	II0	1	619	-	-	2/21/67/67	0/2/2/2

The worst 5 of 2699 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	d	408	8CT	C02-C03	14.93	1.59	1.34
31	D	409	8CT	C02-C03	14.90	1.59	1.34
31	b	622	8CT	C02-C03	14.84	1.59	1.34
31	h	102	8CT	C02-C03	14.83	1.59	1.34
31	H	102	8CT	C02-C03	14.83	1.59	1.34

The worst 5 of 2683 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	k	102	8CT	C33-C32-C31	-11.08	114.25	124.83
31	B	622	8CT	C33-C32-C31	-11.06	114.27	124.83
31	M	201	8CT	C33-C32-C31	-11.05	114.28	124.83
31	a	413	8CT	C33-C32-C31	-11.03	114.30	124.83
31	K	101	8CT	C33-C32-C31	-11.01	114.32	124.83

5 of 208 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
32	1	601	CLA	ND
32	1	602	CLA	ND
32	1	603	CLA	ND
32	1	604	CLA	ND
32	1	605	CLA	ND

5 of 3132 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
31	M	201	8CT	C16-C17-C18-C19
31	M	201	8CT	C20-C21-C23-C24
31	M	201	8CT	C22-C21-C23-C24
31	M	201	8CT	C28-C29-C30-C31
31	M	201	8CT	C28-C29-C30-C35

There are no ring outliers.

202 monomers are involved in 390 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
38	L	101	LHG	2	0
37	c	517	LMG	3	0
32	c	502	CLA	1	0
32	B	610	CLA	3	0
32	7	607	CLA	2	0
32	d	403	CLA	1	0
32	1	612	CLA	2	0
32	P	611	CLA	1	0
32	c	505	CLA	3	0
38	d	405	LHG	1	0
32	4	613	CLA	1	0
47	v	201	HEM	3	0
45	H	101	DGD	6	0
32	0	608	CLA	3	0
38	a	402	LHG	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	p	304	CLA	1	0
32	B	603	CLA	4	0
32	c	501	CLA	1	0
32	g	102	CLA	2	0
32	4	607	CLA	4	0
32	5	304	CLA	1	0
32	c	506	CLA	1	0
32	0	603	CLA	1	0
32	1	603	CLA	1	0
45	c	514	DGD	1	0
32	2	605	CLA	2	0
32	c	507	CLA	1	0
32	B	609	CLA	4	0
38	l	102	LHG	2	0
32	4	604	CLA	1	0
32	8	603	CLA	2	0
32	7	603	CLA	1	0
32	8	607	CLA	1	0
39	A	606	SQD	5	0
32	b	611	CLA	2	0
32	8	608	CLA	3	0
32	b	614	CLA	1	0
32	s	303	CLA	1	0
38	D	406	LHG	1	0
32	0	601	CLA	1	0
47	E	101	HEM	2	0
32	B	613	CLA	2	0
32	4	606	CLA	1	0
32	8	609	CLA	1	0
32	C	501	CLA	1	0
38	a	403	LHG	6	0
32	C	502	CLA	2	0
32	C	504	CLA	4	0
32	P	607	CLA	1	0
32	7	612	CLA	2	0
32	p	305	CLA	2	0
32	p	308	CLA	1	0
34	0	616	II0	1	0
32	b	615	CLA	1	0
39	p	318	SQD	3	0
32	D	404	CLA	2	0
32	1	607	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	3	607	CLA	3	0
41	a	407	PHO	1	0
32	S	303	CLA	1	0
32	C	505	CLA	2	0
45	c	515	DGD	4	0
36	1	618	IHT	1	0
32	a	406	CLA	3	0
32	3	606	CLA	2	0
32	B	612	CLA	3	0
34	7	614	II0	1	0
32	0	602	CLA	3	0
32	2	603	CLA	2	0
37	A	607	LMG	2	0
32	2	609	CLA	1	0
32	C	506	CLA	1	0
32	5	307	CLA	2	0
32	P	610	CLA	1	0
32	4	612	CLA	1	0
32	4	602	CLA	3	0
32	3	609	CLA	3	0
32	B	616	CLA	3	0
37	2	617	LMG	1	0
32	8	605	CLA	1	0
32	B	617	CLA	4	0
32	P	604	CLA	1	0
47	f	101	HEM	3	0
32	p	303	CLA	2	0
32	C	503	CLA	4	0
37	D	411	LMG	1	0
32	9	602	CLA	1	0
32	b	616	CLA	2	0
31	Z	101	8CT	1	0
32	S	302	CLA	4	0
32	4	608	CLA	3	0
32	7	605	CLA	2	0
45	C	514	DGD	2	0
32	P	602	CLA	3	0
32	b	604	CLA	2	0
32	9	606	CLA	2	0
41	d	410	PHO	3	0
32	C	507	CLA	3	0
45	C	516	DGD	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	b	607	CLA	2	0
45	C	515	DGD	4	0
32	b	605	CLA	3	0
32	b	606	CLA	4	0
32	C	512	CLA	1	0
32	G	101	CLA	1	0
32	6	610	CLA	1	0
32	p	306	CLA	1	0
39	B	620	SQD	1	0
32	c	510	CLA	2	0
32	C	509	CLA	1	0
34	1	614	II0	1	0
32	5	306	CLA	2	0
38	b	621	LHG	3	0
32	C	508	CLA	1	0
45	A	614	DGD	1	0
32	a	408	CLA	2	0
32	9	609	CLA	3	0
32	b	610	CLA	2	0
34	4	616	II0	1	0
37	a	410	LMG	3	0
32	1	602	CLA	4	0
32	B	615	CLA	1	0
32	9	607	CLA	4	0
32	c	512	CLA	2	0
39	b	601	SQD	1	0
32	b	603	CLA	4	0
32	4	603	CLA	2	0
32	0	607	CLA	4	0
32	D	403	CLA	3	0
32	3	604	CLA	1	0
32	c	509	CLA	1	0
32	0	613	CLA	1	0
32	9	604	CLA	1	0
32	6	602	CLA	3	0
38	A	612	LHG	5	0
32	1	606	CLA	3	0
32	0	604	CLA	1	0
32	a	405	CLA	4	0
32	A	602	CLA	5	0
41	D	402	PHO	3	0
32	B	604	CLA	2	0

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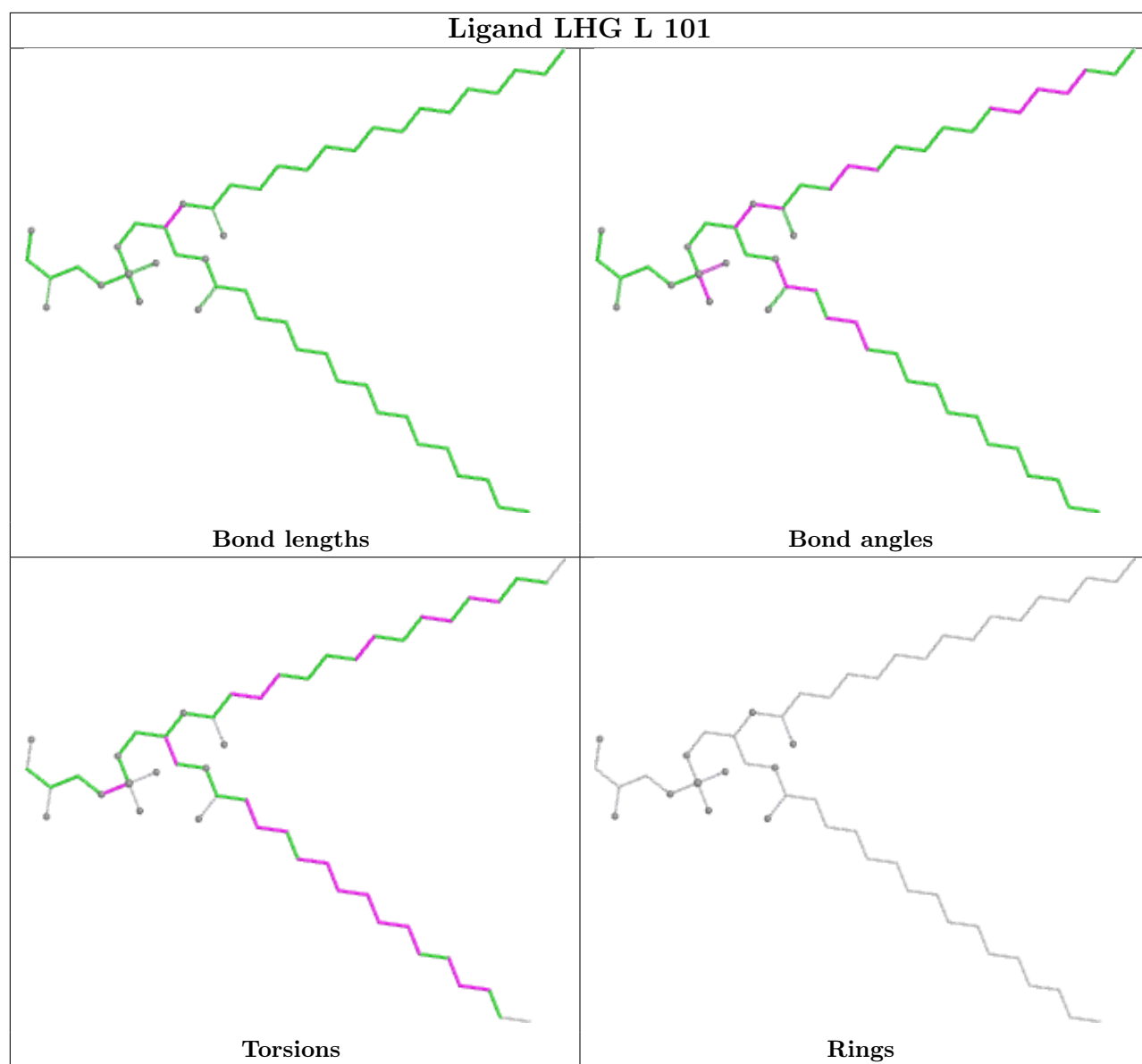
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32	B	607	CLA	3	0
32	5	305	CLA	2	0
32	c	513	CLA	2	0
32	7	606	CLA	2	0
32	b	612	CLA	3	0
32	5	303	CLA	2	0
32	C	511	CLA	3	0
32	4	601	CLA	1	0
33	P	605	KC2	3	0
32	7	608	CLA	1	0
32	C	510	CLA	2	0
32	c	511	CLA	4	0
32	b	613	CLA	2	0
38	A	613	LHG	5	0
39	a	409	SQD	6	0
32	0	612	CLA	1	0
32	2	602	CLA	1	0
47	V	201	HEM	3	0
32	8	606	CLA	5	0
32	B	606	CLA	6	0
32	1	605	CLA	1	0
37	d	401	LMG	1	0
41	A	604	PHO	1	0
32	1	613	CLA	1	0
32	b	617	CLA	2	0
32	B	614	CLA	1	0
32	6	611	CLA	1	0
38	B	621	LHG	3	0
37	b	618	LMG	1	0
32	6	607	CLA	1	0
37	8	617	LMG	2	0
32	7	602	CLA	4	0
32	C	513	CLA	2	0
32	d	402	CLA	1	0
32	2	607	CLA	1	0
32	9	605	CLA	1	0
39	5	318	SQD	4	0
32	2	608	CLA	3	0
39	B	601	SQD	2	0

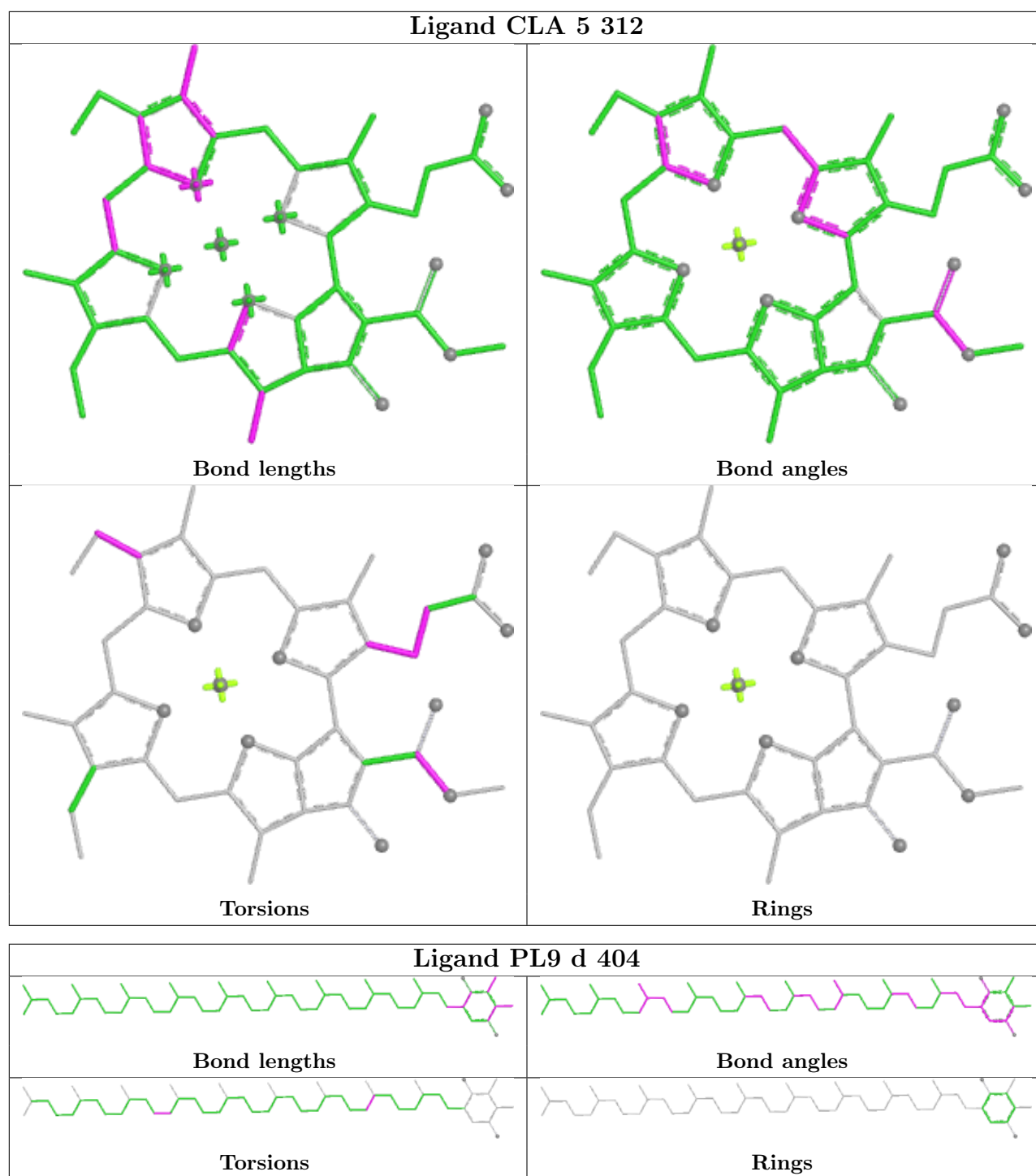
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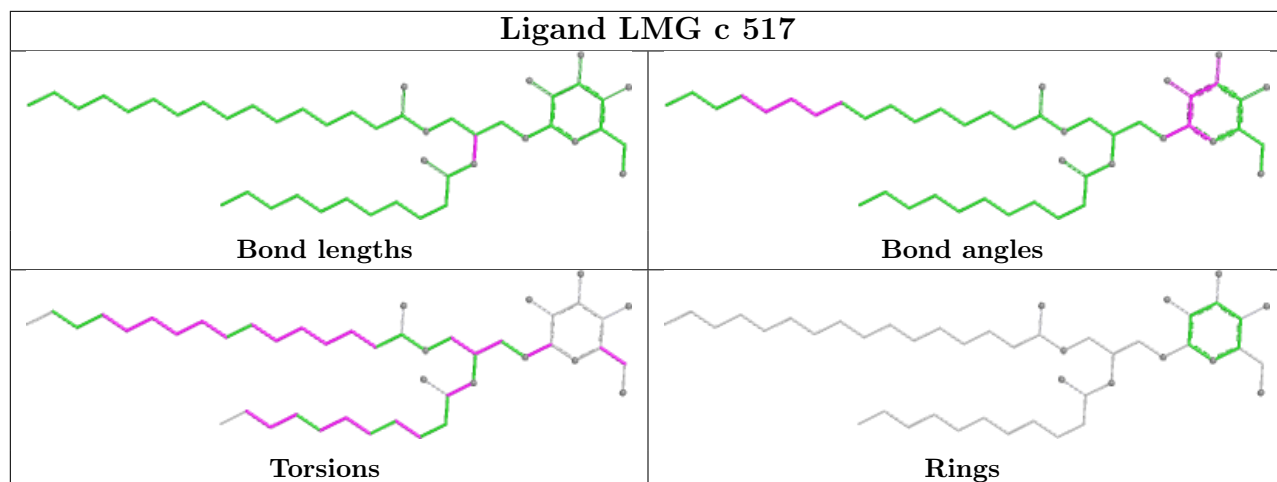
Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	B	611	CLA	2	0
32	A	605	CLA	3	0
37	L	102	LMG	1	0
39	b	620	SQD	1	0
32	p	307	CLA	2	0
32	2	606	CLA	5	0
37	C	517	LMG	3	0
38	s	301	LHG	1	0
32	s	302	CLA	3	0
38	S	301	LHG	1	0
45	c	516	DGD	3	0
32	3	605	CLA	1	0
32	b	609	CLA	4	0
32	B	605	CLA	3	0
32	8	602	CLA	1	0
32	A	603	CLA	3	0
32	3	602	CLA	1	0
32	1	608	CLA	1	0
45	h	101	DGD	5	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 than 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.

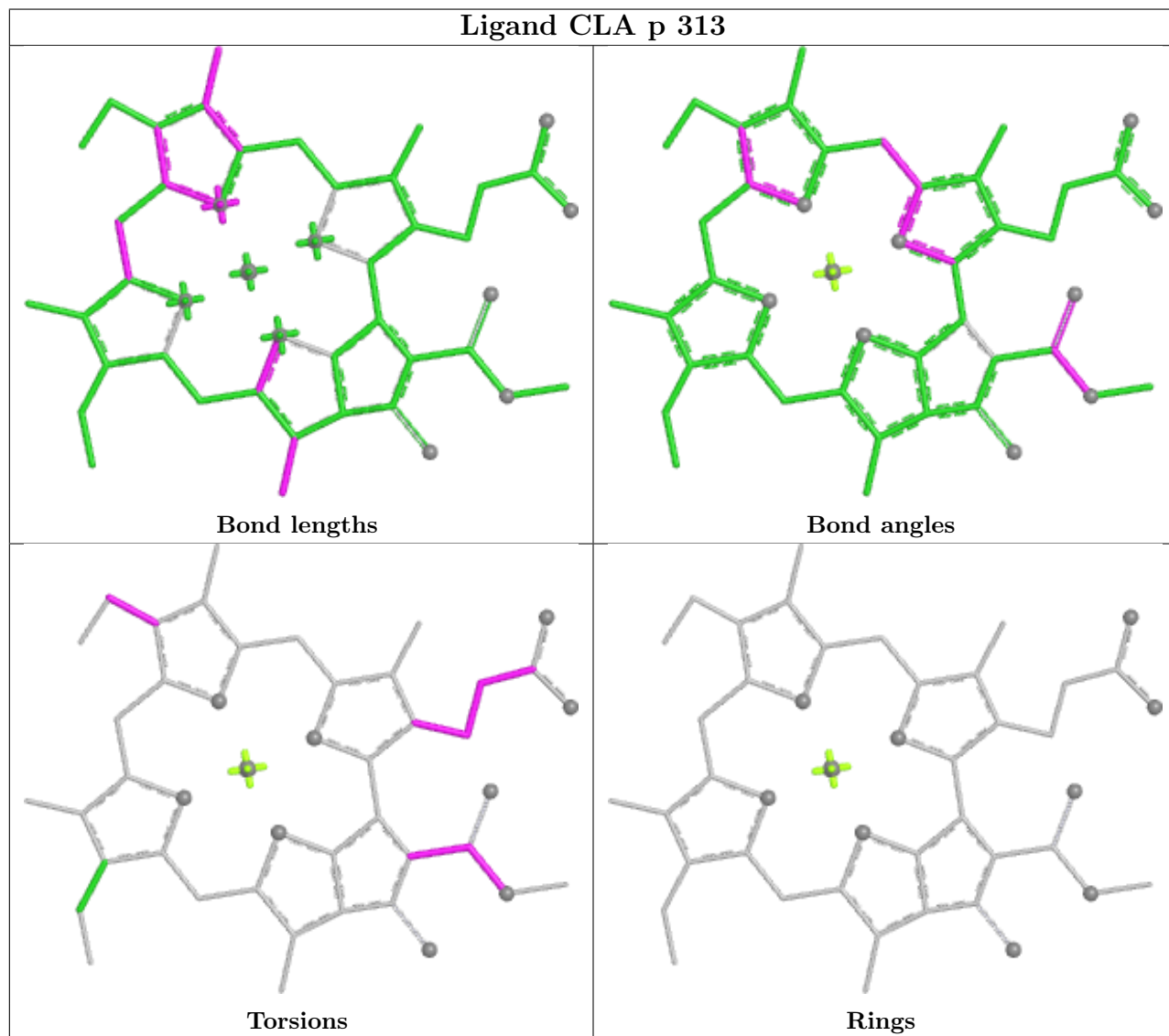




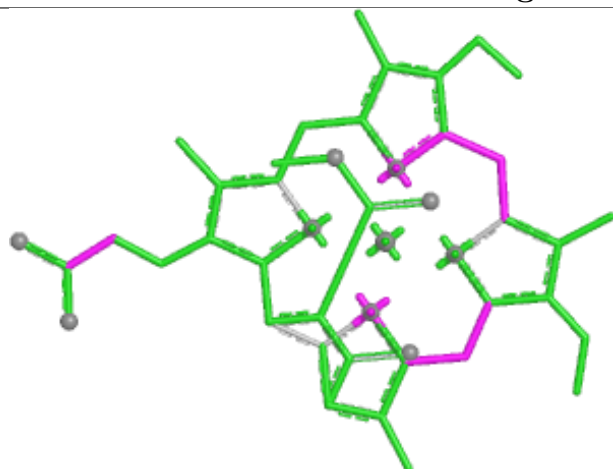
Ligand LMG c 517



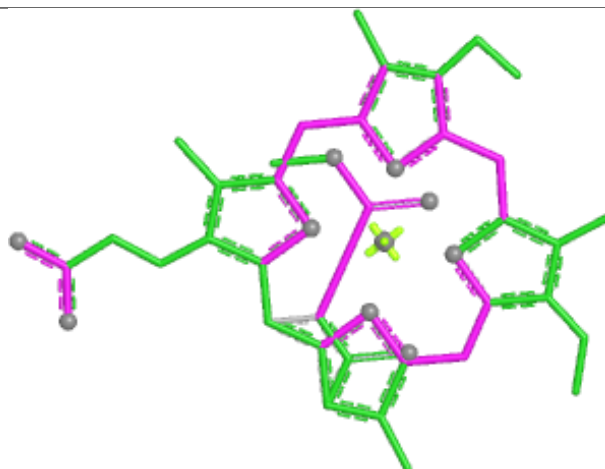
Ligand CLA p 313



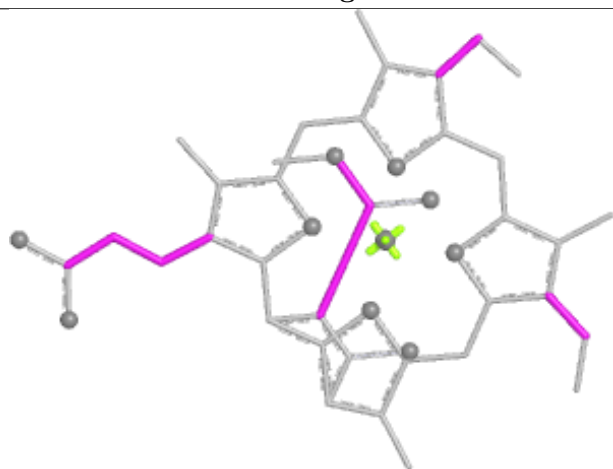
Ligand KC2 P 609



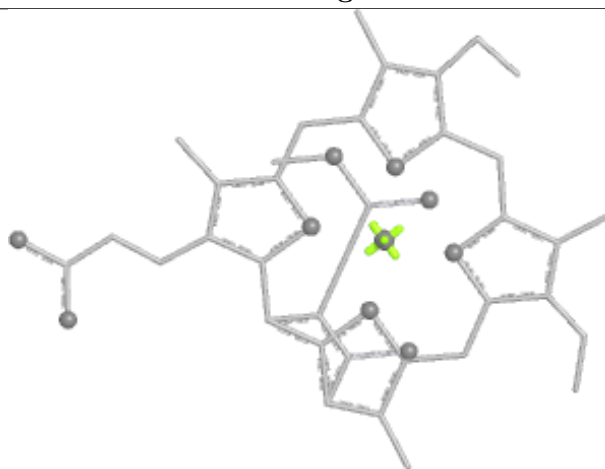
Bond lengths



Bond angles

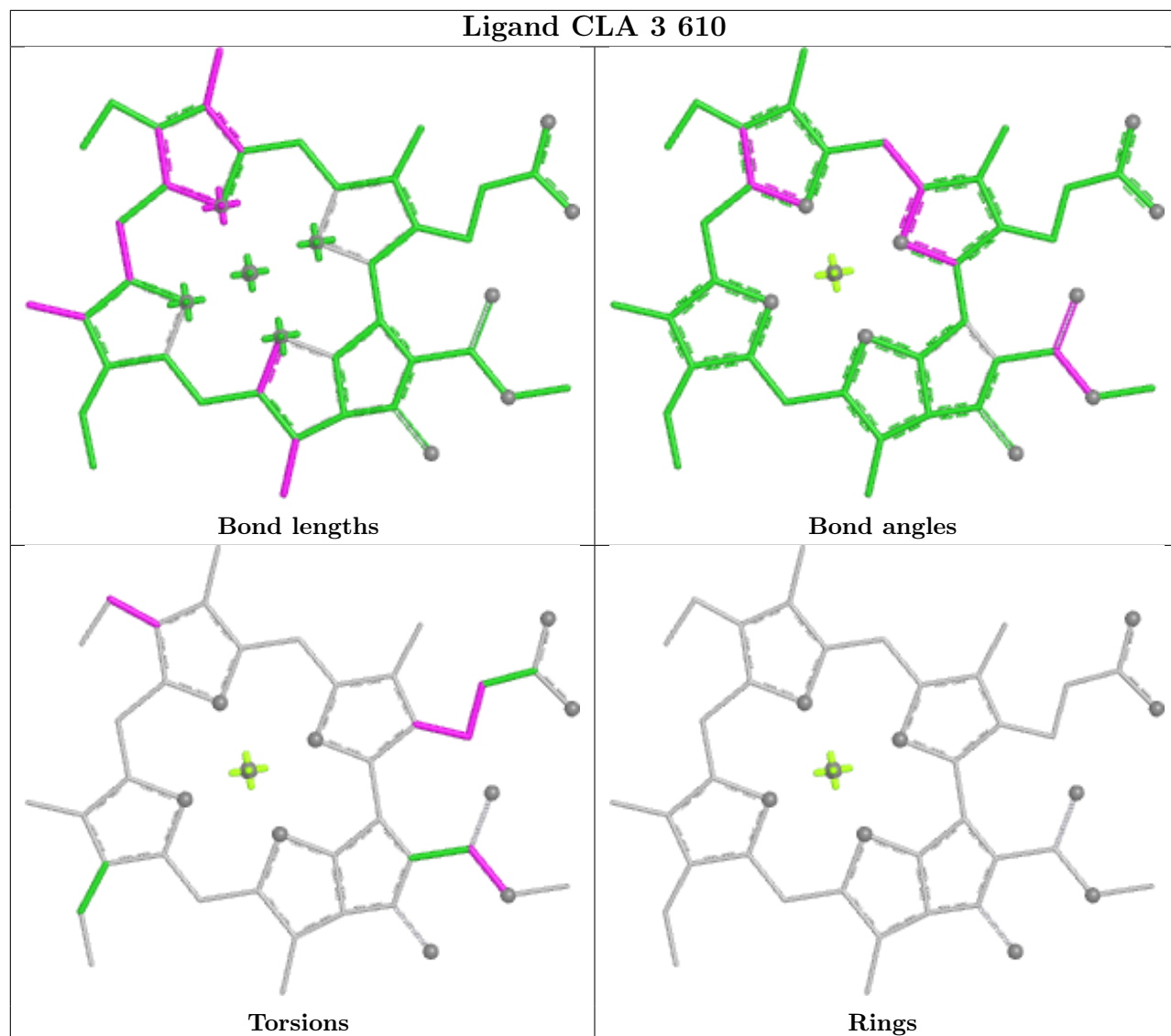


Torsions

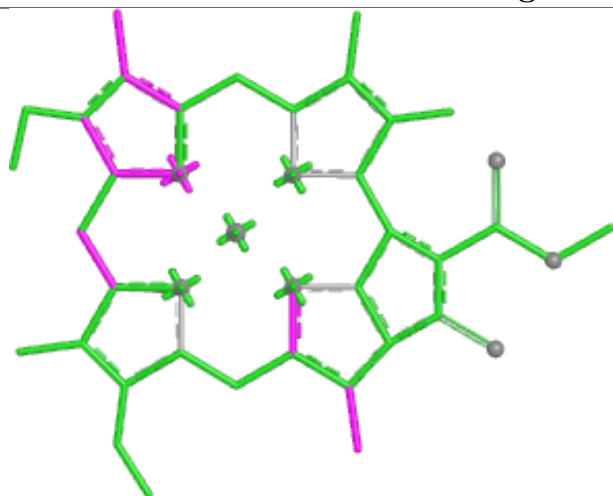


Rings

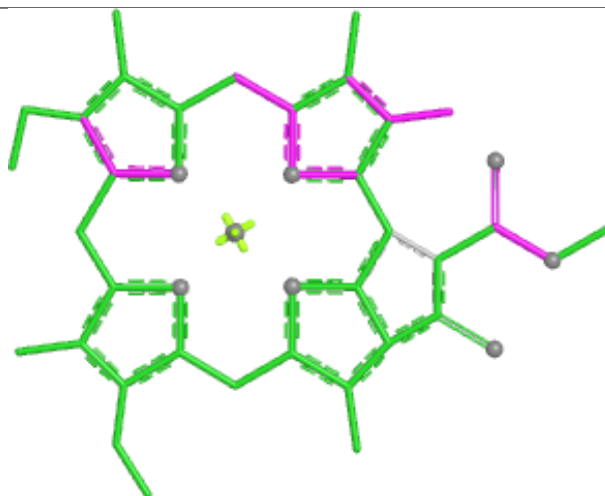
Ligand CLA 3 610



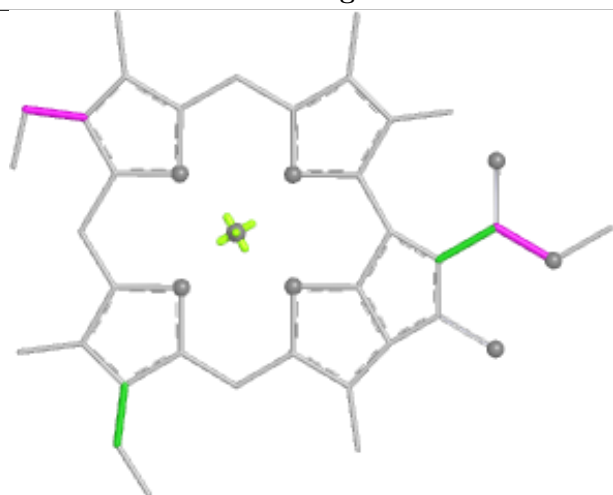
Ligand CLA 1 609



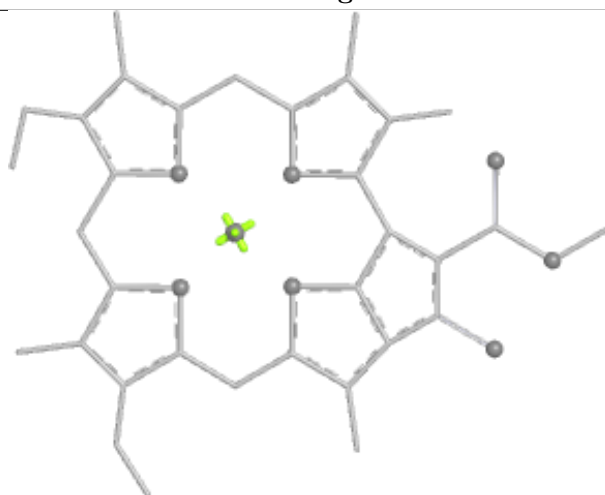
Bond lengths



Bond angles

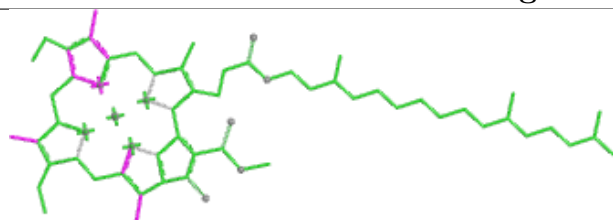


Torsions

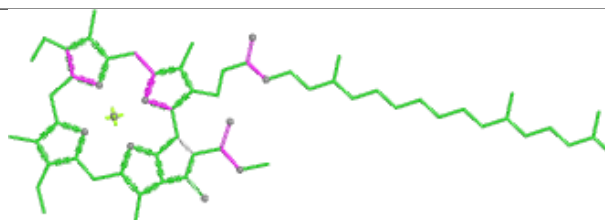


Rings

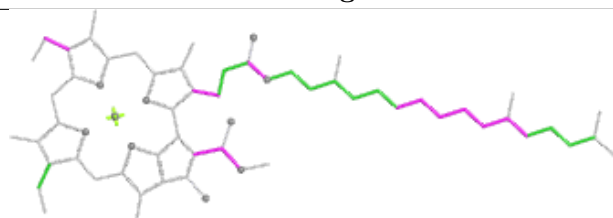
Ligand CLA c 502



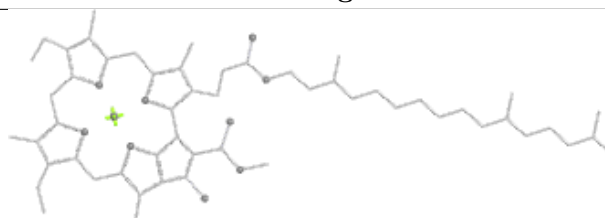
Bond lengths



Bond angles

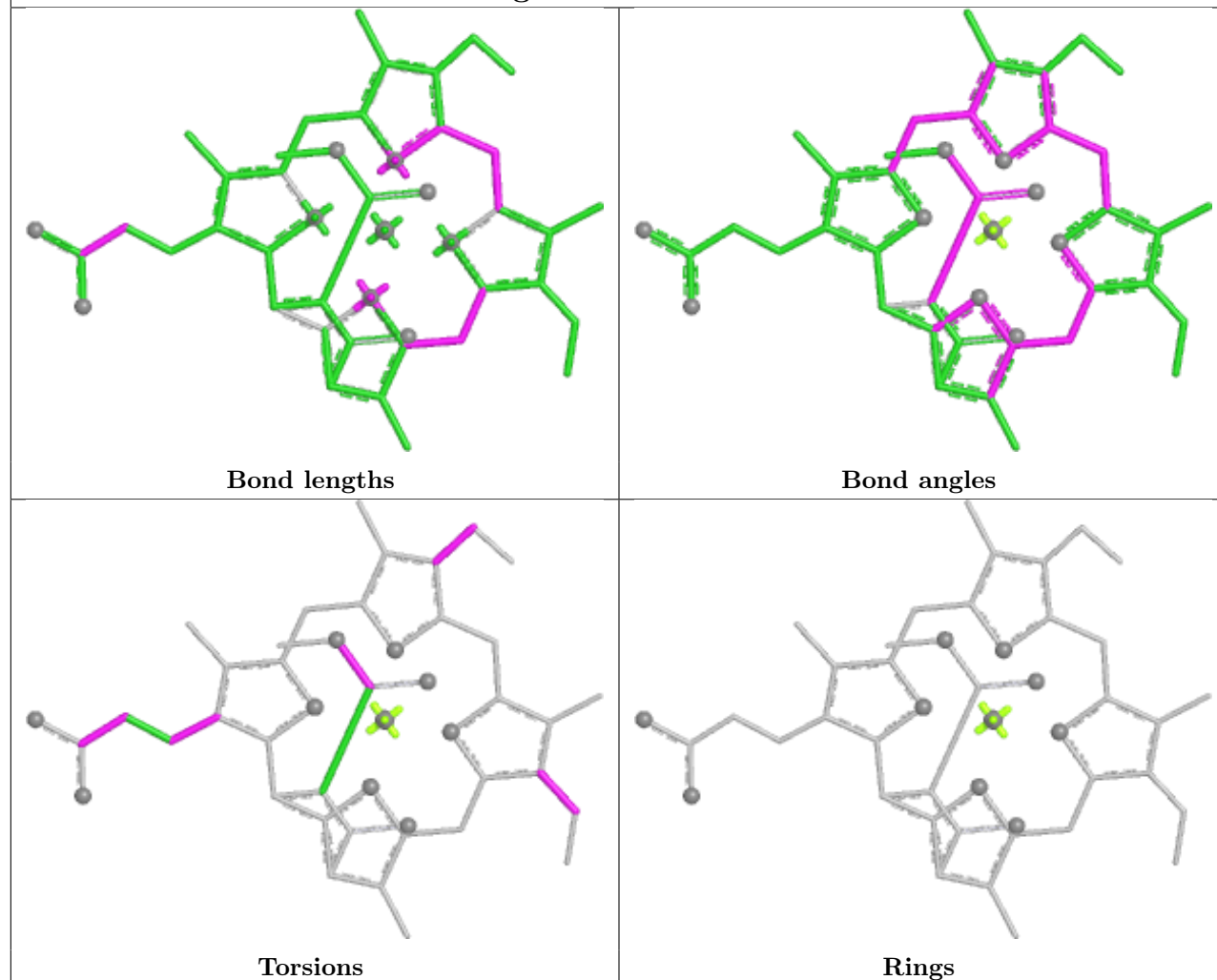


Torsions

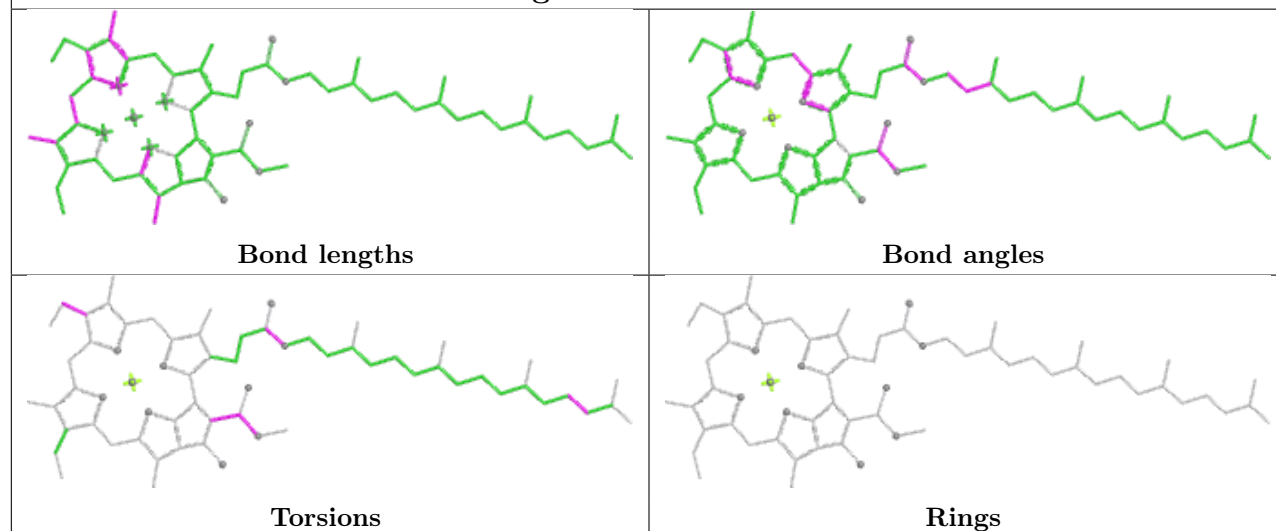


Rings

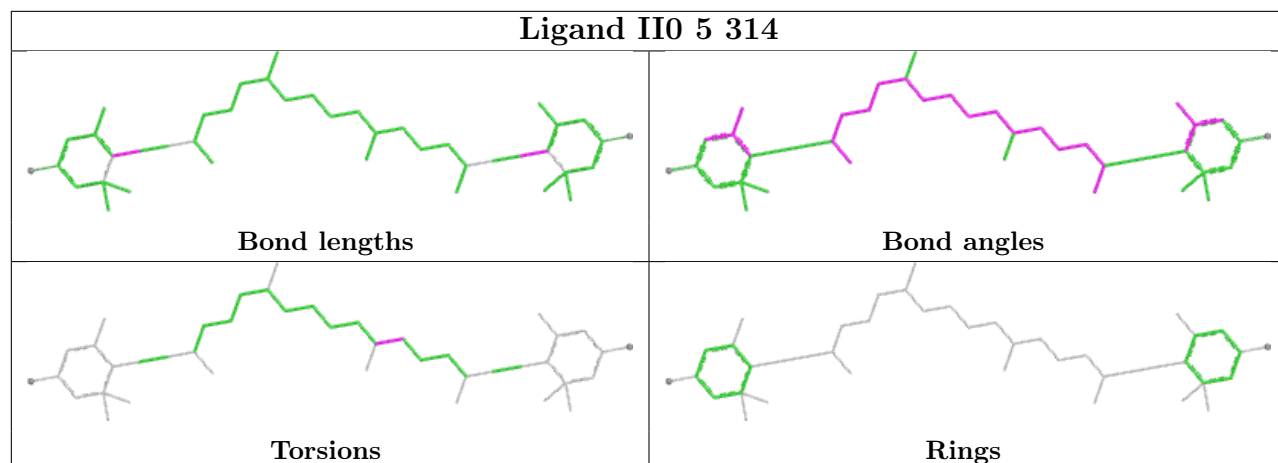
Ligand KC2 6 605



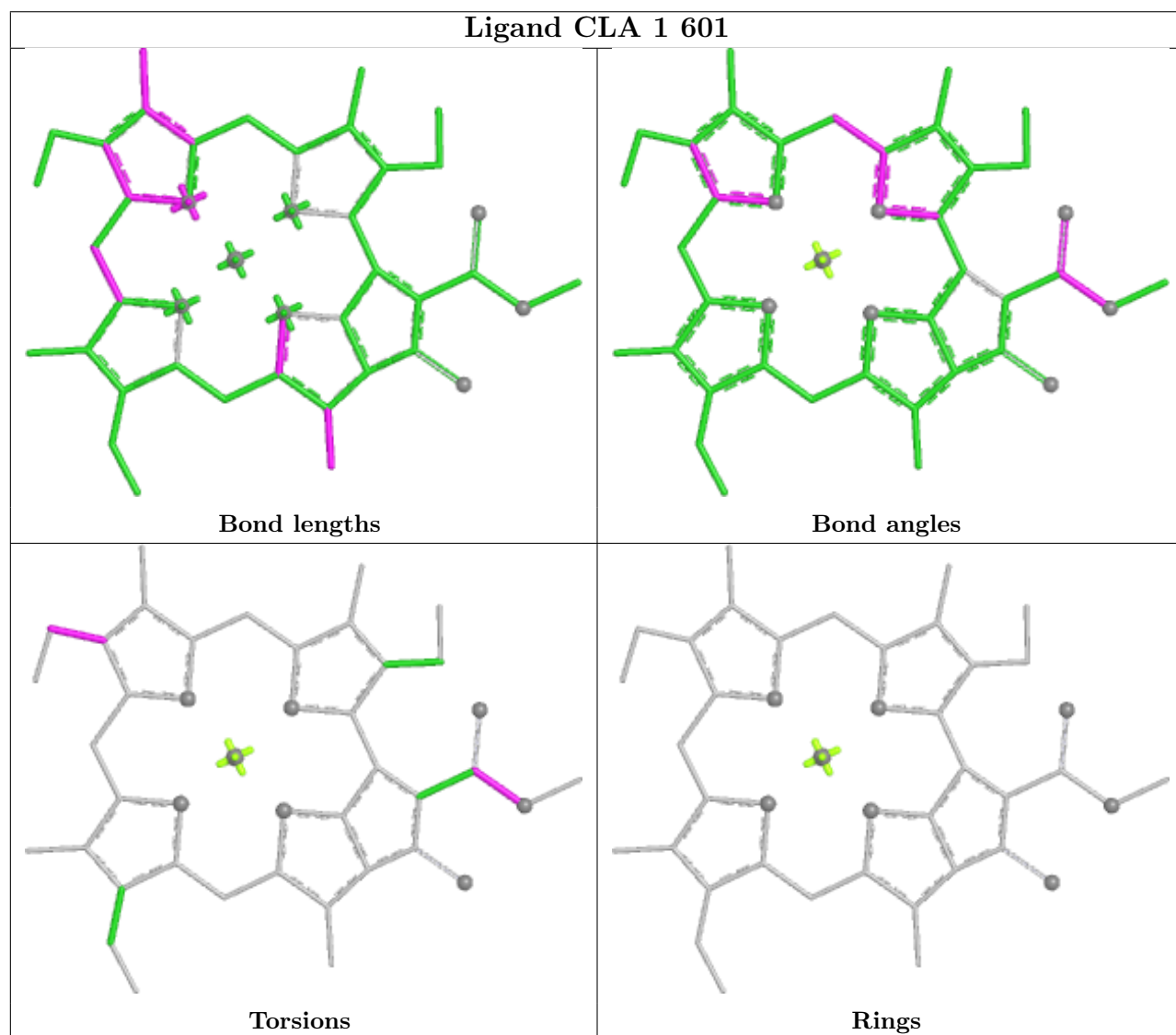
Ligand CLA B 610



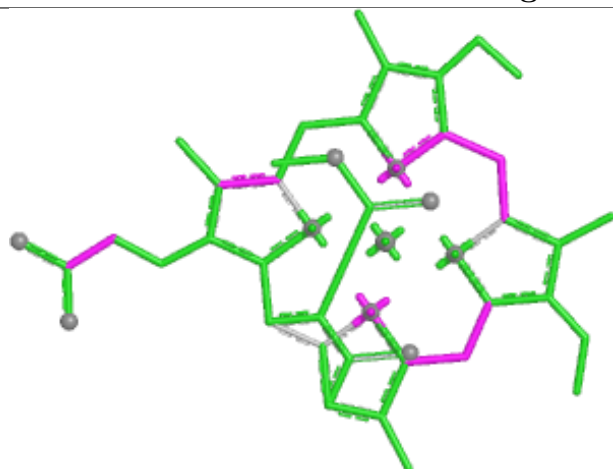
Ligand II0 5 314



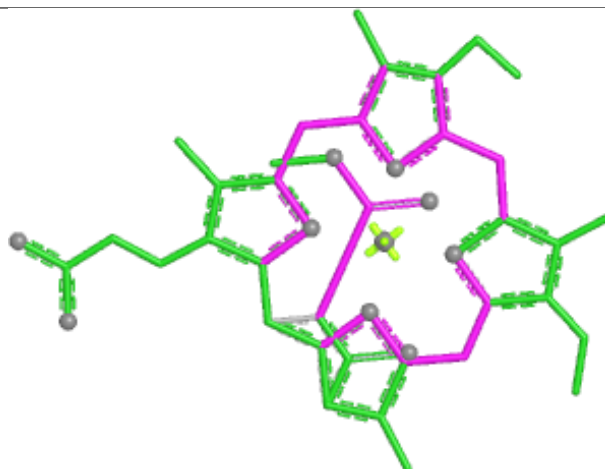
Ligand CLA 1 601



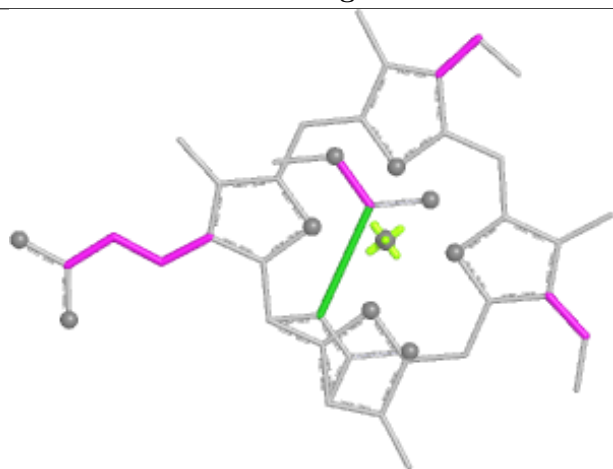
Ligand KC2 8 610



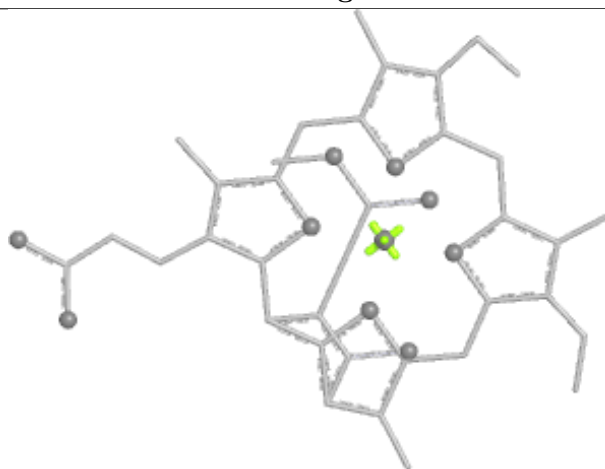
Bond lengths



Bond angles

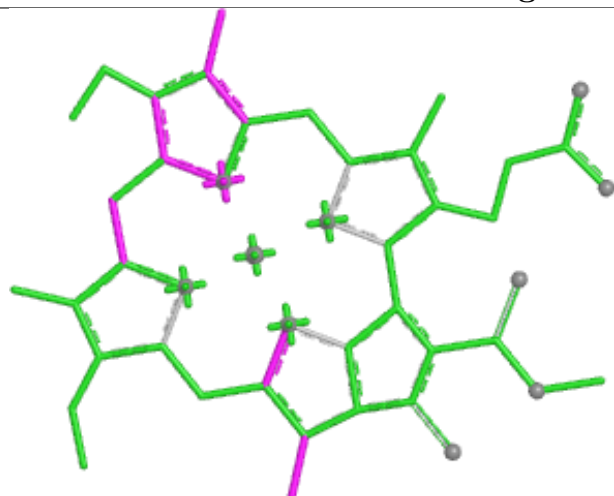


Torsions

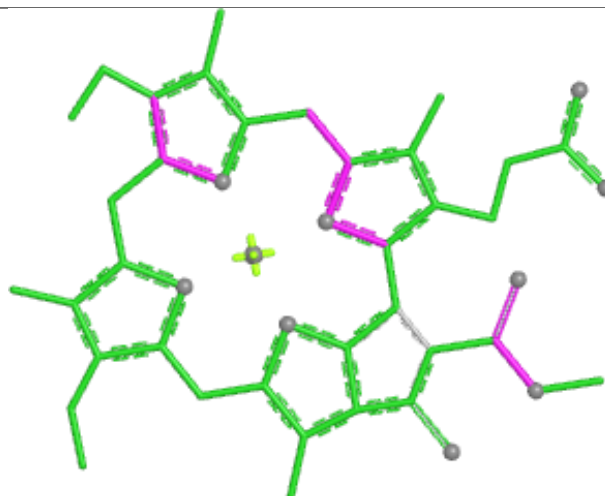


Rings

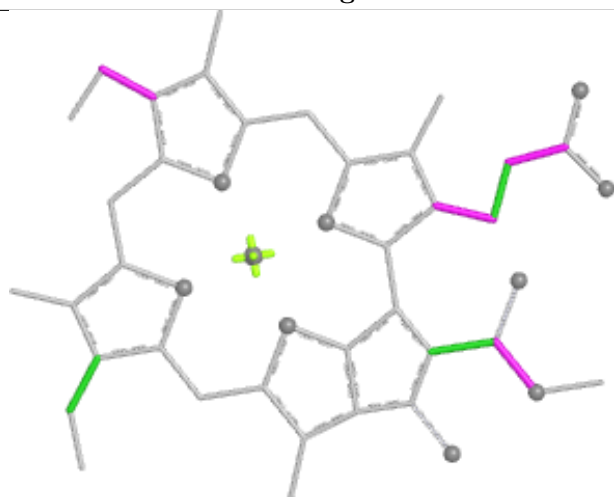
Ligand CLA 7 607



Bond lengths



Bond angles

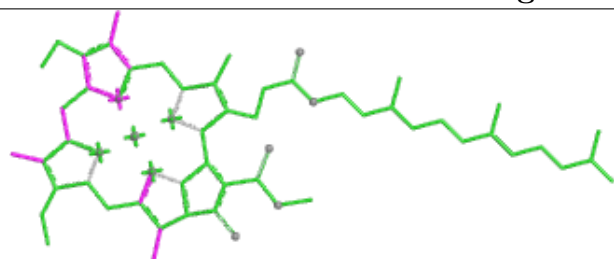


Torsions

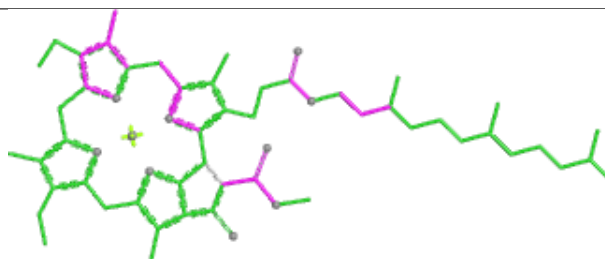


Rings

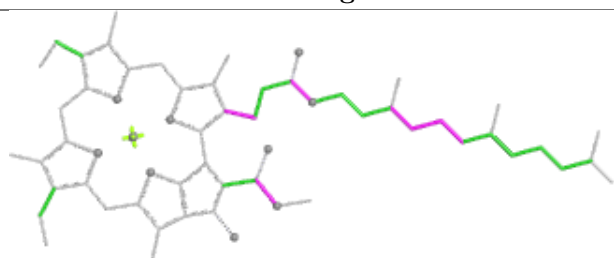
Ligand CLA d 403



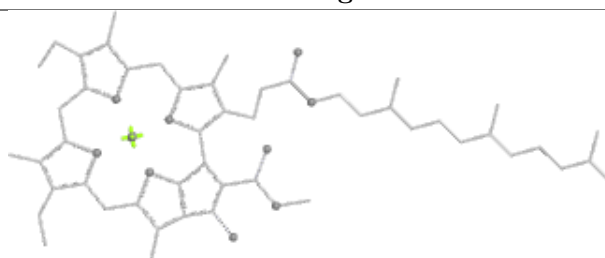
Bond lengths



Bond angles

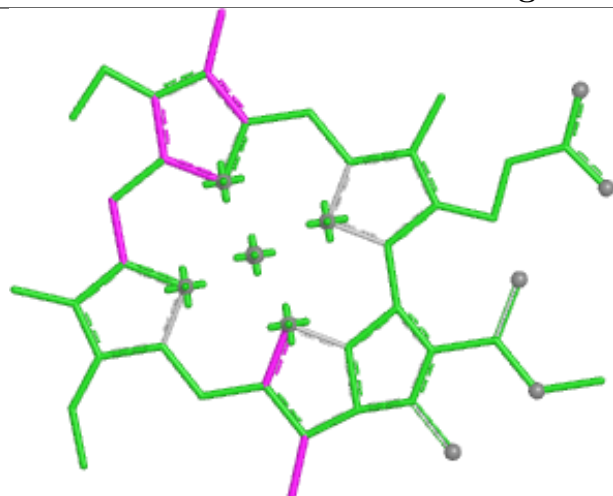


Torsions

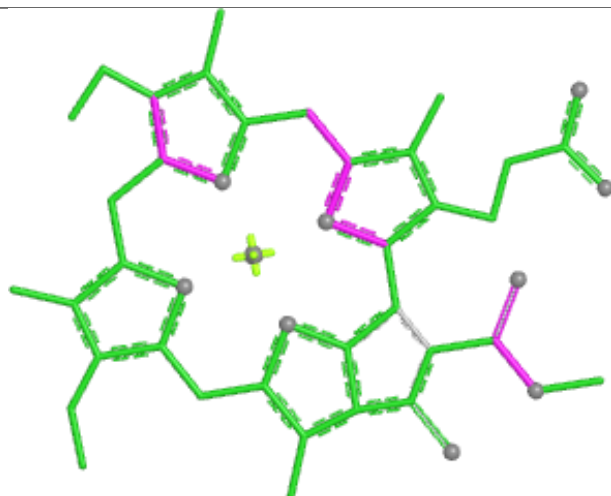


Rings

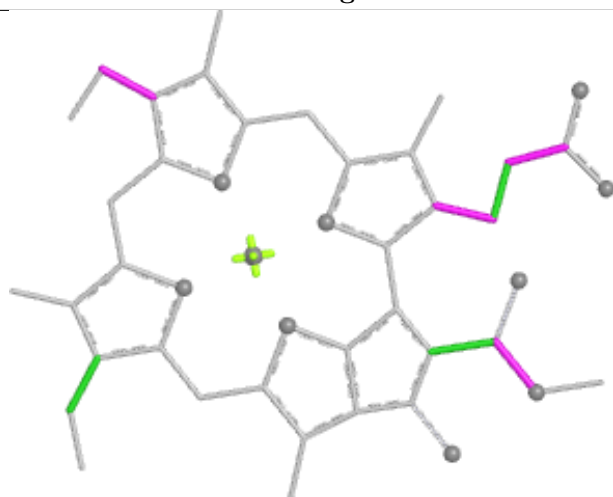
Ligand CLA 1 612



Bond lengths



Bond angles

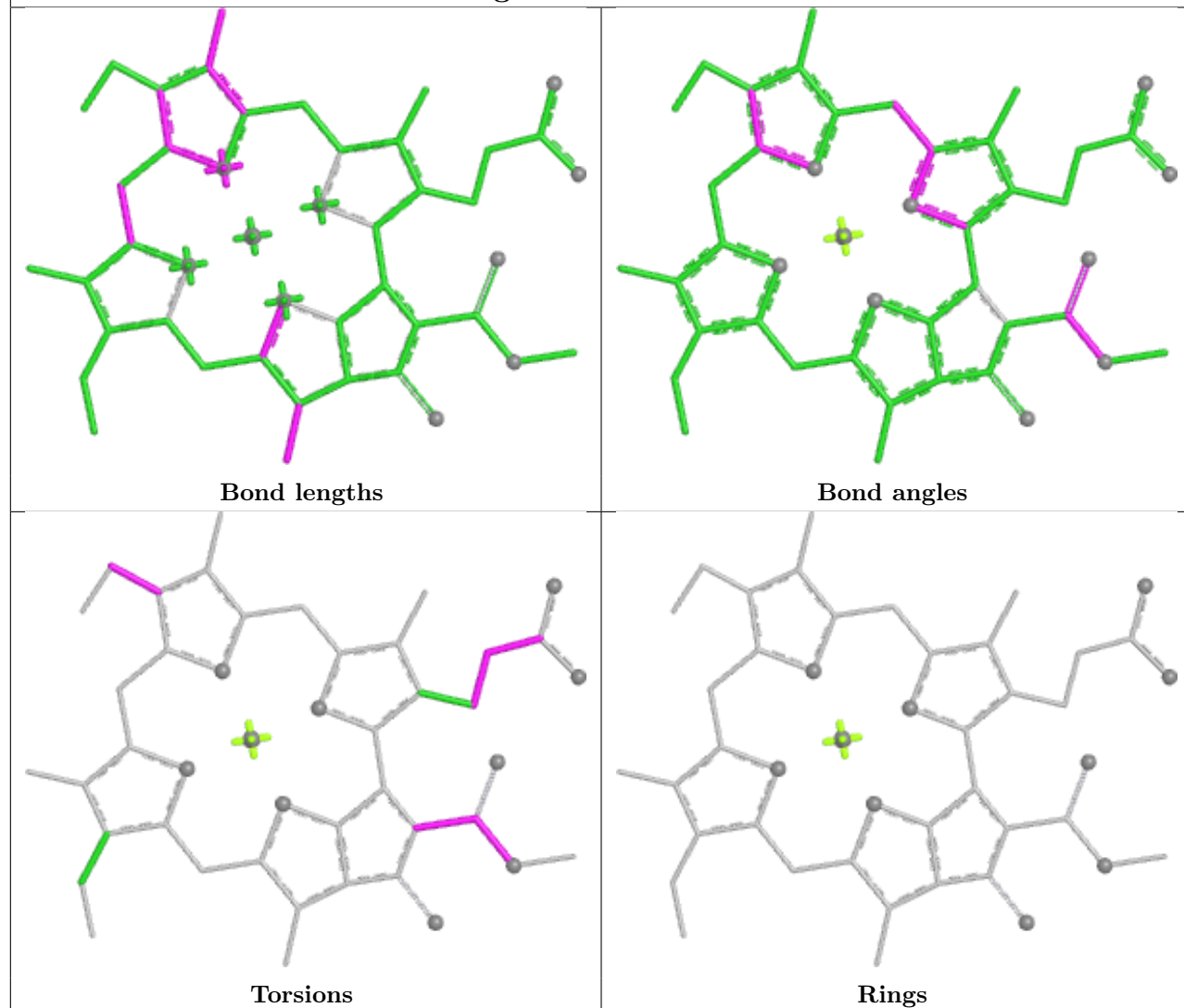


Torsions

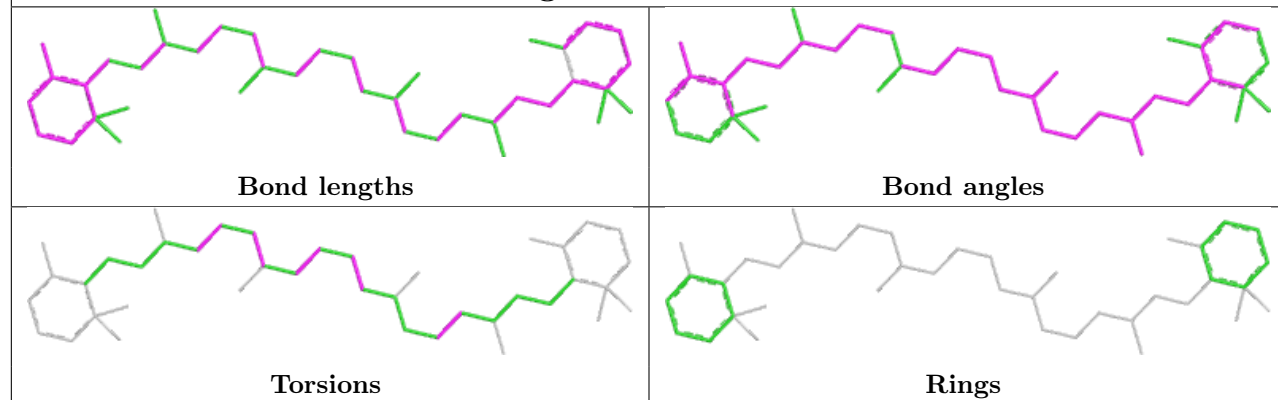


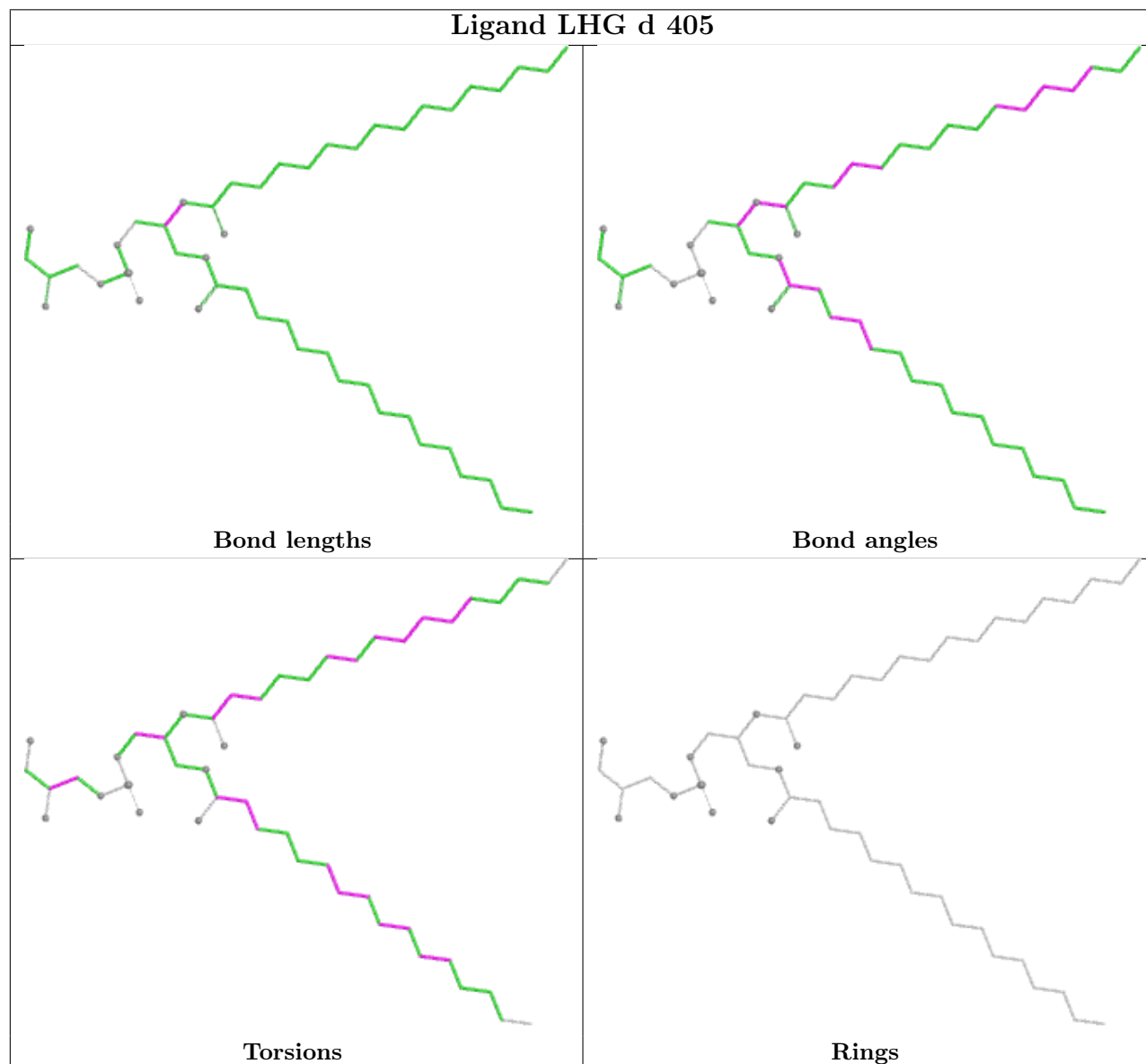
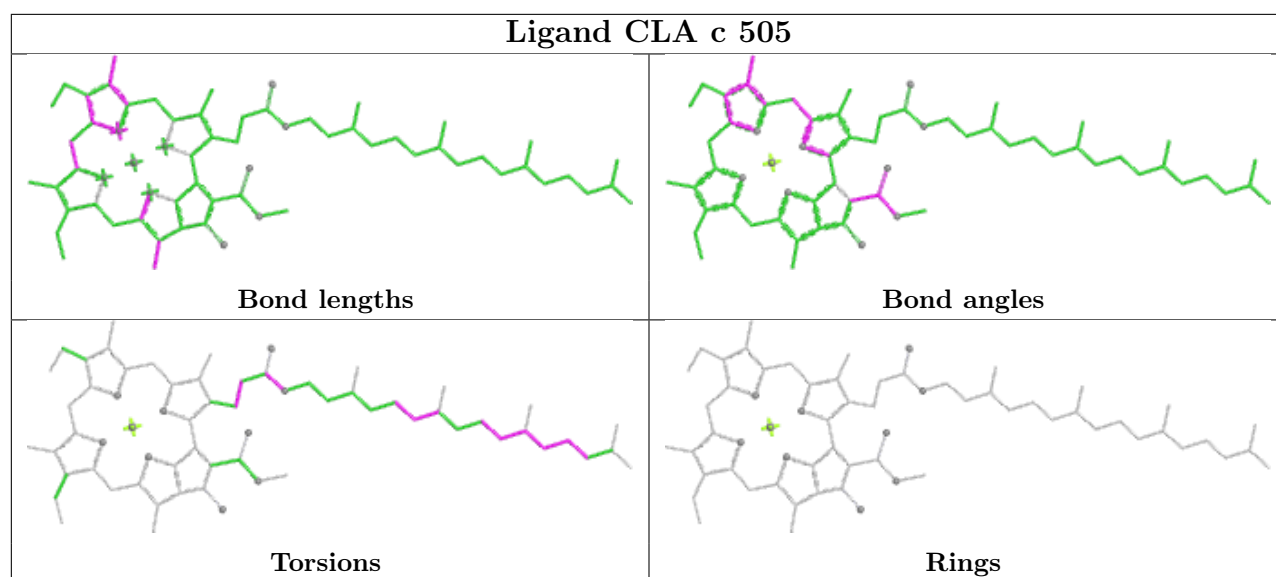
Rings

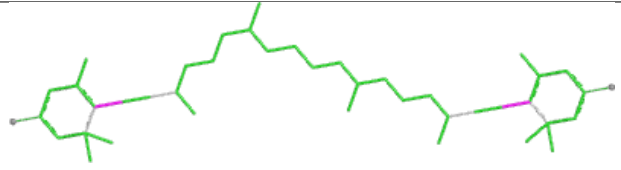
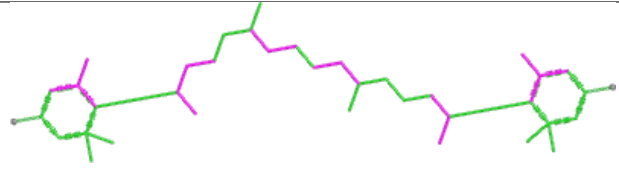
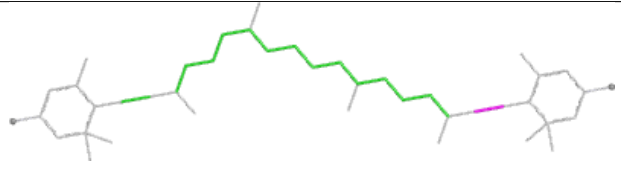
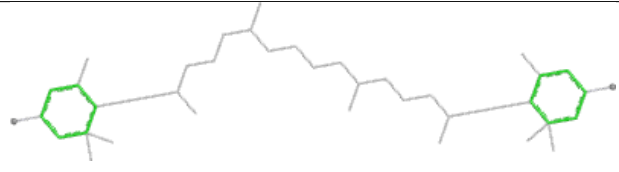
Ligand CLA P 611

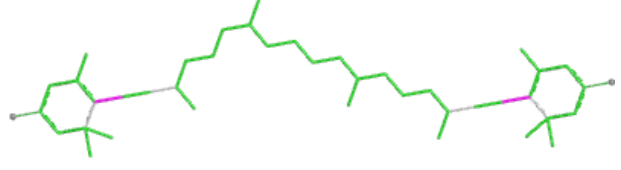
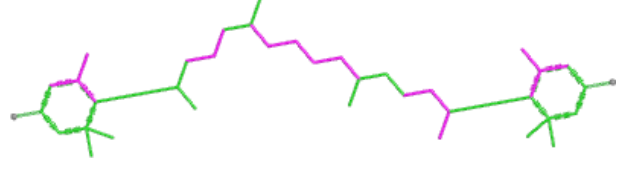
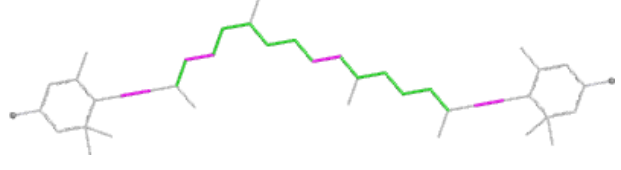
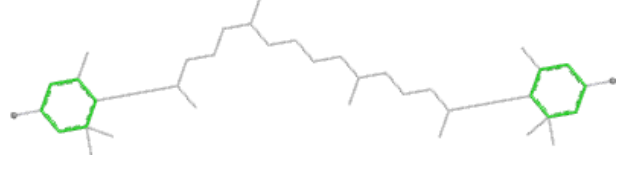


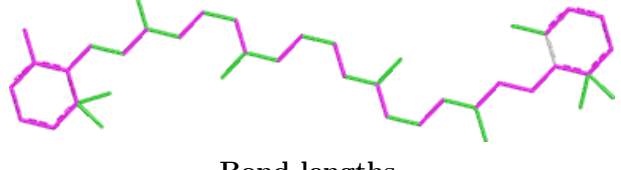
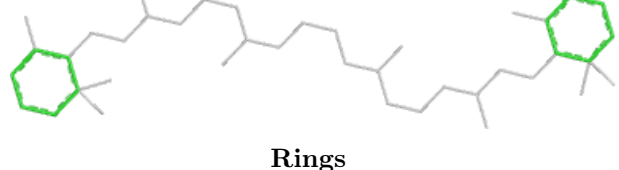
Ligand 8CT k 101



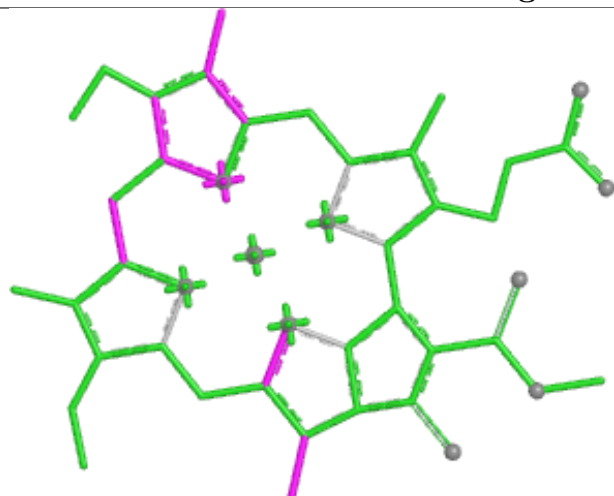


Ligand II0 7 619	
	
Bond lengths	Bond angles
	
Torsions	Rings

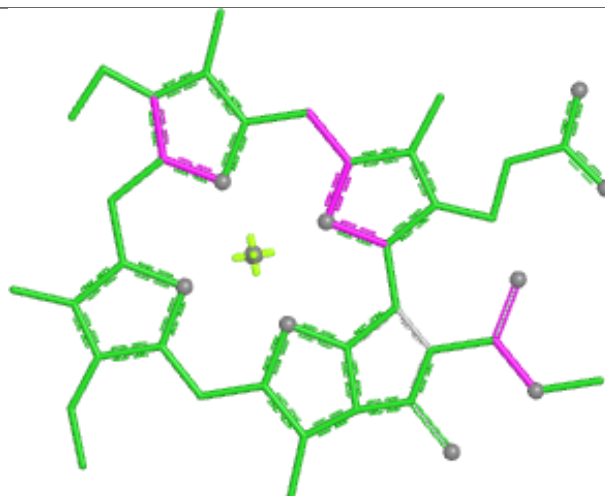
Ligand II0 p 315	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand 8CT B 624	
	
Bond lengths	Bond angles
	
Torsions	Rings

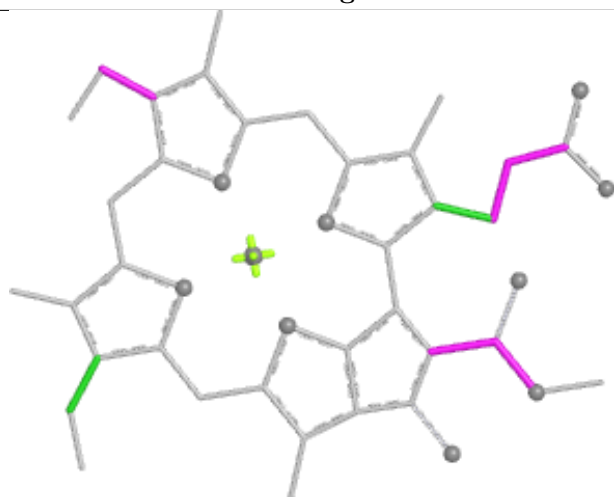
Ligand CLA 4 613



Bond lengths



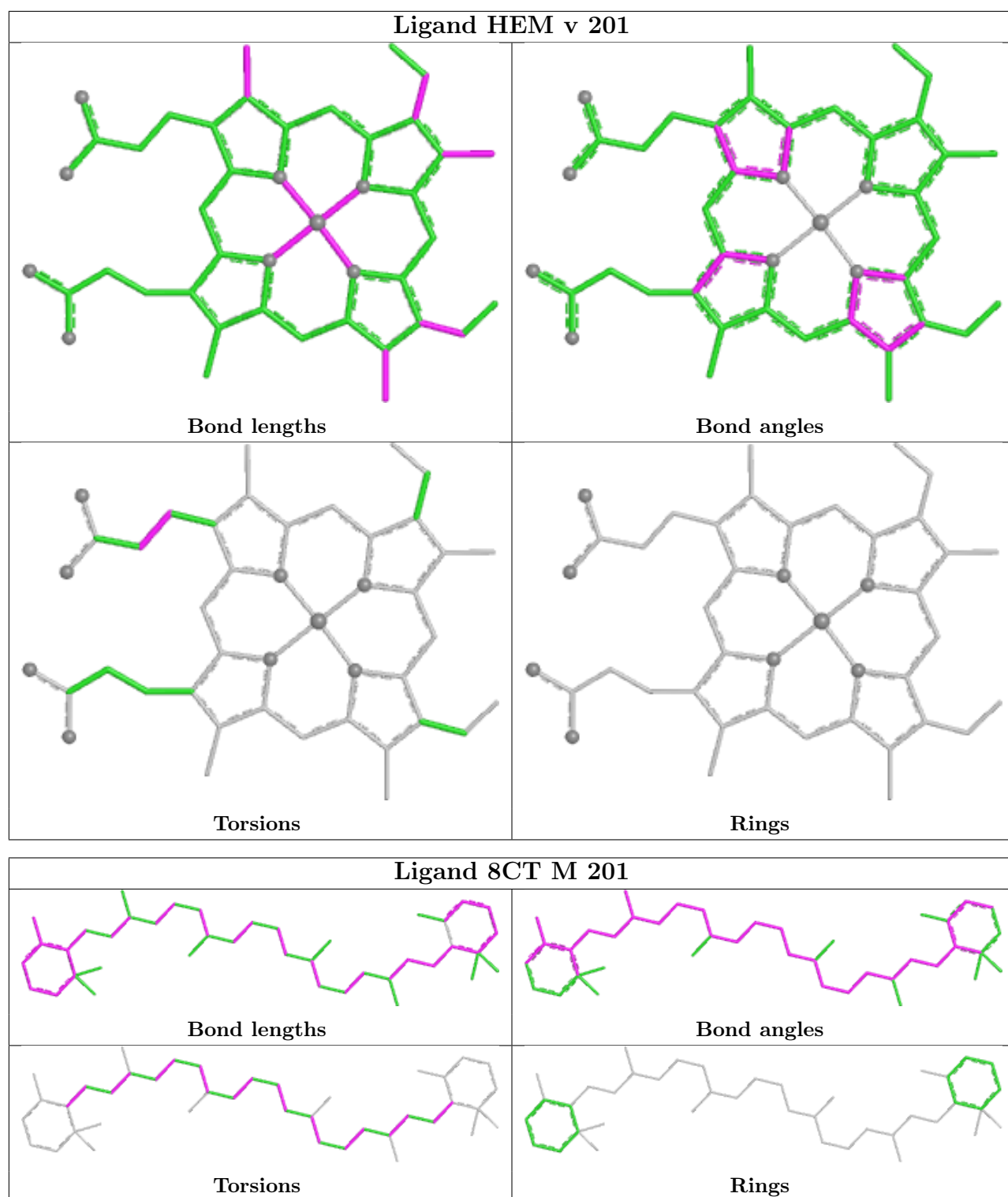
Bond angles

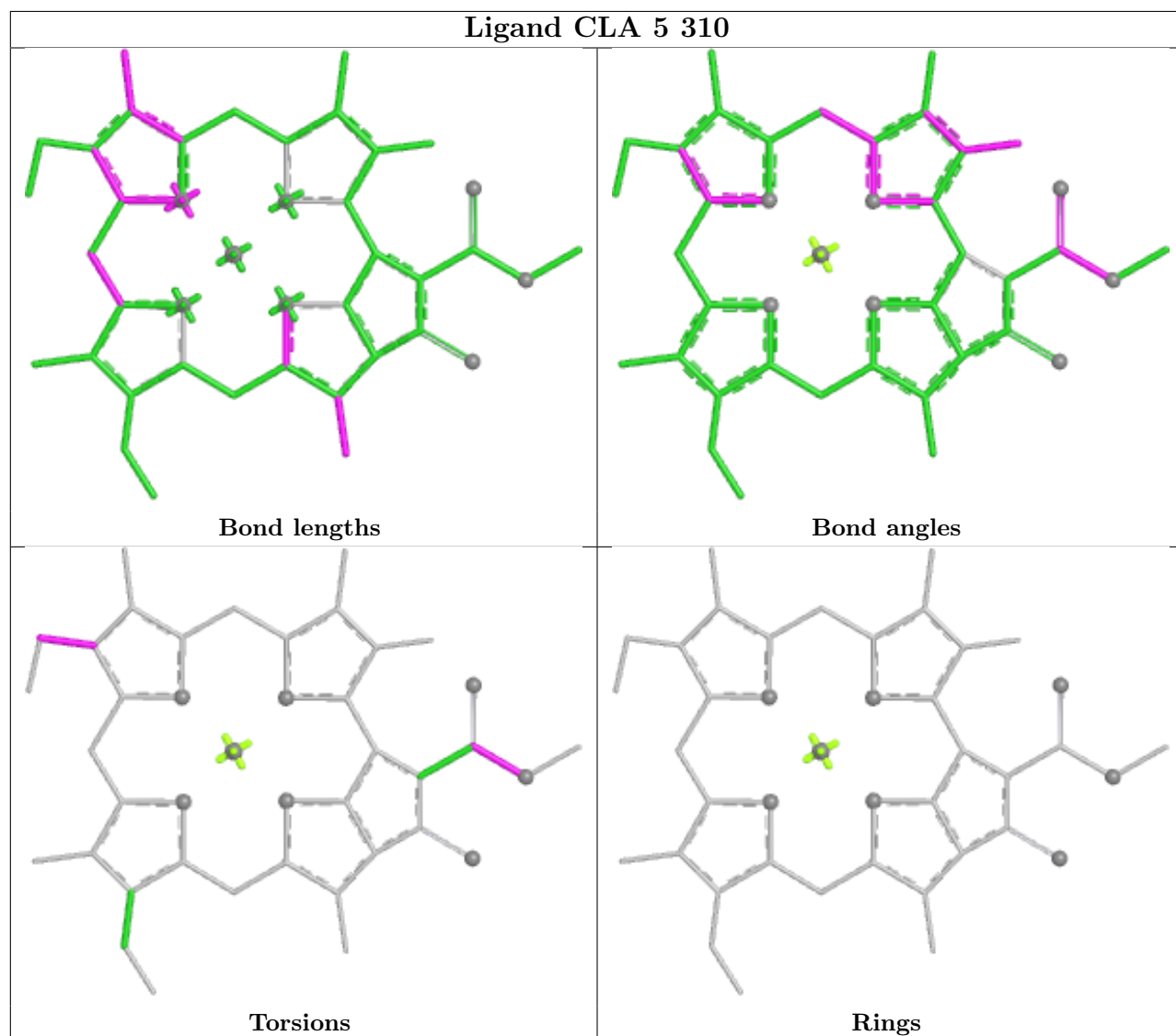
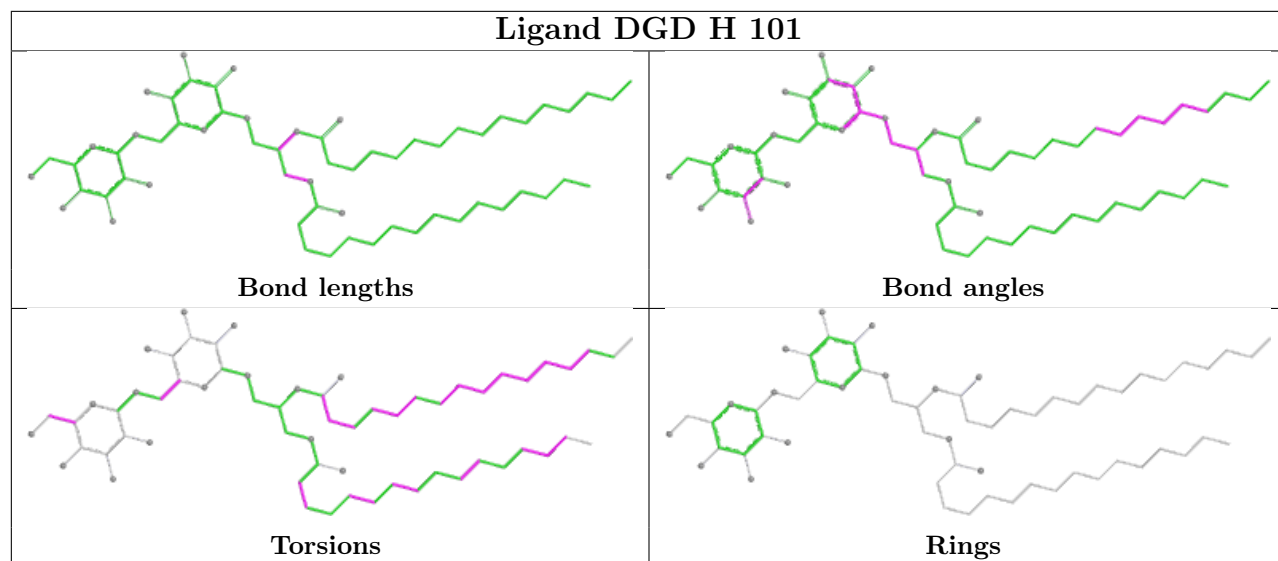


Torsions

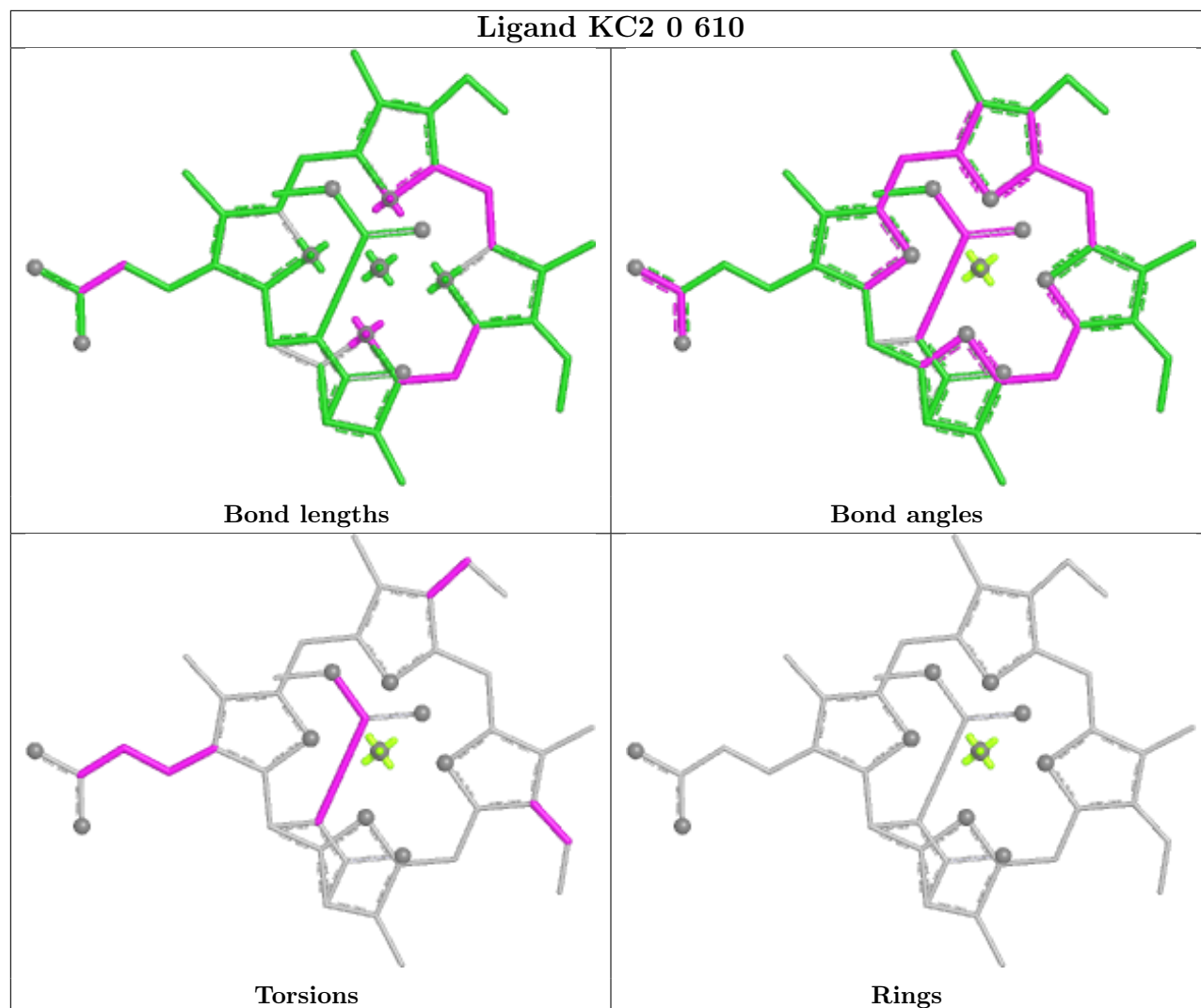


Rings

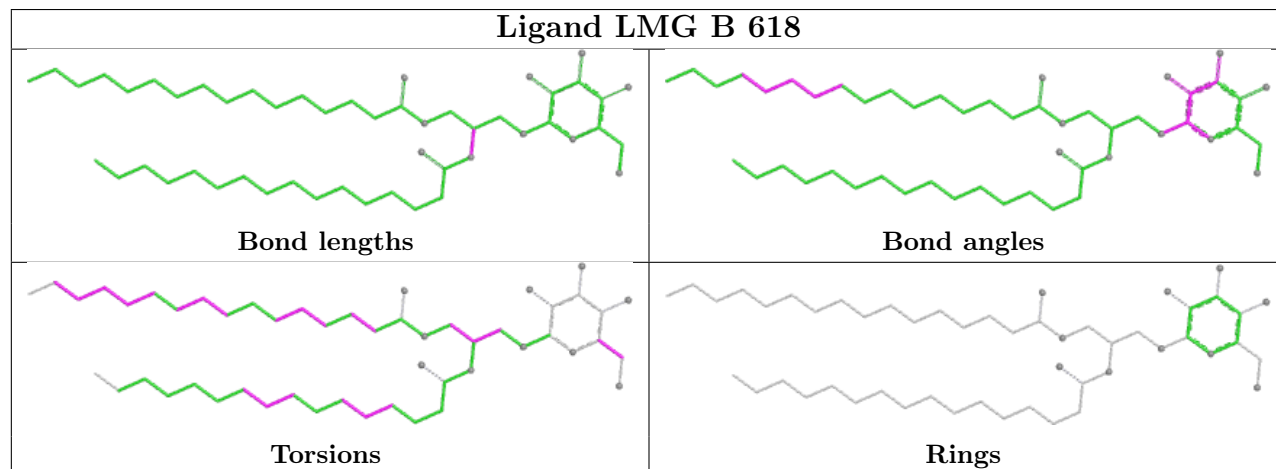




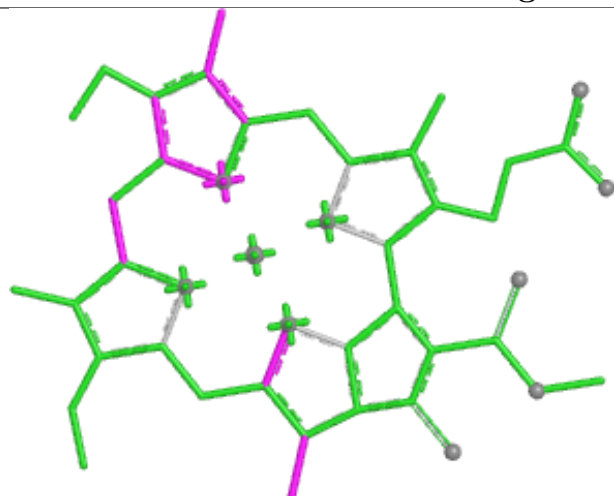
Ligand KC2 0 610



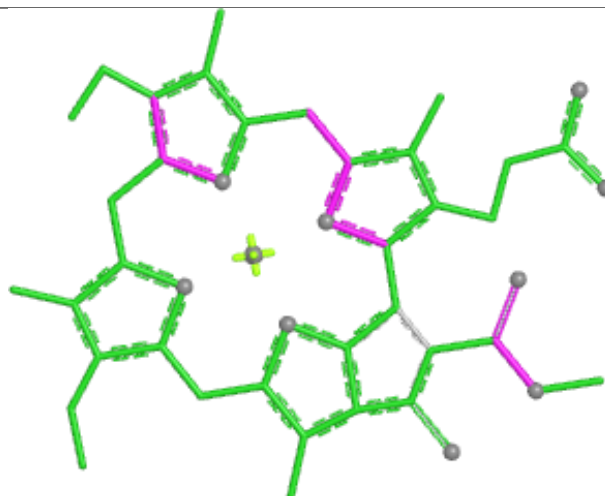
Ligand LMG B 618



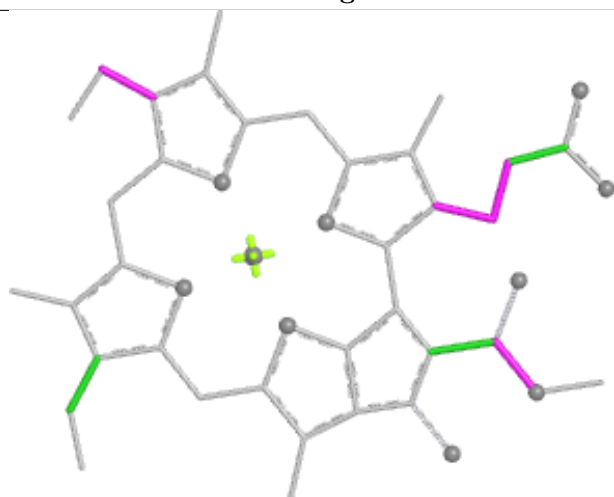
Ligand CLA 9 610



Bond lengths



Bond angles

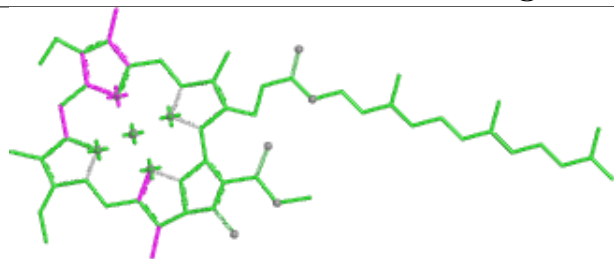


Torsions

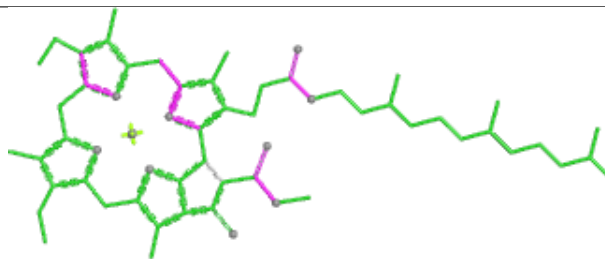


Rings

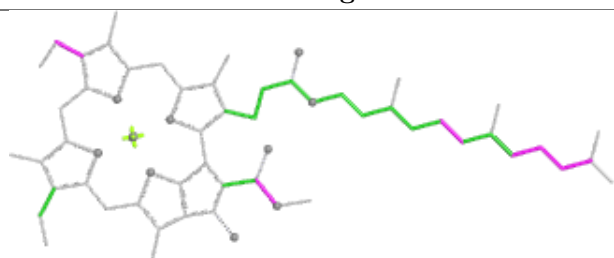
Ligand CLA 0 608



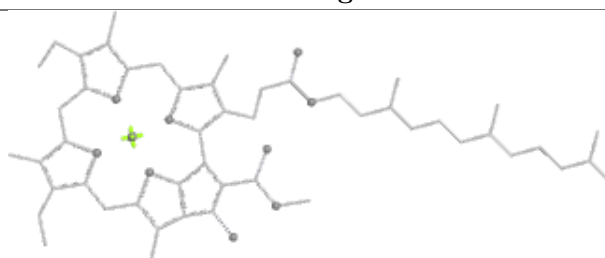
Bond lengths



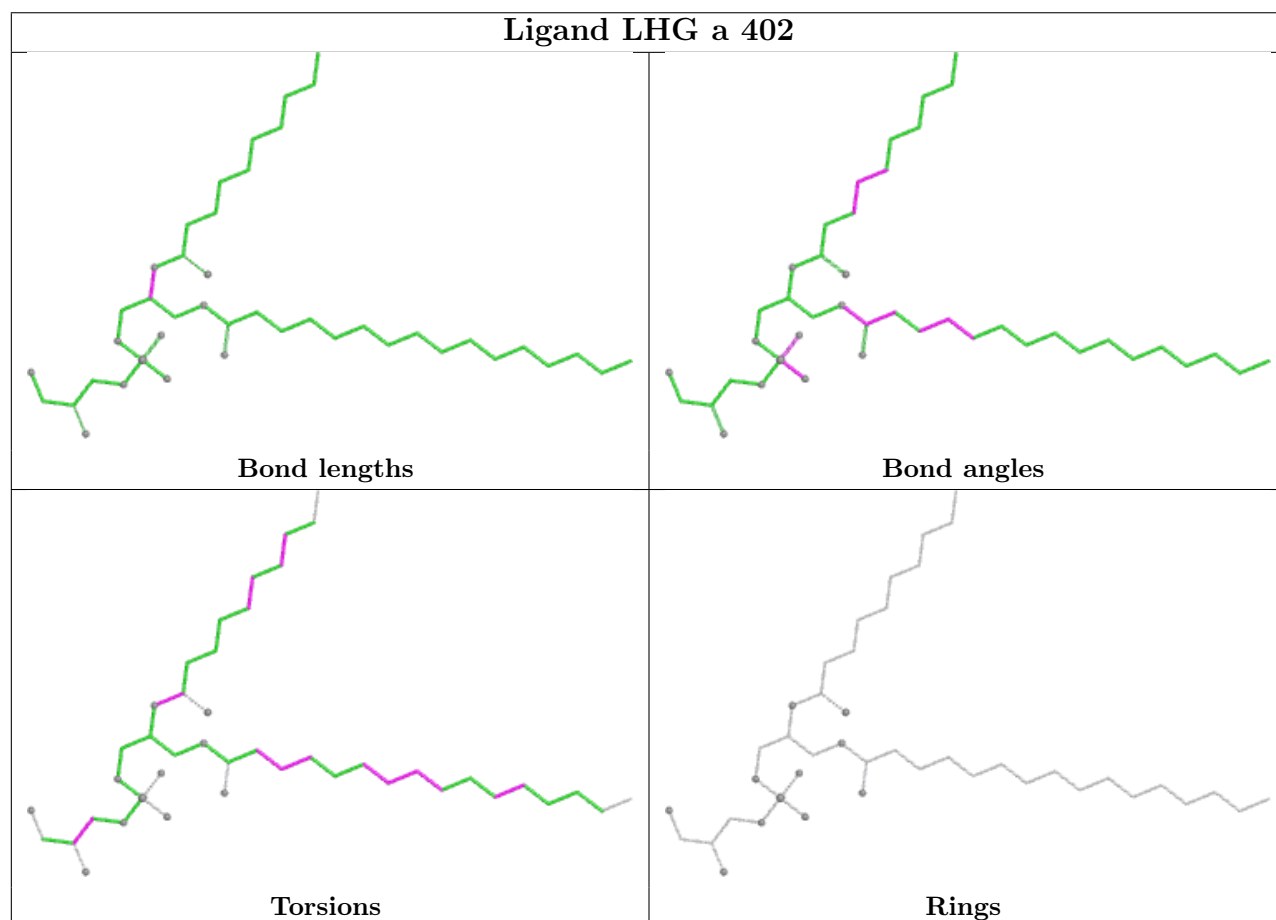
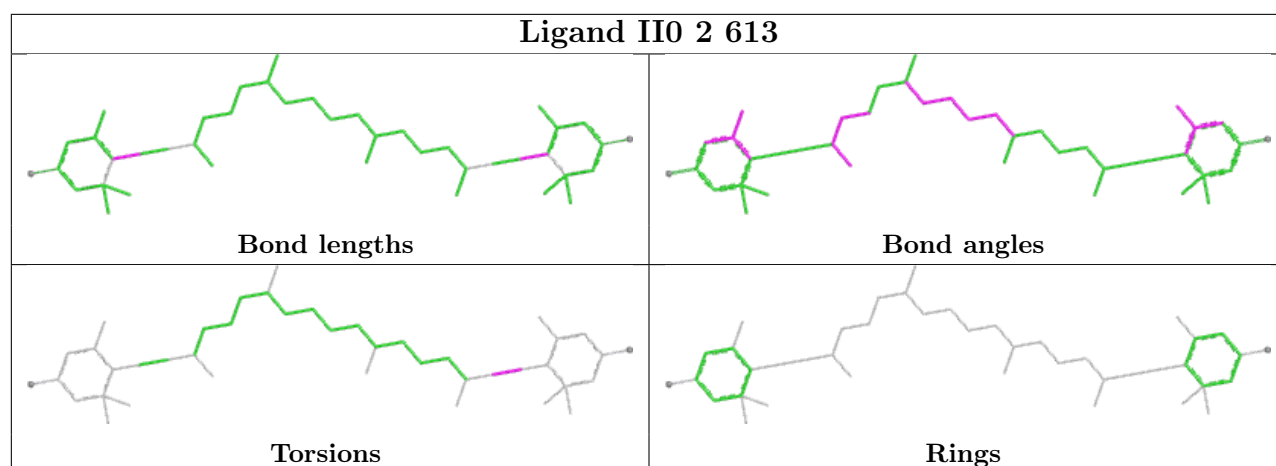
Bond angles



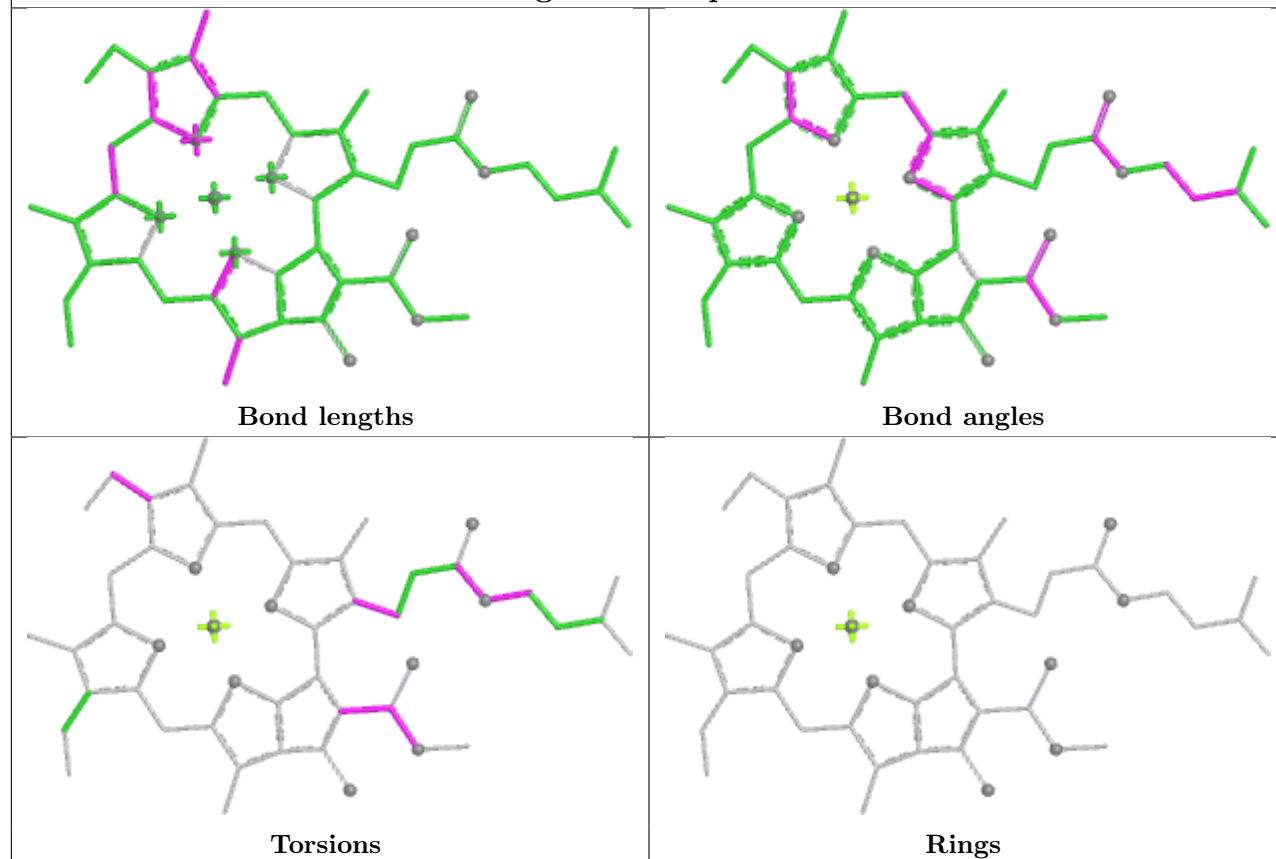
Torsions



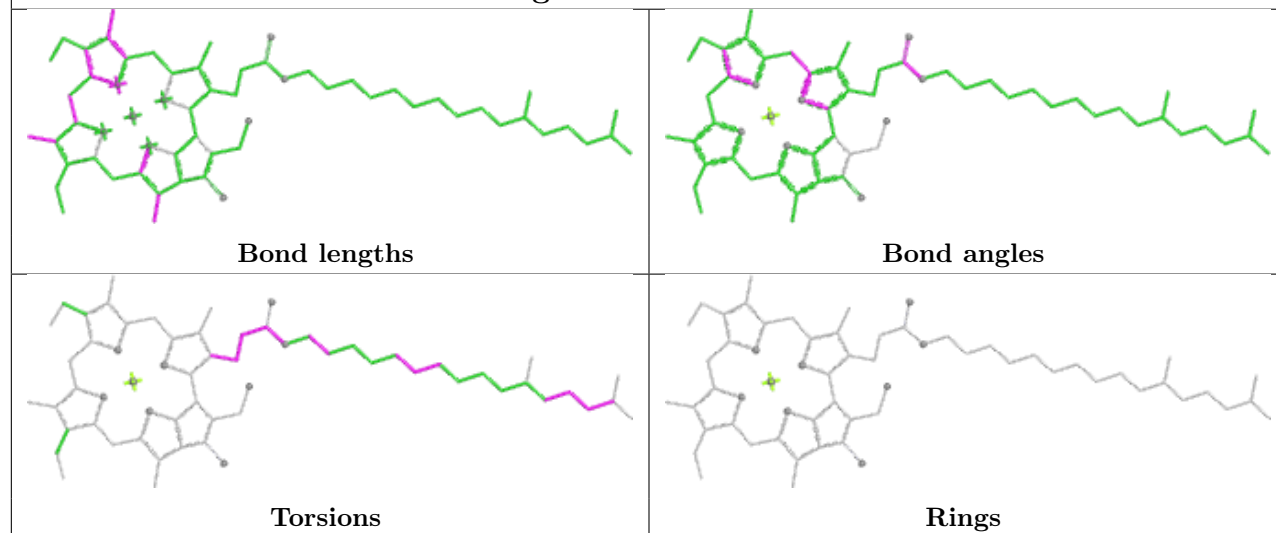
Rings



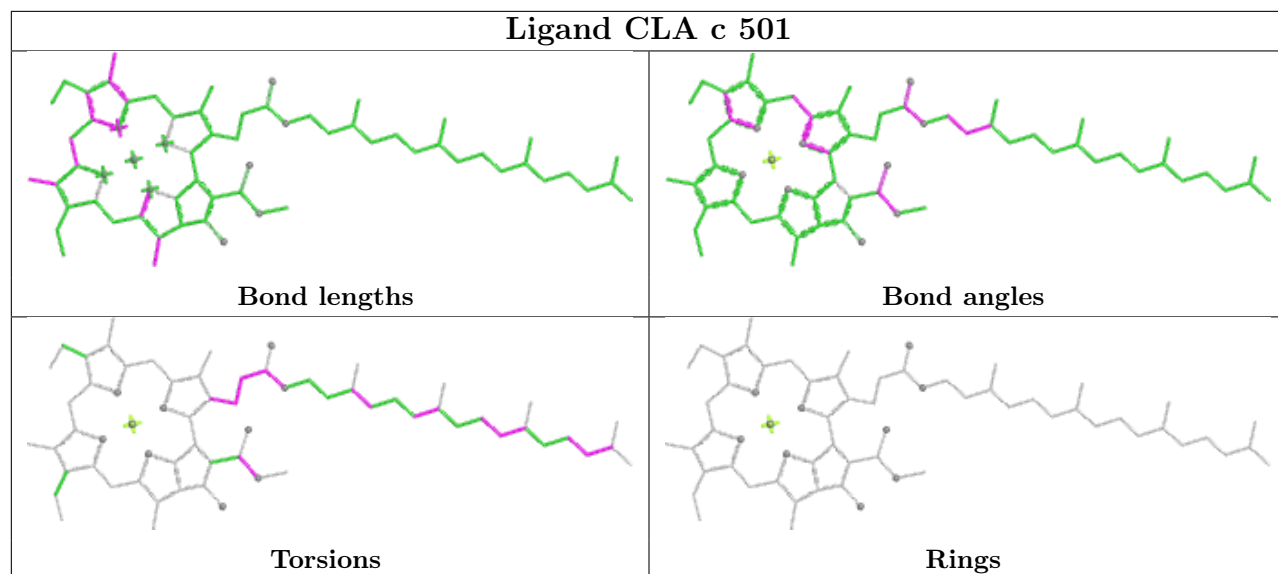
Ligand CLA p 304



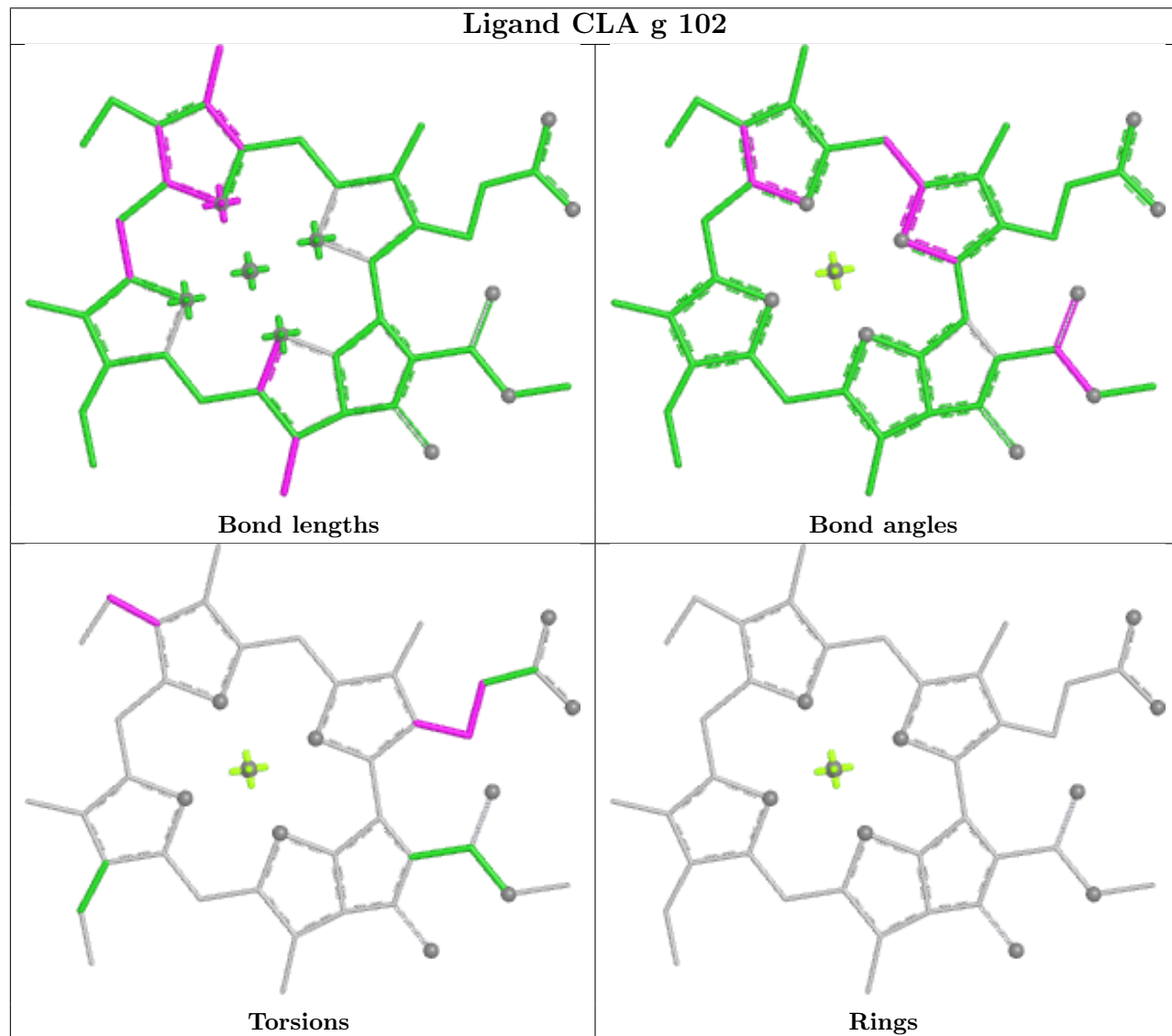
Ligand CLA B 603



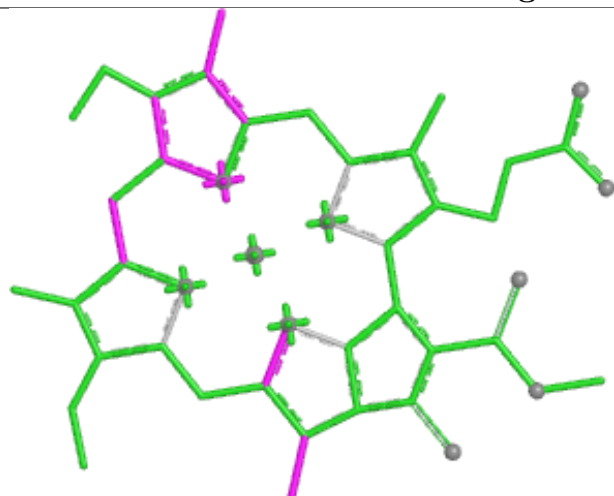
Ligand CLA c 501



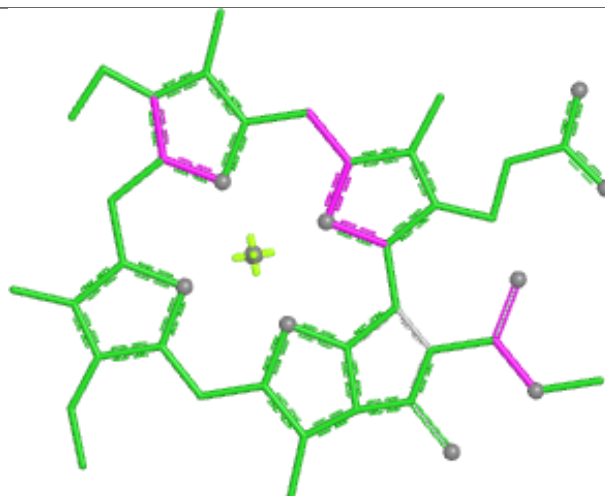
Ligand CLA g 102



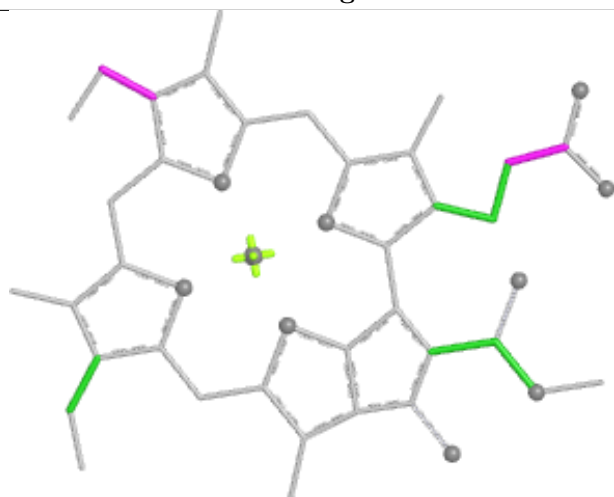
Ligand CLA 4 607



Bond lengths



Bond angles

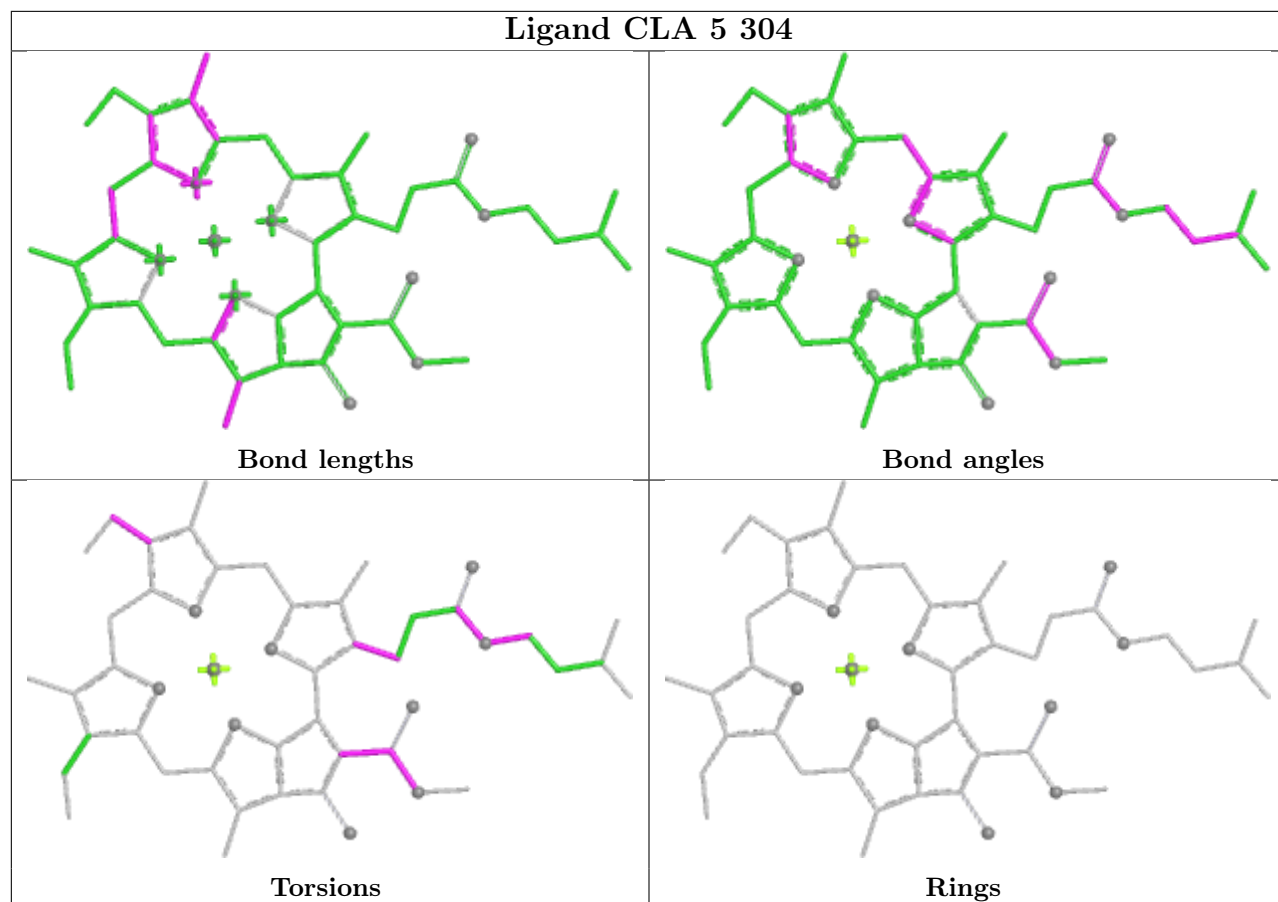


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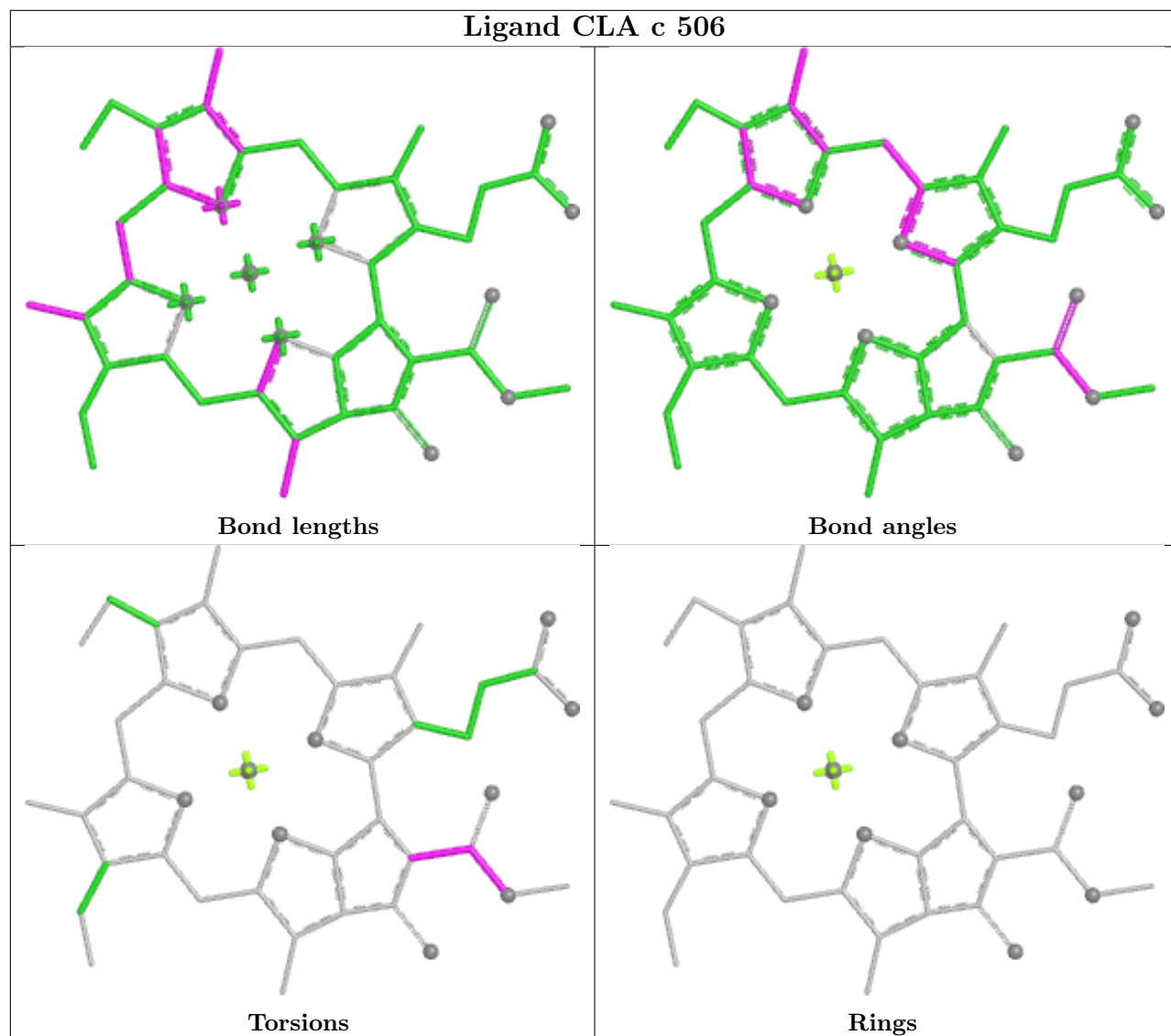


Rings

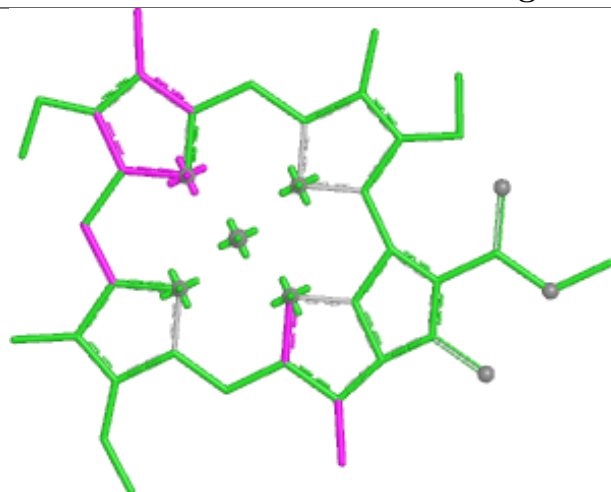
Ligand CLA 5 304



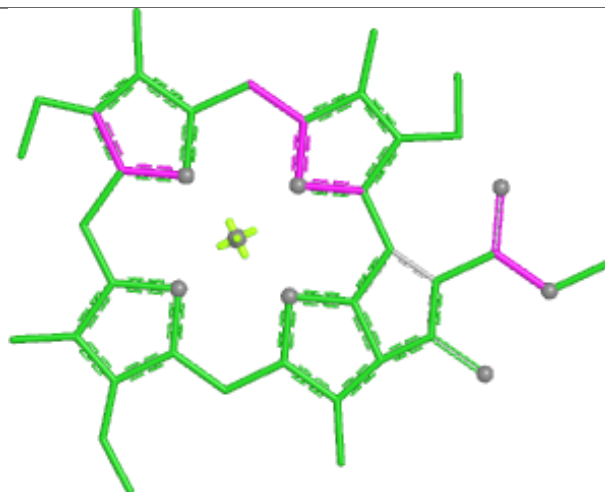
Ligand CLA c 506



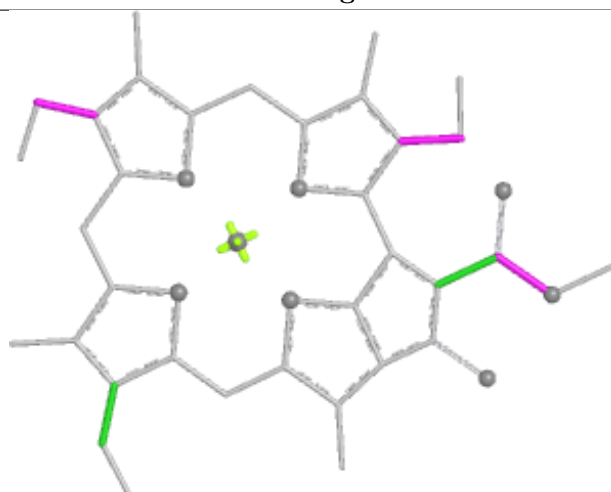
Ligand CLA 7 601



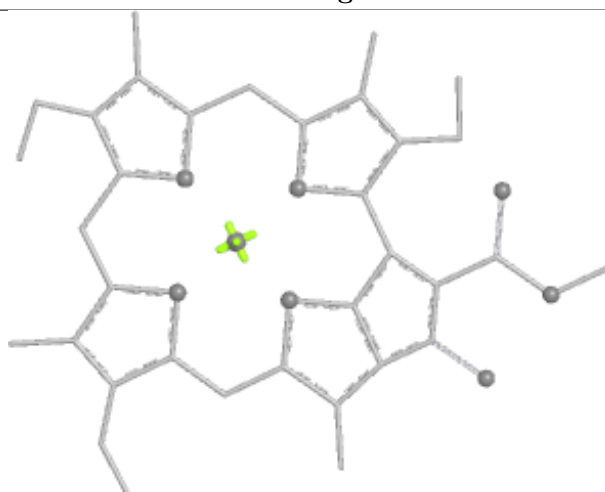
Bond lengths



Bond angles

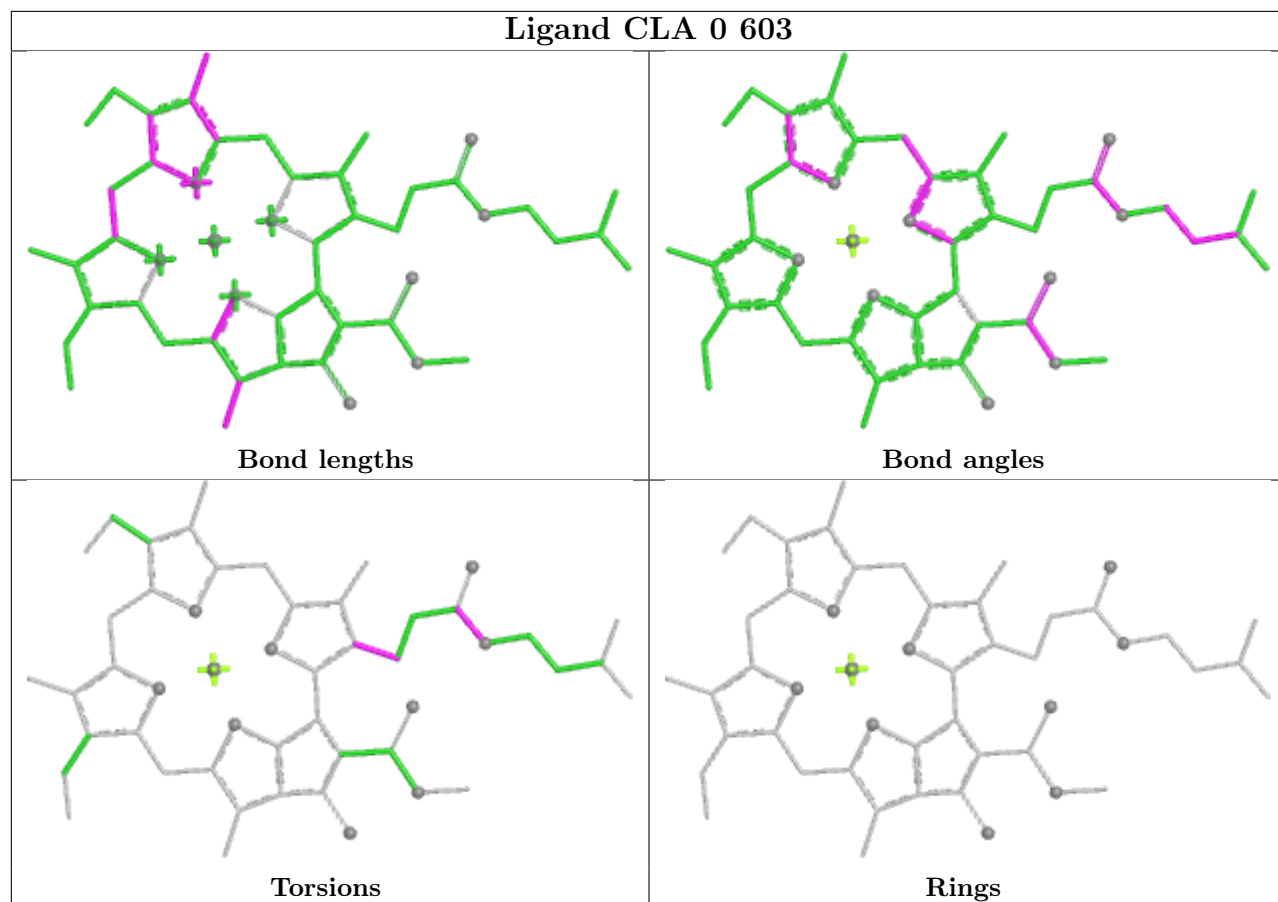


Torsions

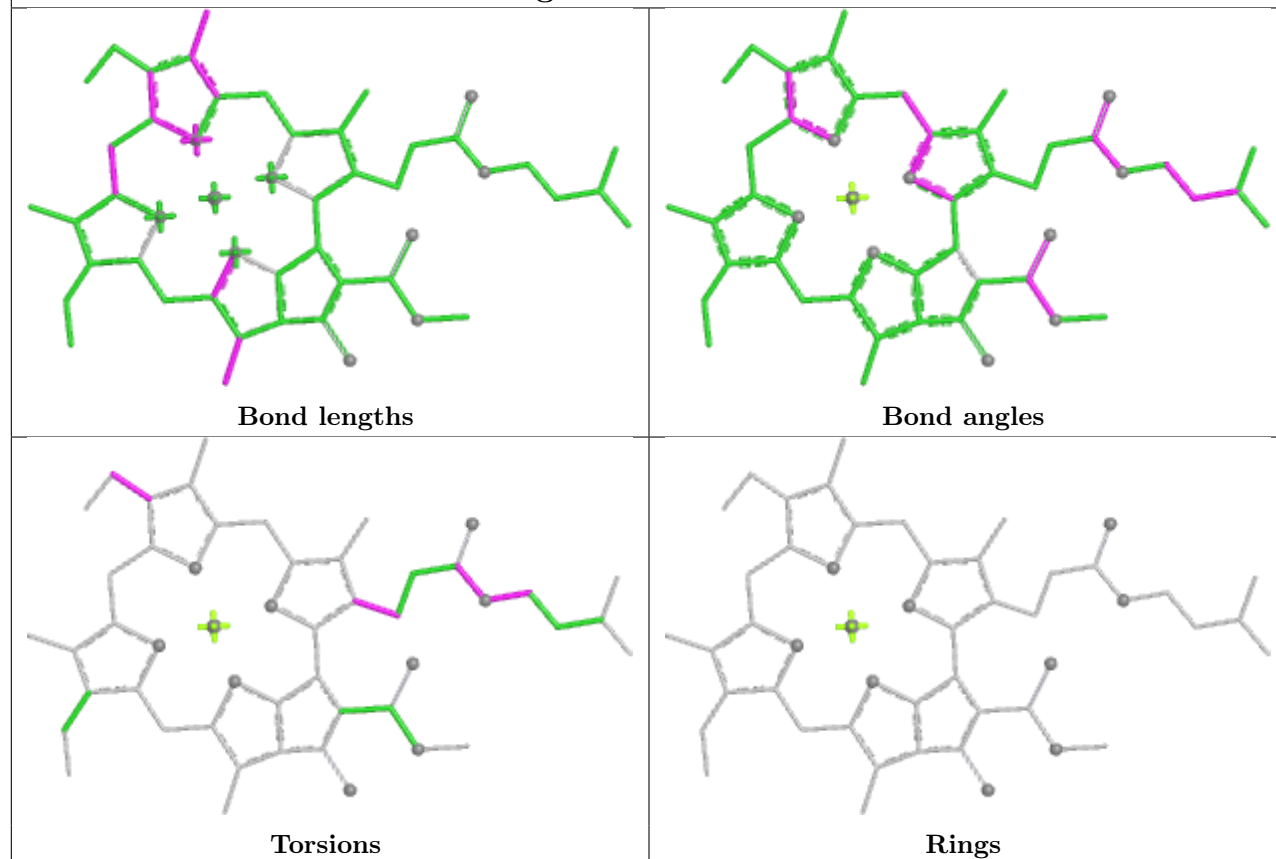


Rings

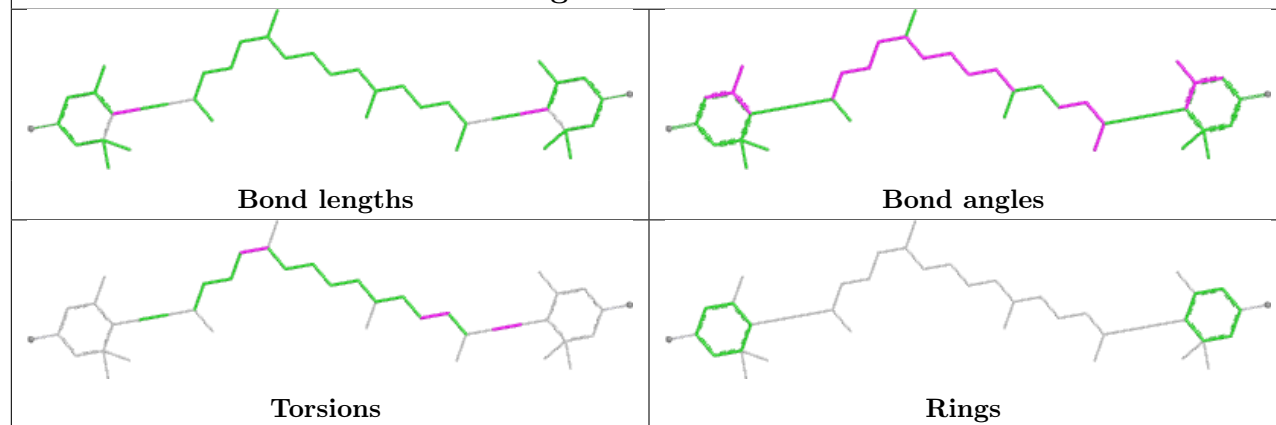
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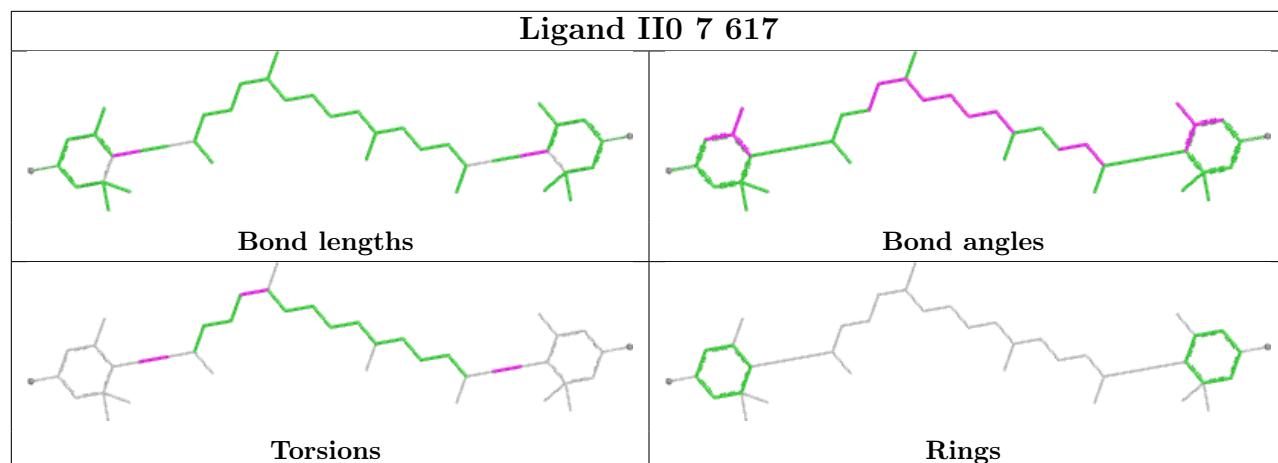
Ligand CLA 1 603



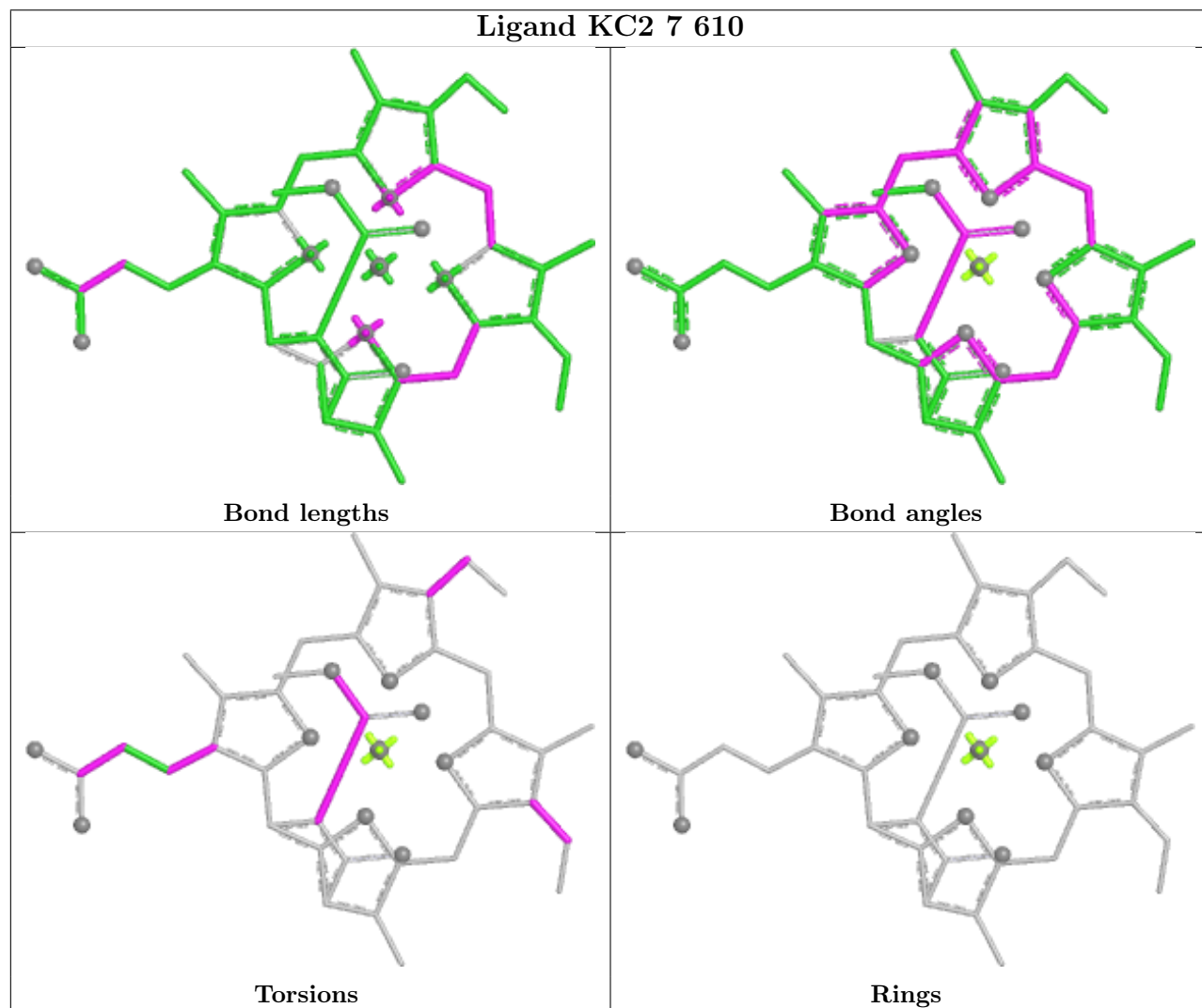
Ligand II0 1 616



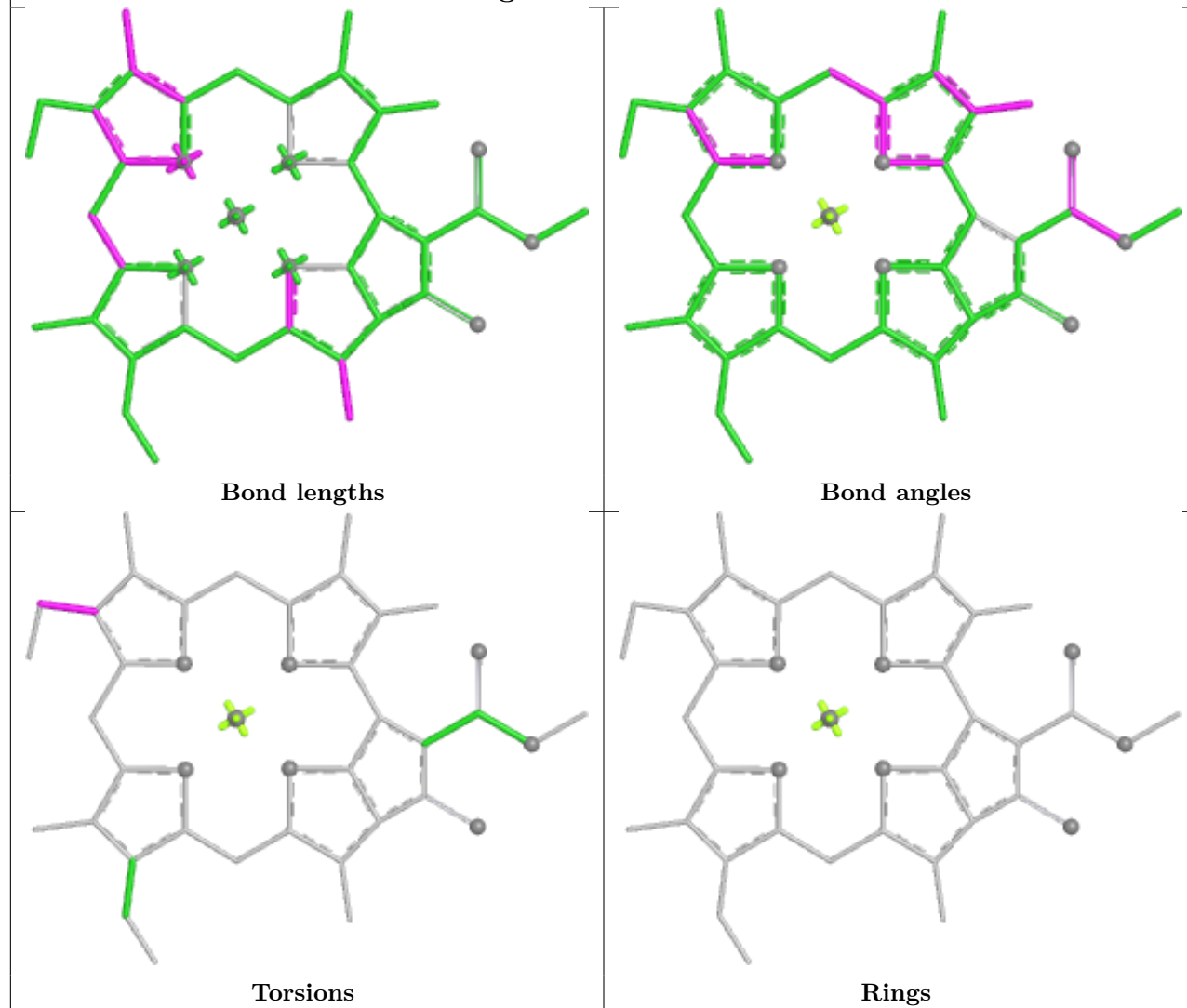
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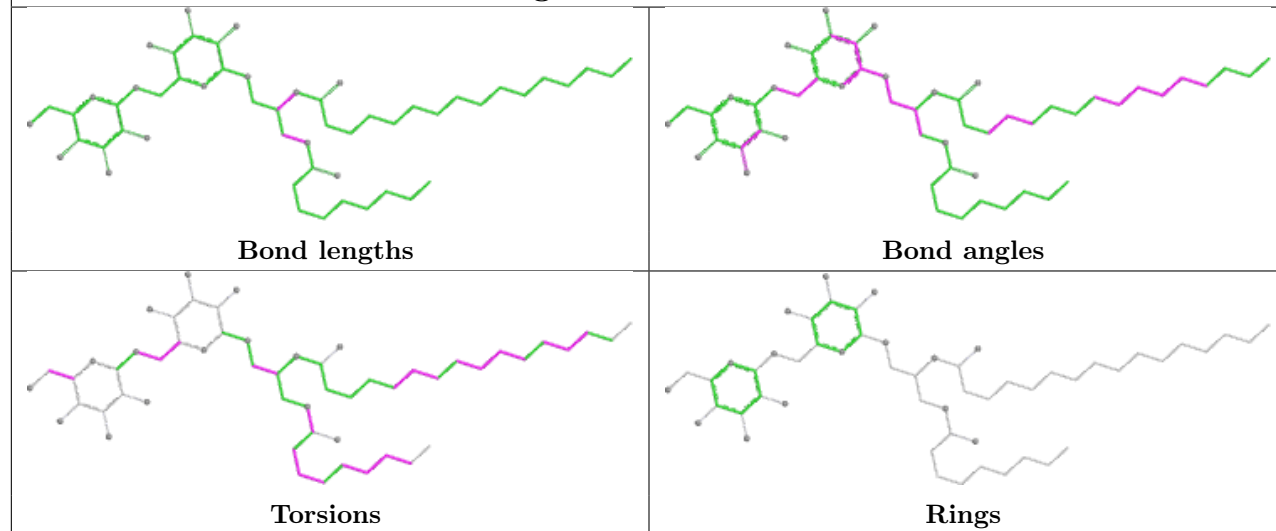
Ligand KC2 7 610

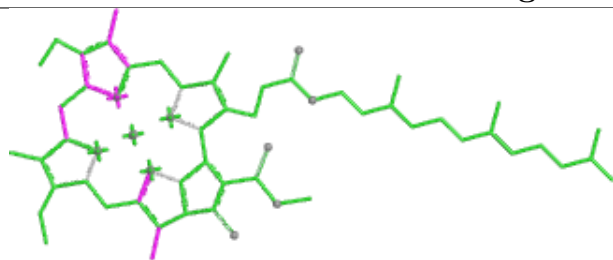
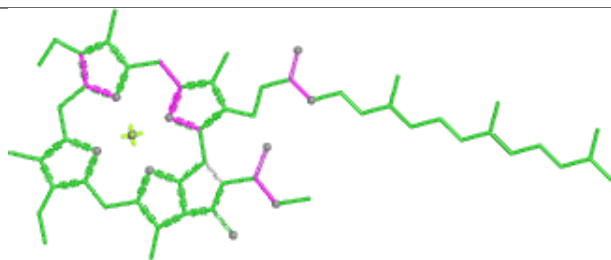
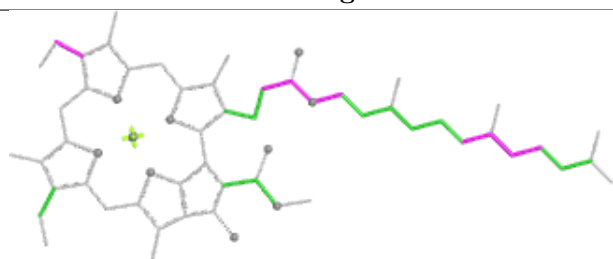
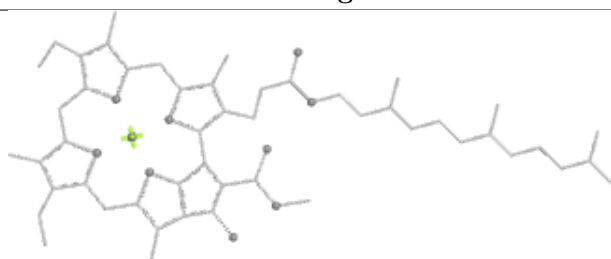
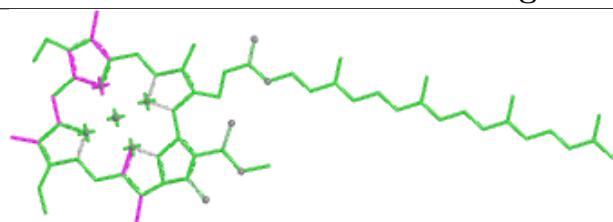
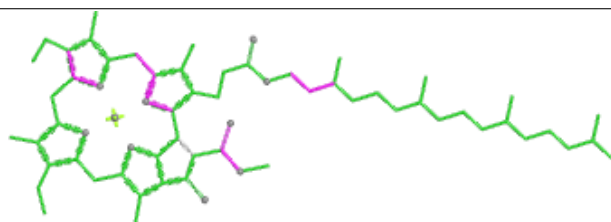
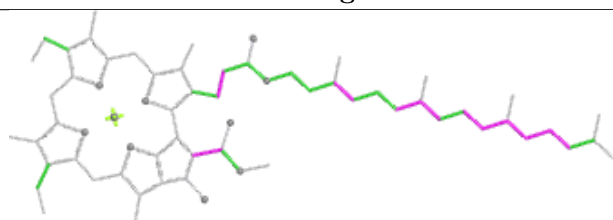
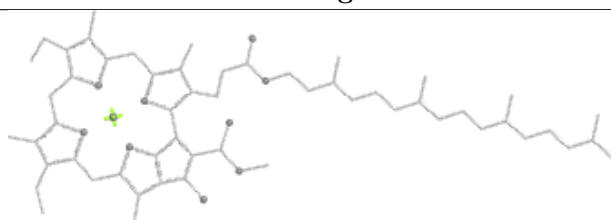


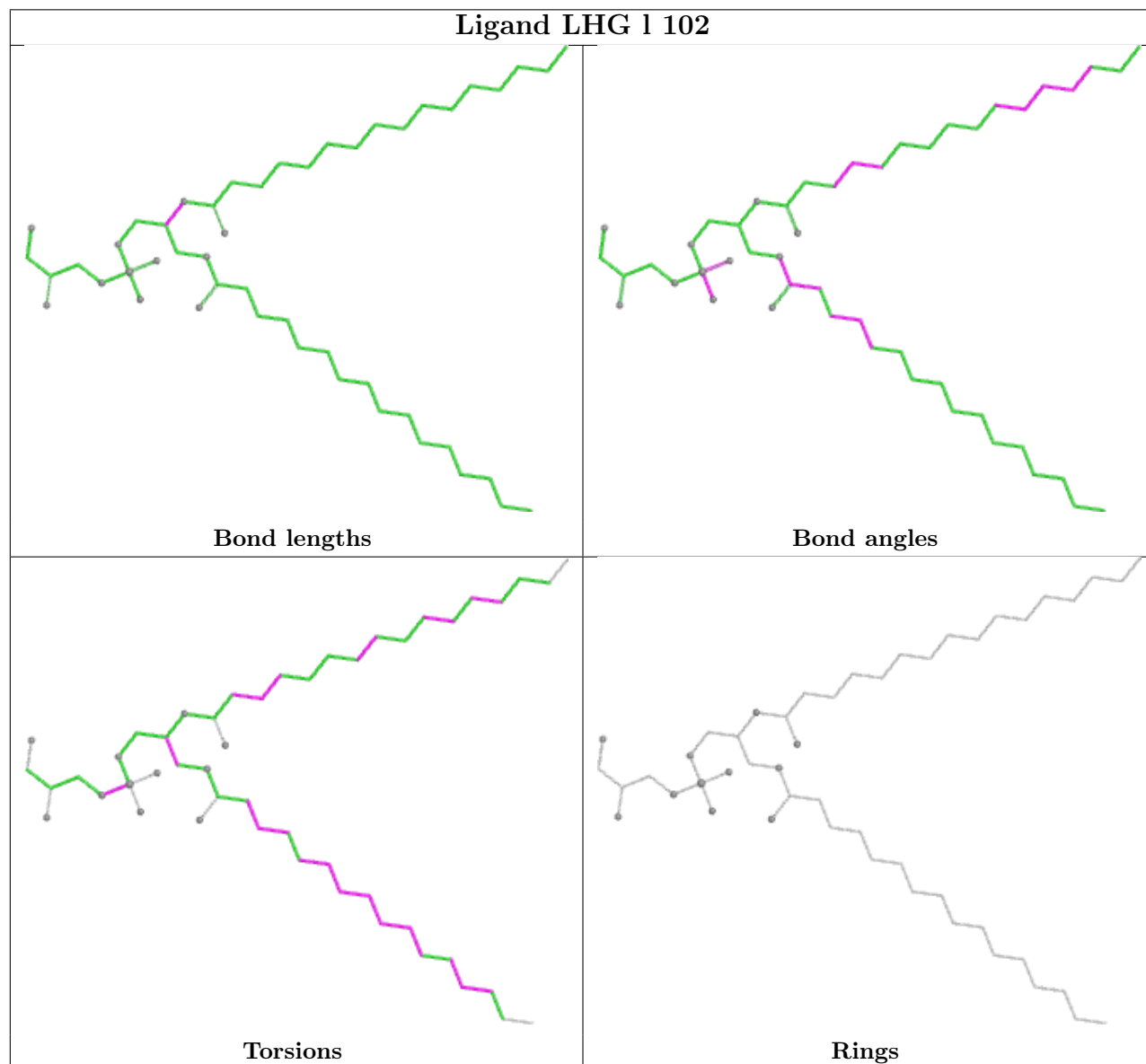
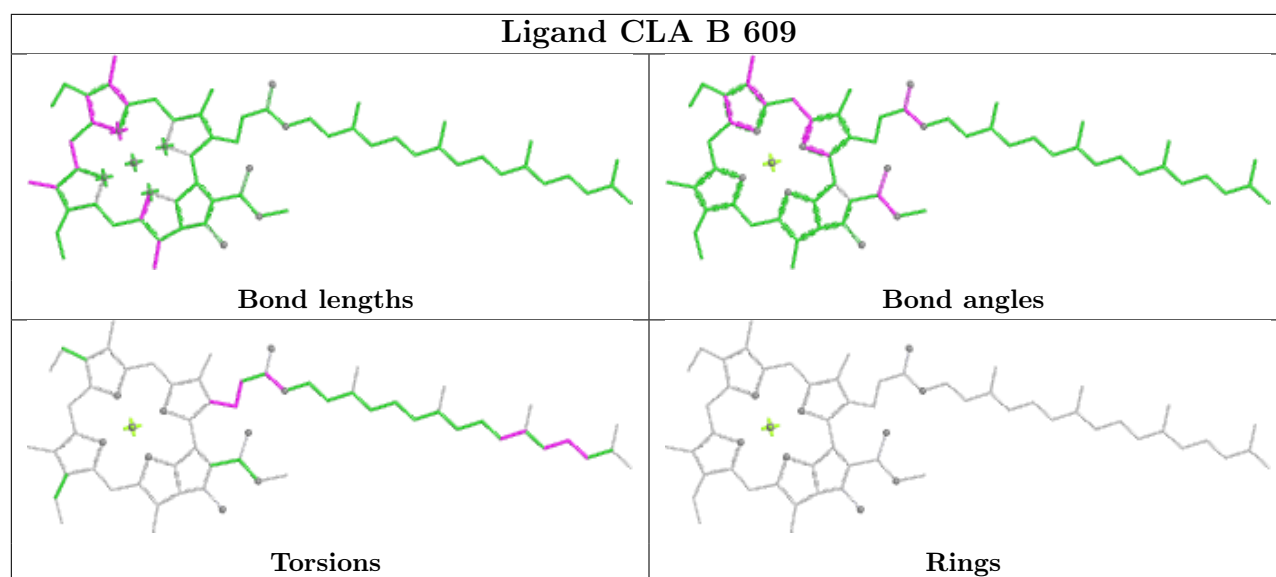
Ligand CLA 0 609

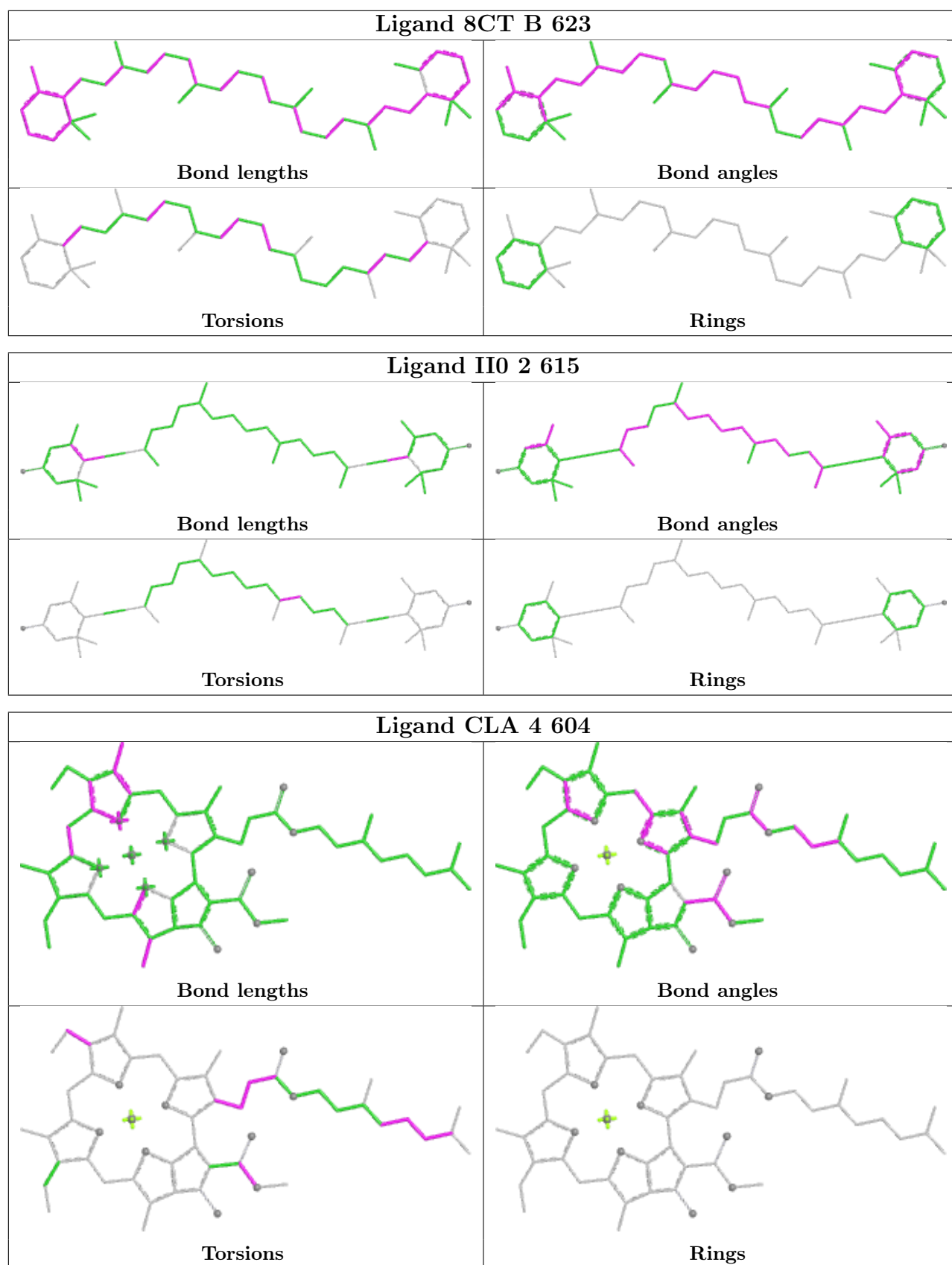


Ligand DGD c 514

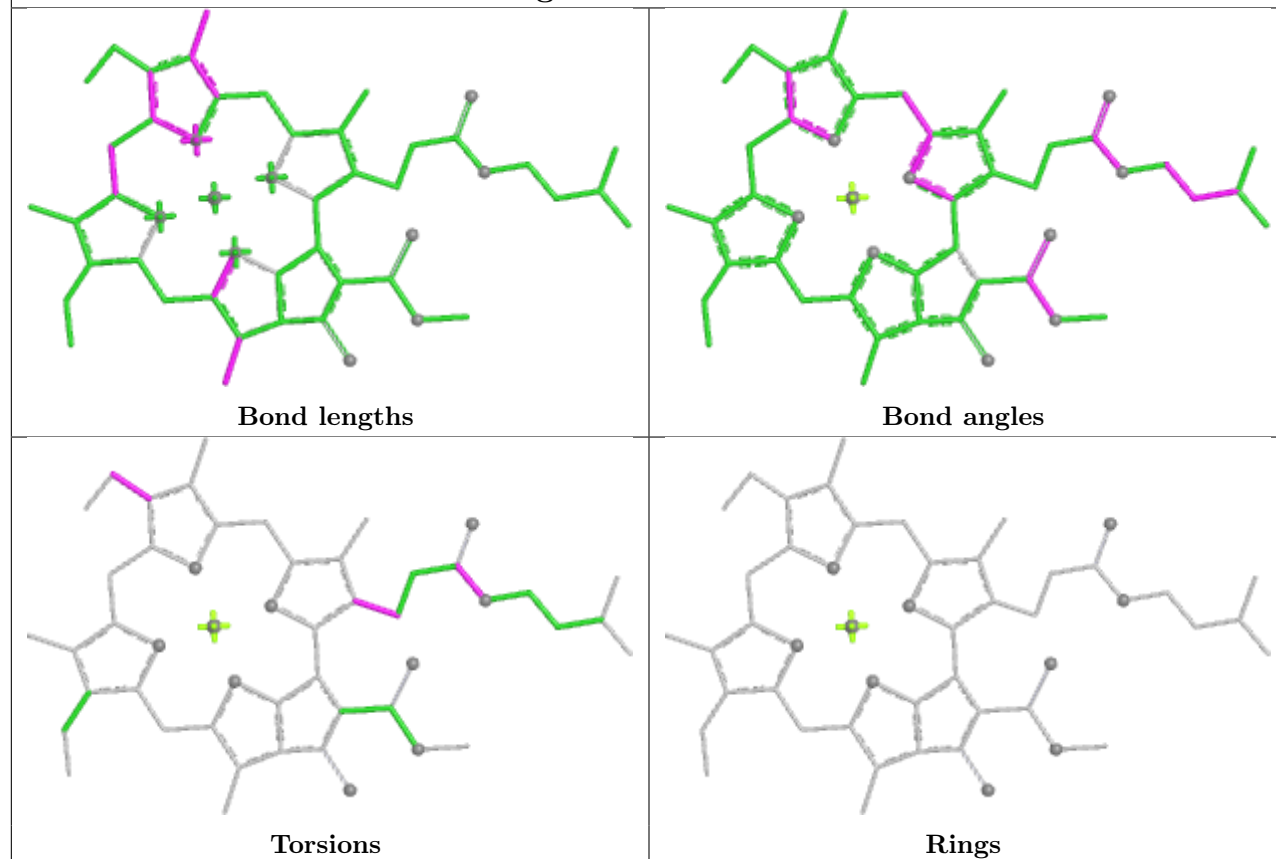


Ligand CLA 2 605**Bond lengths****Bond angles****Torsions****Rings****Ligand CLA c 507****Bond lengths****Bond angles****Torsions****Rings**

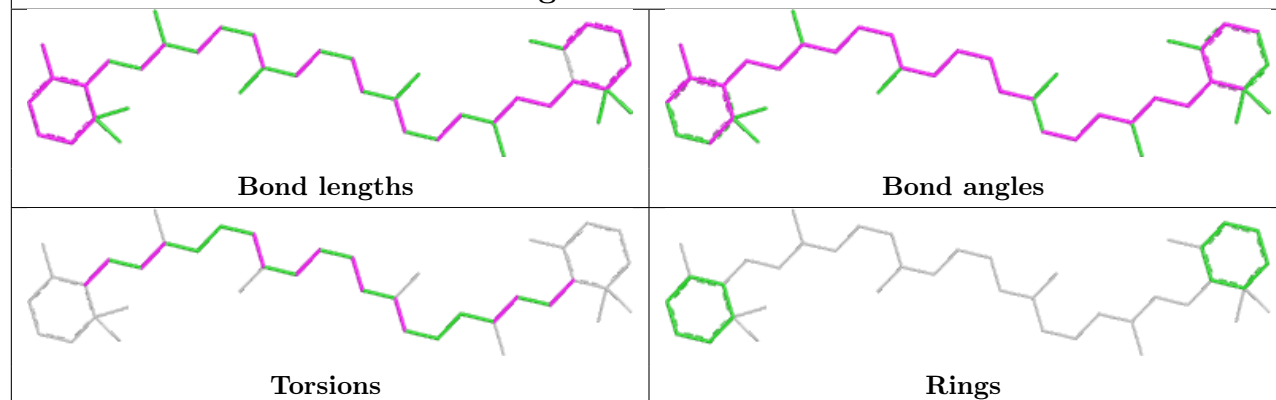




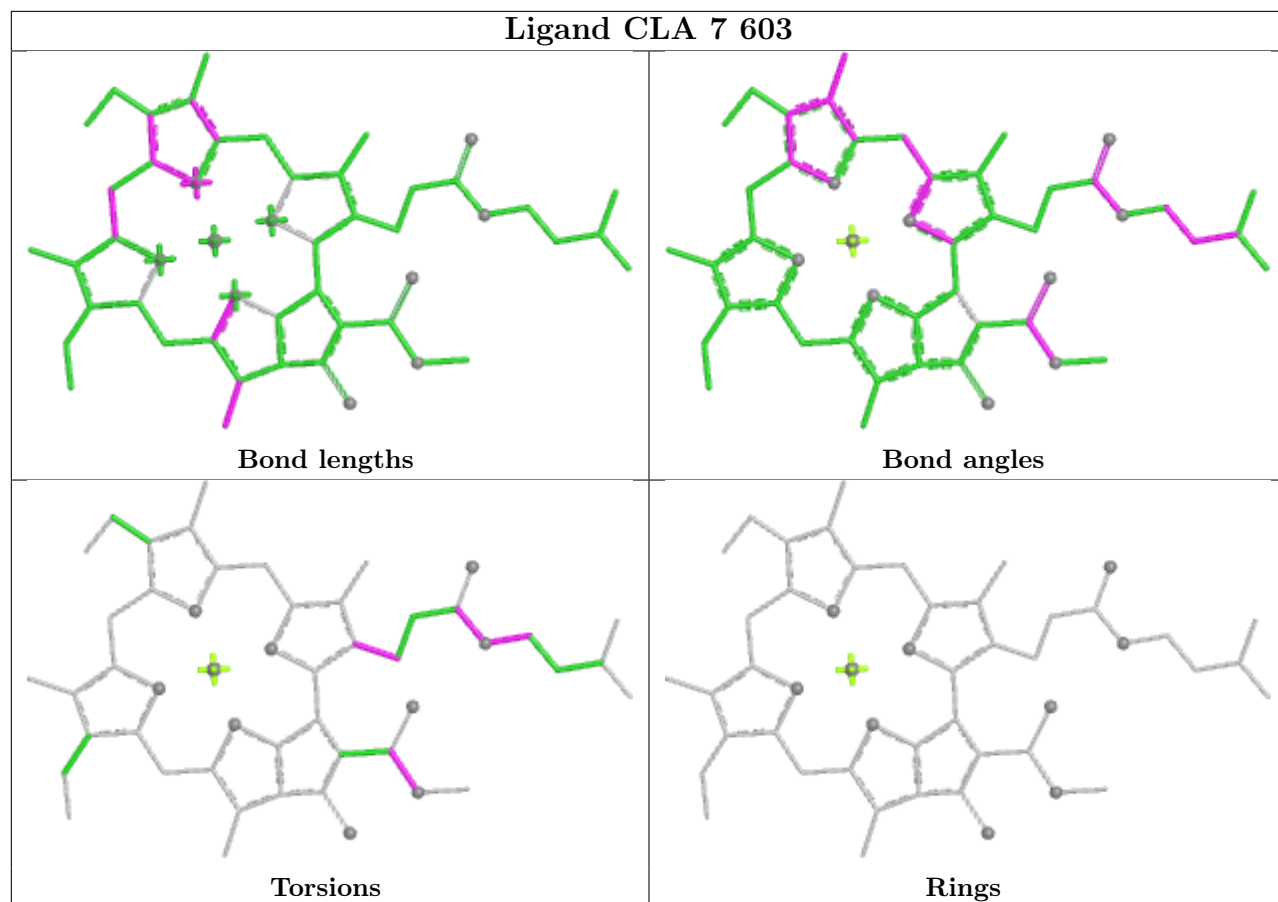
Ligand CLA 8 603



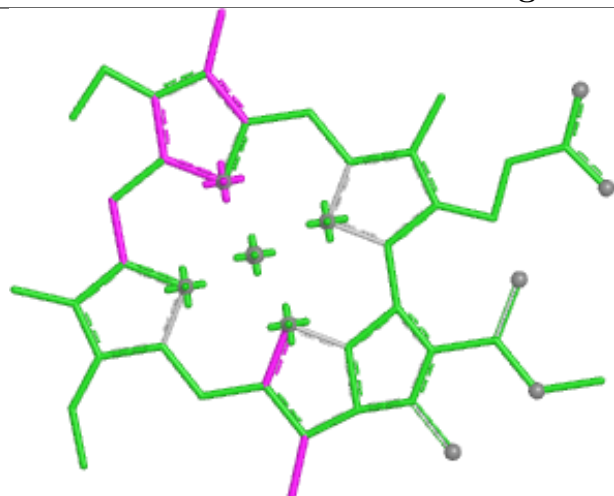
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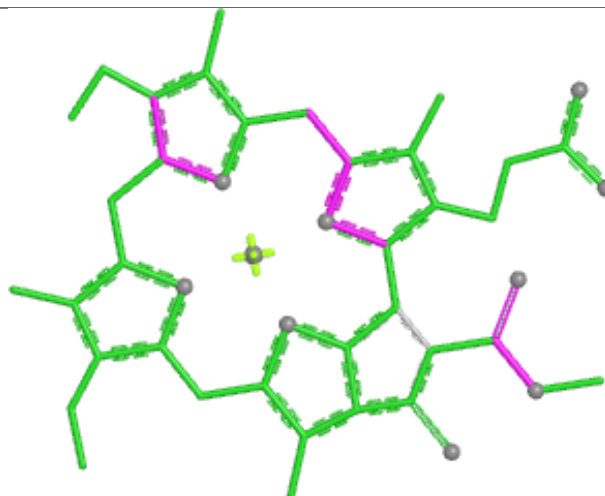
Ligand CLA 7 603



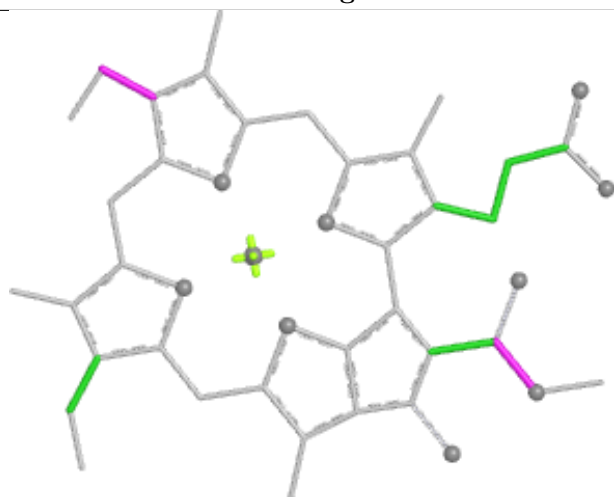
Ligand CLA 8 607



Bond lengths



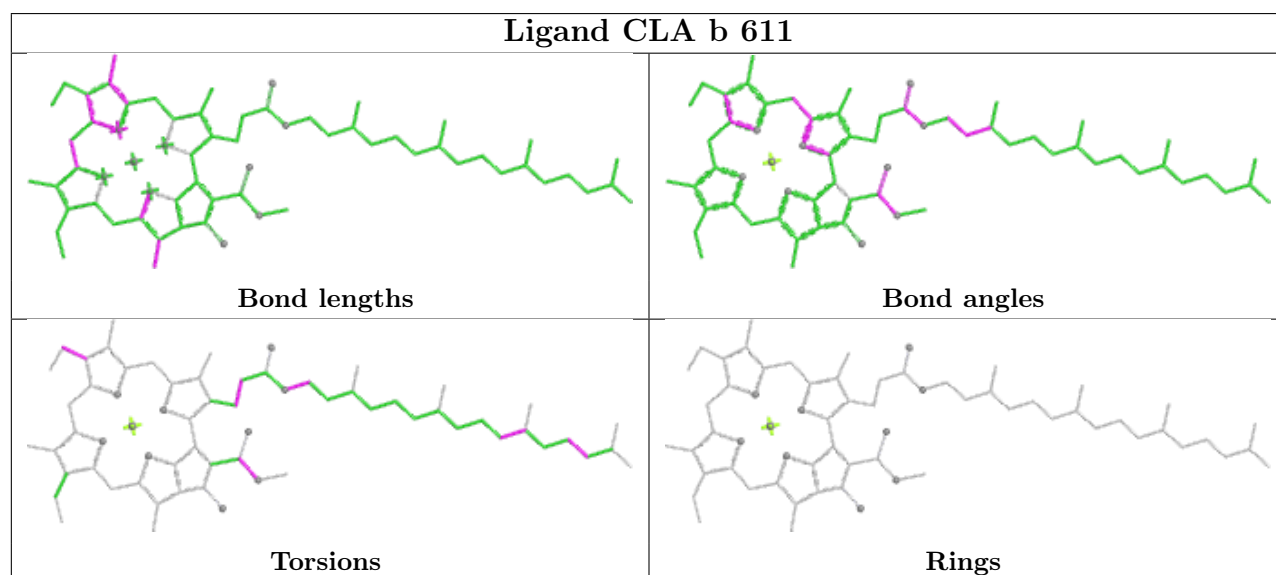
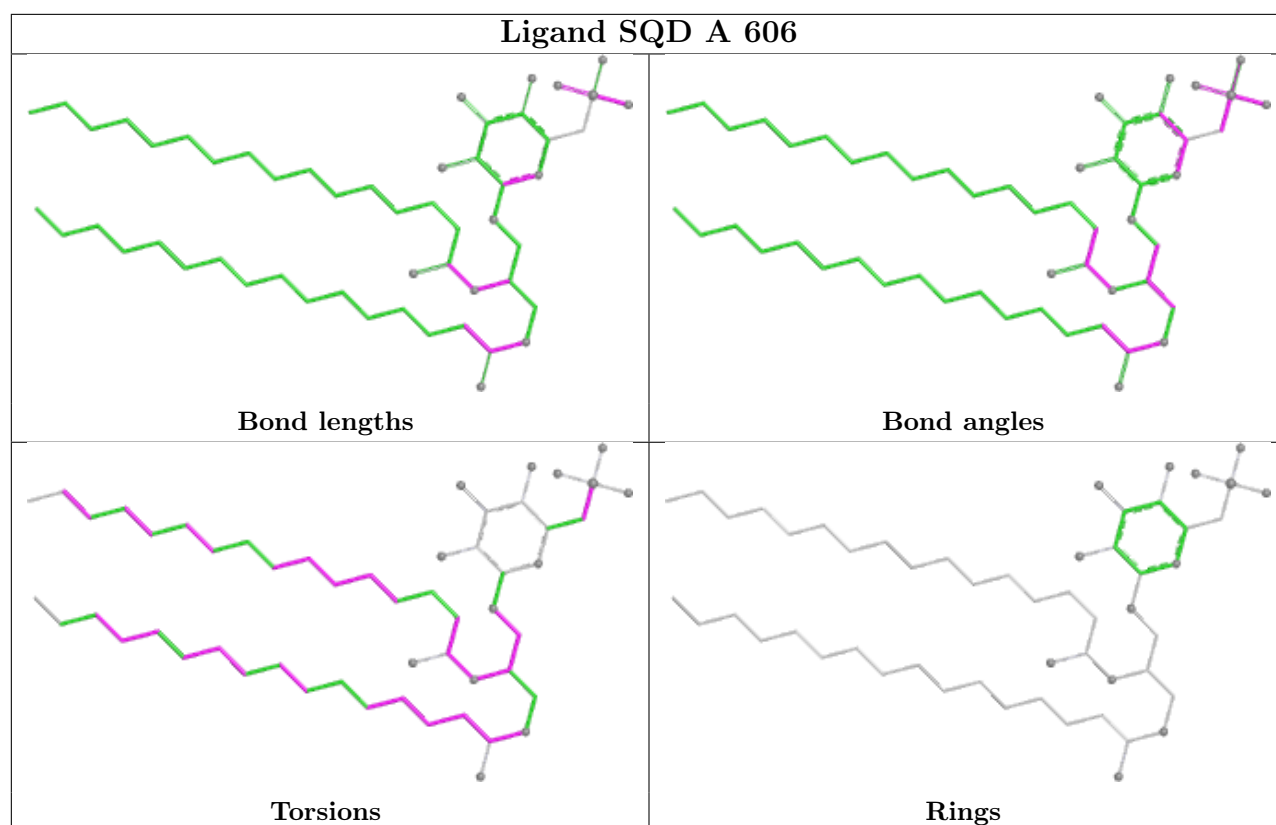
Bond angles



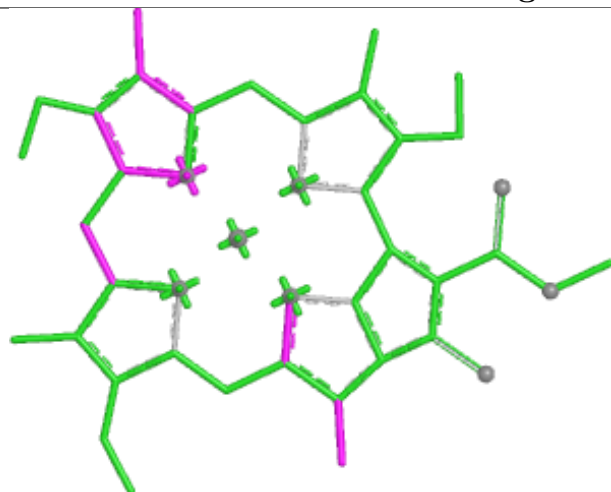
Torsions



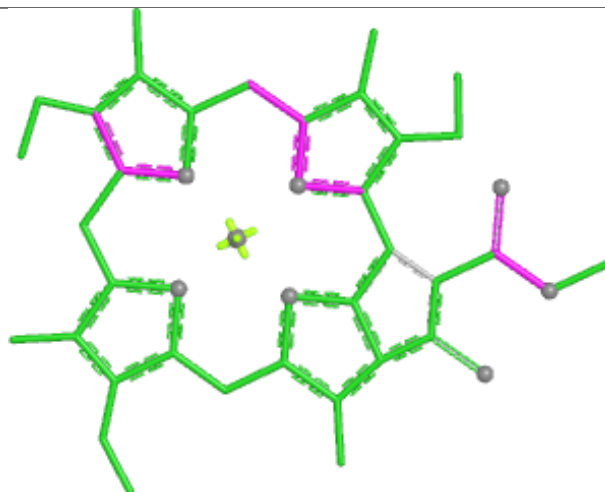
Rings



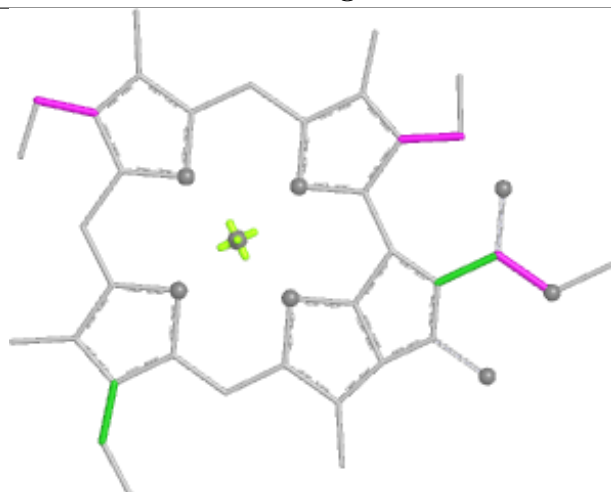
Ligand CLA 3 601



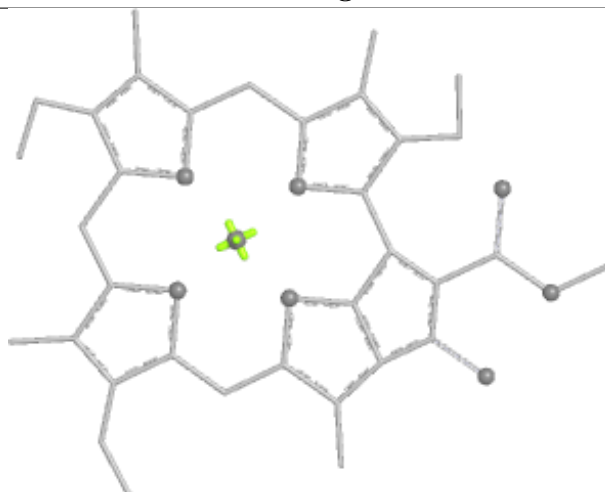
Bond lengths



Bond angles

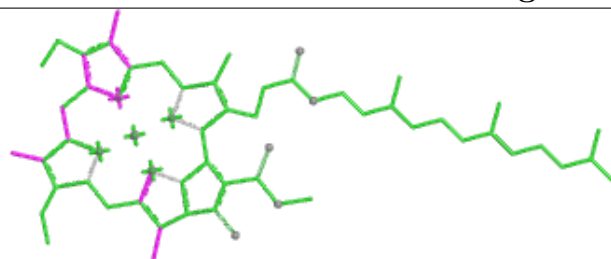


Torsions

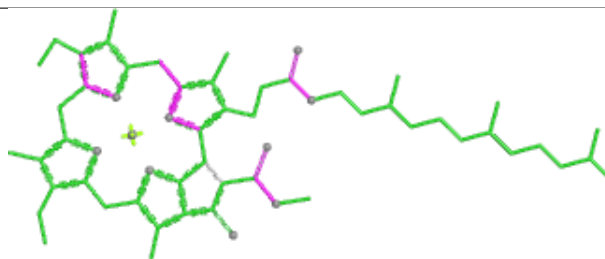


Rings

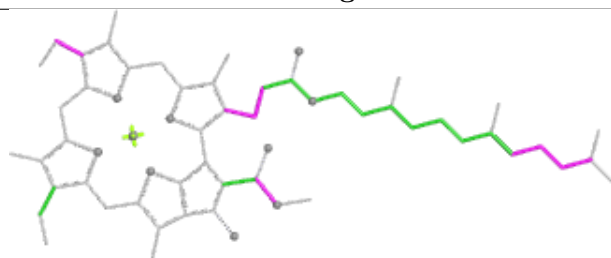
Ligand CLA 8 608



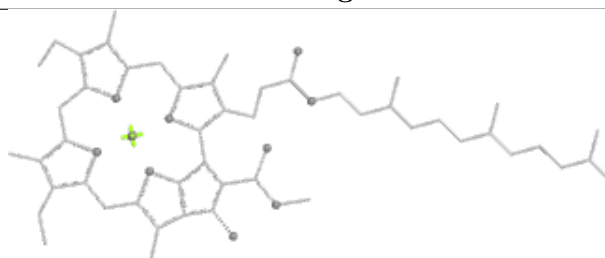
Bond lengths



Bond angles

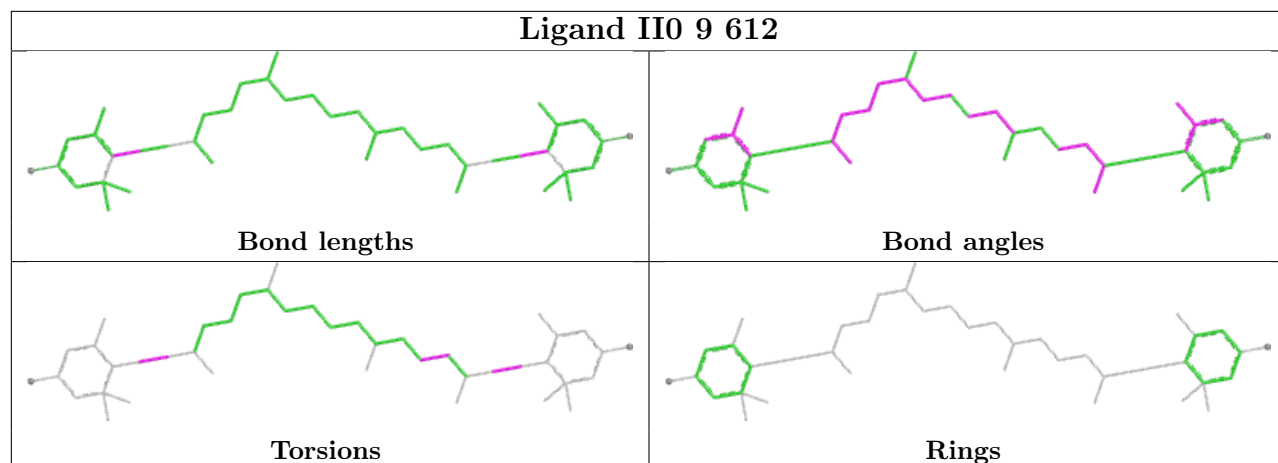


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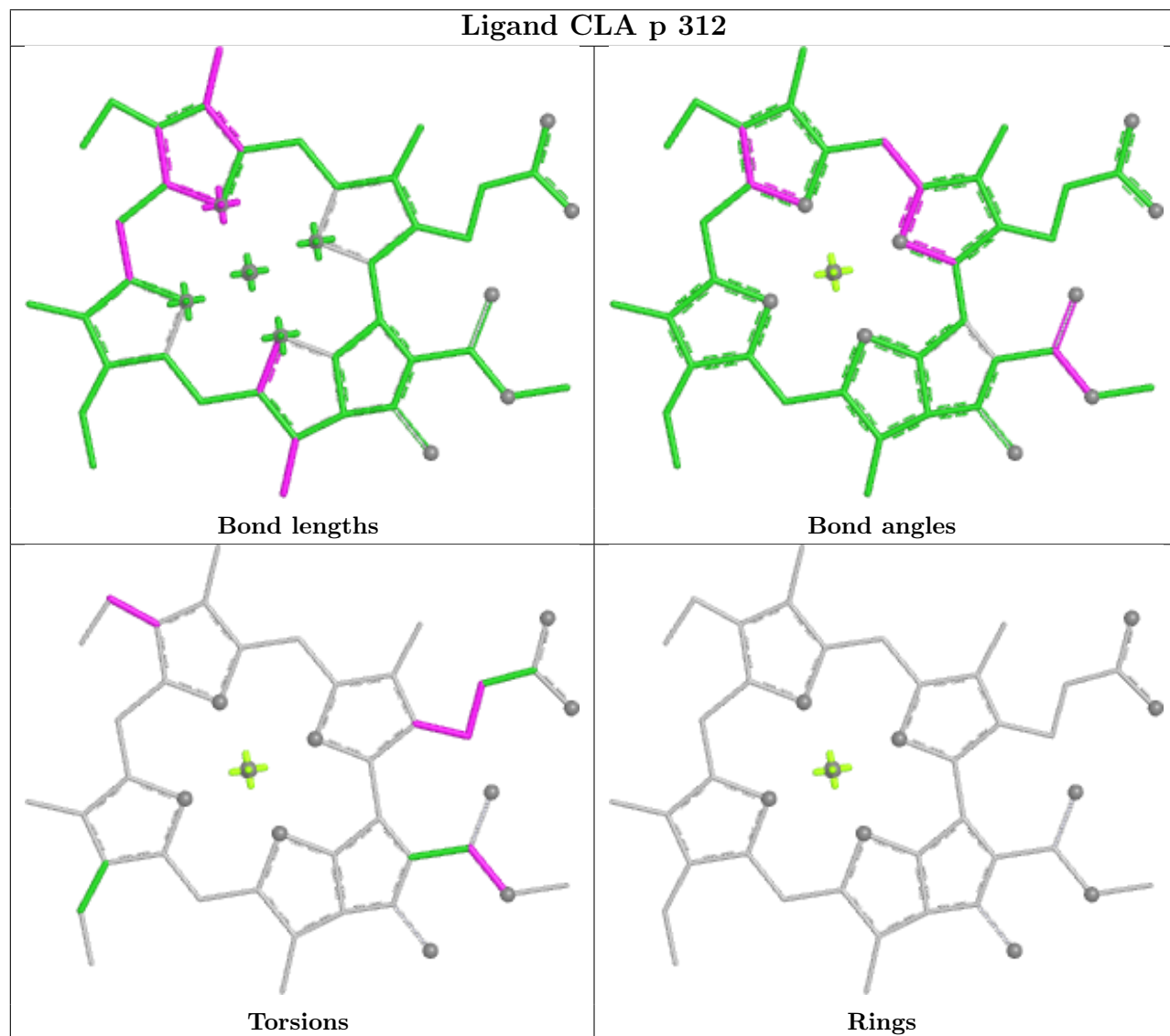


Rings

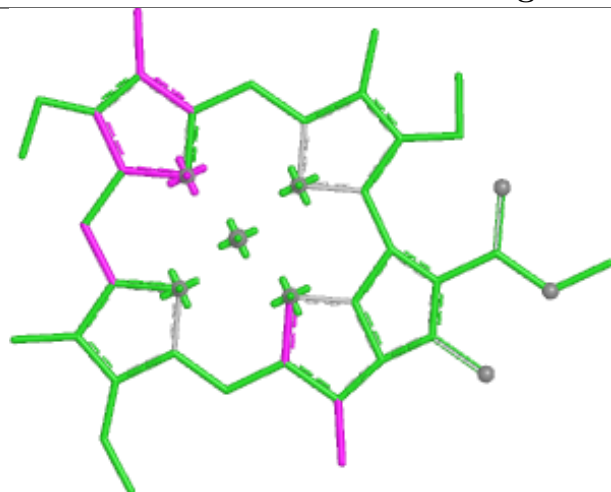
Ligand II0 9 612



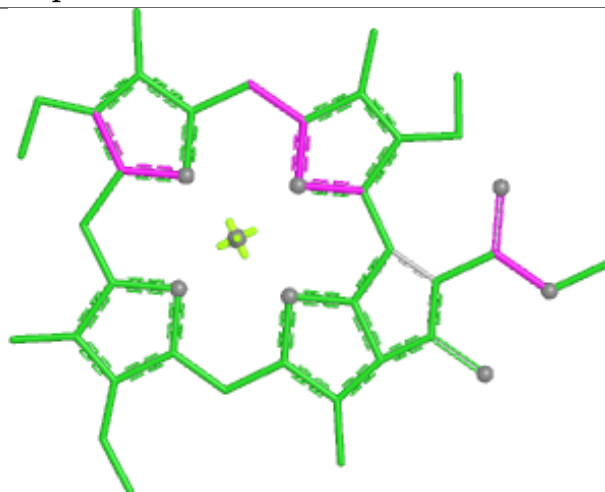
Ligand CLA p 312



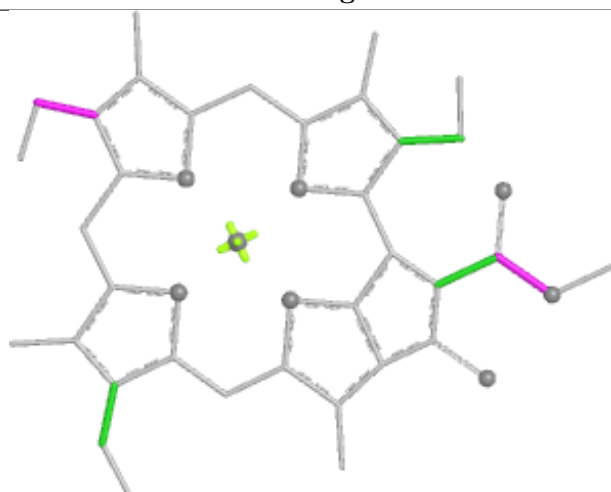
Ligand CLA p 302



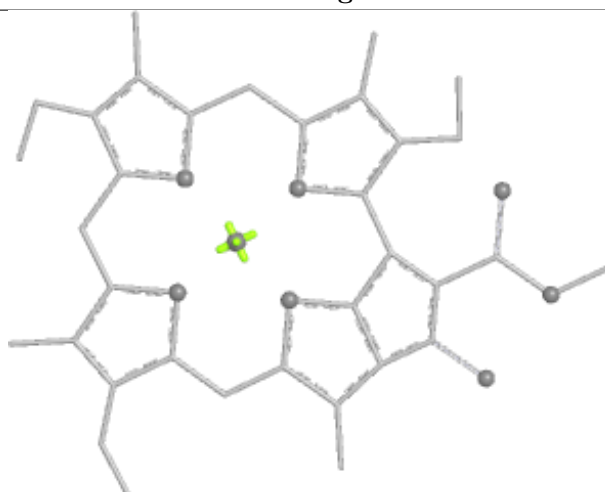
Bond lengths



Bond angles

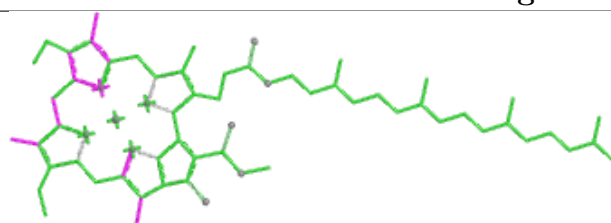


Torsions

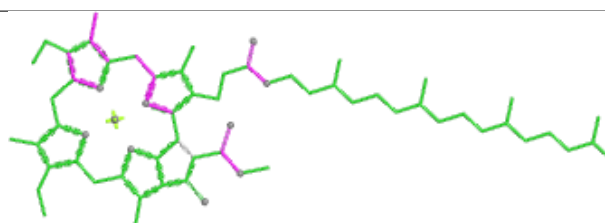


Rings

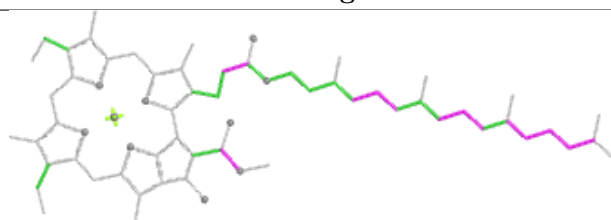
Ligand CLA b 614



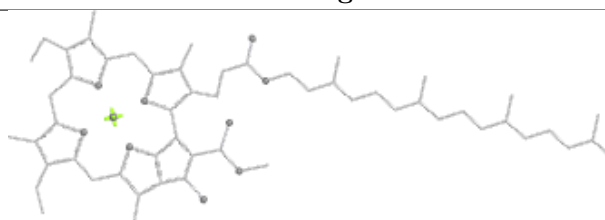
Bond lengths



Bond angles

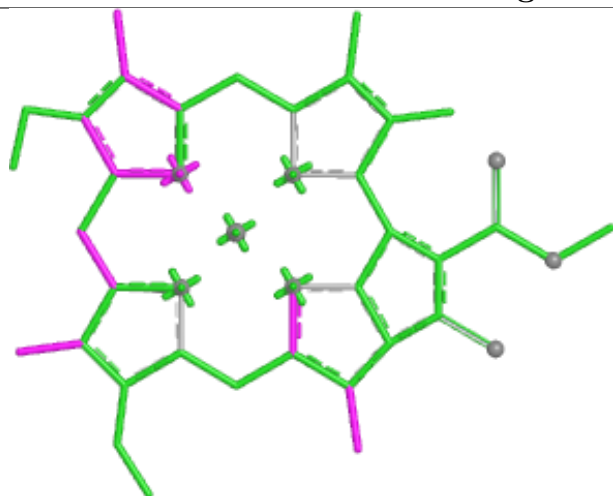


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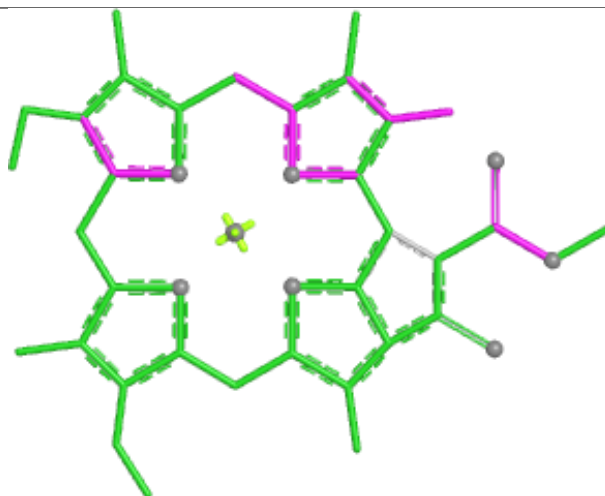


Rings

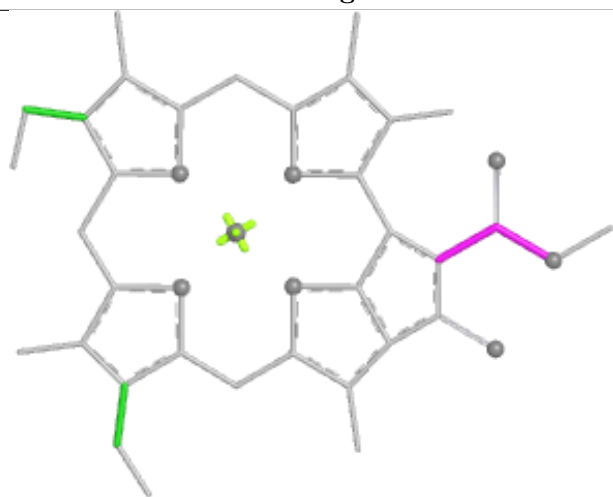
Ligand CLA b 608



Bond lengths



Bond angles

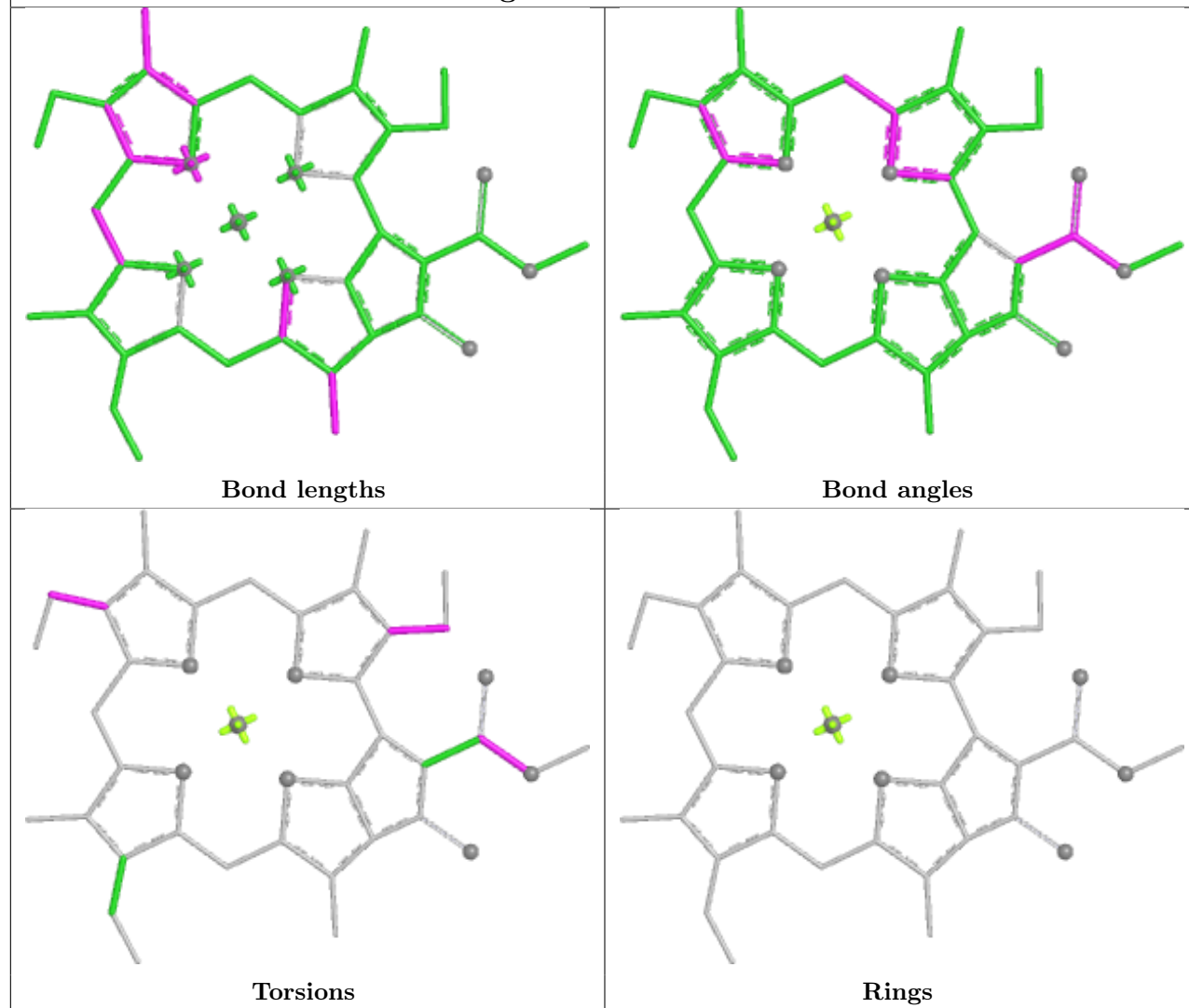


Torsions

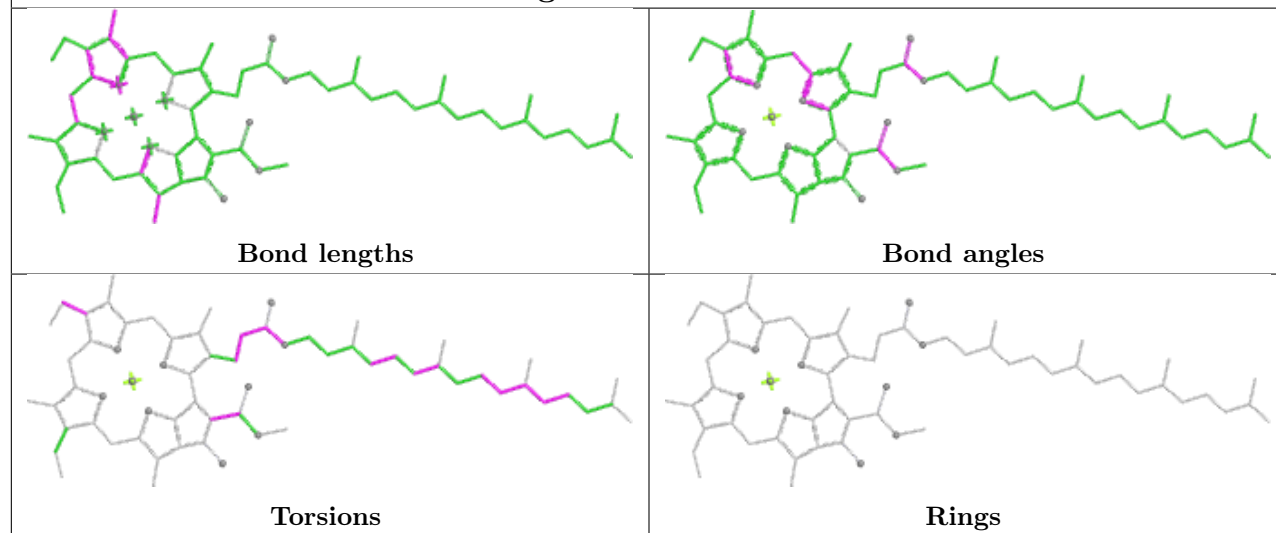


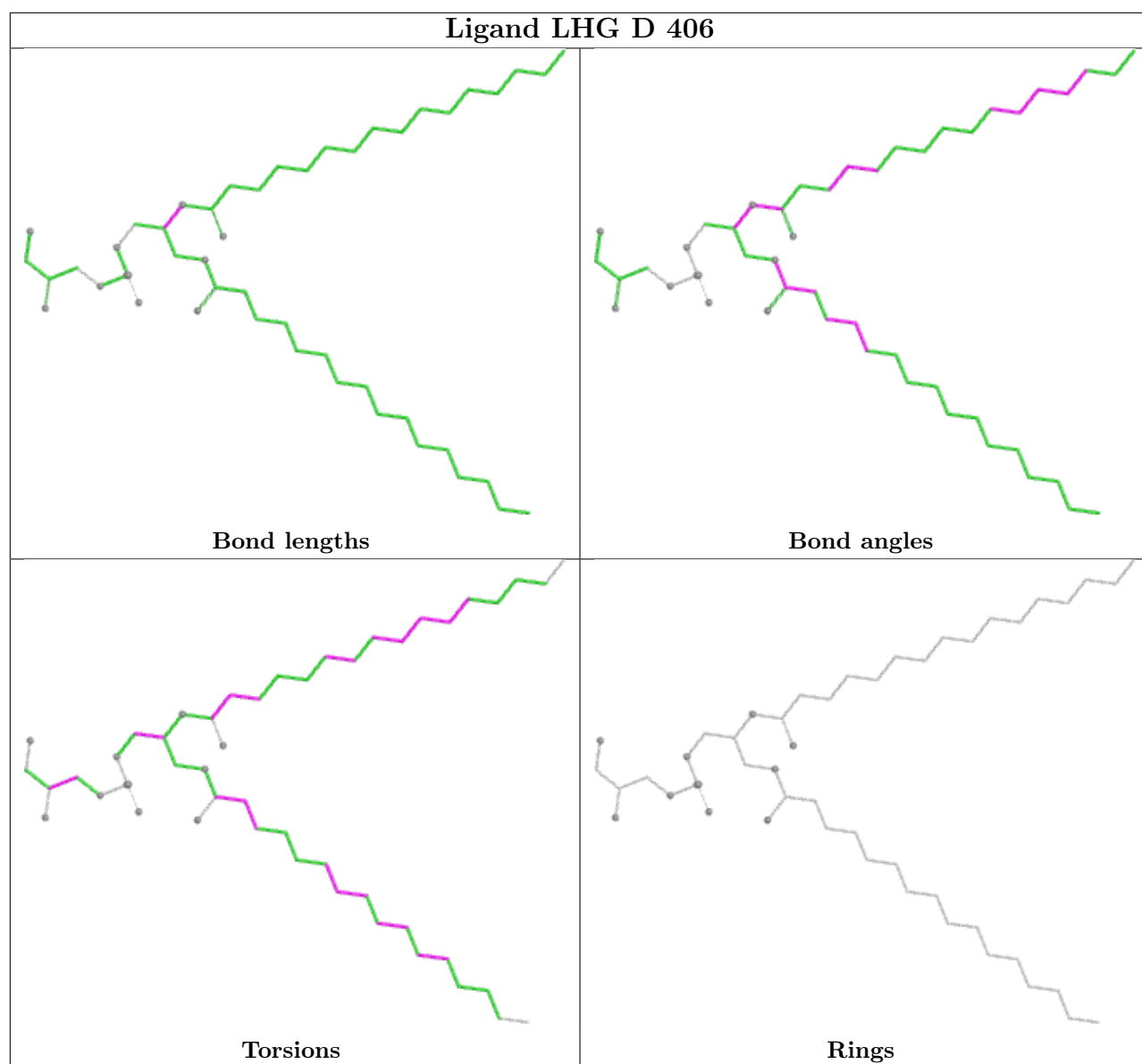
Rings

Ligand CLA 9 601

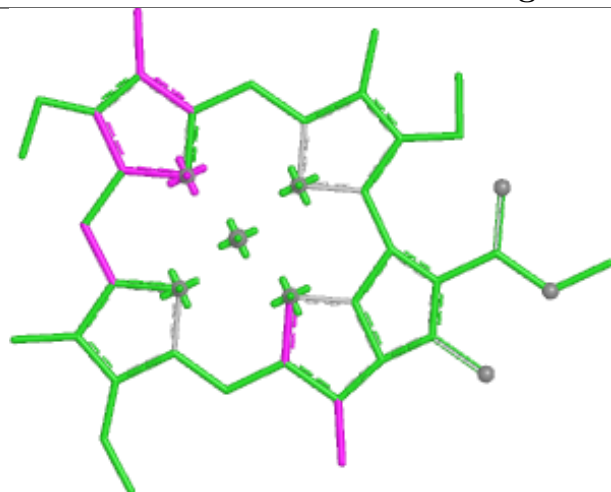


Ligand CLA s 303

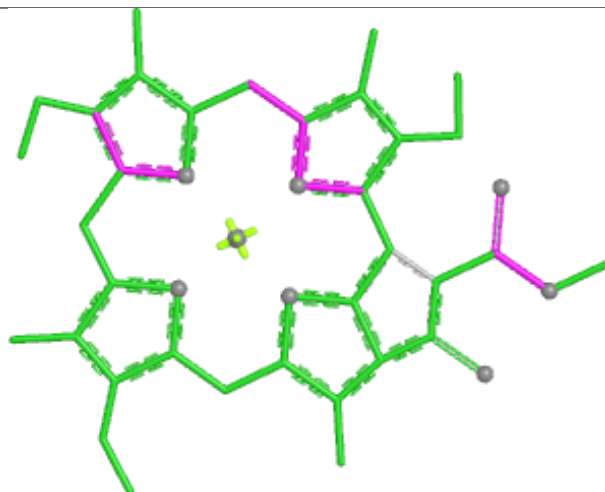




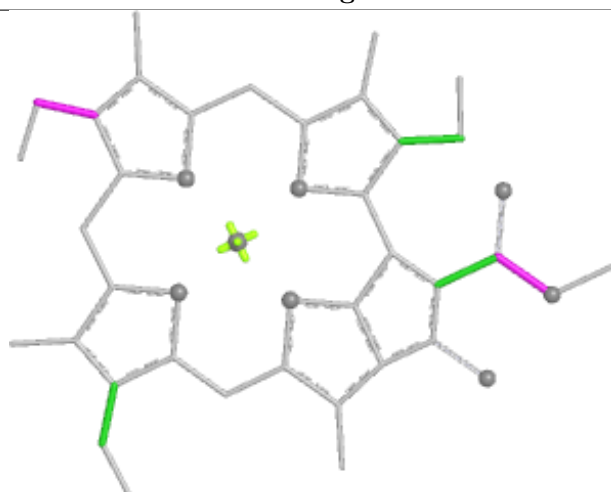
Ligand CLA 5 302



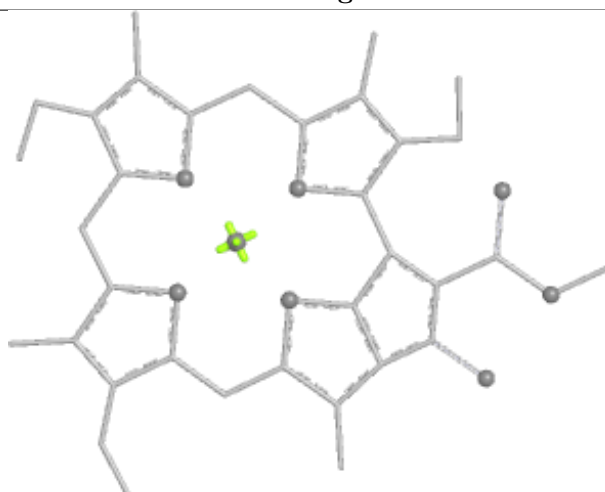
Bond lengths



Bond angles

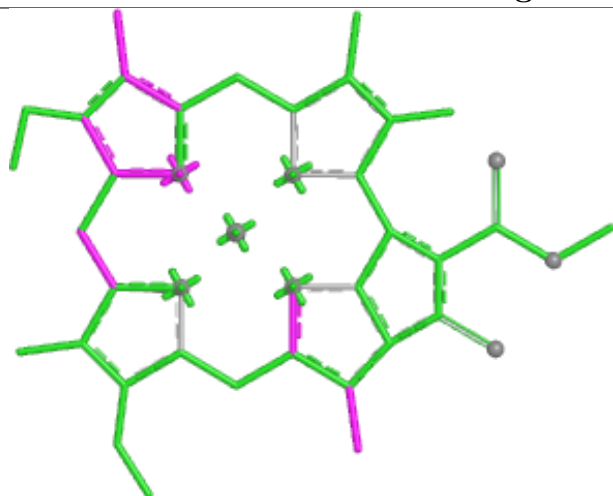


Torsions

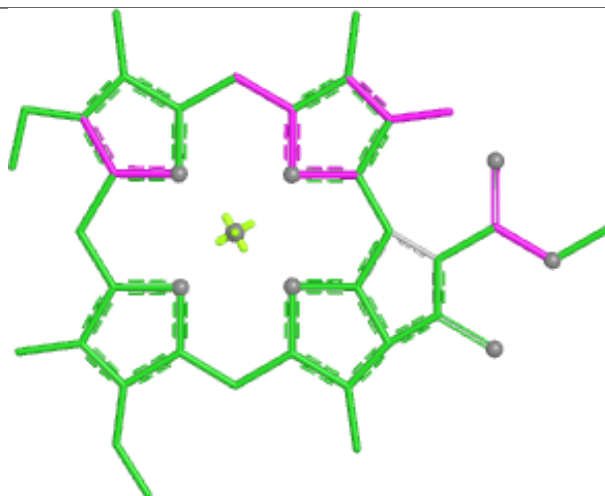


Rings

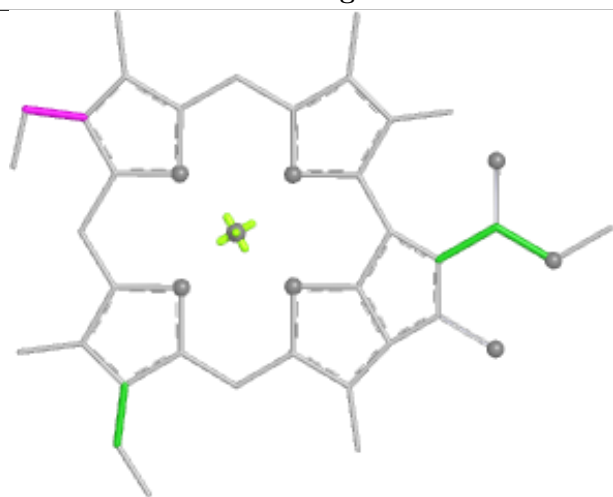
Ligand CLA P 608



Bond lengths



Bond angles

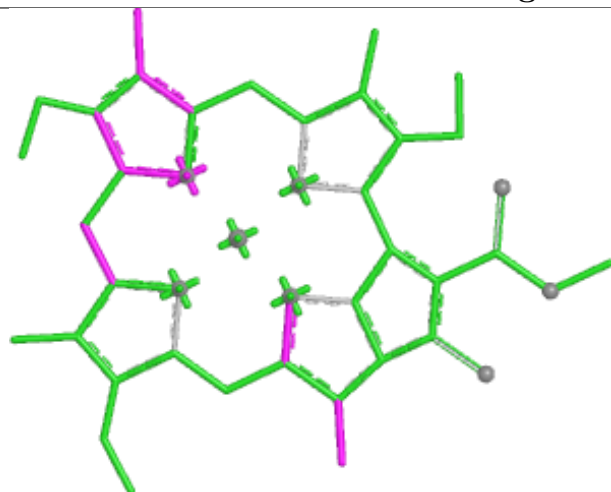


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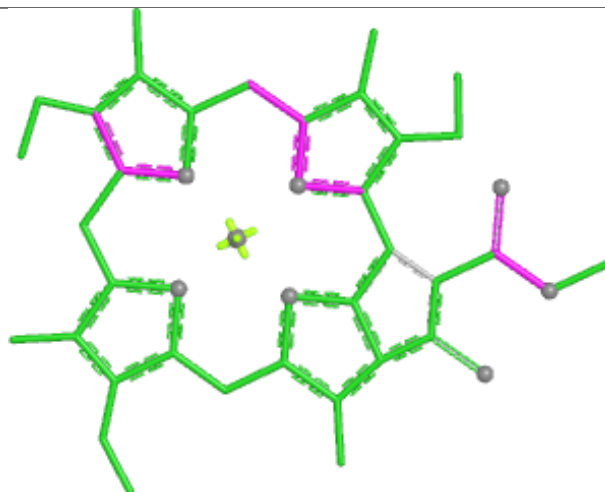


Rings

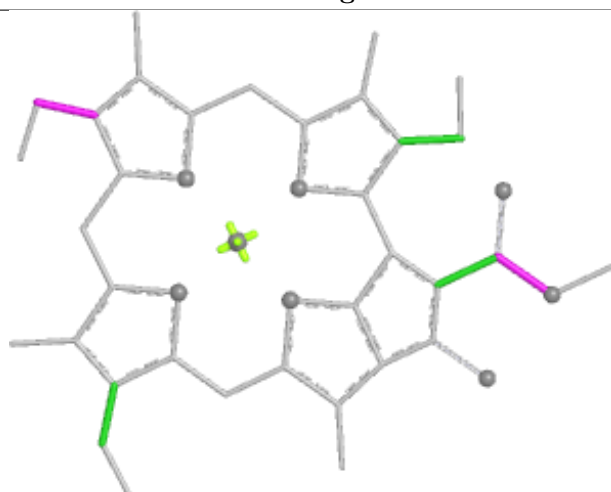
Ligand CLA 0 601



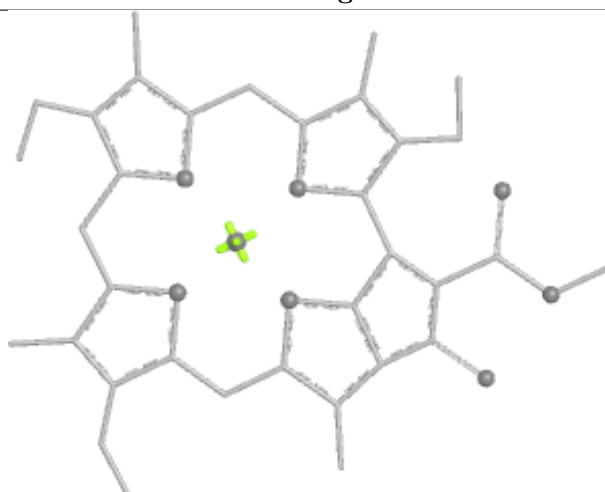
Bond lengths



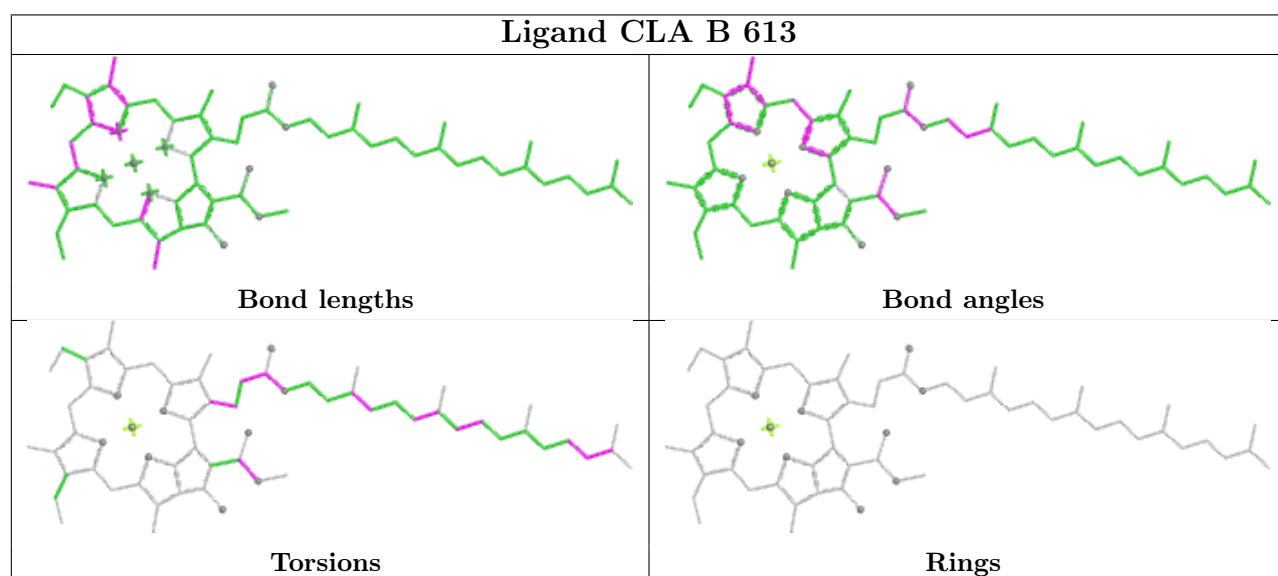
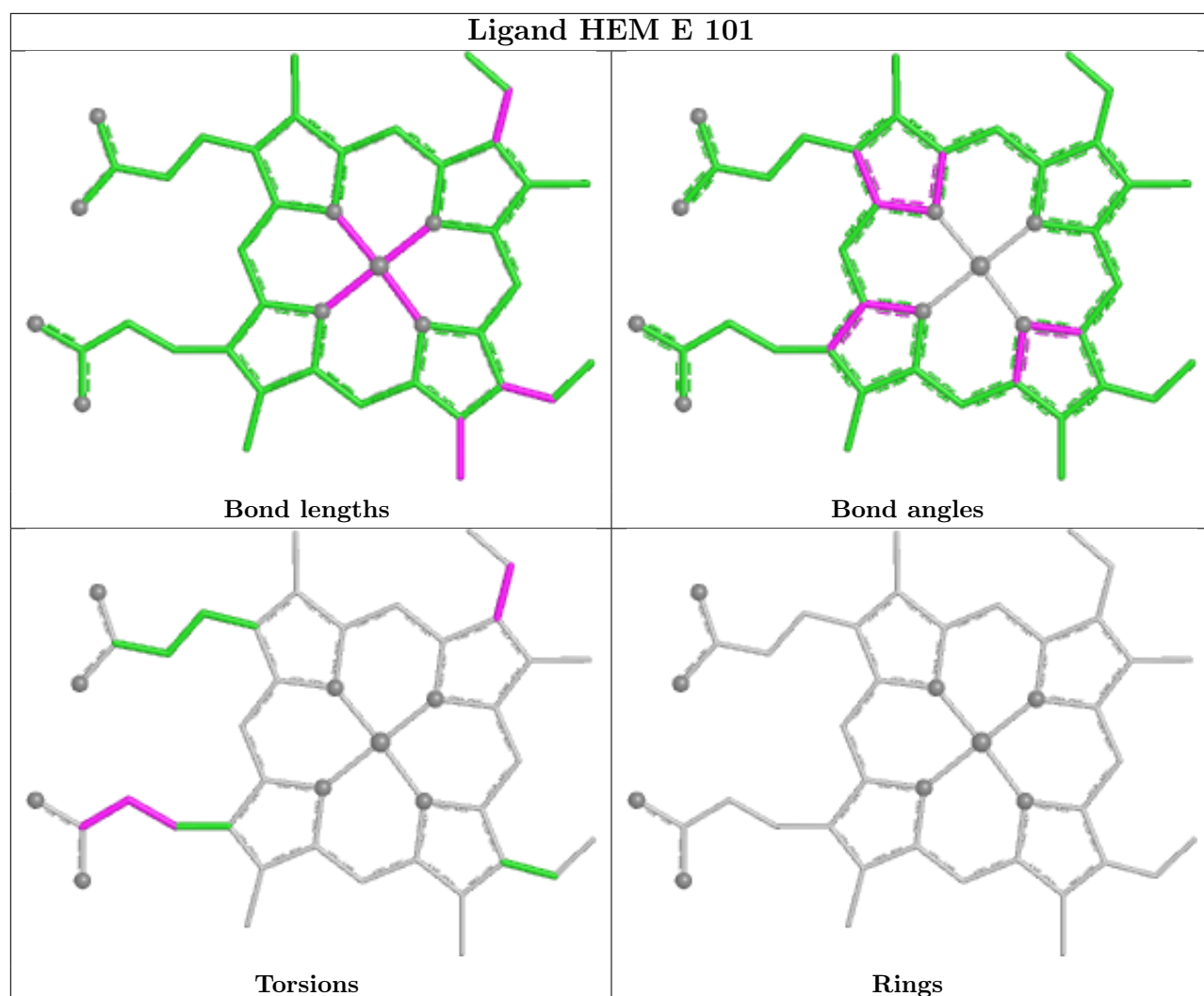
Bond angles



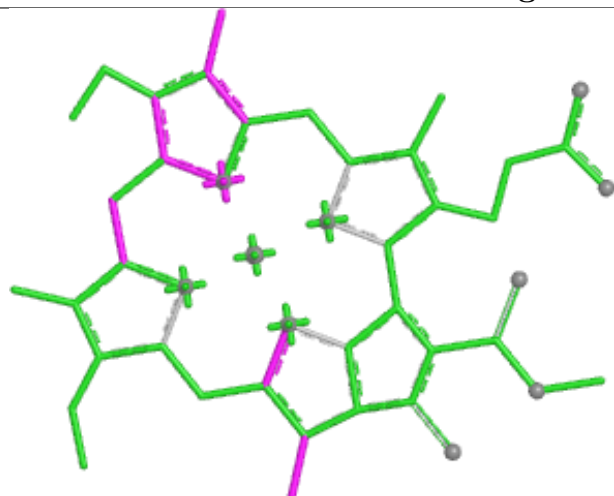
Torsions



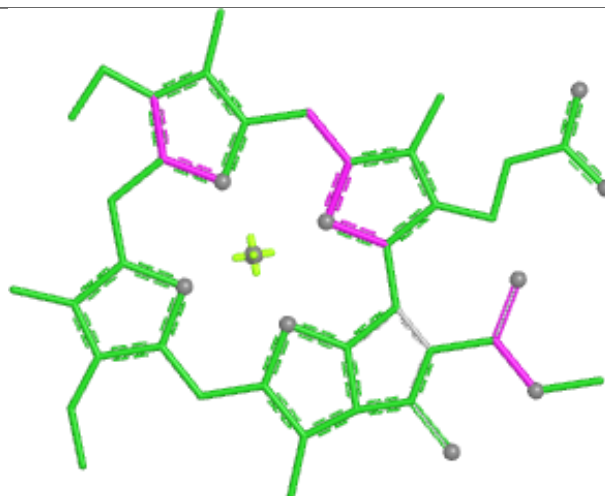
Rings



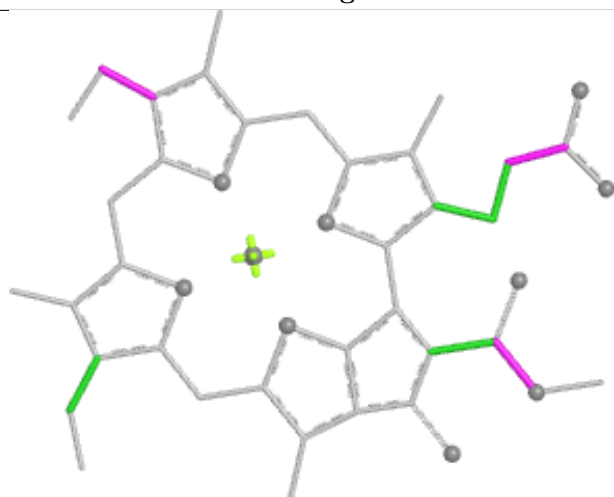
Ligand CLA 4 606



Bond lengths



Bond angles

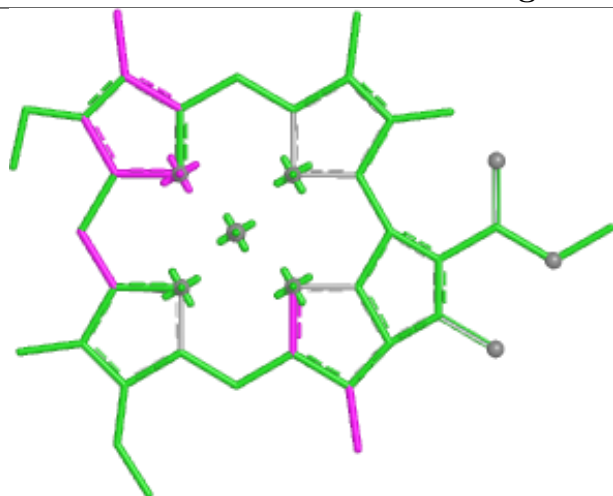


Torsions

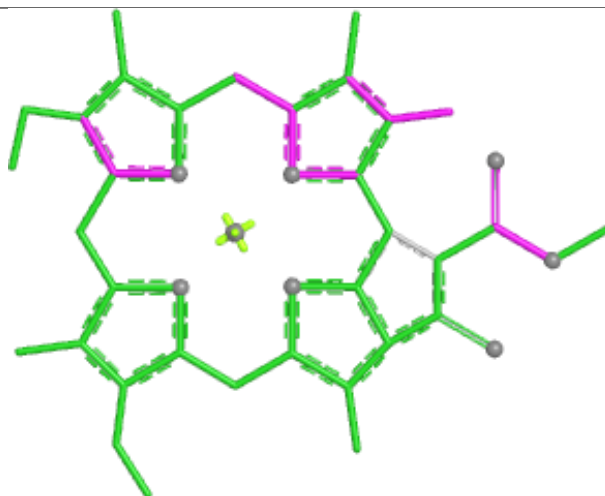


Rings

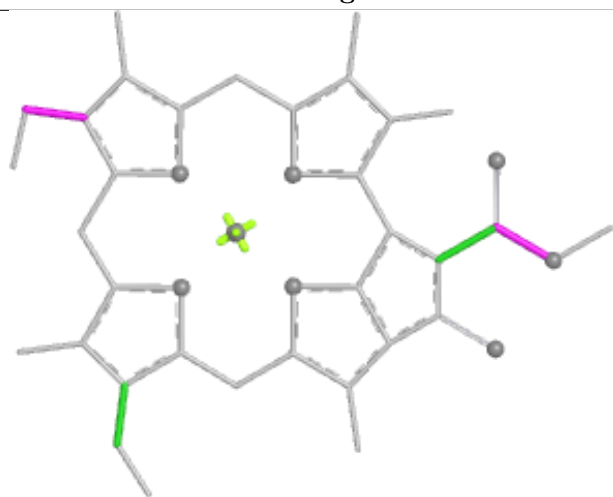
Ligand CLA 8 609



Bond lengths



Bond angles

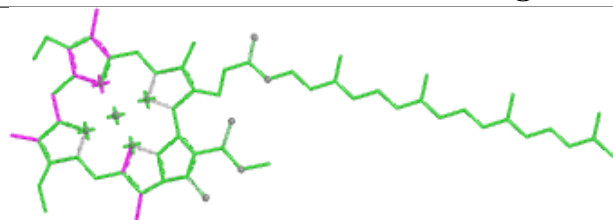


Torsions

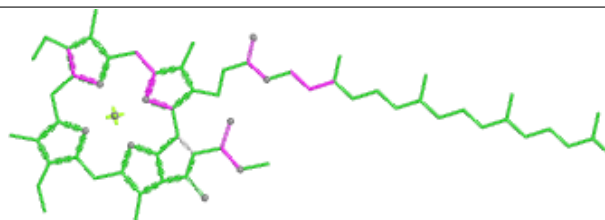


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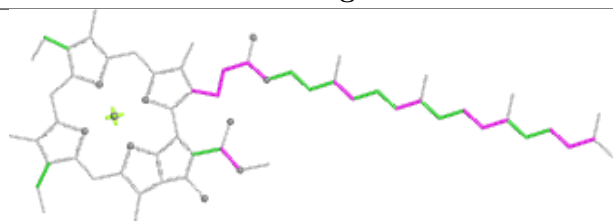
Ligand CLA C 501



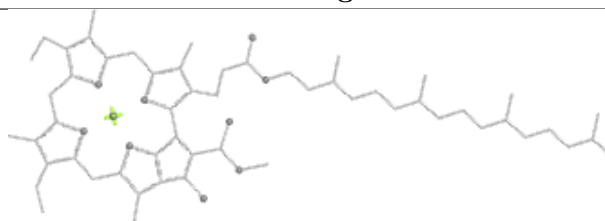
Bond lengths



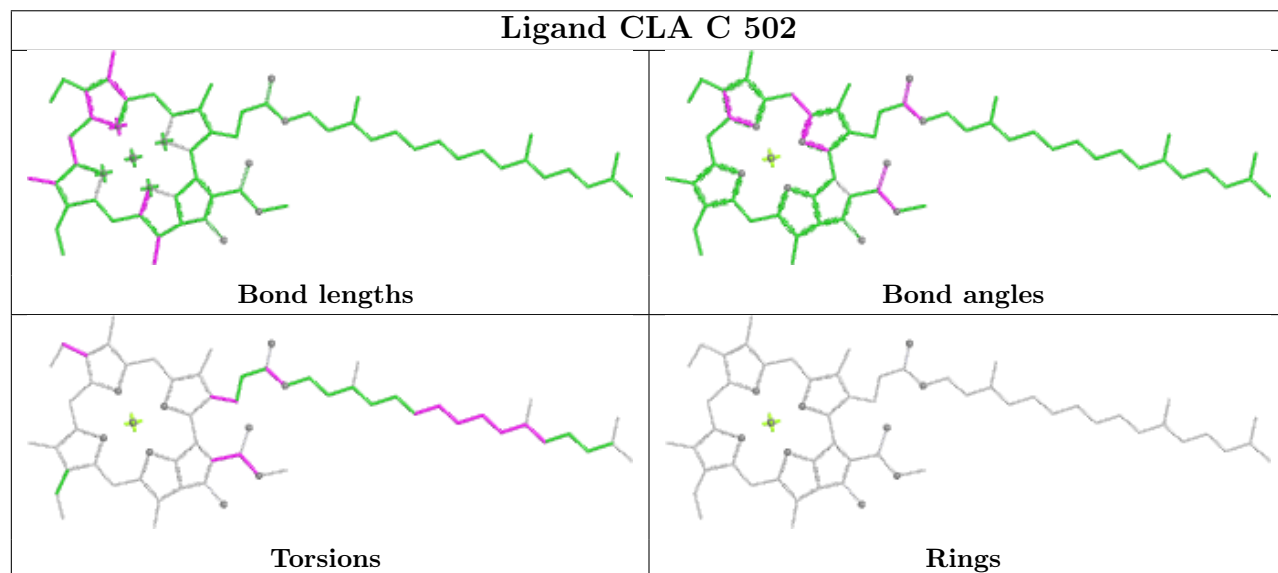
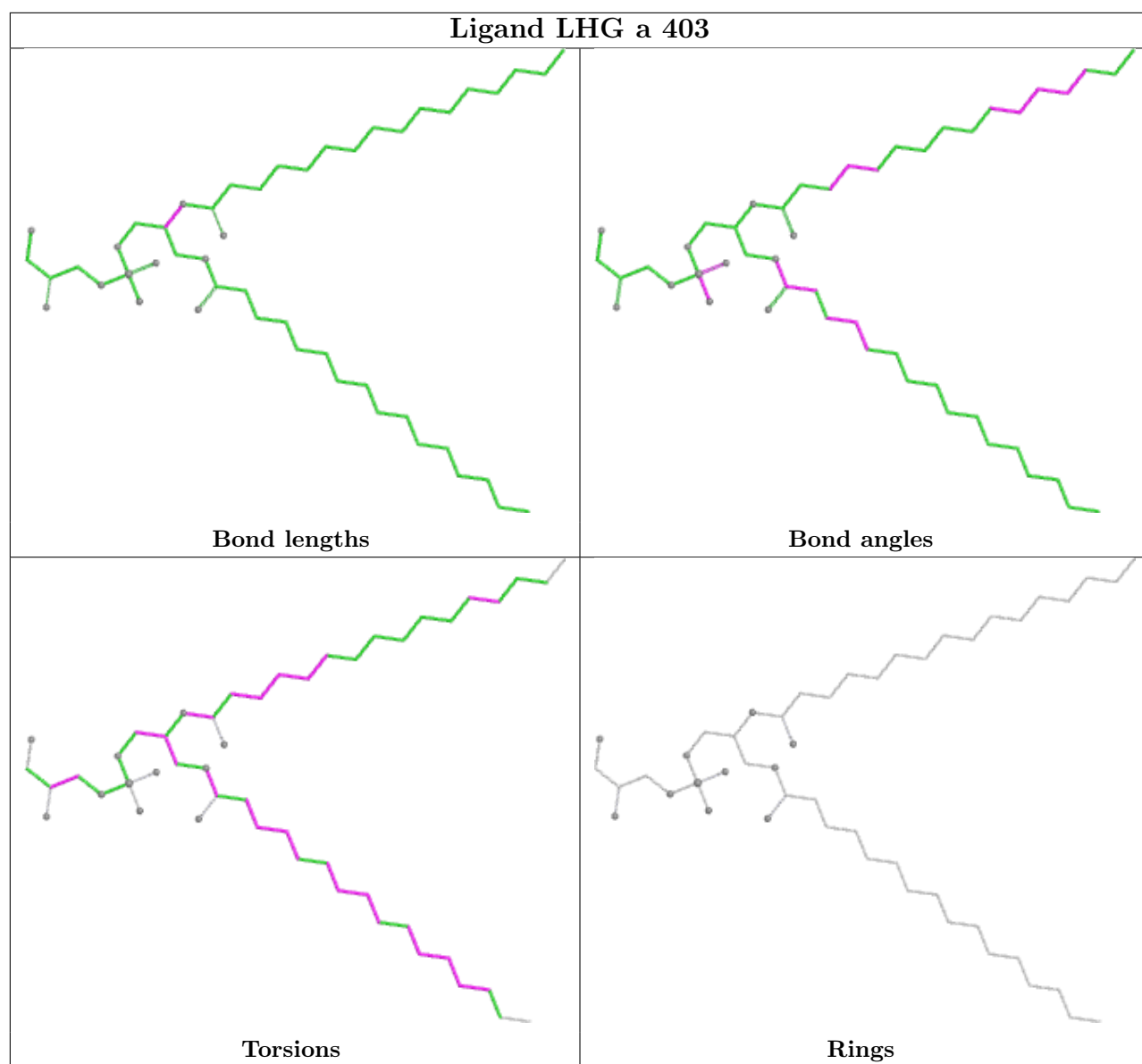
Bond angles

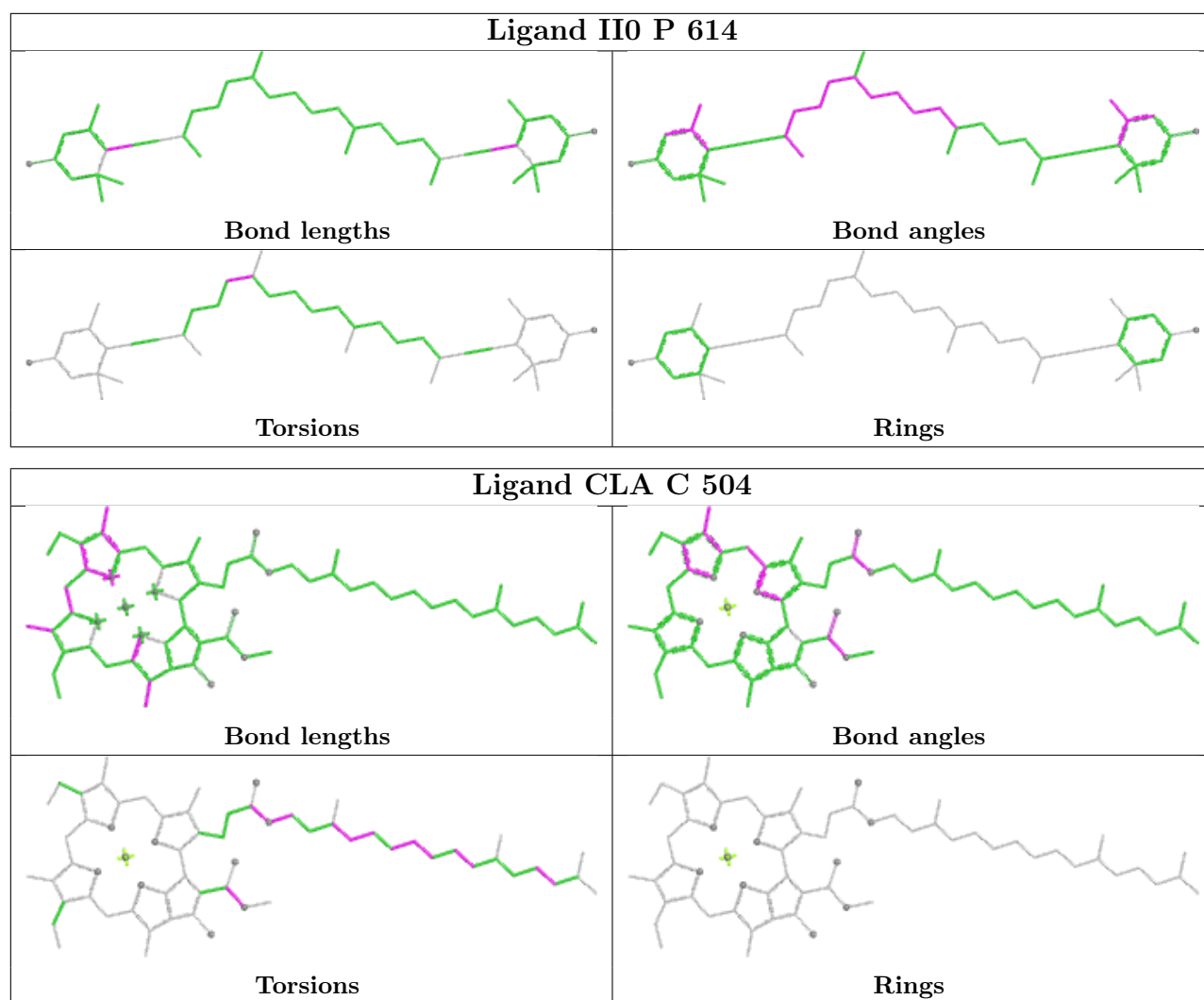


Torsions

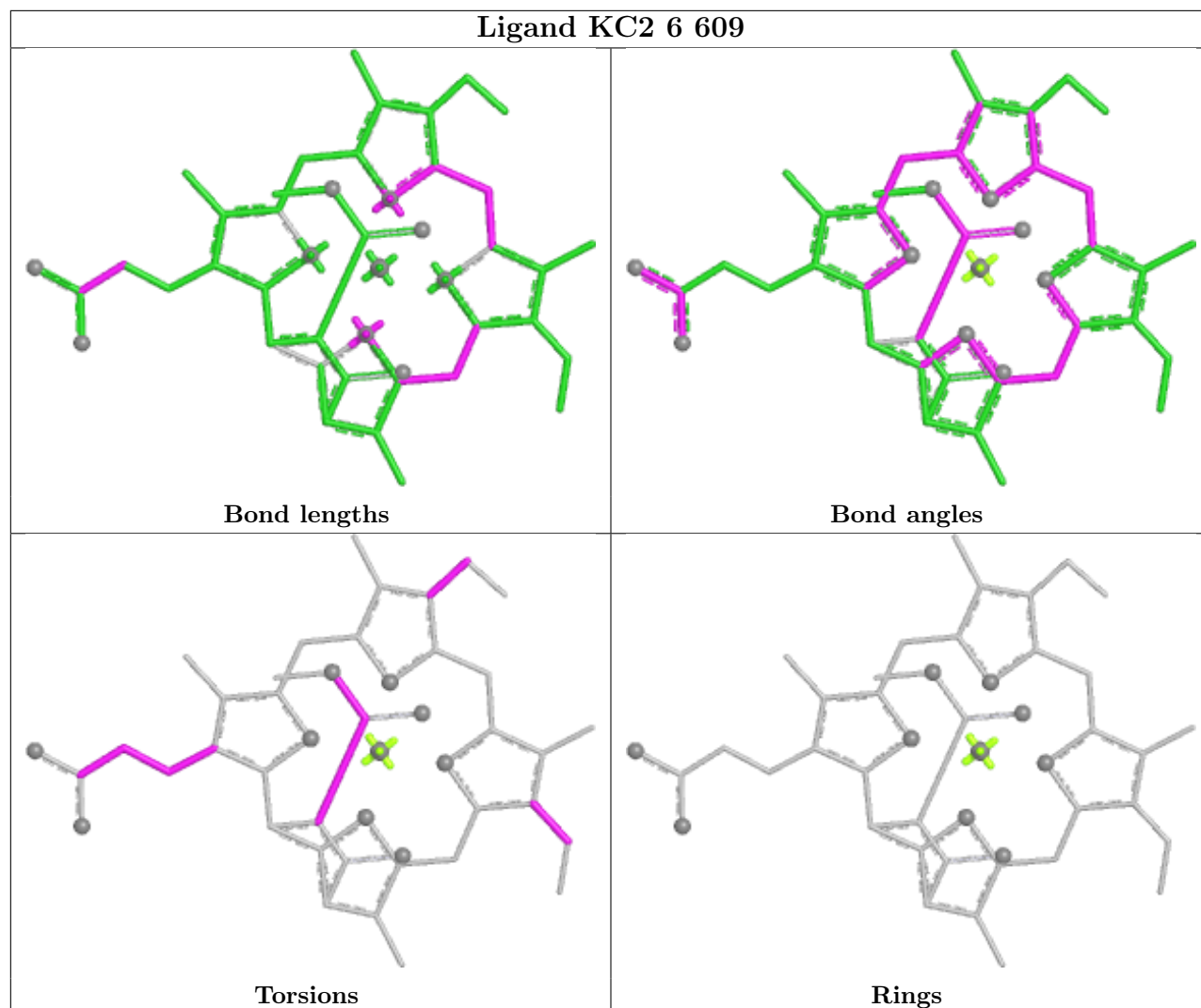


Rings

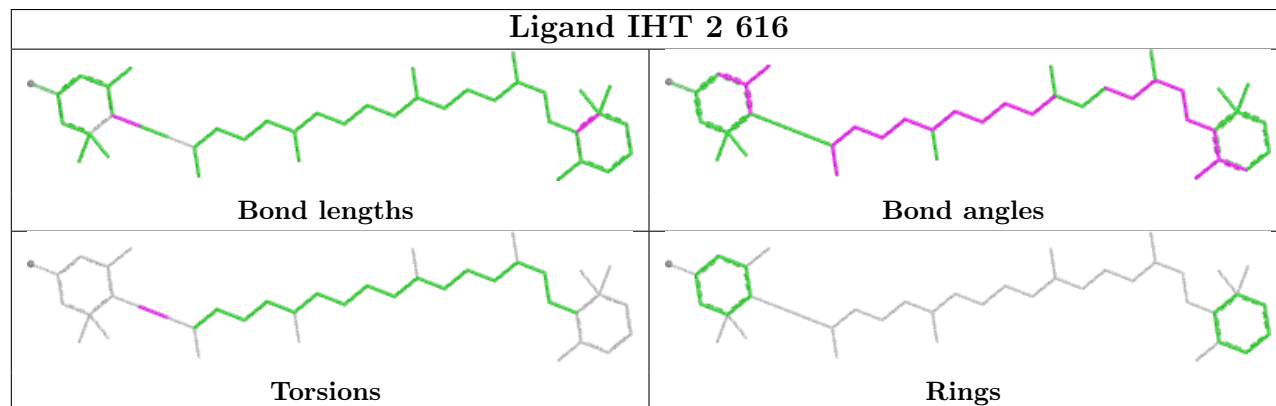




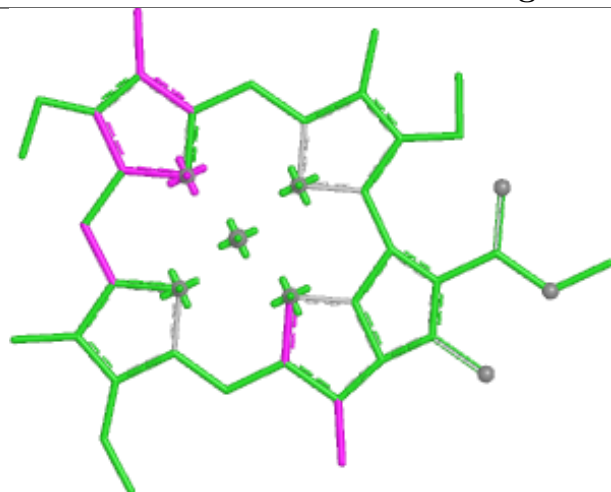
Ligand KC2 6 609



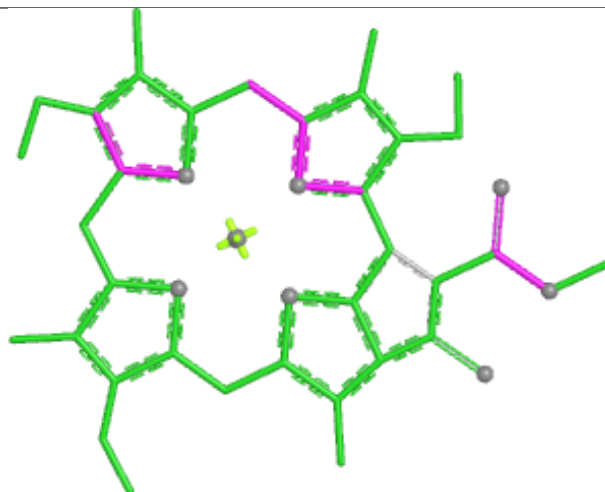
Ligand IHT 2 616



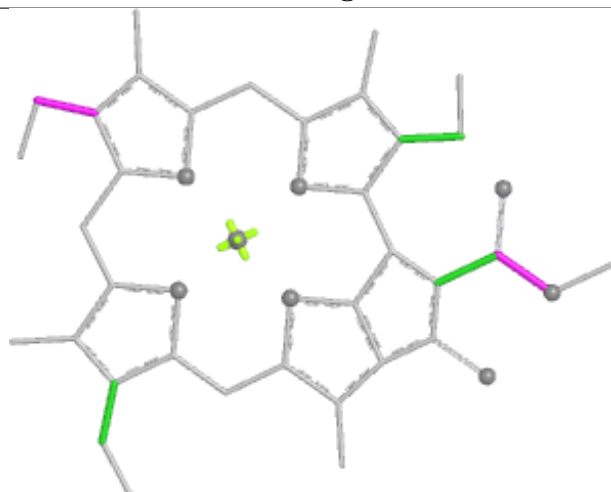
Ligand CLA 8 601



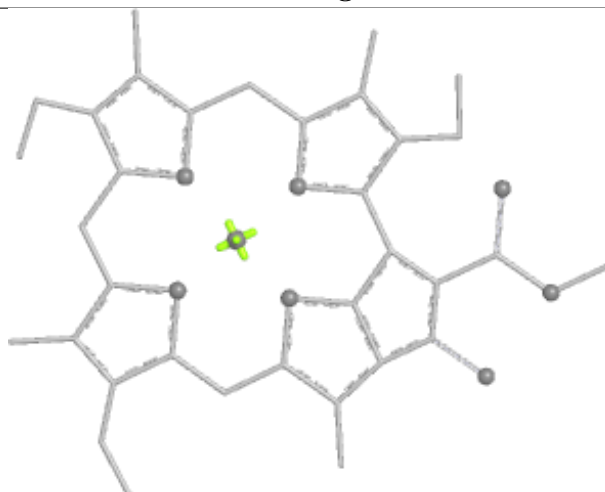
Bond lengths



Bond angles

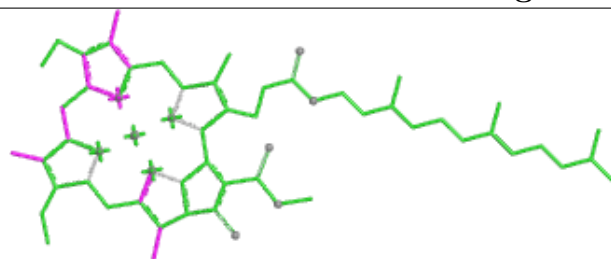


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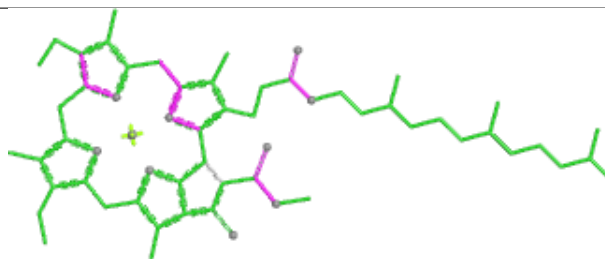


Rings

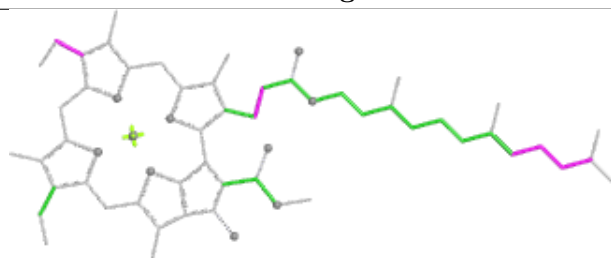
Ligand CLA P 607



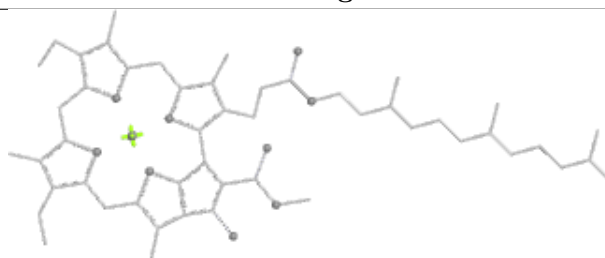
Bond lengths



Bond angles

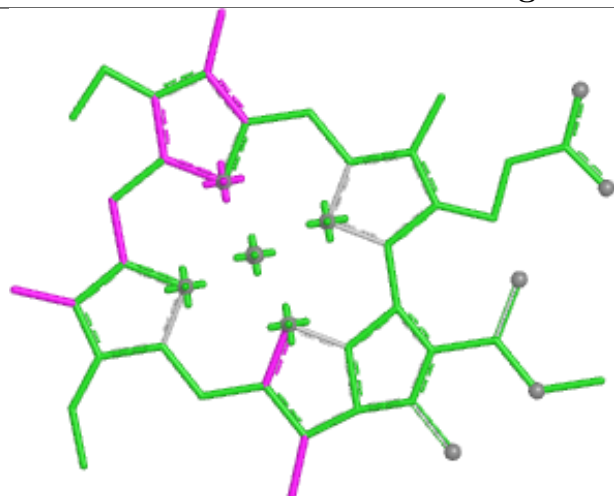


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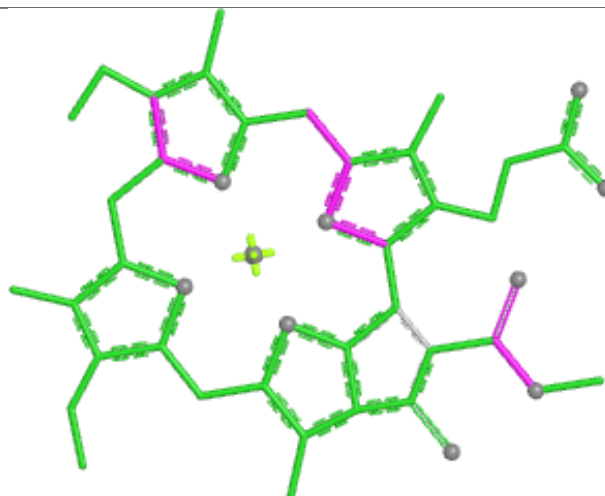


Rings

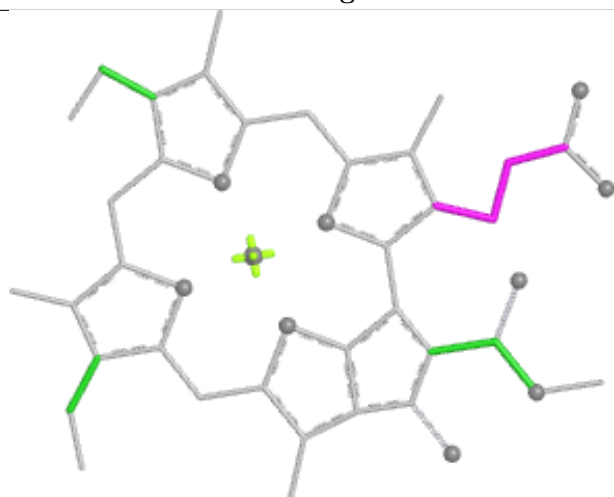
Ligand CLA 5 308



Bond lengths



Bond angles

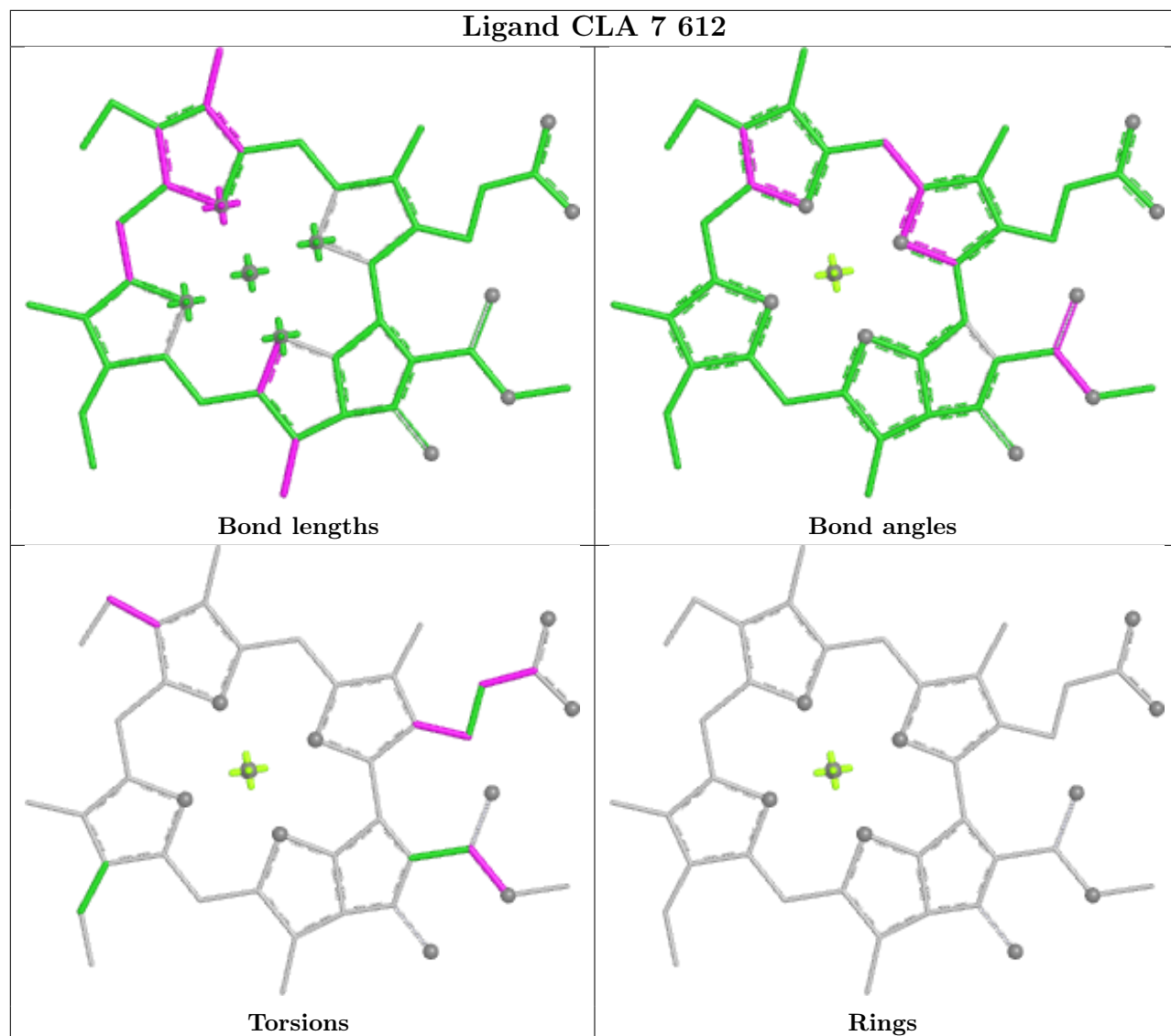


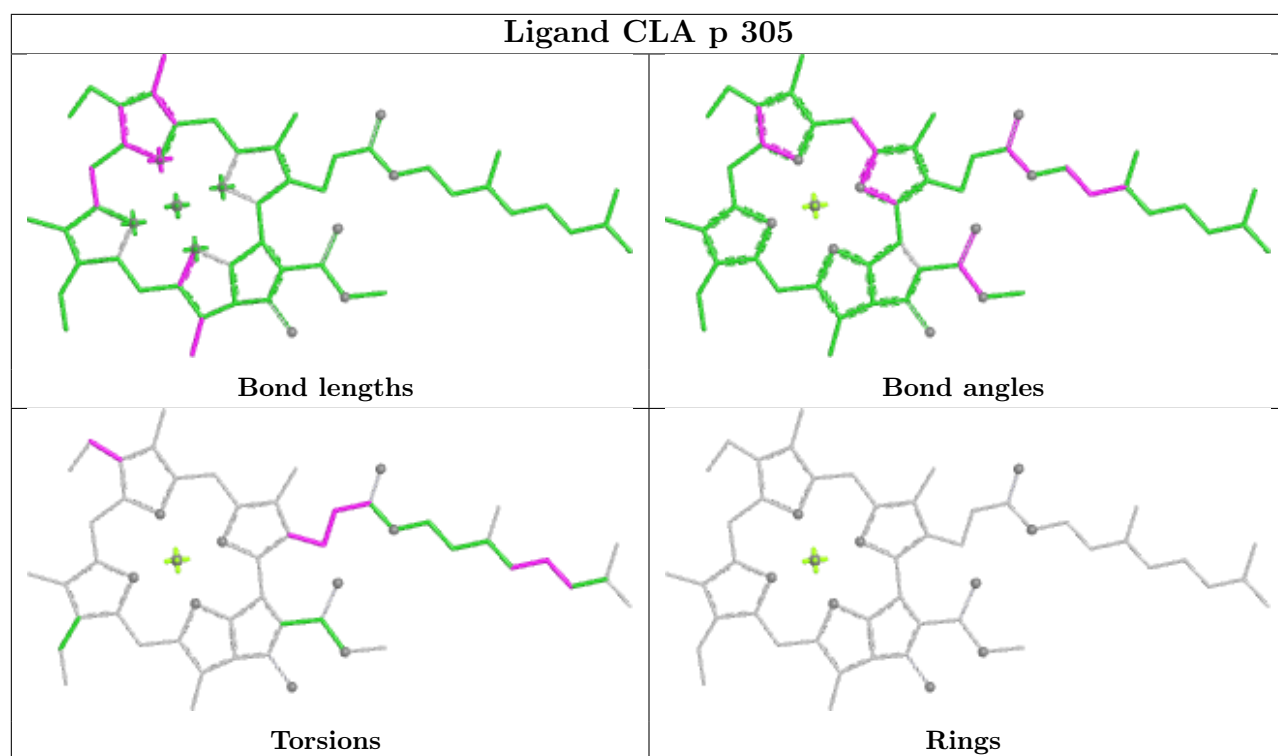
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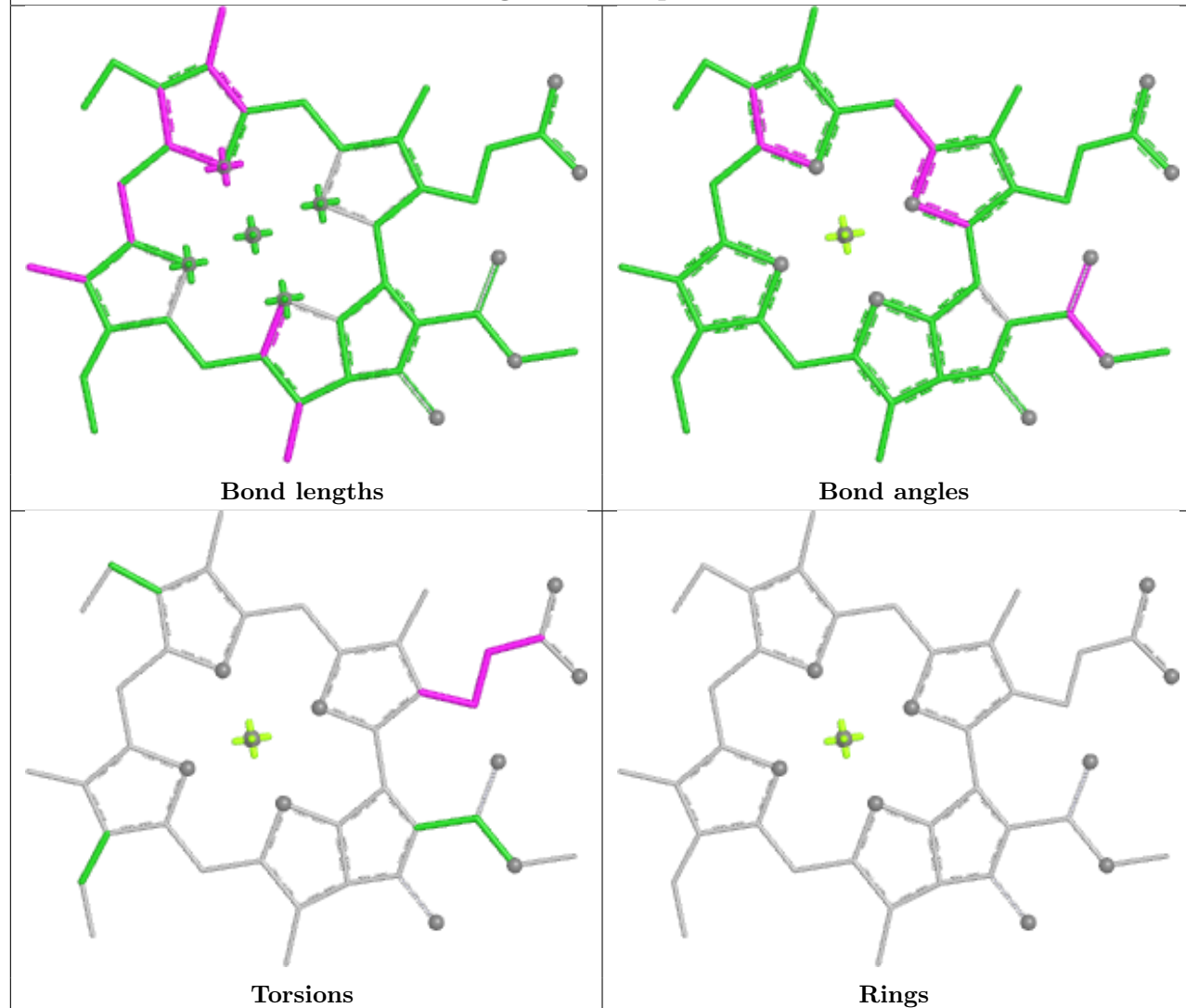
Rings

Ligand CLA 7 612

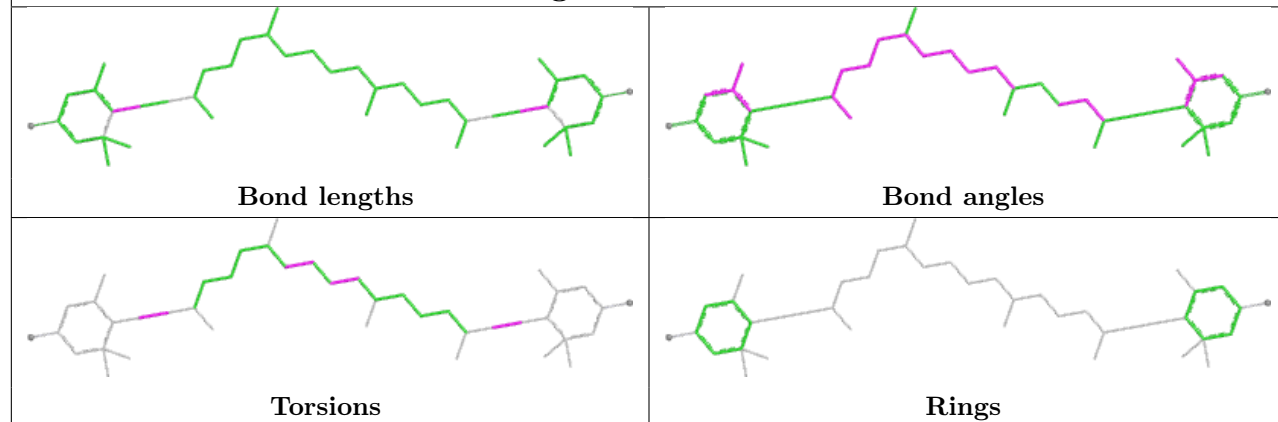




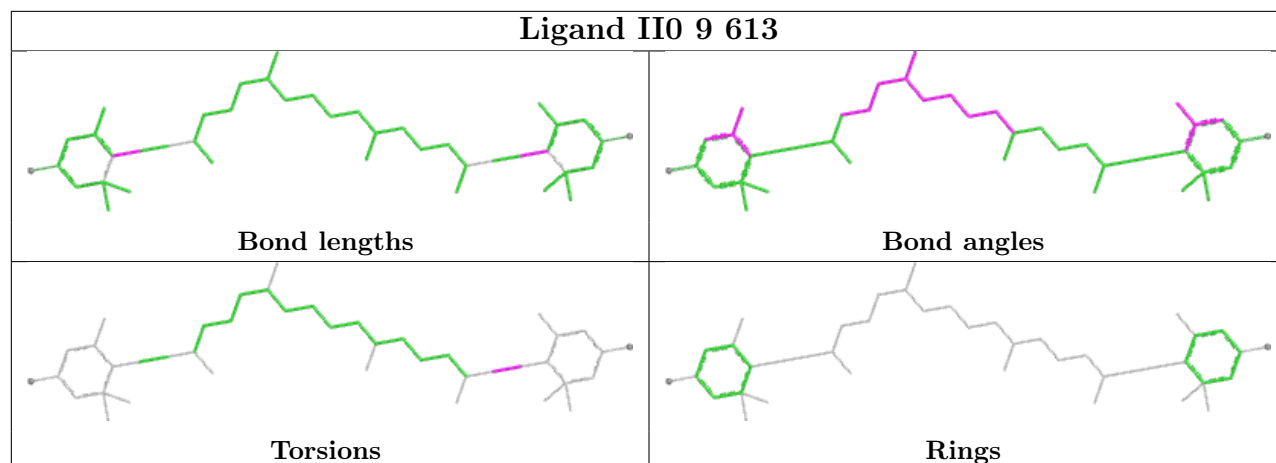
Ligand CLA p 308



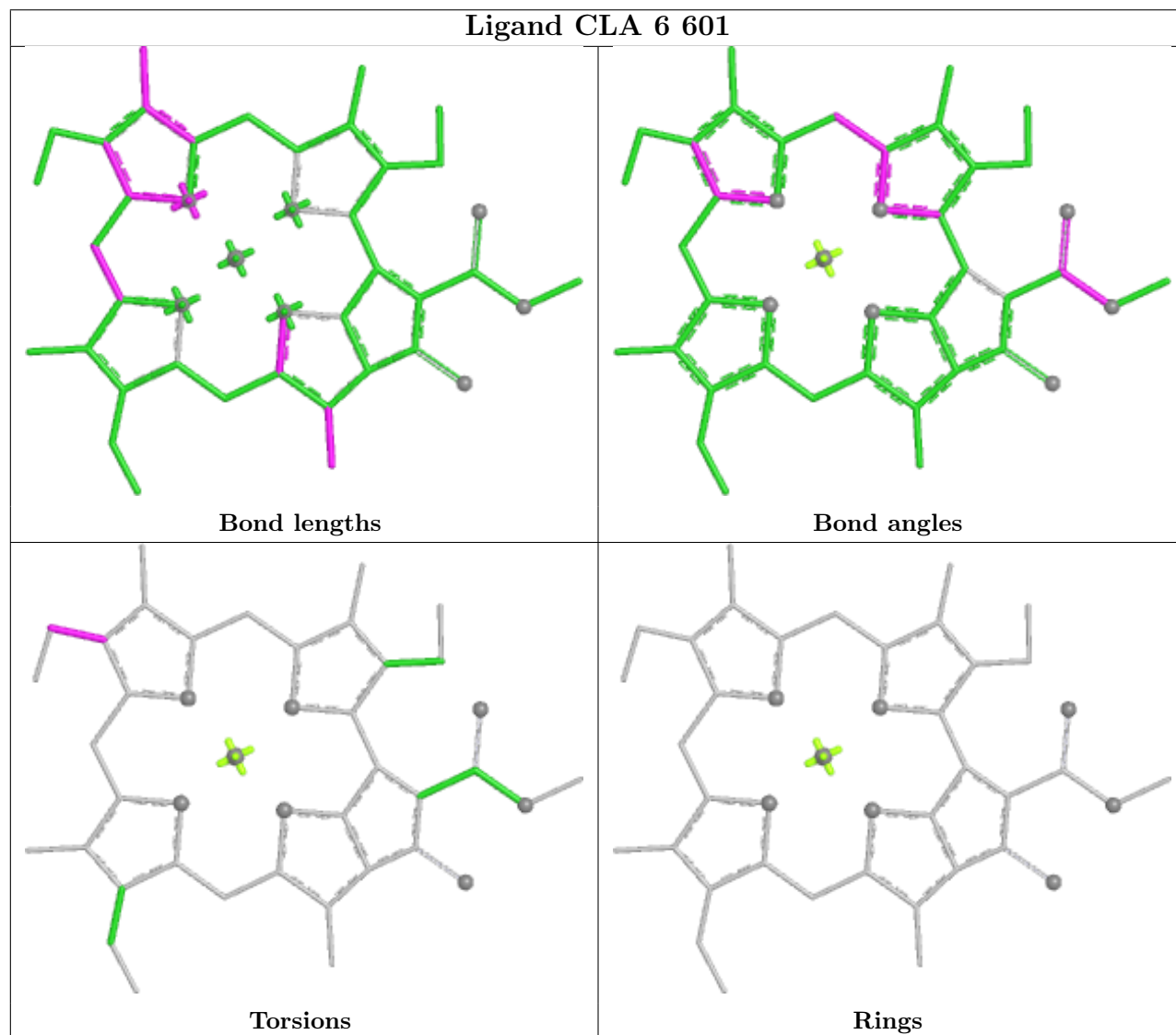
Ligand II0 0 616



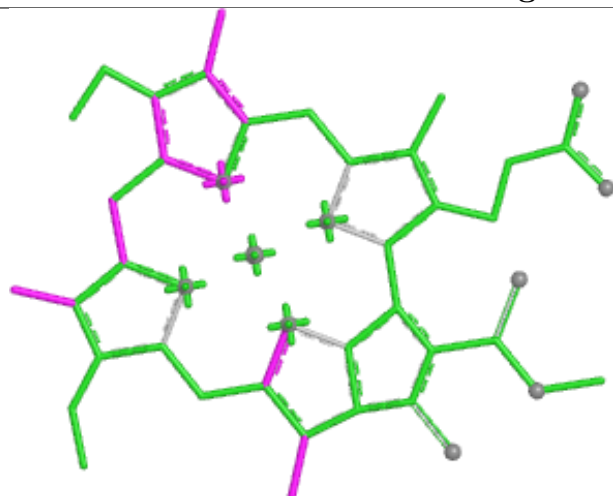
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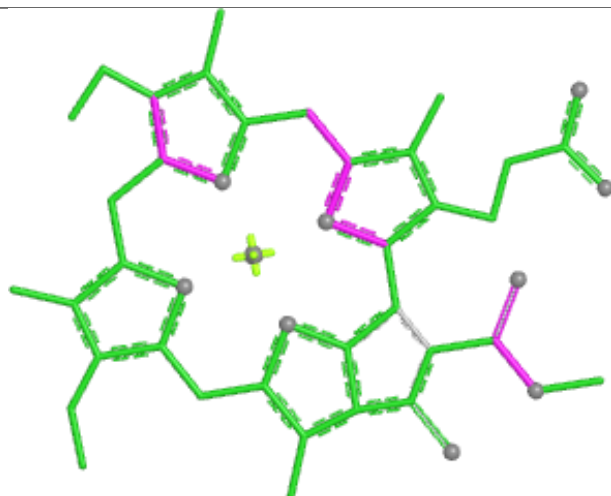
Ligand CLA 6 601



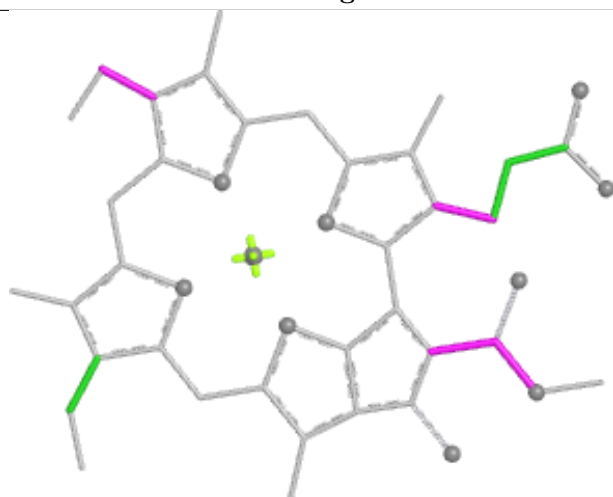
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Bond lengths



Bond angles

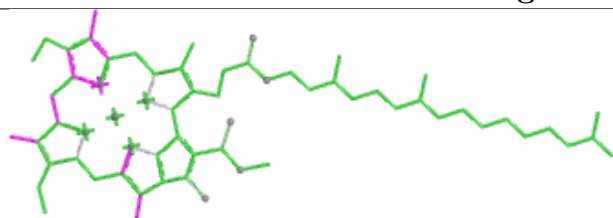


Torsions

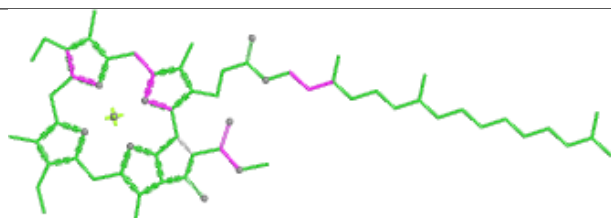


Rings

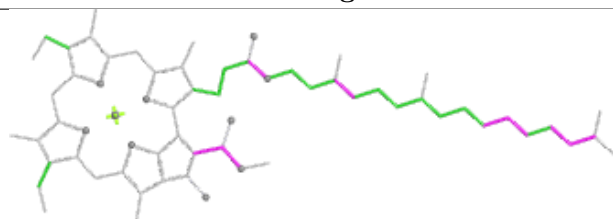
Ligand CLA b 615



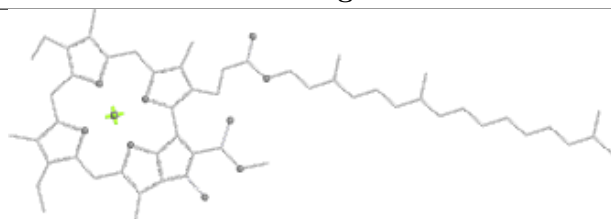
Bond lengths



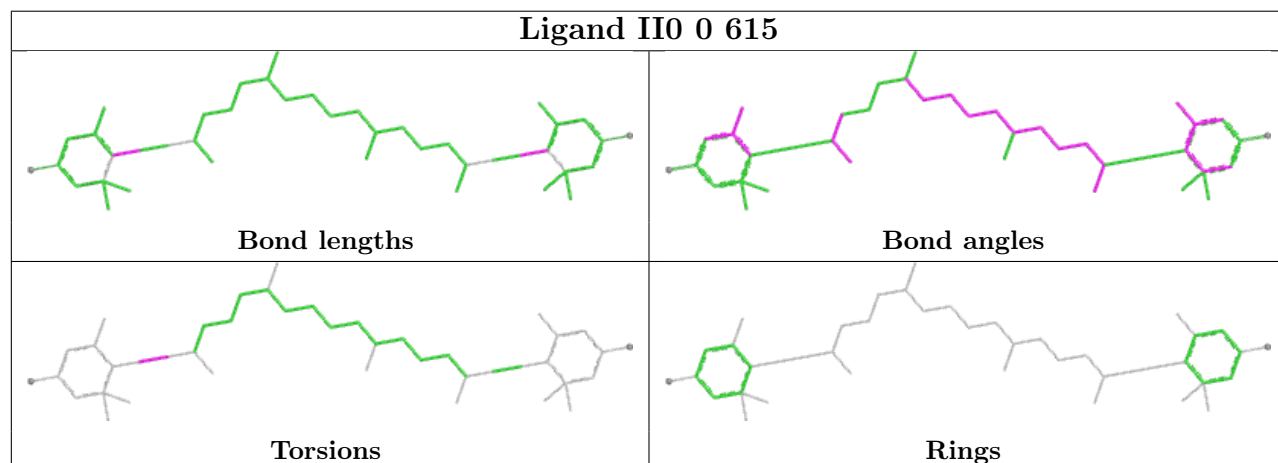
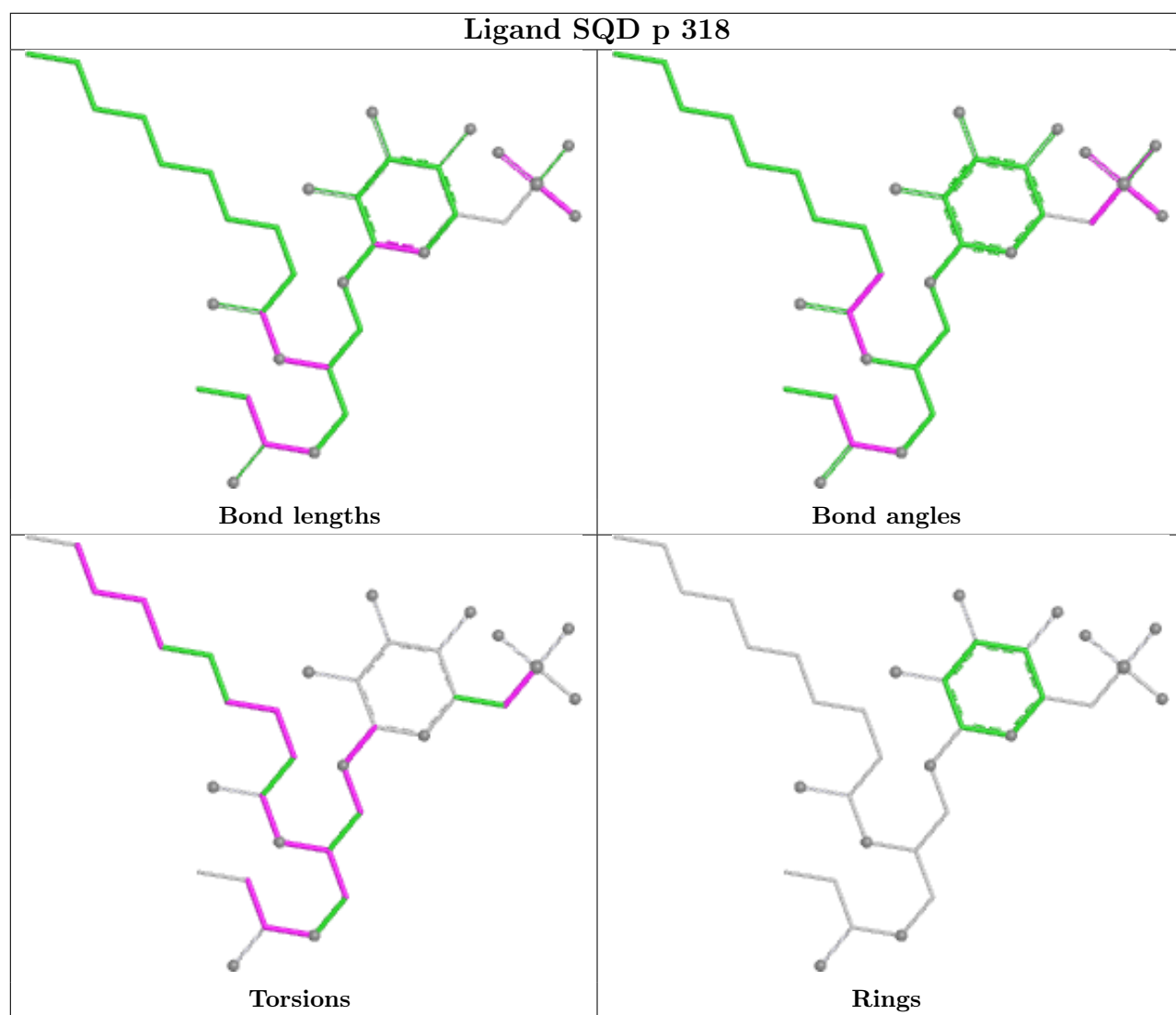
Bond angles

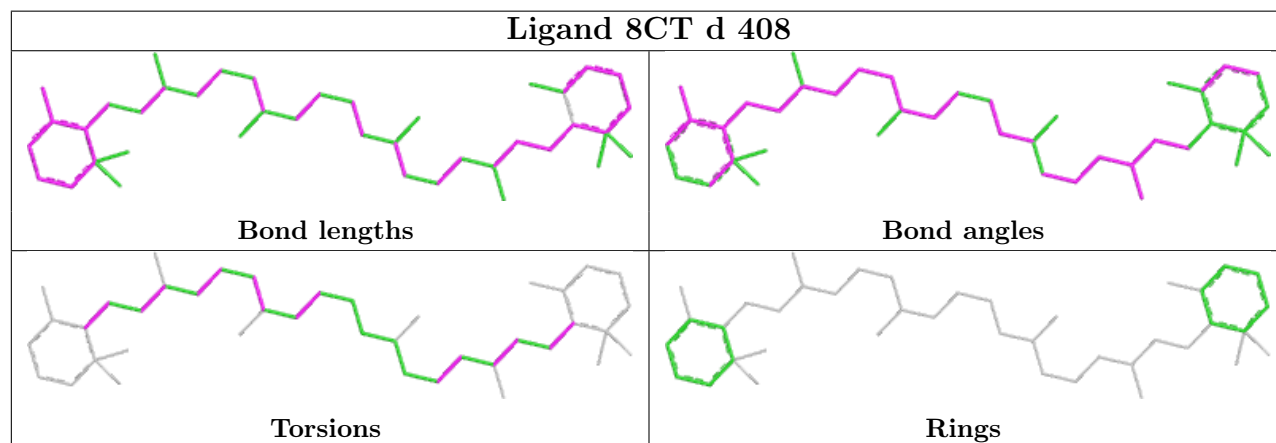
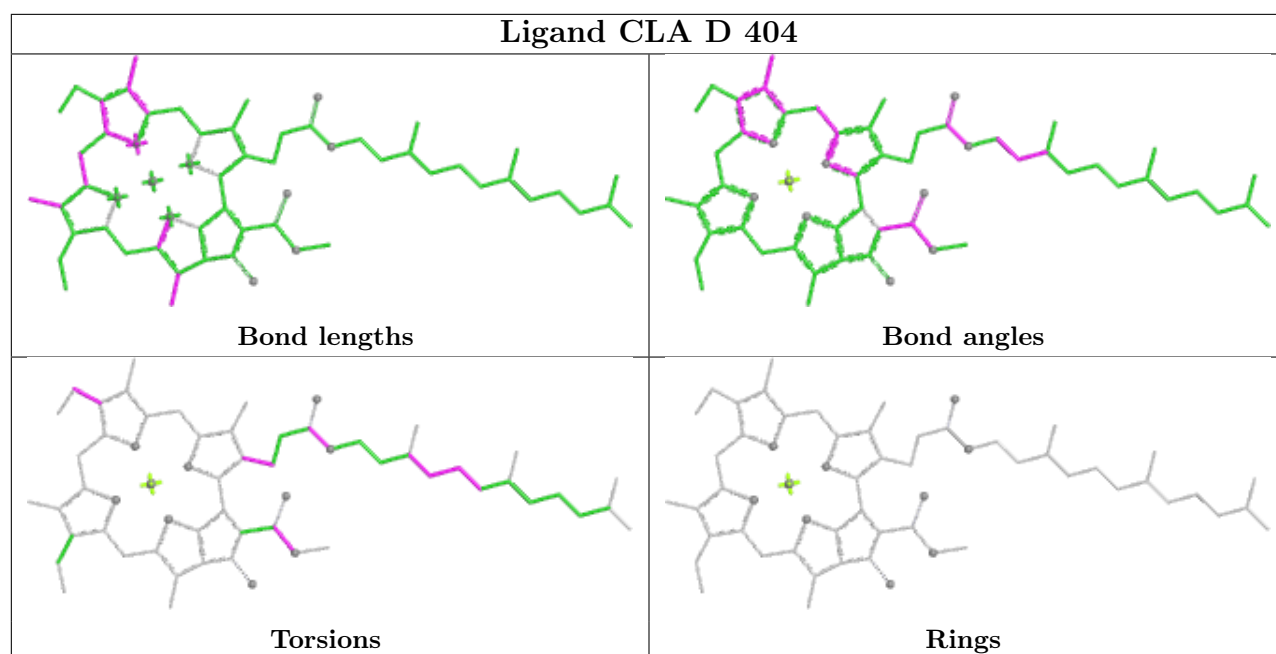


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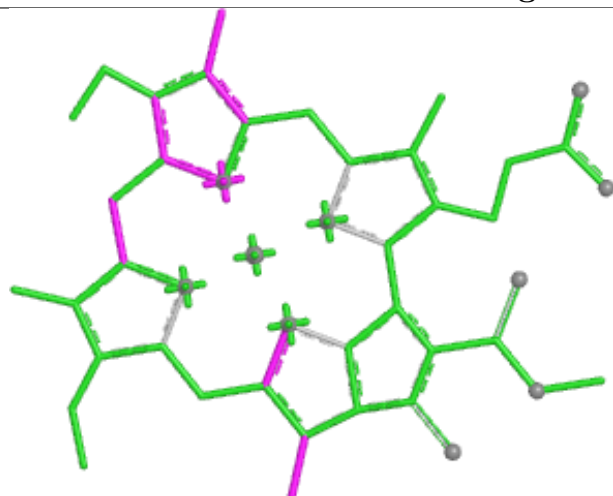


Rings

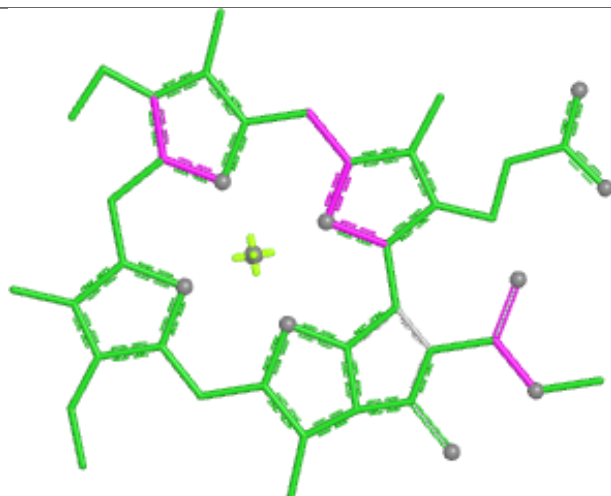




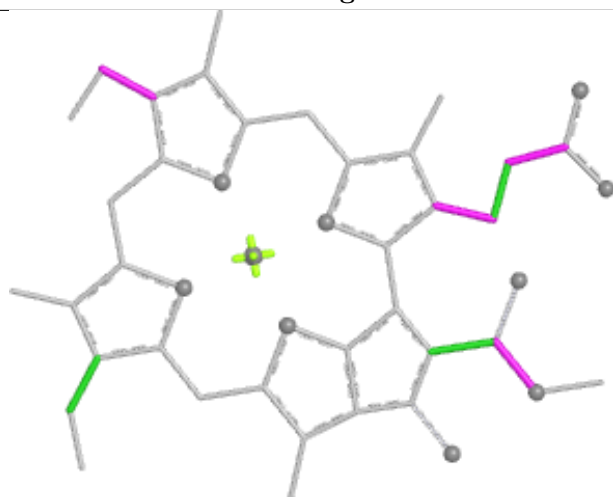
Ligand CLA 1 607



Bond lengths



Bond angles

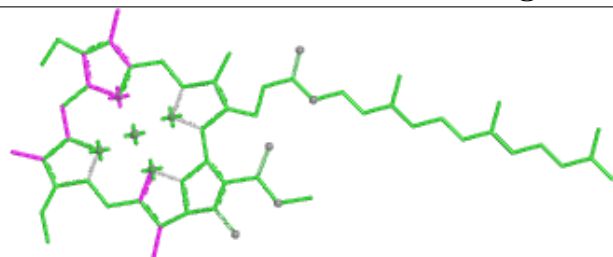


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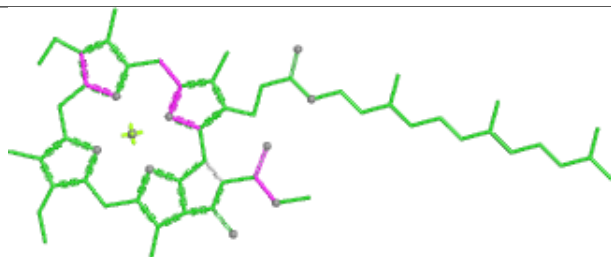


Rings

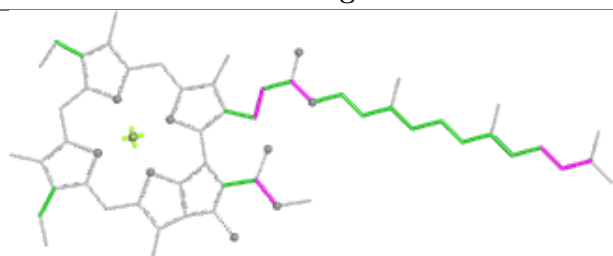
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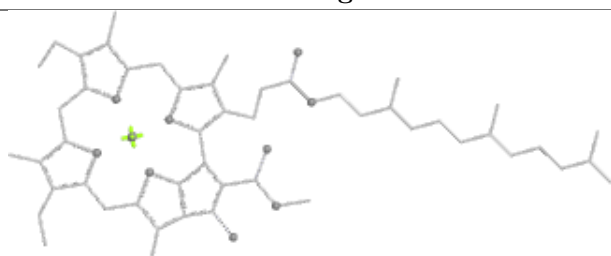
Bond lengths



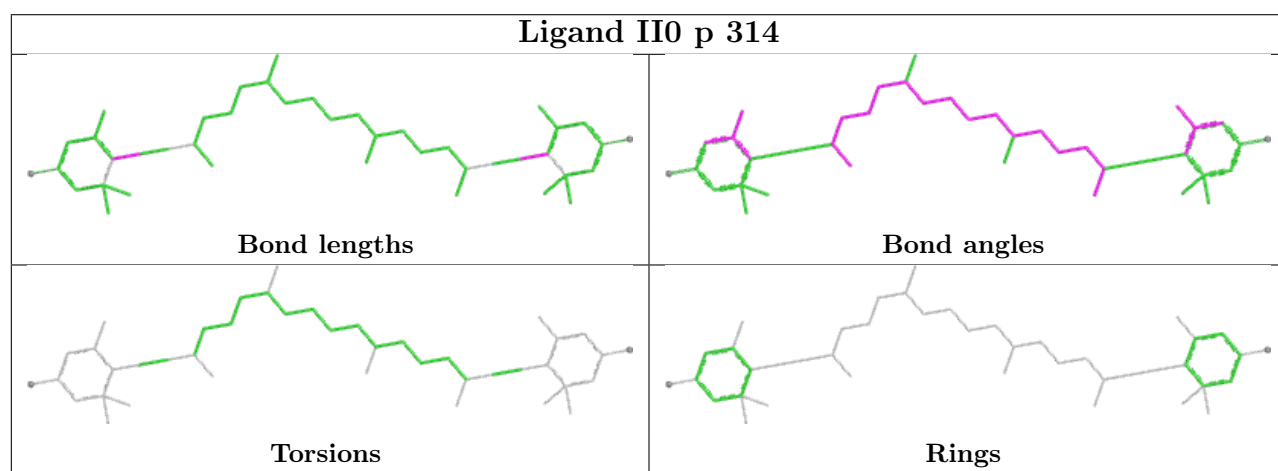
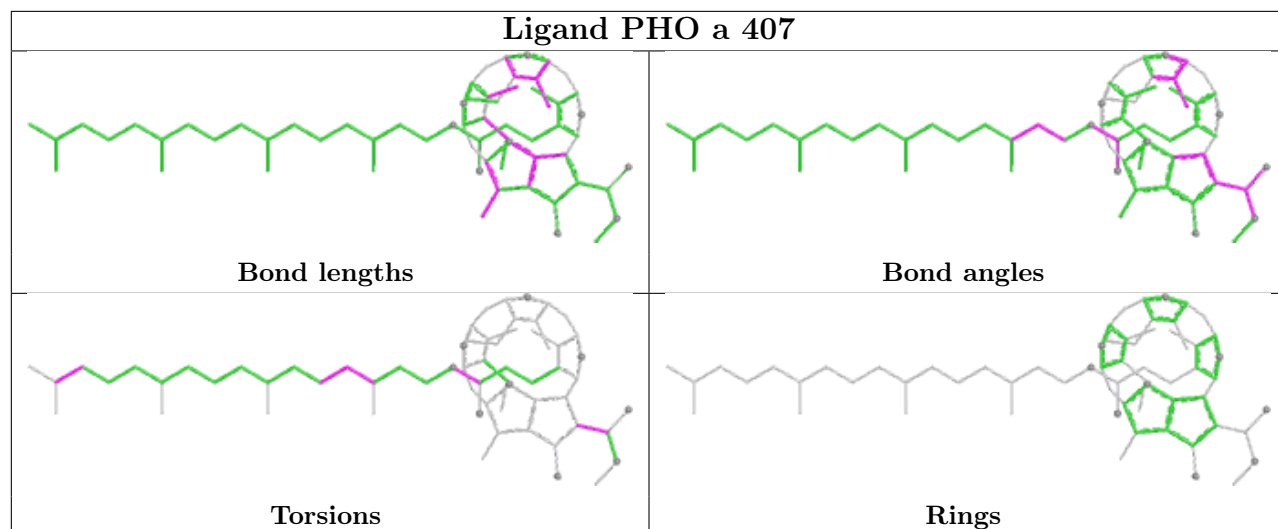
Bond angles



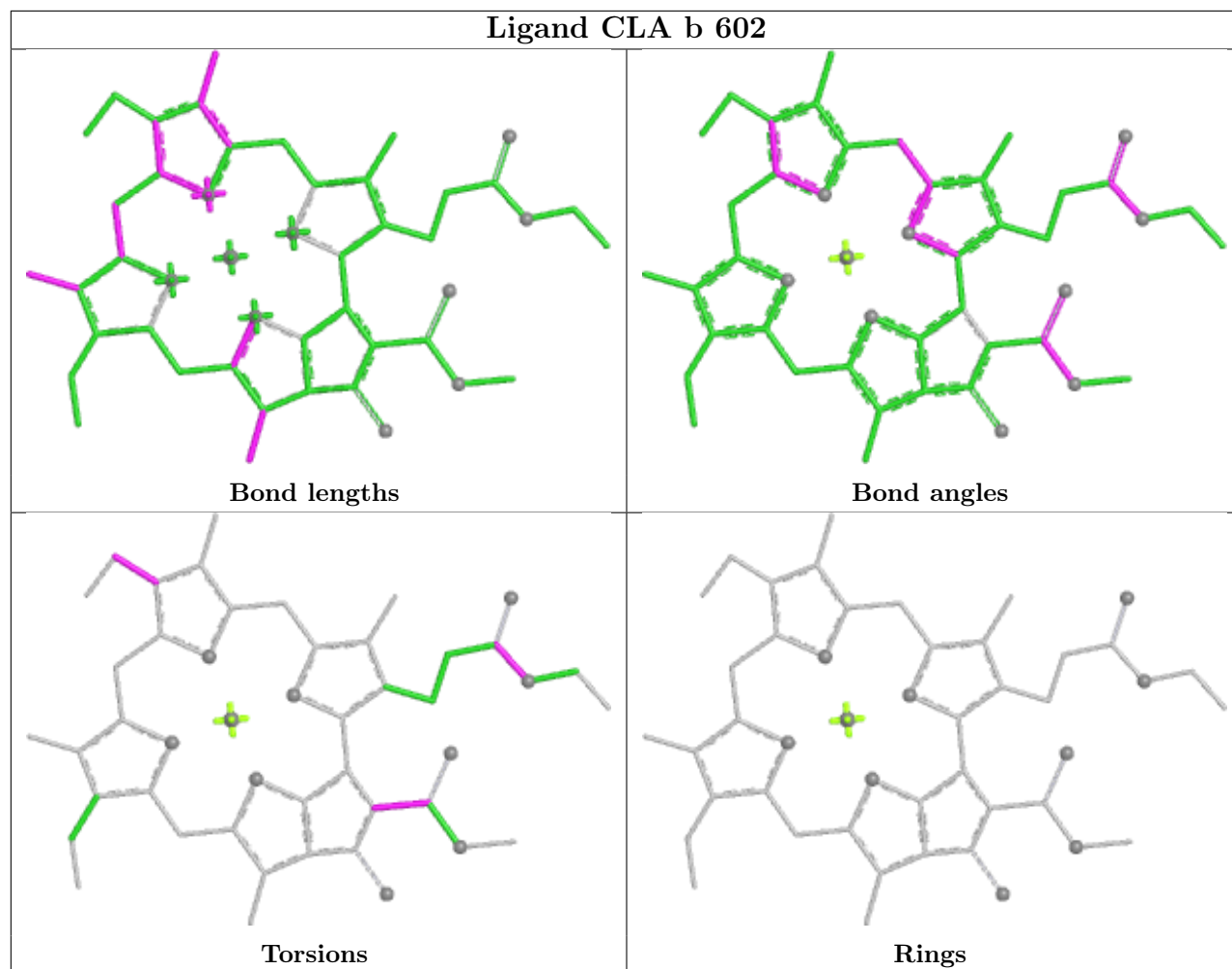
Torsions



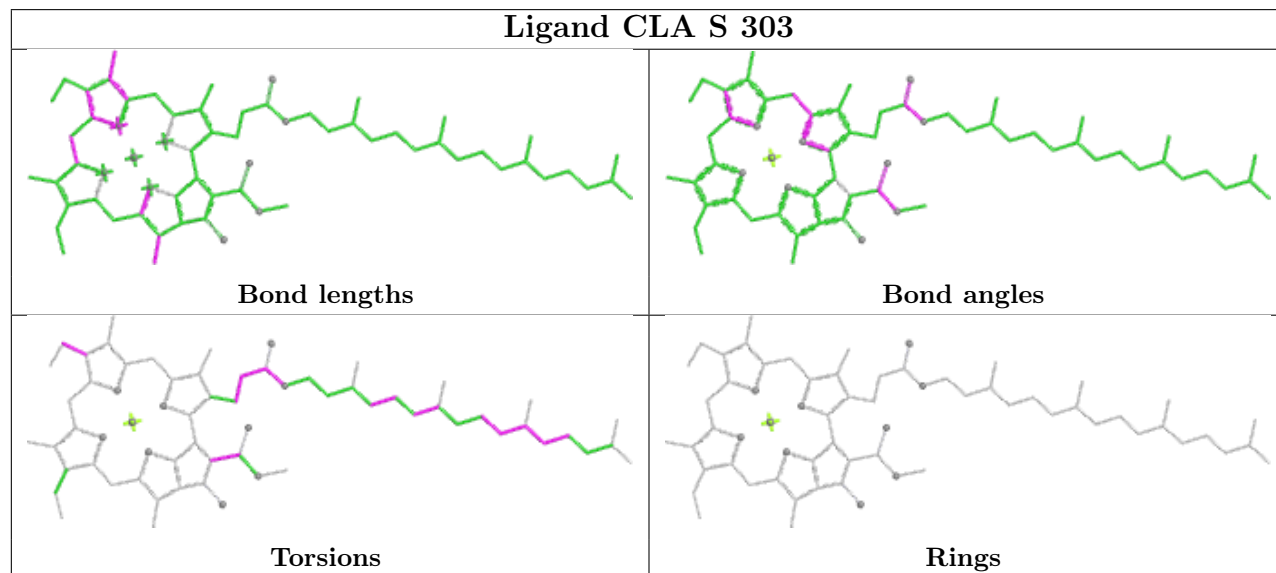
Rings

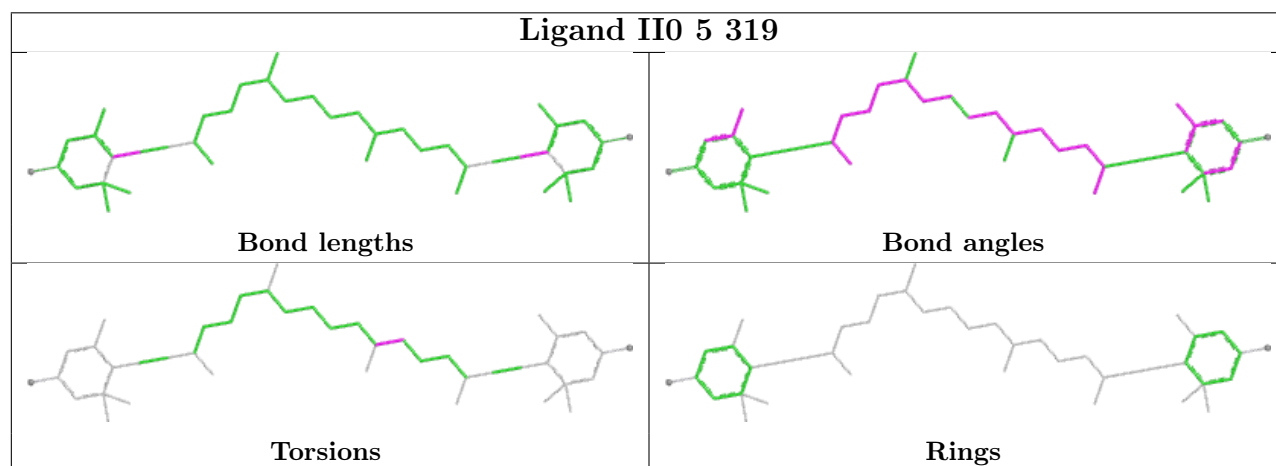
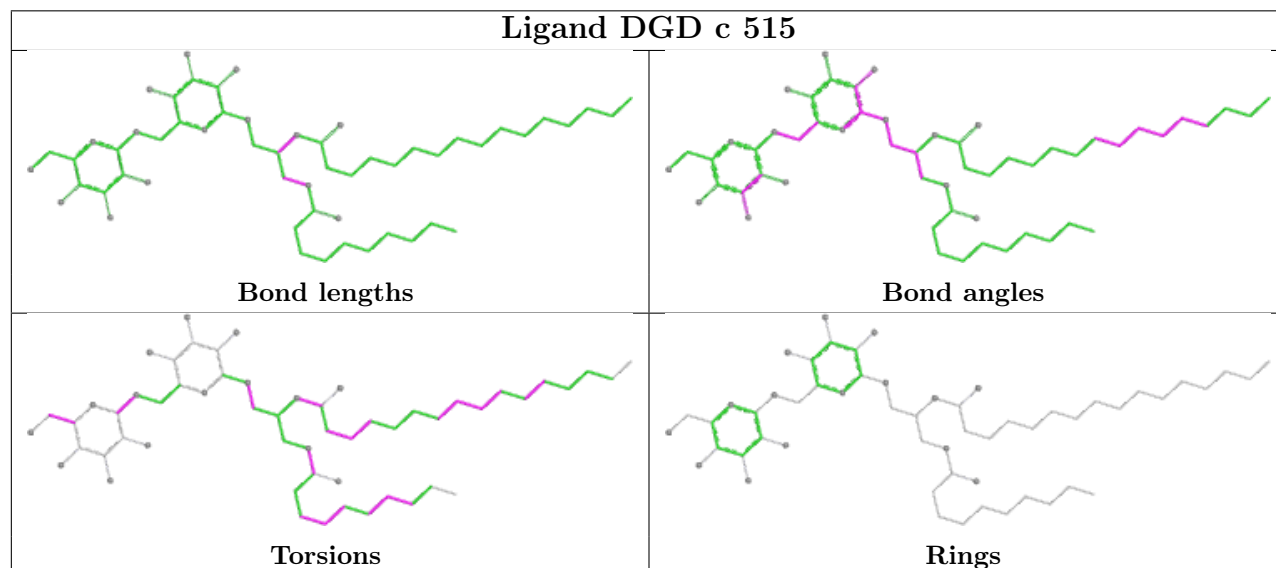
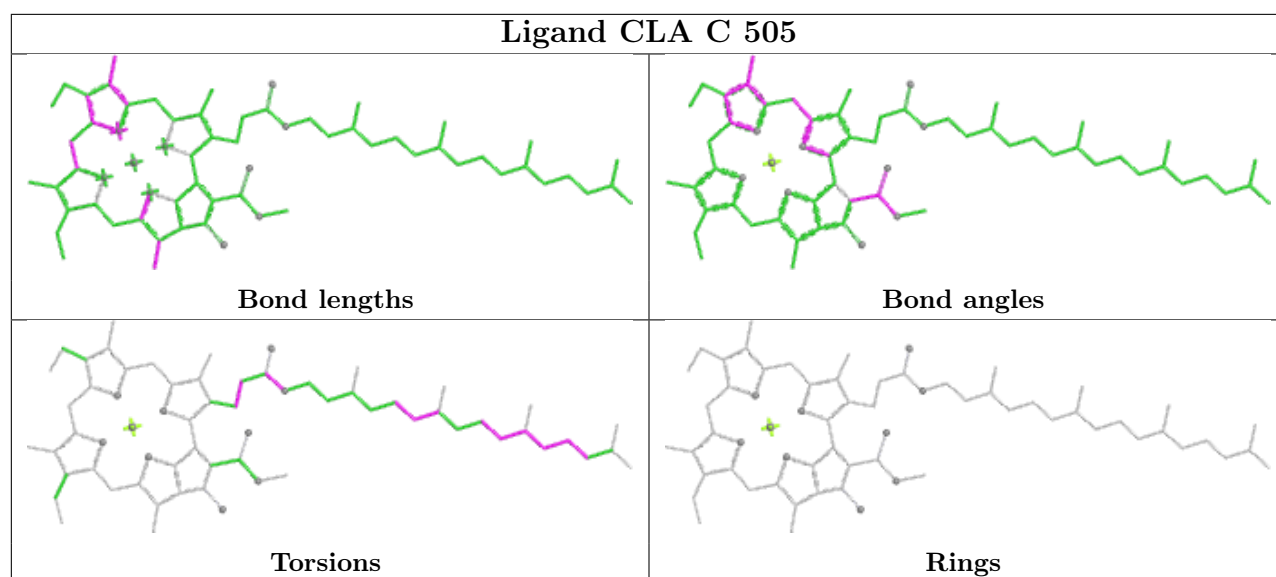


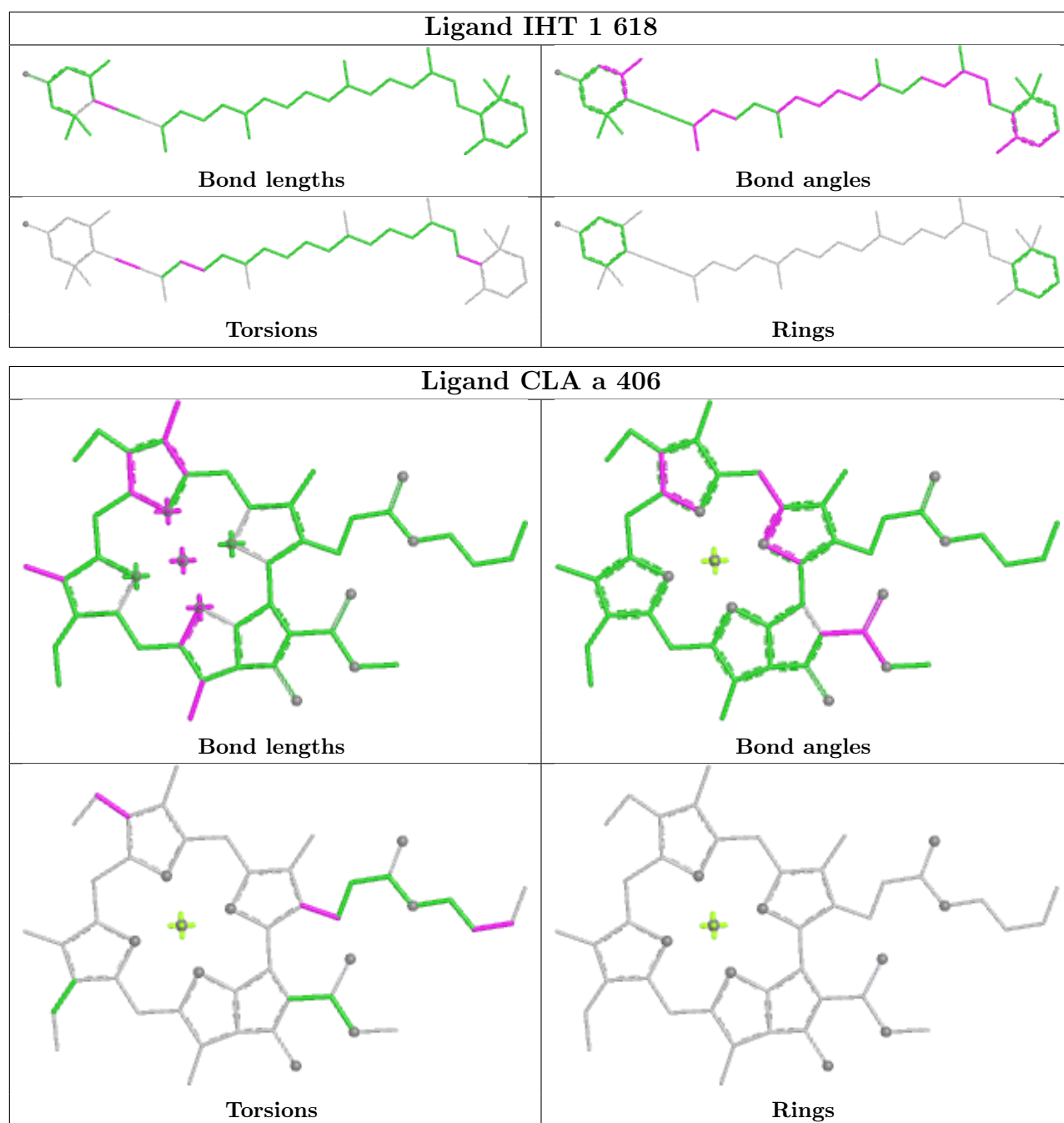
Ligand CLA b 602



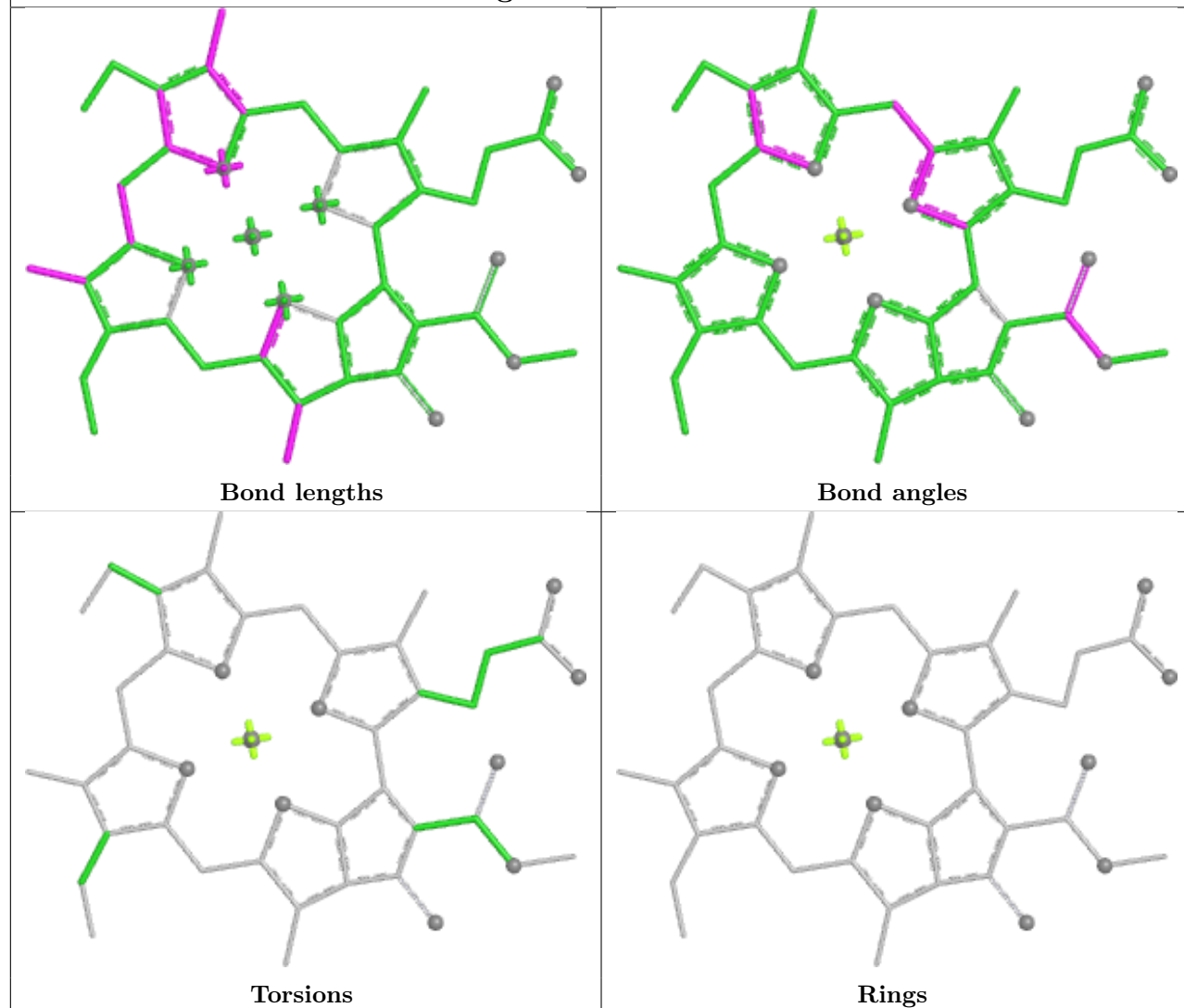
Ligand CLA S 303



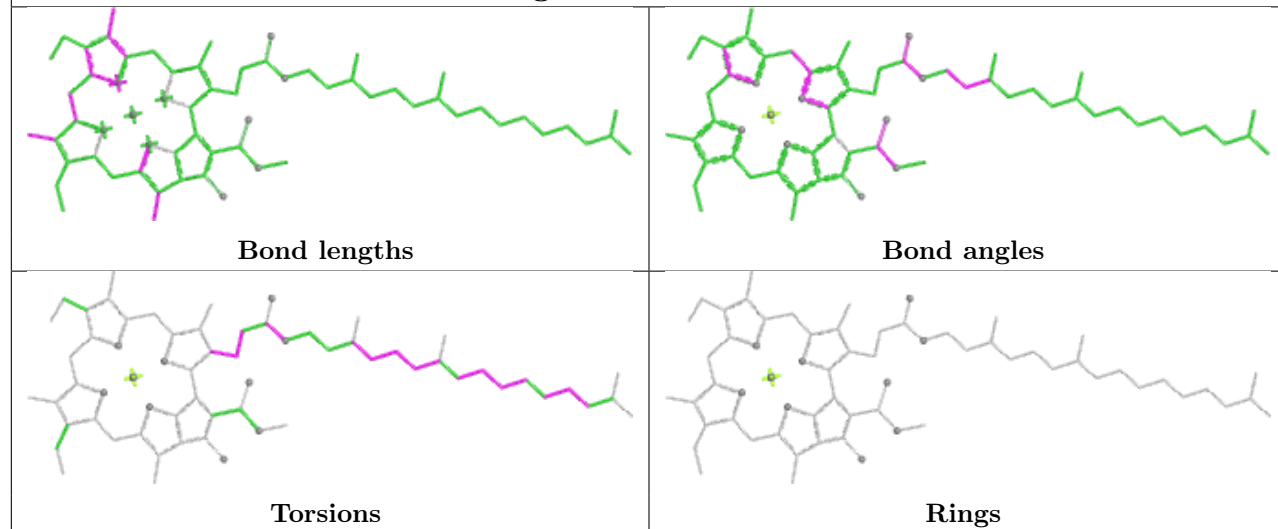


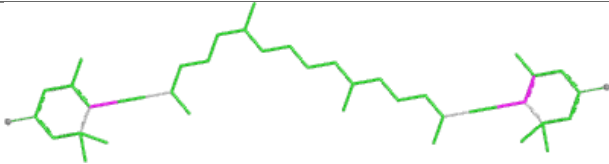
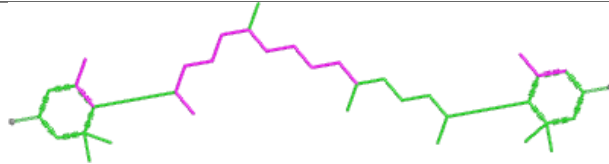
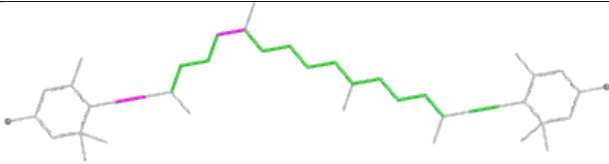
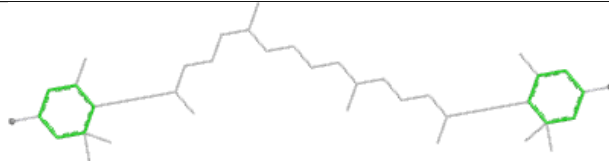


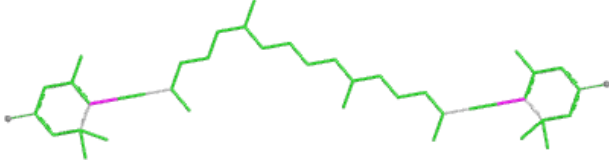
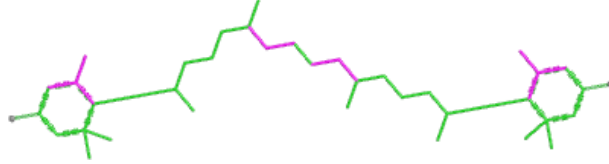
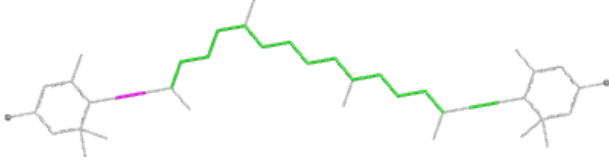
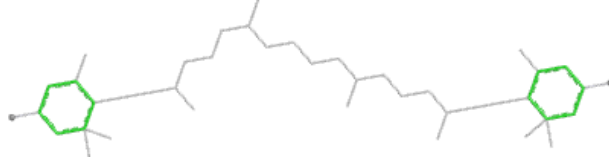
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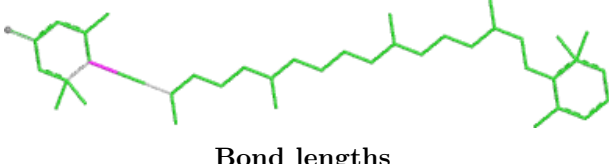
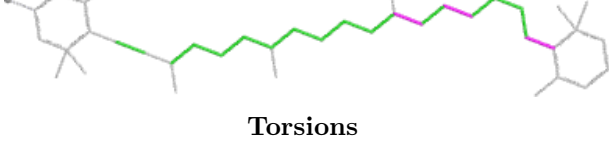
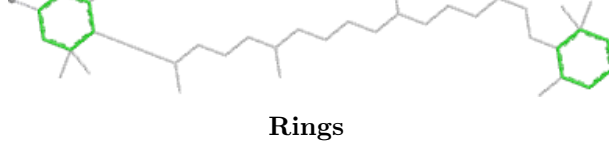


Ligand CLA B 612

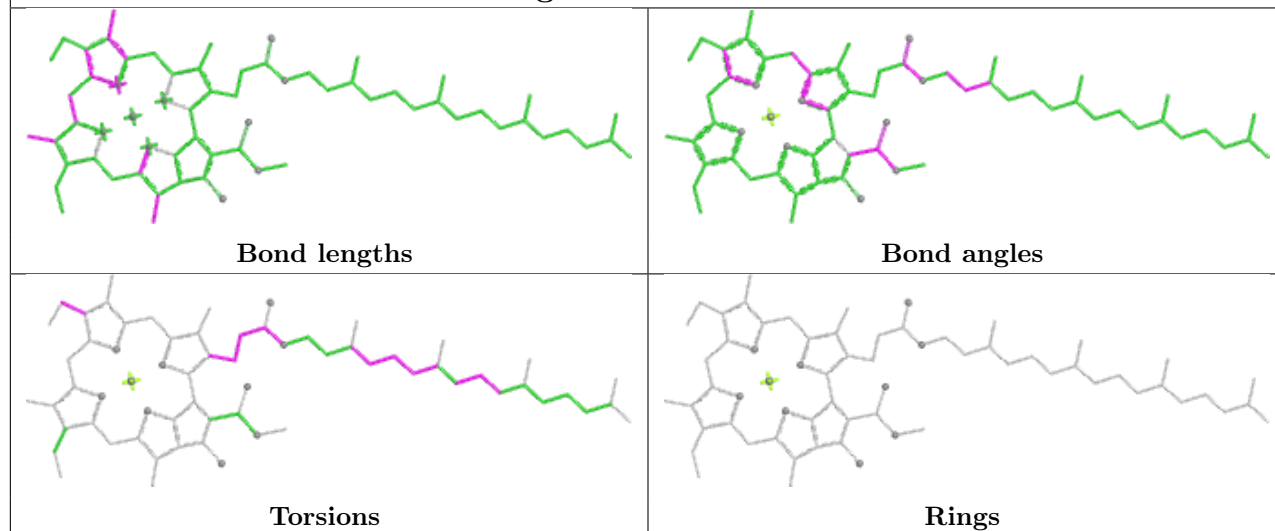


Ligand II0 6 614	
	
Bond lengths	Bond angles
	
Torsions	Rings

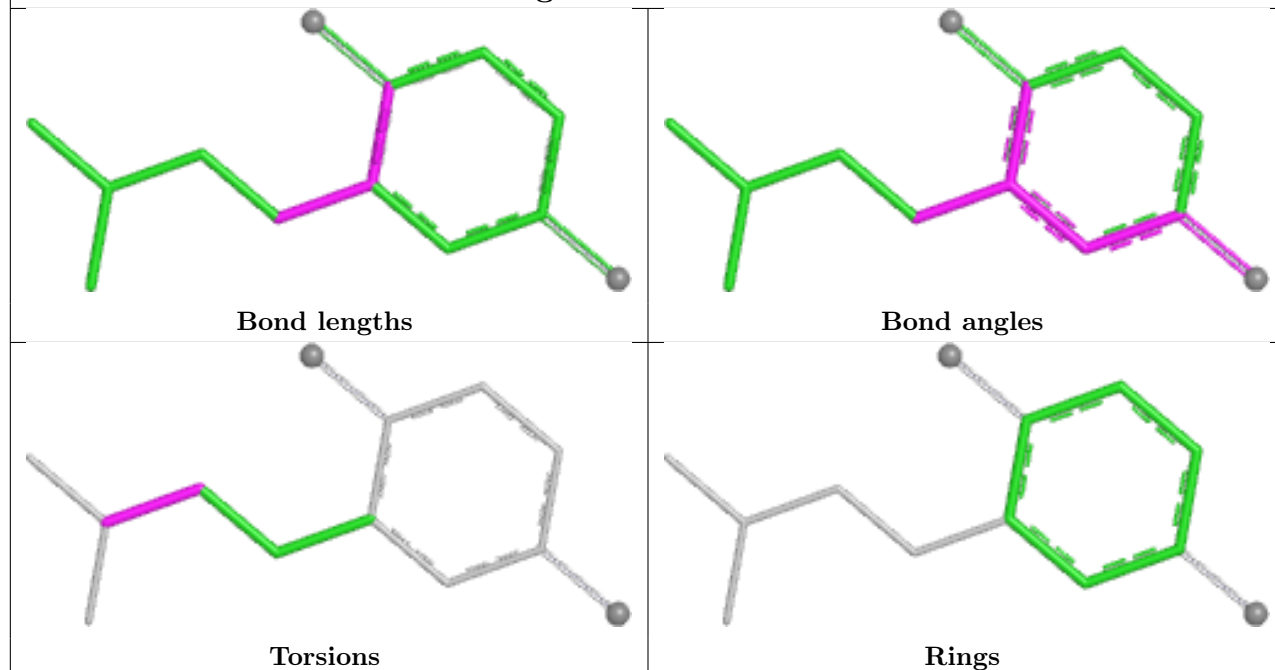
Ligand II0 7 614	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand IHT 4 614	
	
Bond lengths	Bond angles
	
Torsions	Rings

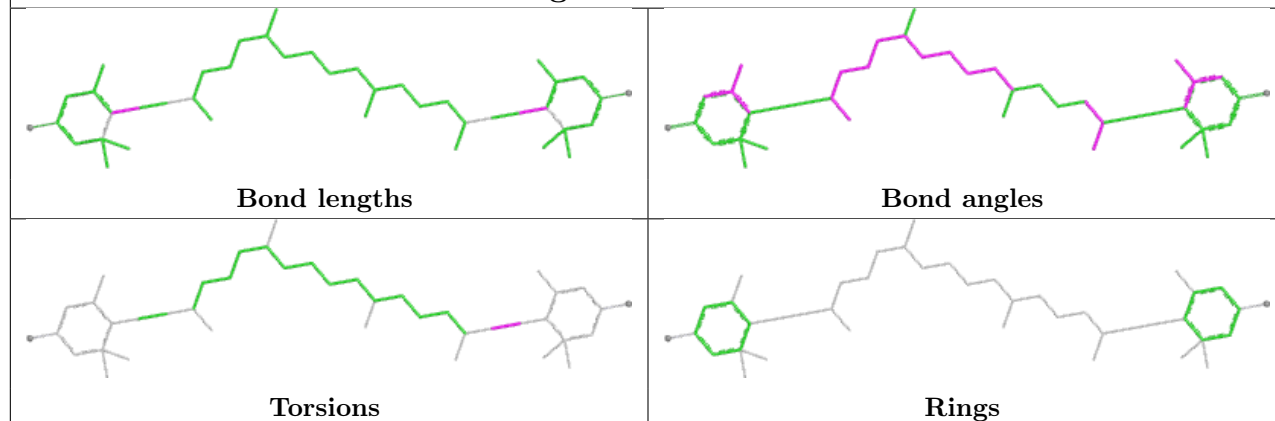
Ligand CLA c 503

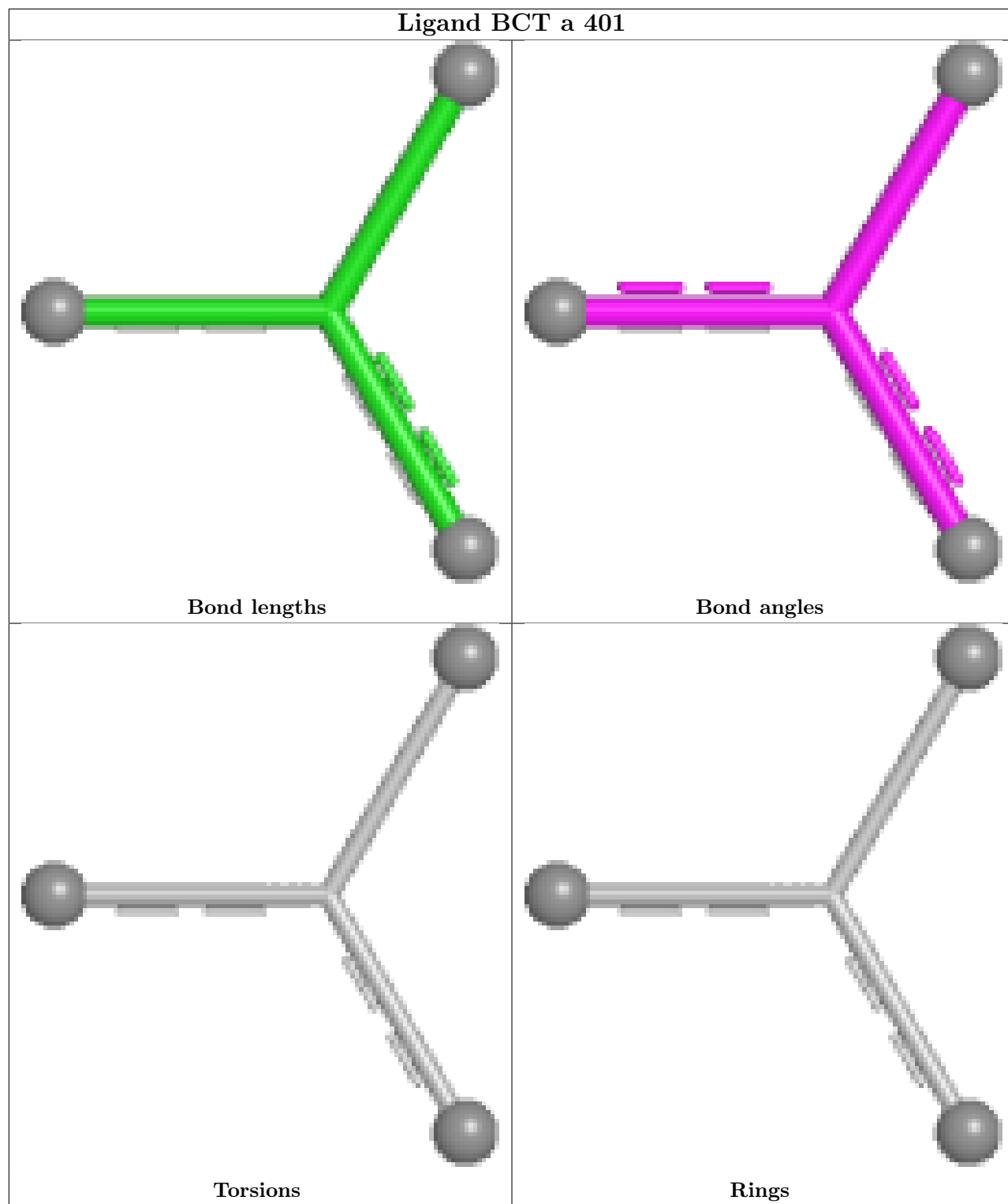


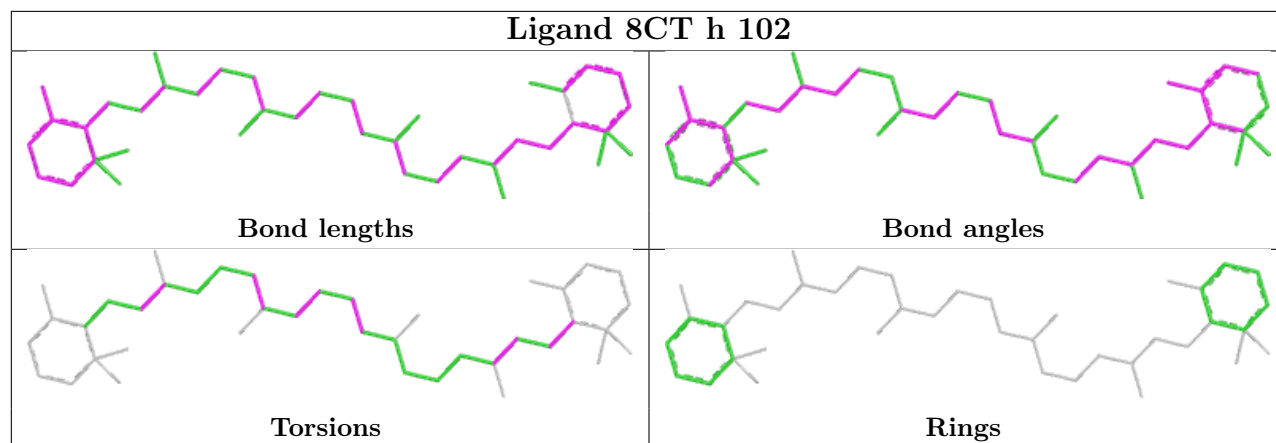
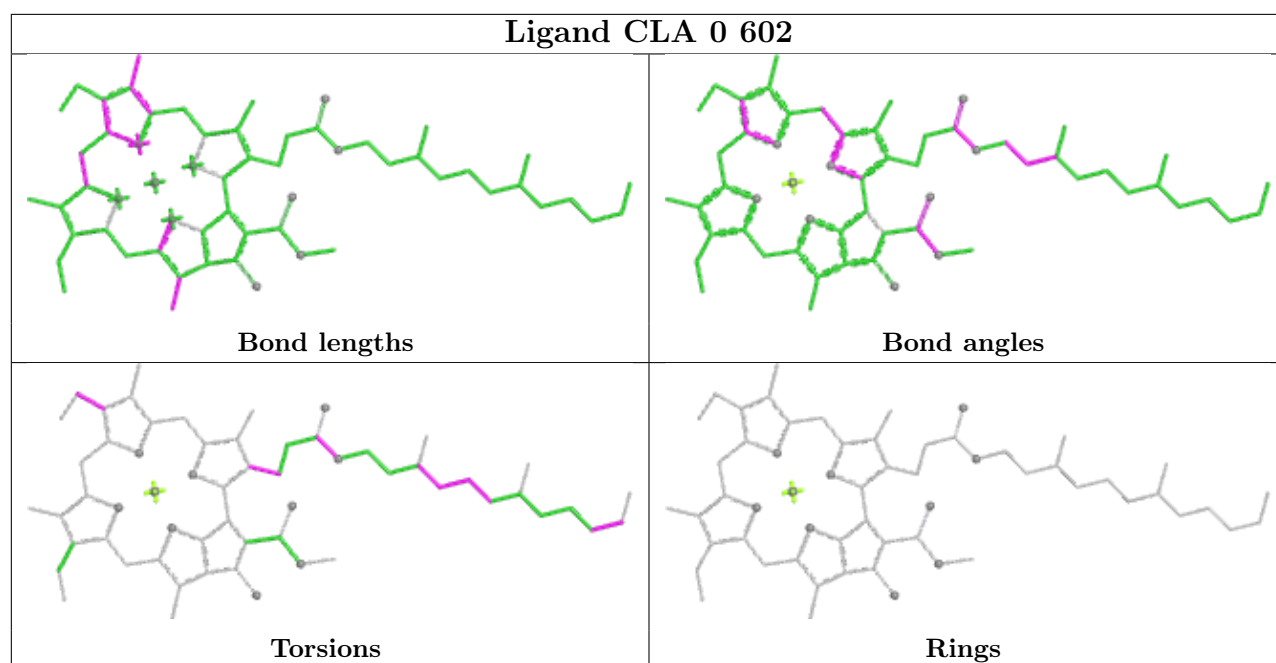
Ligand PL9 A 609



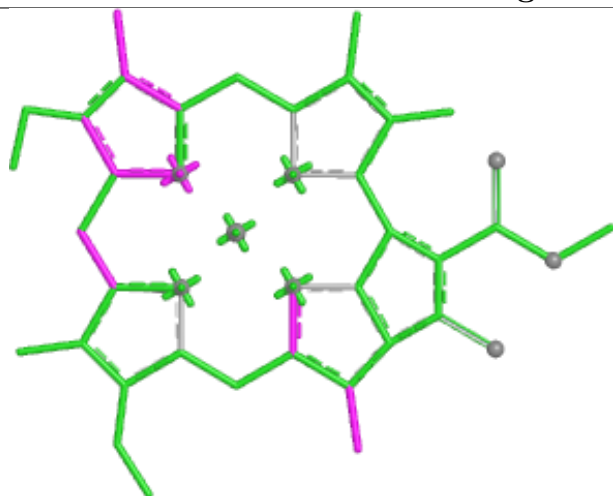
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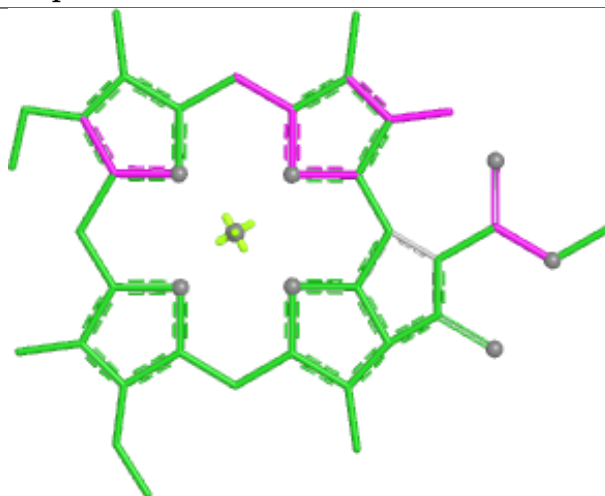




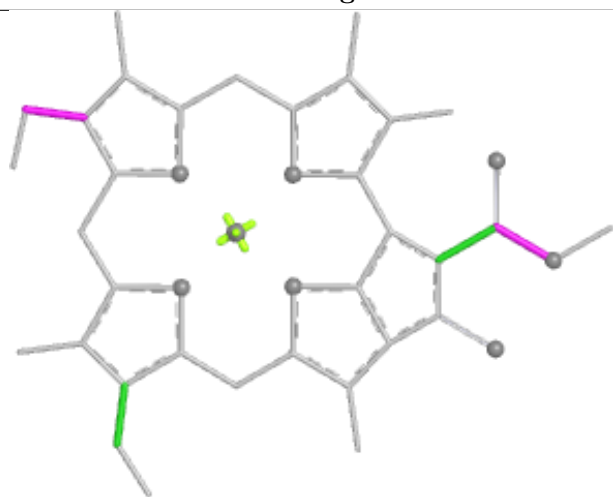
Ligand CLA p 310



Bond lengths



Bond angles

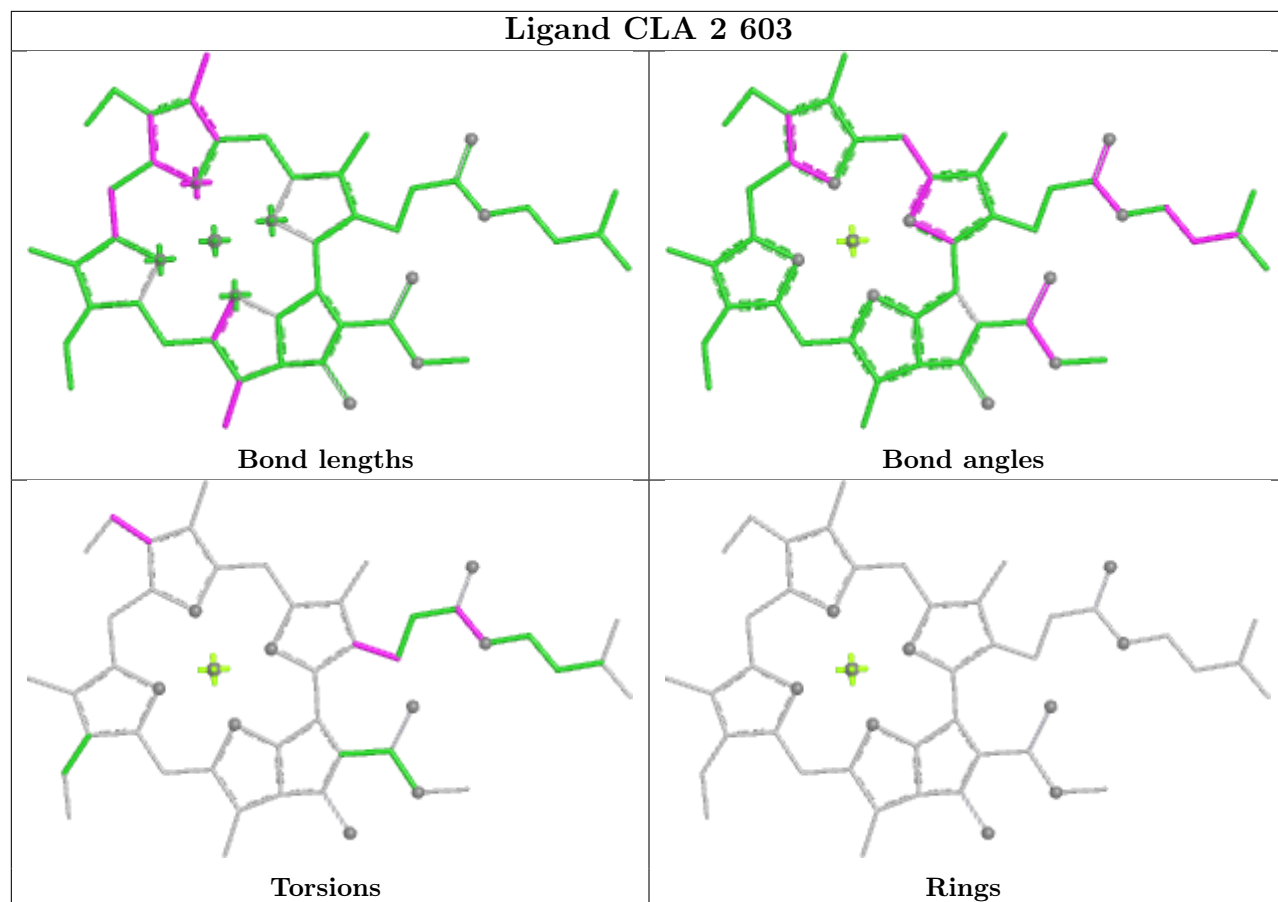


Torsions

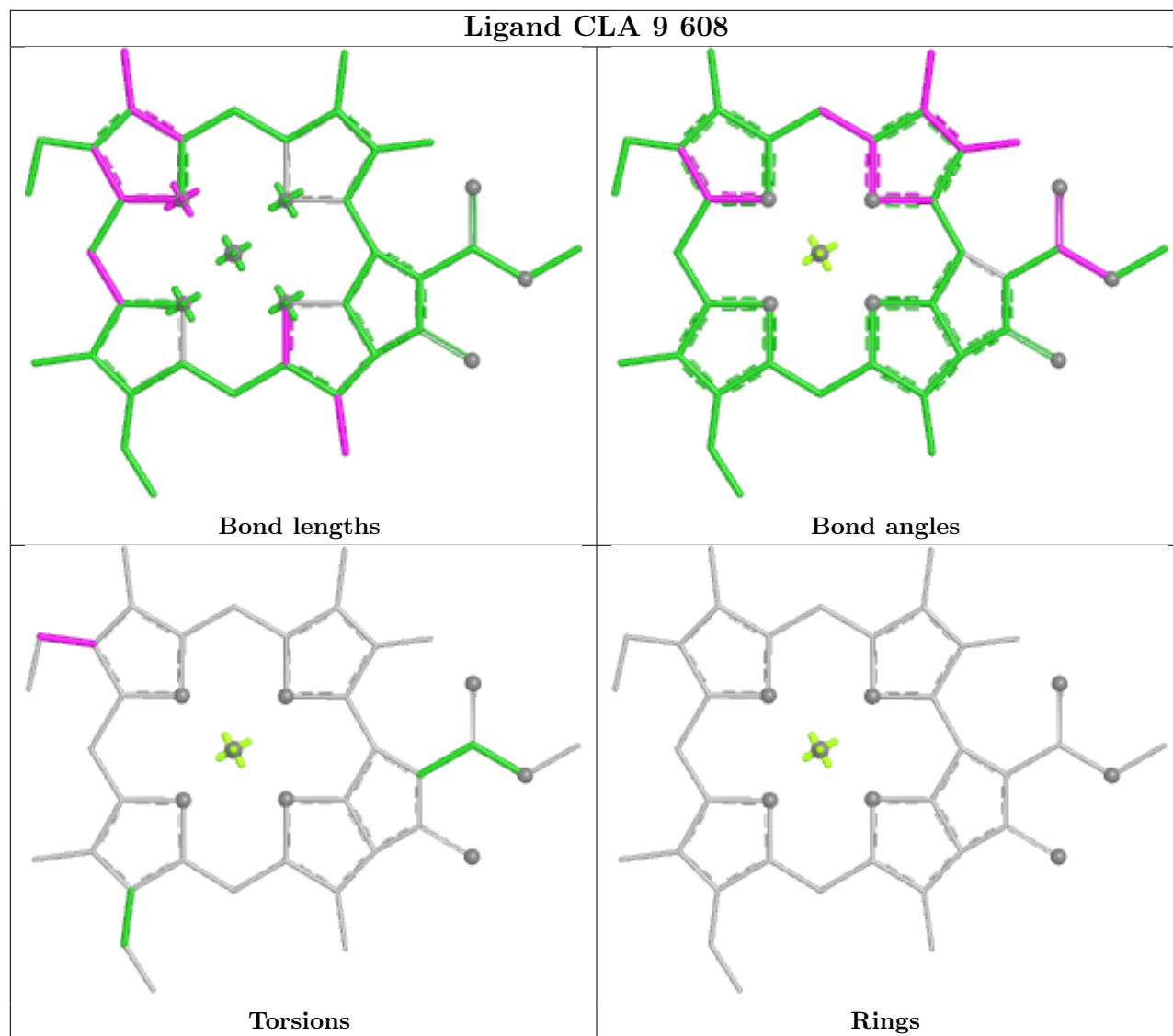


Rings

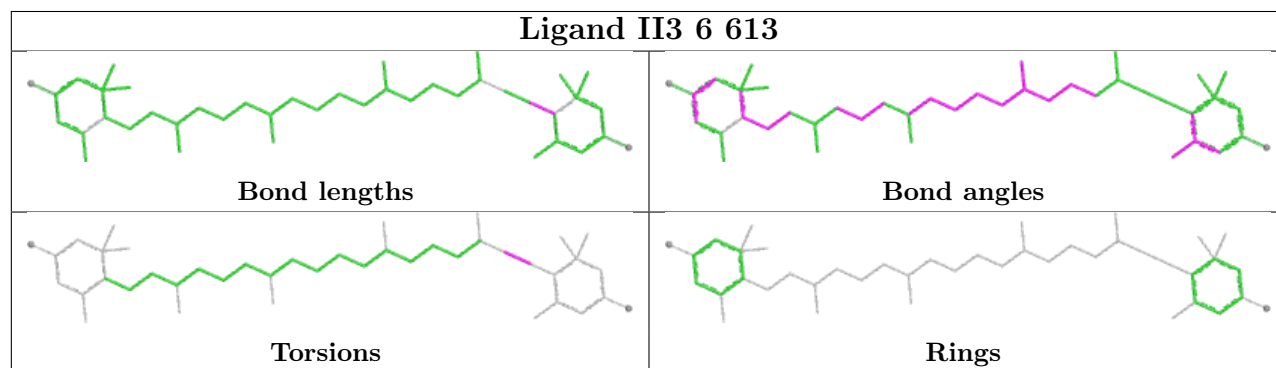
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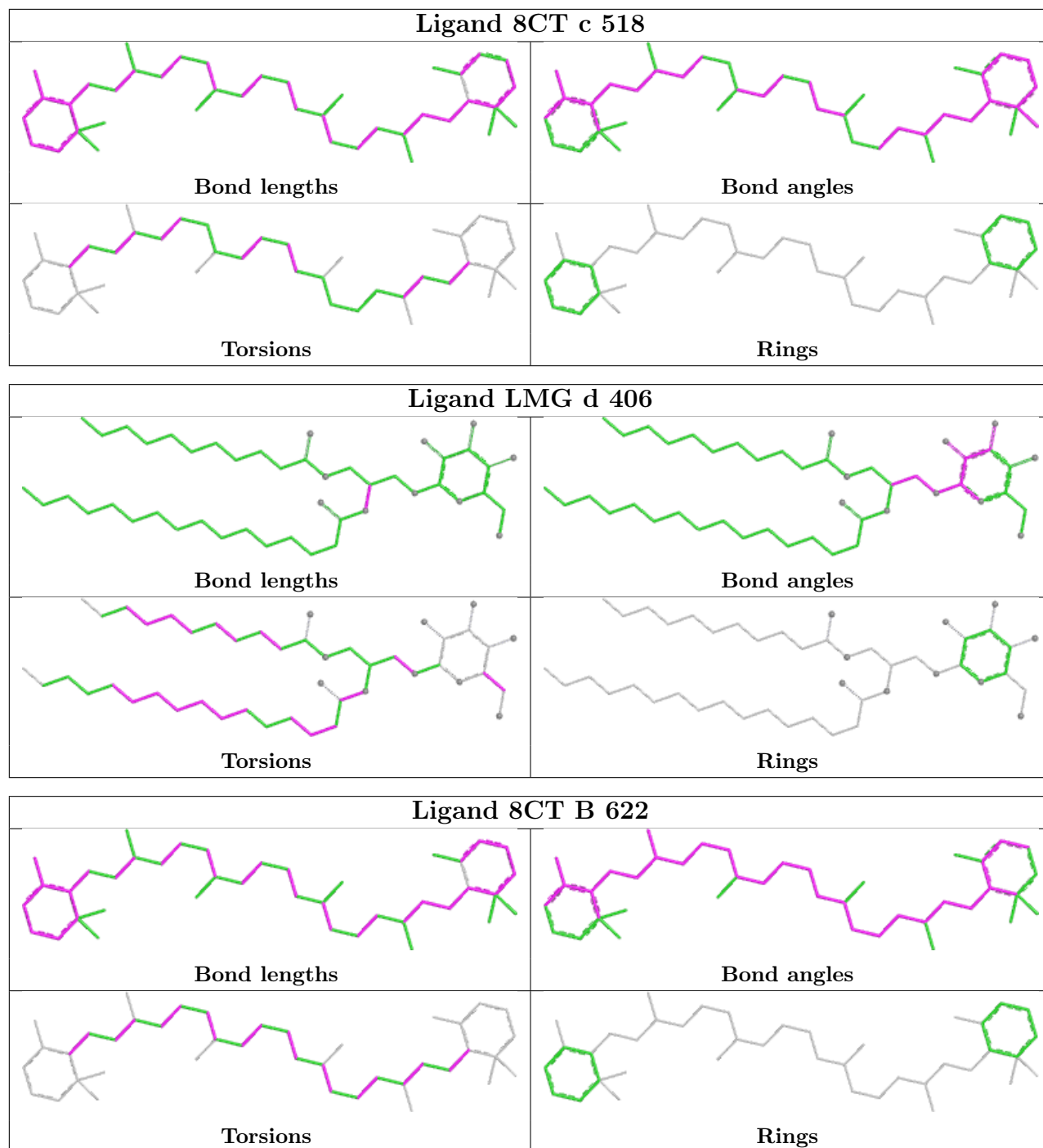


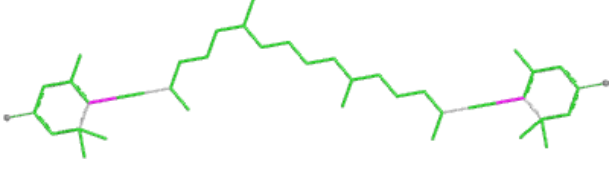
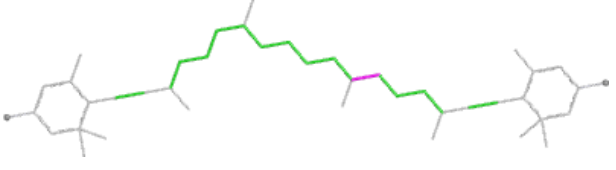
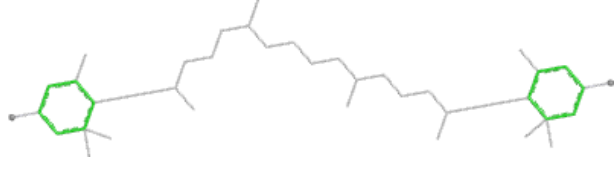
Ligand CLA 9 608

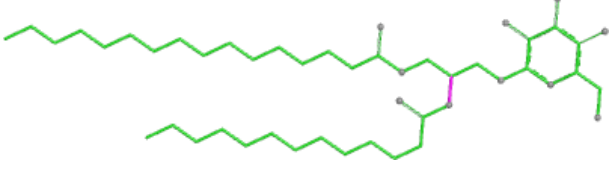
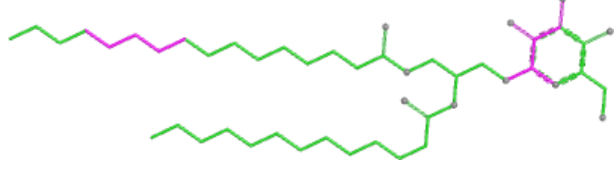
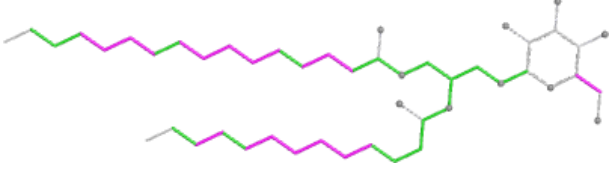
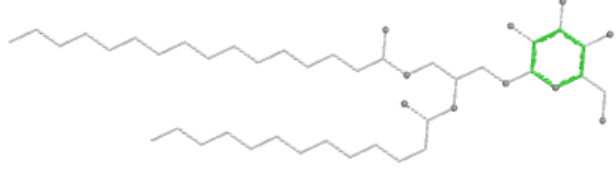


Ligand II3 6 613

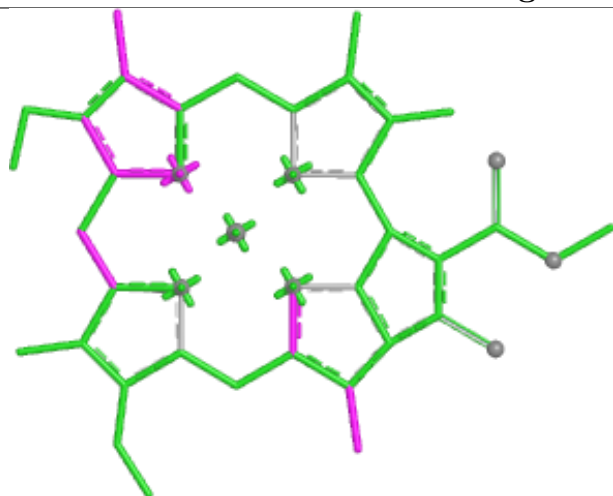




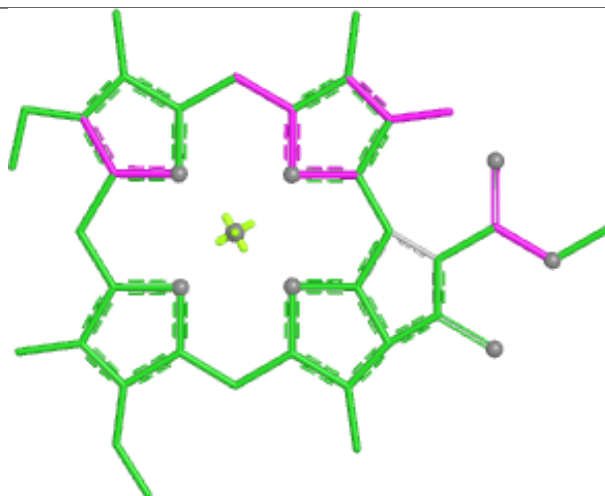
Ligand II0 8 615			
			
Bond lengths	Bond angles		
			
Torsions	Rings		

Ligand LMG A 607			
			
Bond lengths	Bond angles		
			
Torsions	Rings		

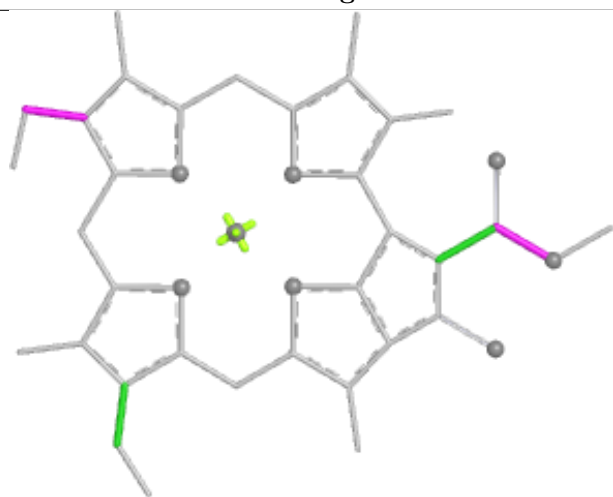
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Bond lengths



Bond angles

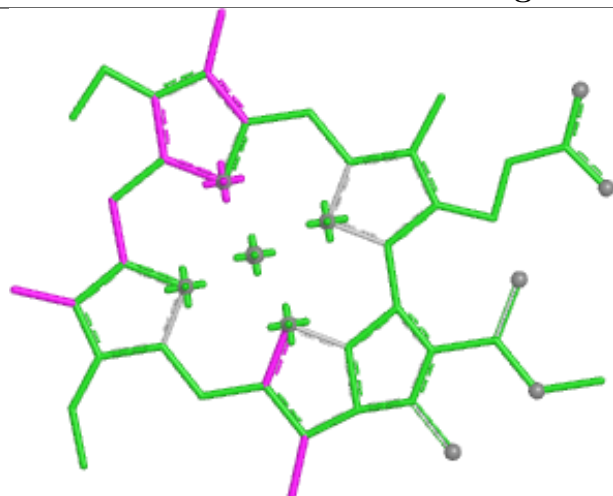


Torsions

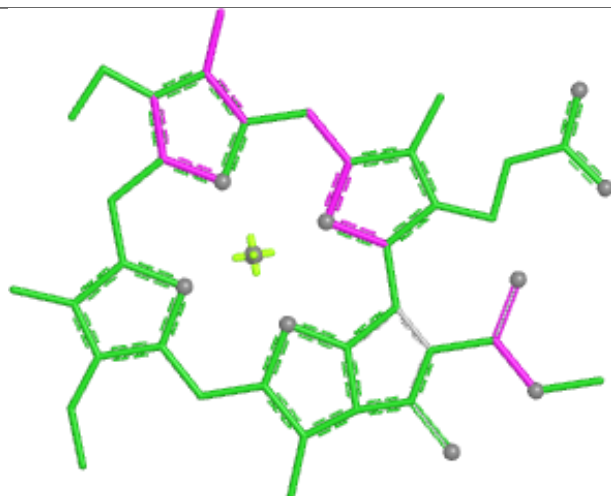


Rings

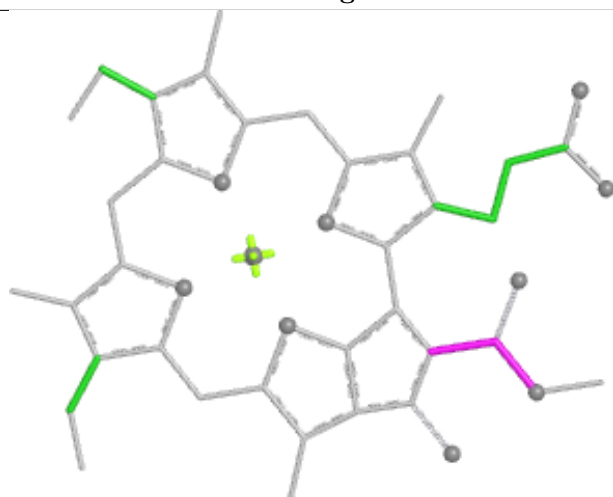
Ligand CLA C 506



Bond lengths



Bond angles

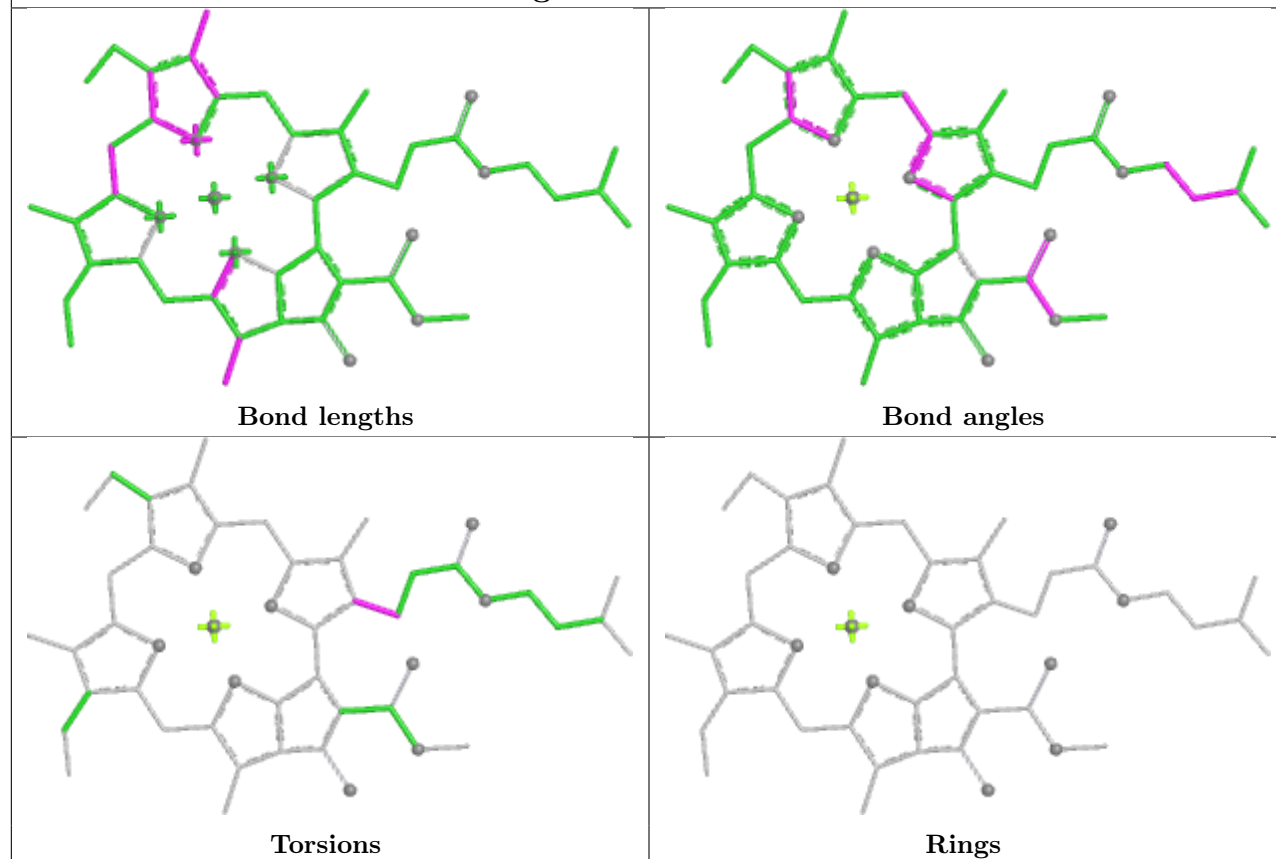


Torsions

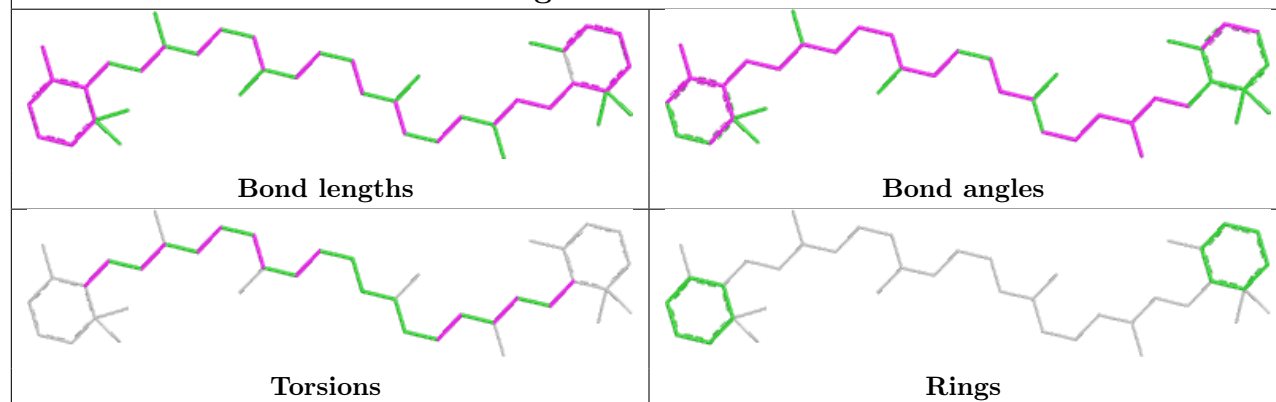


Rings

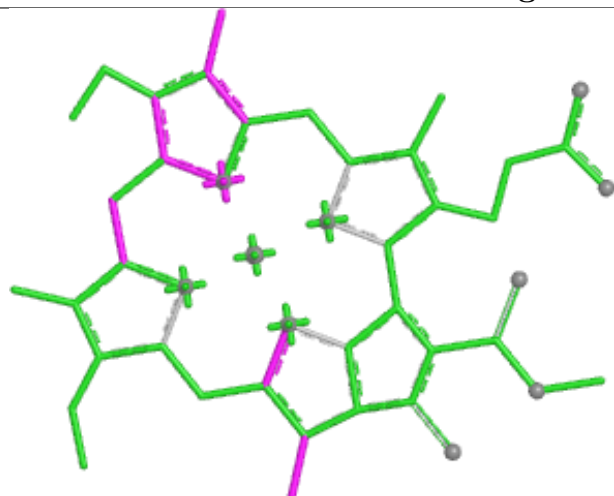
Ligand CLA P 603



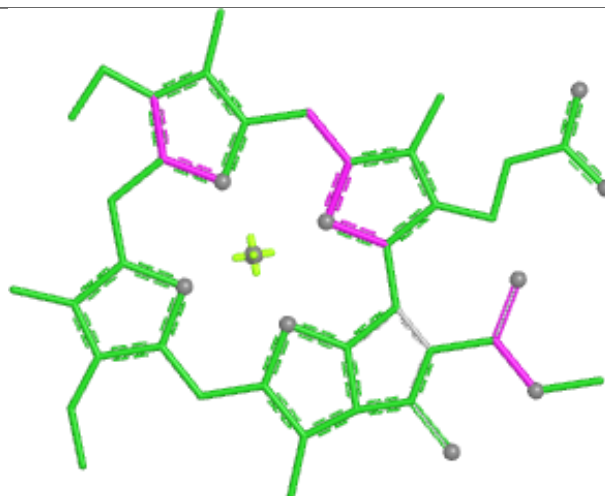
Ligand 8CT D 409



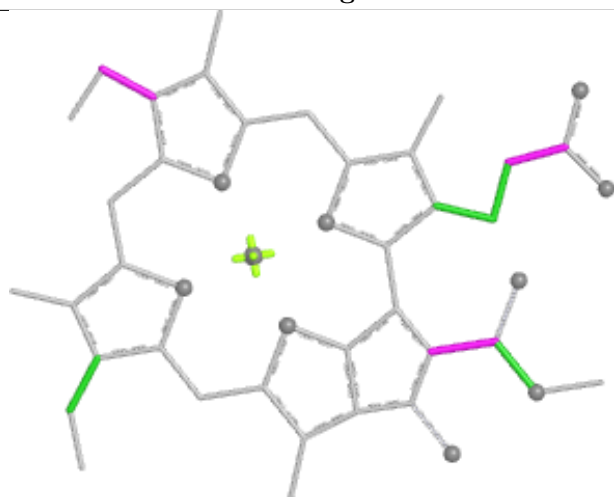
Ligand CLA 5 307



Bond lengths



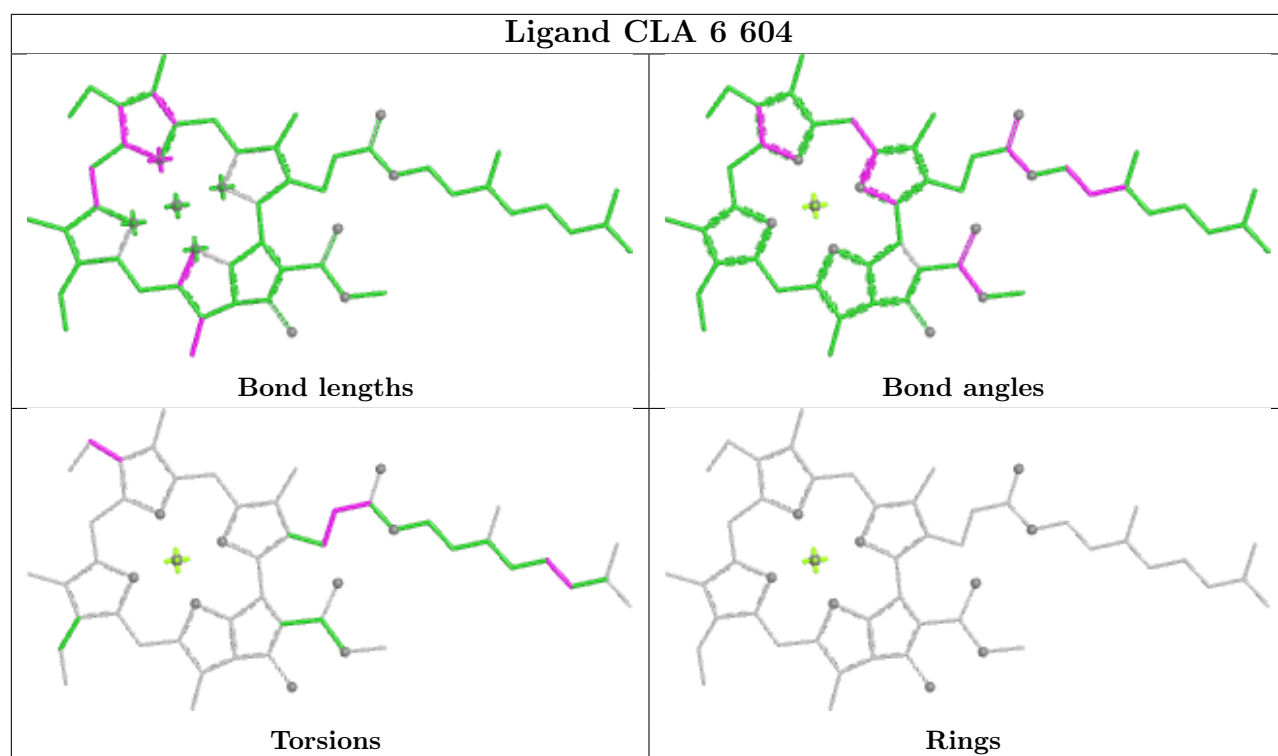
Bond angles



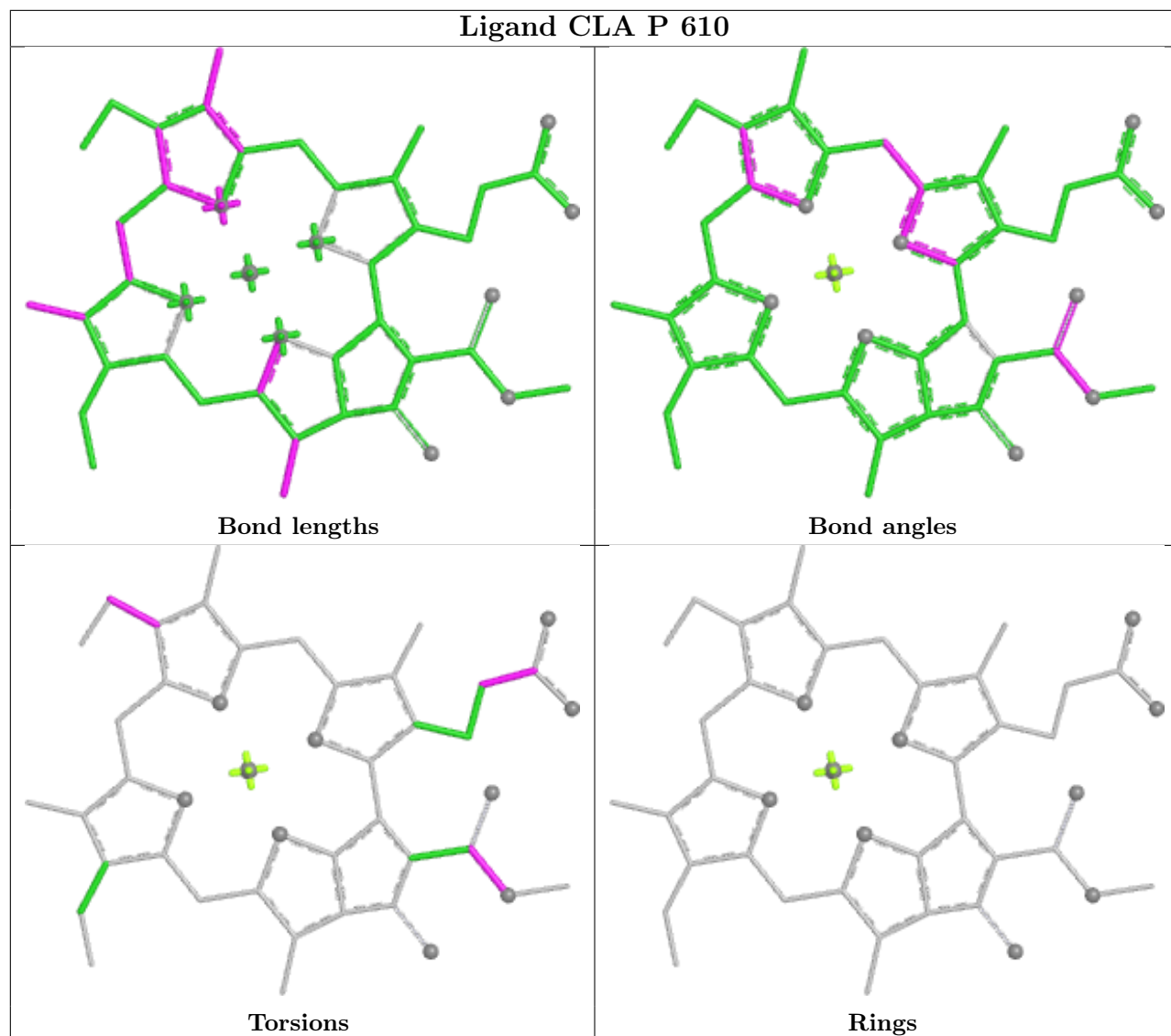
Torsions



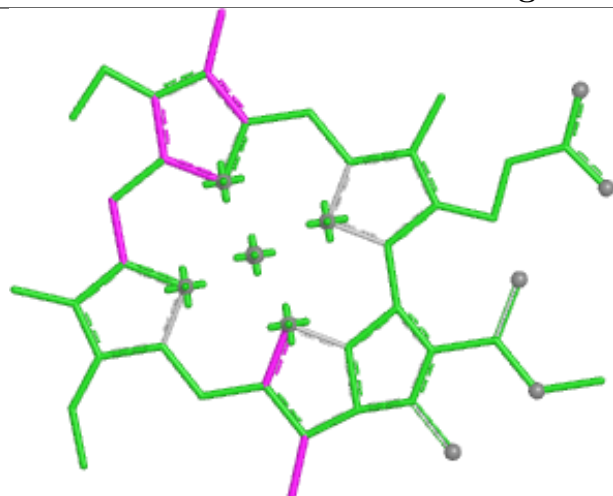
Rings



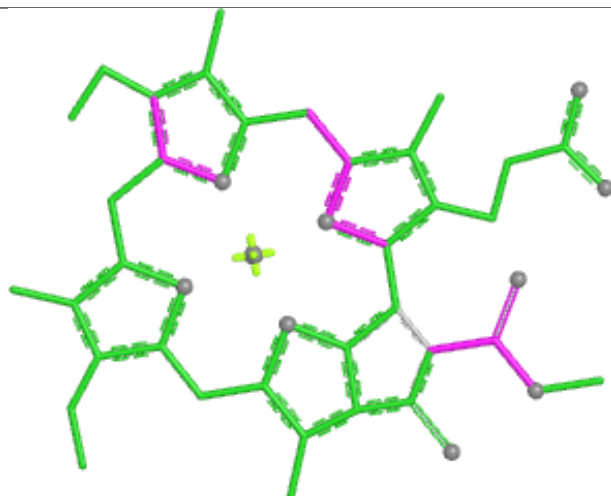
Ligand CLA P 610



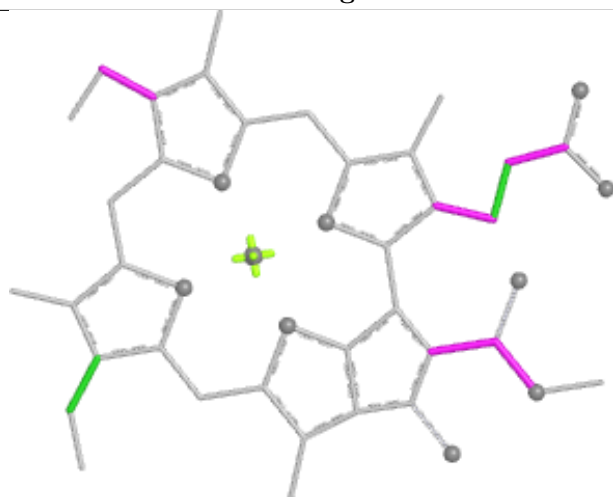
Ligand CLA 4 612



Bond lengths



Bond angles

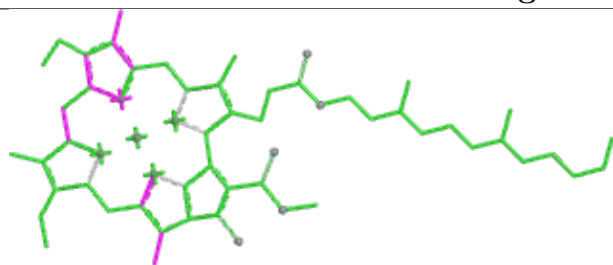


Torsions

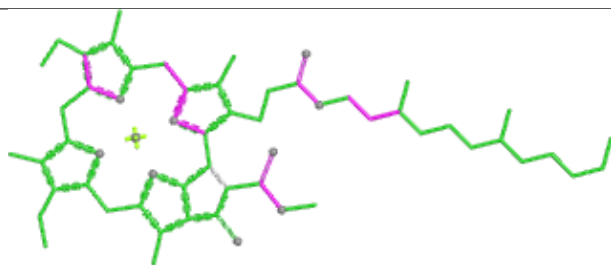


Rings

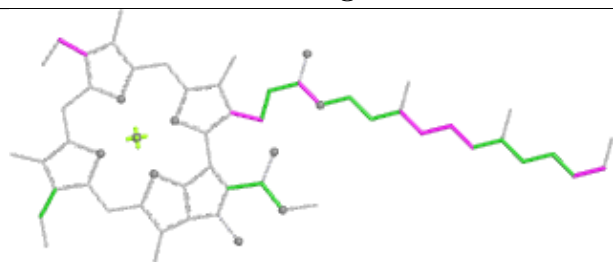
Ligand CLA 4 602



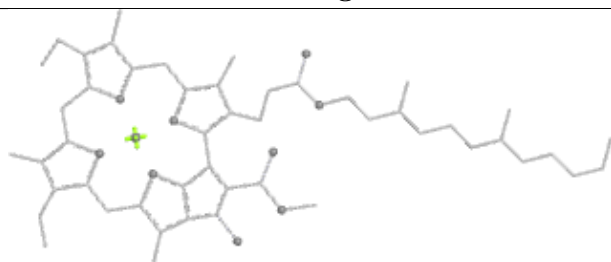
Bond lengths



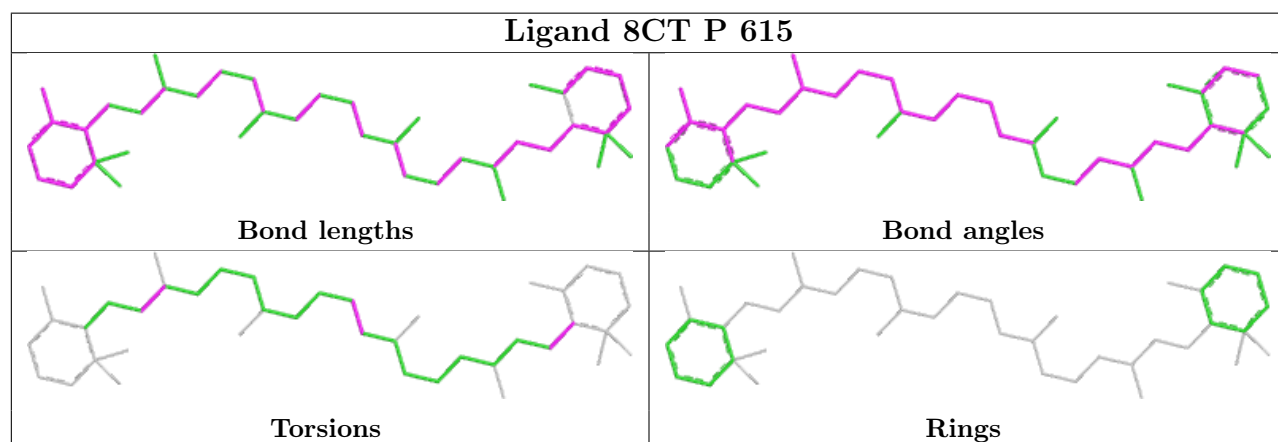
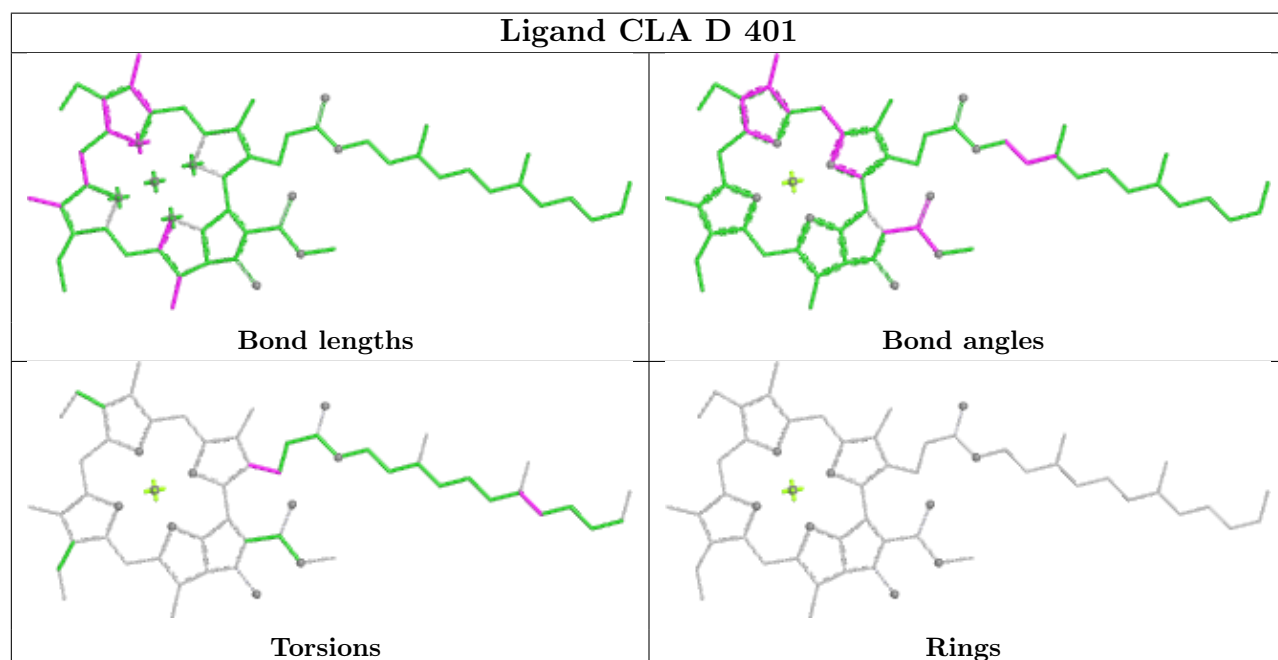
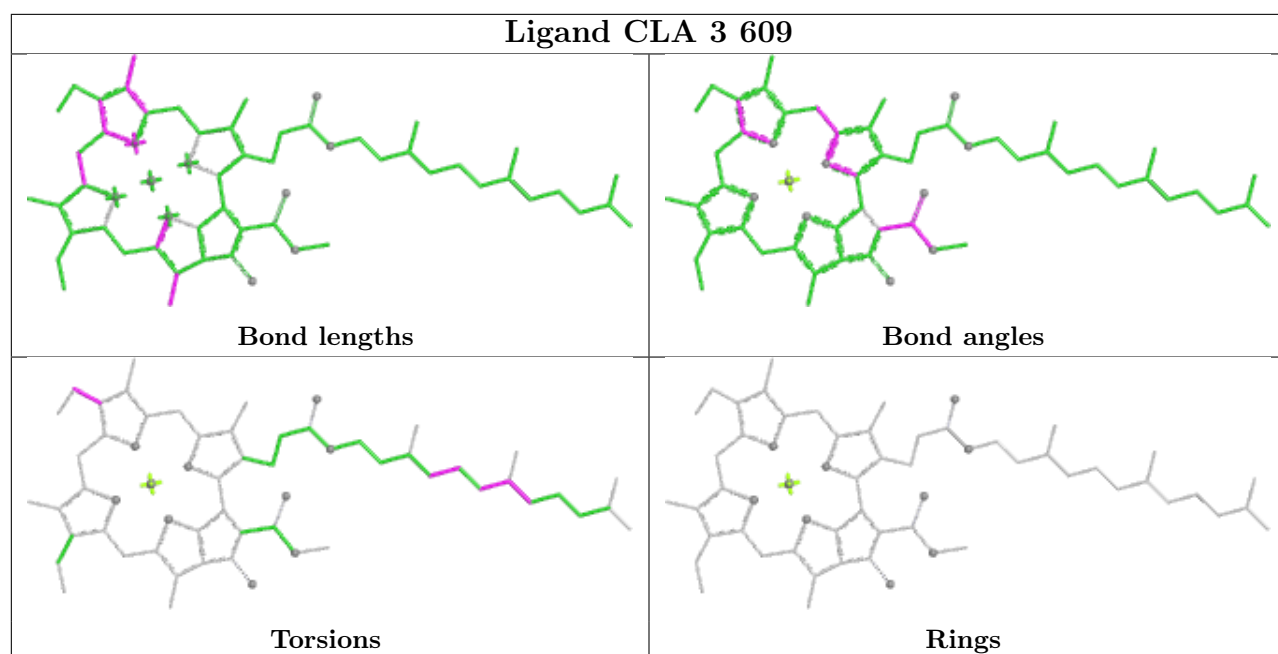
Bond angles

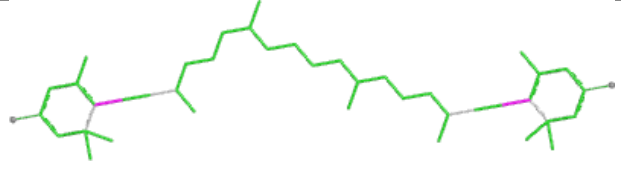
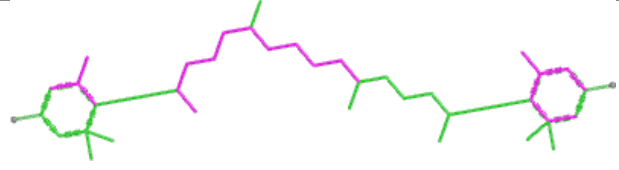
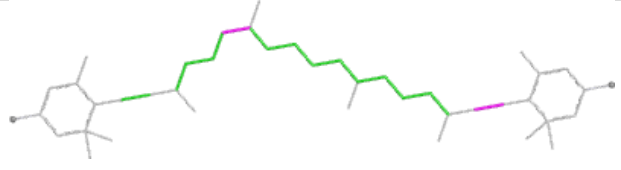
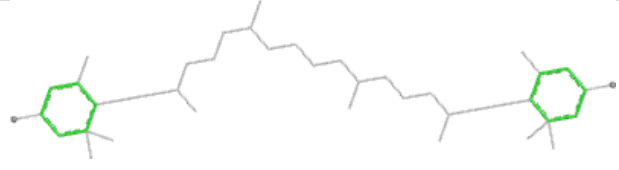


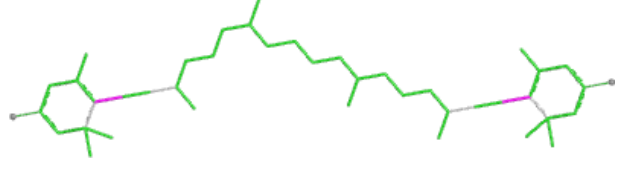
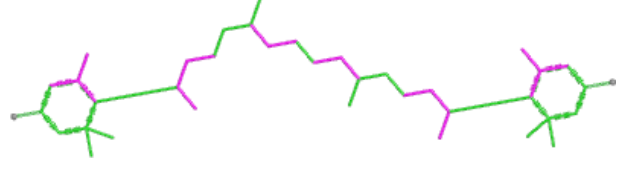
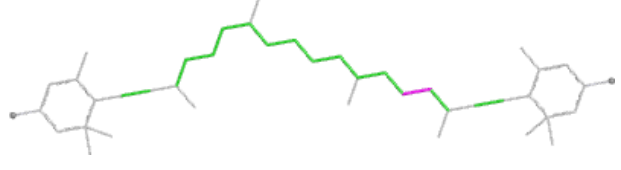
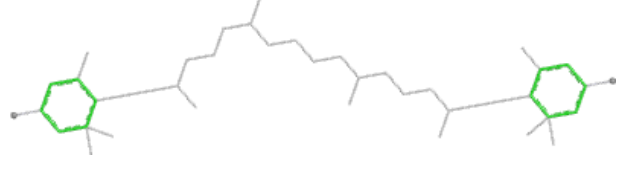
Torsions

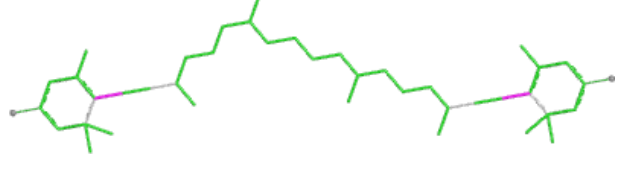
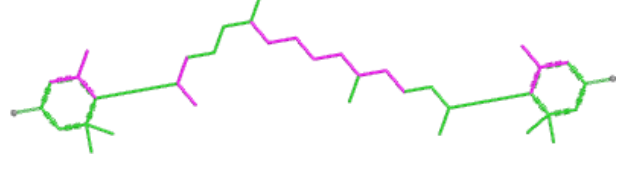
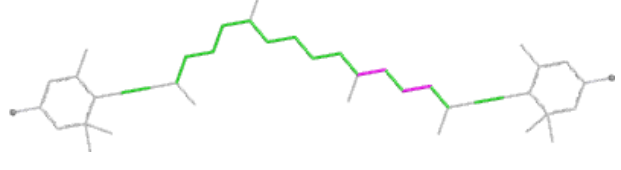
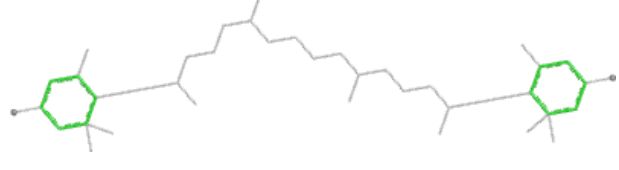


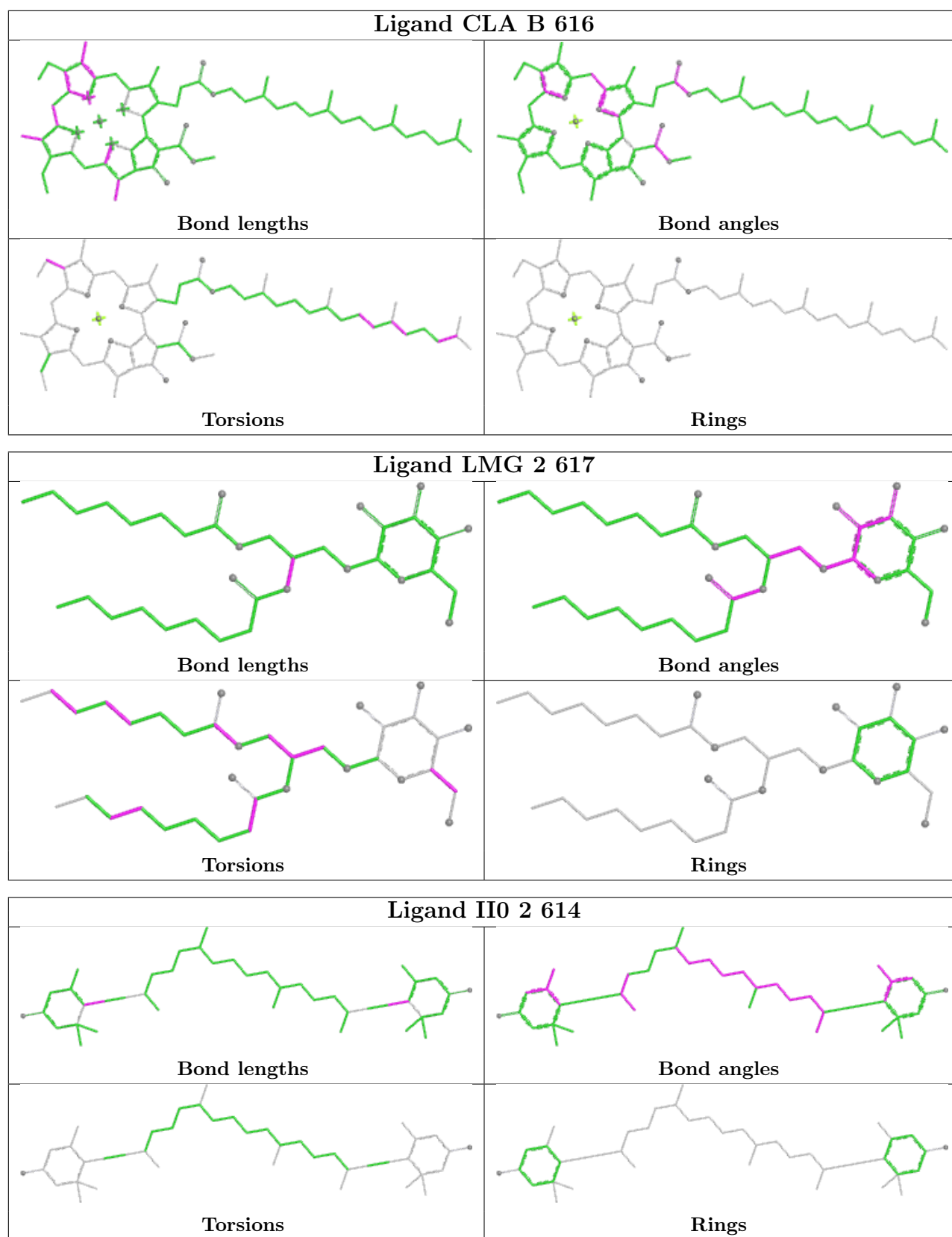
Rings



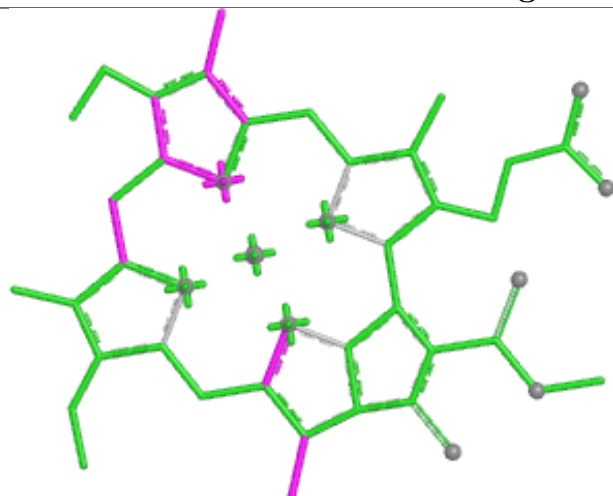
Ligand II0 9 614	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand II0 8 619	
	
Bond lengths	Bond angles
	
Torsions	Rings

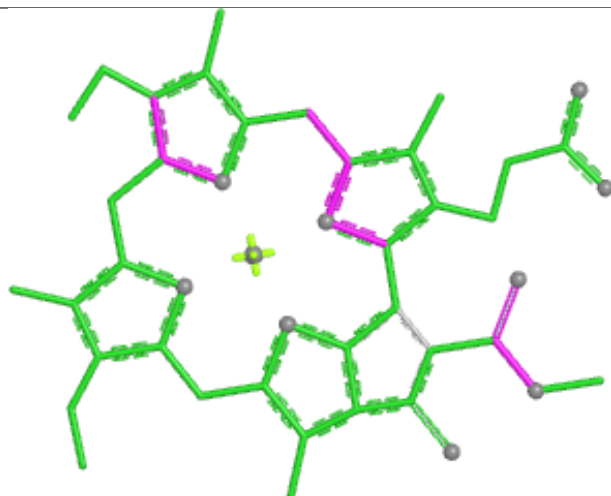
Ligand II0 p 316	
	
Bond lengths	Bond angles
	
Torsions	Rings



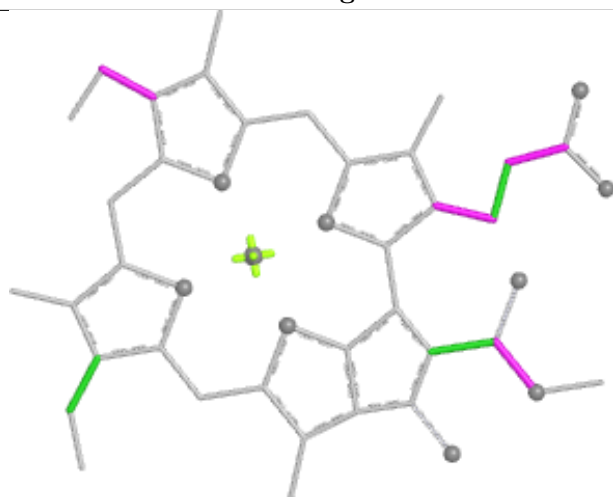
Ligand CLA 8 612



Bond lengths



Bond angles

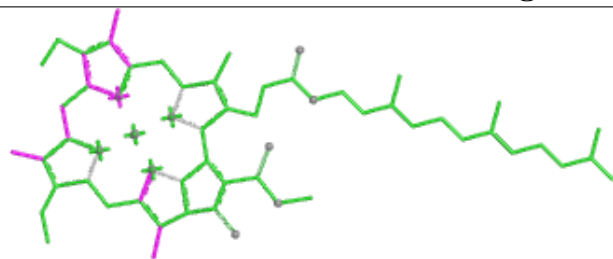


Torsions

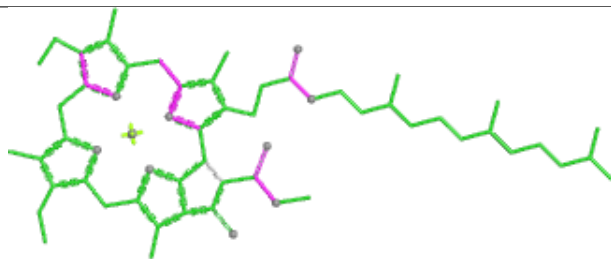


Rings

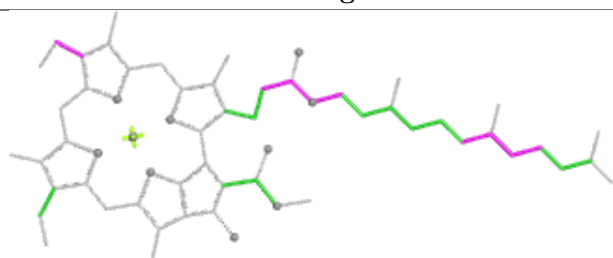
Ligand CLA 8 605



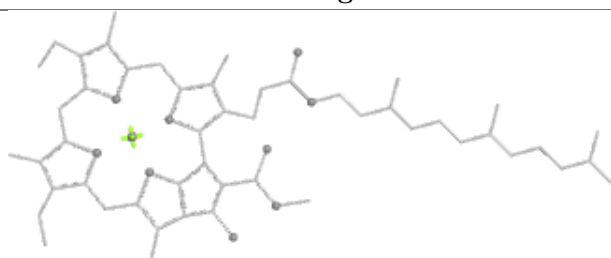
Bond lengths



Bond angles

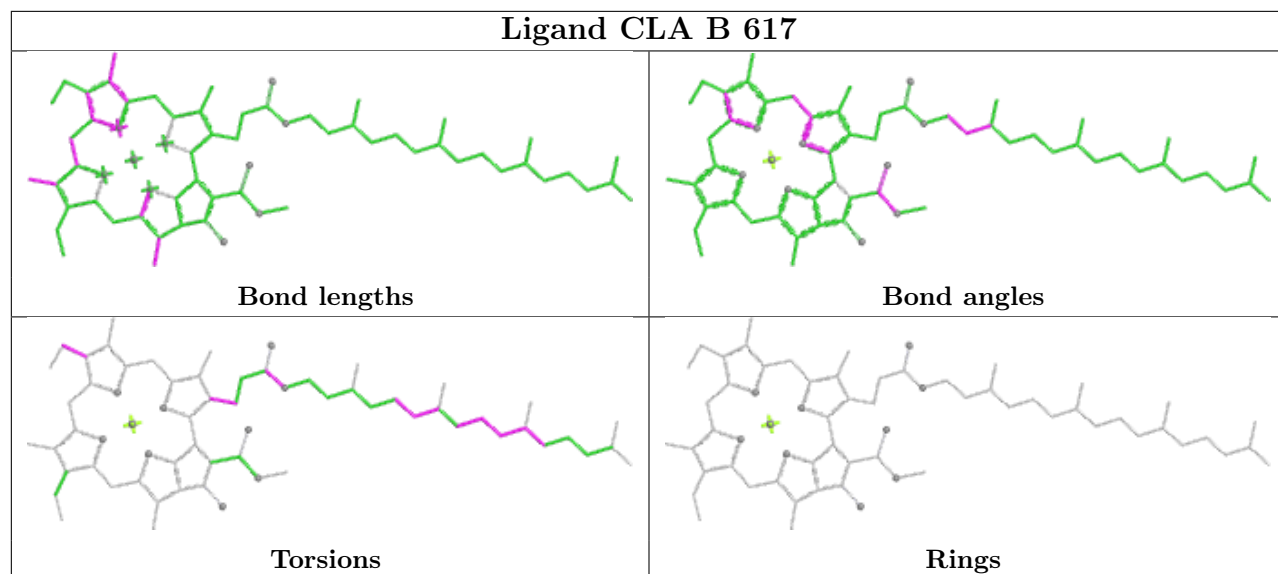


Torsions

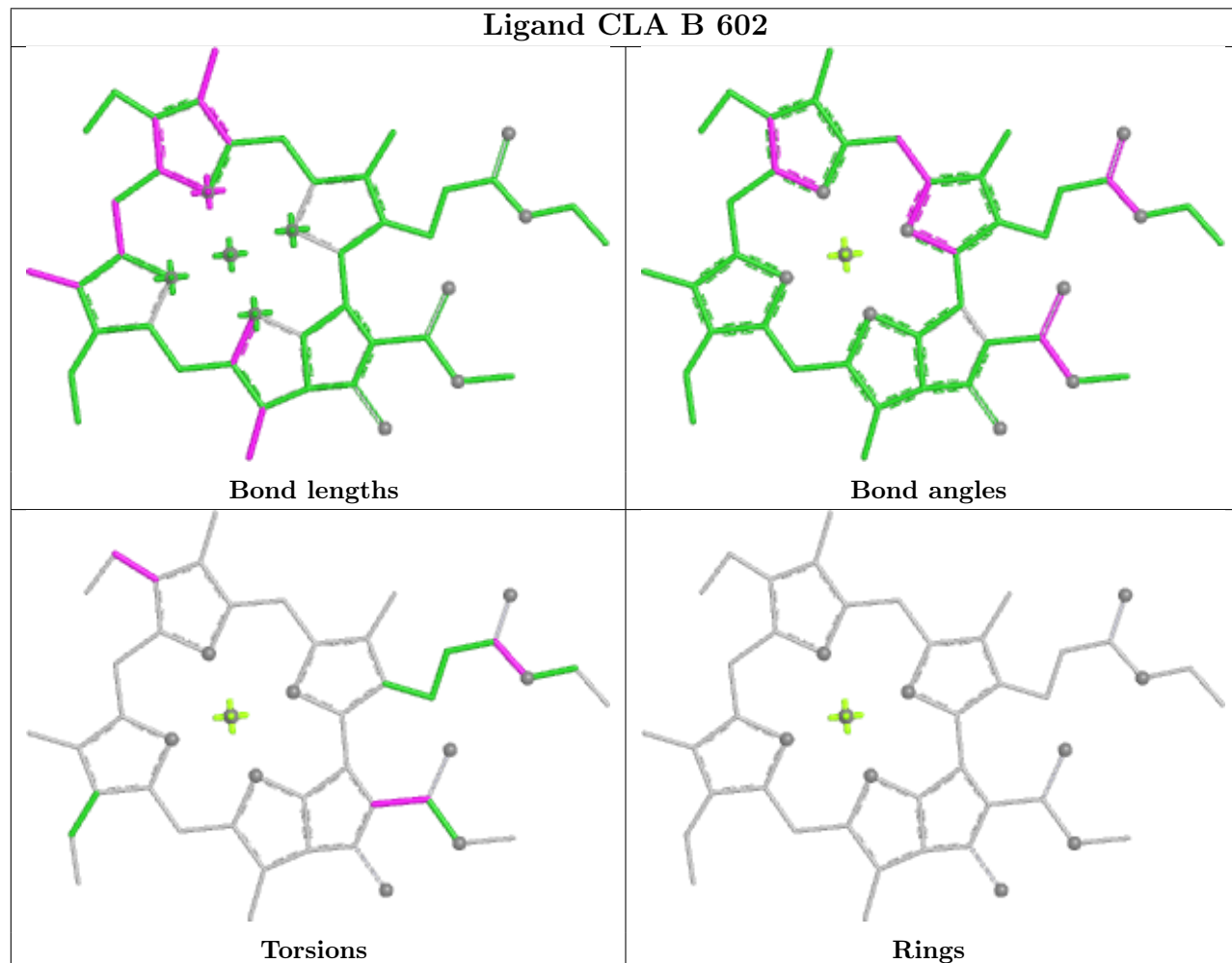


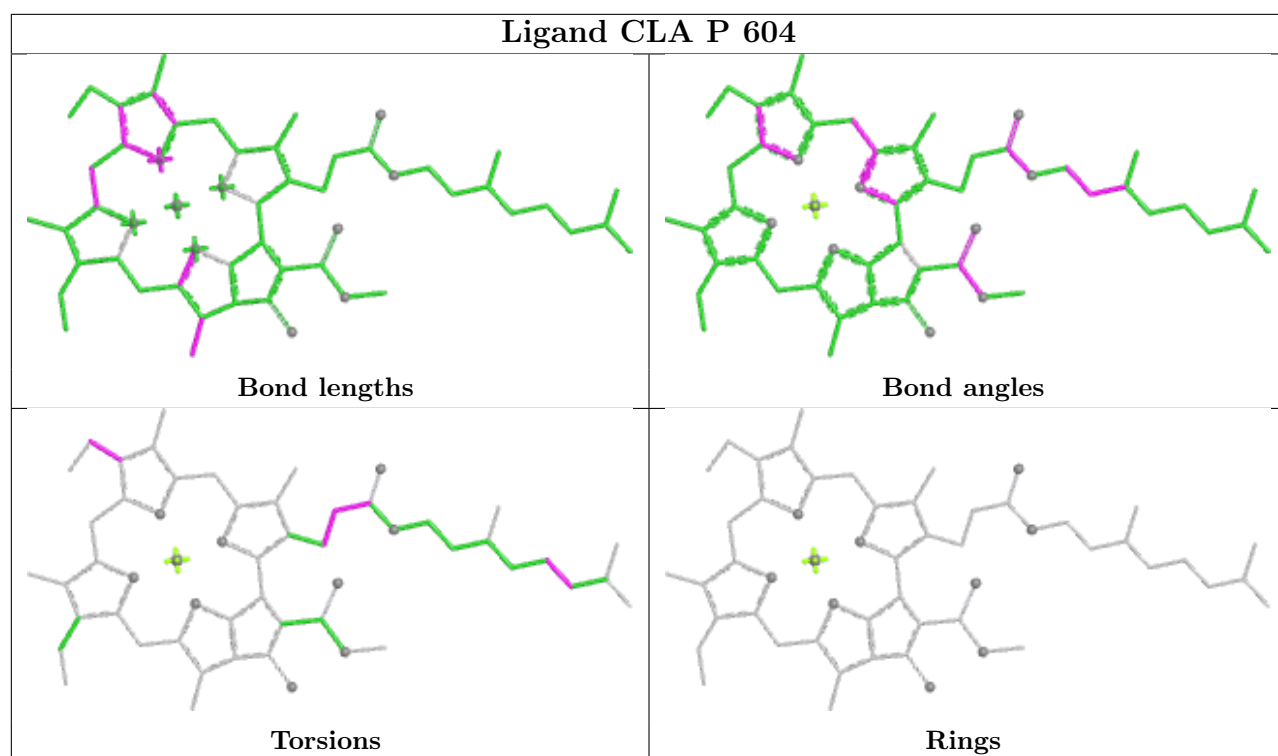
Rings

Ligand CLA B 617

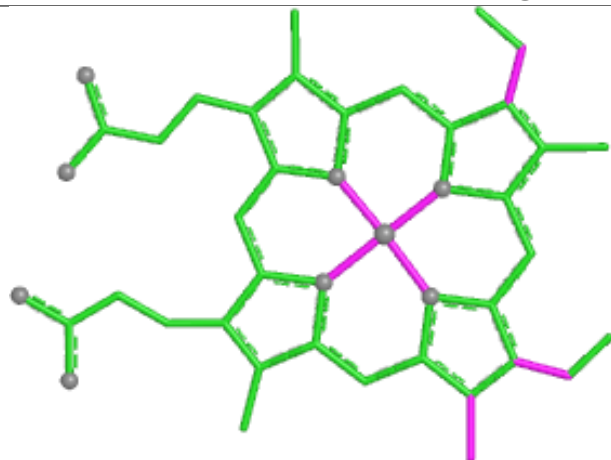


Ligand CLA B 602

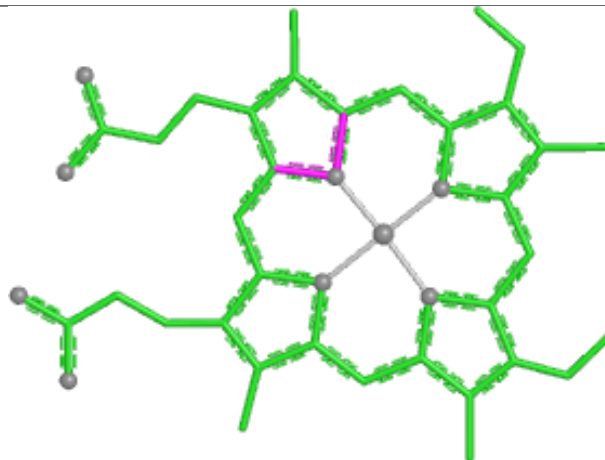




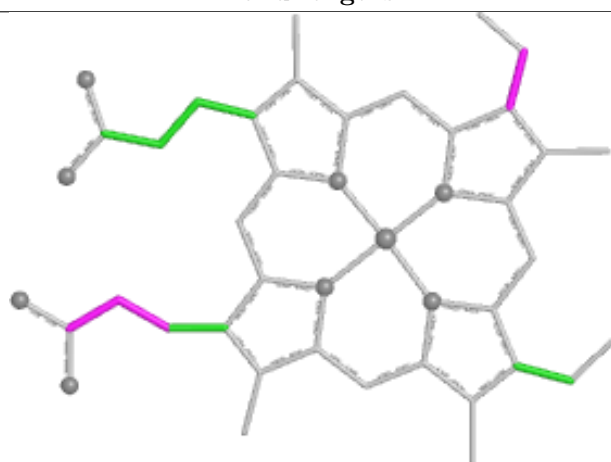
Ligand HEM f 101



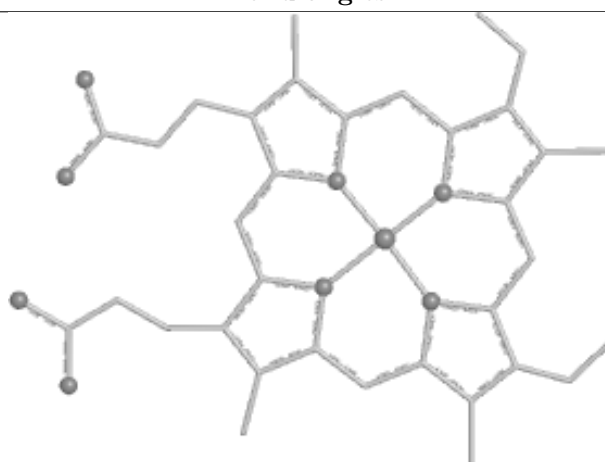
Bond lengths



Bond angles

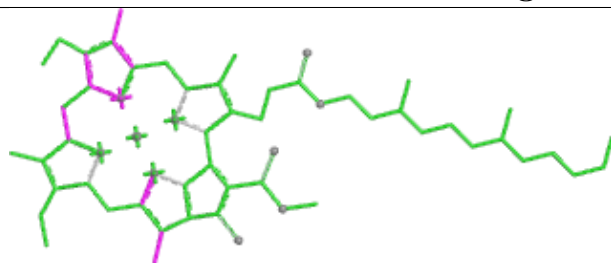


Torsions

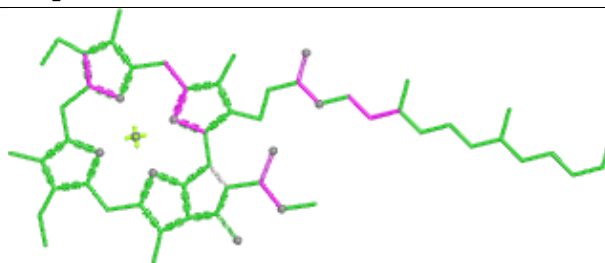


Rings

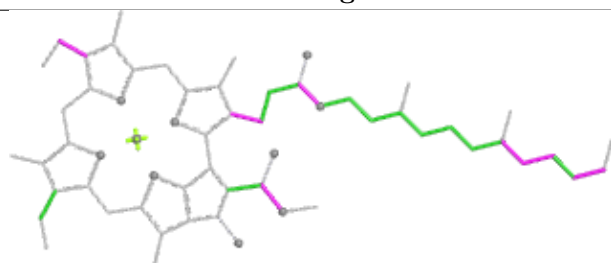
Ligand CLA p 303



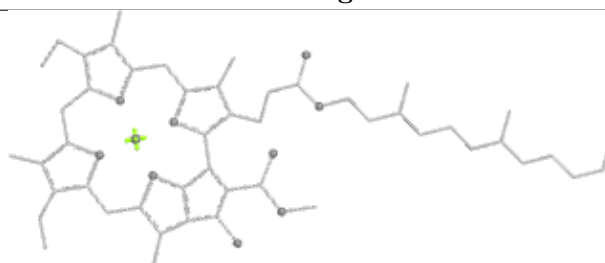
Bond lengths



Bond angles

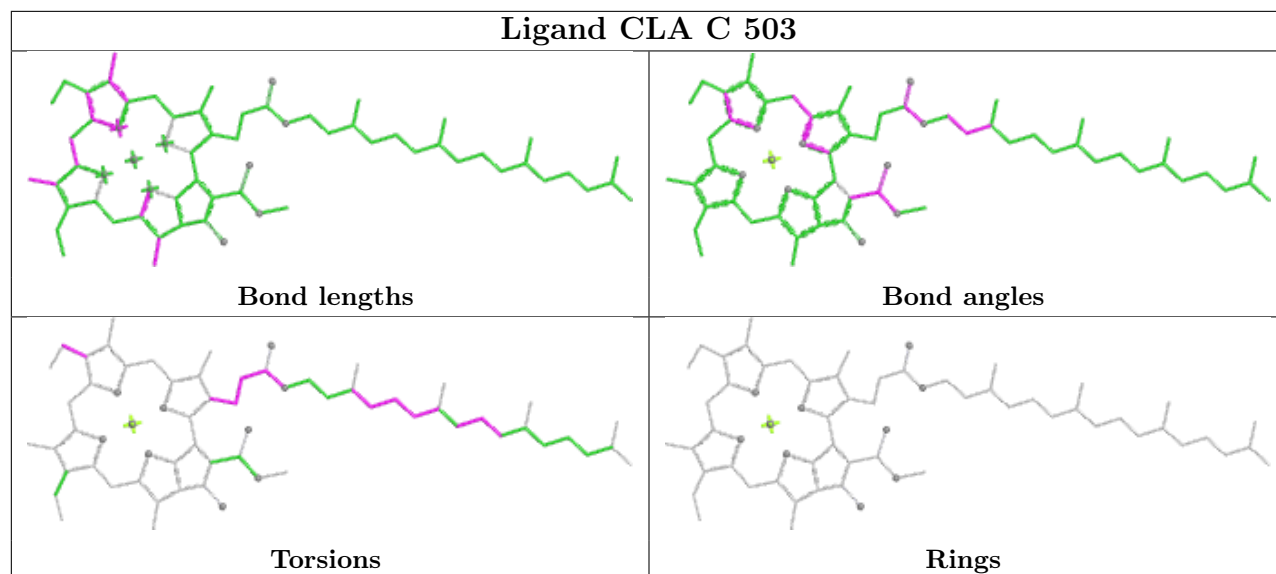


Torsions

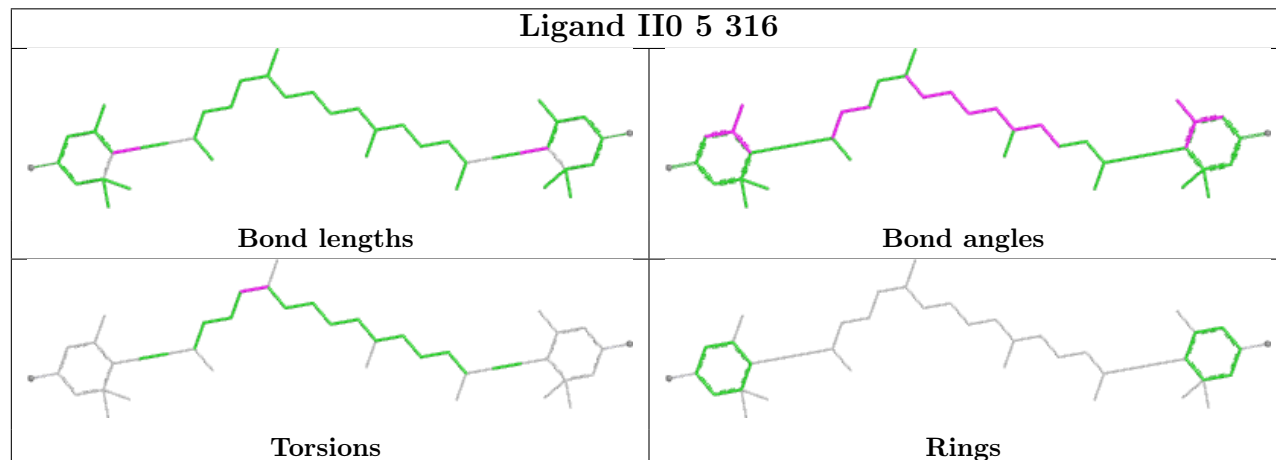


Rings

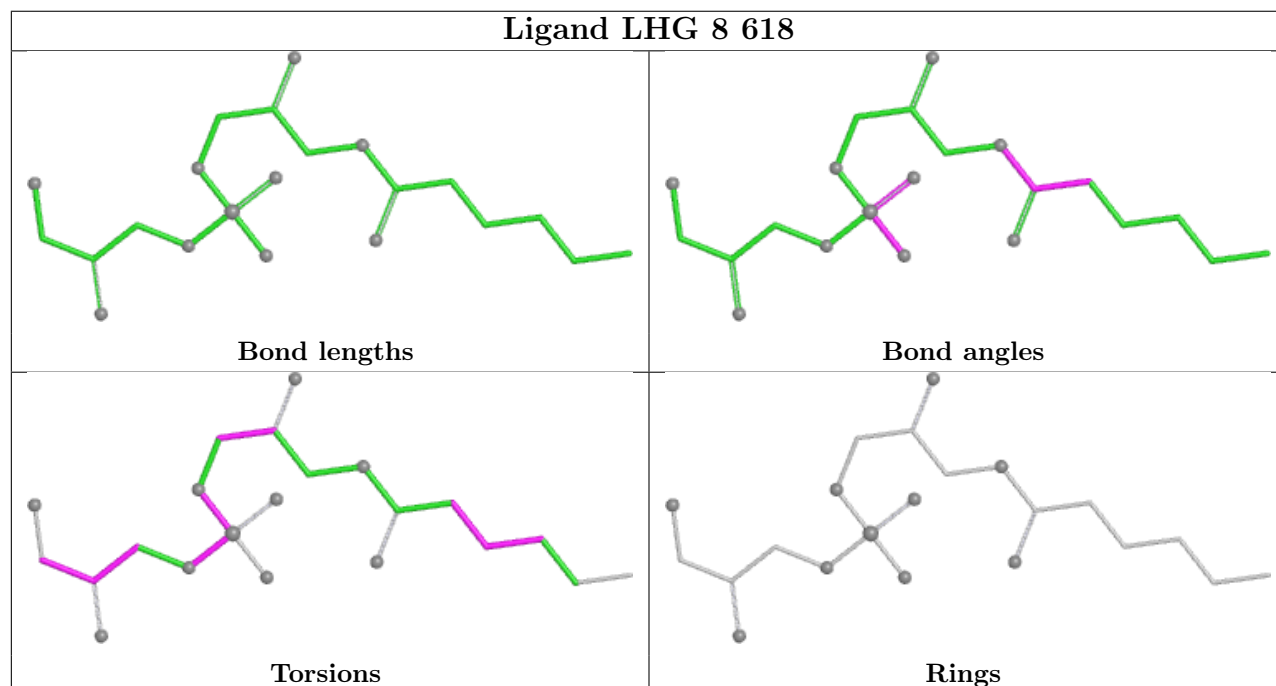
Ligand CLA C 503

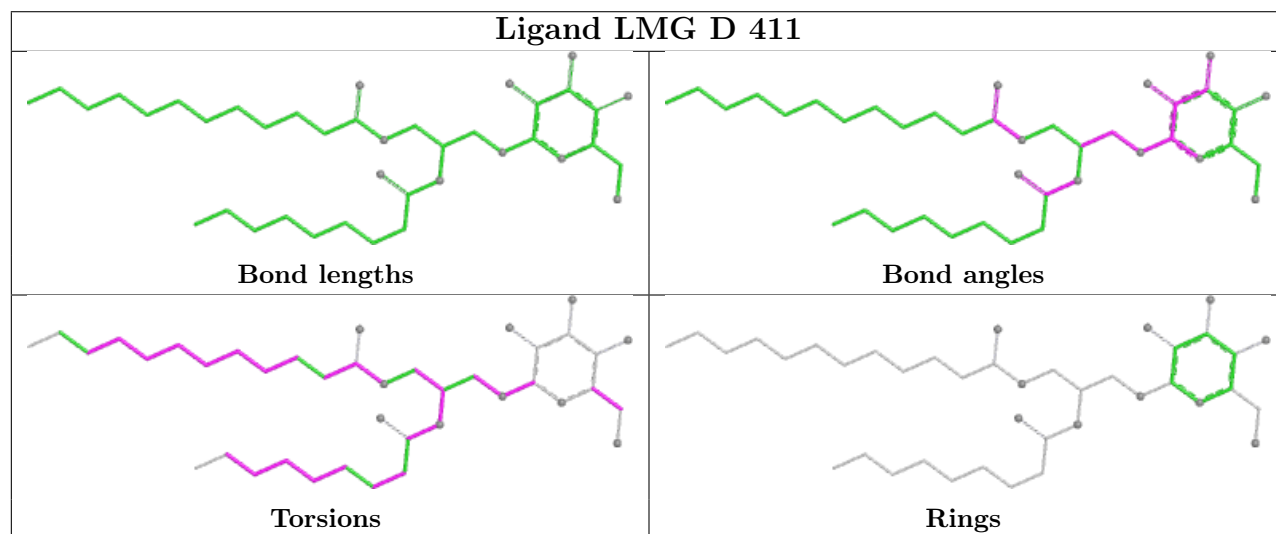
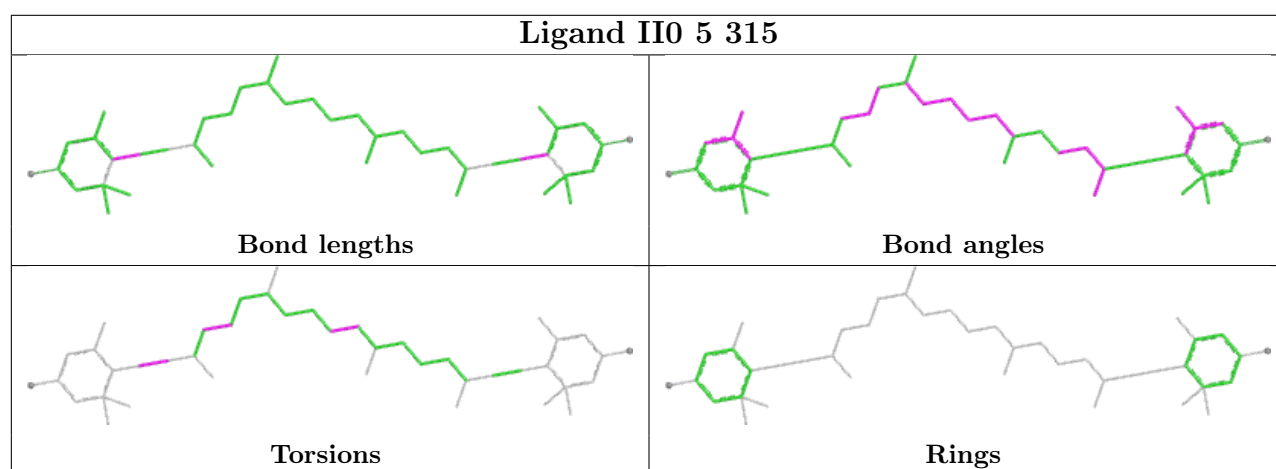
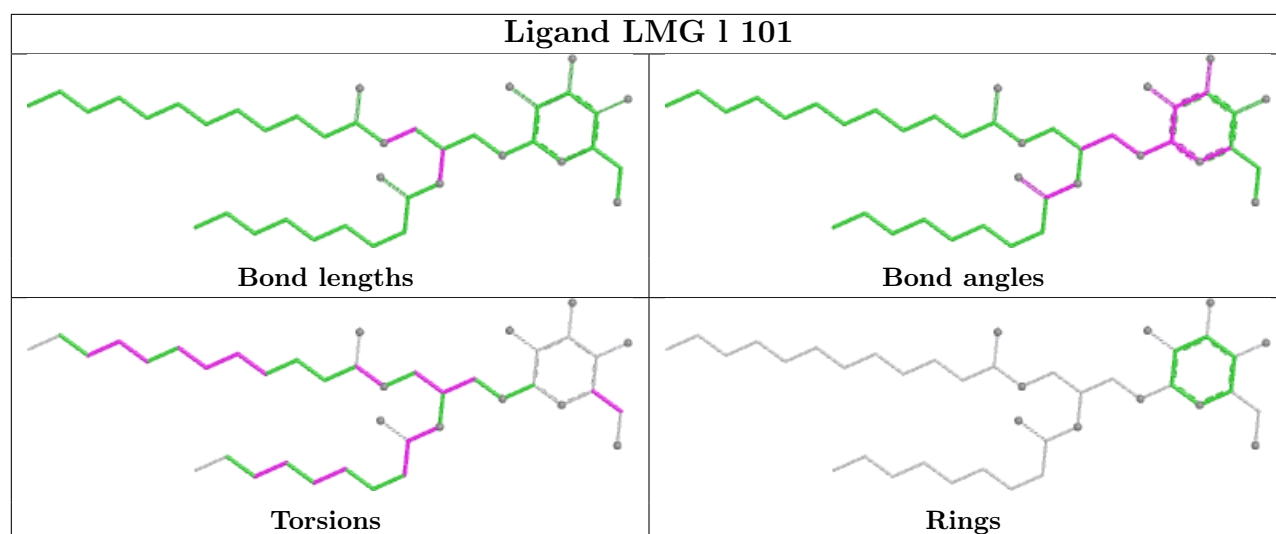


Ligand II0 5 316

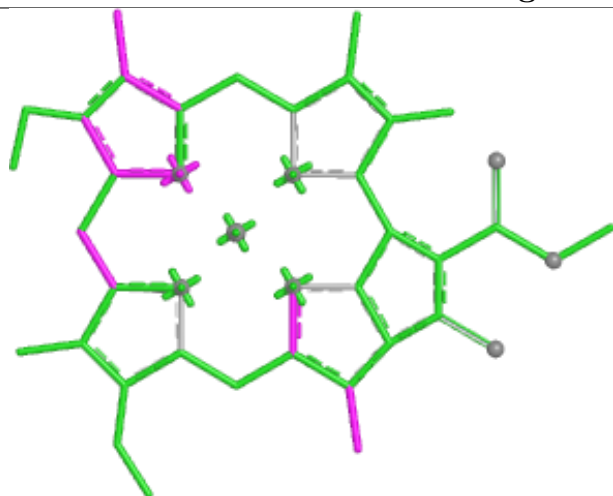


Ligand LHG 8 618

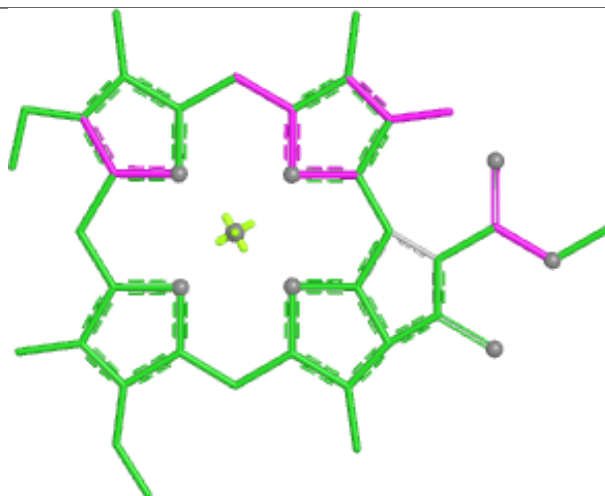




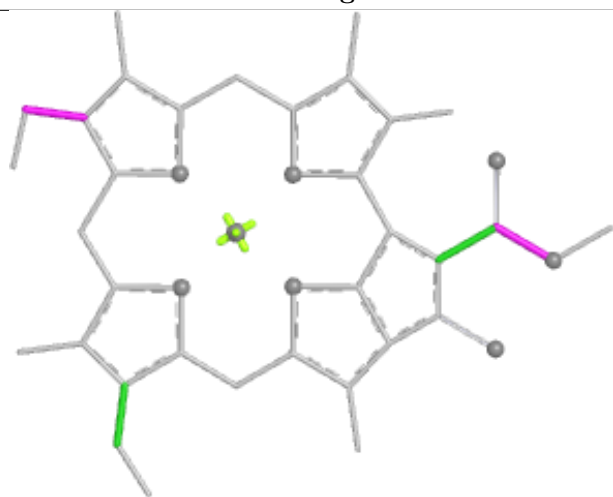
Ligand CLA 7 609



Bond lengths



Bond angles

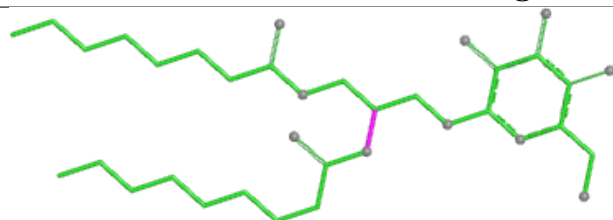


Torsions

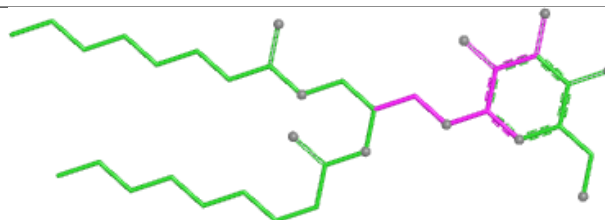


Rings

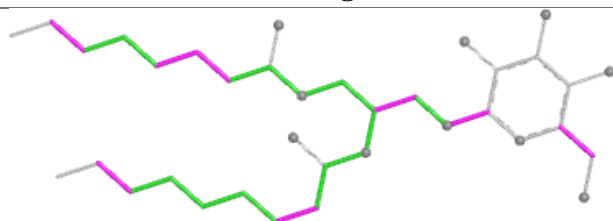
Ligand LMG 0 619



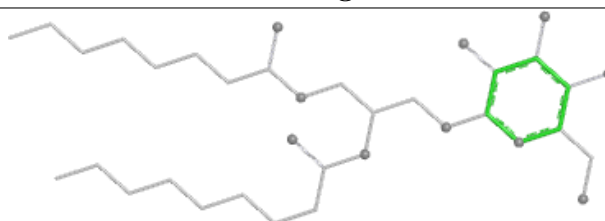
Bond lengths



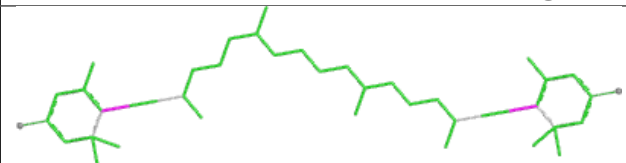
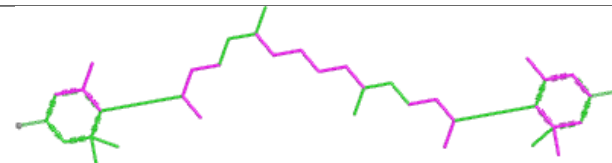
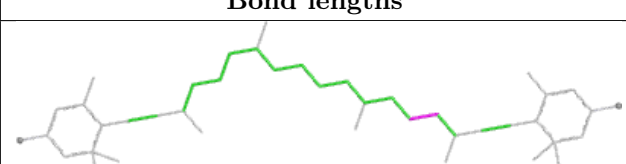
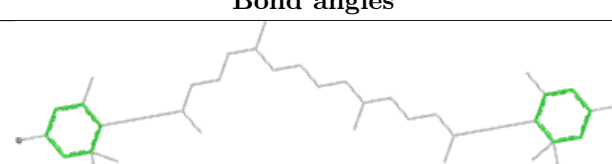
Bond angles

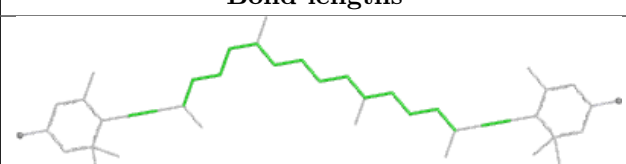
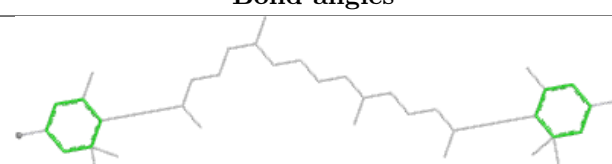


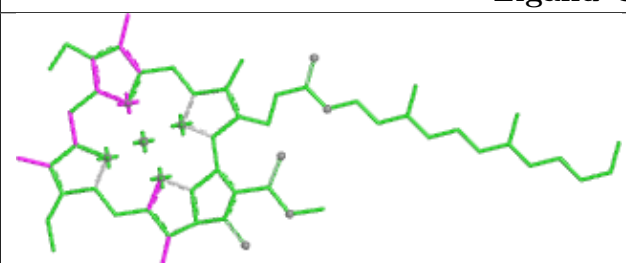
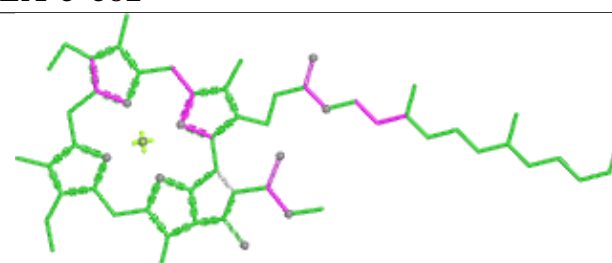
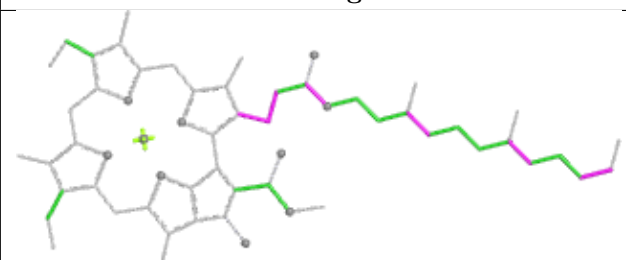
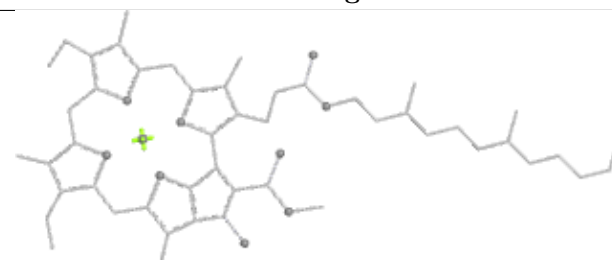
Torsions



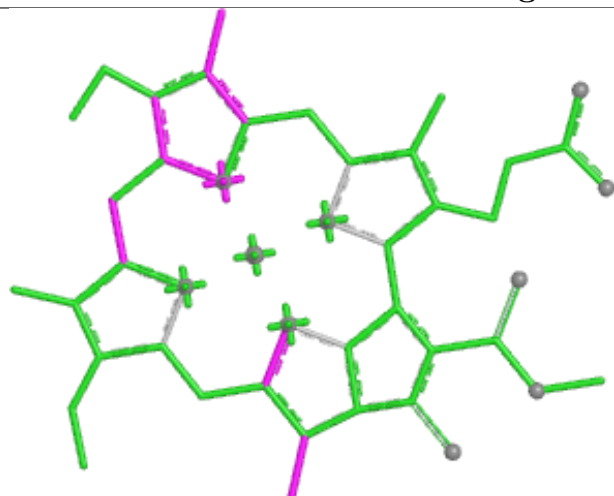
Rings

Ligand II0 0 620	
	
Bond lengths	Bond angles
	
Torsions	Rings

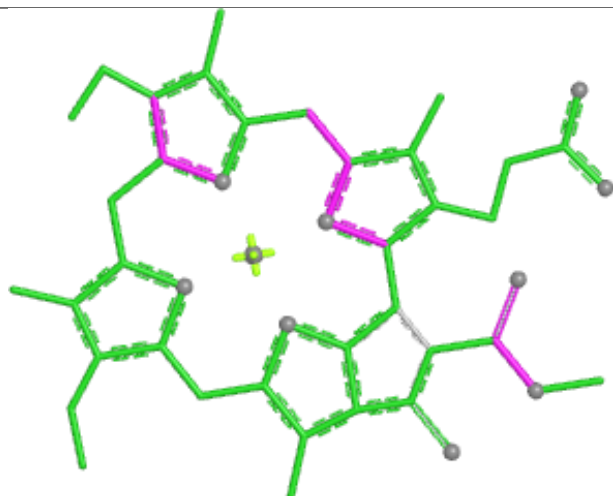
Ligand II0 3 613	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA 9 602	
	
Bond lengths	Bond angles
	
Torsions	Rings

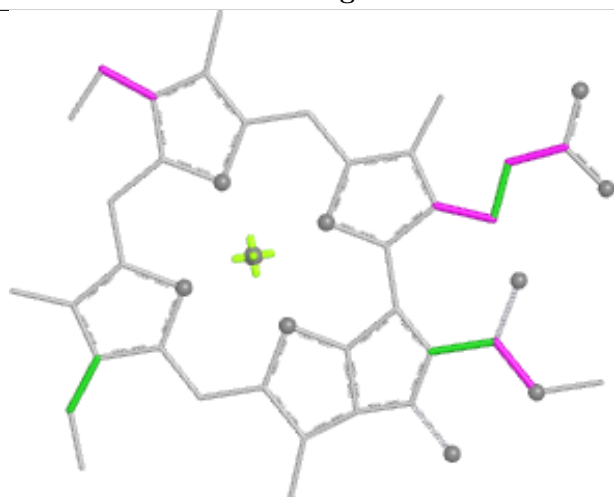
Ligand CLA 2 612



Bond lengths



Bond angles

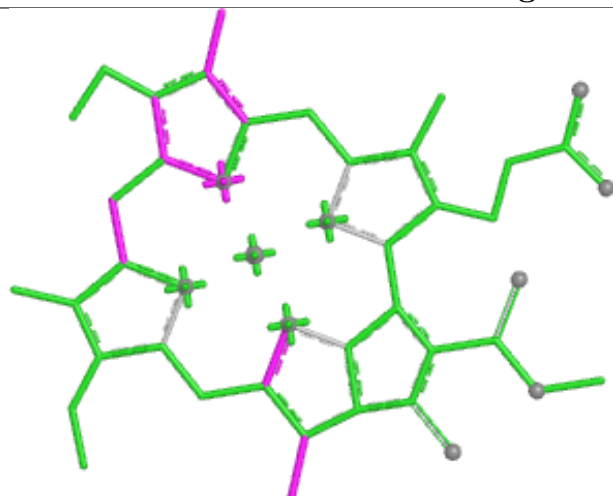


Torsions

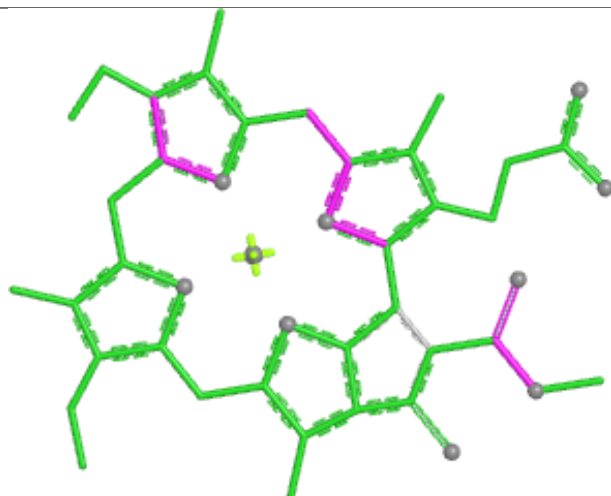


Rings

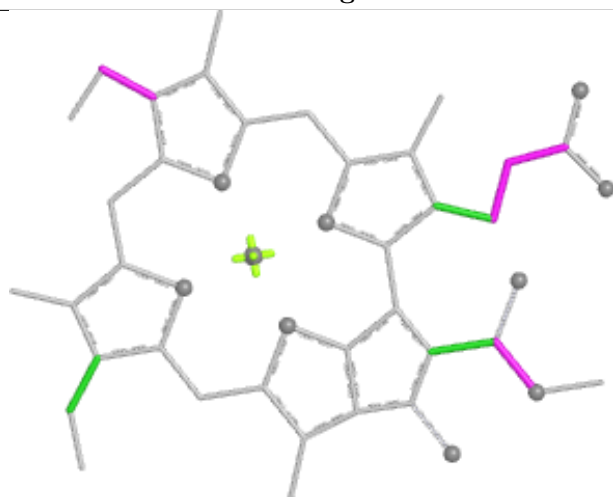
Ligand CLA 4 611



Bond lengths



Bond angles

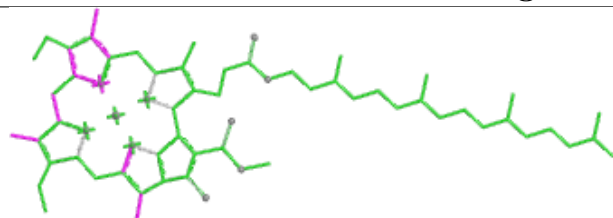


Torsions

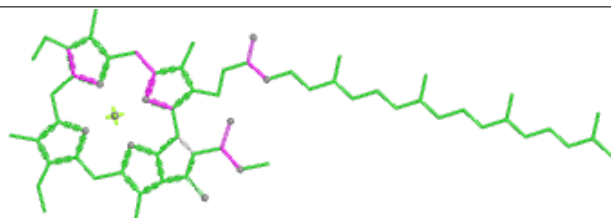


Rings

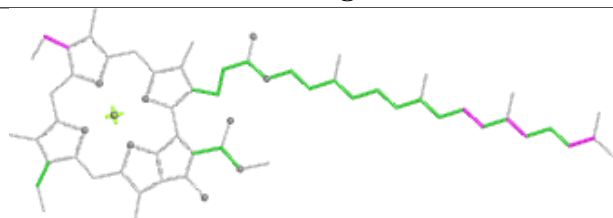
Ligand CLA b 616



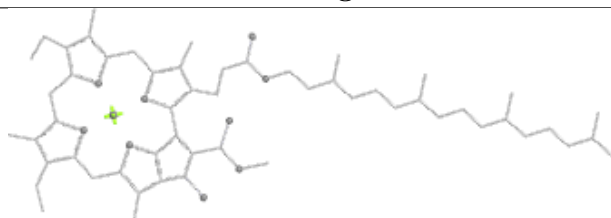
Bond lengths



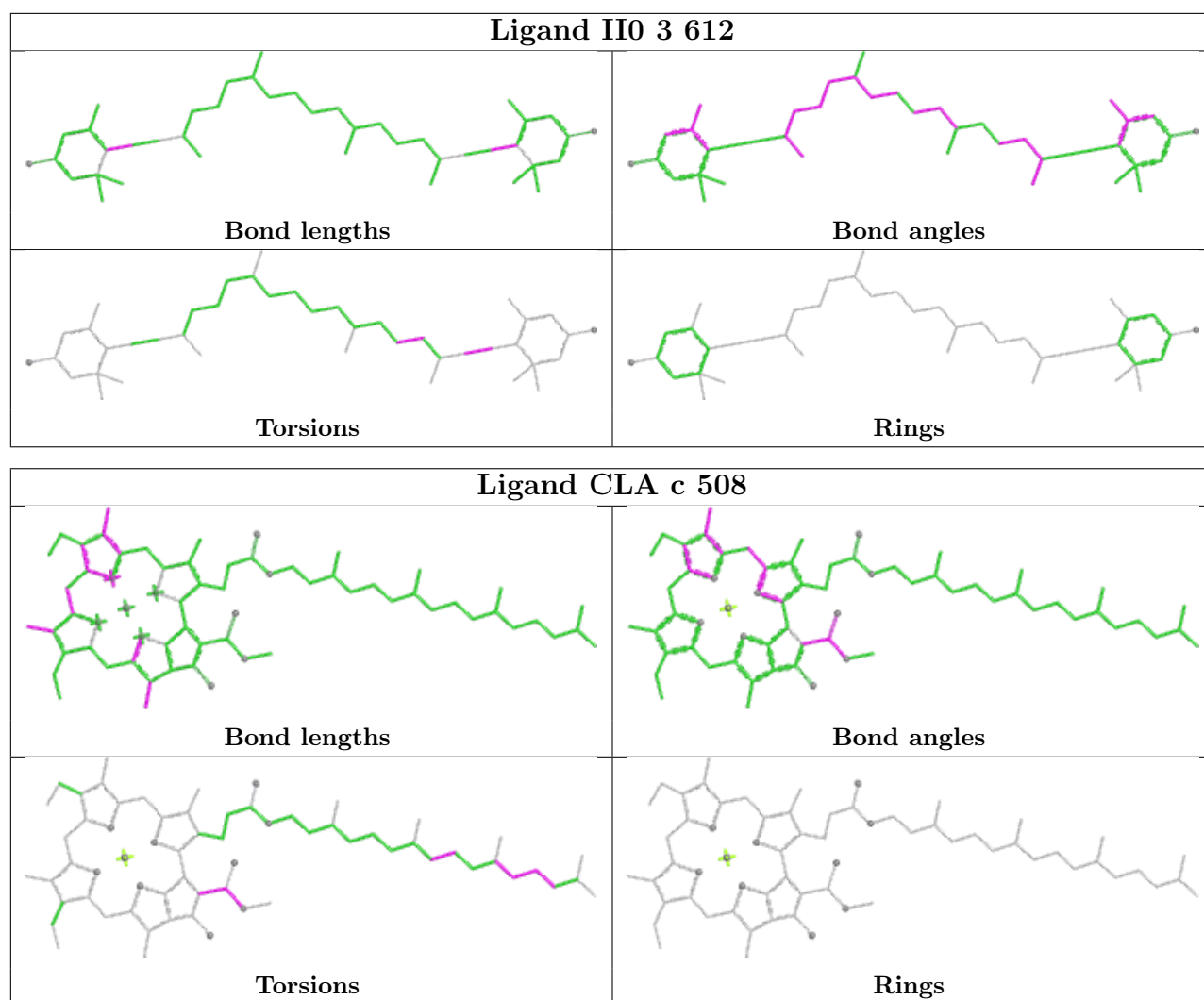
Bond angles

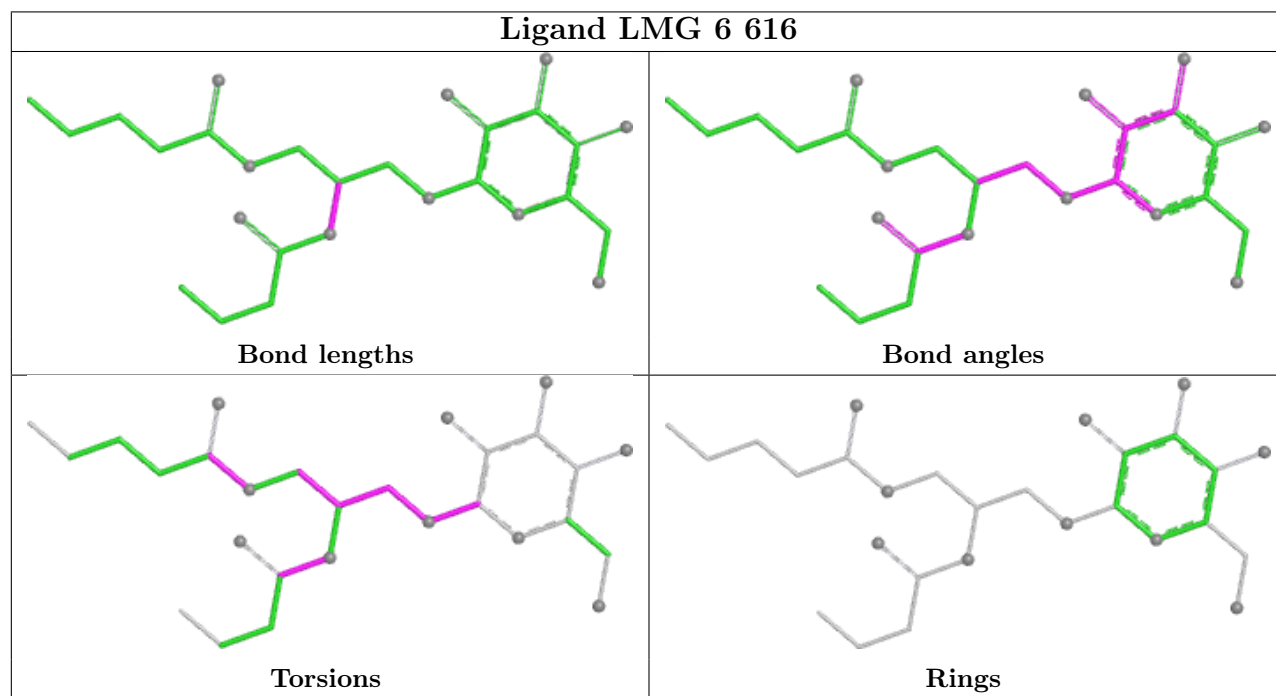
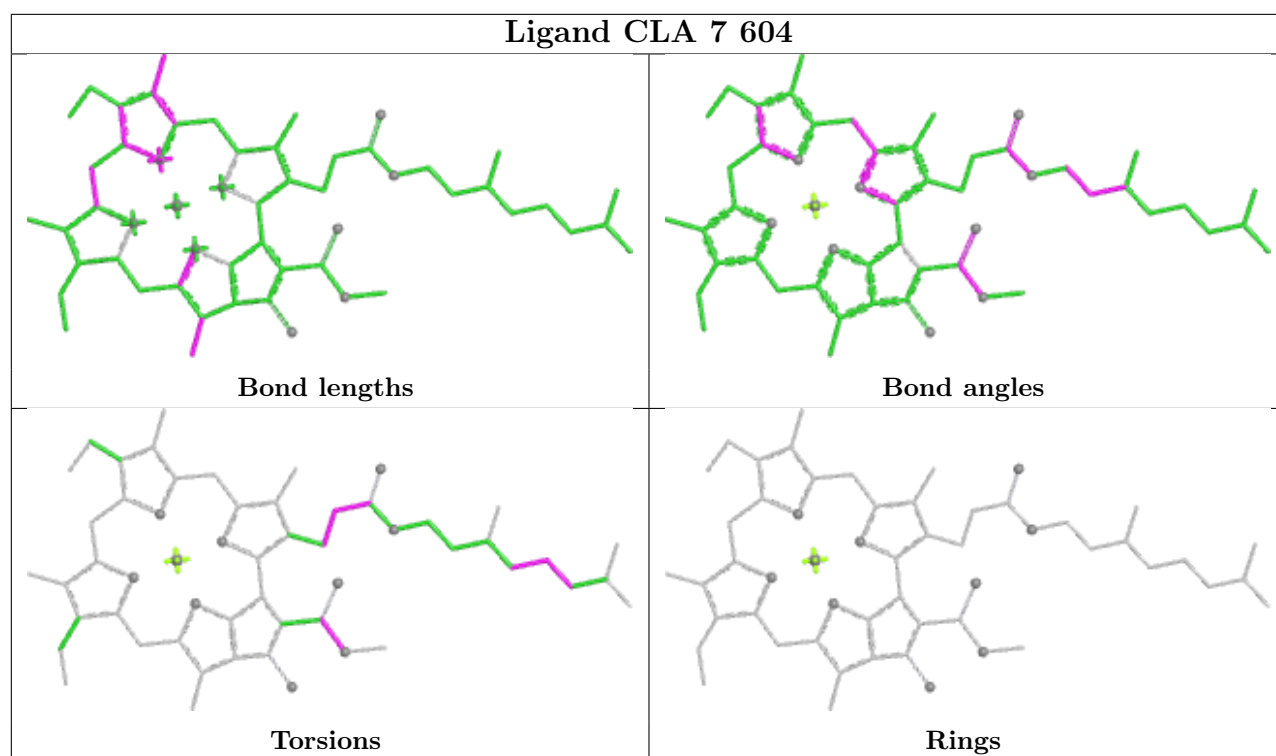


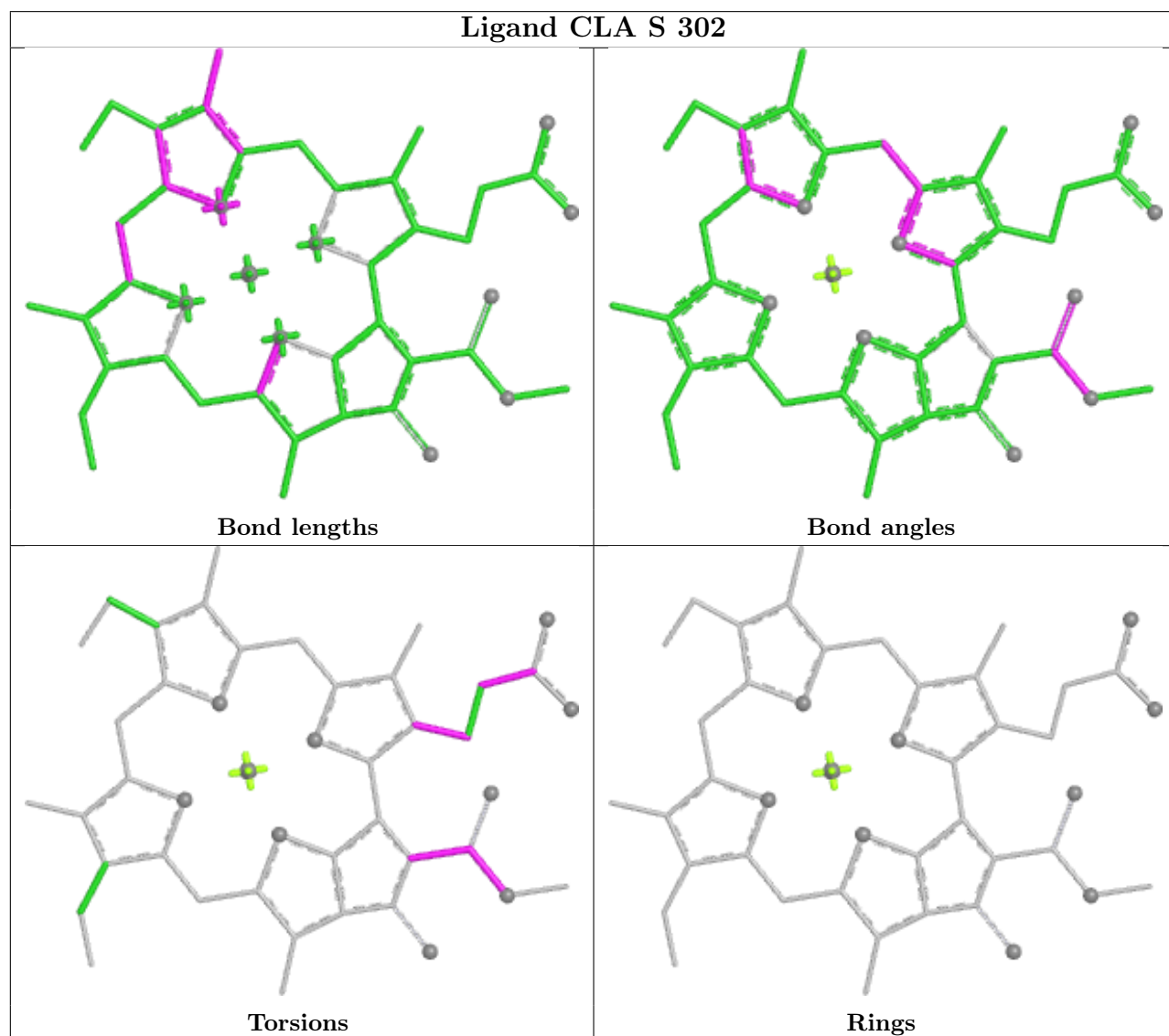
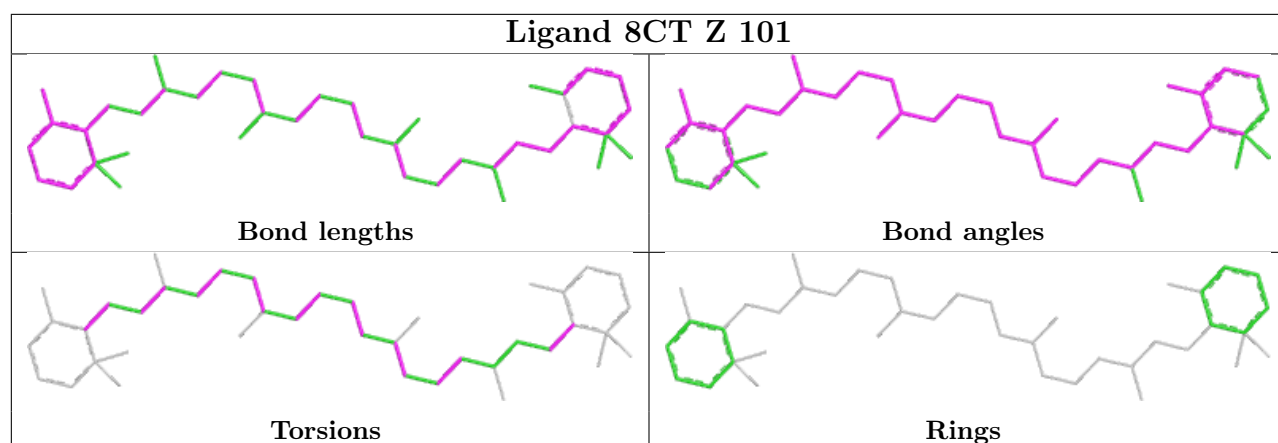
Torsions

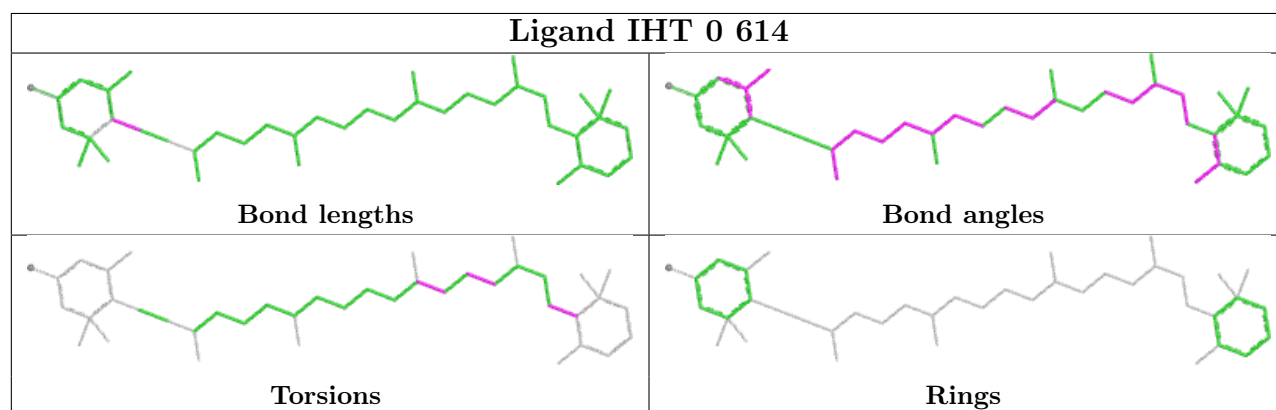
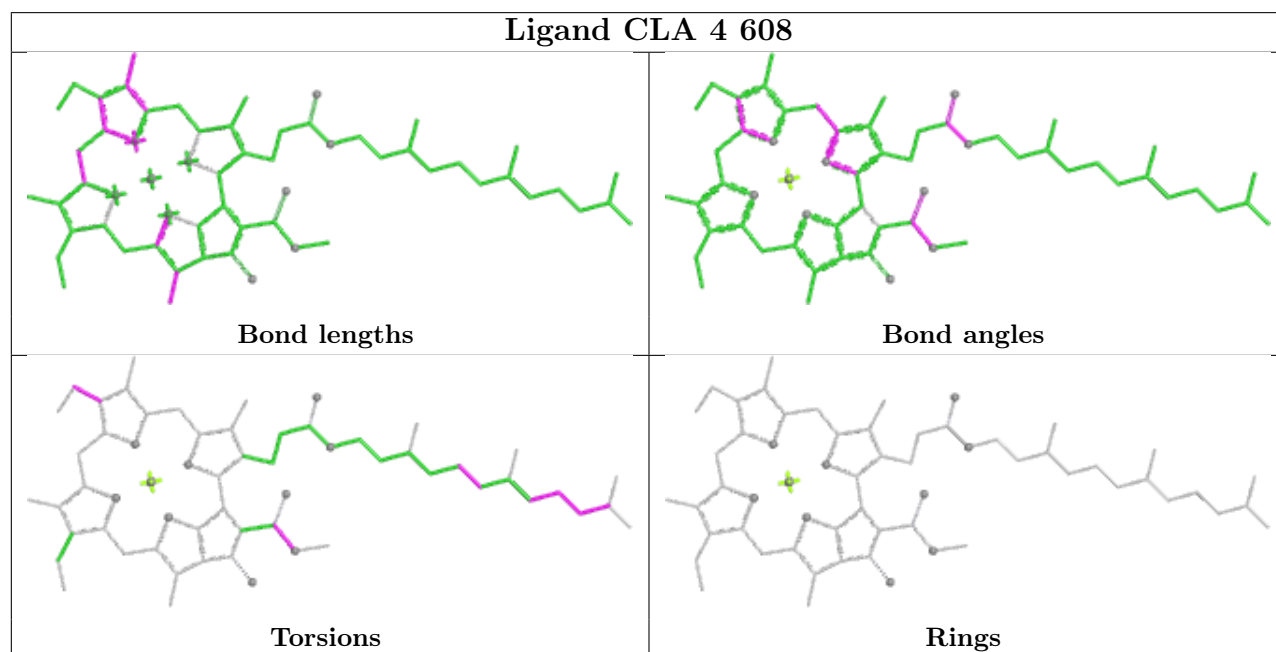
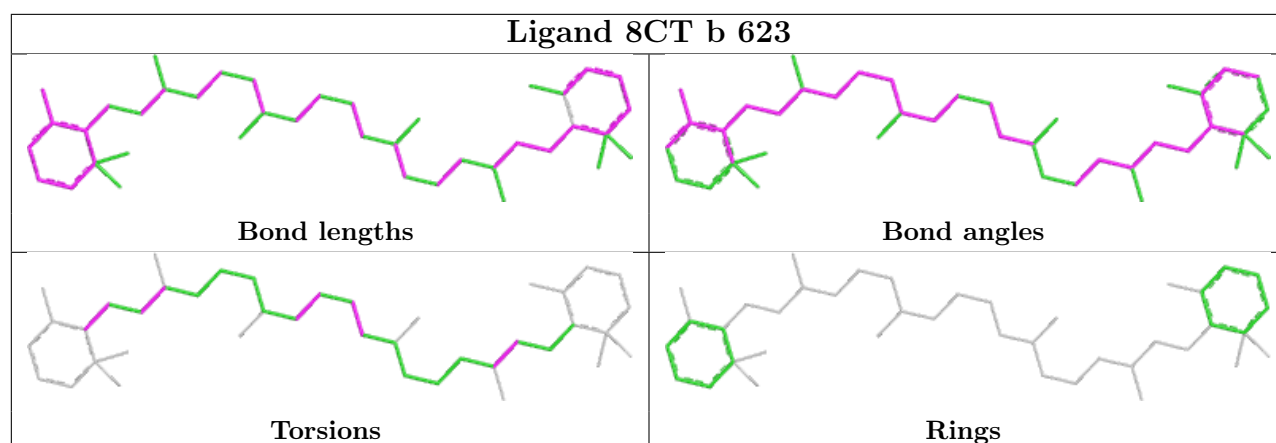


Rings

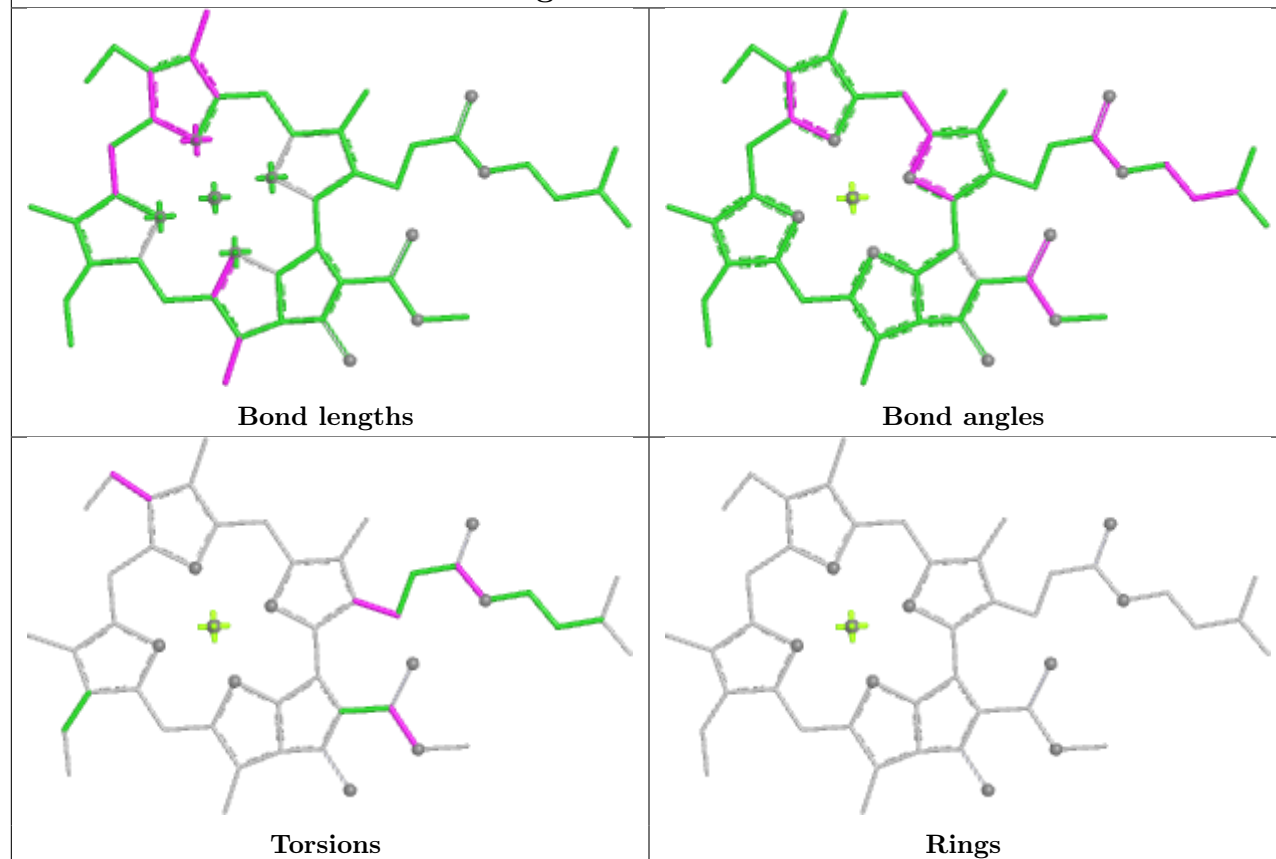




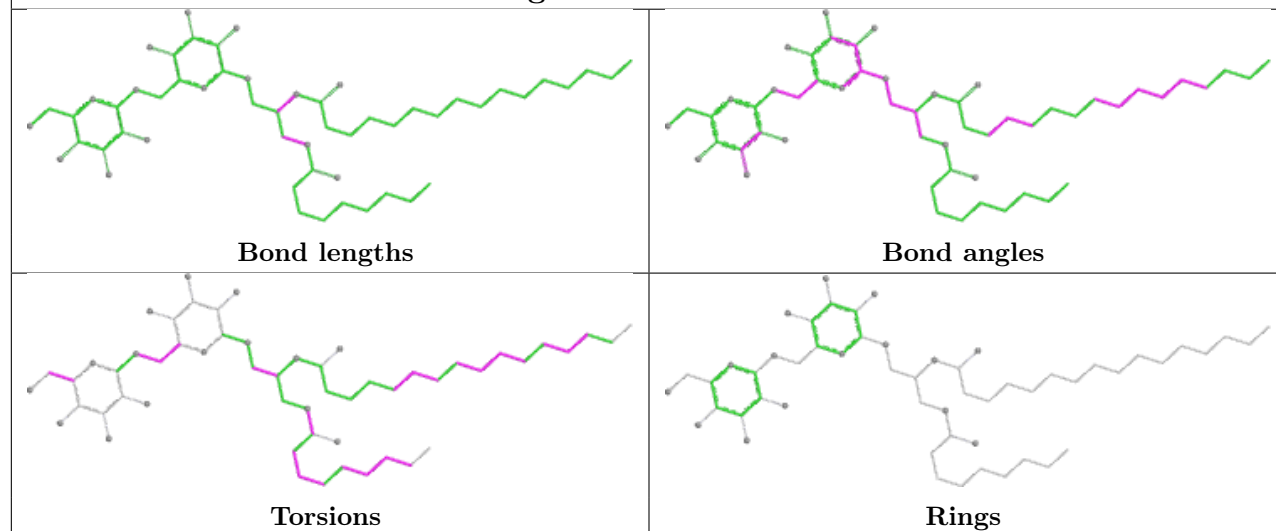


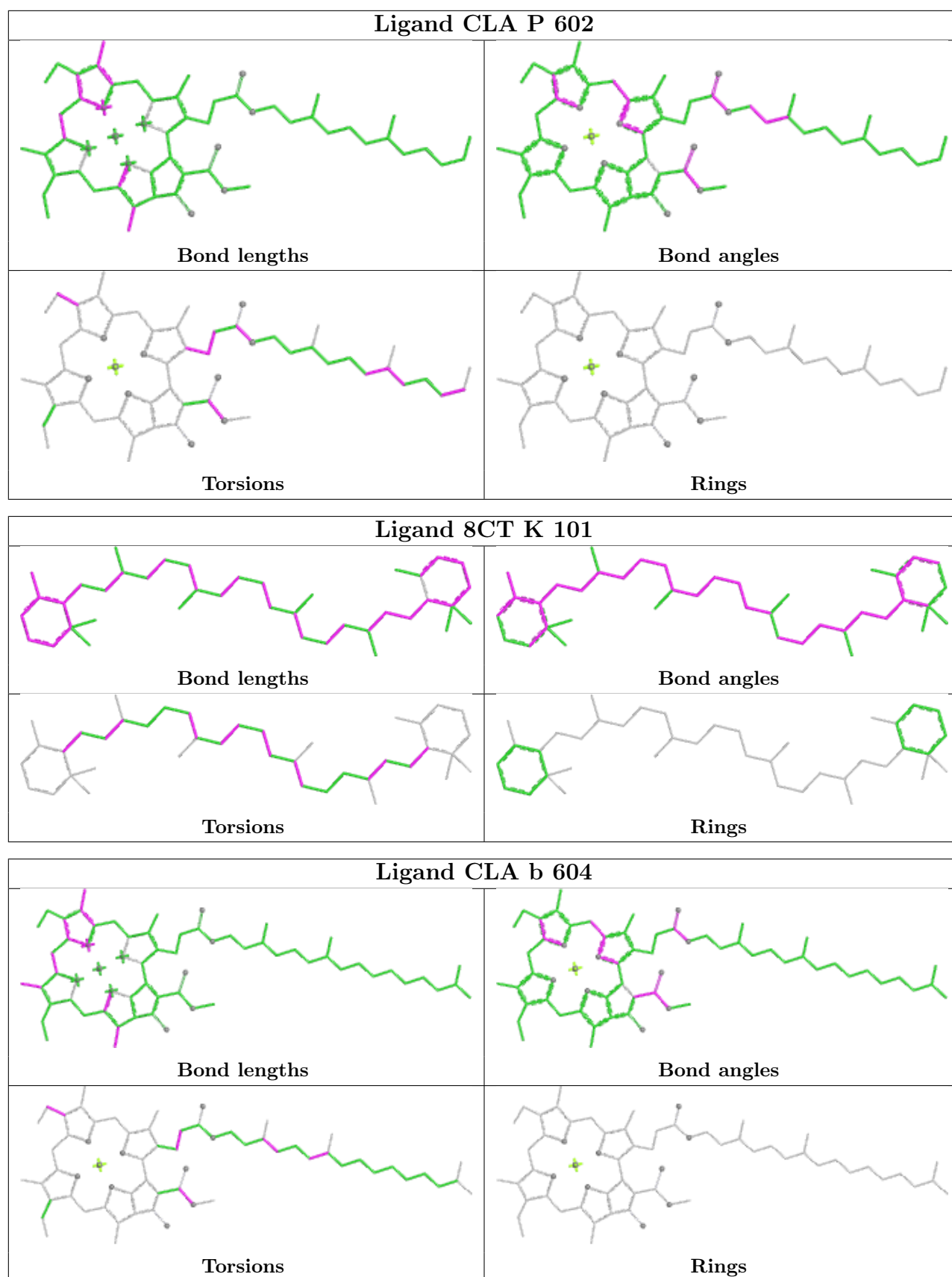


Ligand CLA 7 605

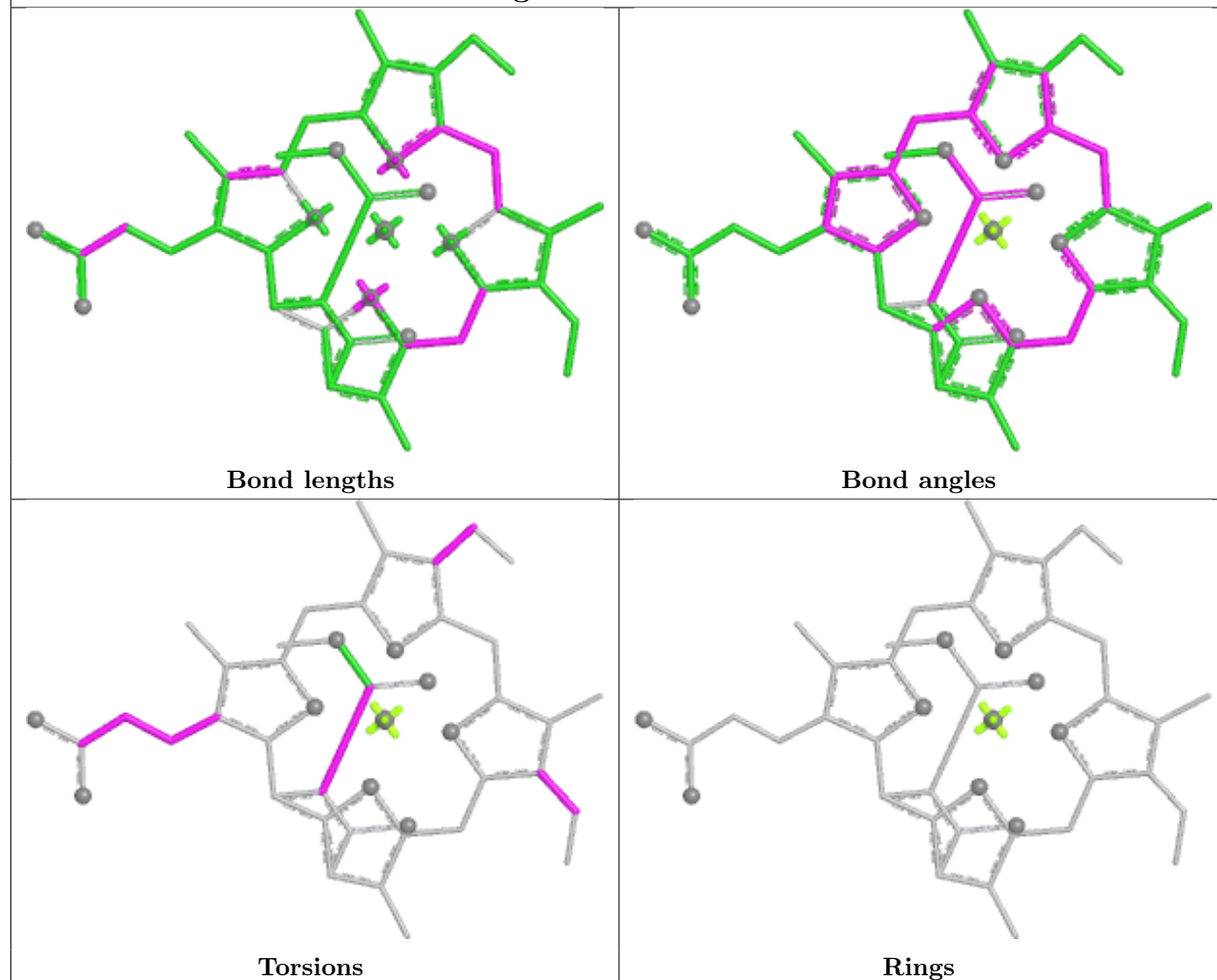


Ligand DGD C 514

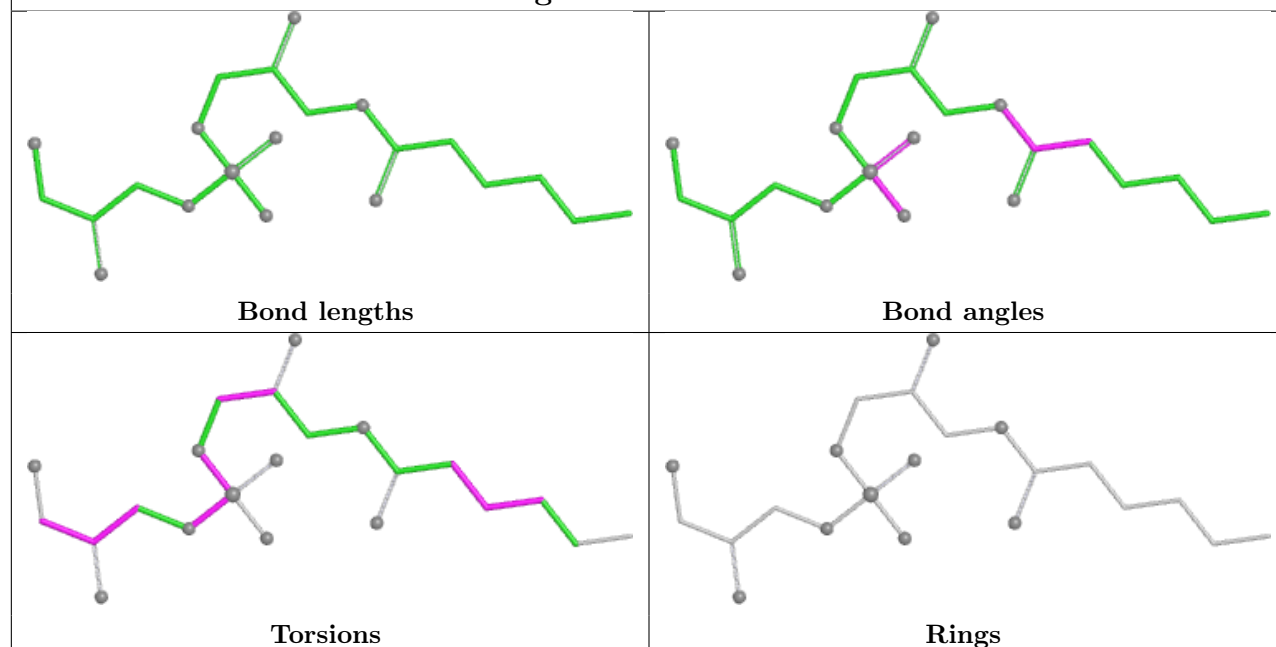




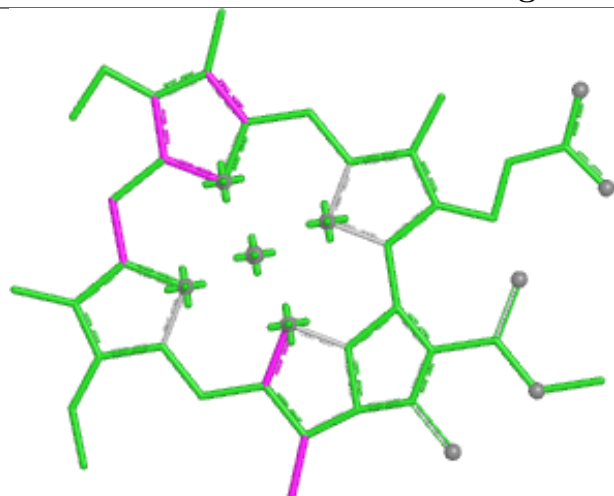
Ligand KC2 5 311



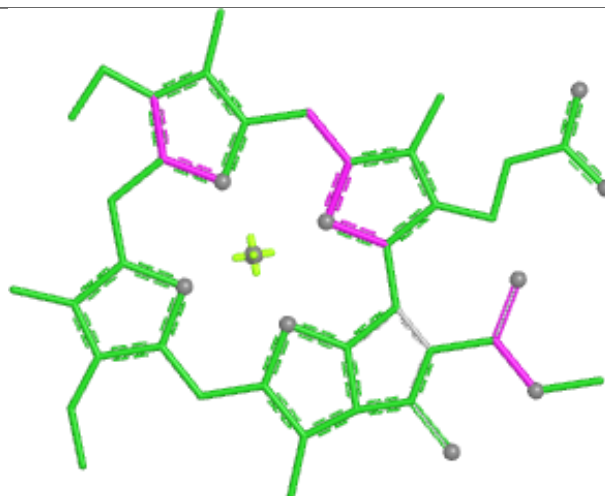
Ligand LHG 2 618



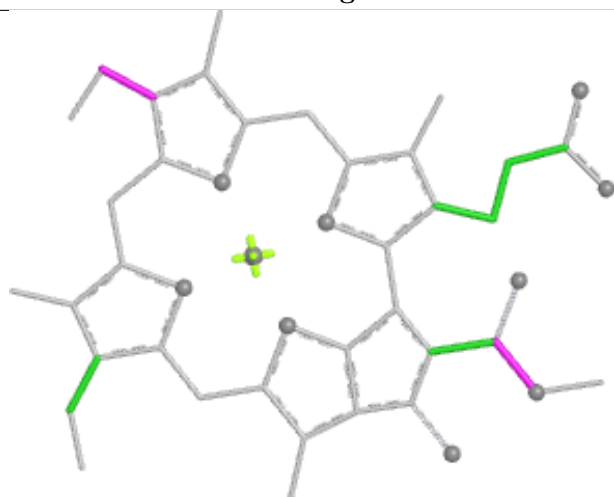
Ligand CLA 6 606



Bond lengths



Bond angles

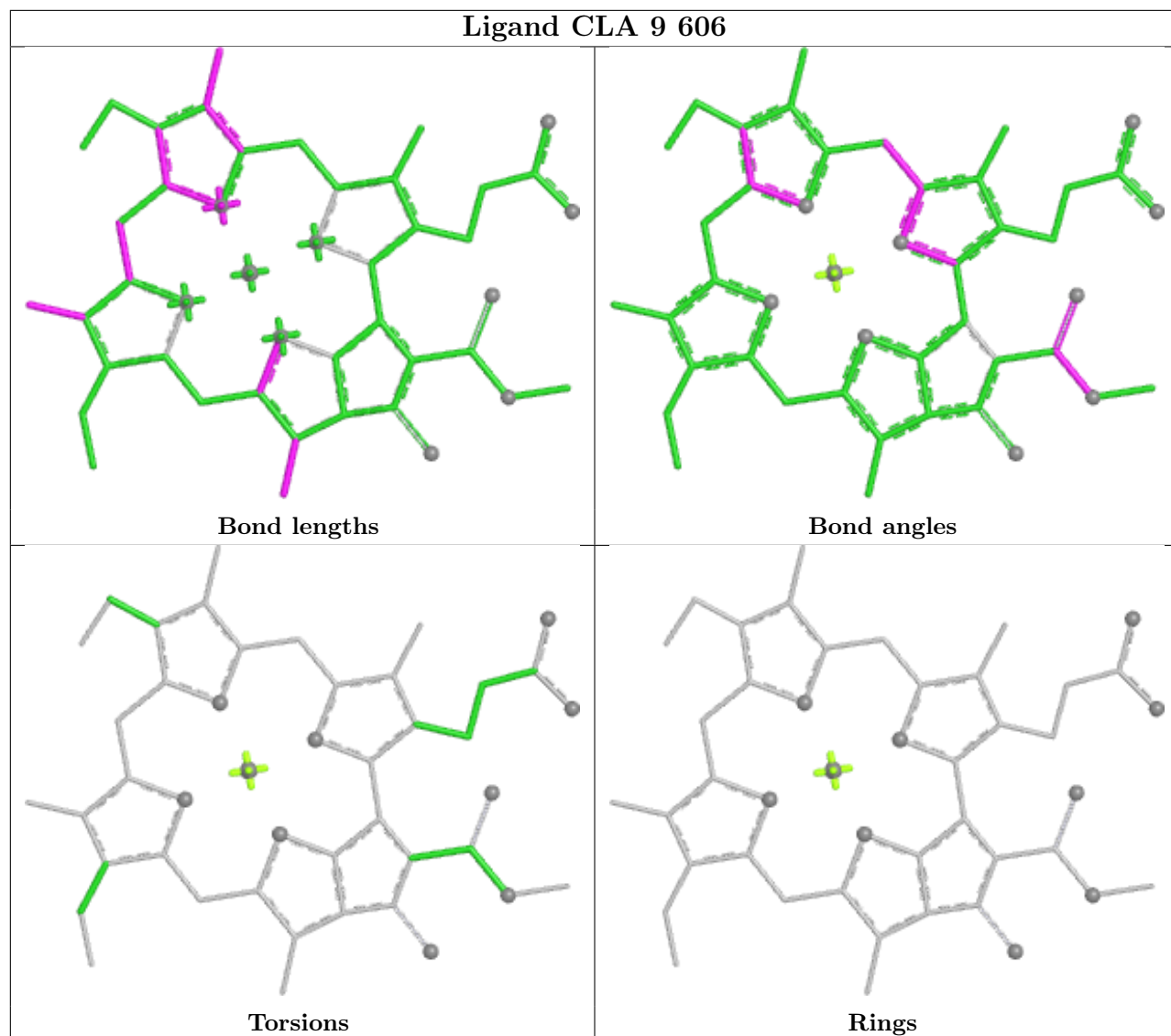


Torsions

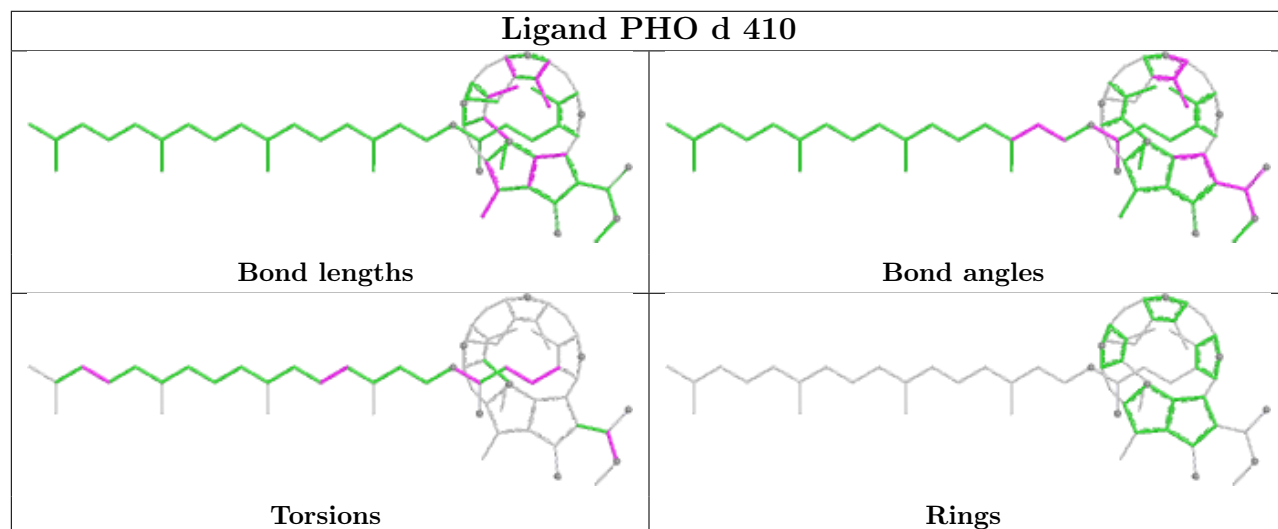


Rings

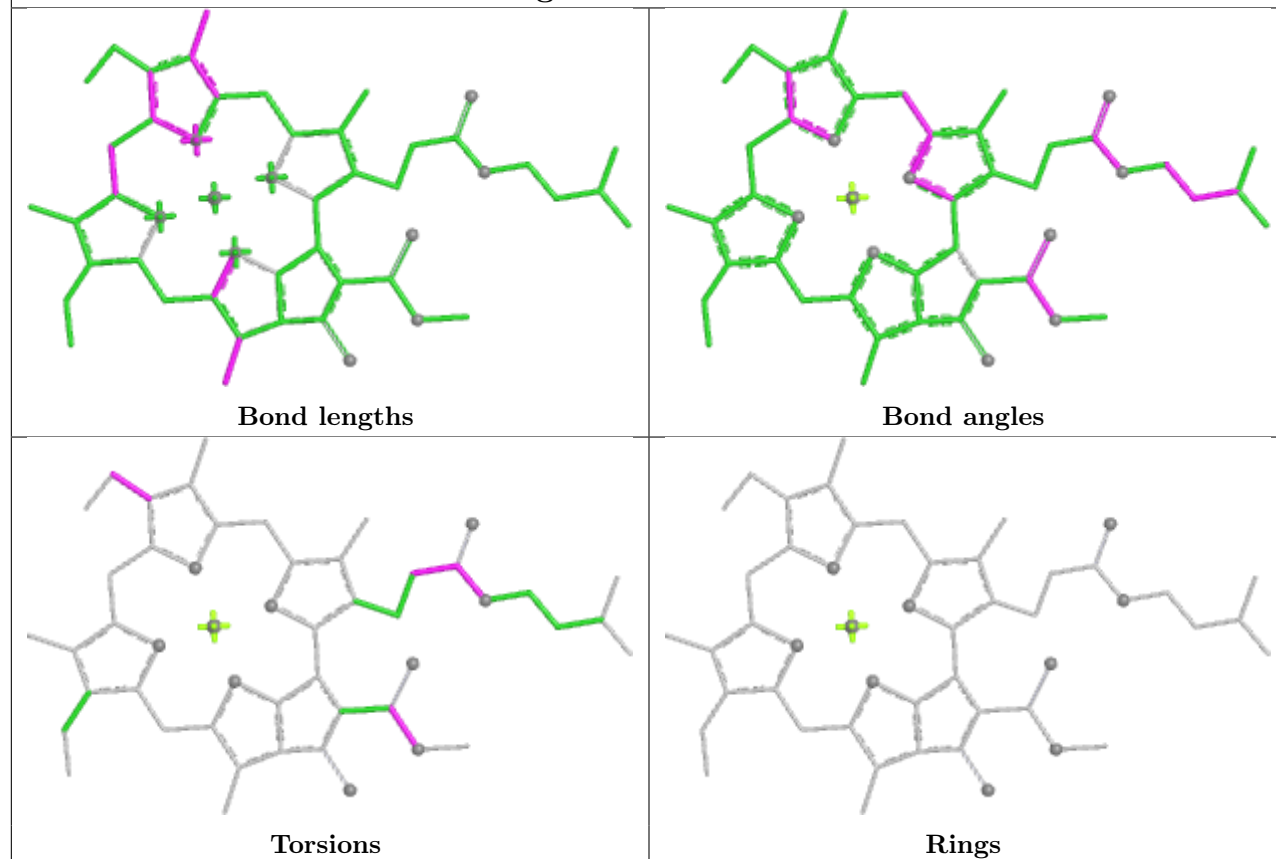
Ligand CLA 9 606



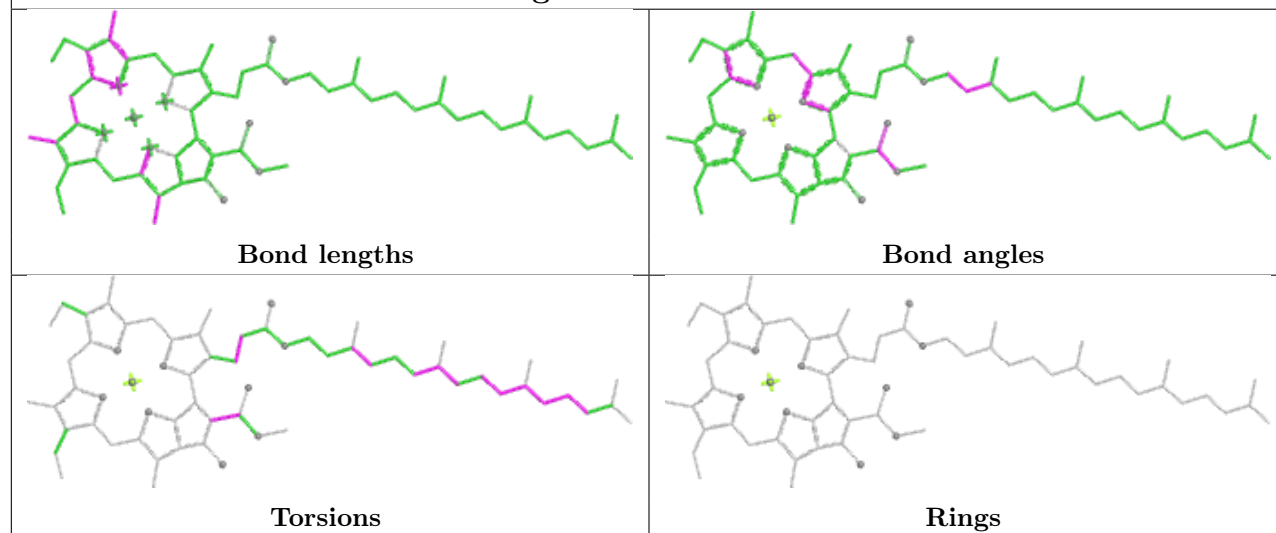
Ligand PHO d 410

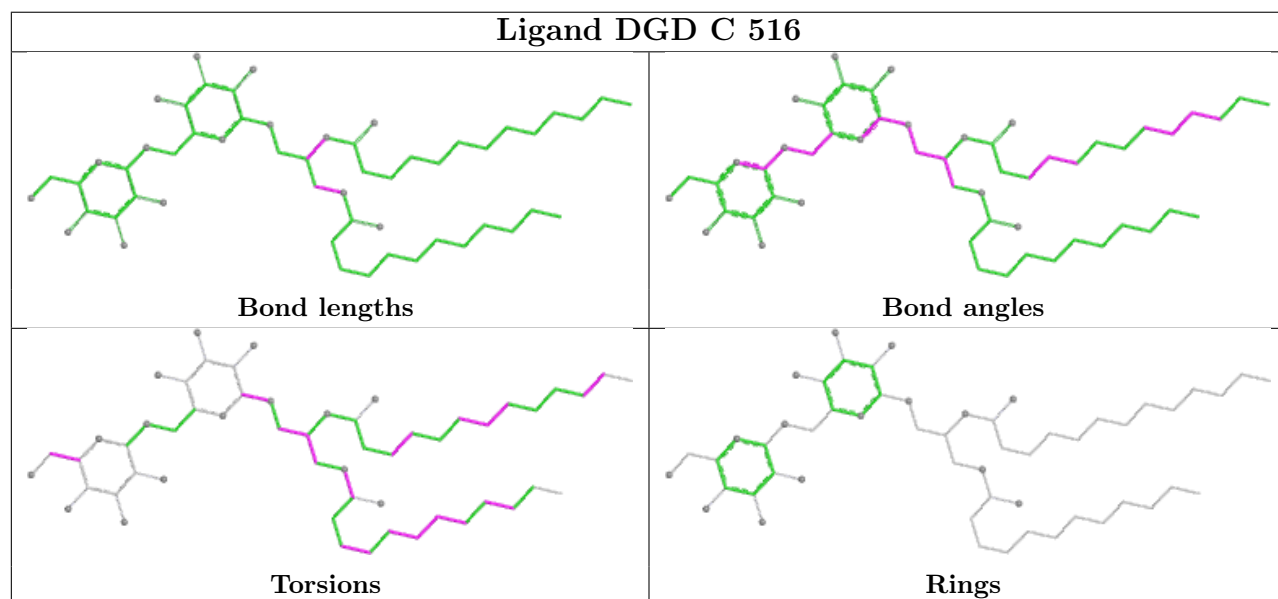
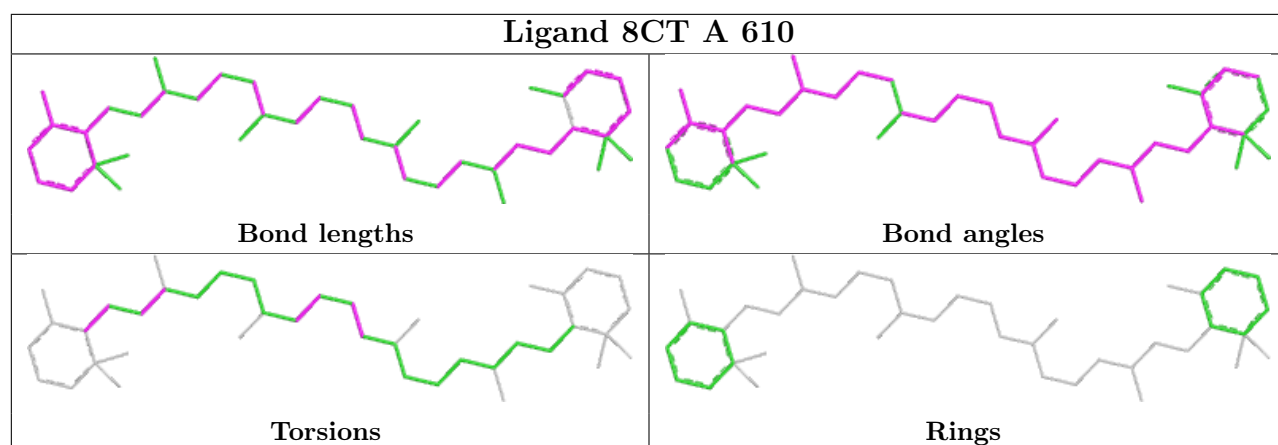


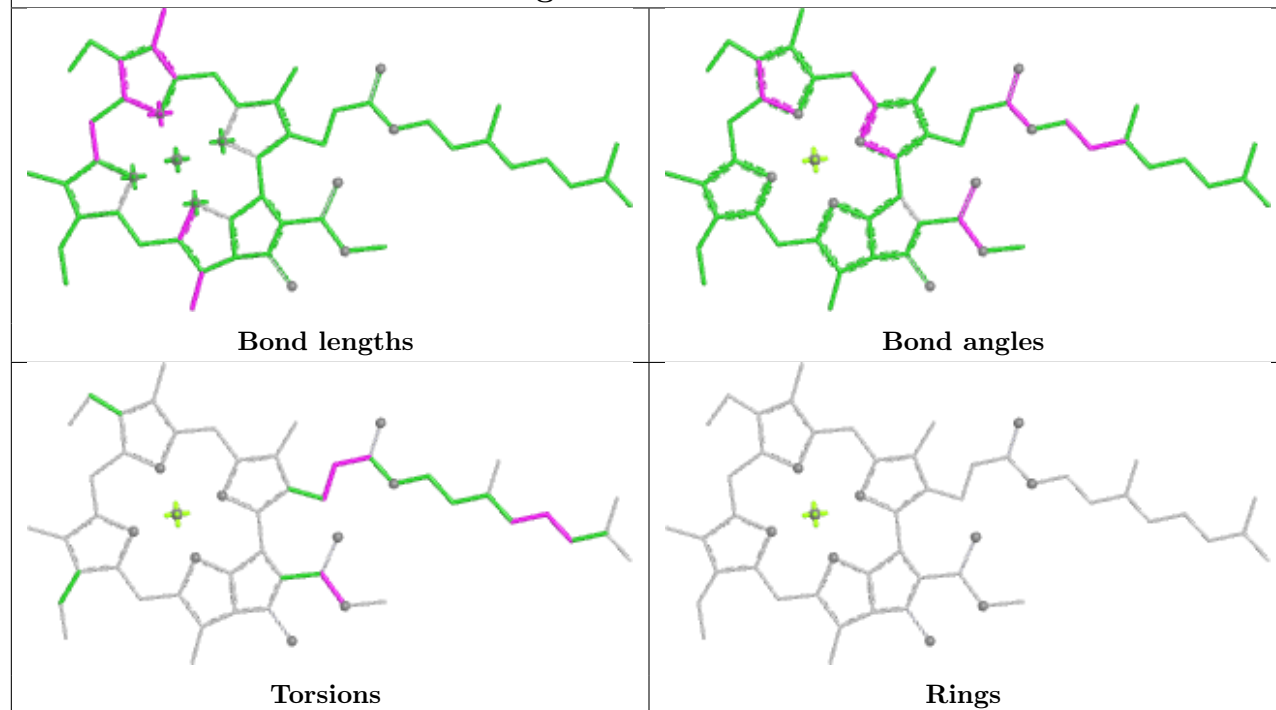
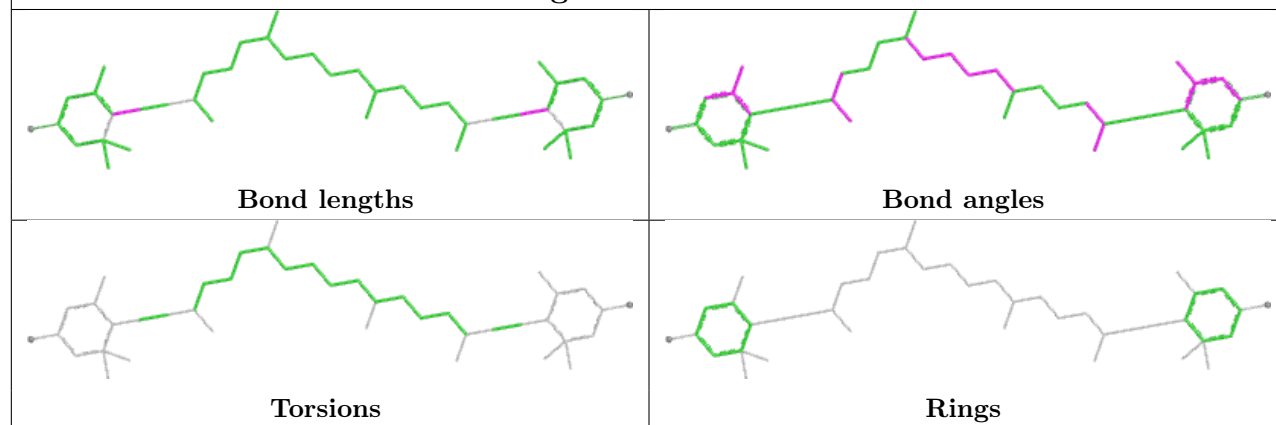
Ligand CLA 4 605

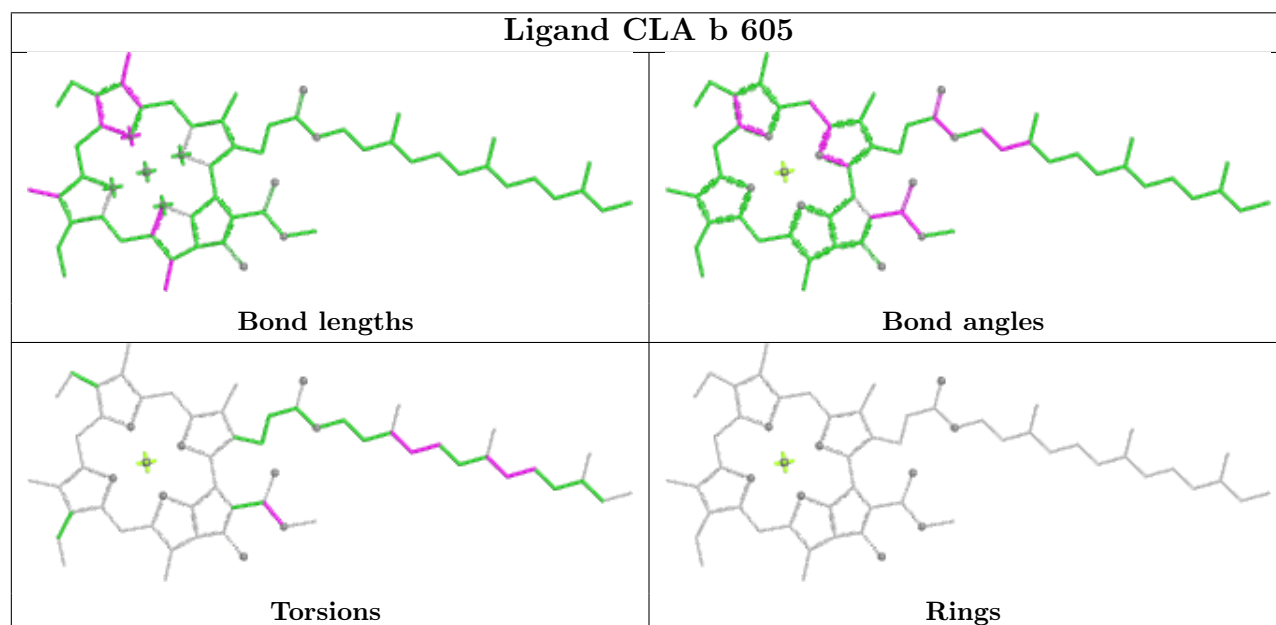
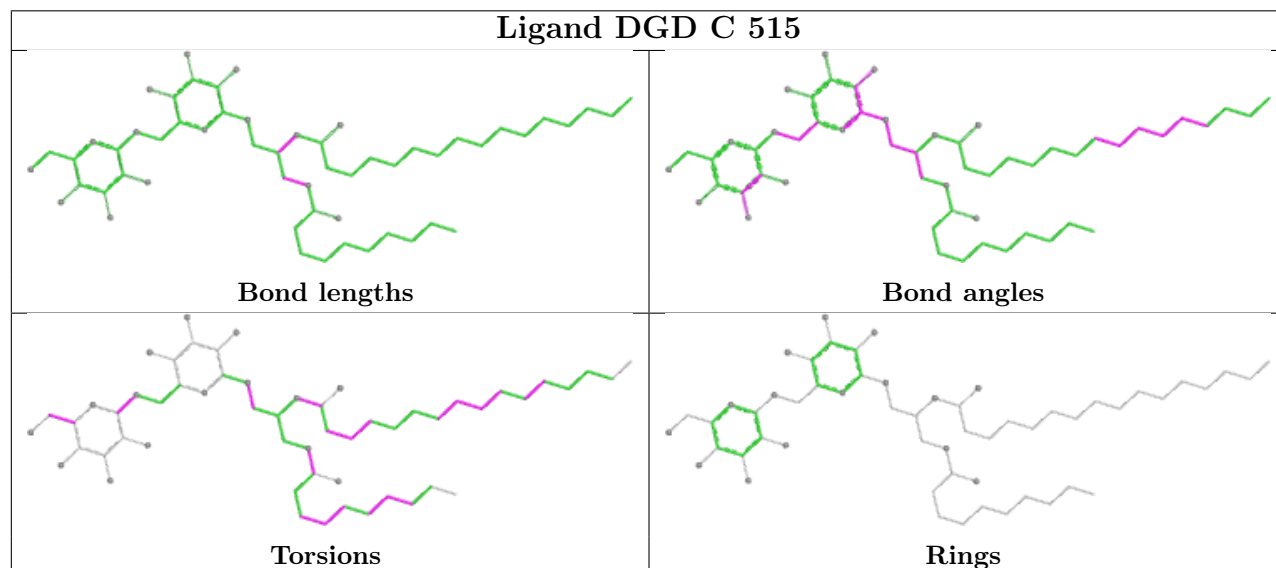
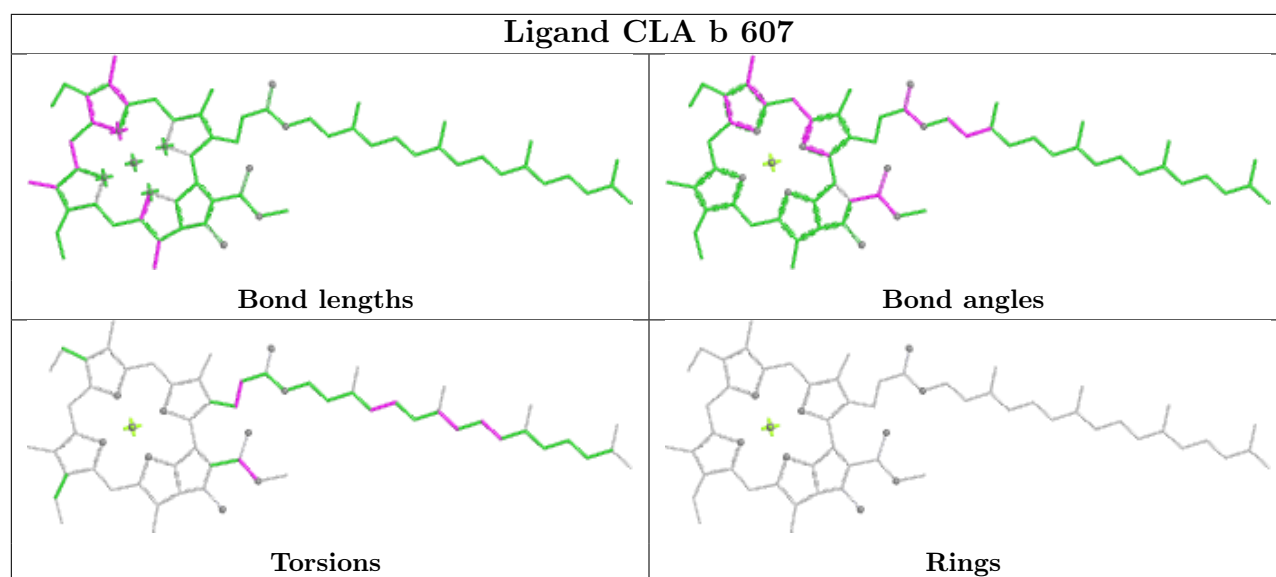


Ligand CLA C 507

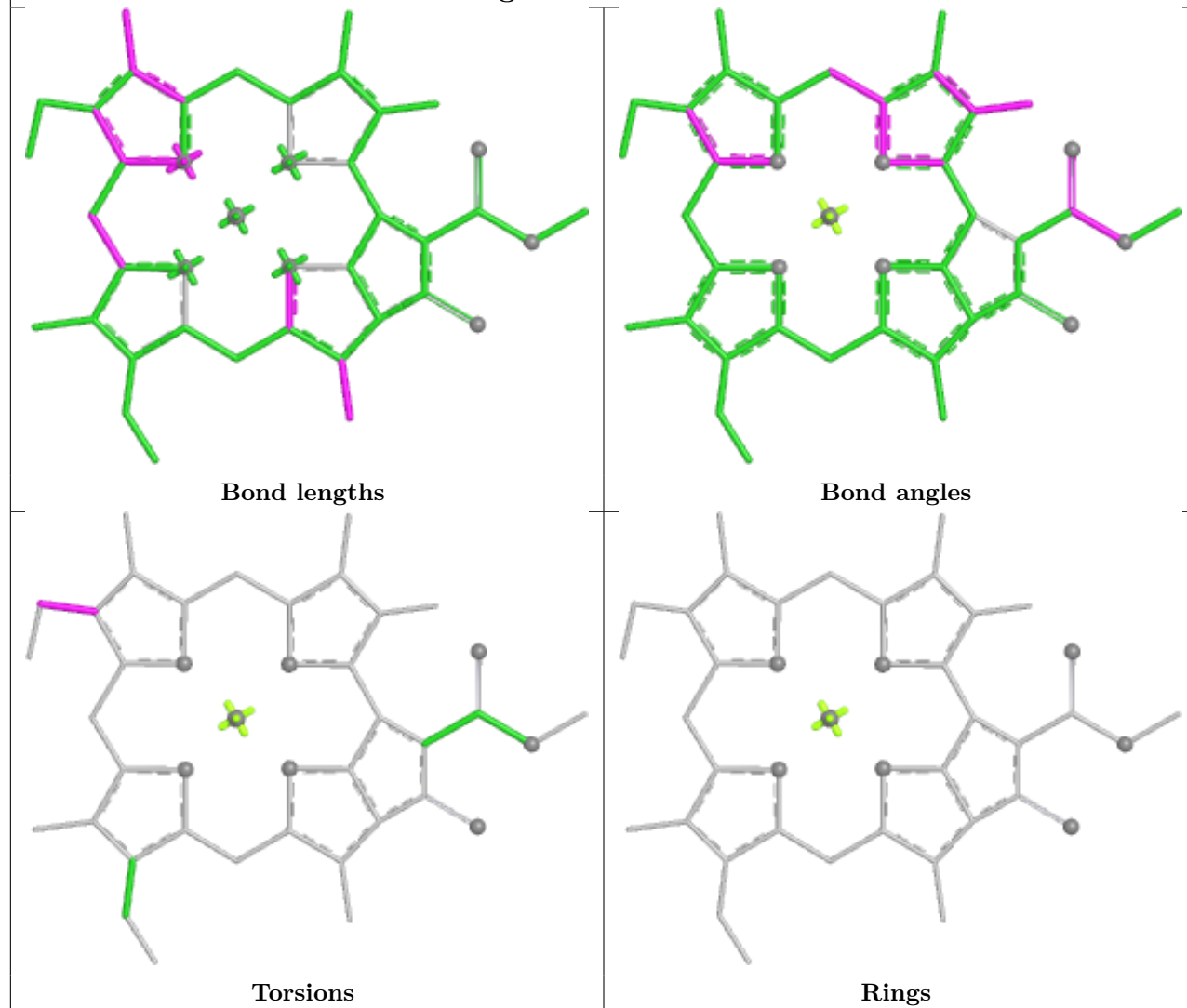




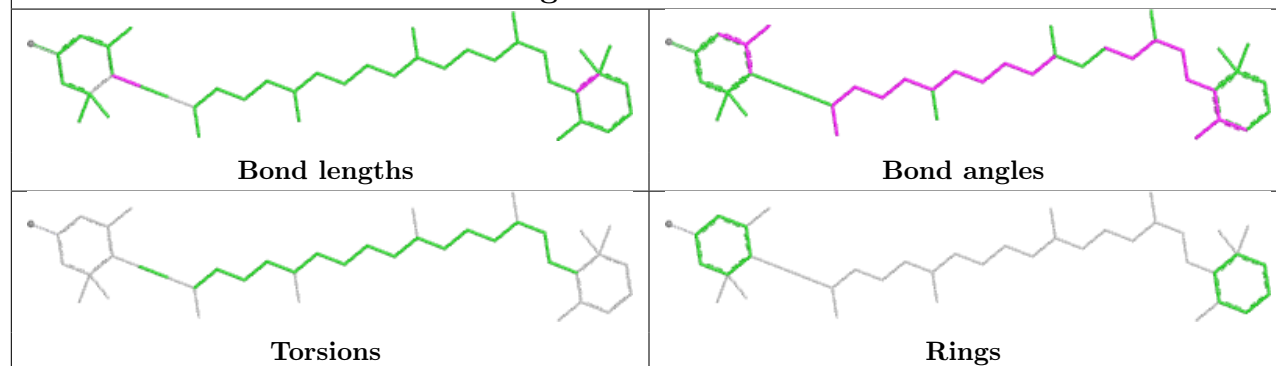
Ligand CLA 1 604**Ligand II0 4 615**

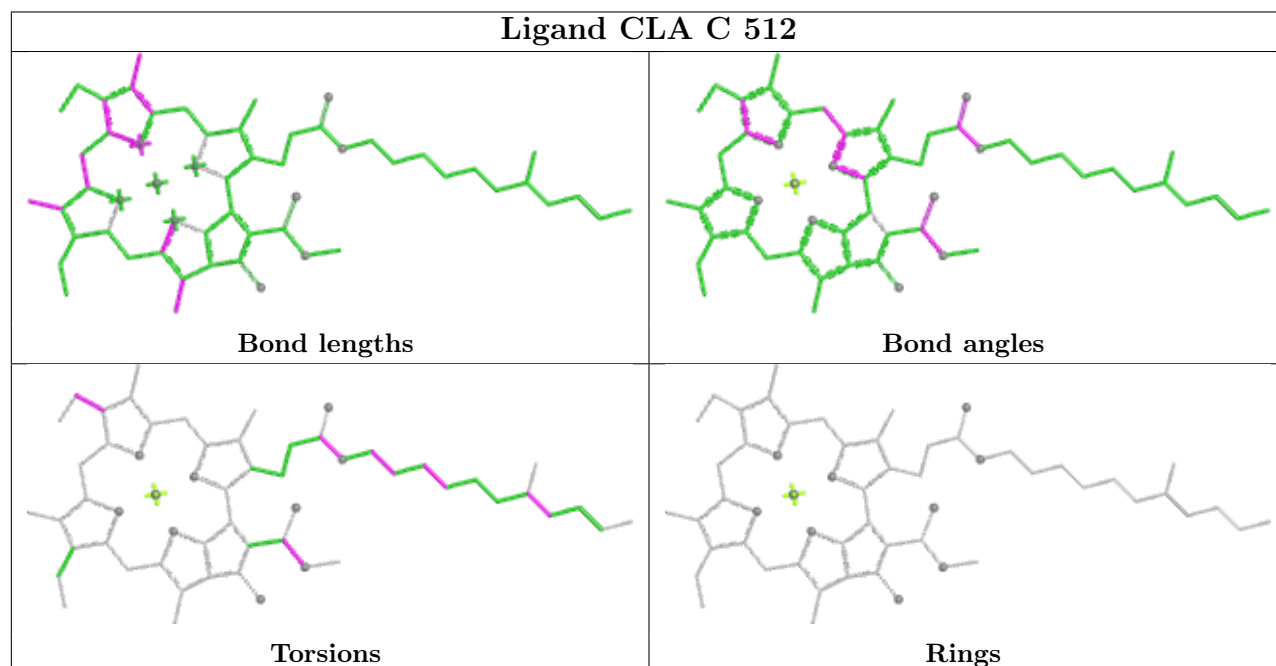
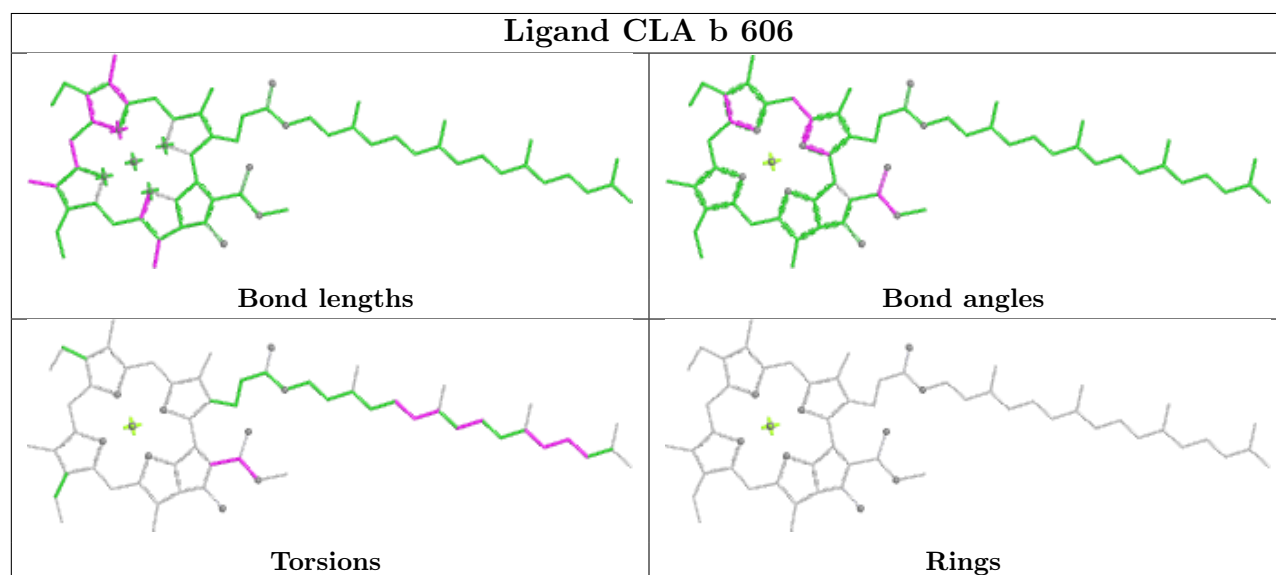
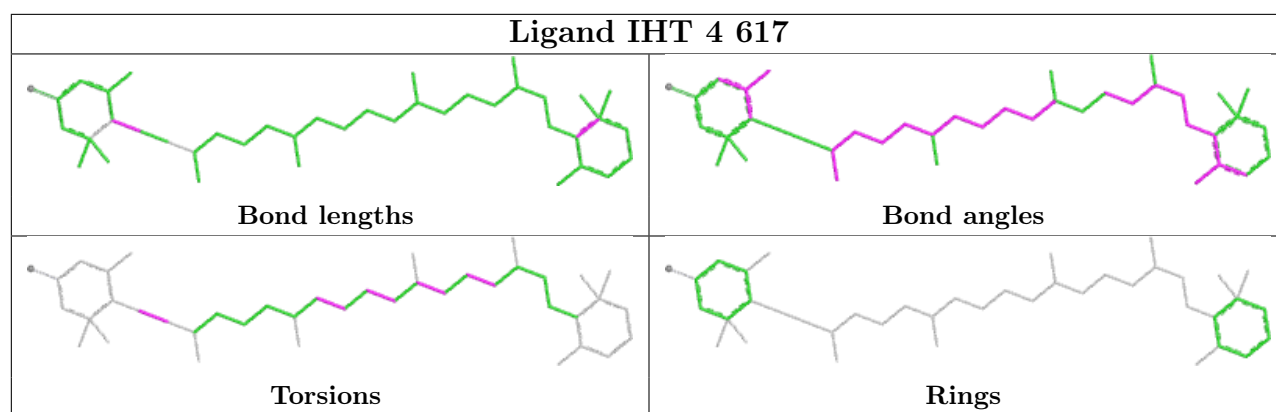


Ligand CLA 4 609

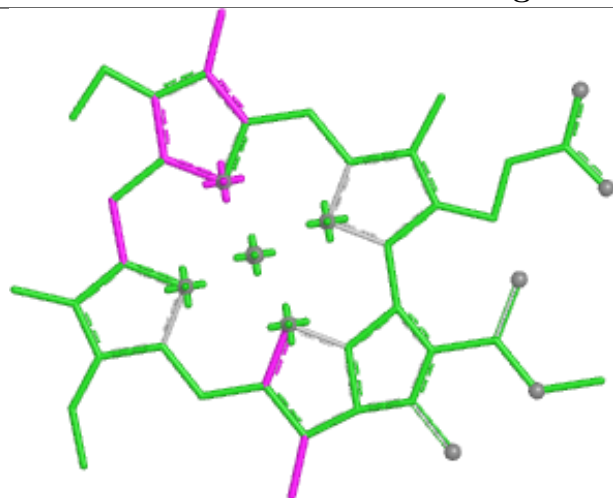


Ligand IHT 8 616

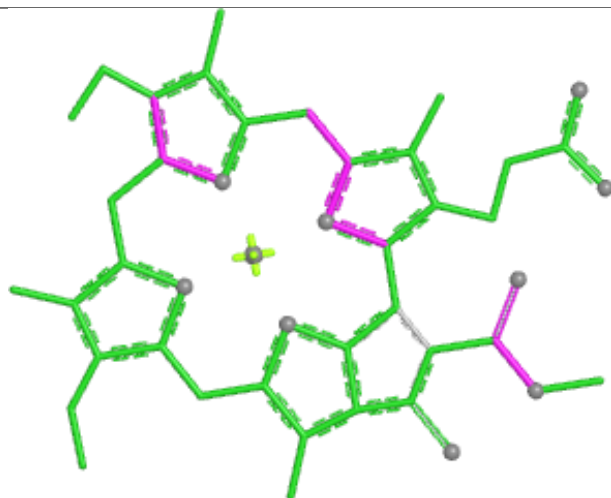




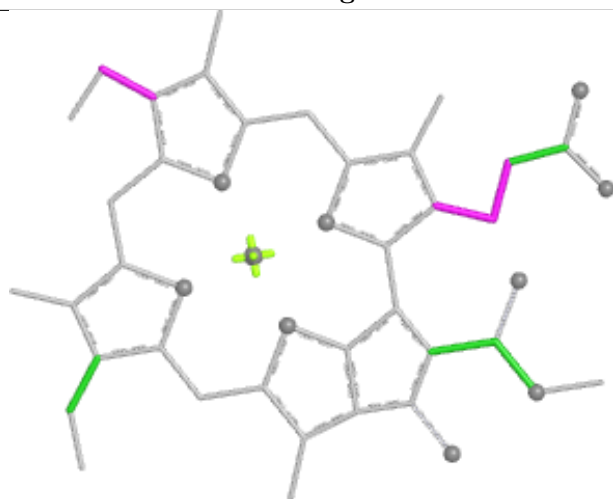
Ligand CLA G 101



Bond lengths



Bond angles

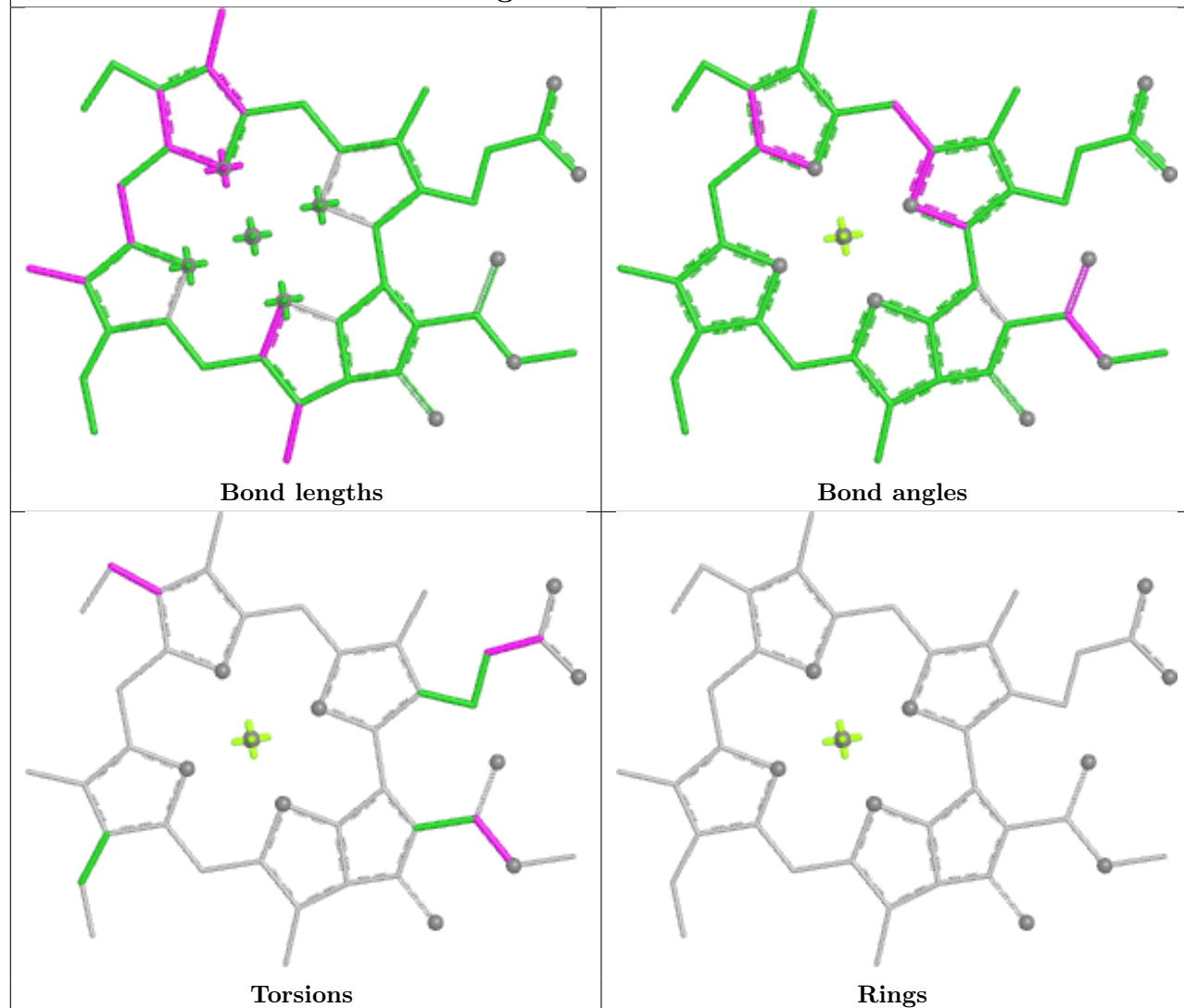


Torsions

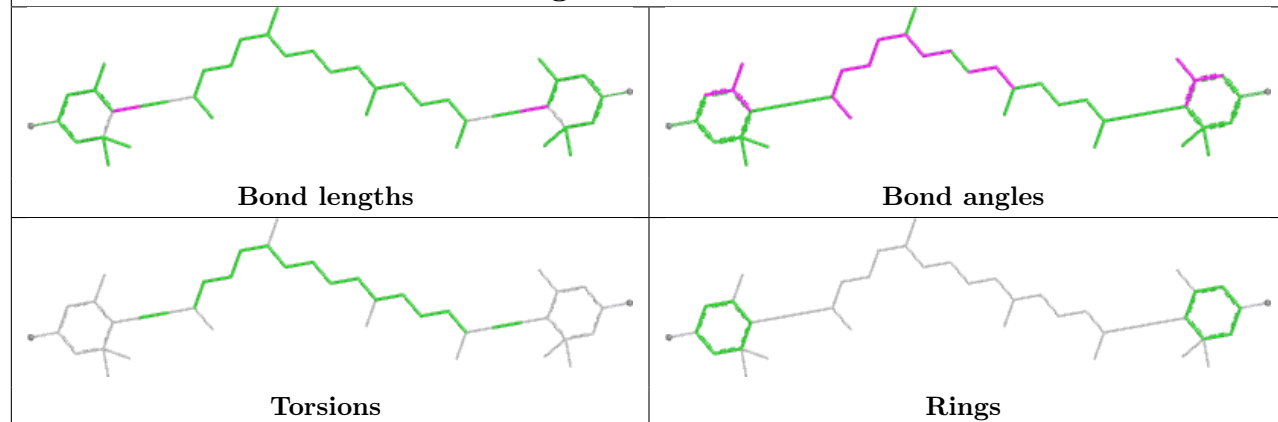


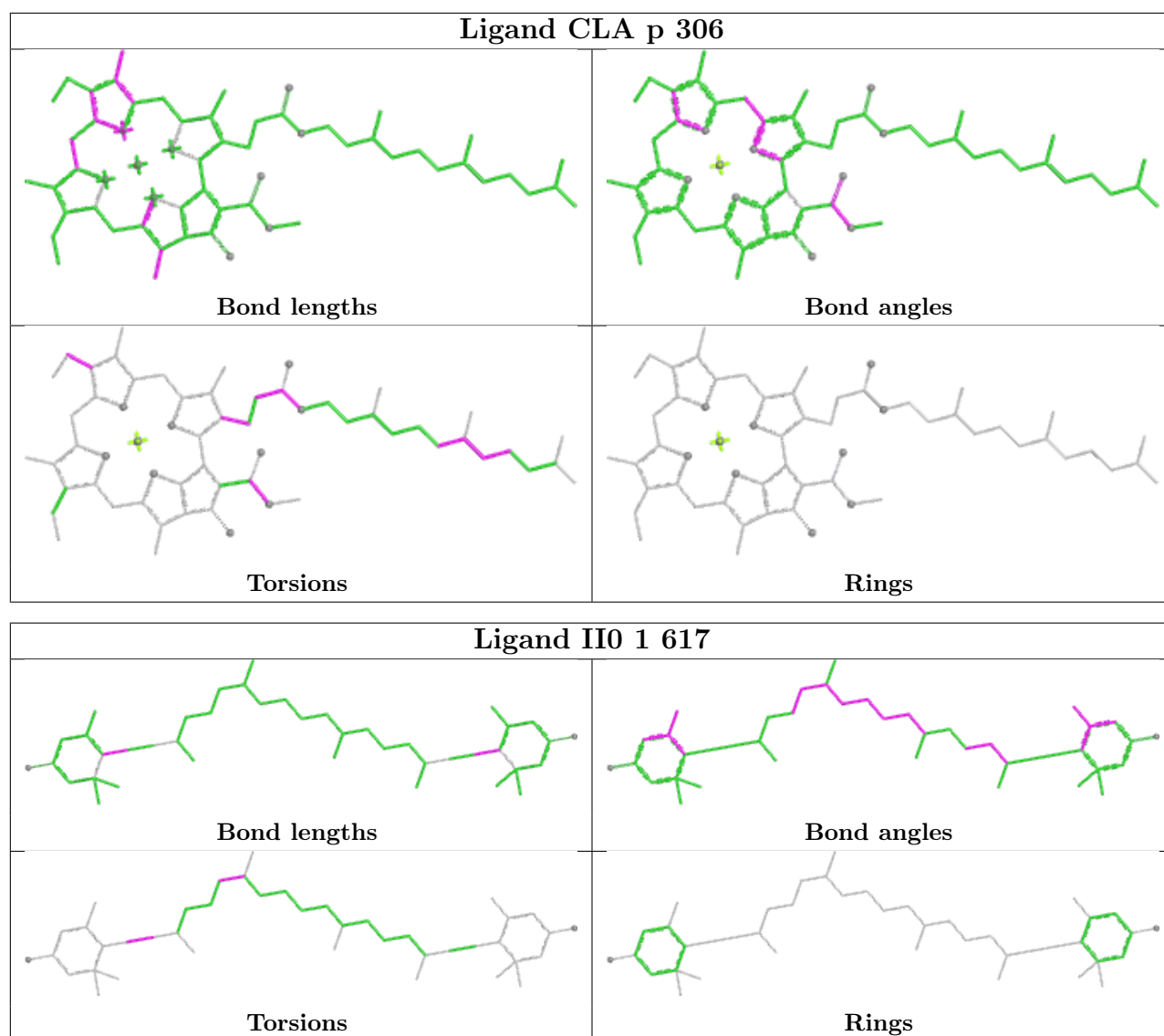
Rings

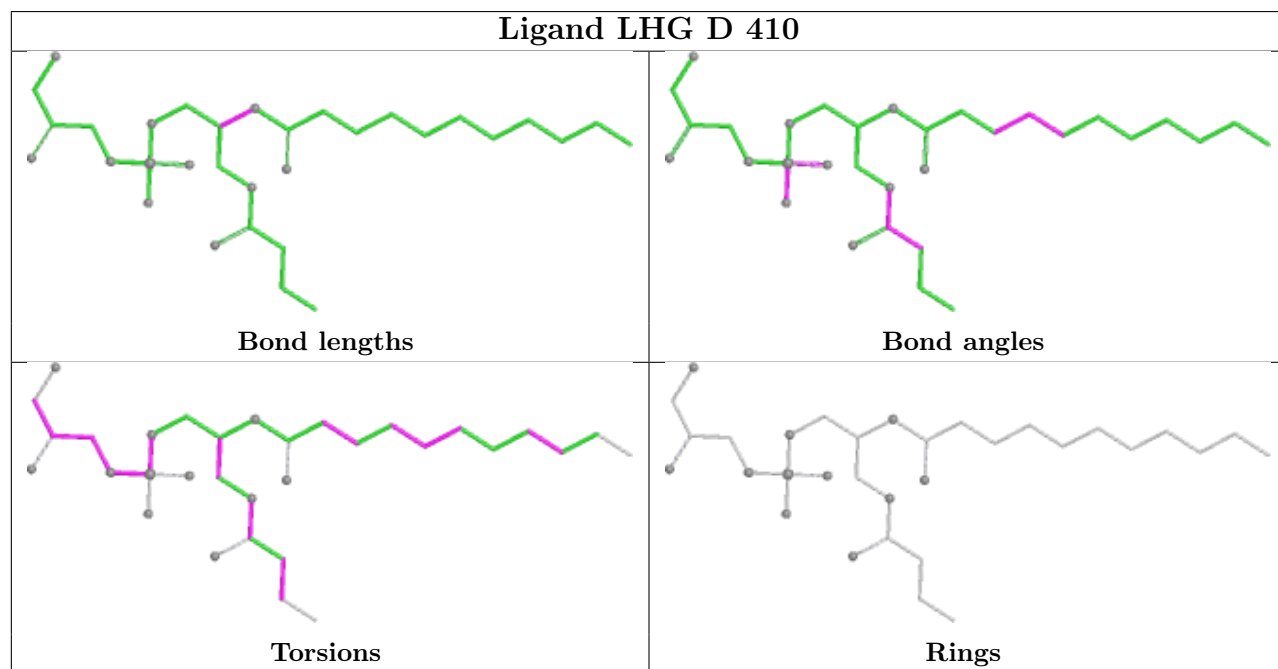
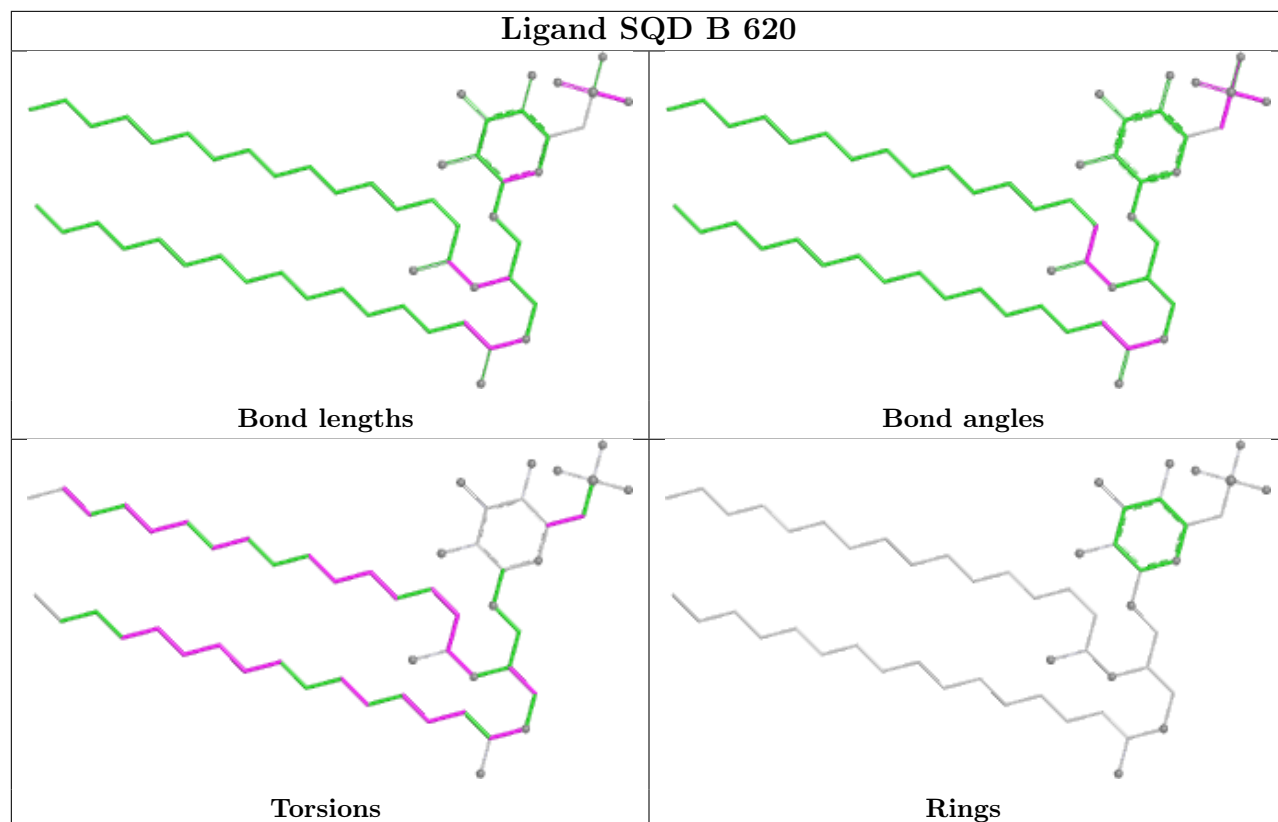
Ligand CLA 6 610



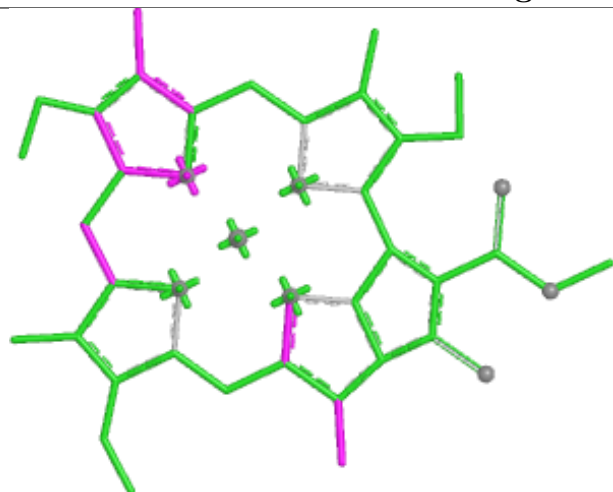
Ligand II0 8 613



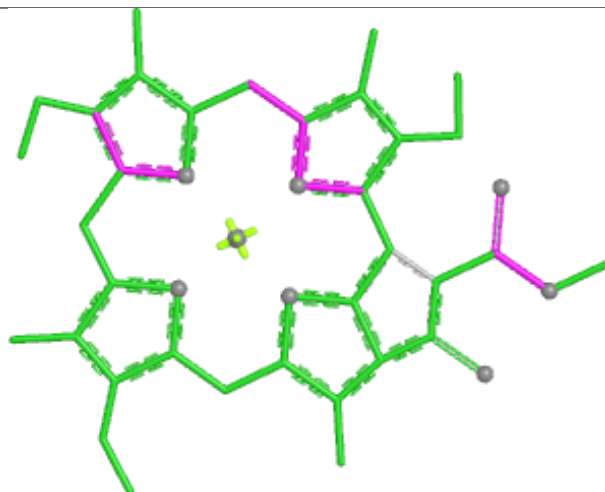




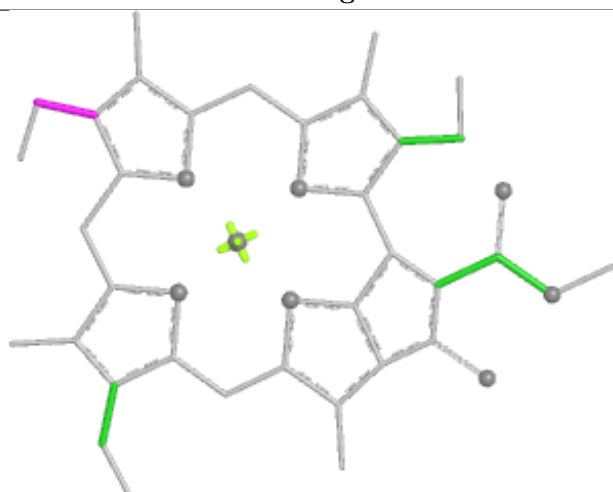
Ligand CLA P 601



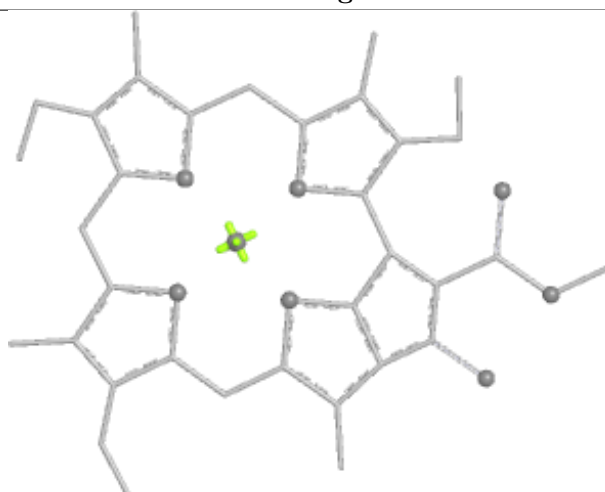
Bond lengths



Bond angles

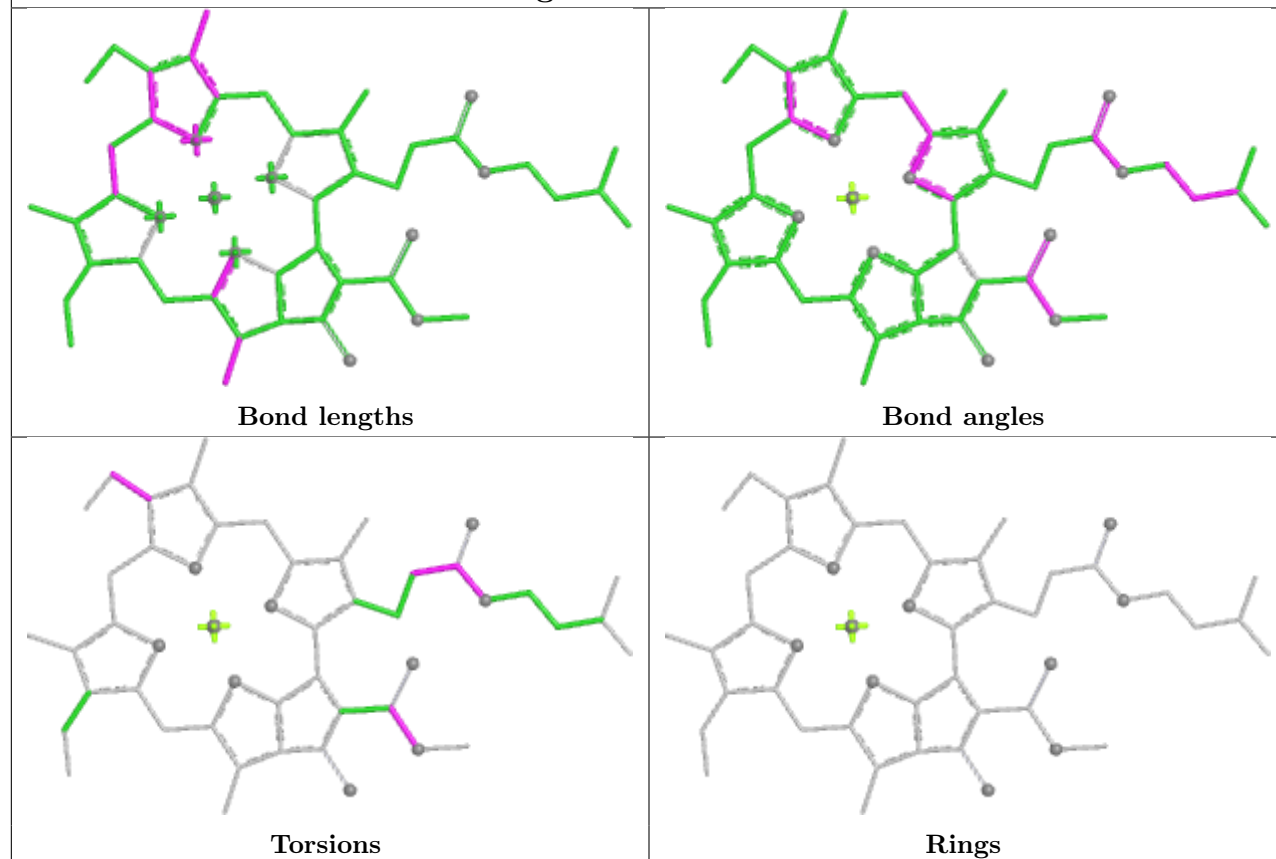


Torsions

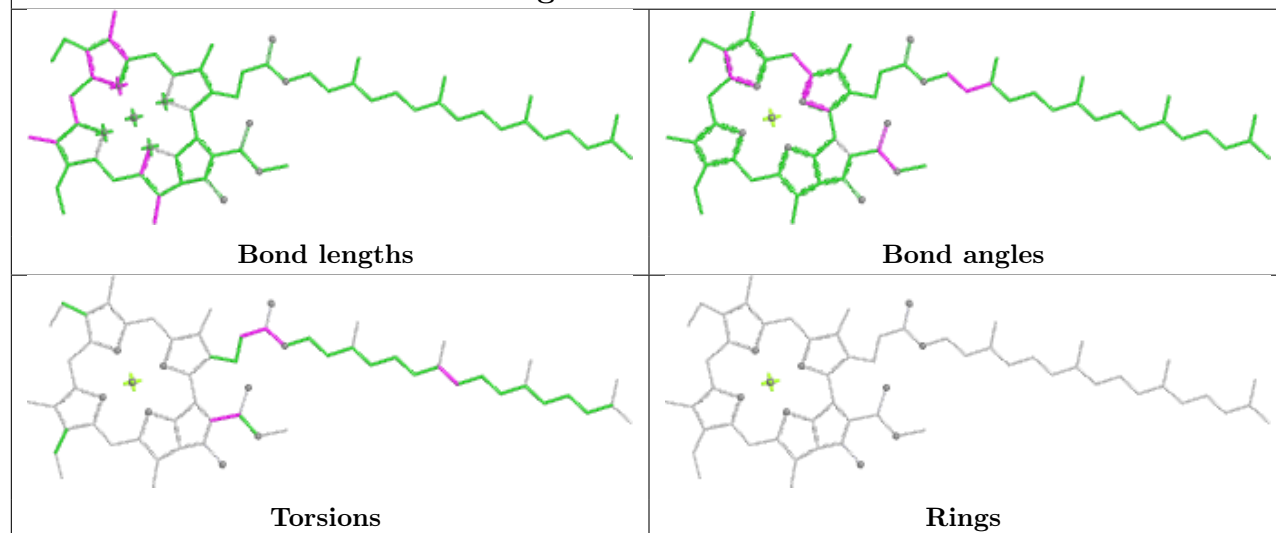


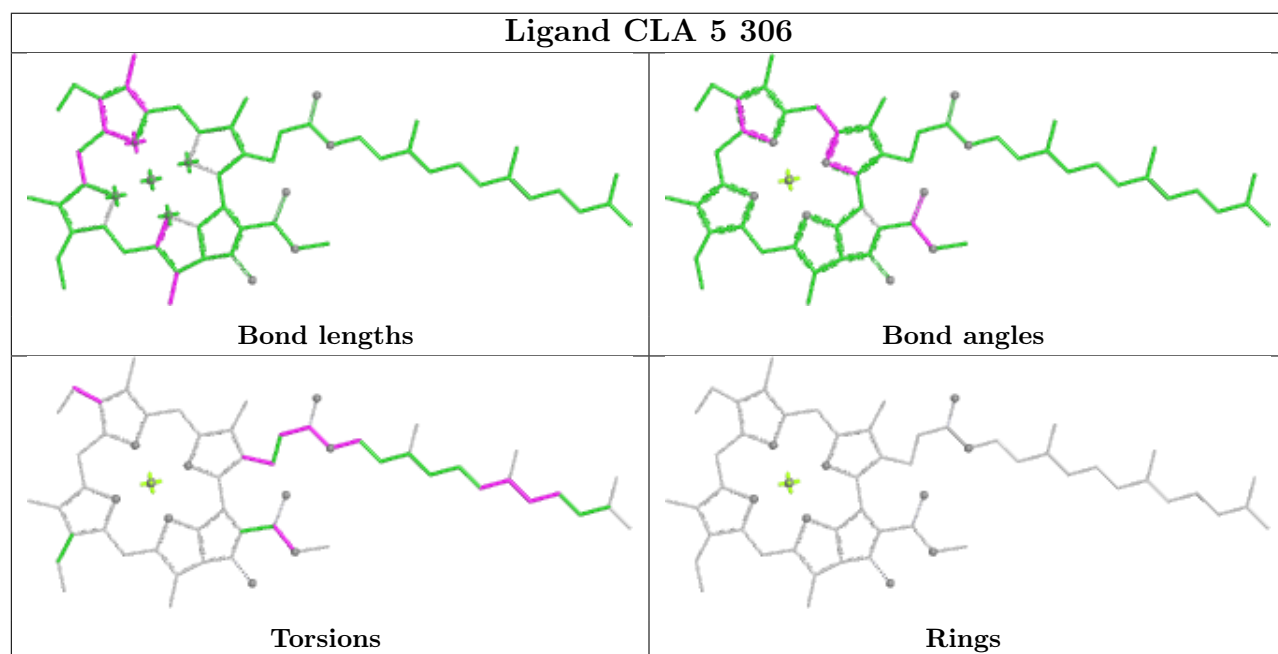
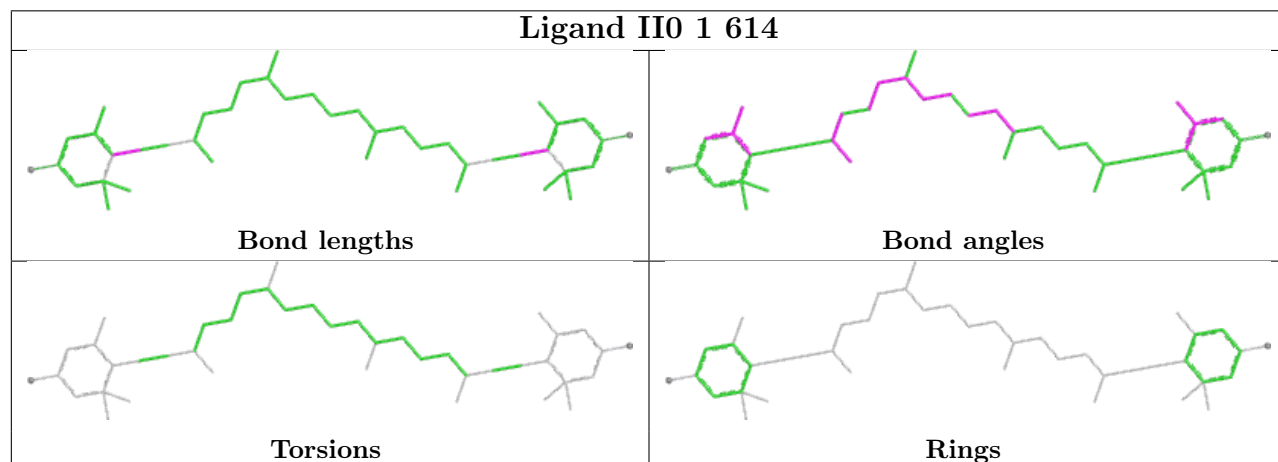
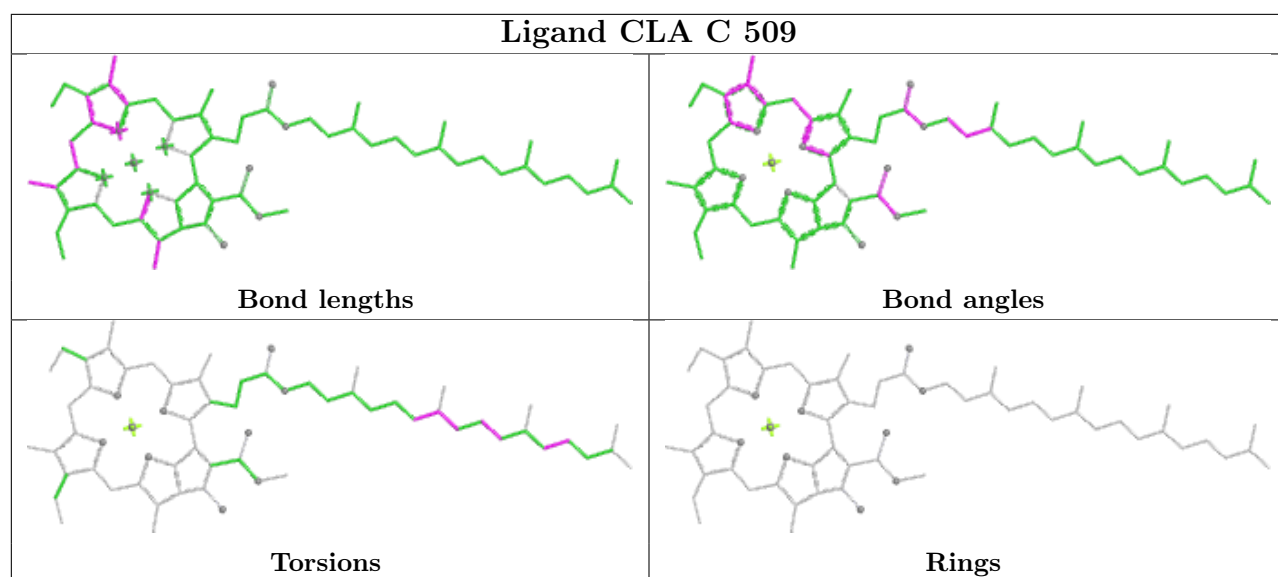
Rings

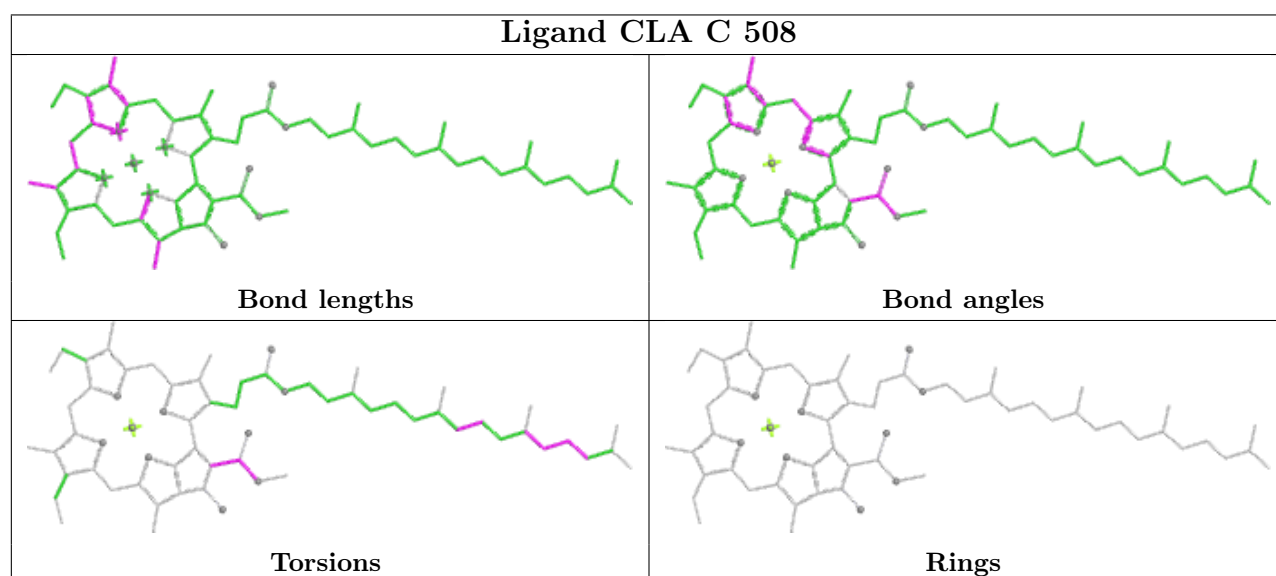
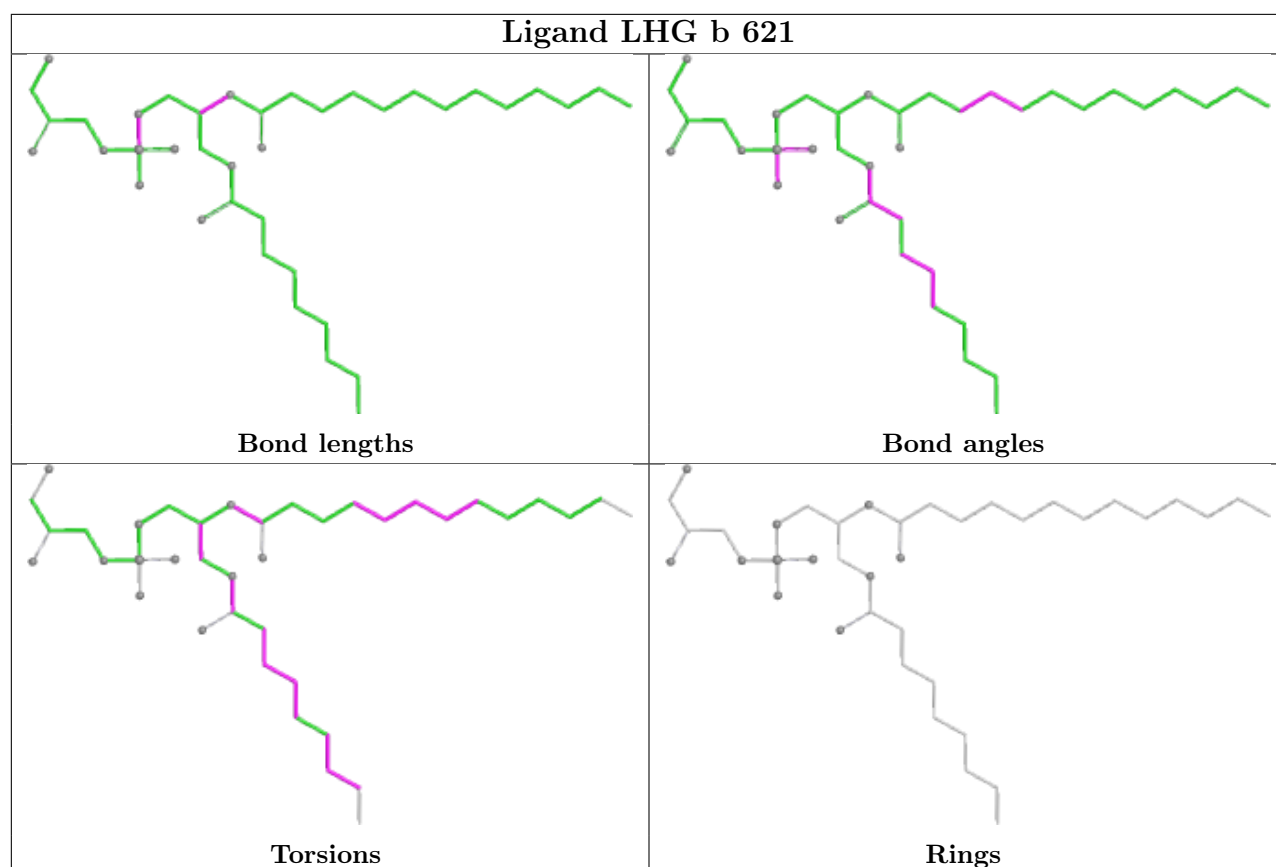
Ligand CLA 0 605

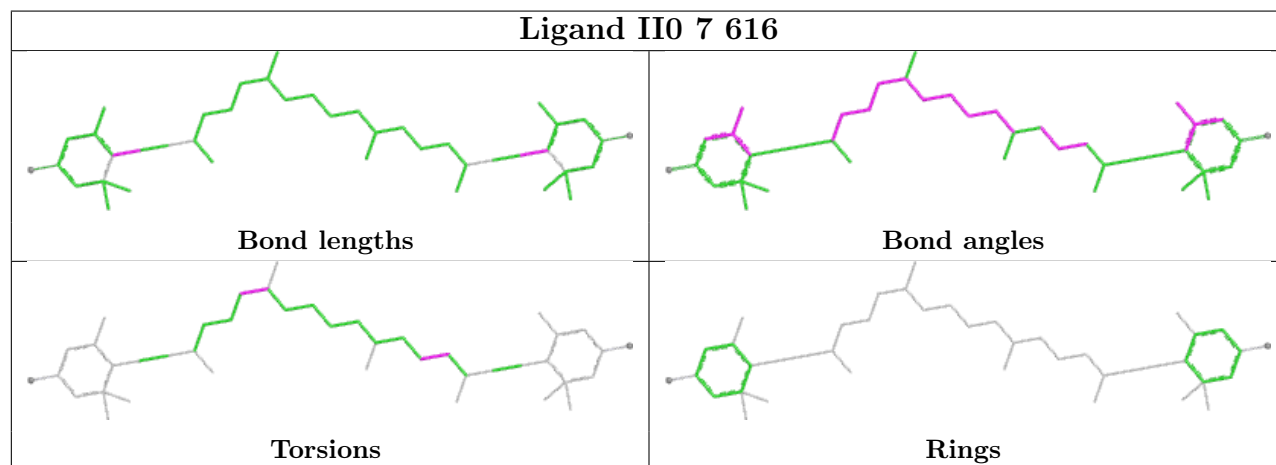
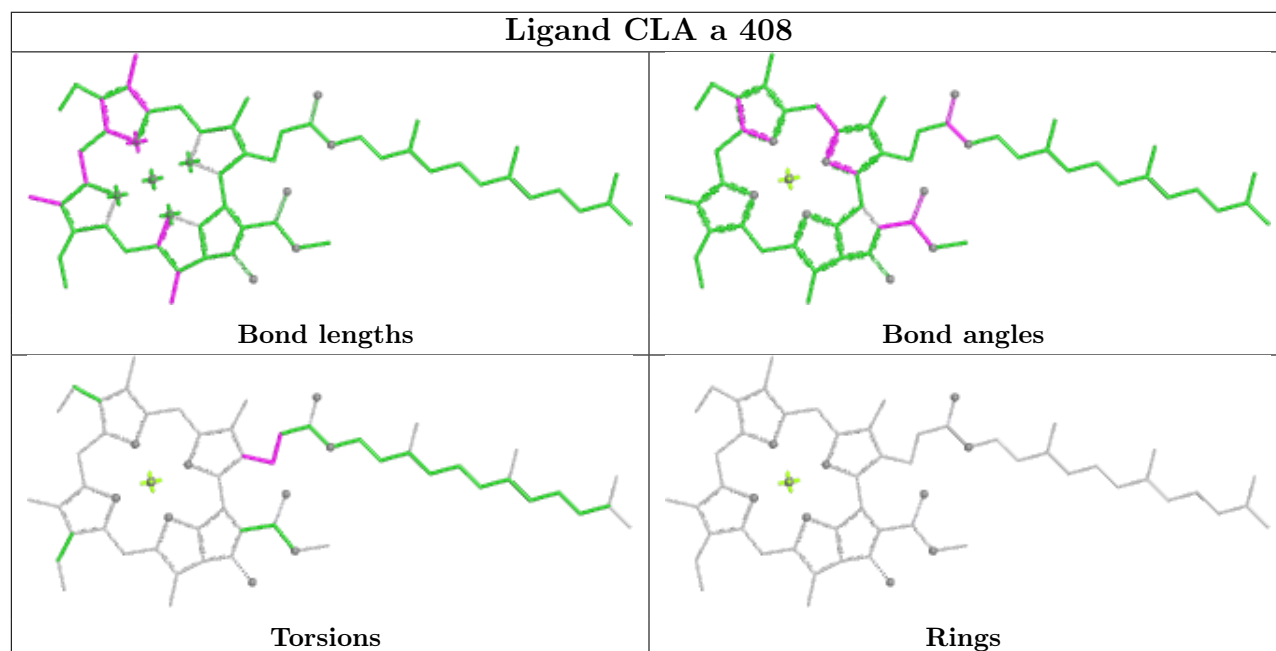
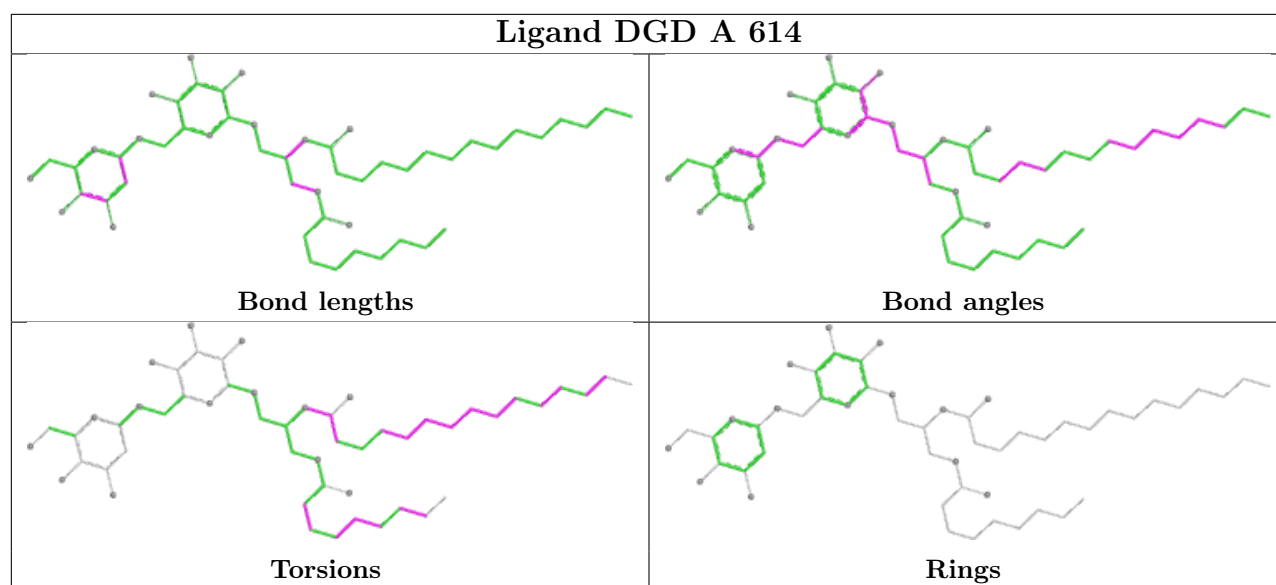


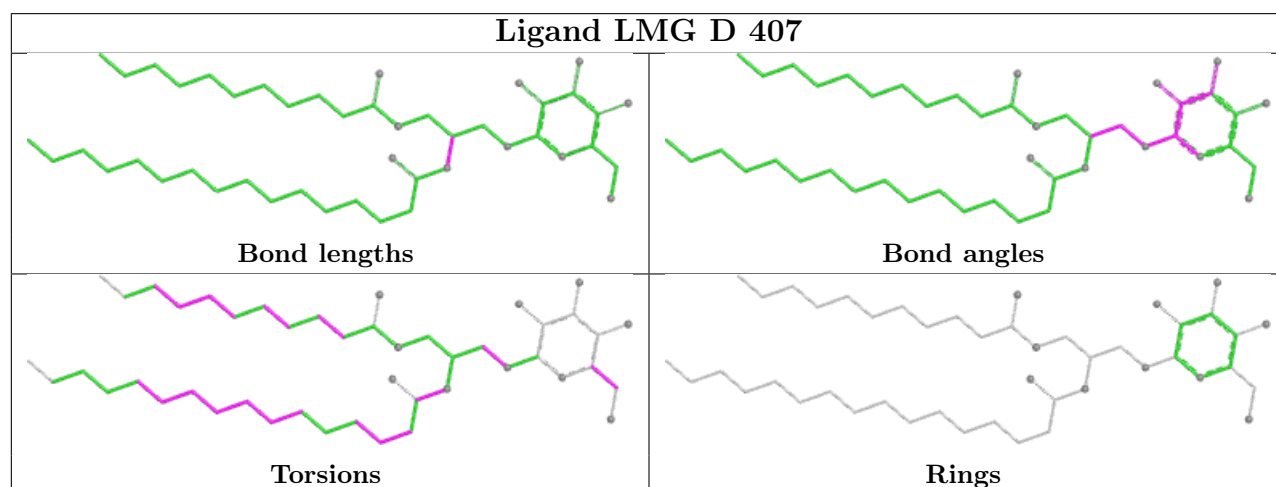
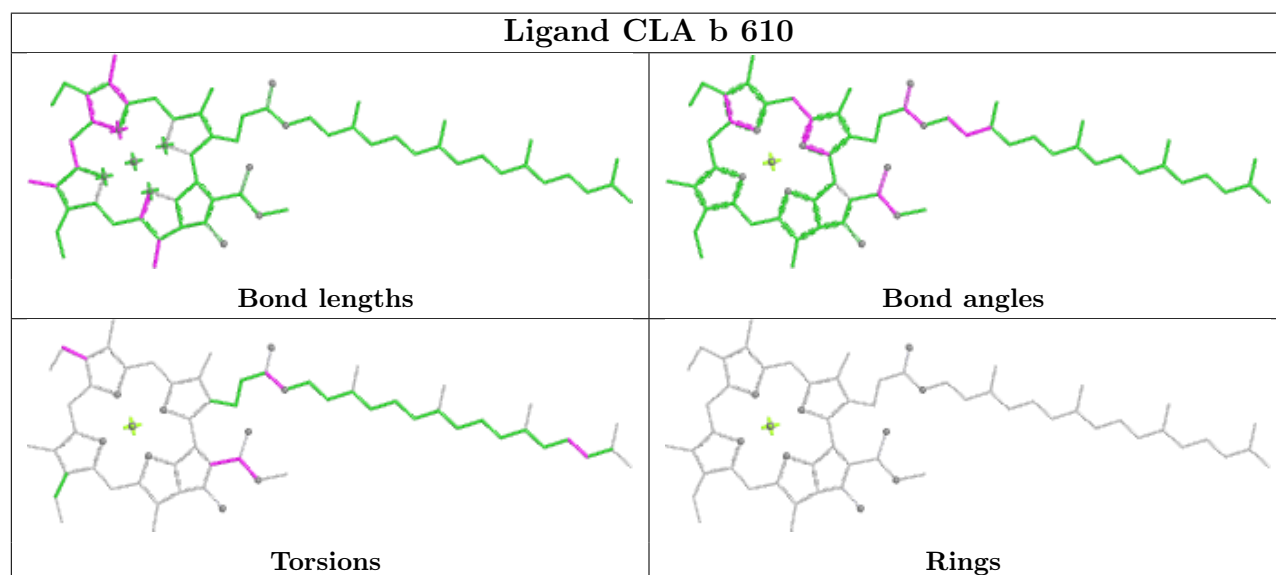
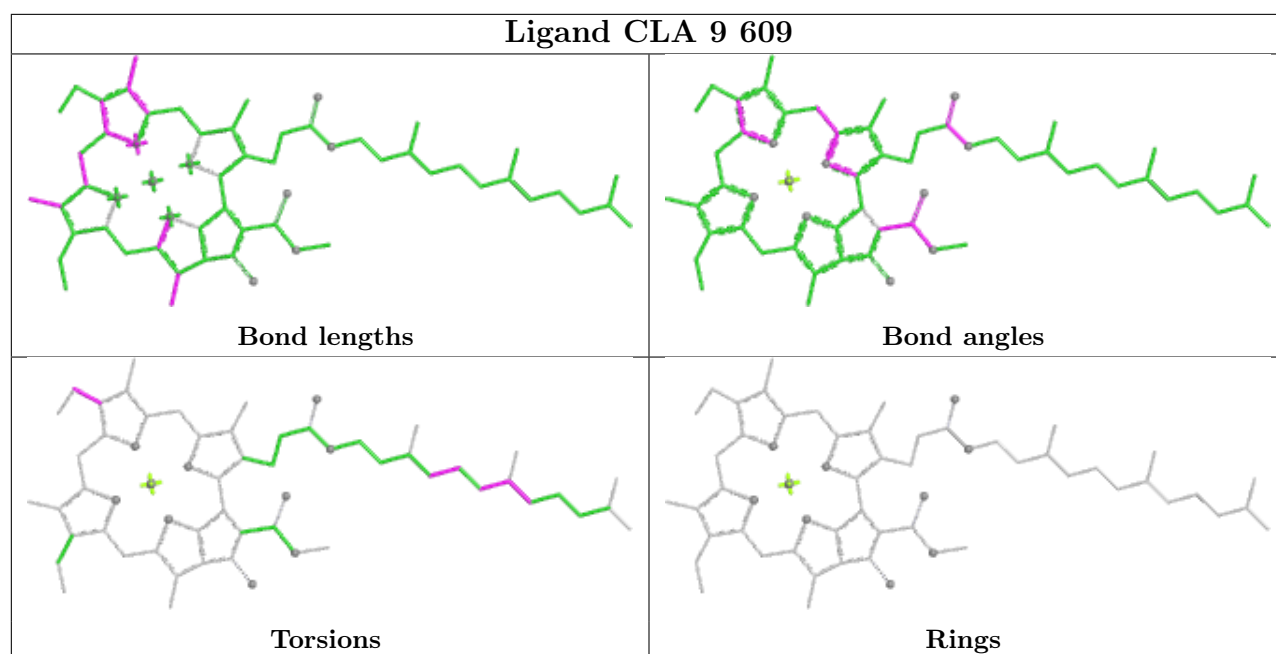
Ligand CLA c 510

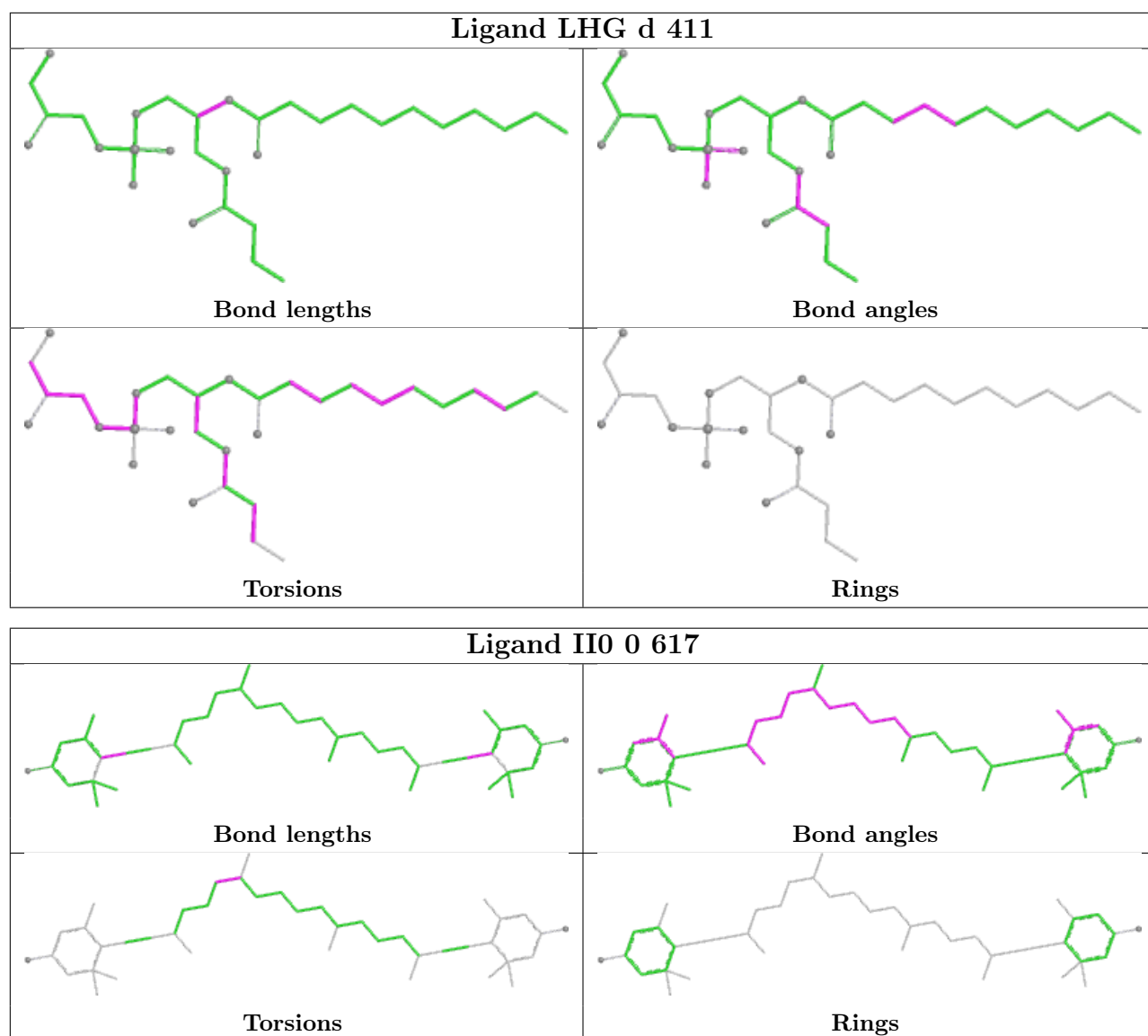




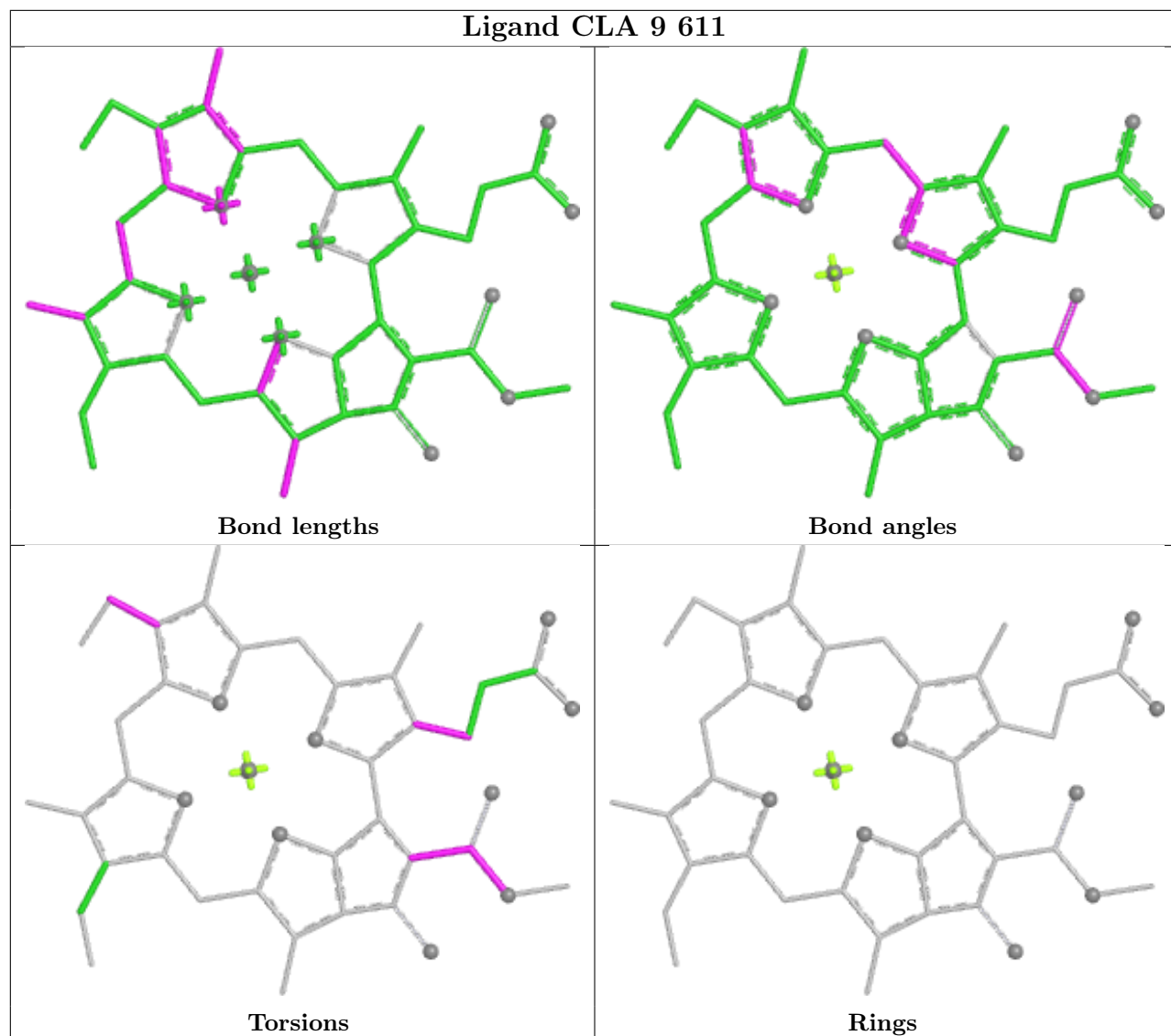




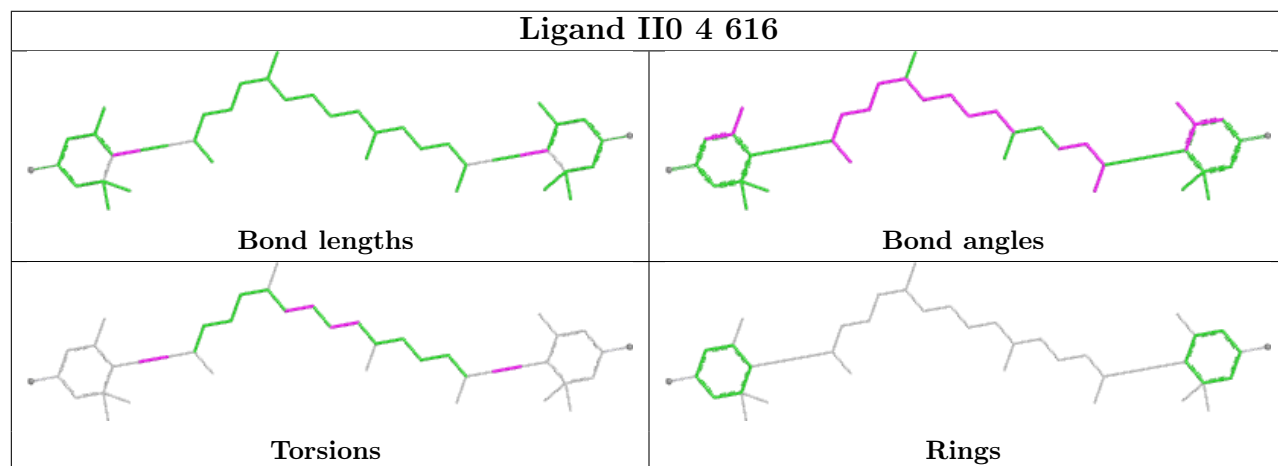


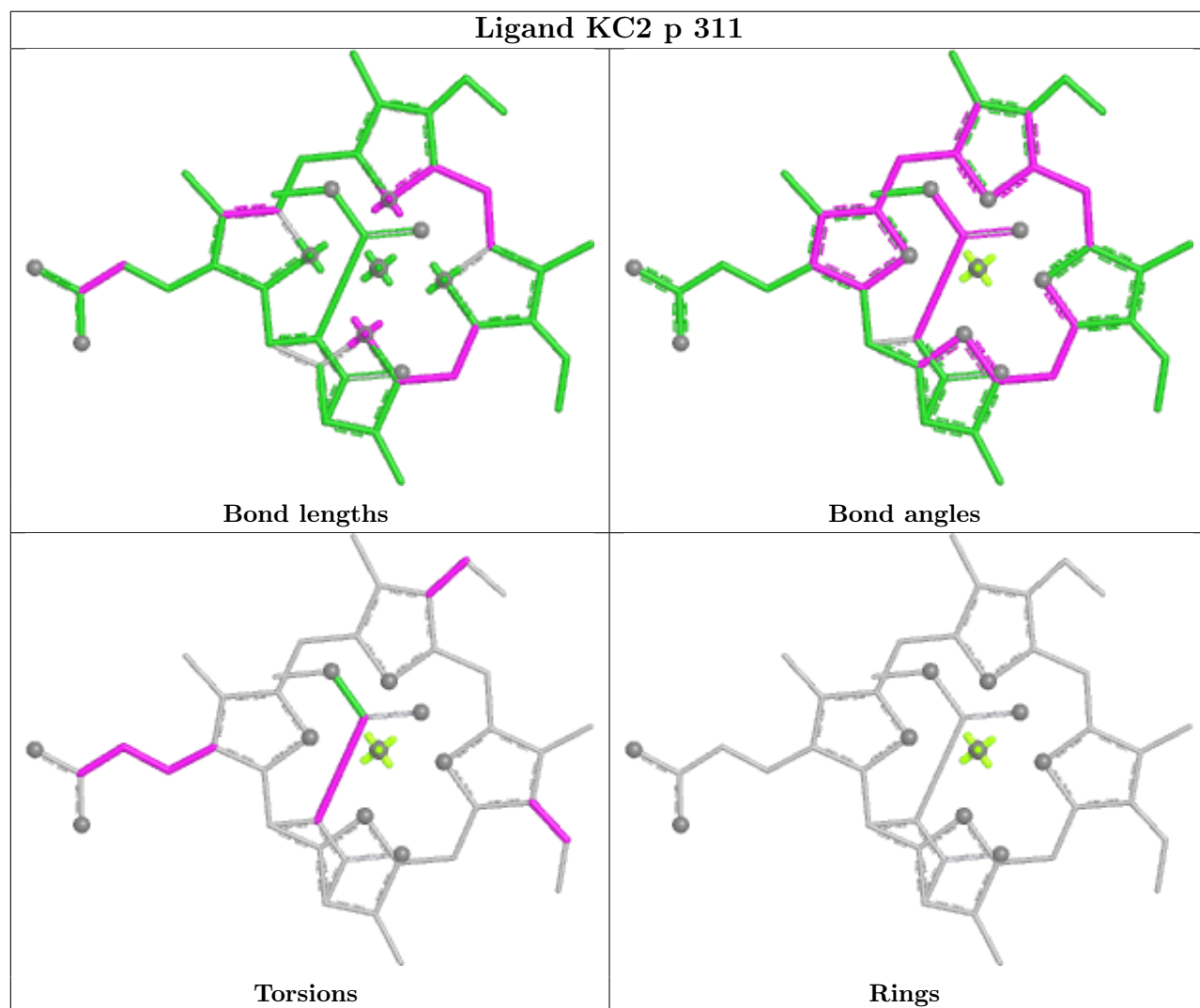
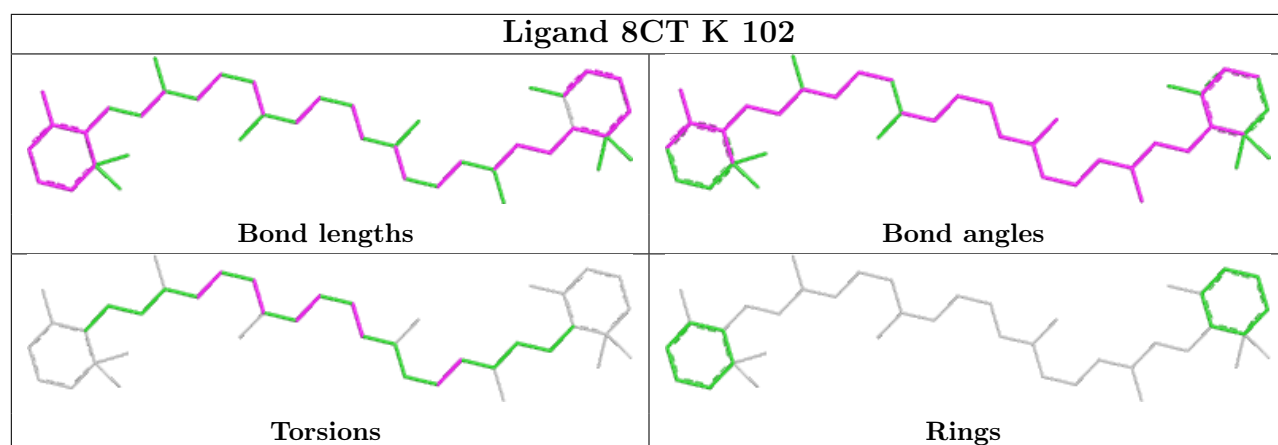


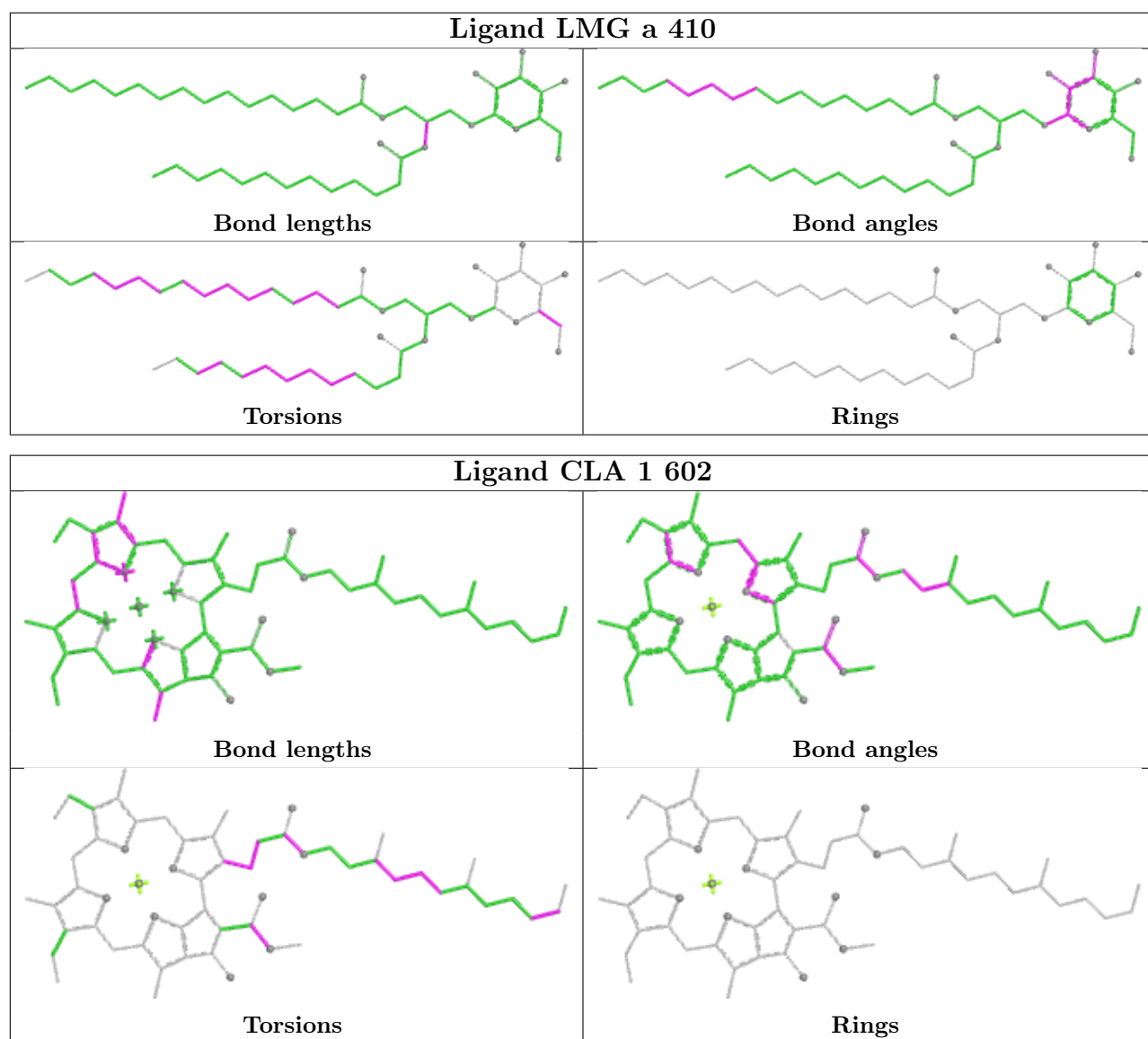
Ligand CLA 9 611



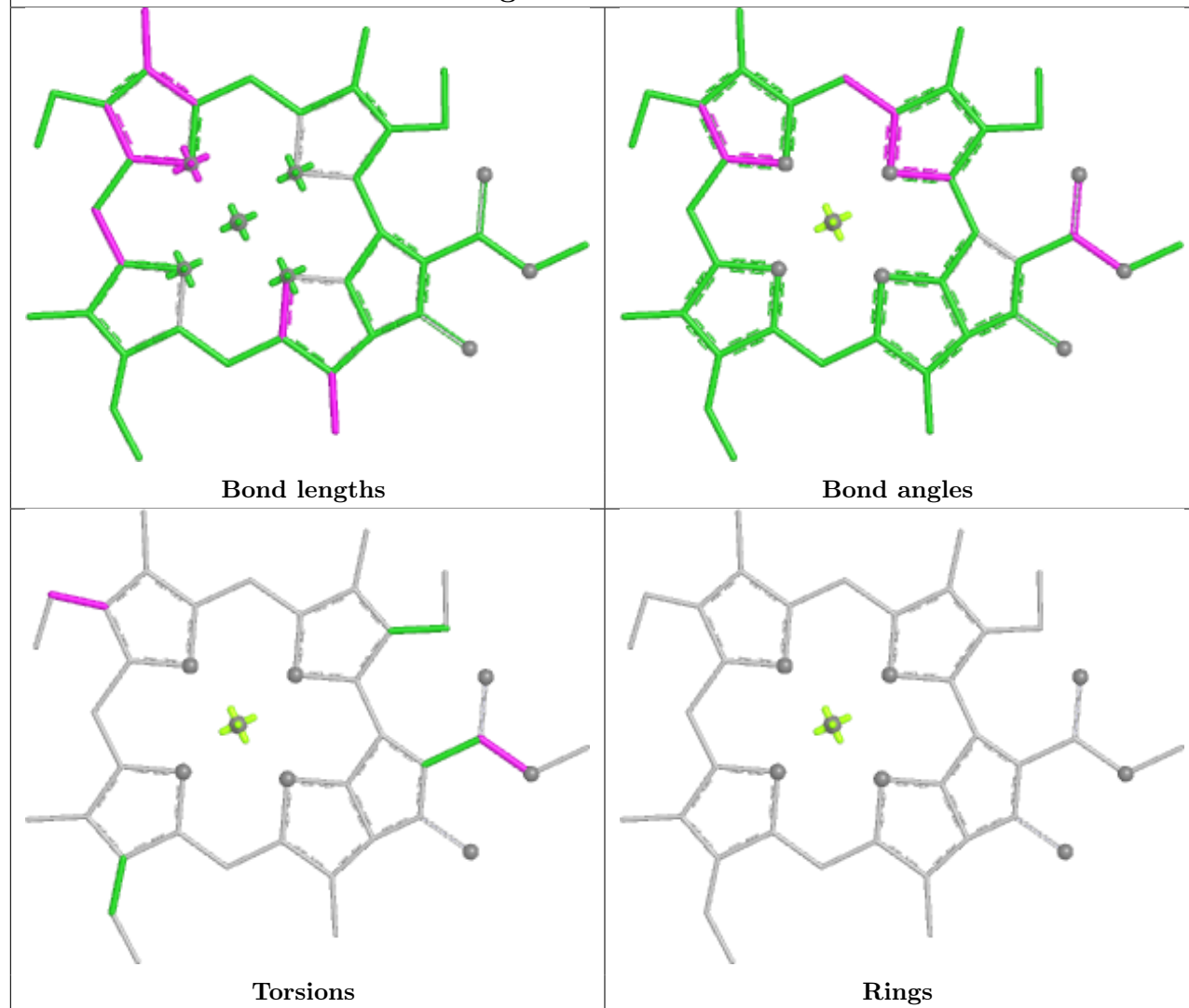
Ligand II0 4 616



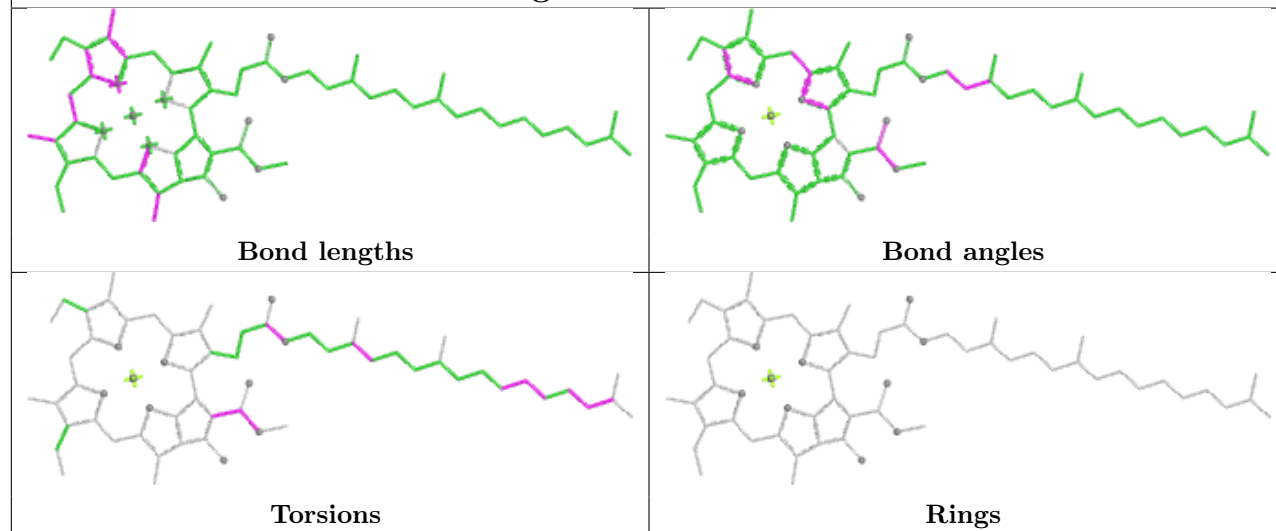


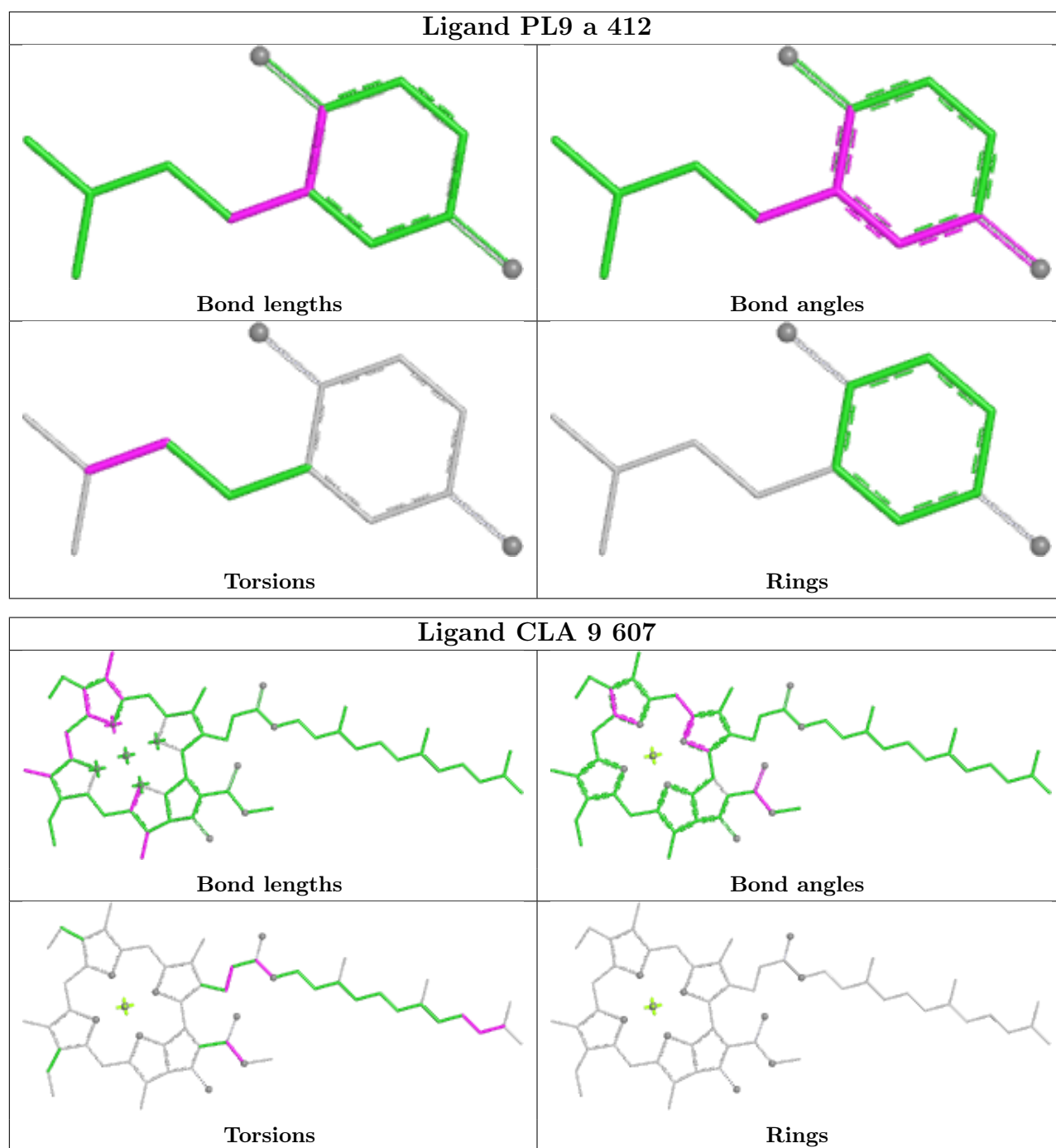


Ligand CLA 2 601

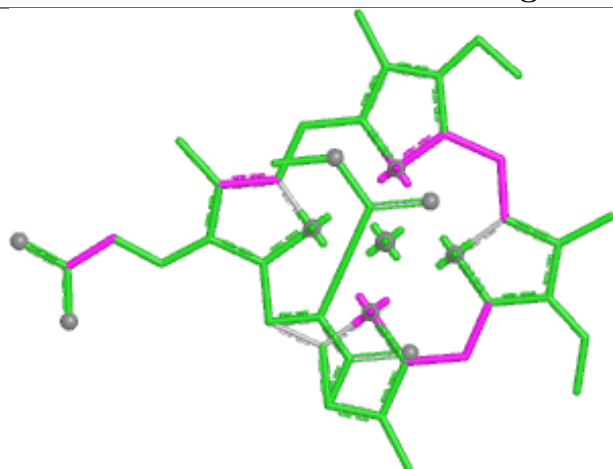


Ligand CLA B 615

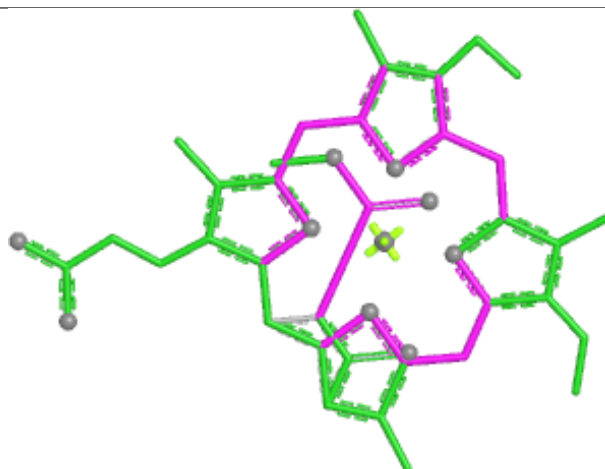




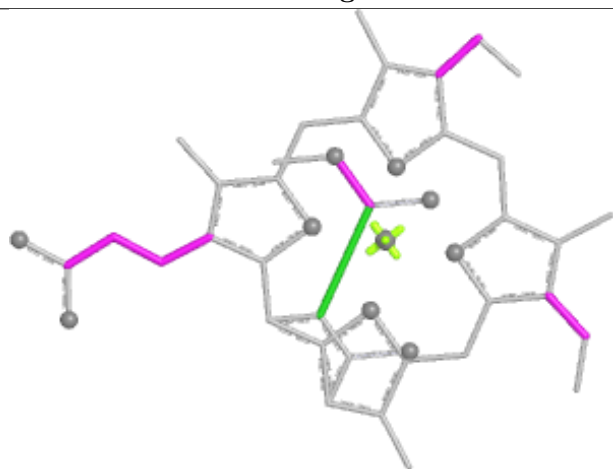
Ligand KC2 2 610



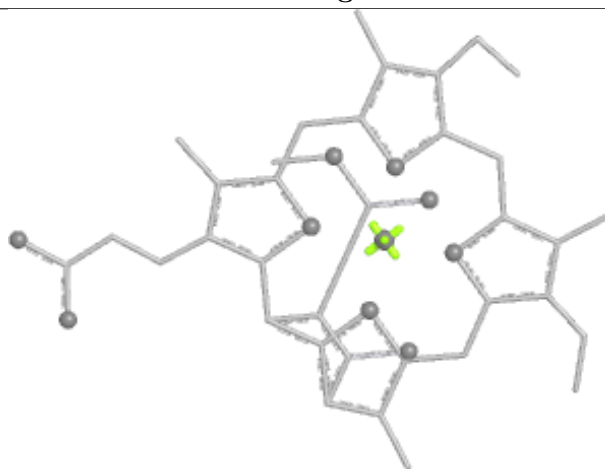
Bond lengths



Bond angles

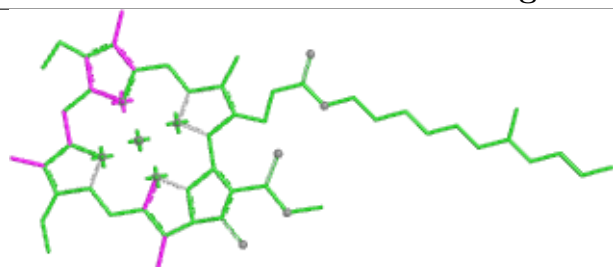


Torsions

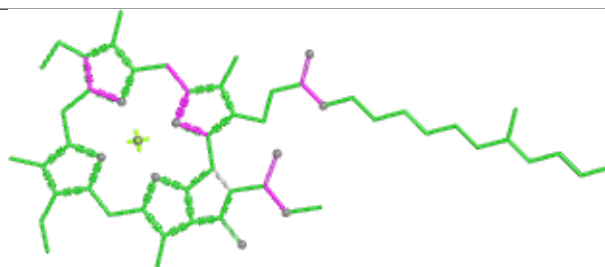


Rings

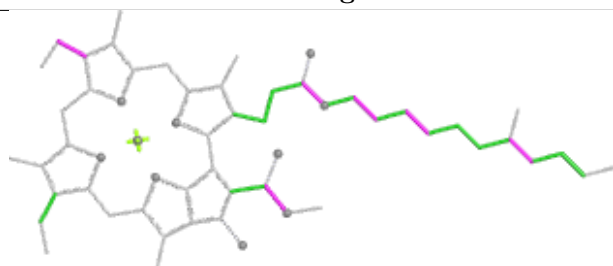
Ligand CLA c 512



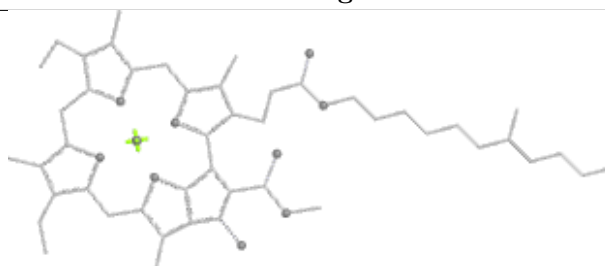
Bond lengths



Bond angles

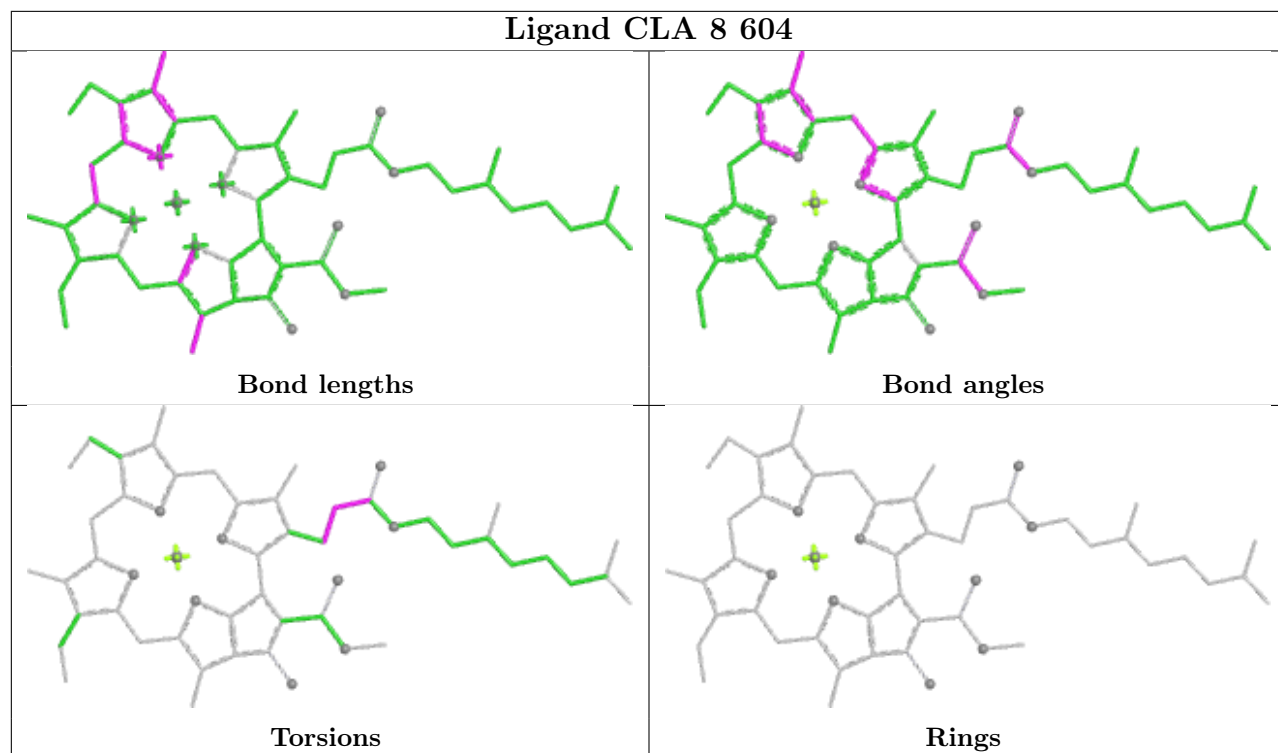


Torsions

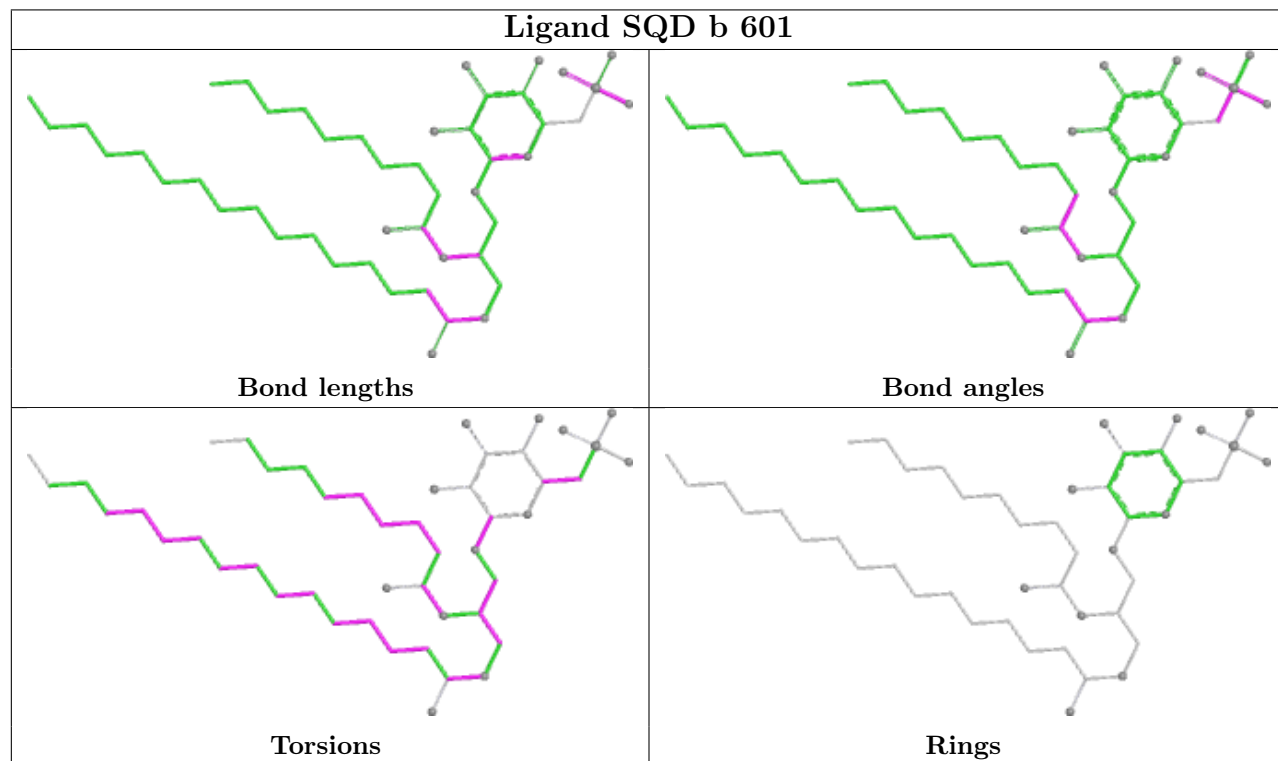


Rings

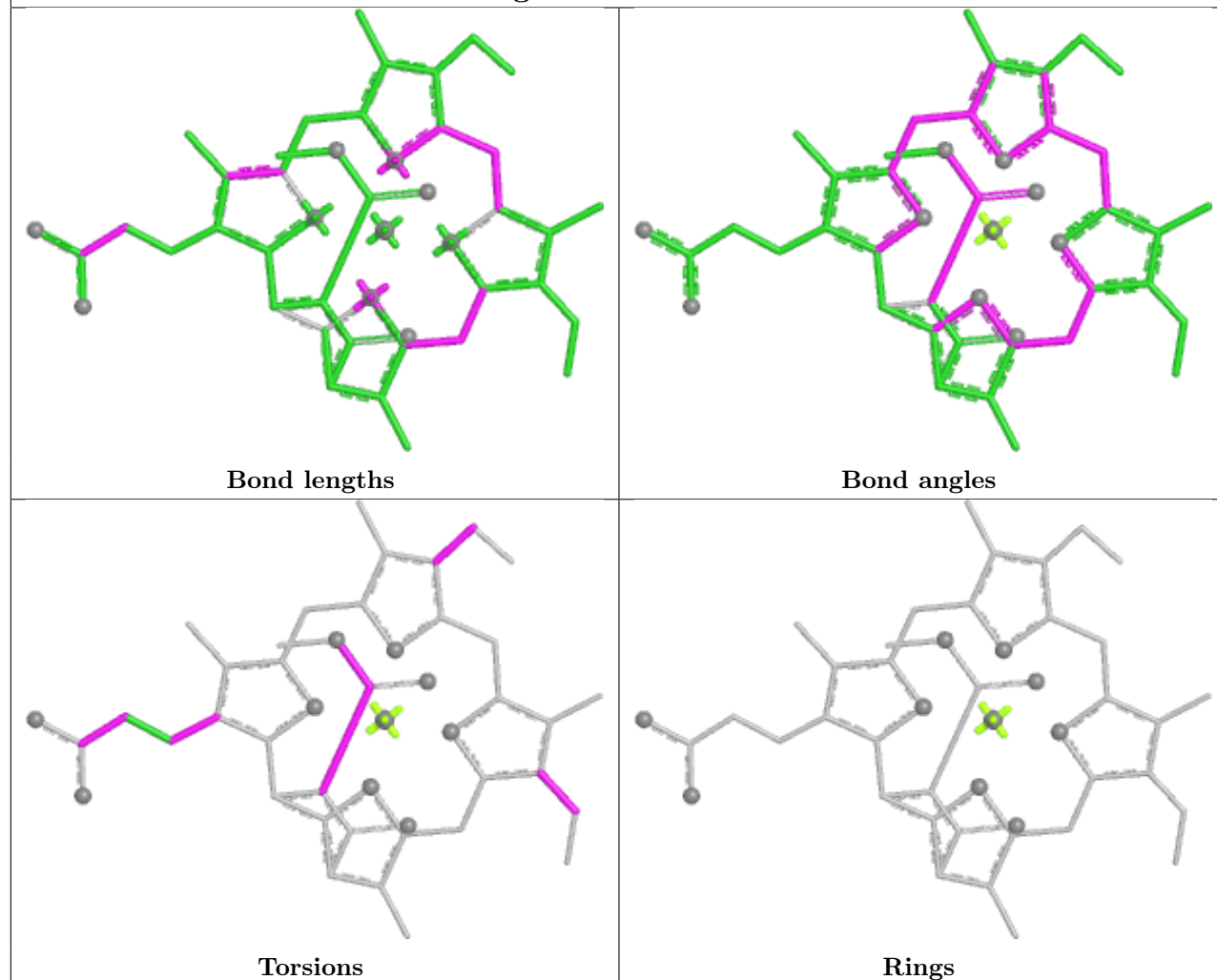
Ligand CLA 8 604



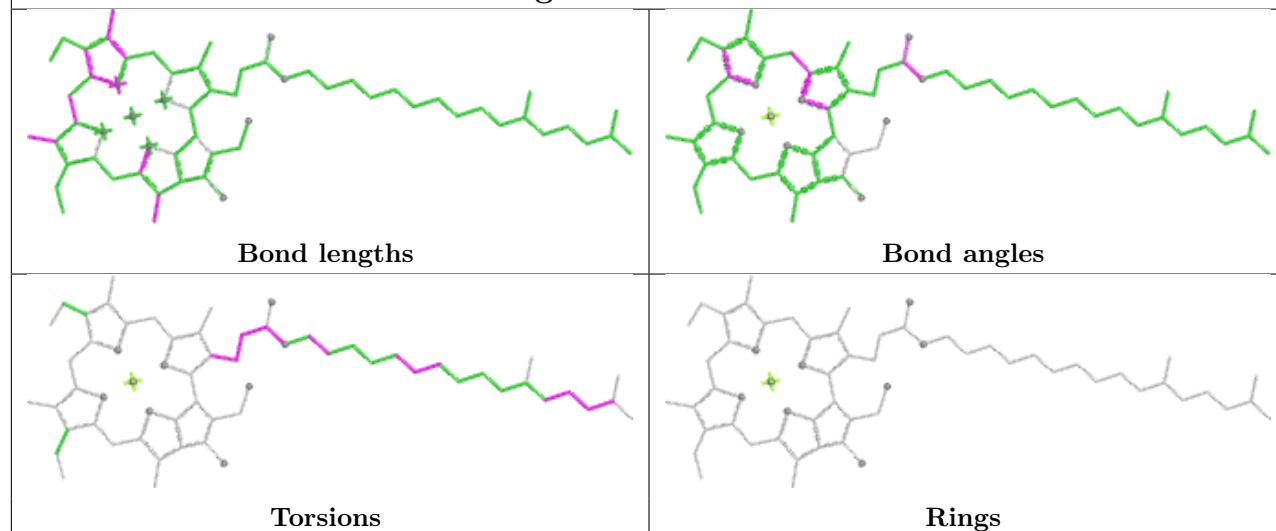
Ligand SQD b 601



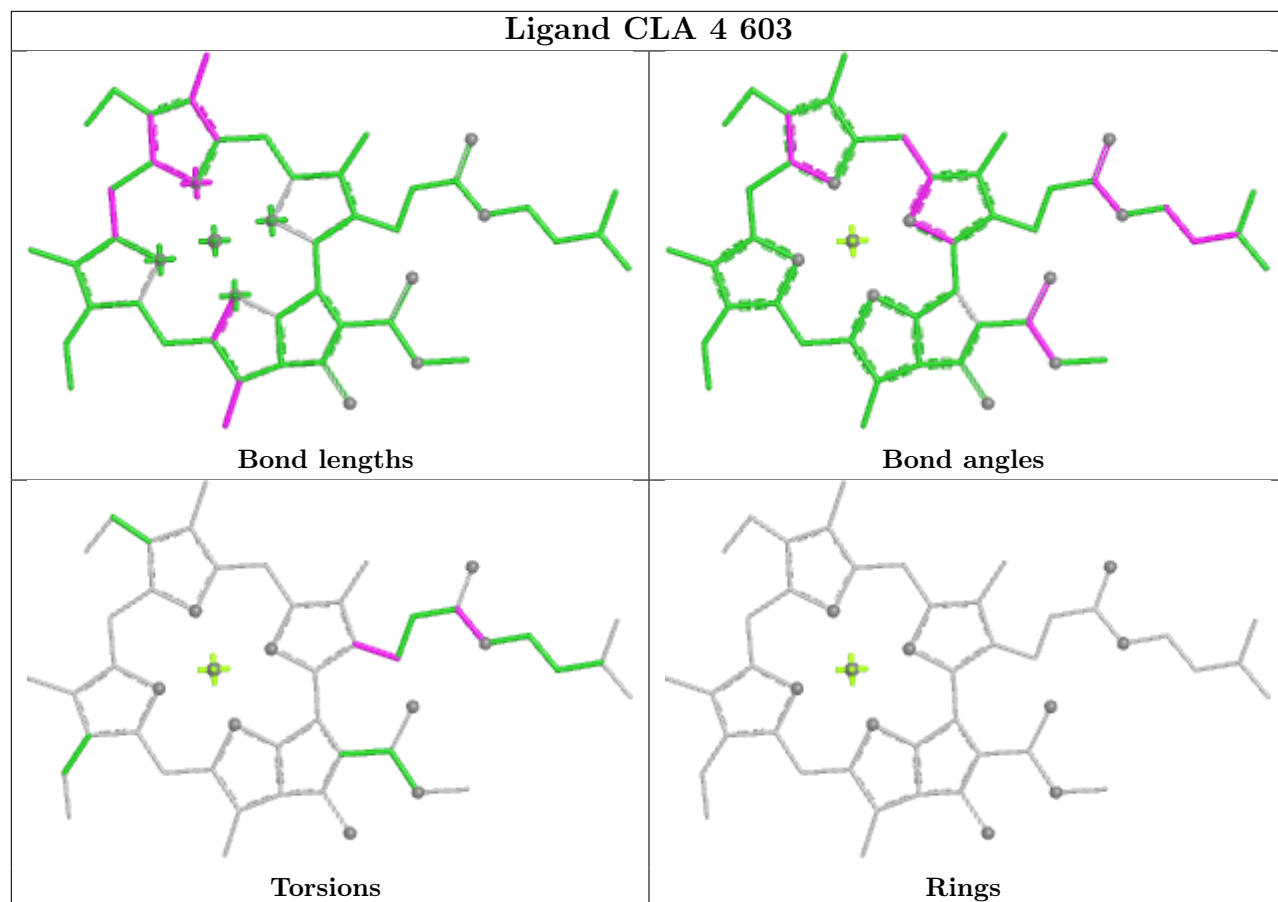
Ligand KC2 1 610



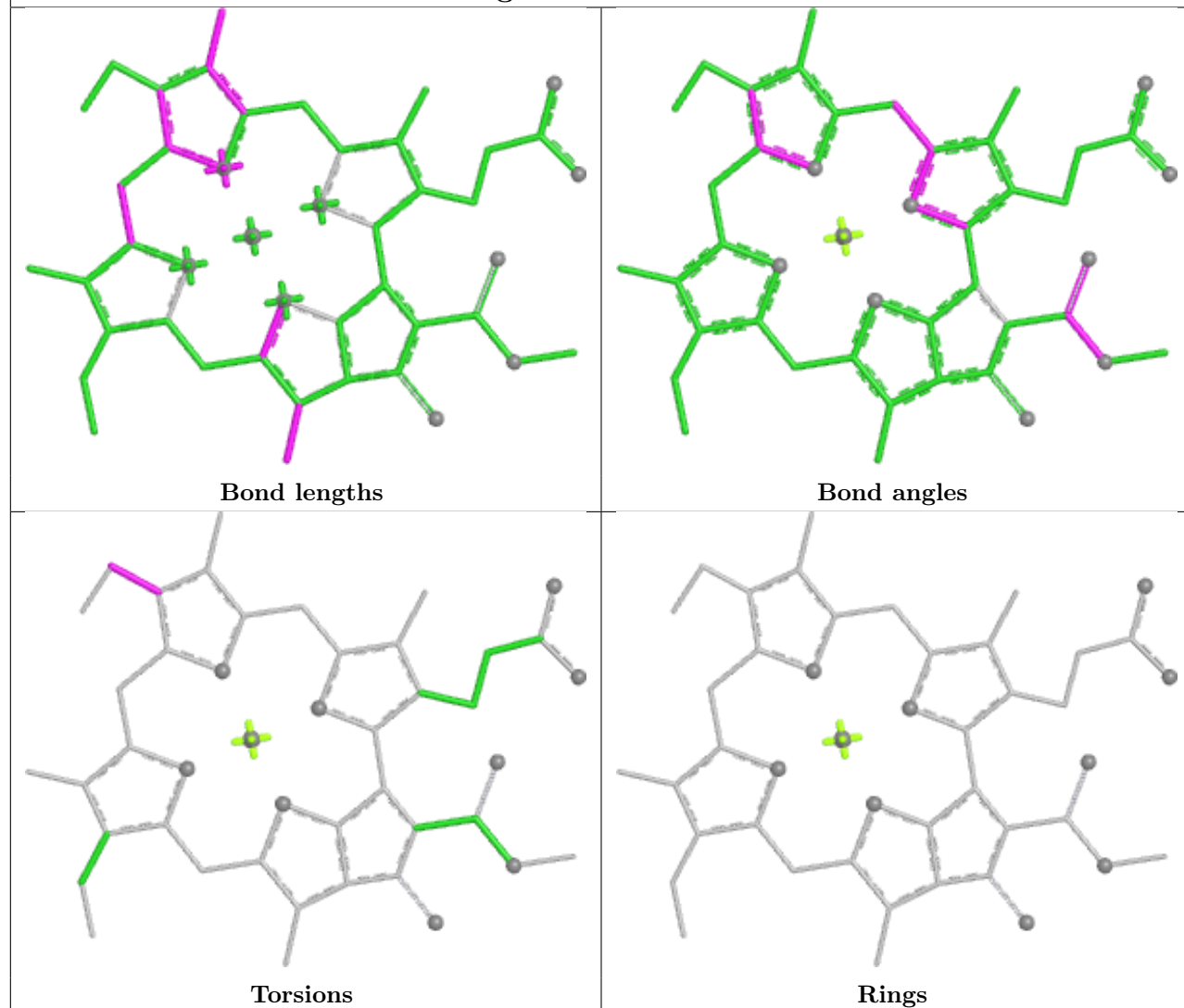
Ligand CLA b 603



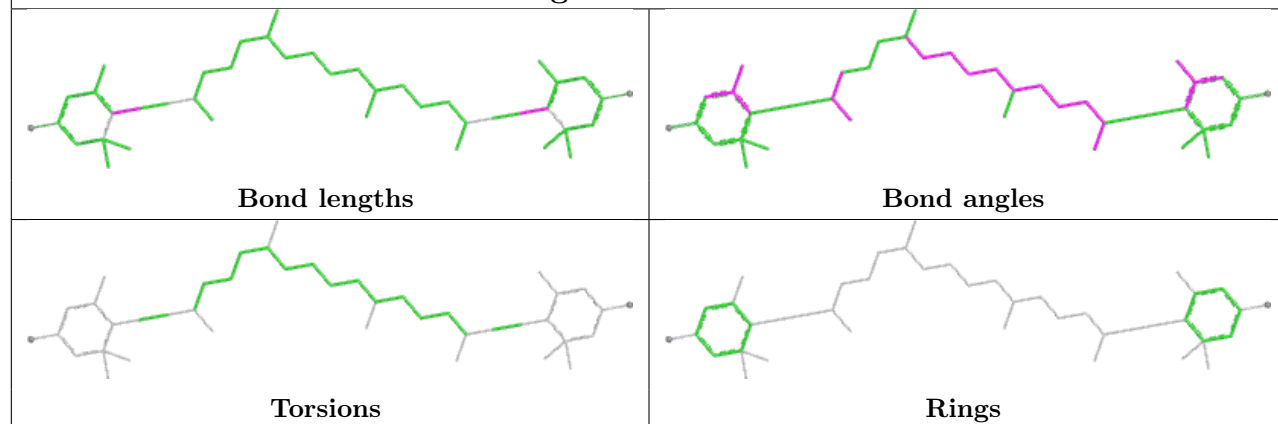
Ligand CLA 4 603

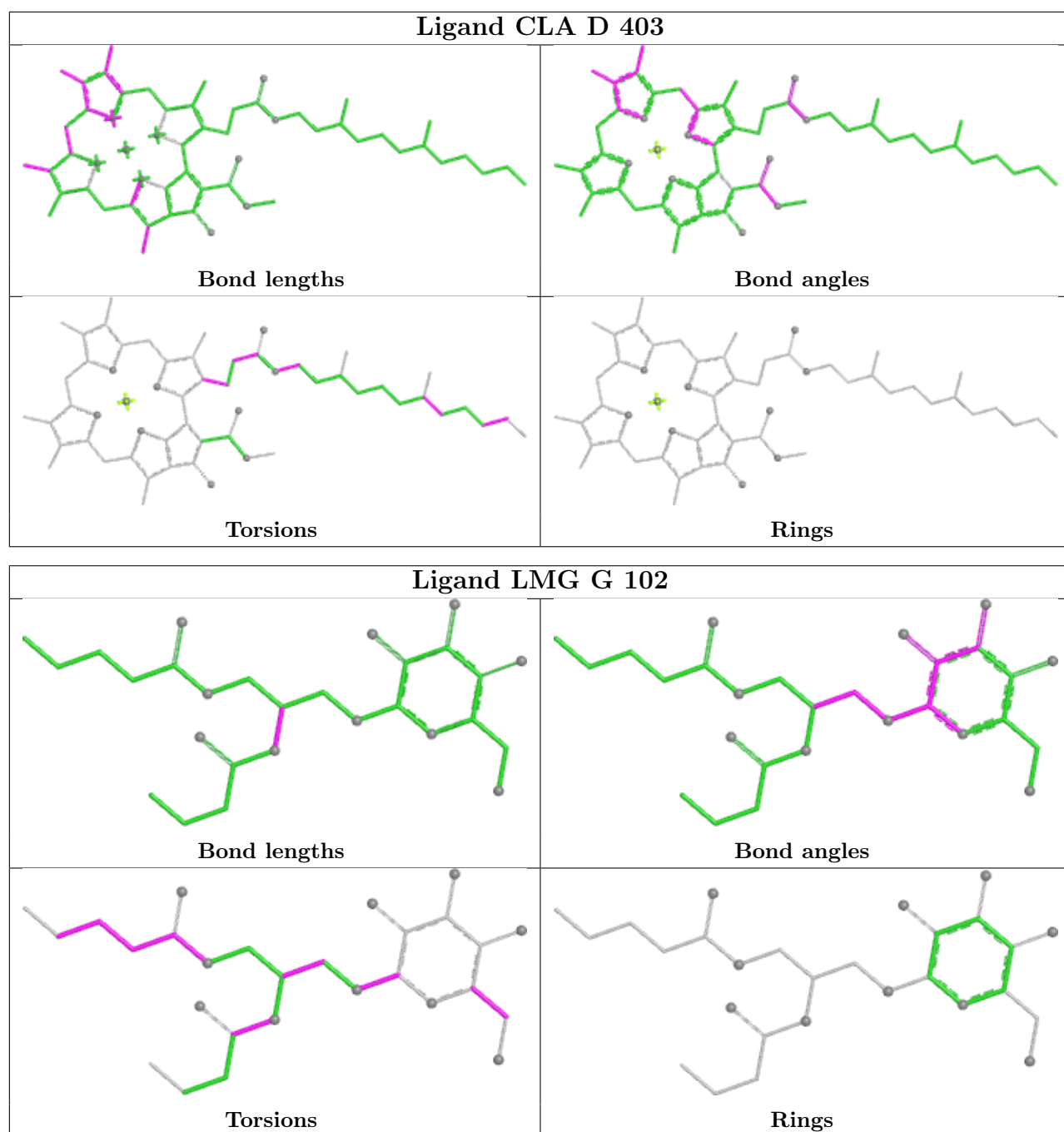


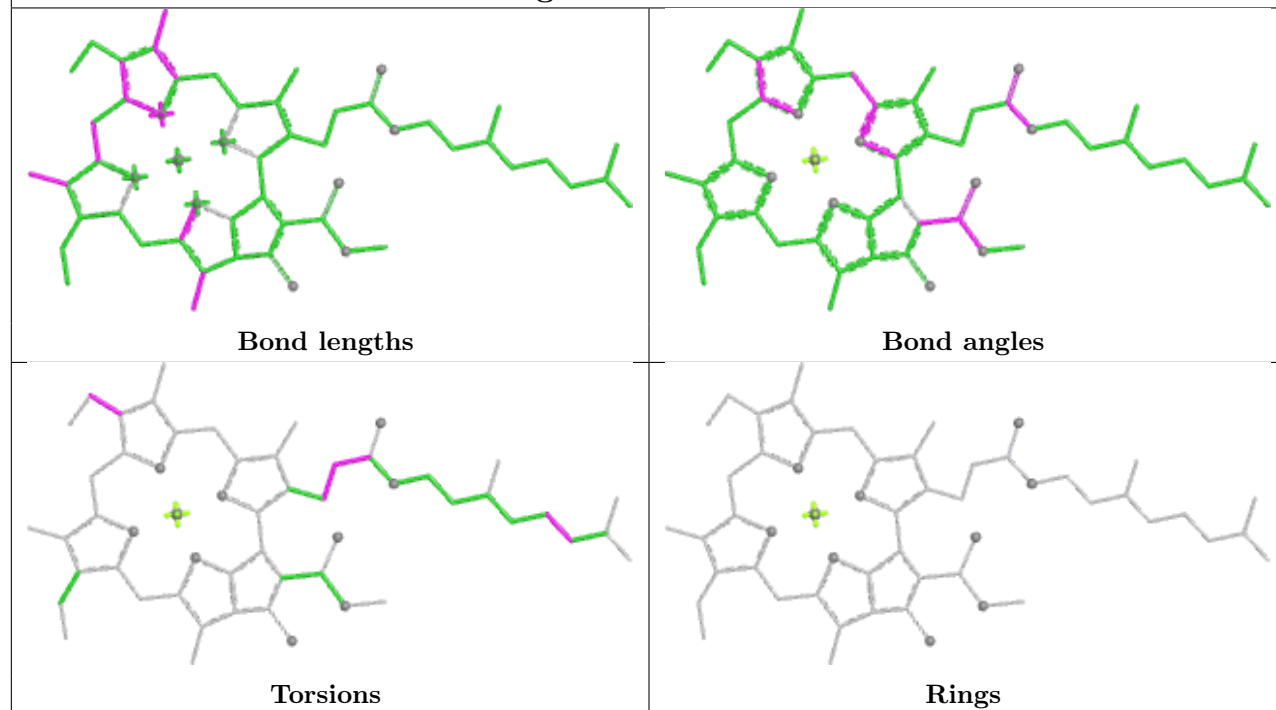
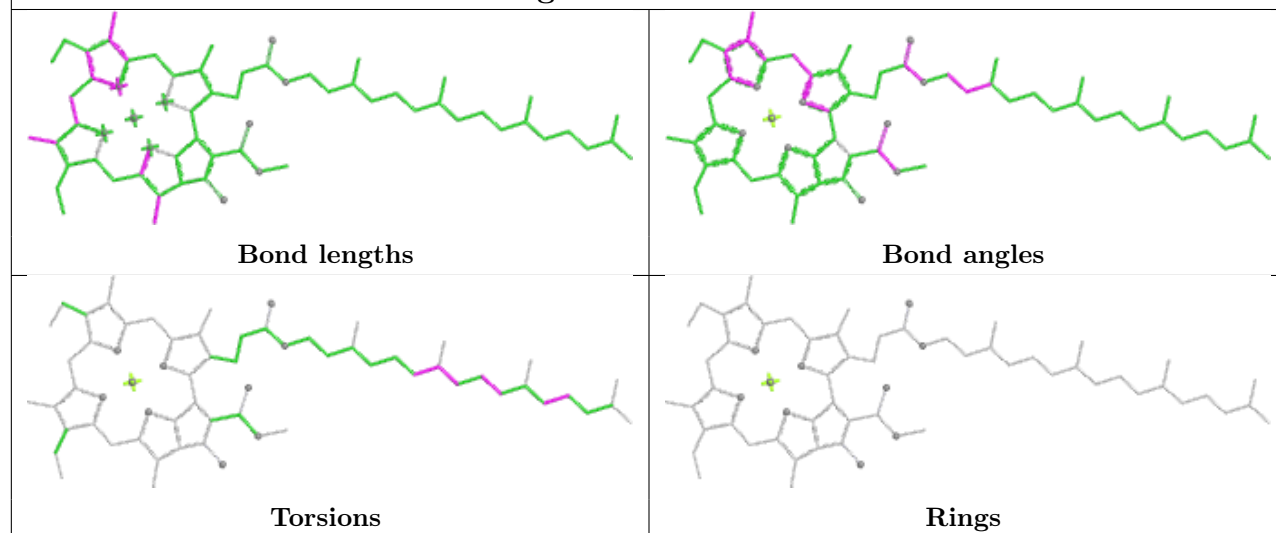
Ligand CLA 0 607



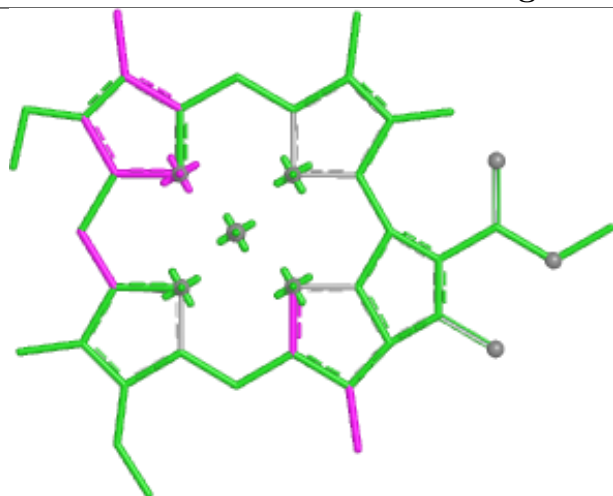
Ligand II0 8 614



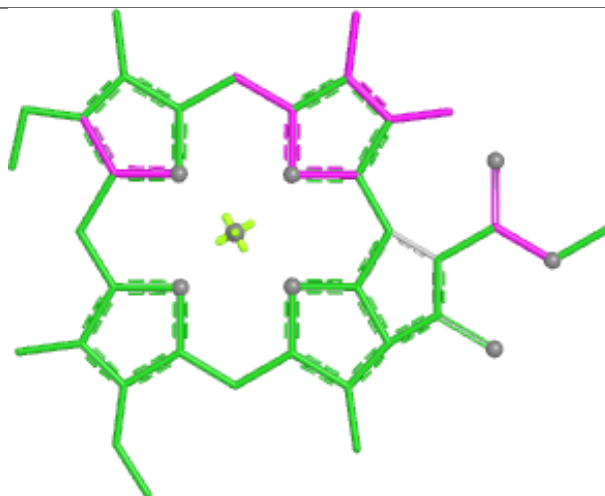


Ligand CLA 3 604**Ligand CLA c 509**

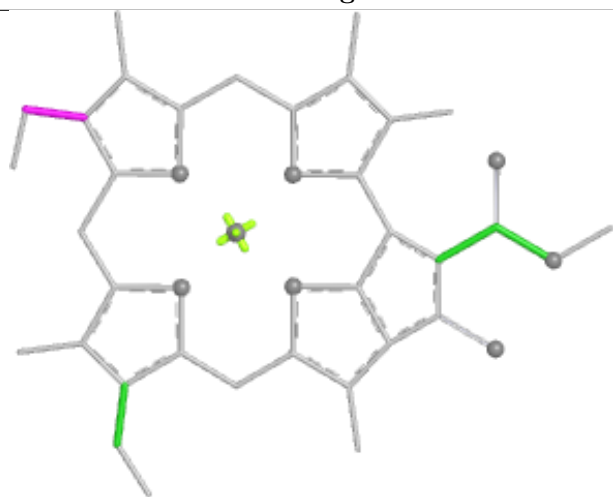
Ligand CLA 3 608



Bond lengths



Bond angles

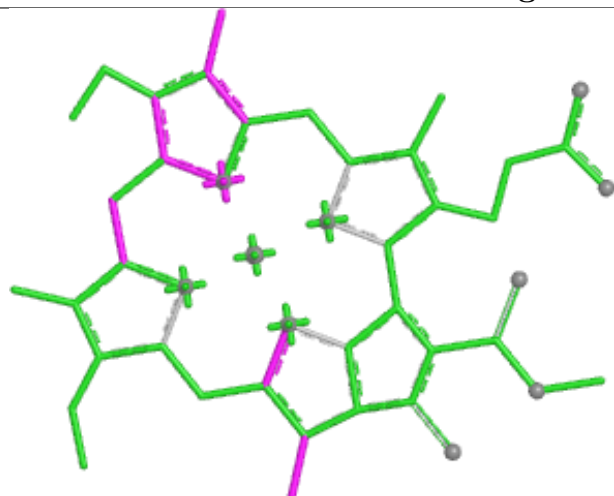


Torsions

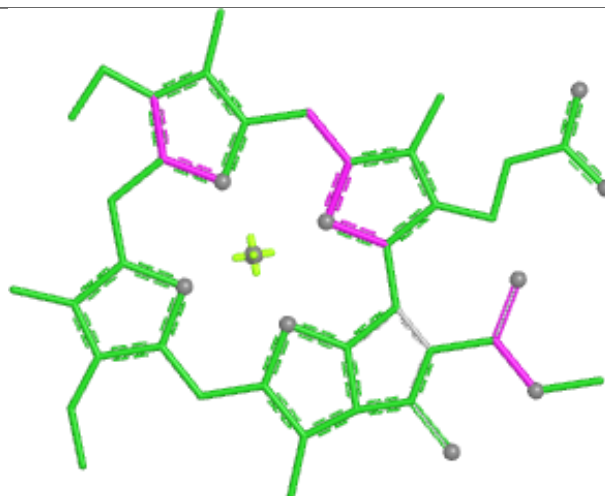


Rings

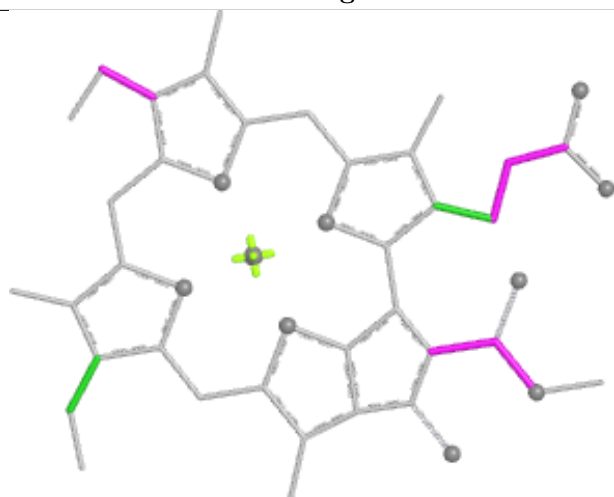
Ligand CLA 0 613



Bond lengths



Bond angles

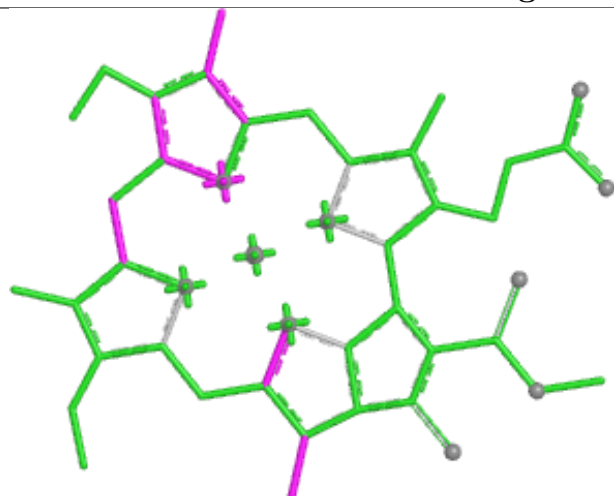


Torsions

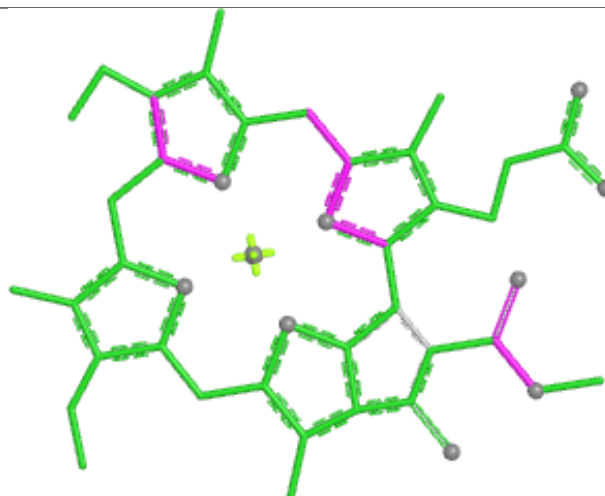


Rings

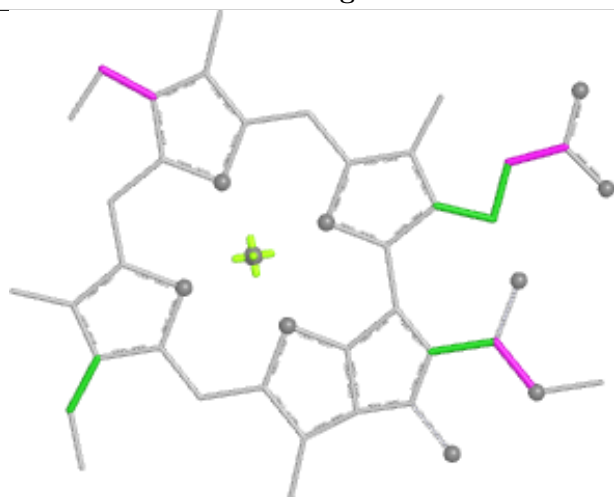
Ligand CLA 7 611



Bond lengths



Bond angles

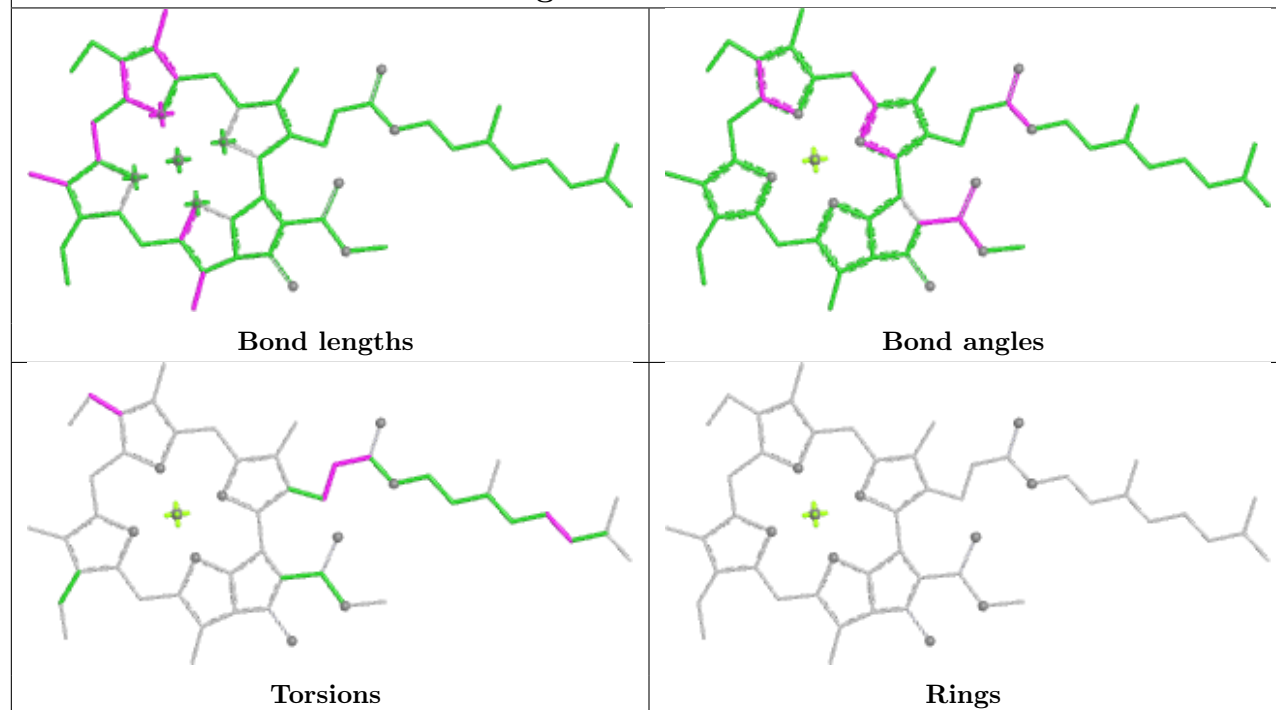


Torsions

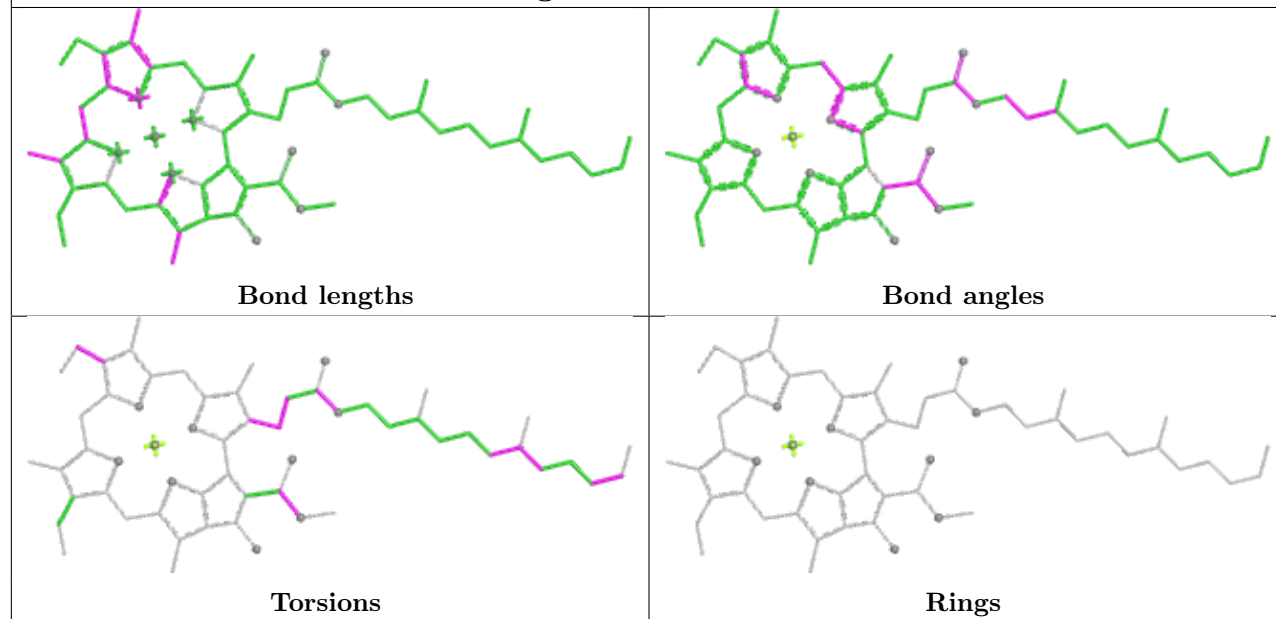


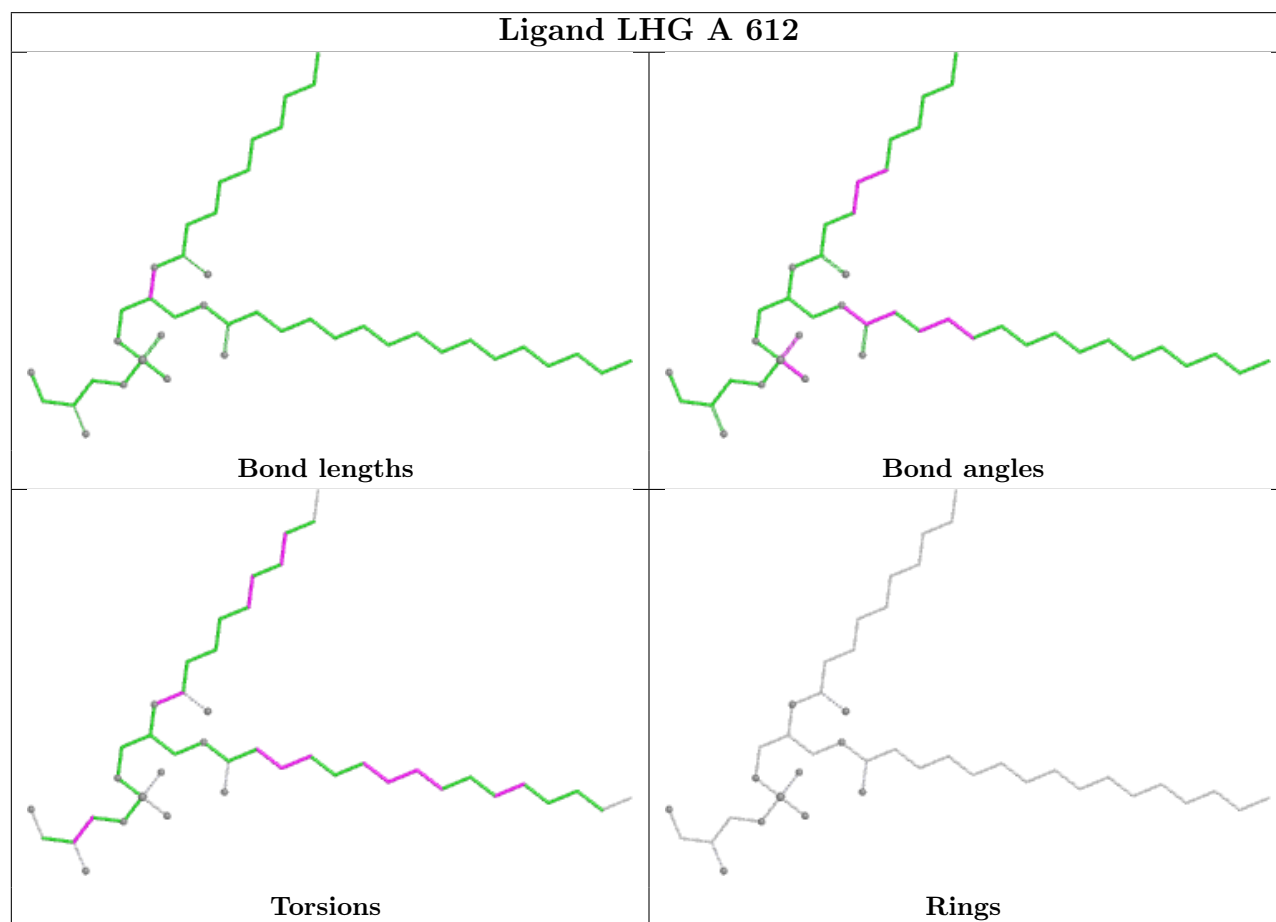
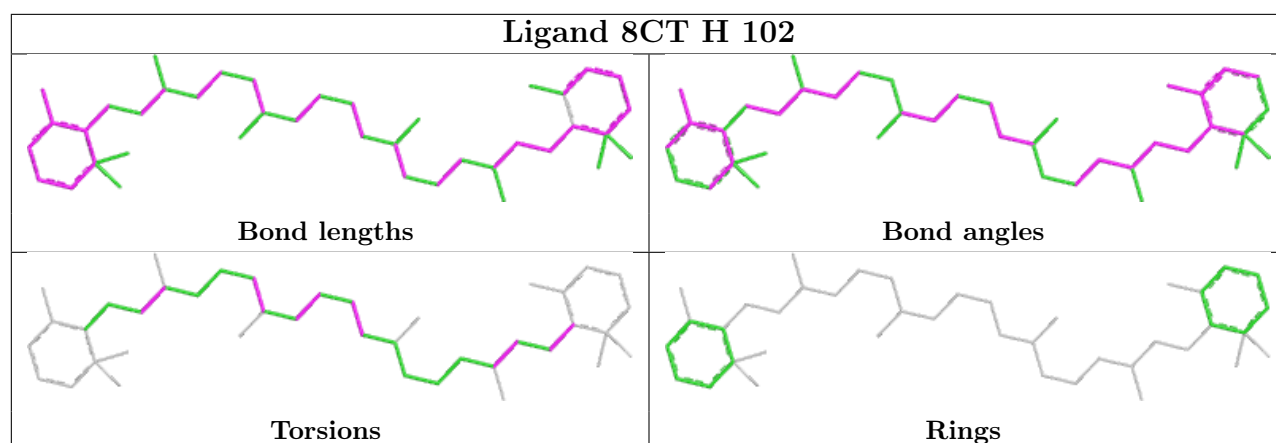
Rings

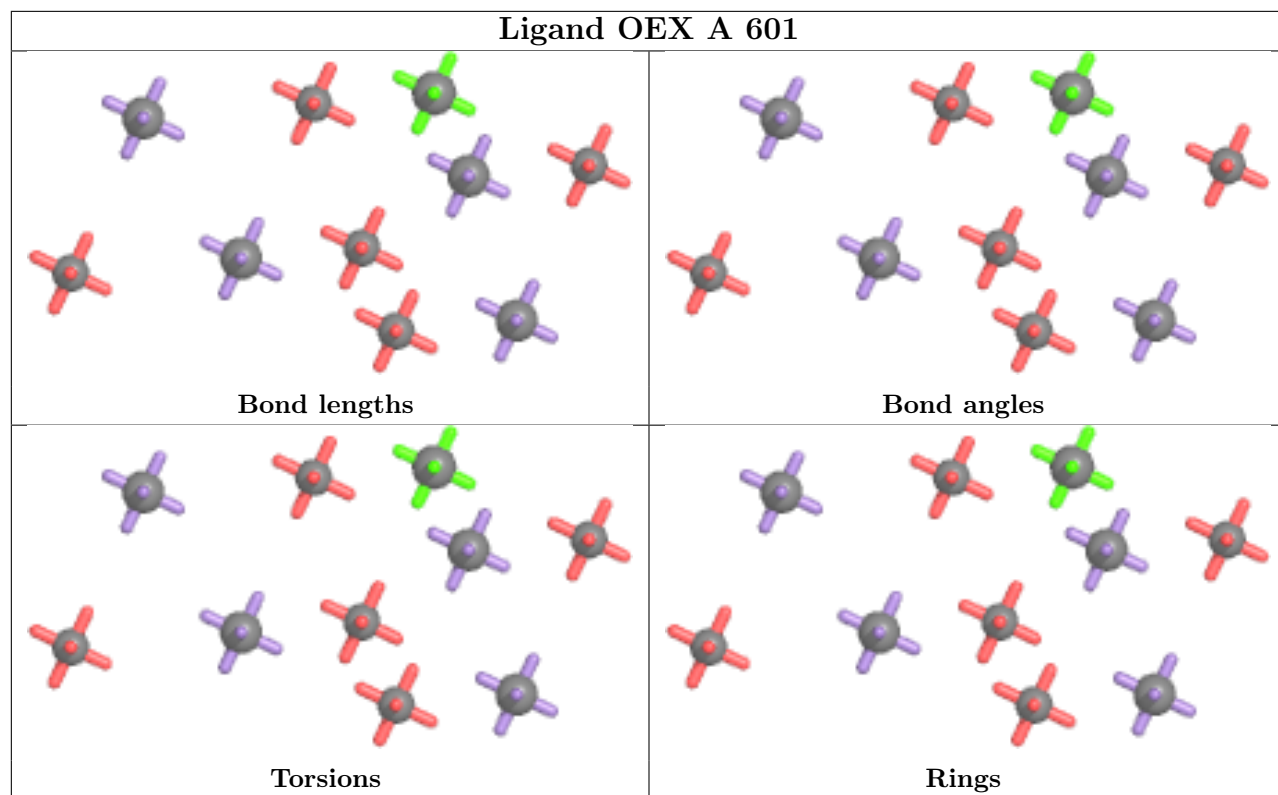
Ligand CLA 9 604



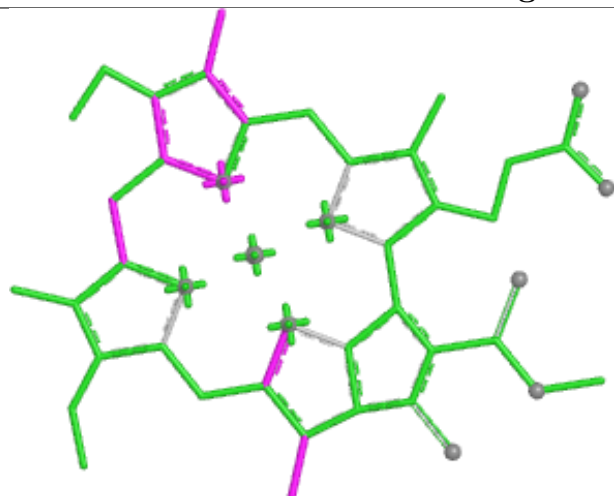
Ligand CLA 6 602



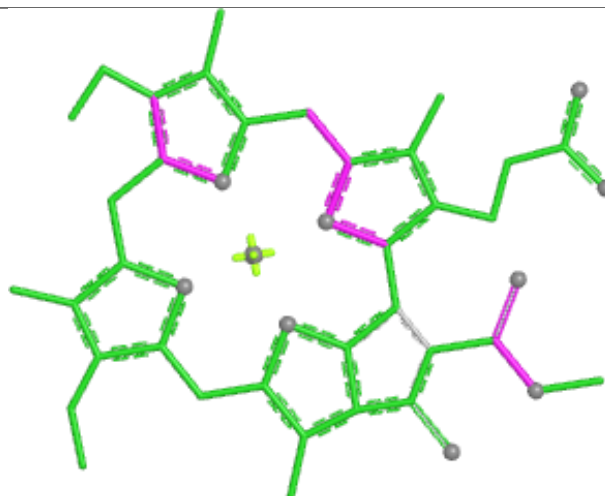




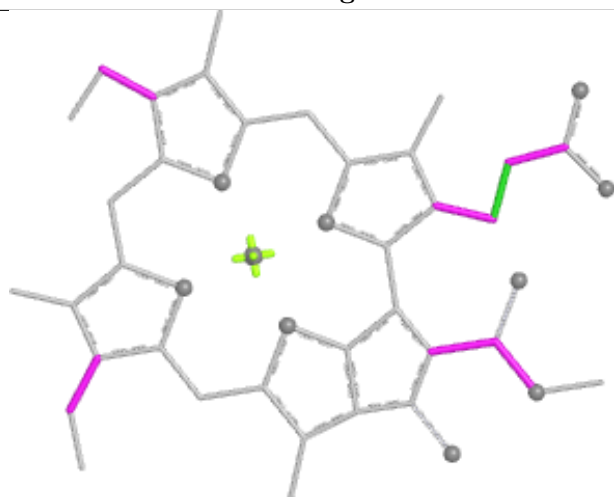
Ligand CLA 1 606



Bond lengths



Bond angles

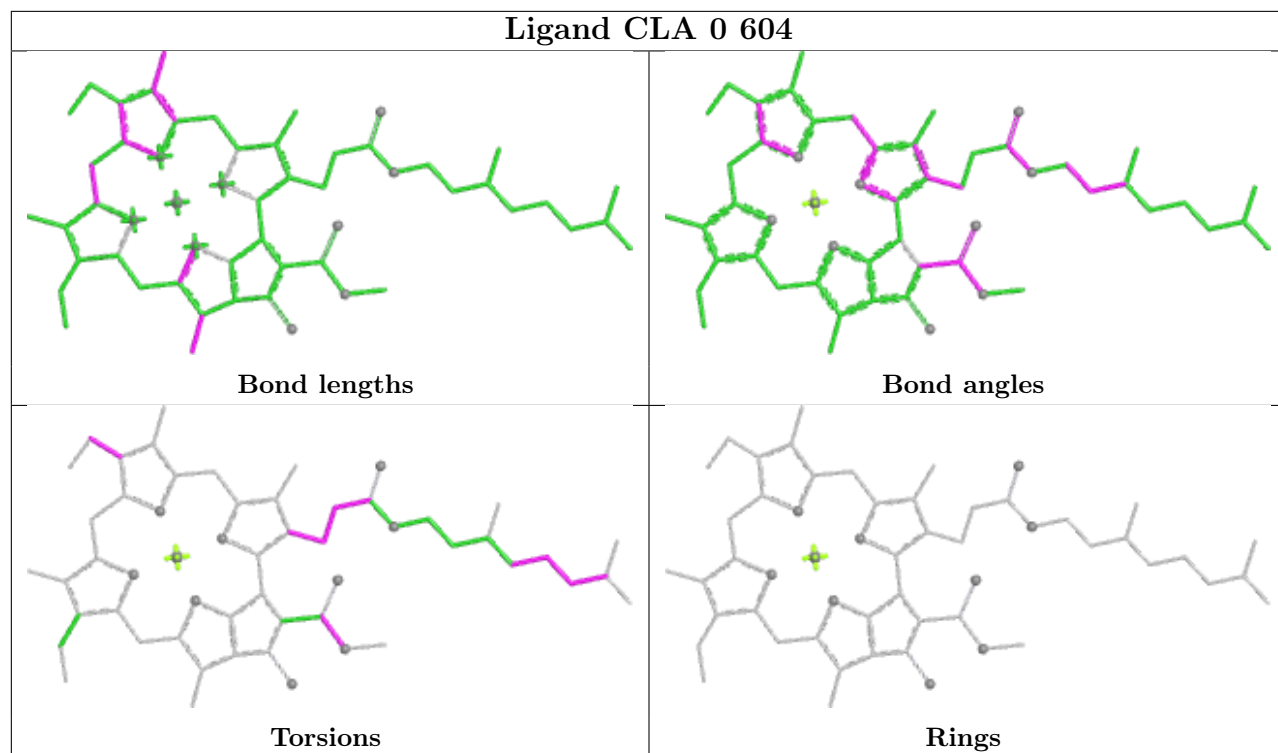


Torsions

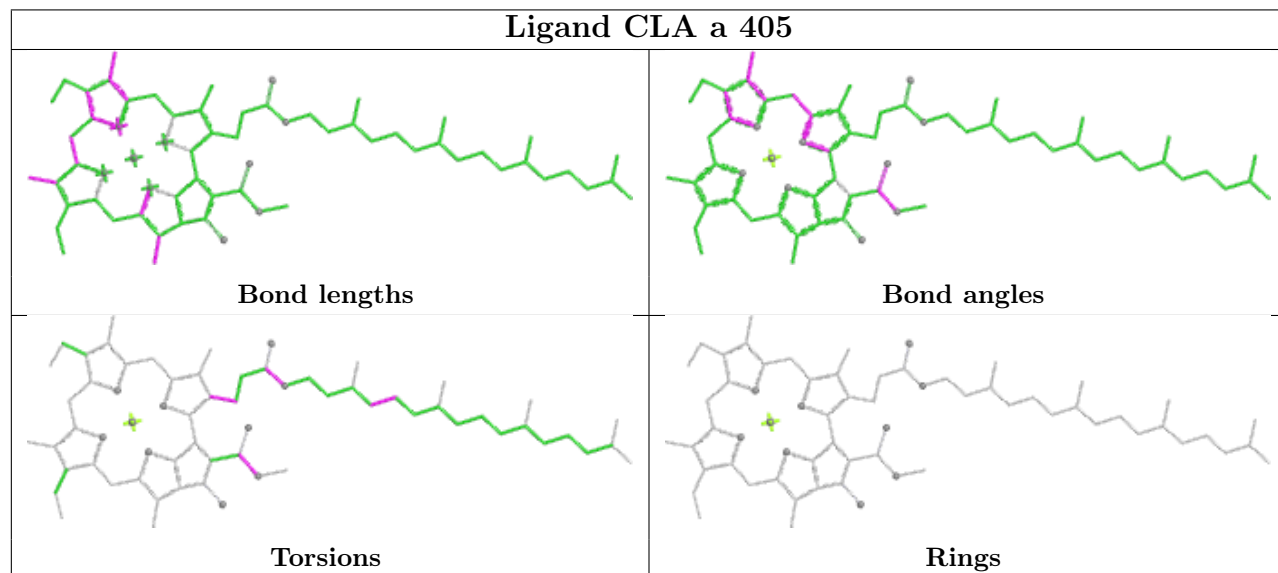


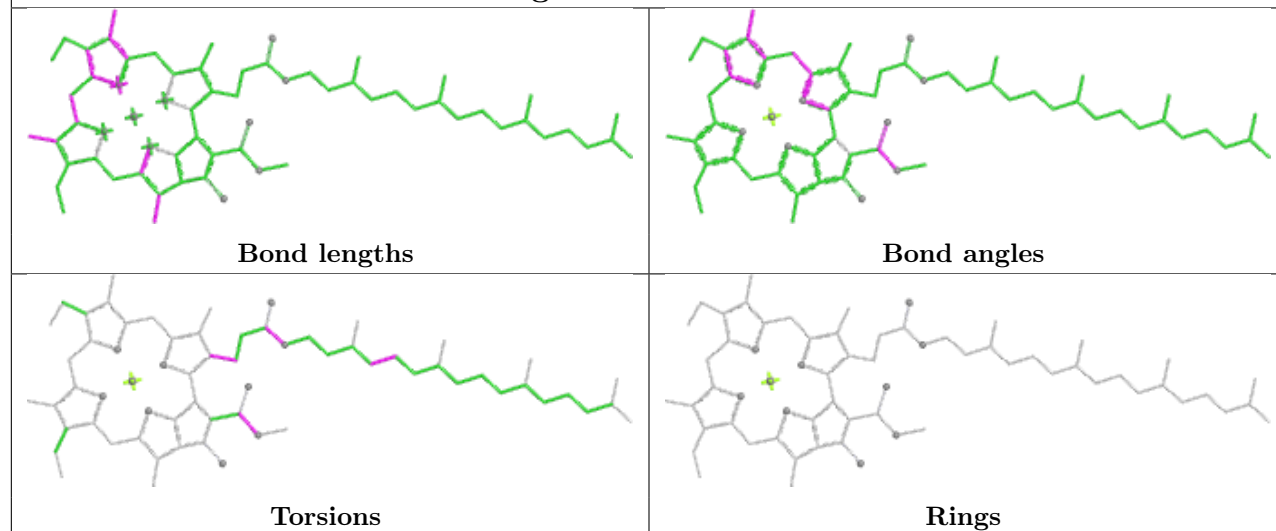
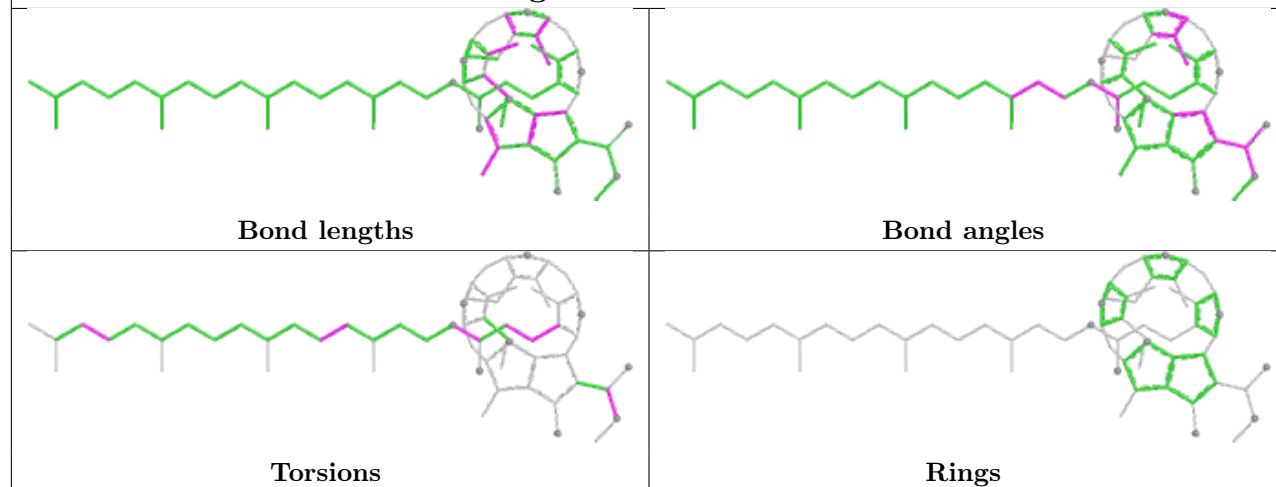
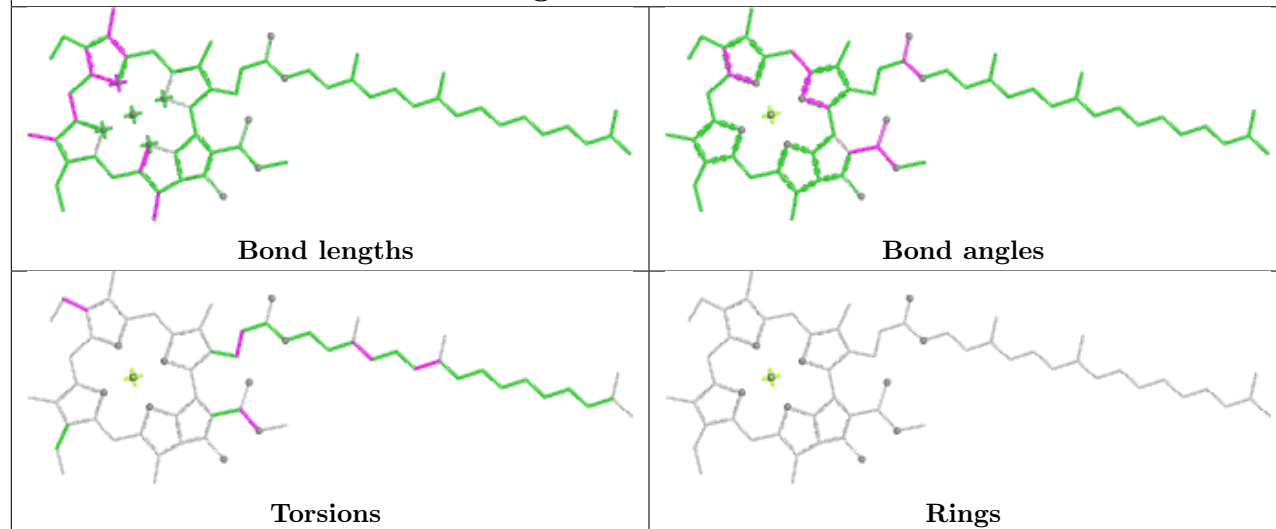
Rings

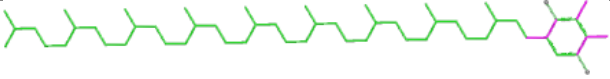
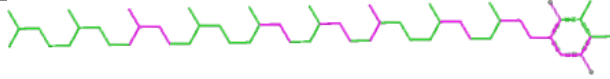
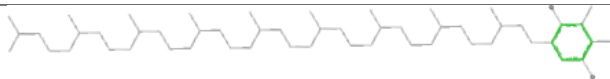
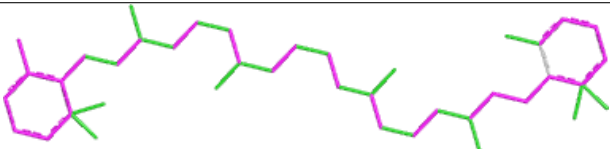
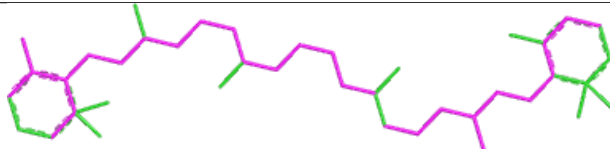
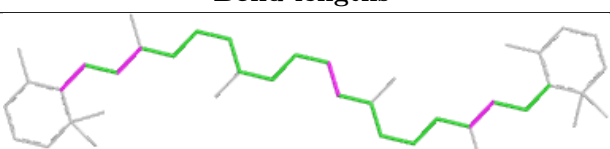
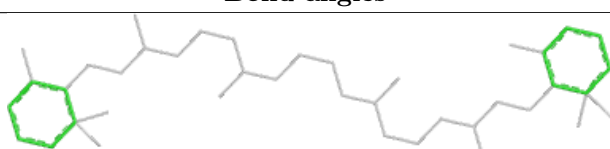
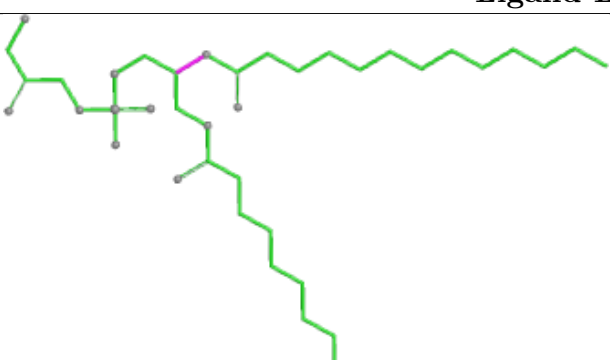
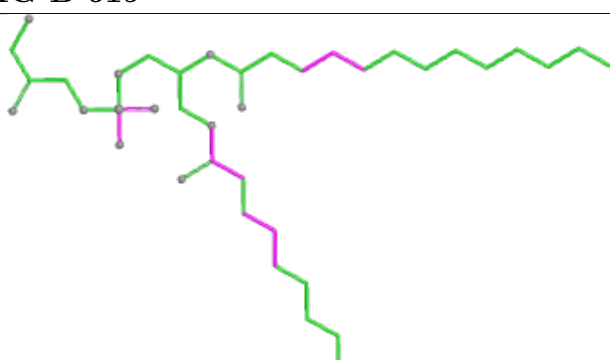
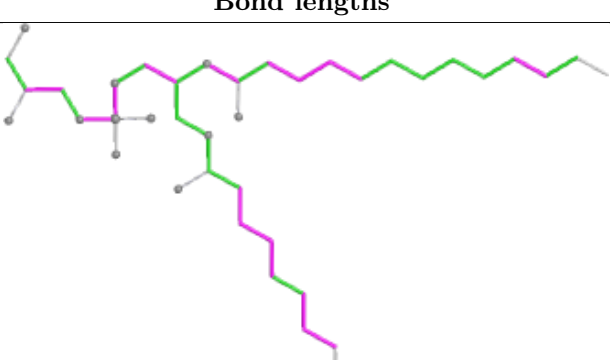
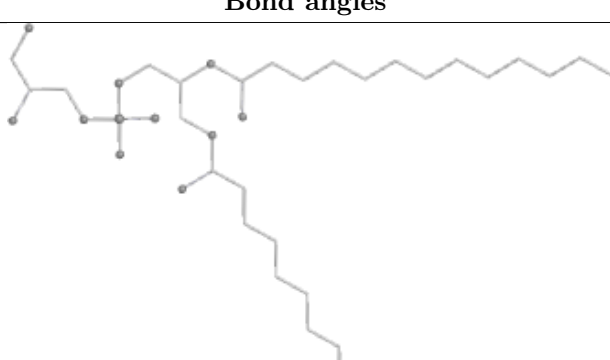
Ligand CLA 0 604

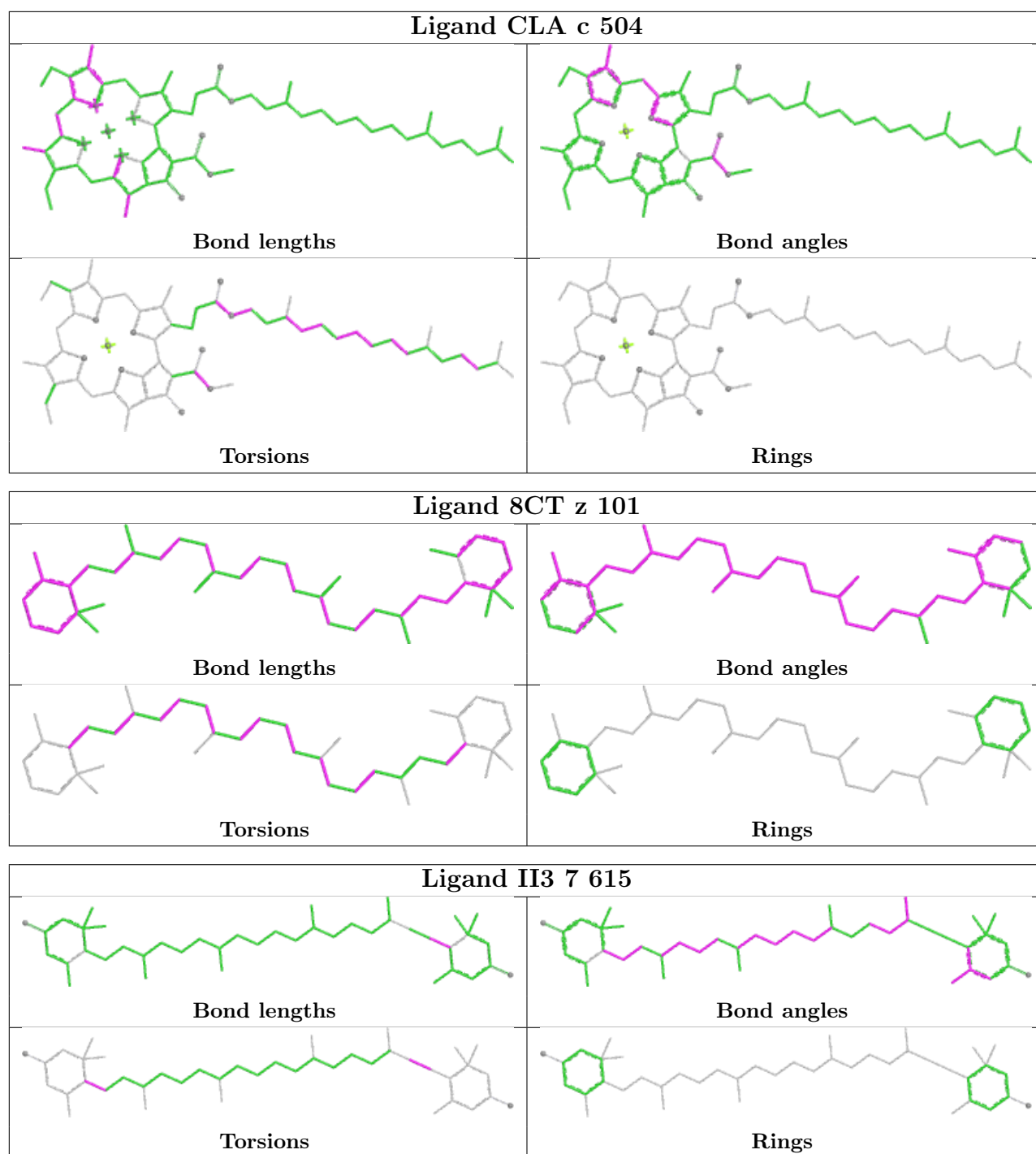


Ligand CLA a 405

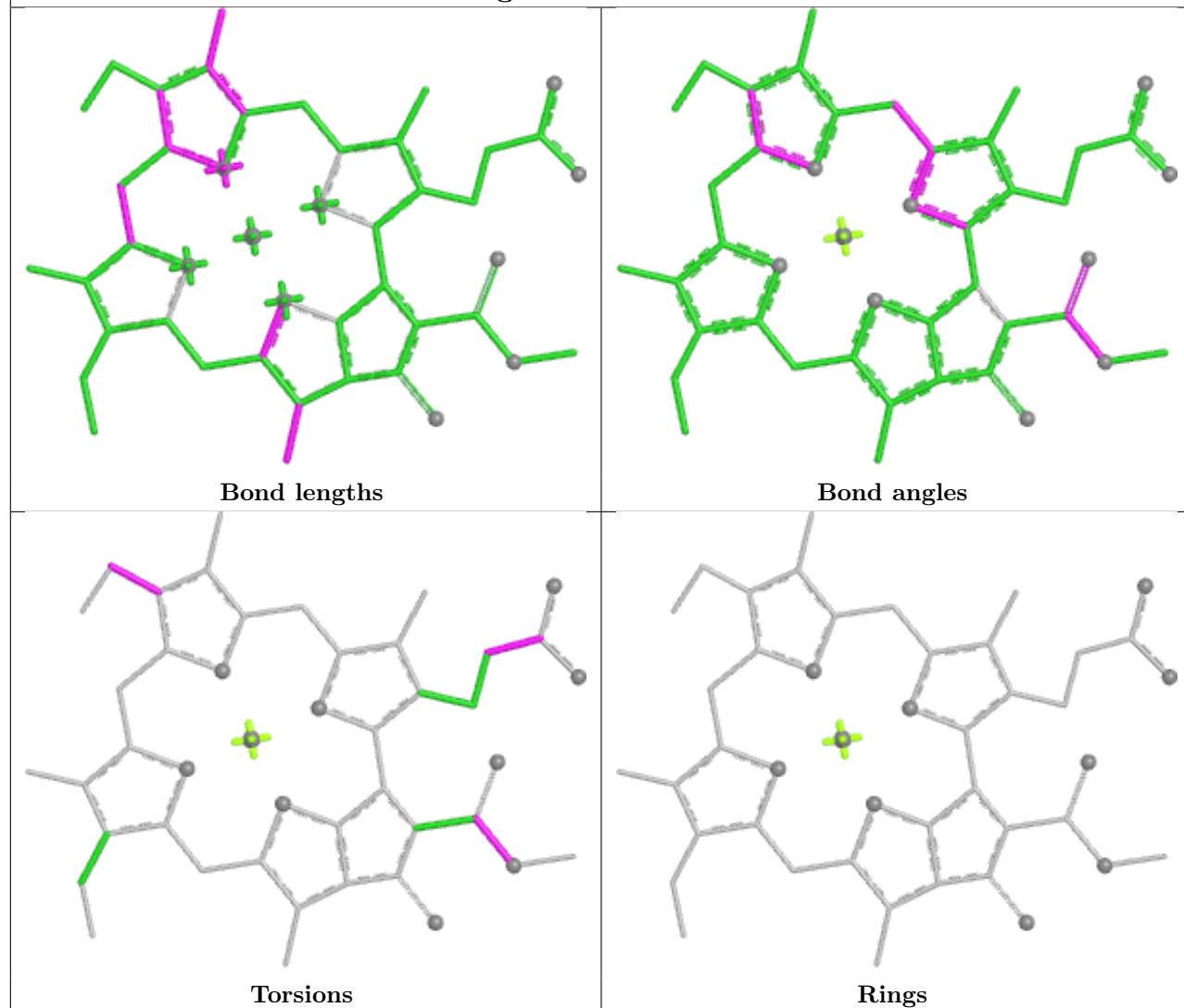


Ligand CLA A 602**Ligand PHO D 402****Ligand CLA B 604**

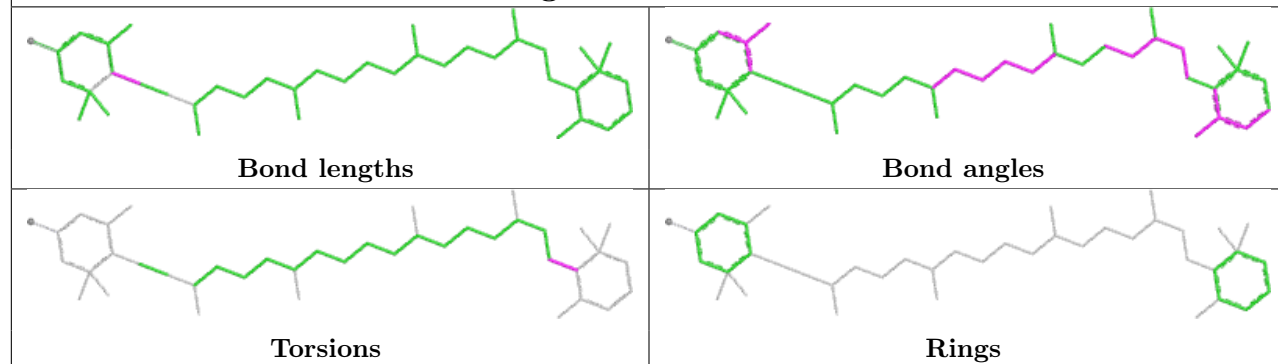
Ligand PL9 D 405	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand 8CT a 413	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand LHG B 619	
 Bond lengths	 Bond angles
 Torsions	 Rings

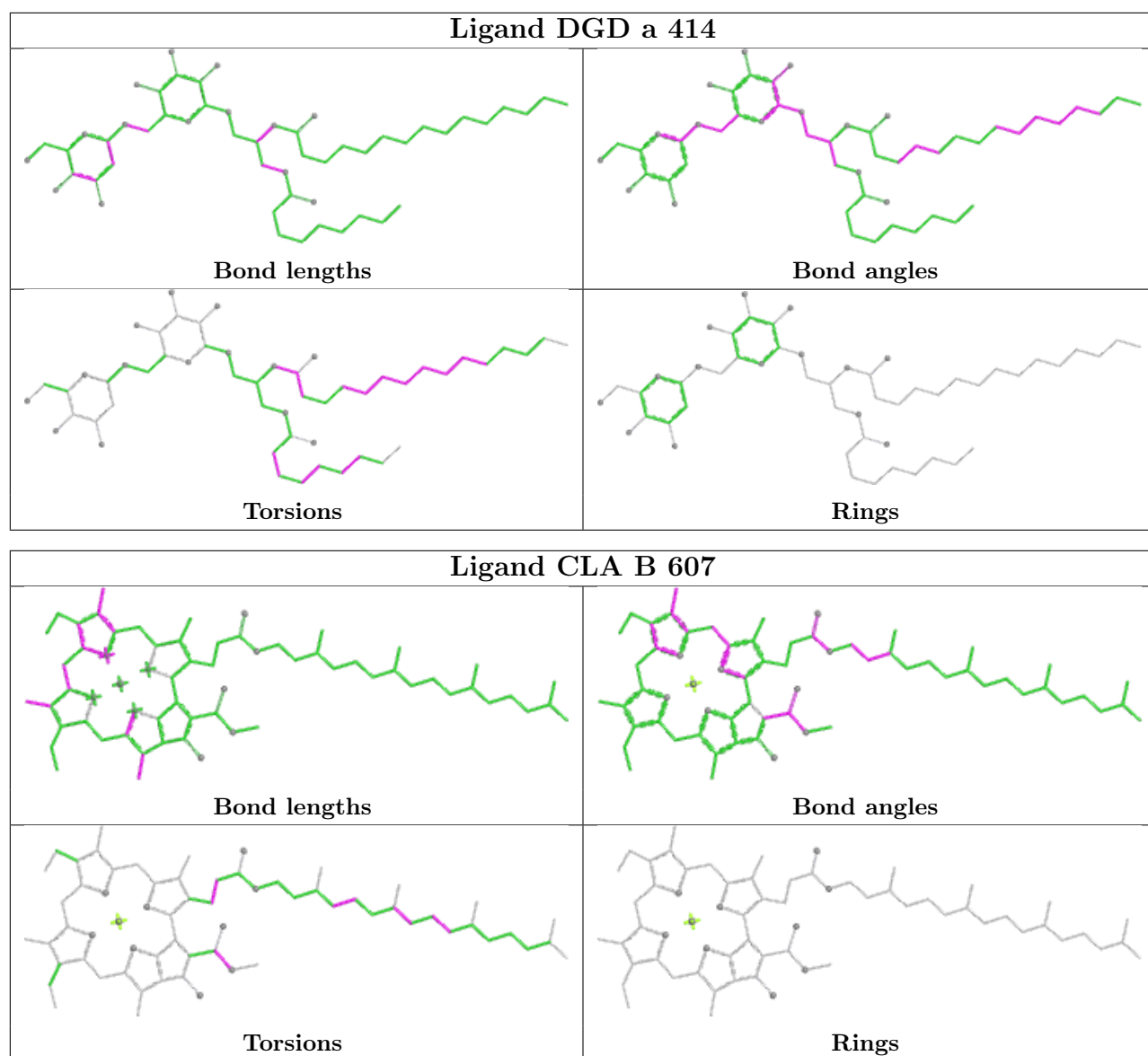


Ligand CLA 0 606

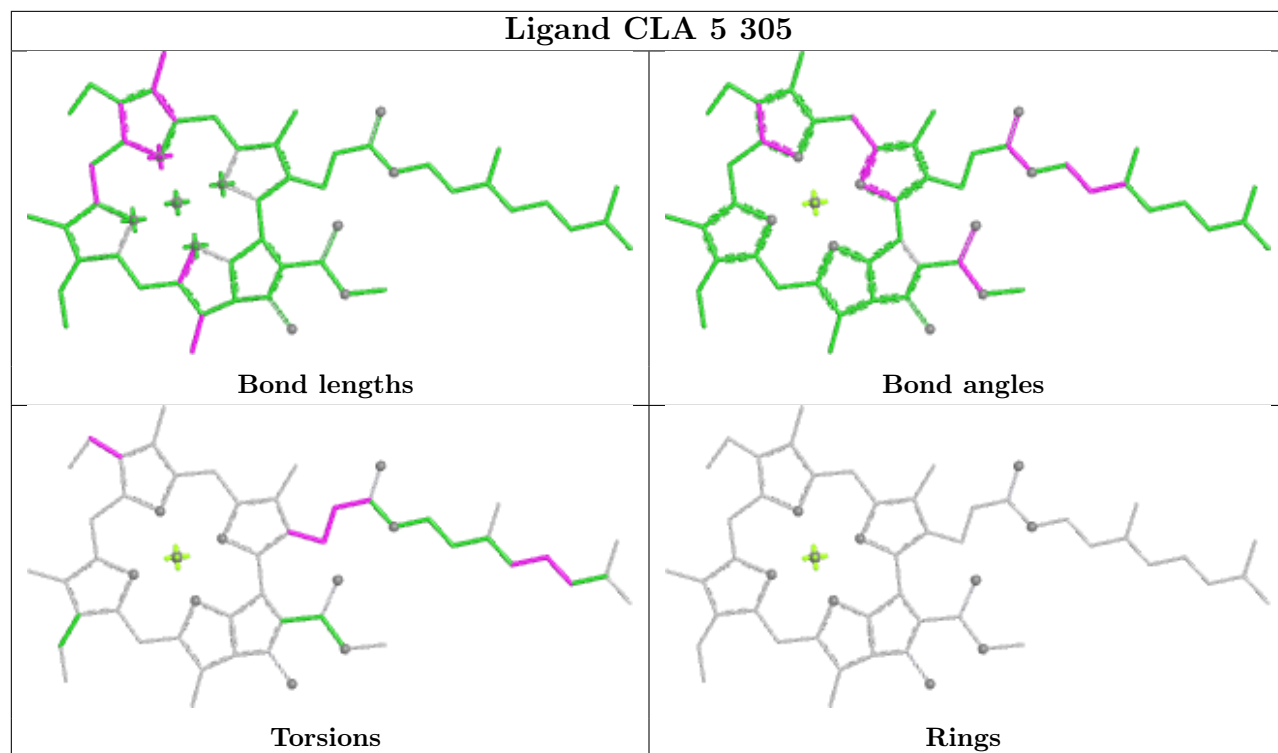


Ligand IHT 7 618

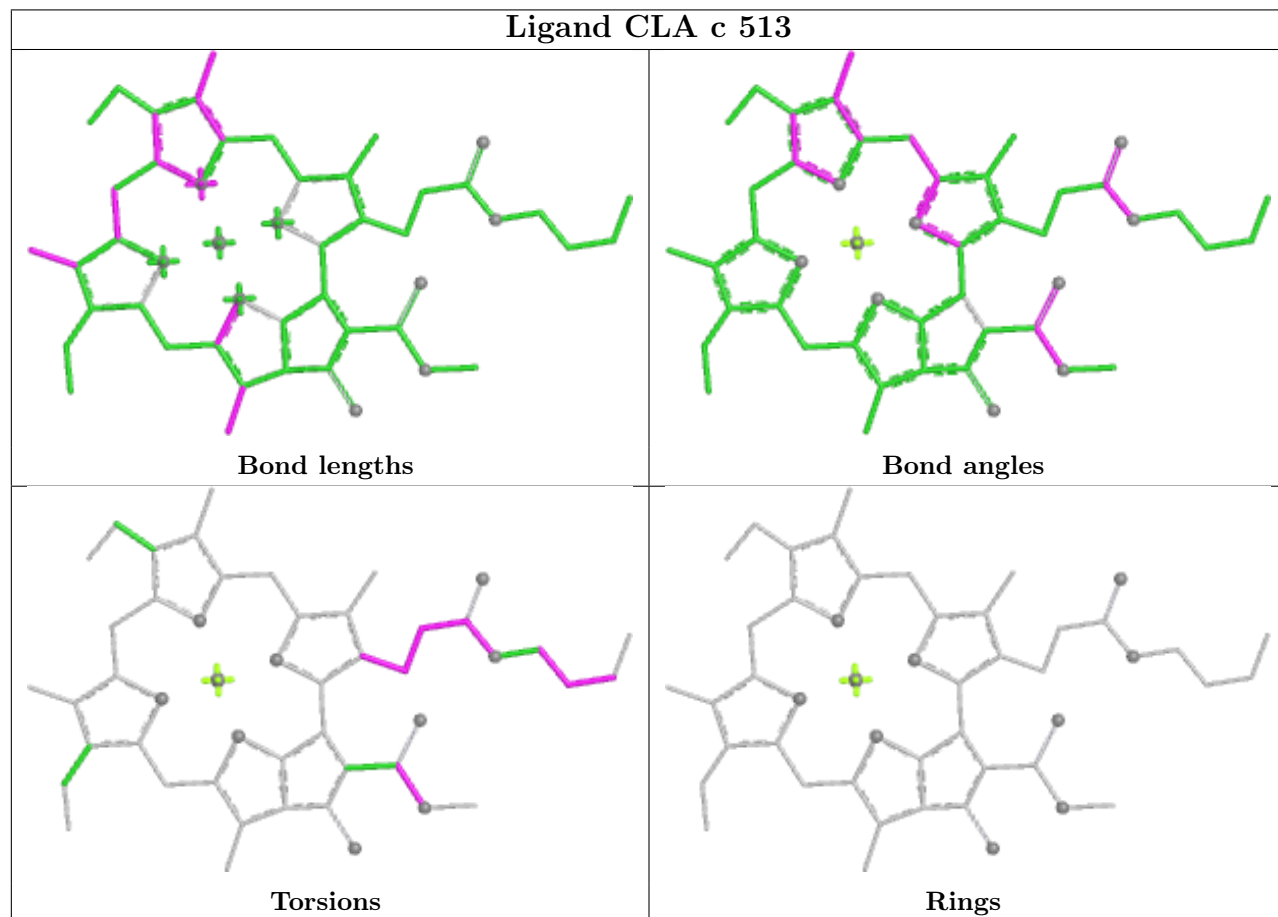




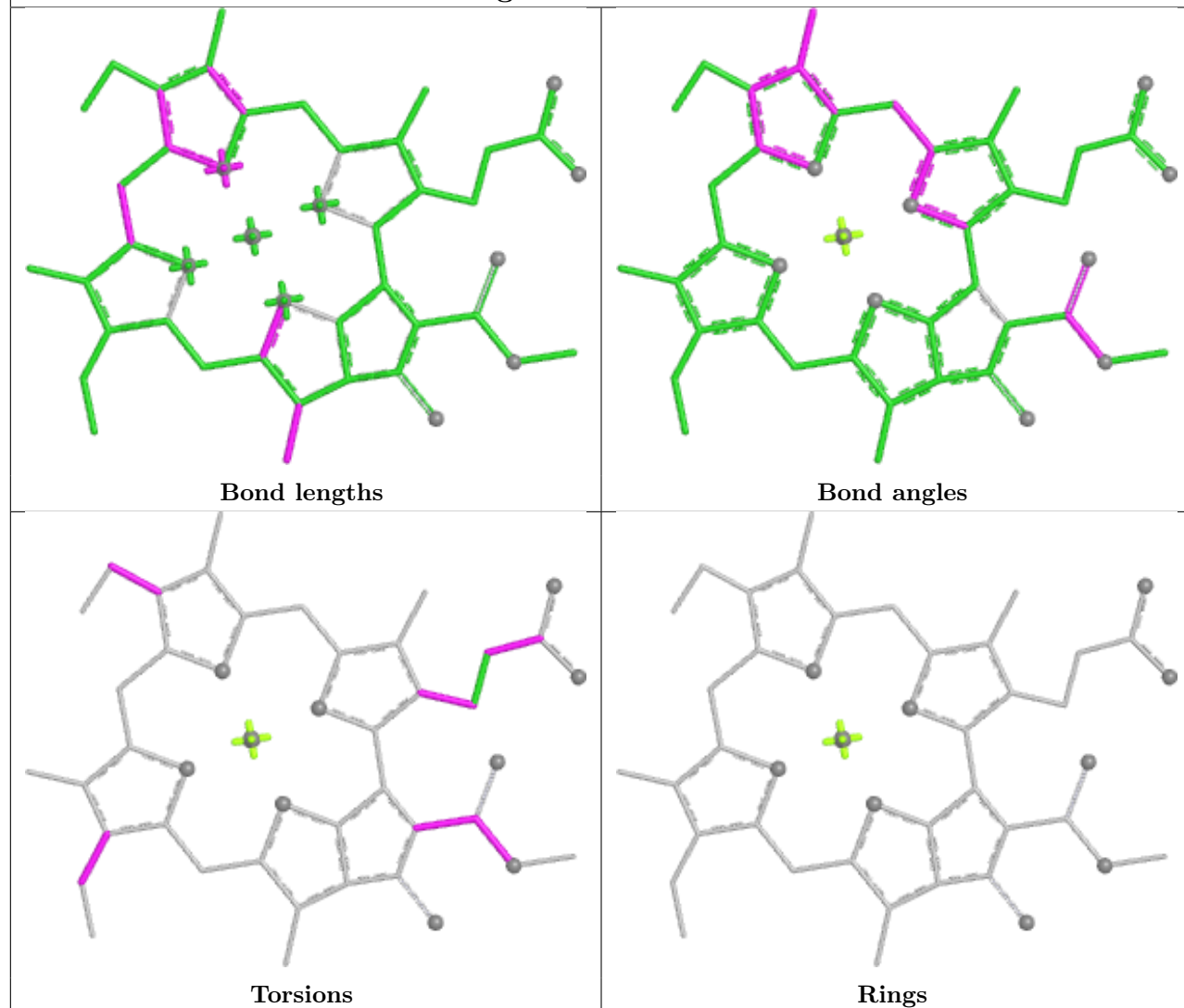
Ligand CLA 5 305



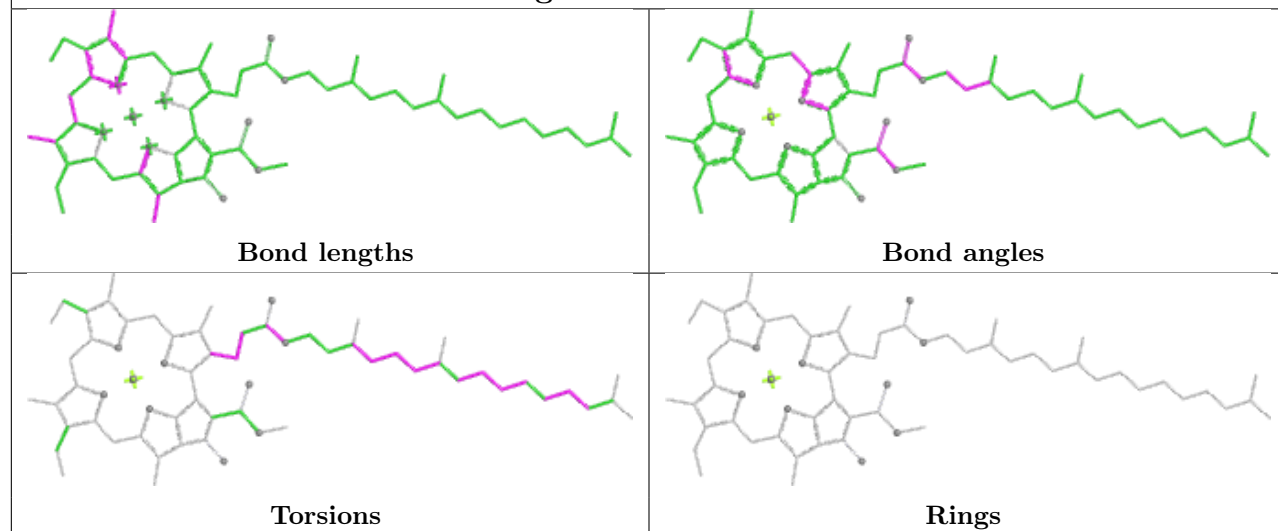
Ligand CLA c 513

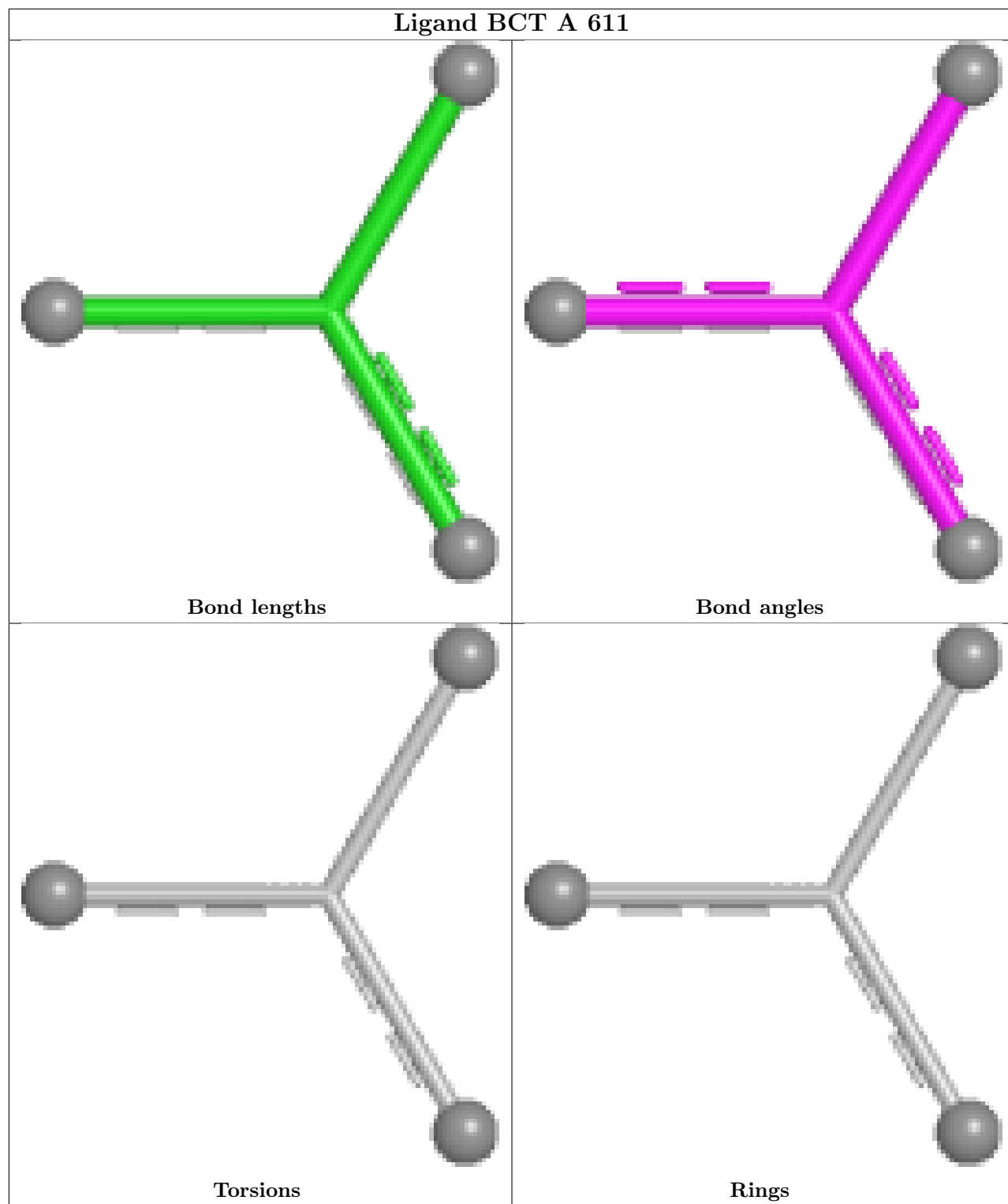


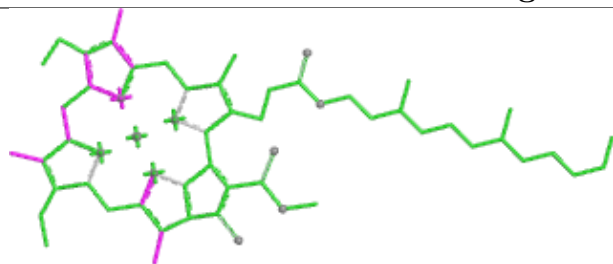
Ligand CLA 7 606



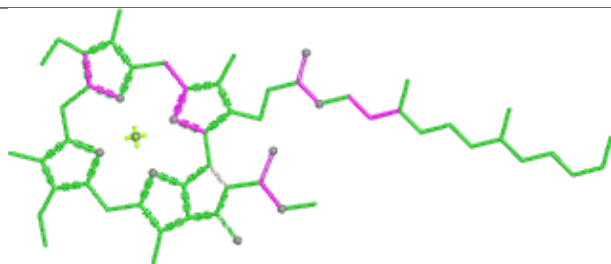
Ligand CLA b 612



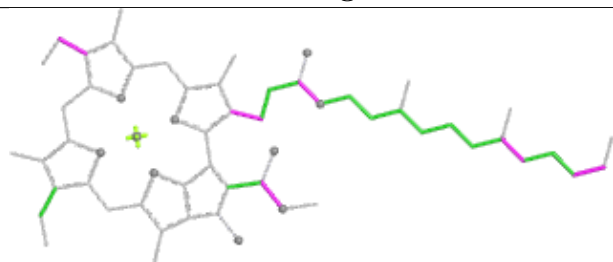


Ligand CLA 5 303

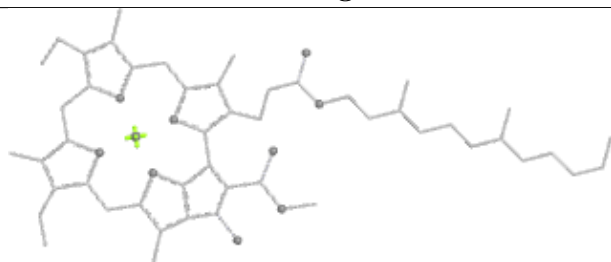
Bond lengths



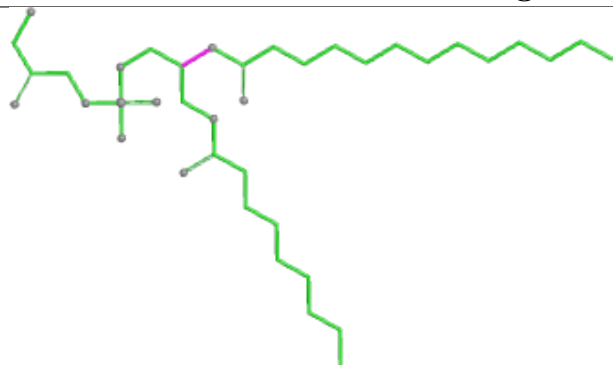
Bond angles



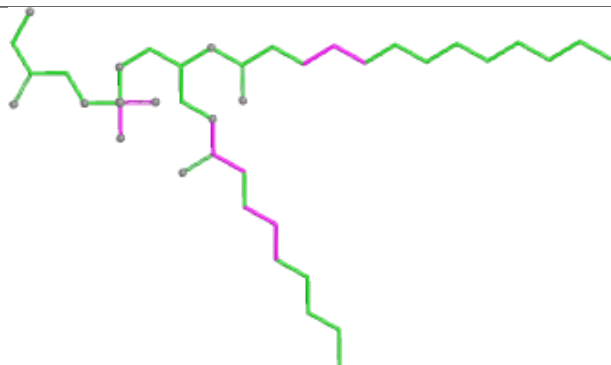
Torsions



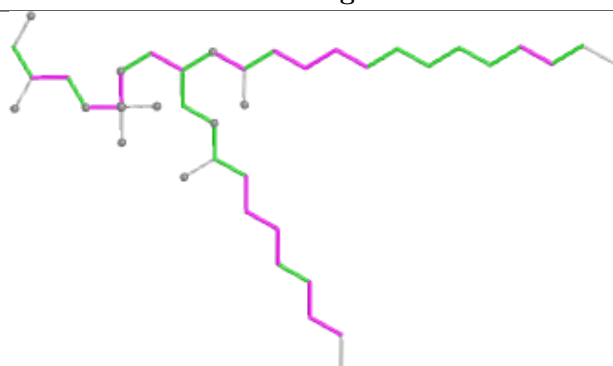
Rings

Ligand LHG b 619

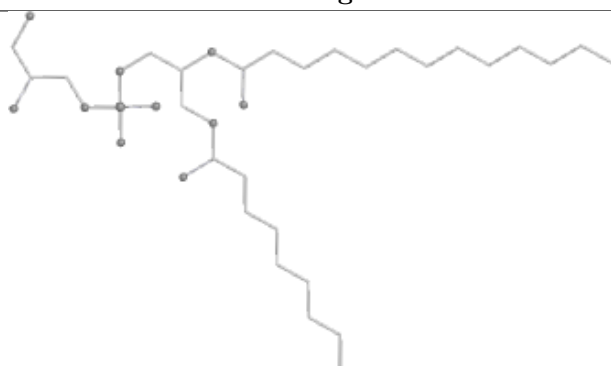
Bond lengths



Bond angles

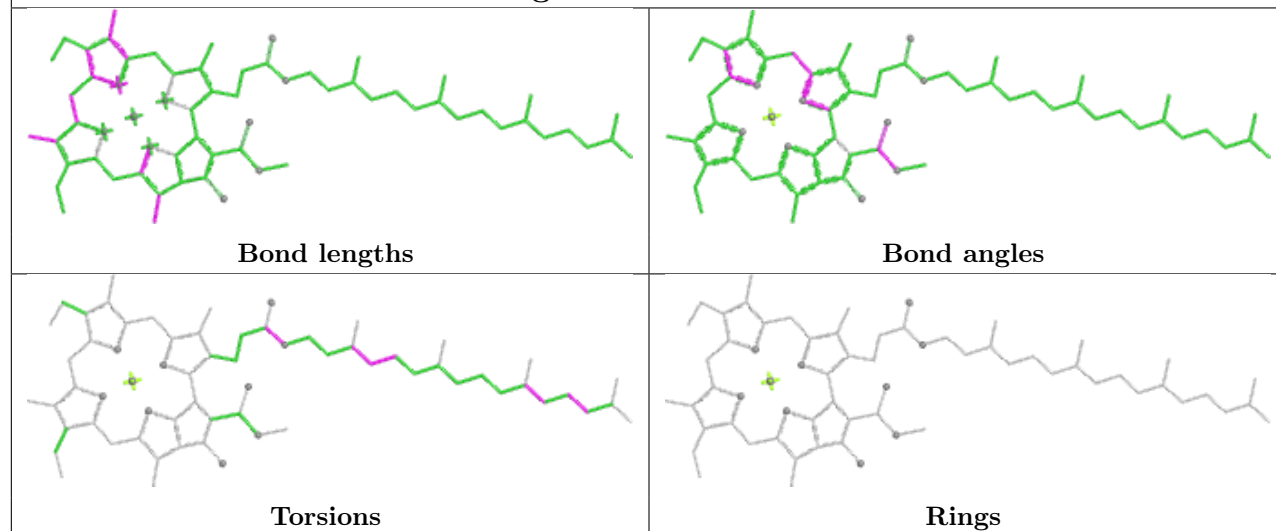


Torsions

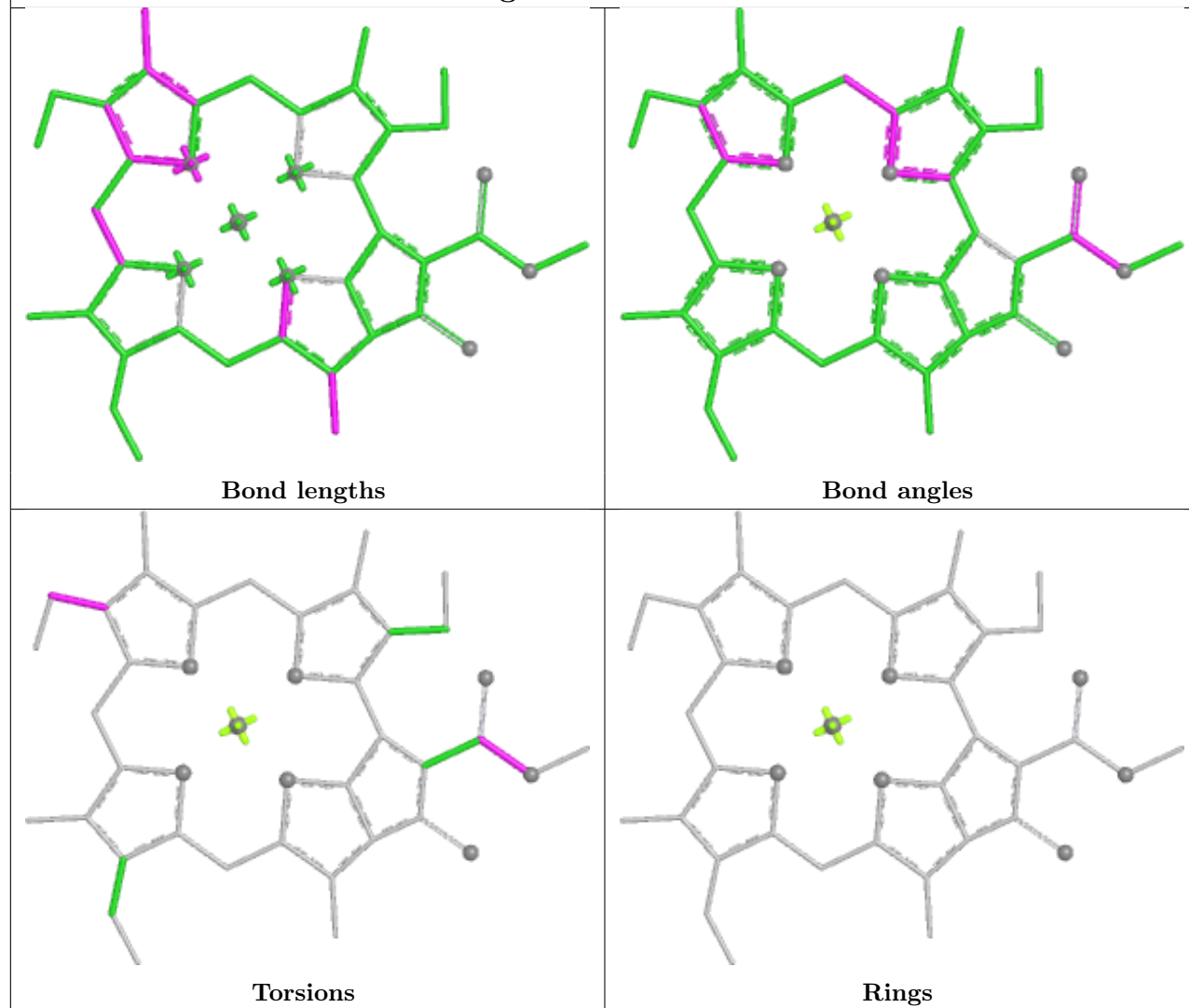


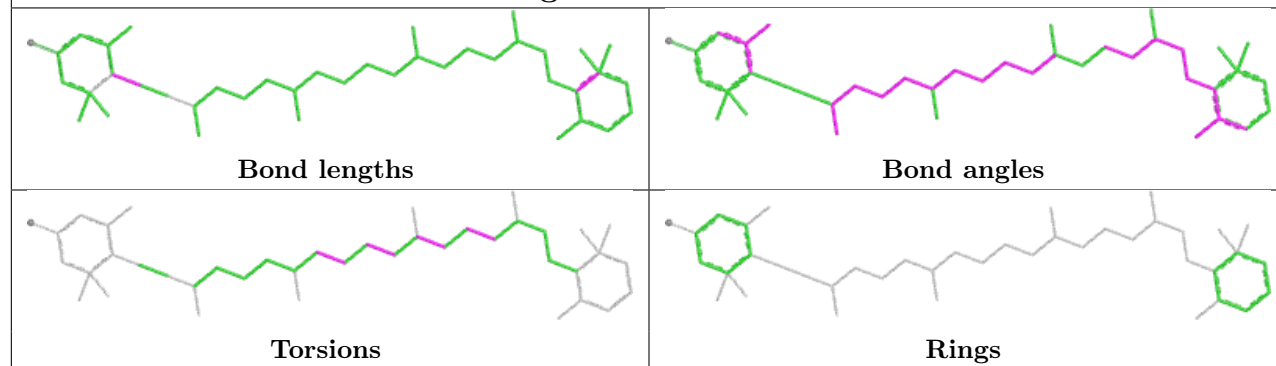
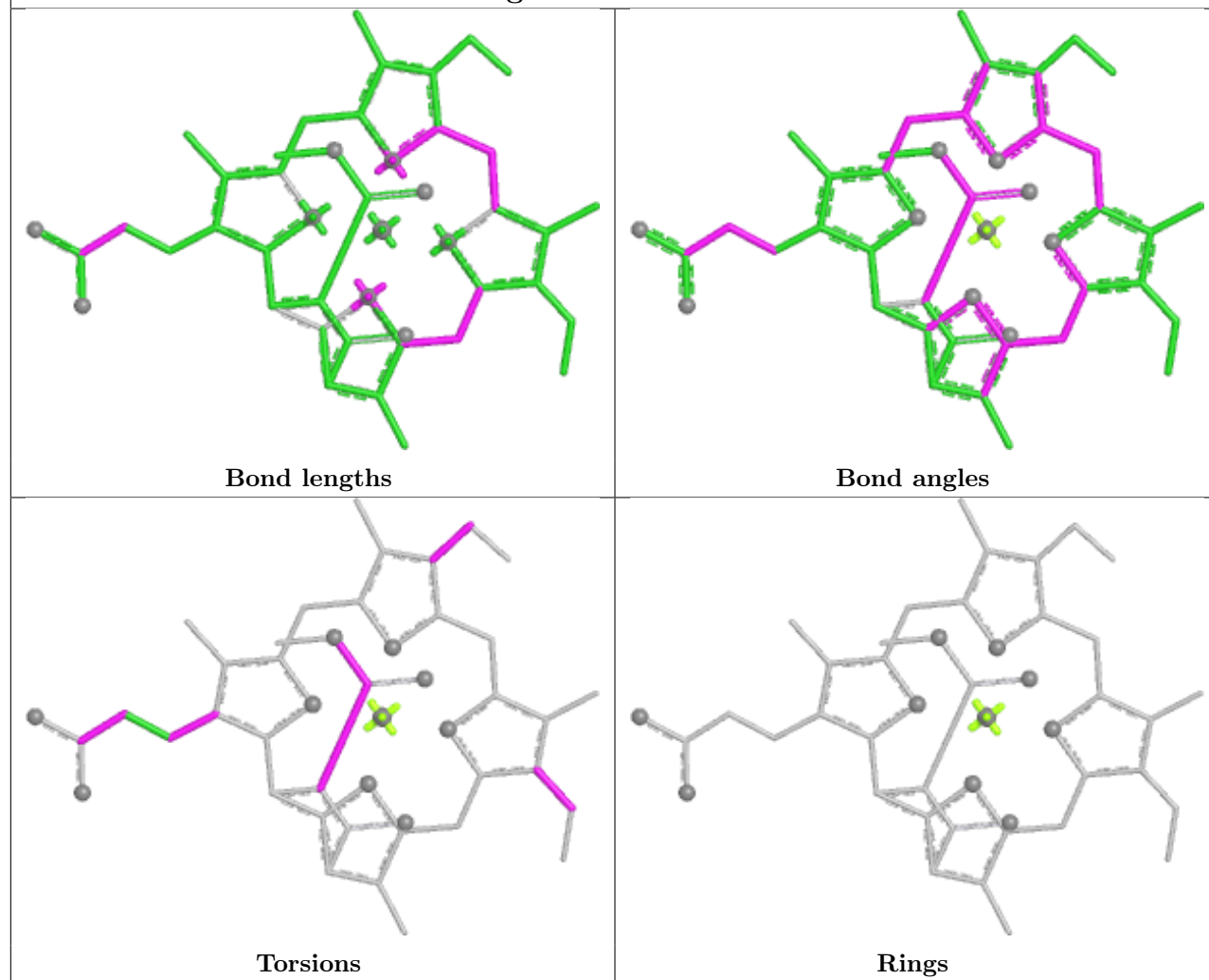
Rings

Ligand CLA C 511

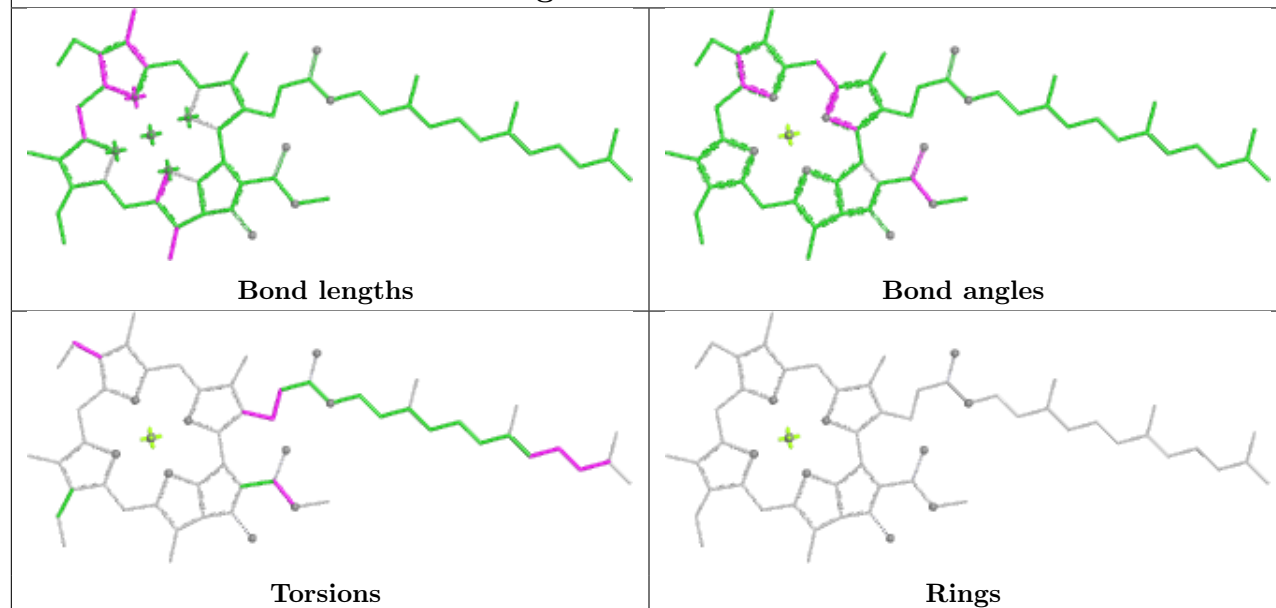


Ligand CLA 4 601

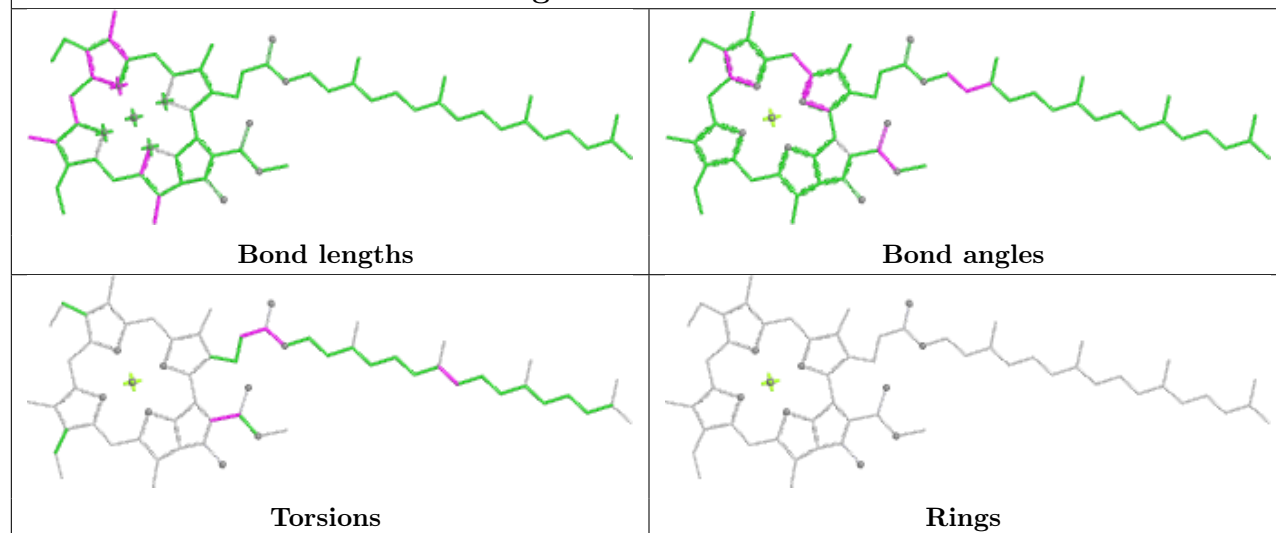


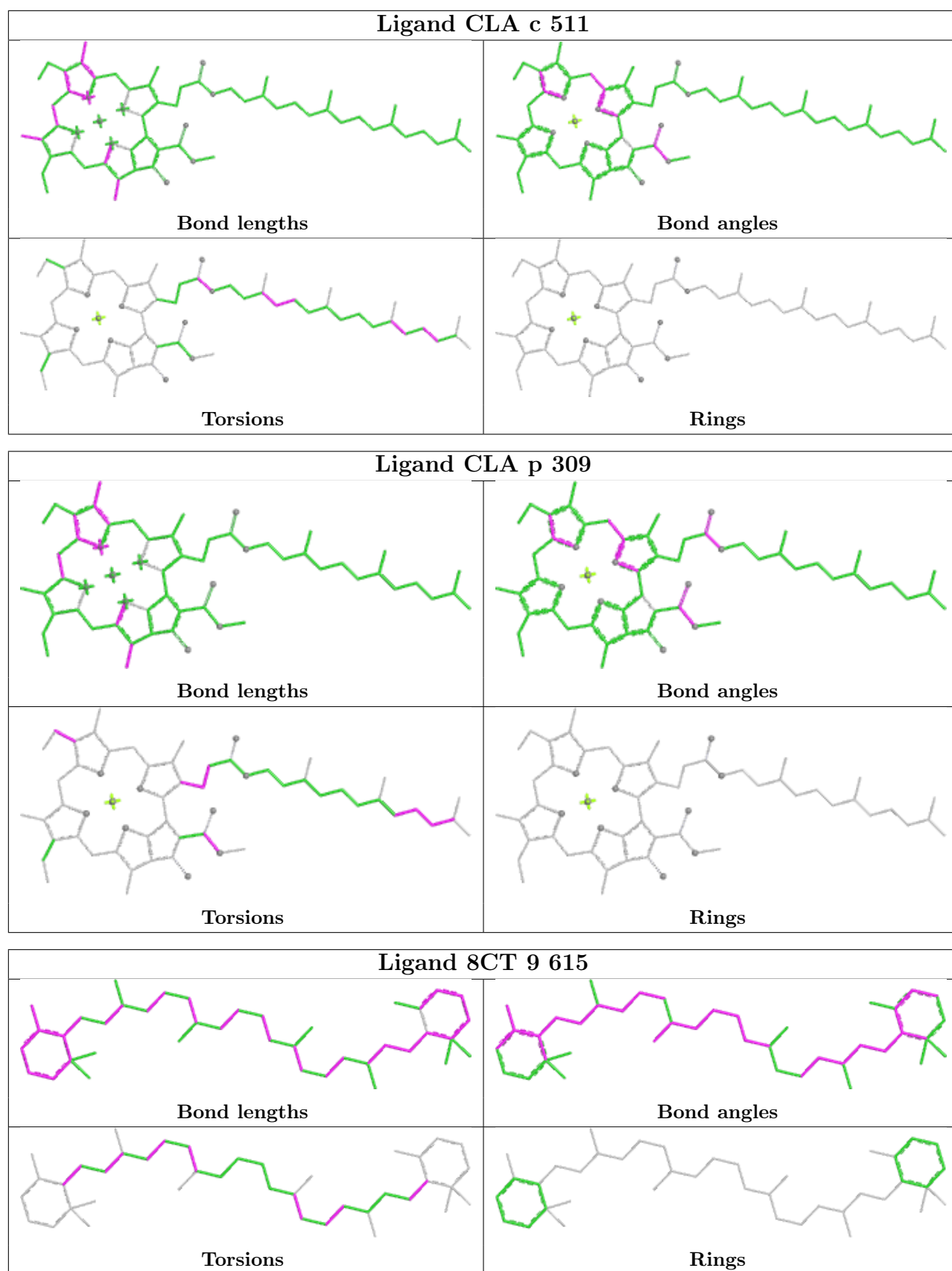
Ligand IHT 0 618**Ligand KC2 P 605**

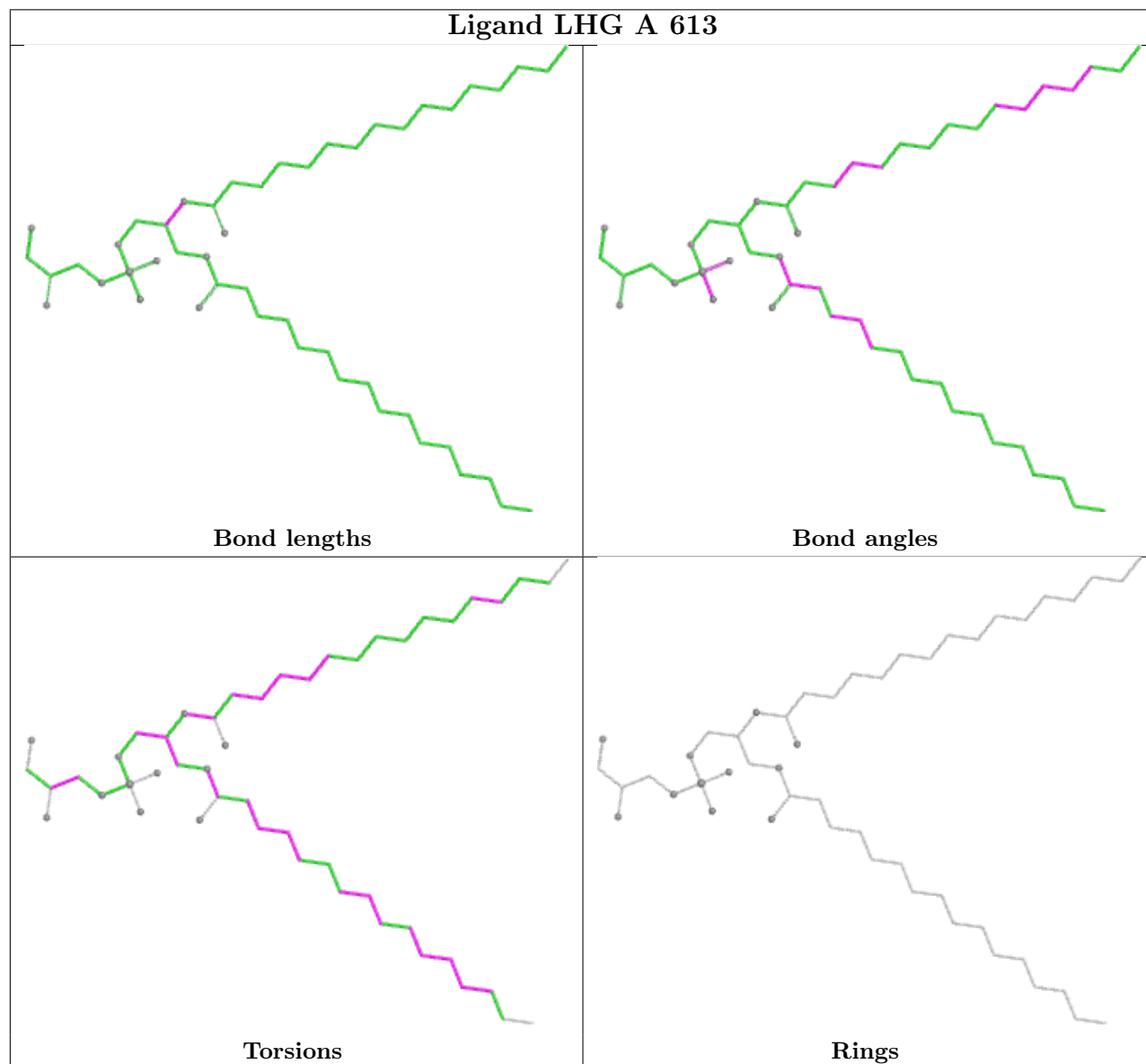
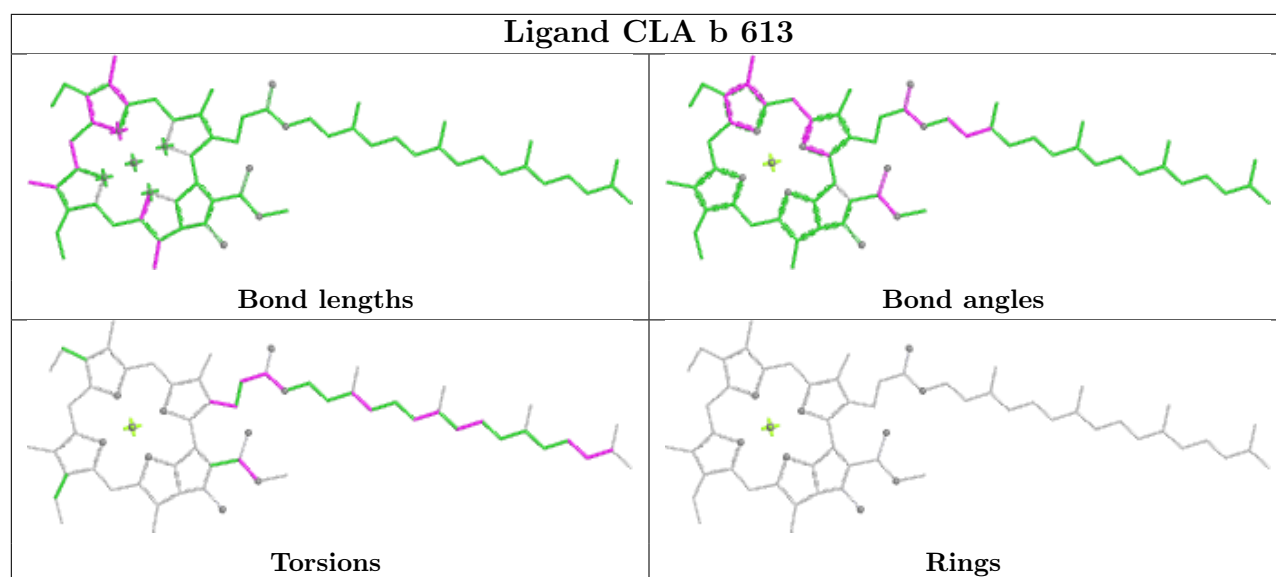
Ligand CLA 7 608

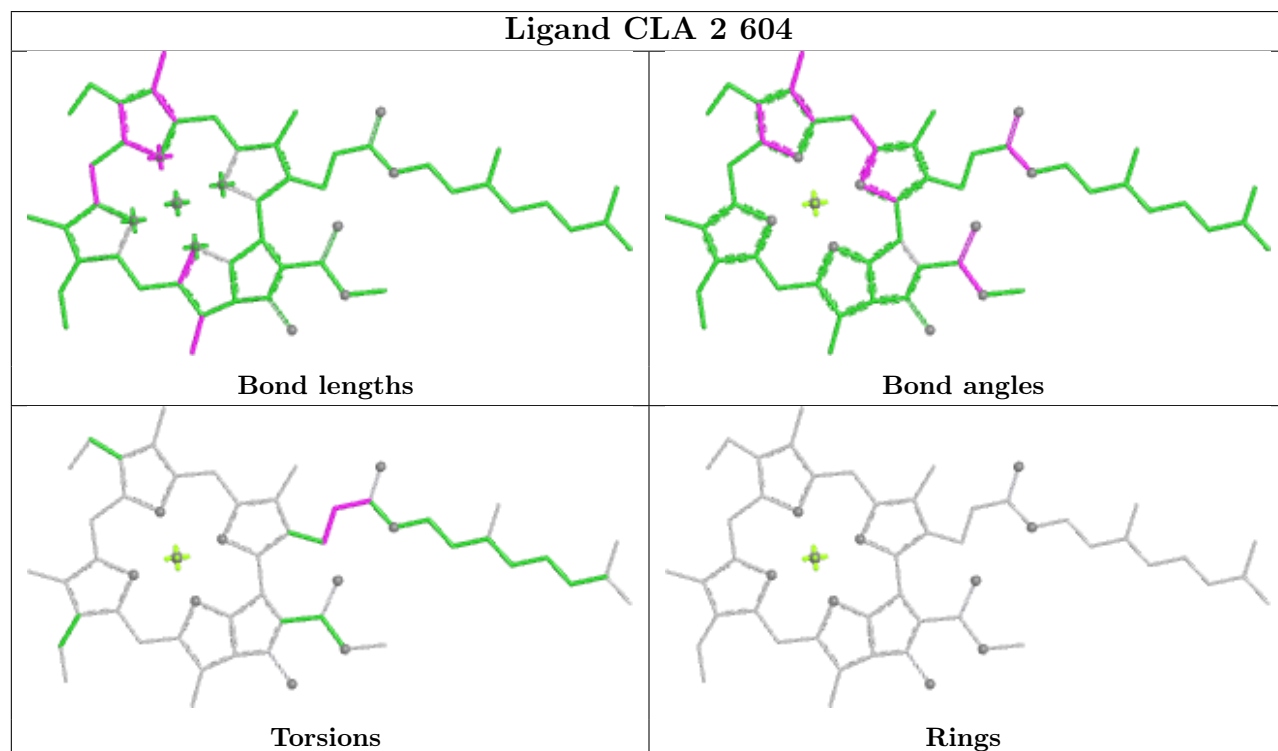
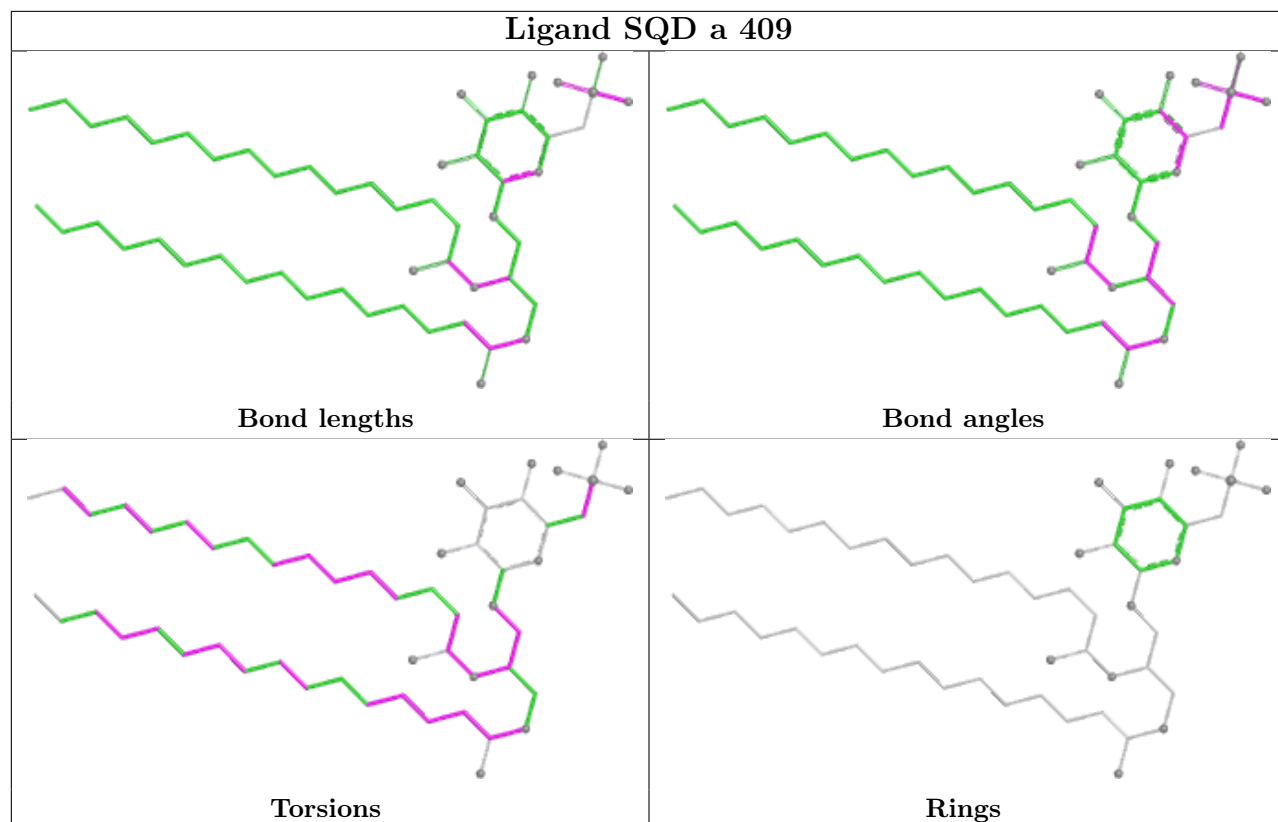


Ligand CLA C 510

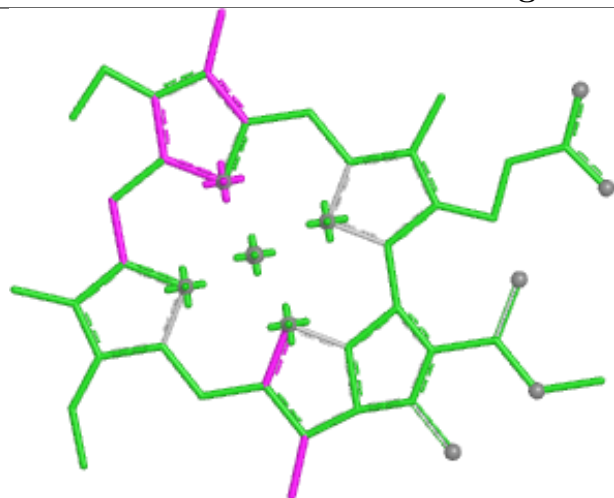




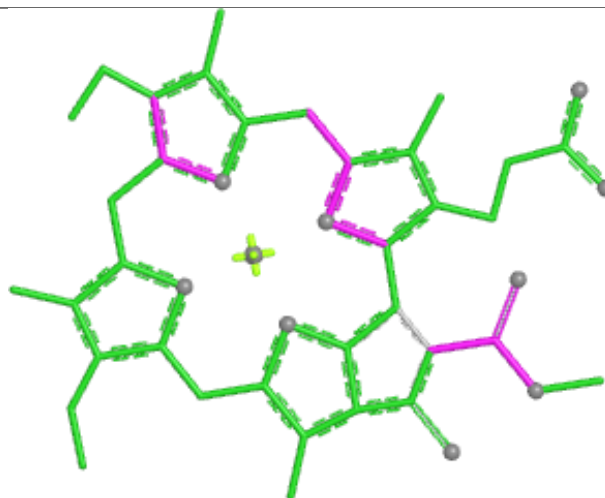




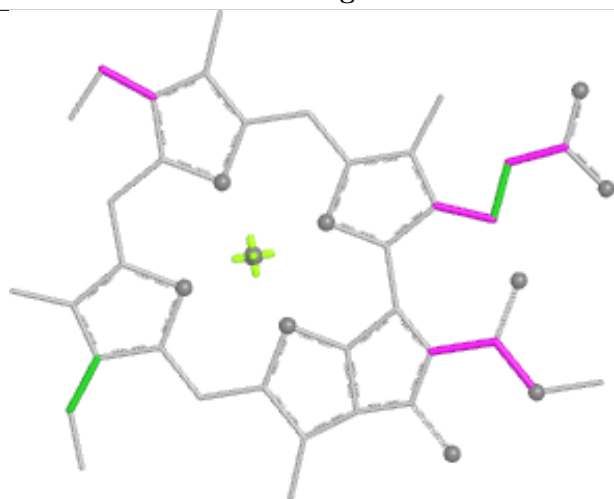
Ligand CLA 0 612



Bond lengths



Bond angles

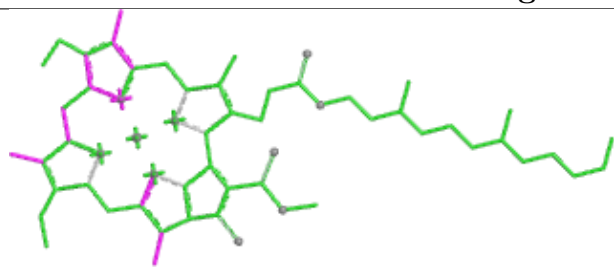


Torsions

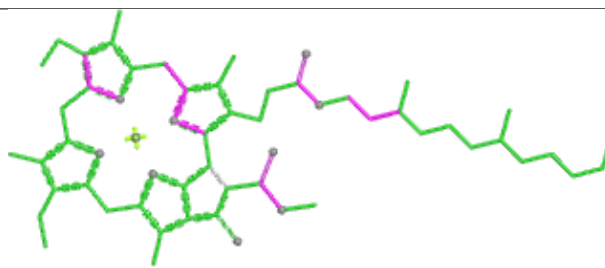


Rings

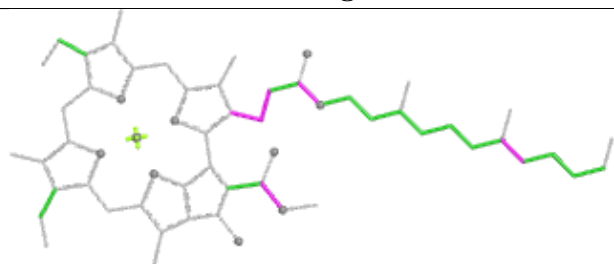
Ligand CLA 2 602



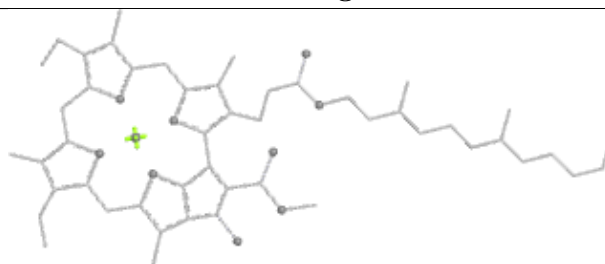
Bond lengths



Bond angles

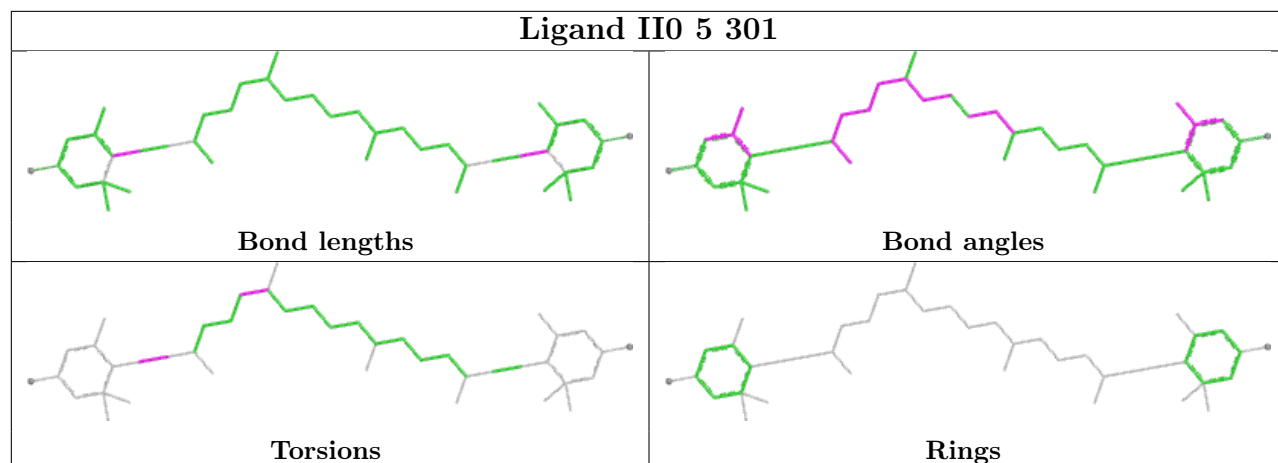


Torsions

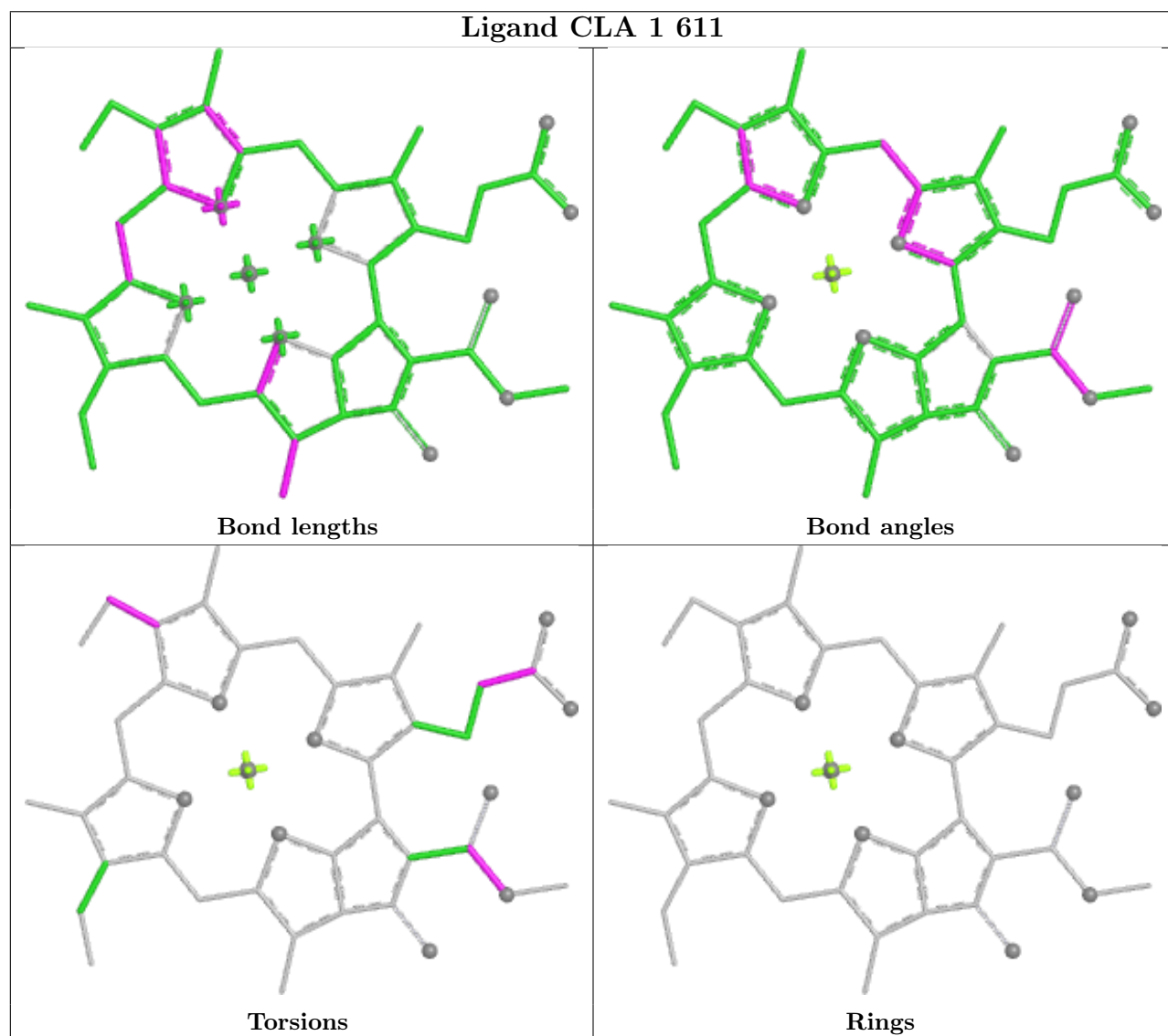


Rings

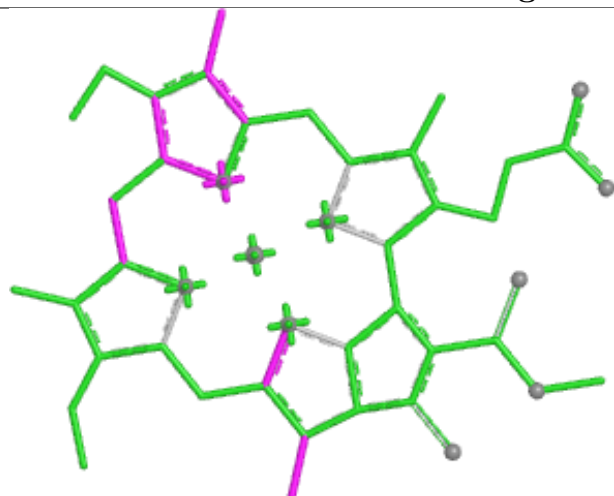
Ligand II0 5 301



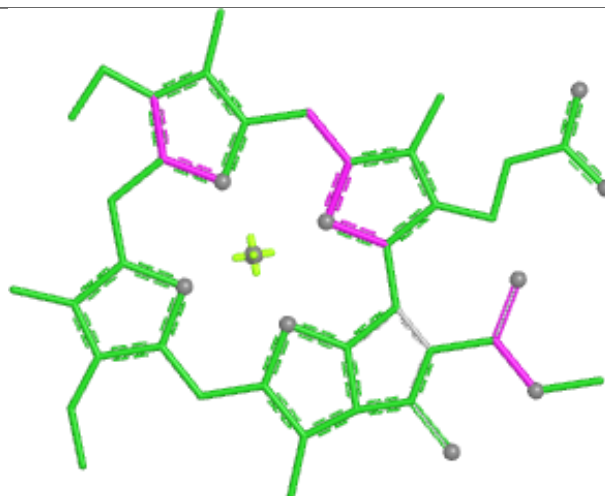
Ligand CLA 1 611



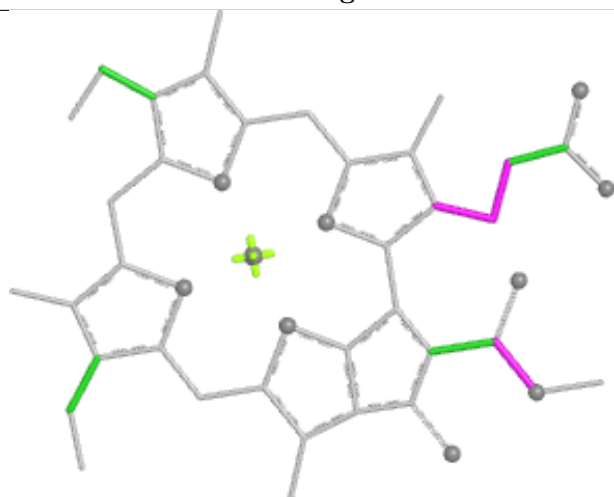
Ligand CLA 8 611



Bond lengths



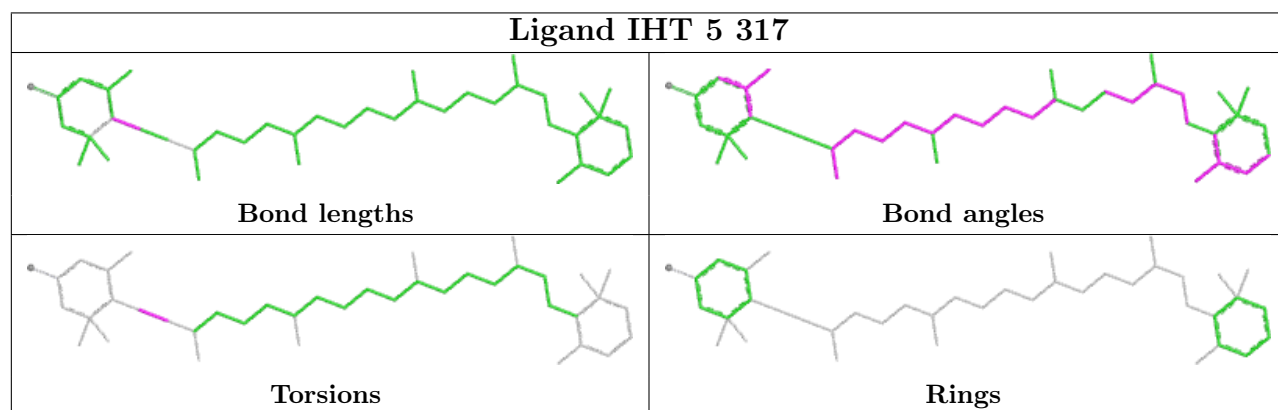
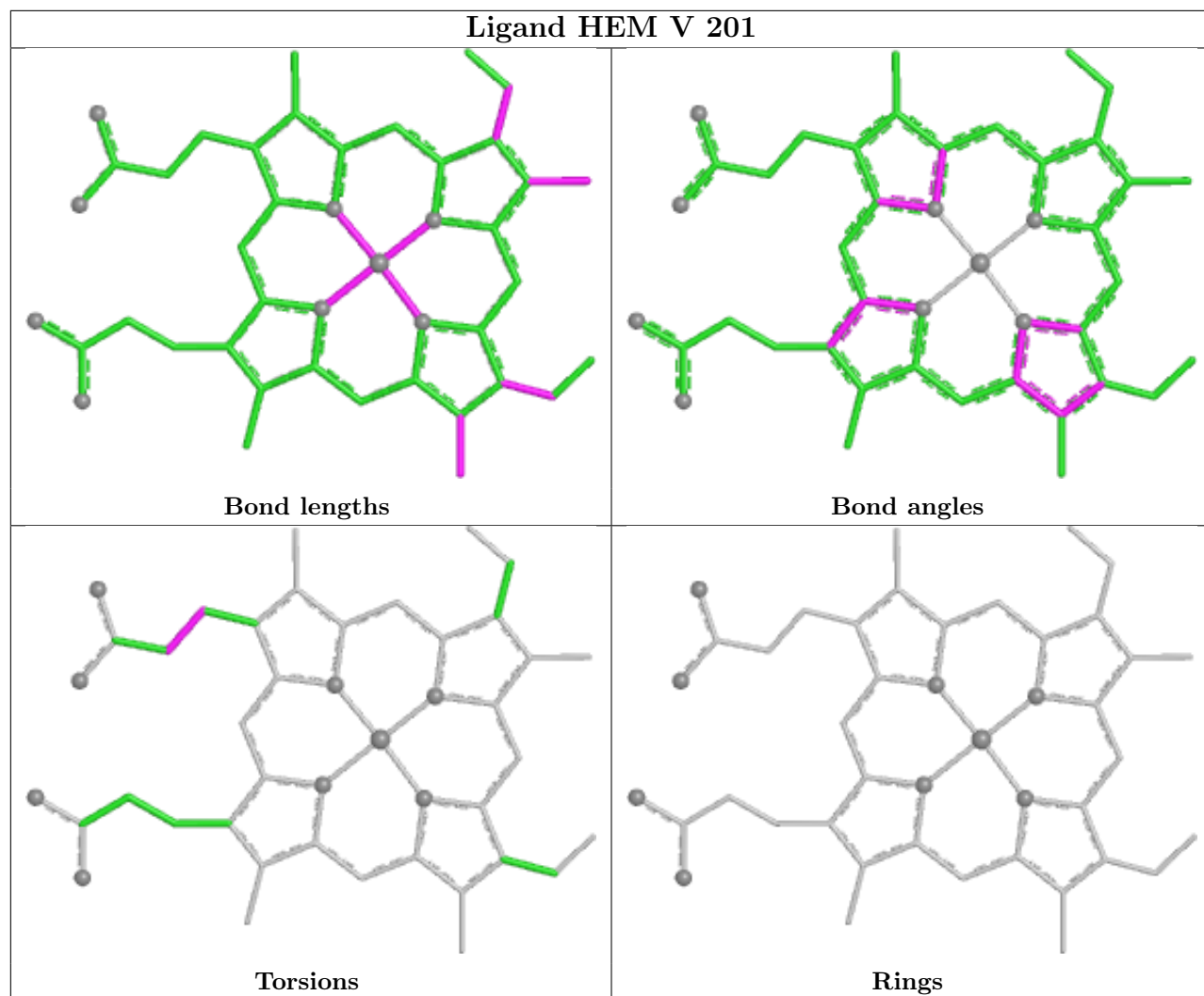
Bond angles



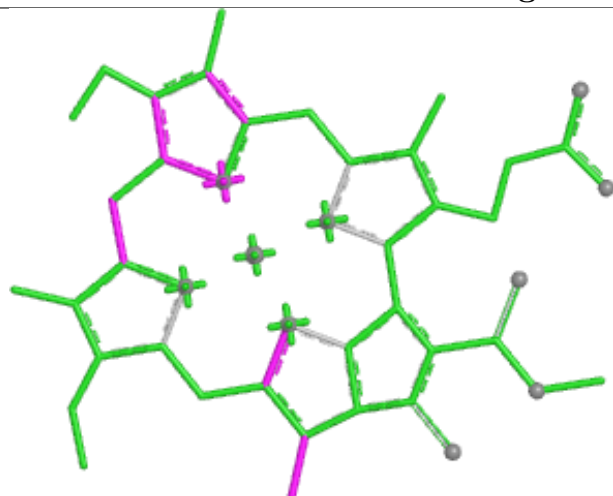
Torsions



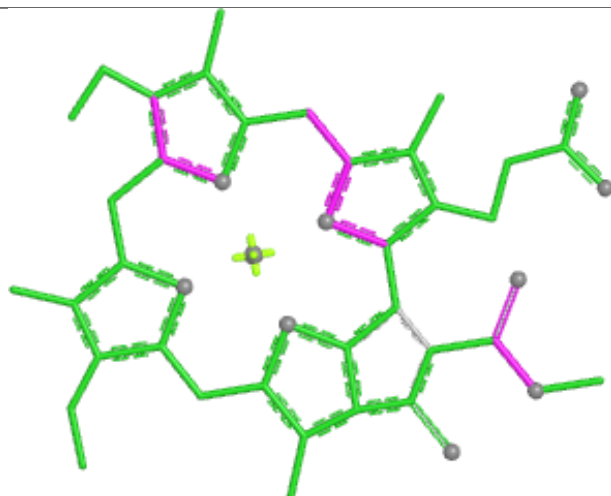
Rings



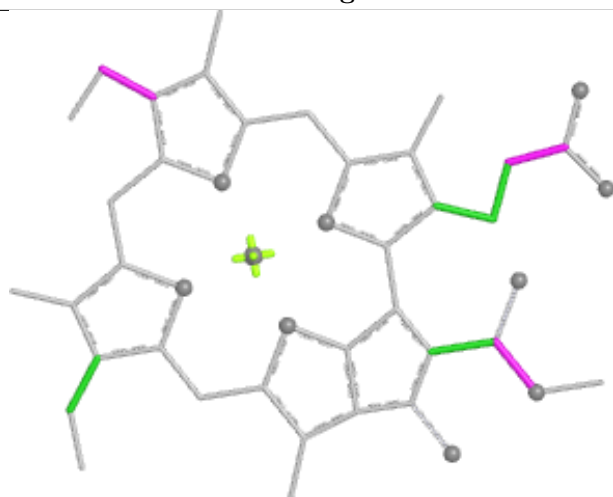
Ligand CLA 7 613



Bond lengths



Bond angles

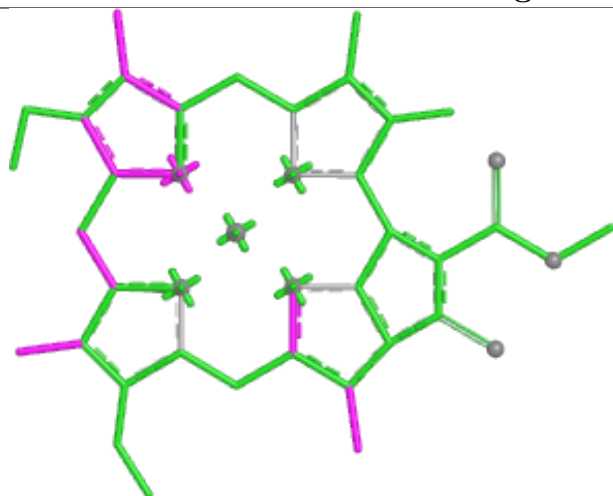


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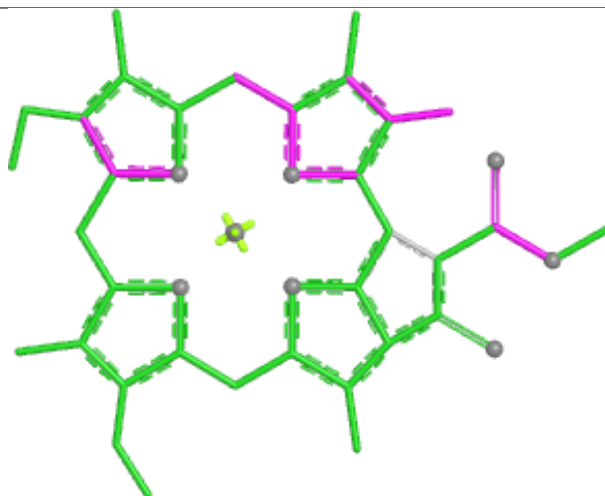


Rings

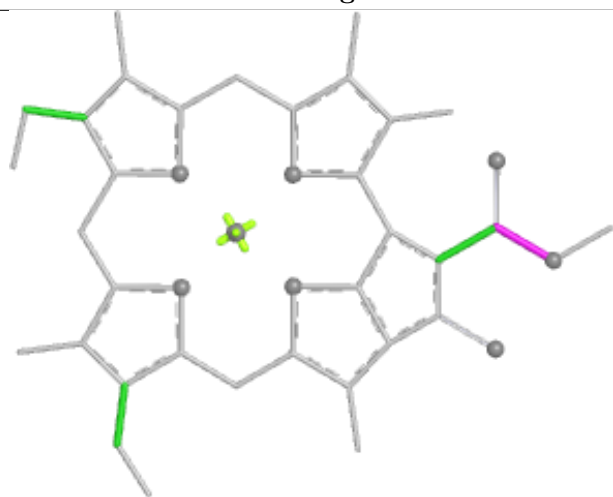
Ligand CLA B 608



Bond lengths



Bond angles

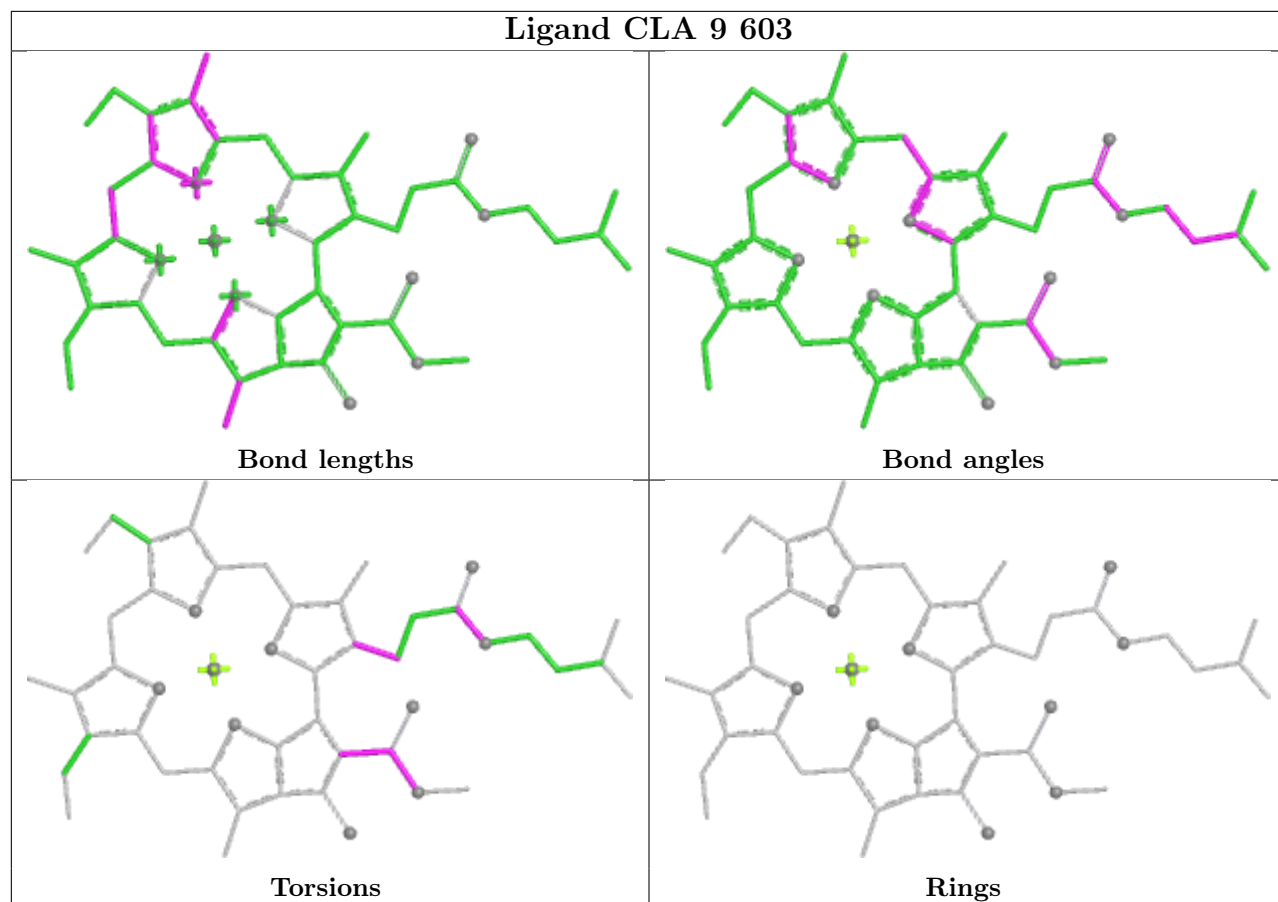


Torsions

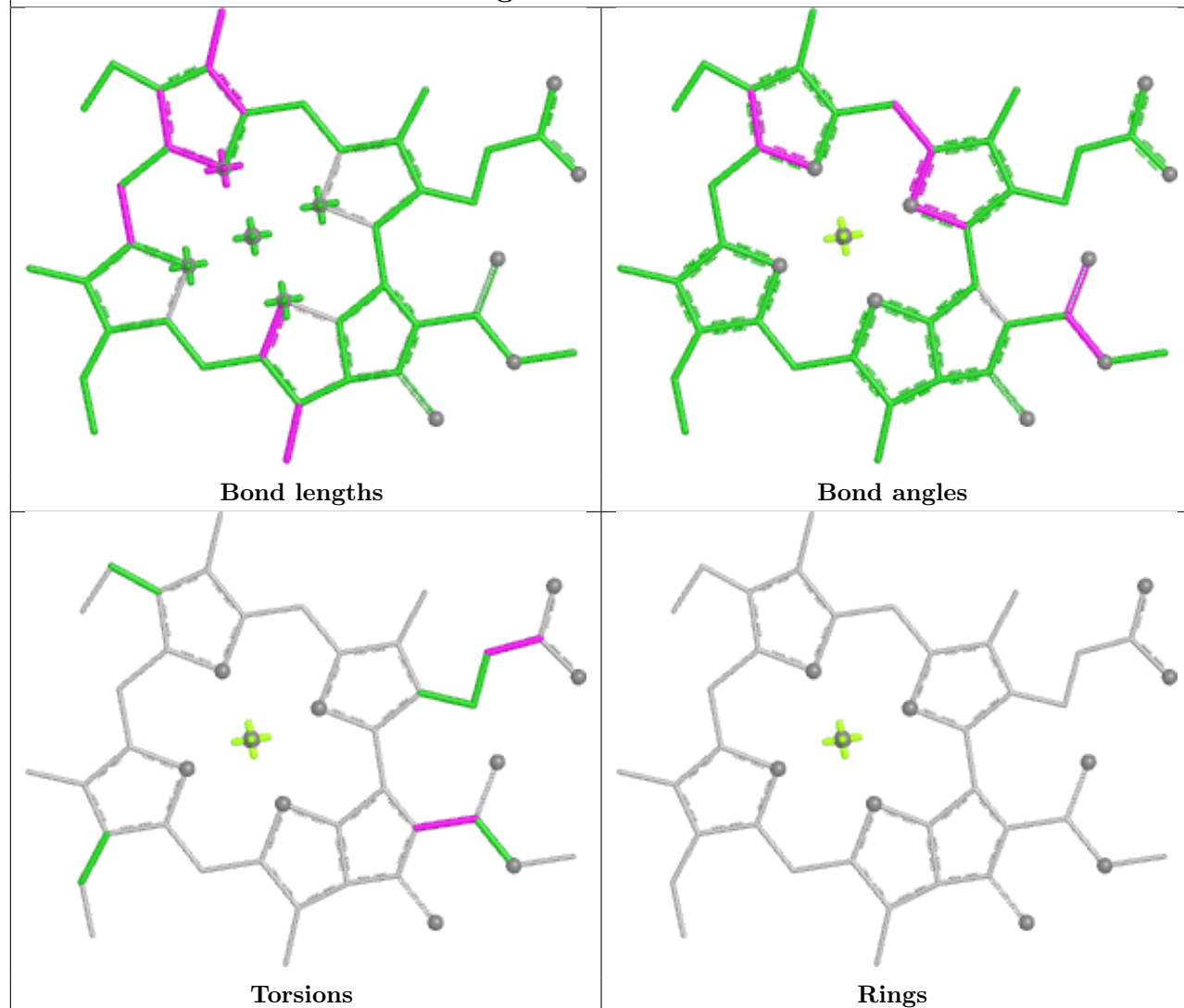


Rings

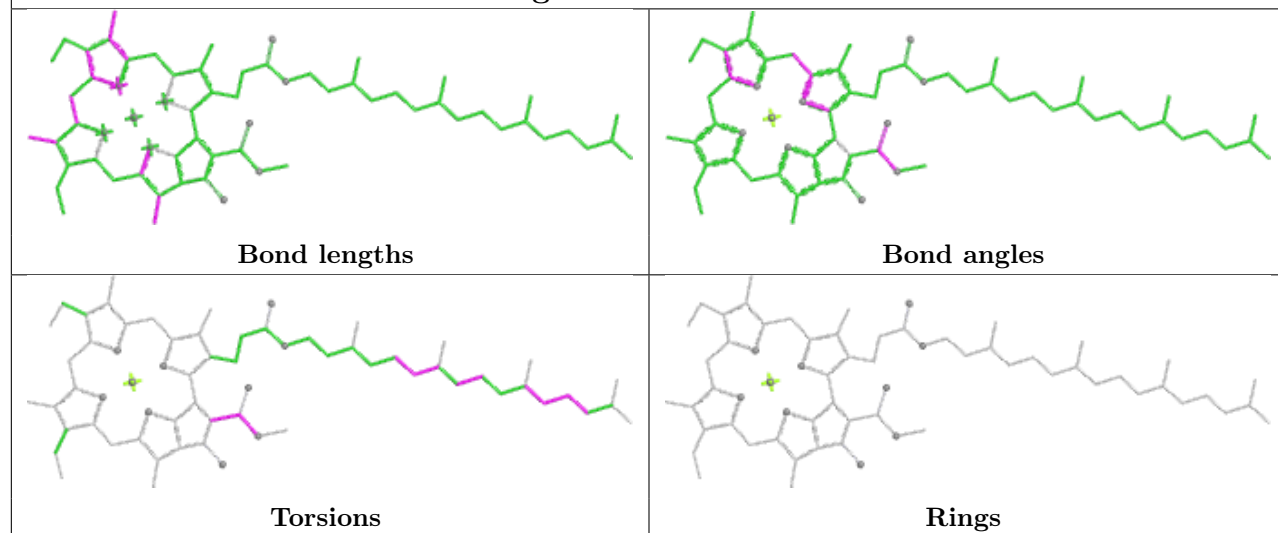
Ligand CLA 9 603



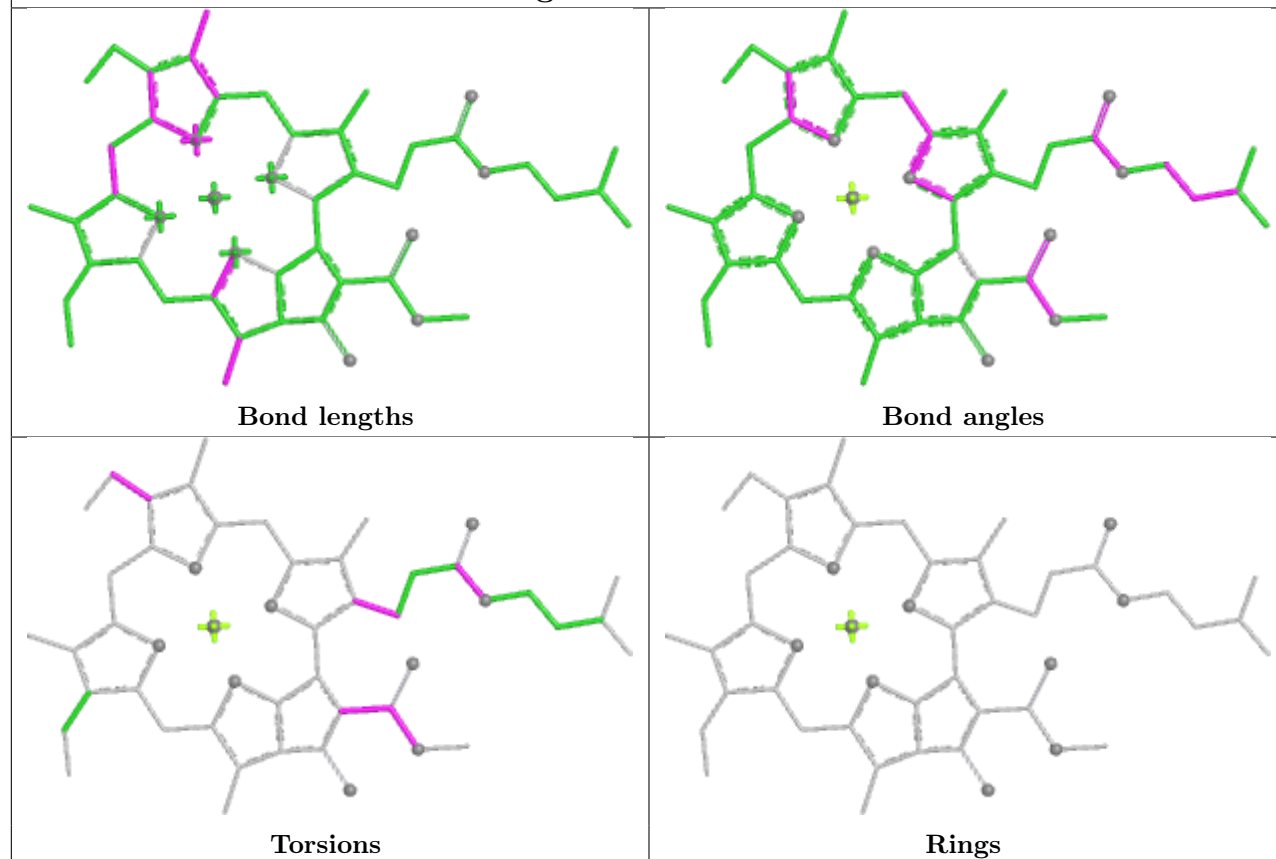
Ligand CLA 8 606



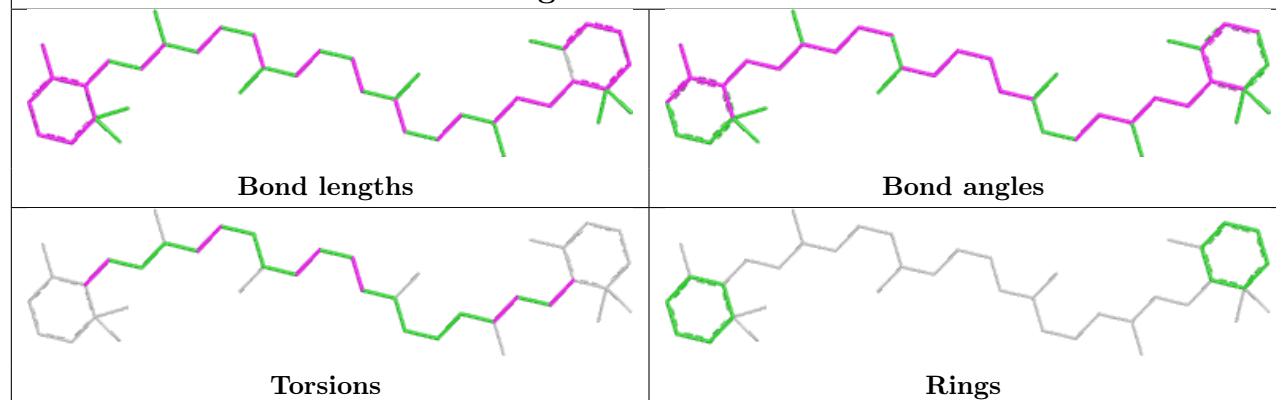
Ligand CLA B 606

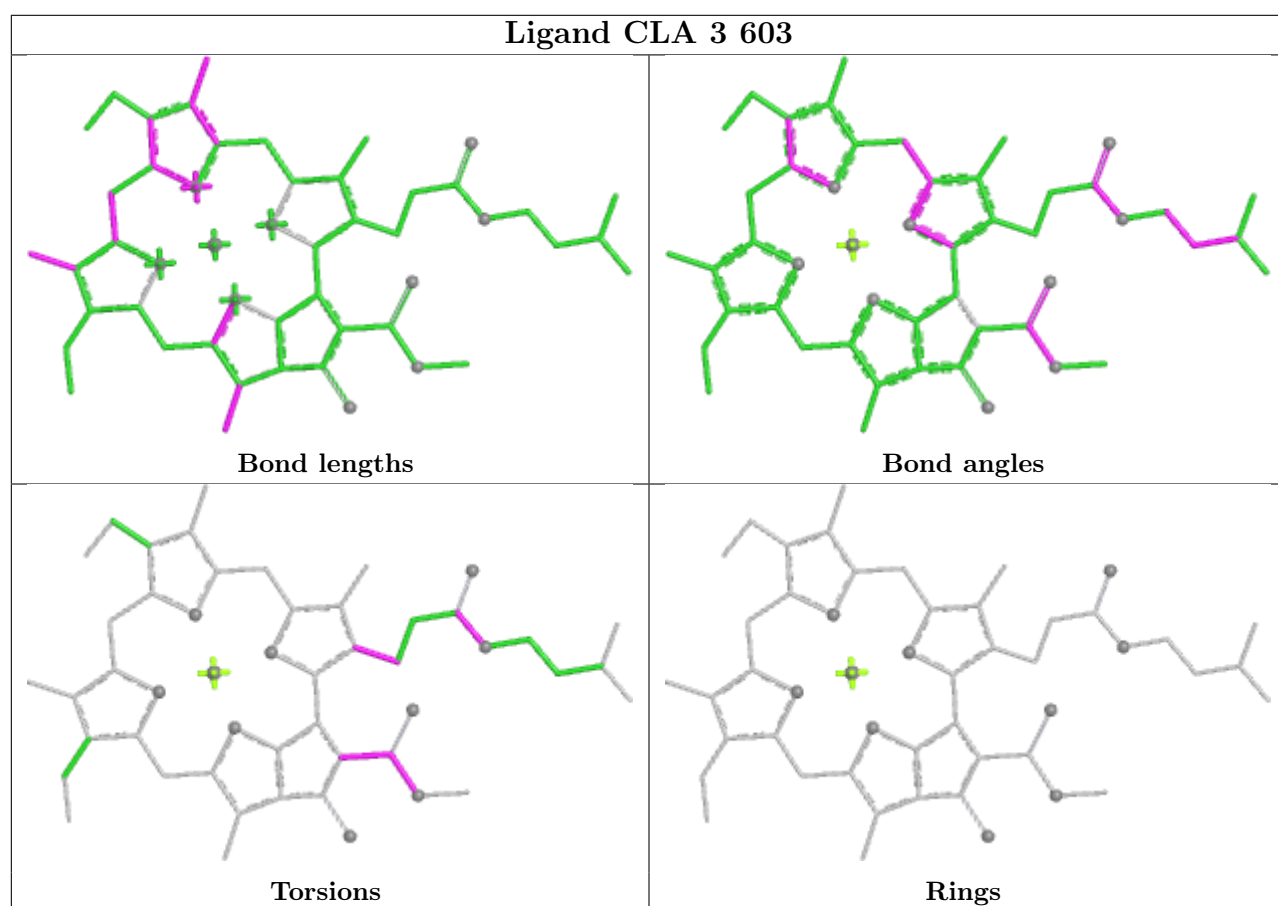
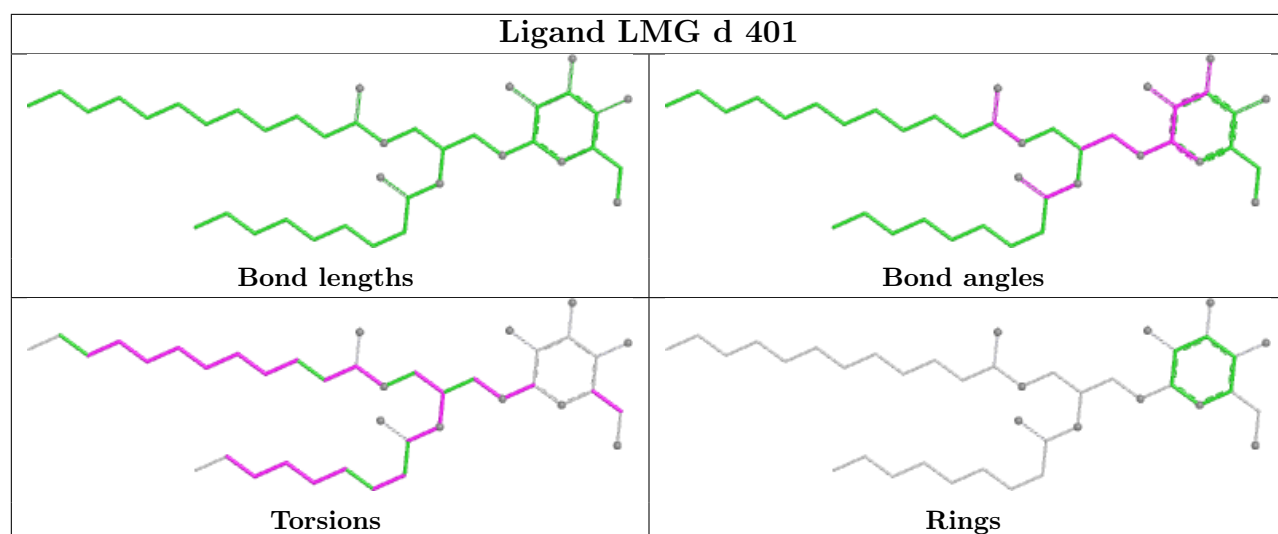


Ligand CLA 1 605

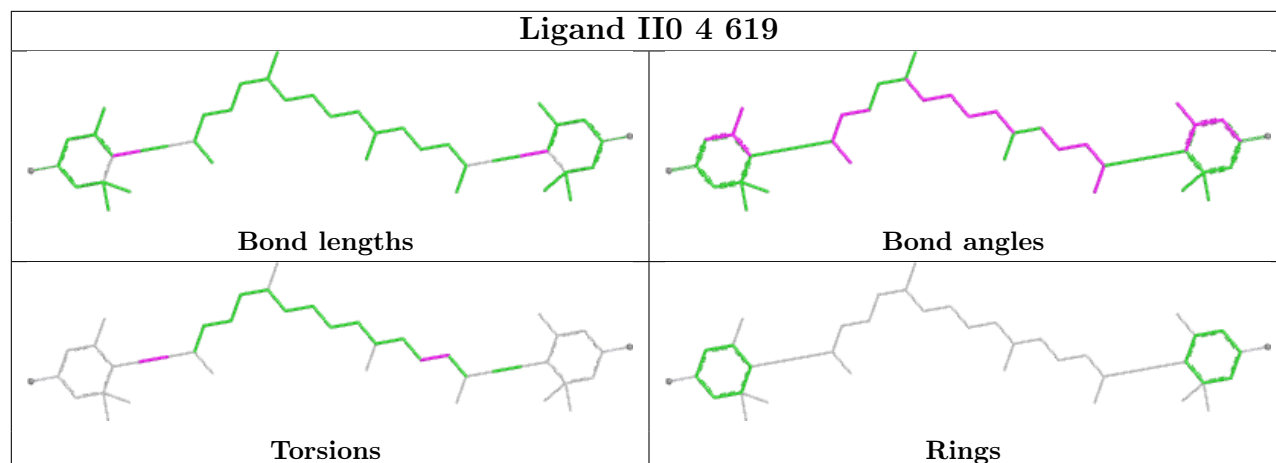


Ligand 8CT b 622

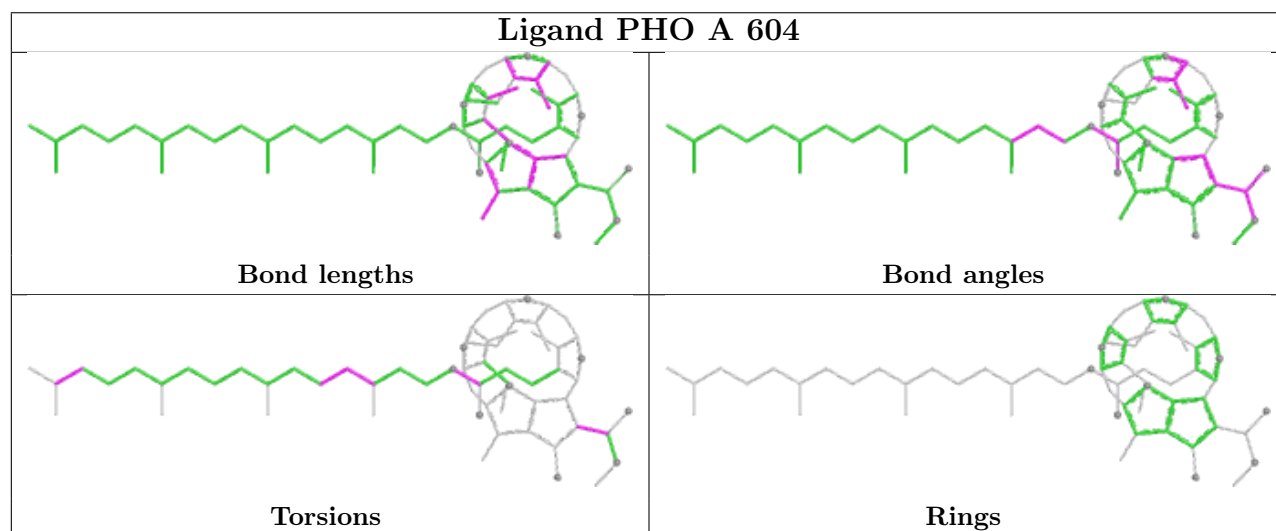




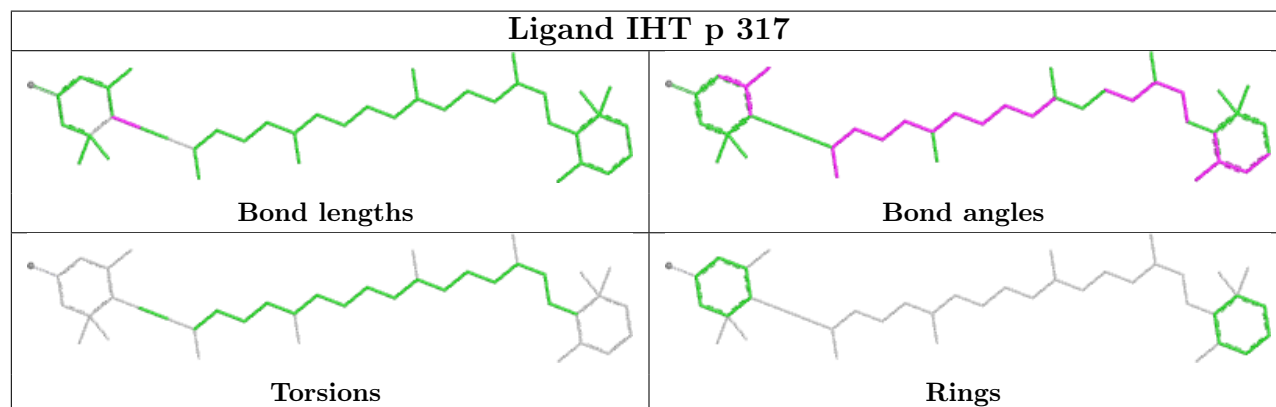
Ligand IIO 4 619



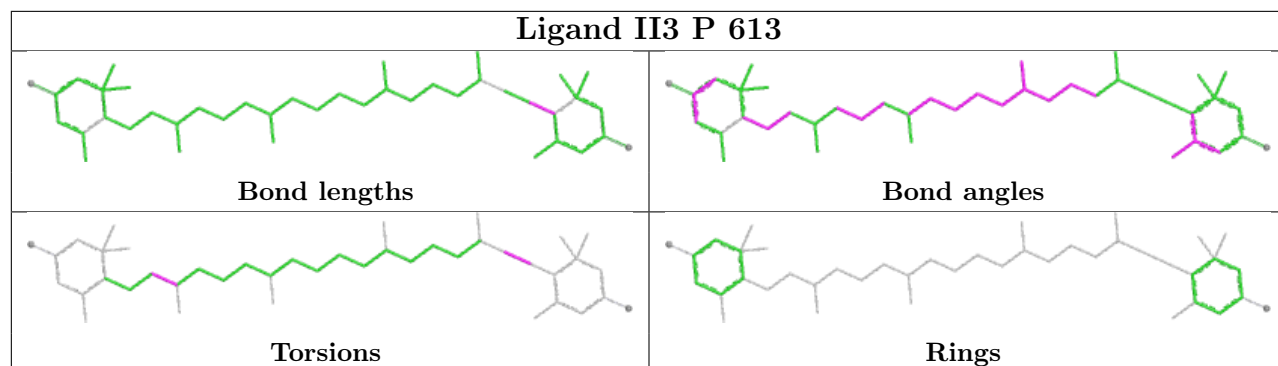
Ligand PHO A 604



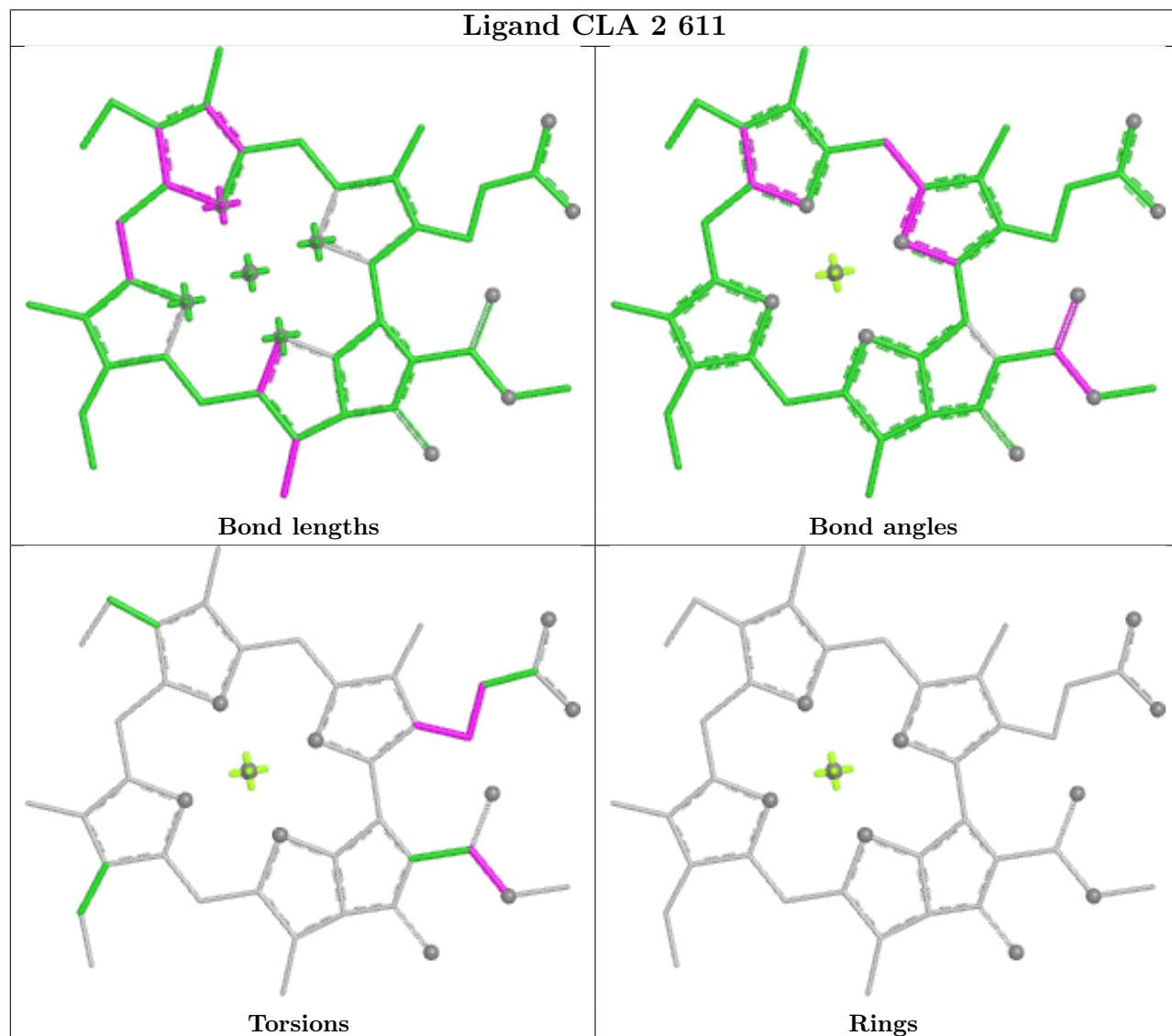
Ligand IHT p 317

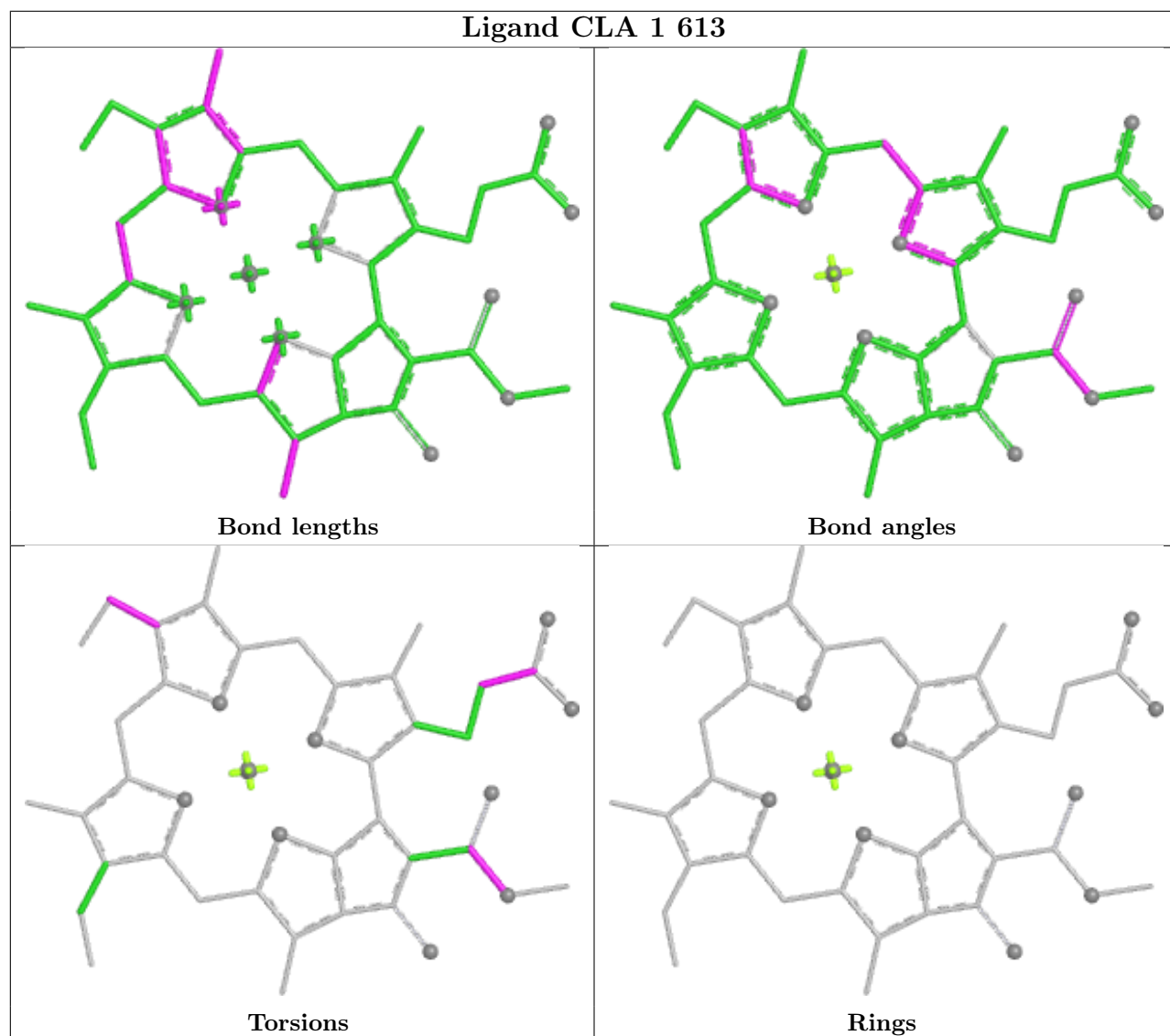
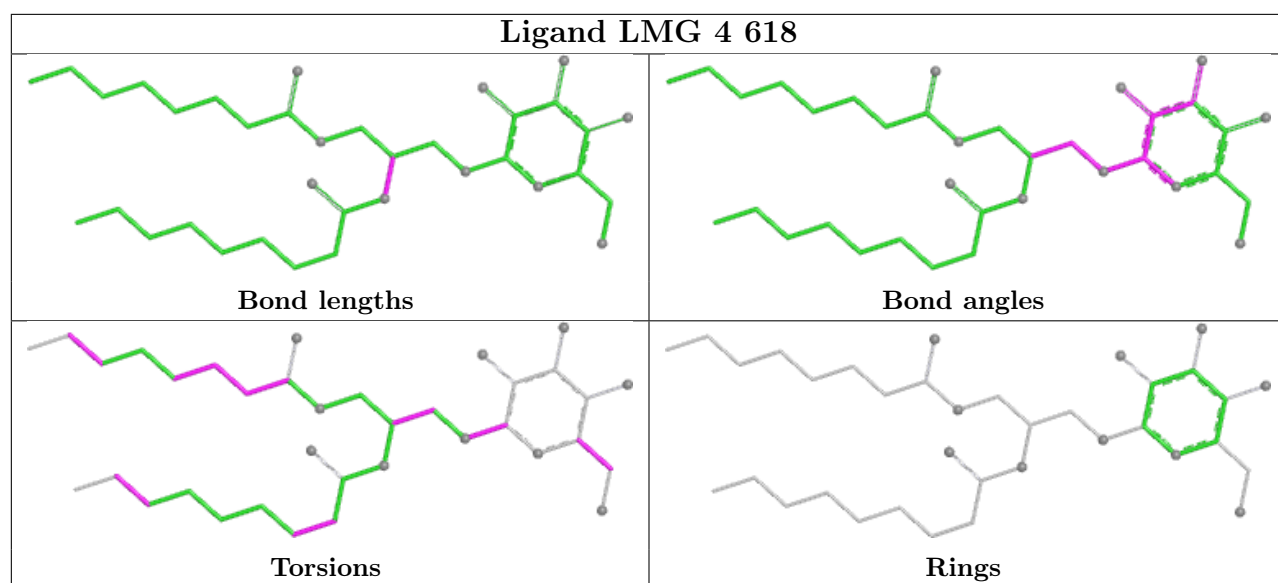


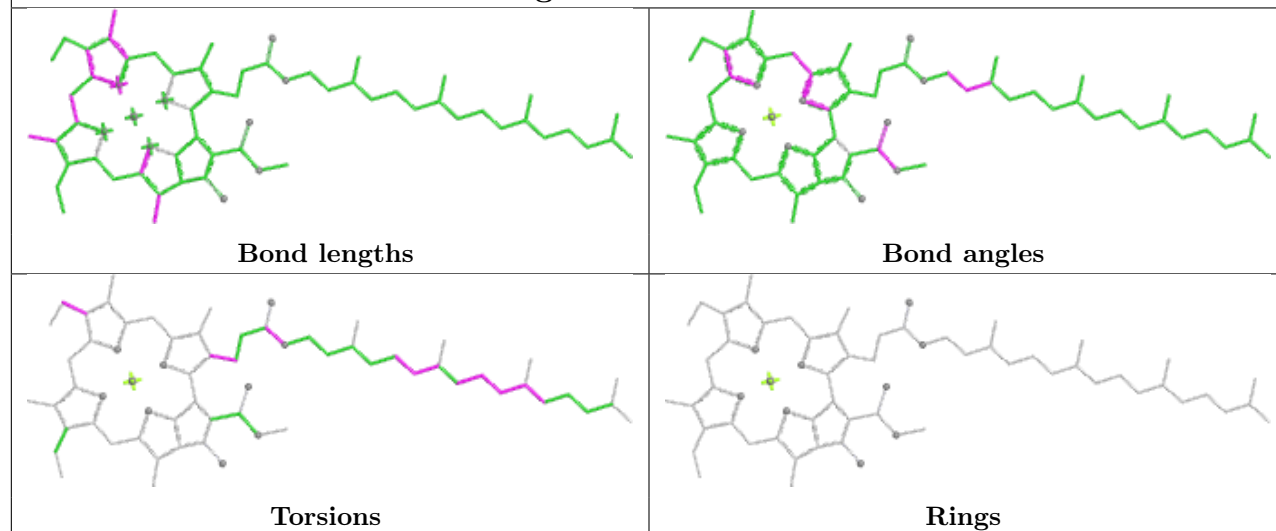
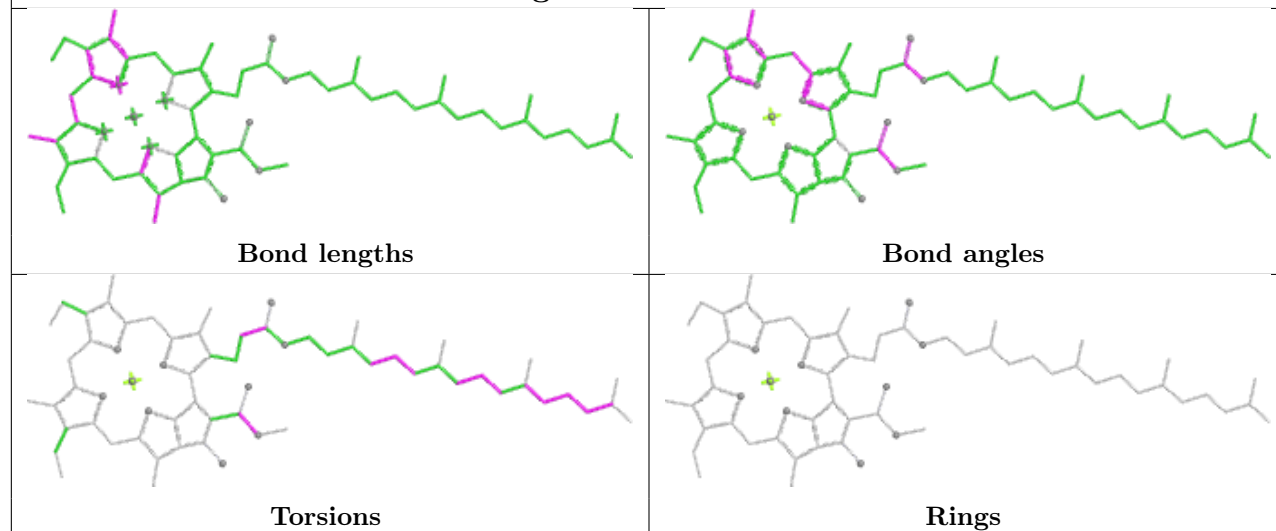
Ligand II3 P 613



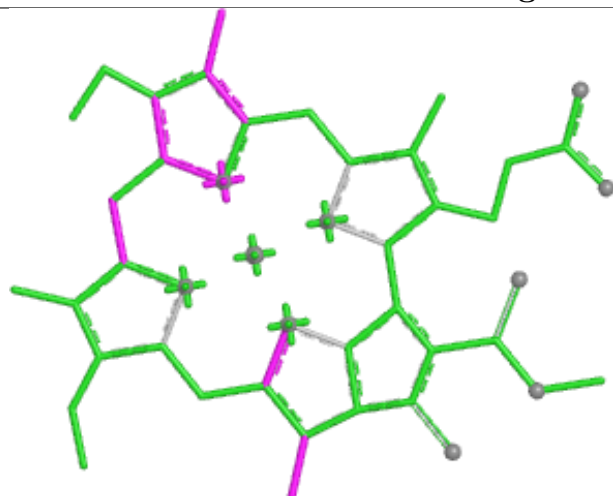
Ligand CLA 2 611



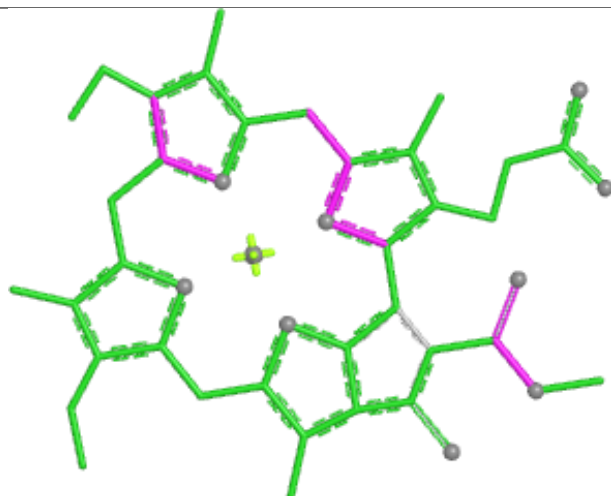


Ligand CLA b 617**Ligand CLA B 614**

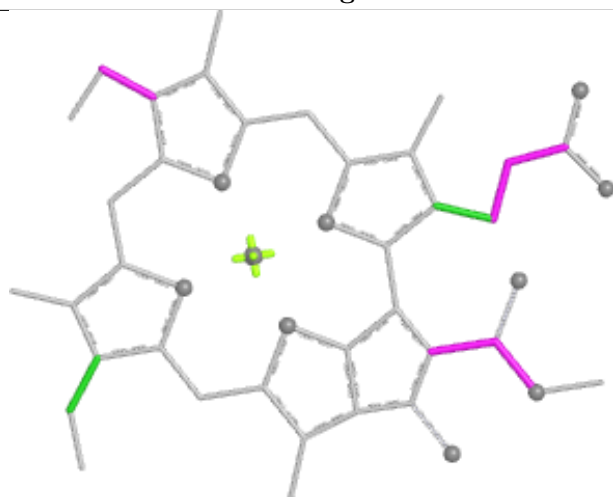
Ligand CLA 6 611



Bond lengths



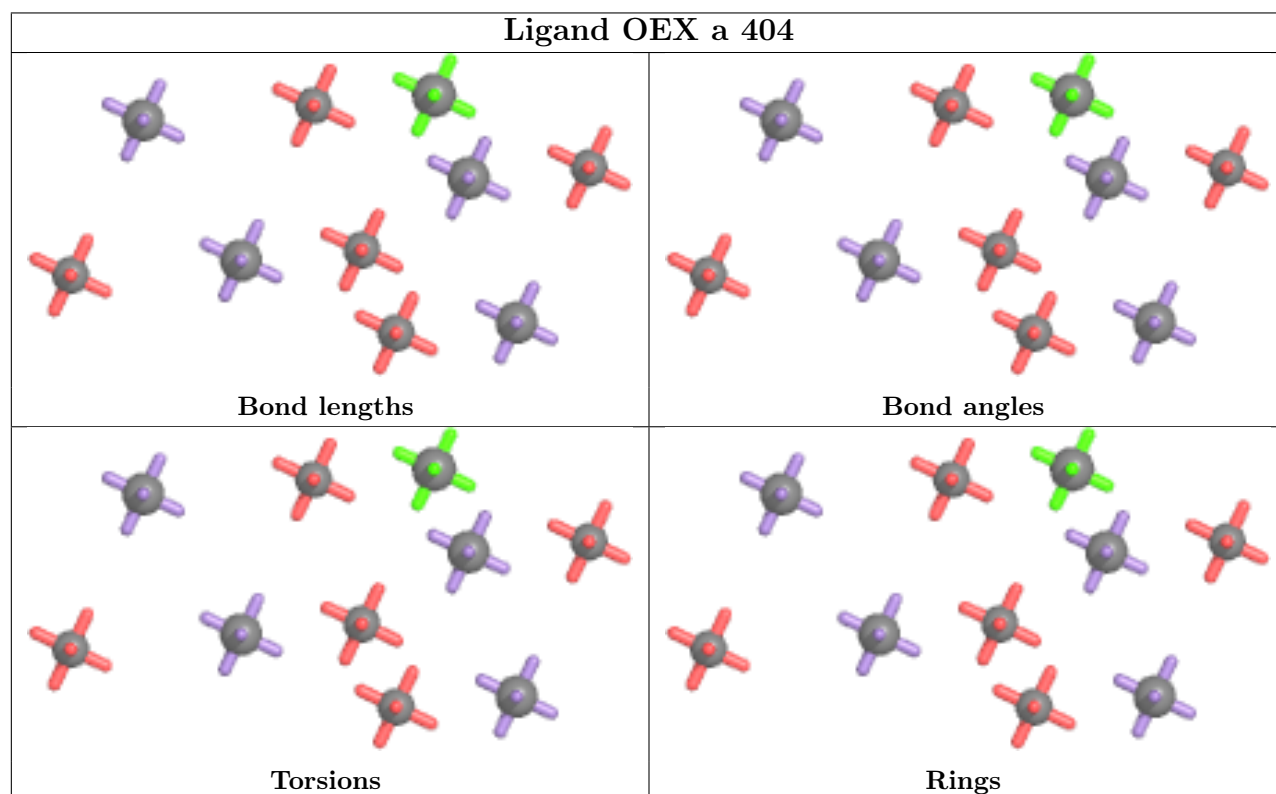
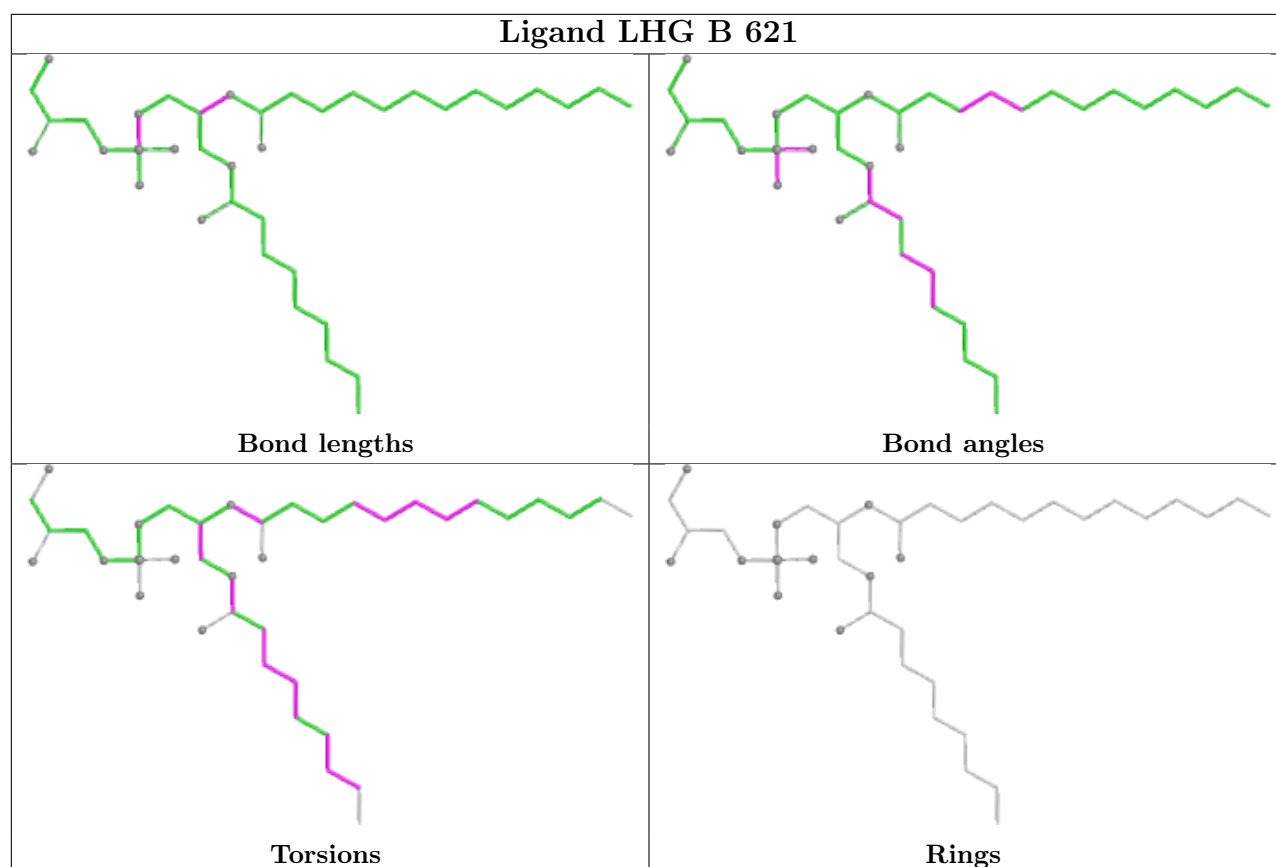
Bond angles

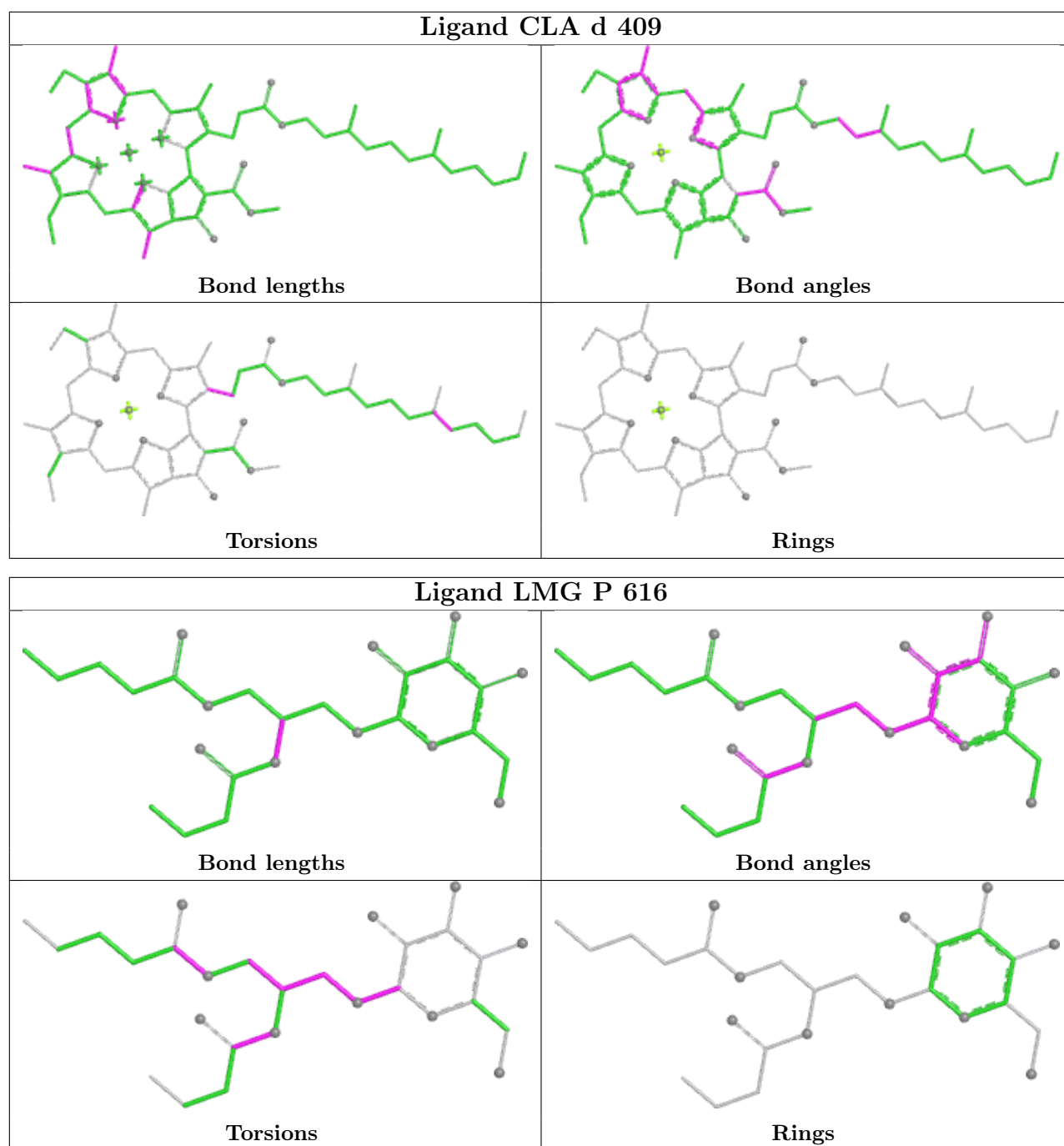


Torsions

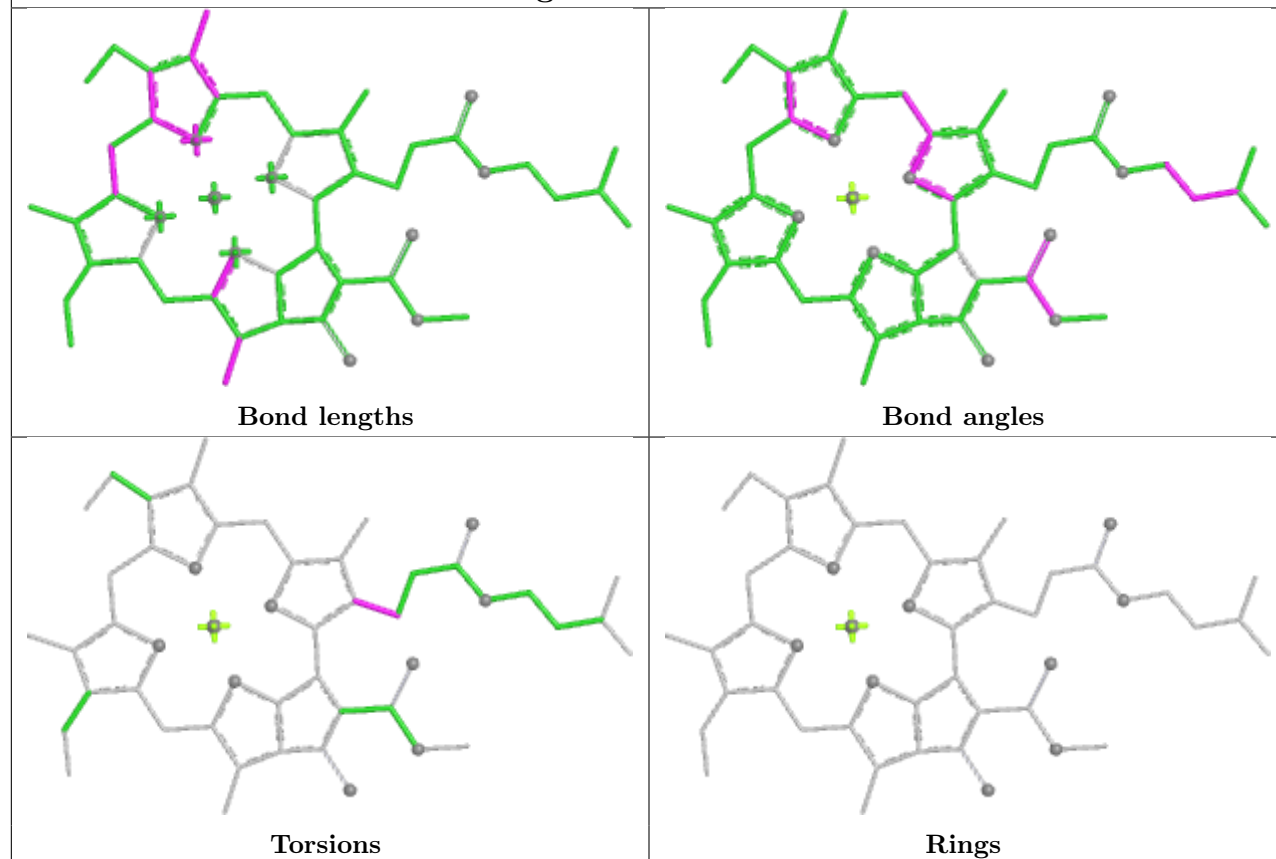


Rings

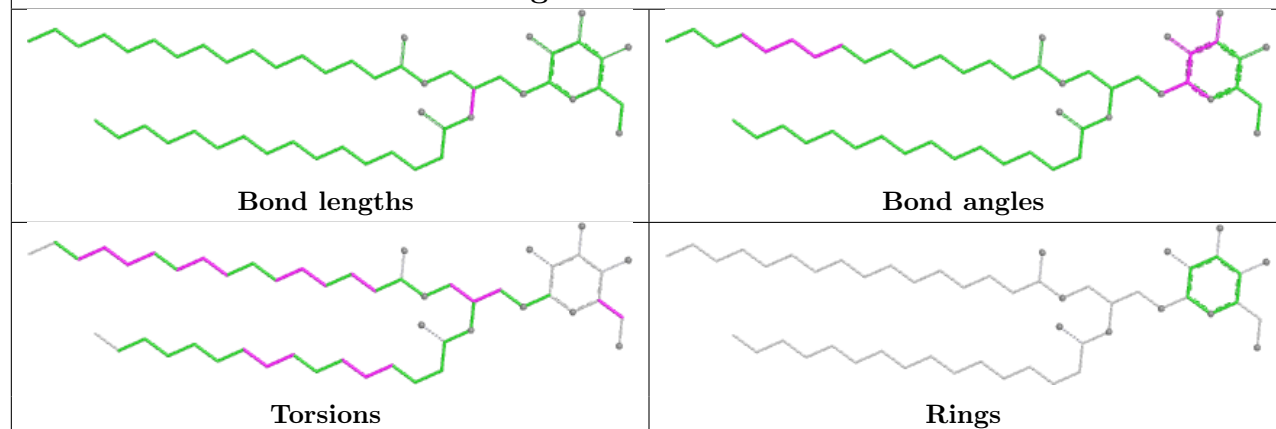




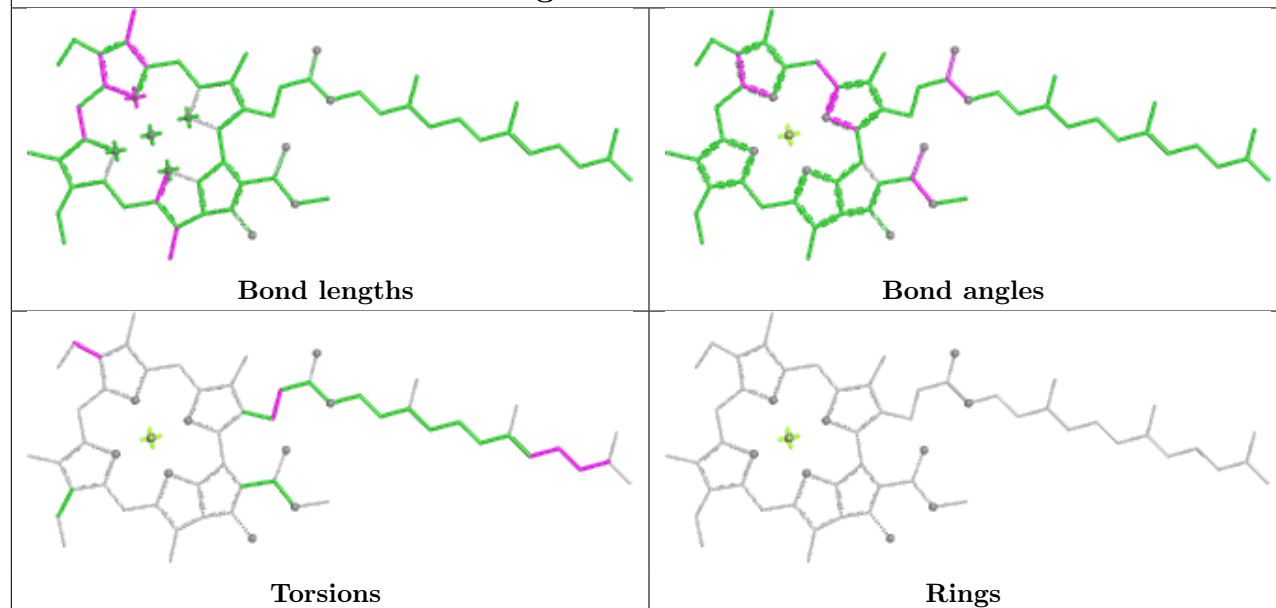
Ligand CLA 6 603



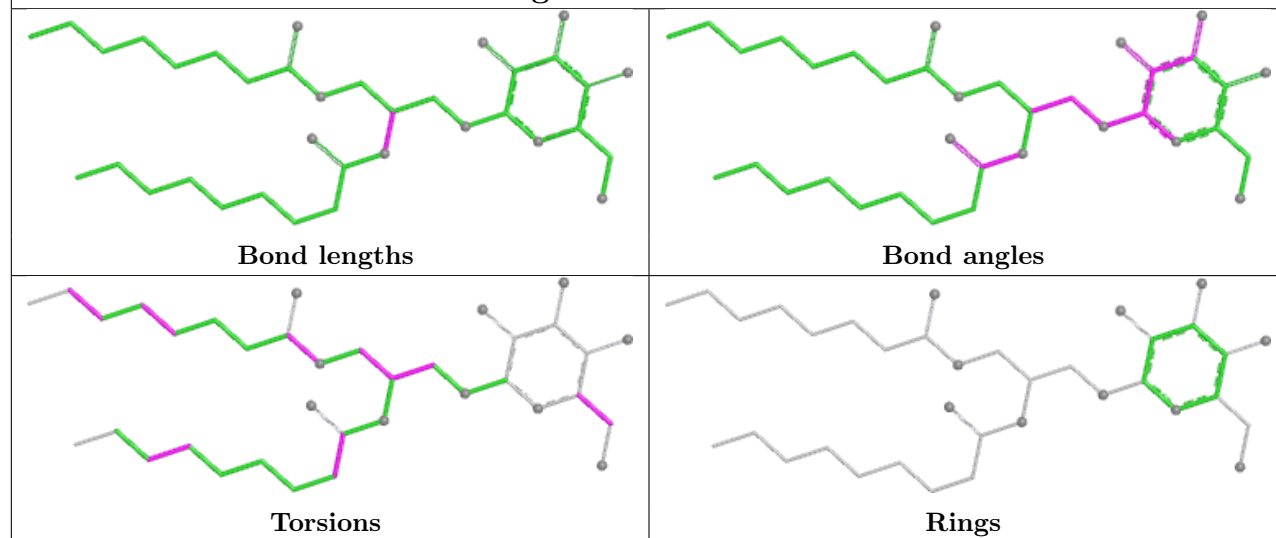
Ligand LMG b 618



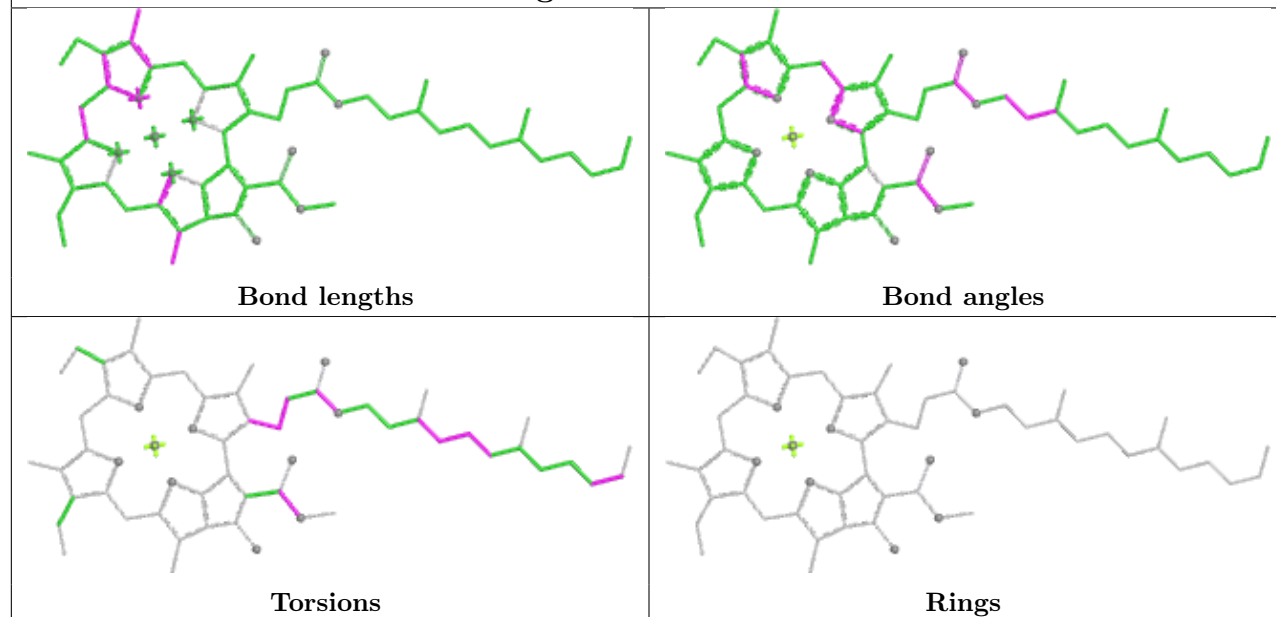
Ligand CLA 6 607



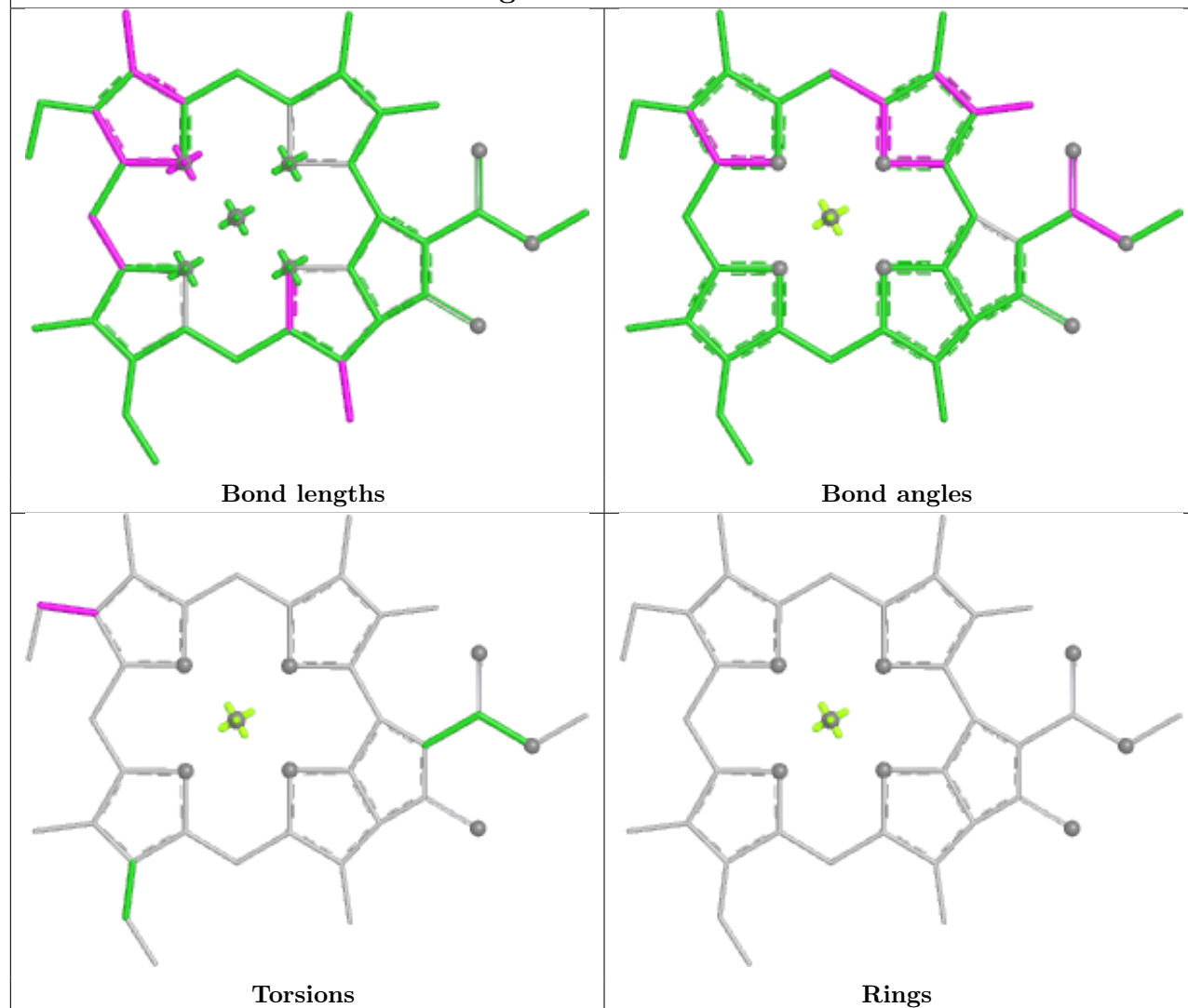
Ligand LMG 8 617



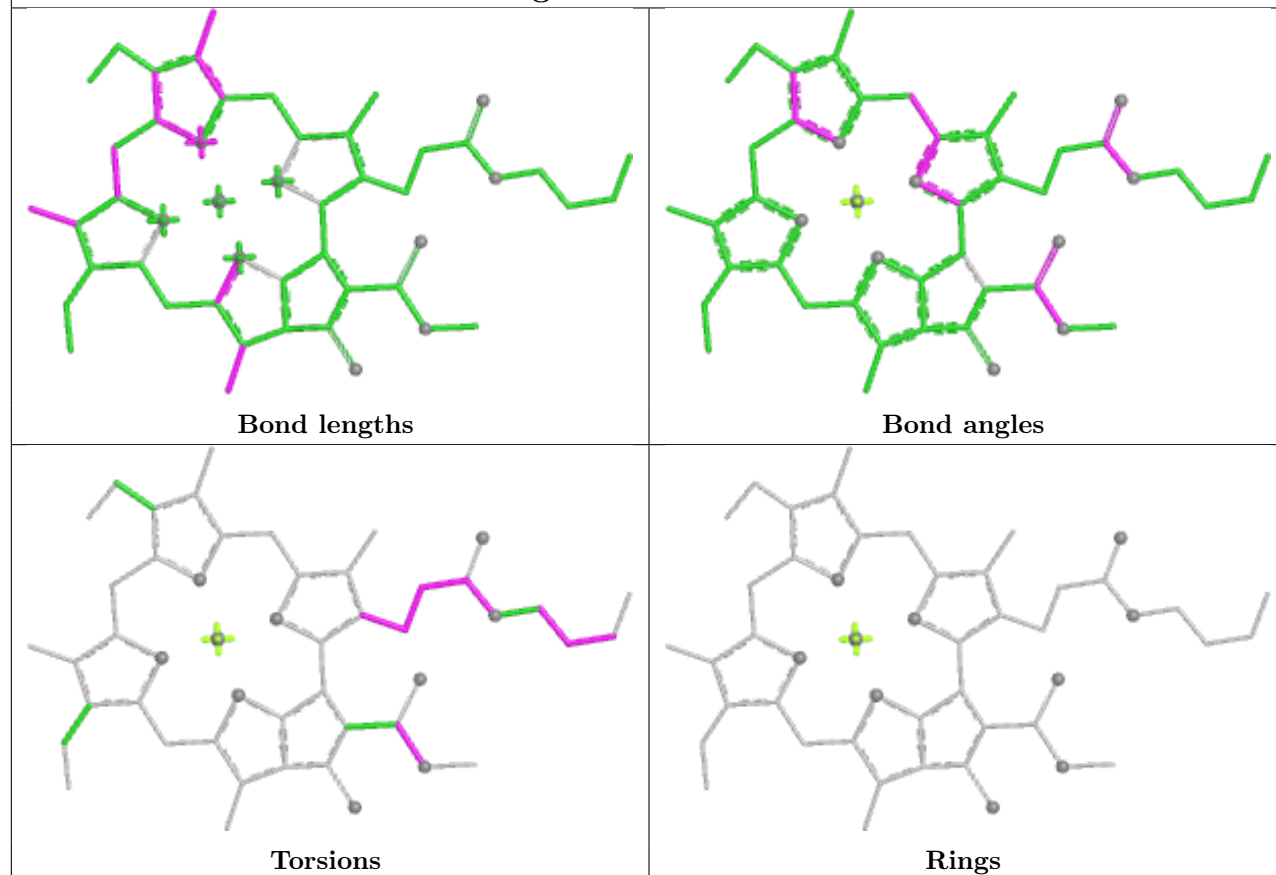
Ligand CLA 7 602



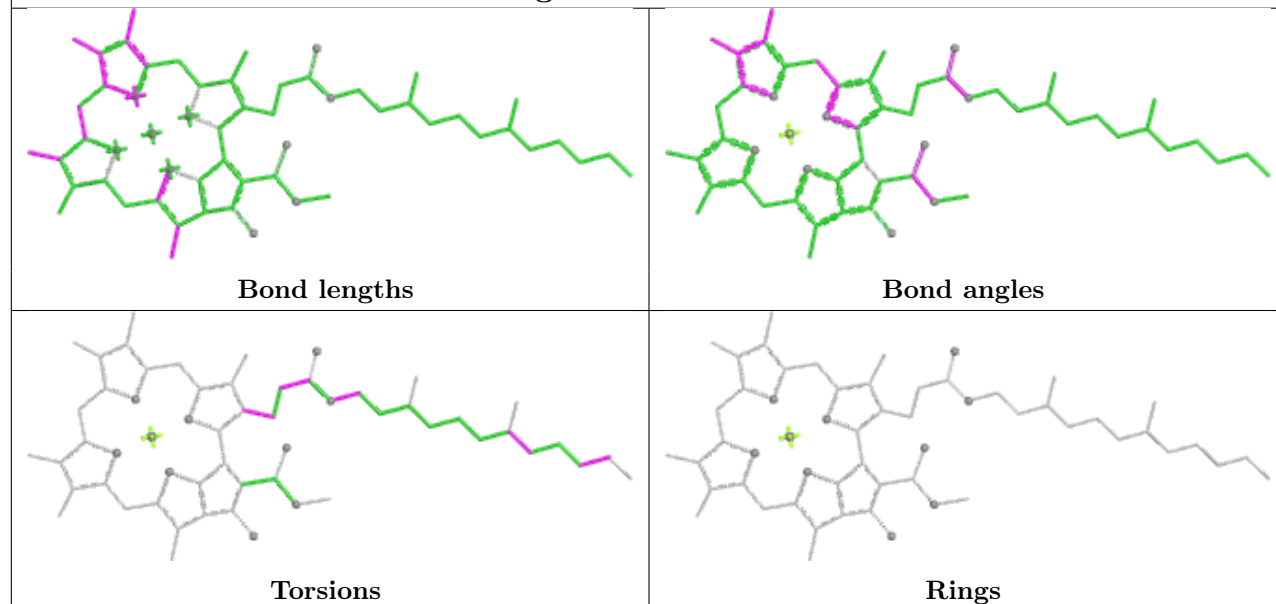
Ligand CLA 6 608



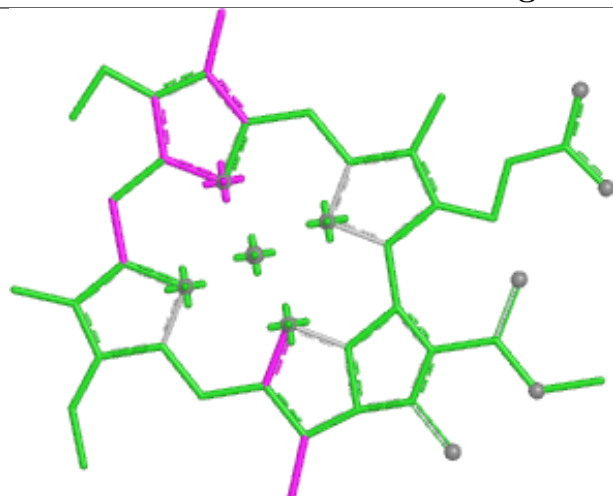
Ligand CLA C 513



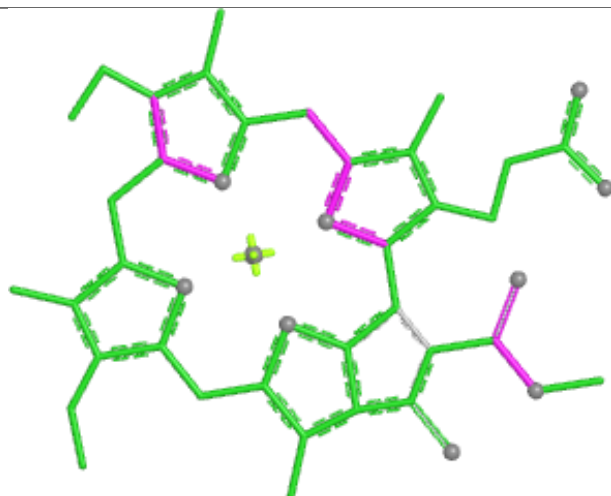
Ligand CLA d 402



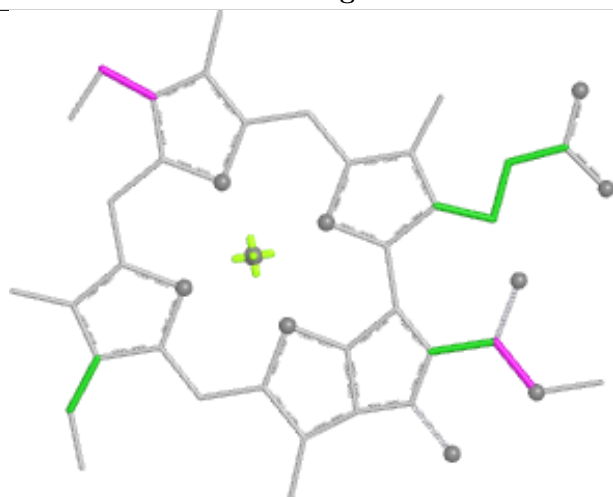
Ligand CLA 2 607



Bond lengths



Bond angles

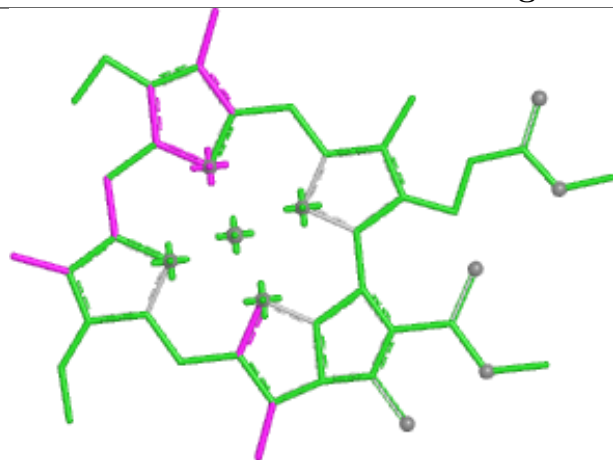


Torsions

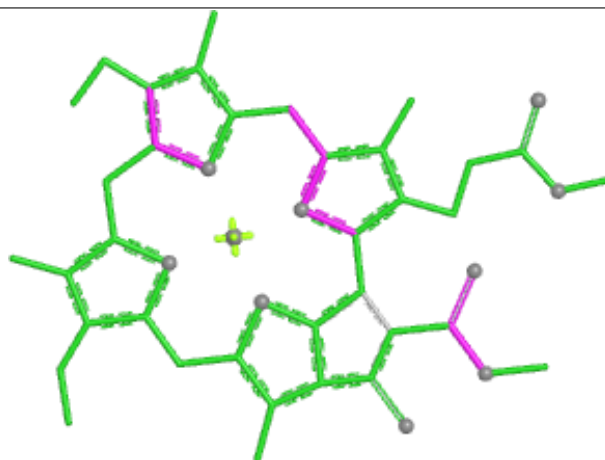


Rings

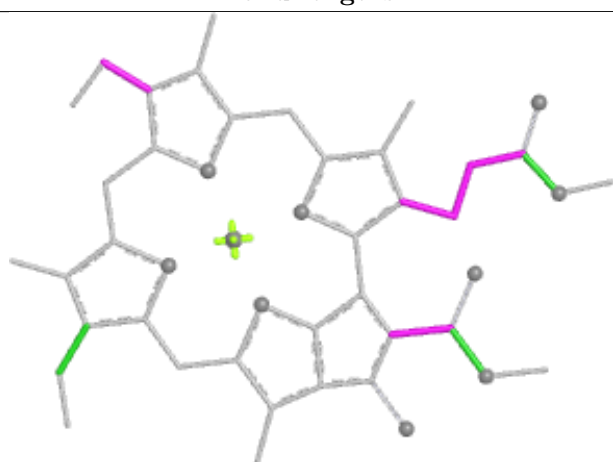
Ligand CLA 9 605



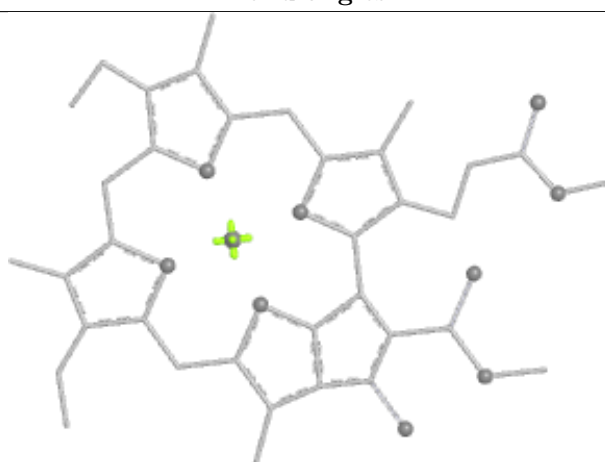
Bond lengths



Bond angles

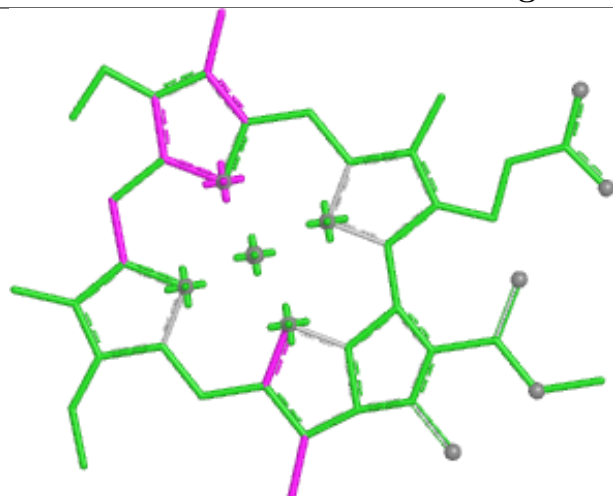


Torsions

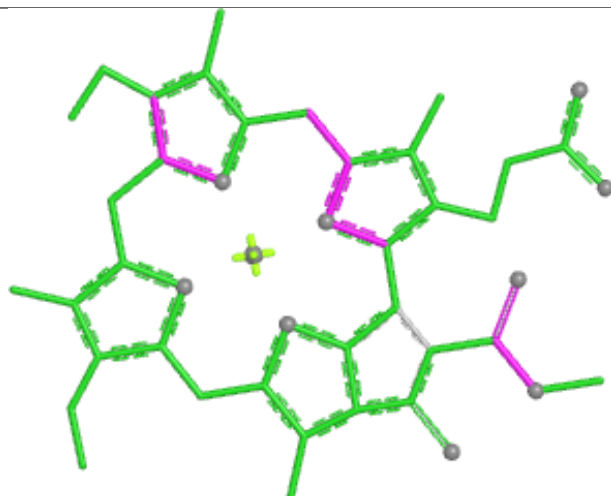


Rings

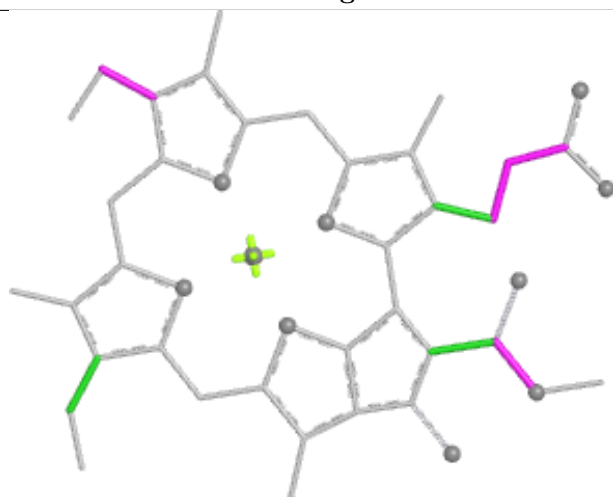
Ligand CLA 0 611



Bond lengths



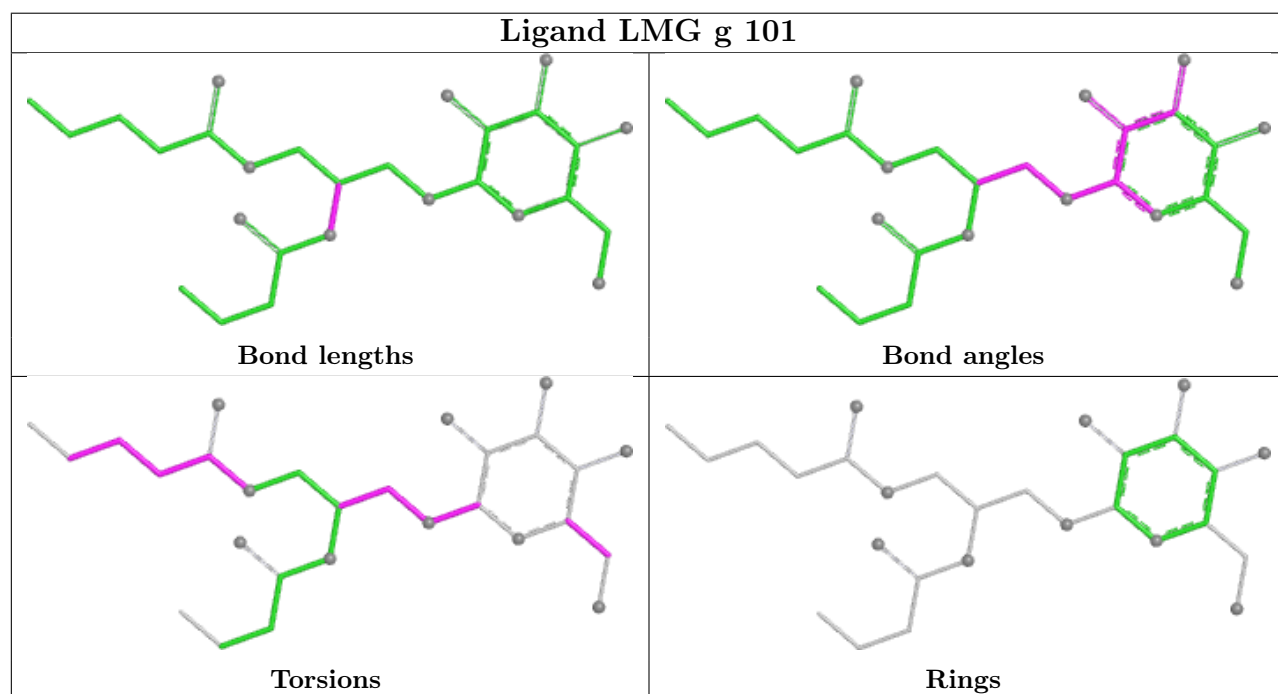
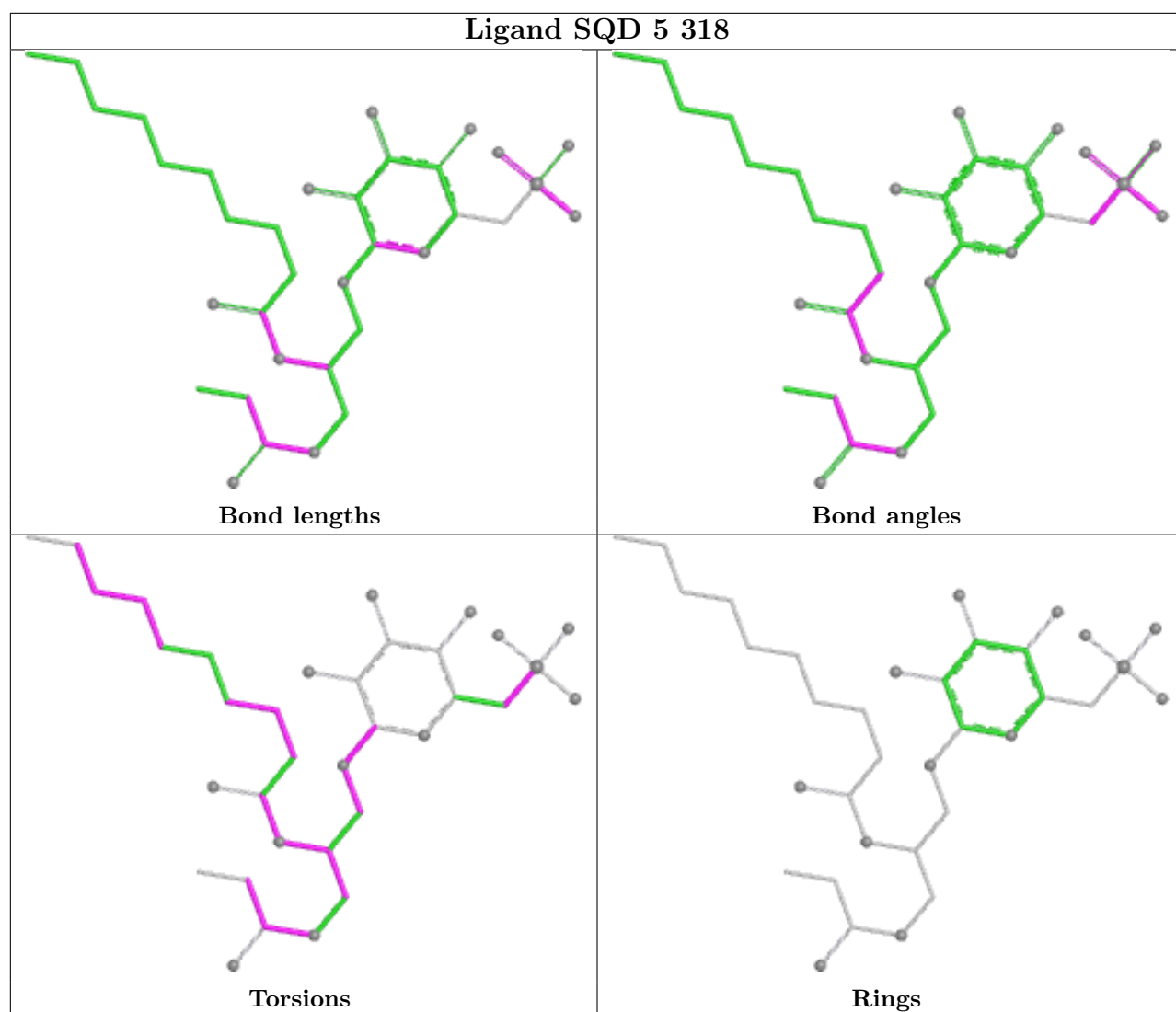
Bond angles

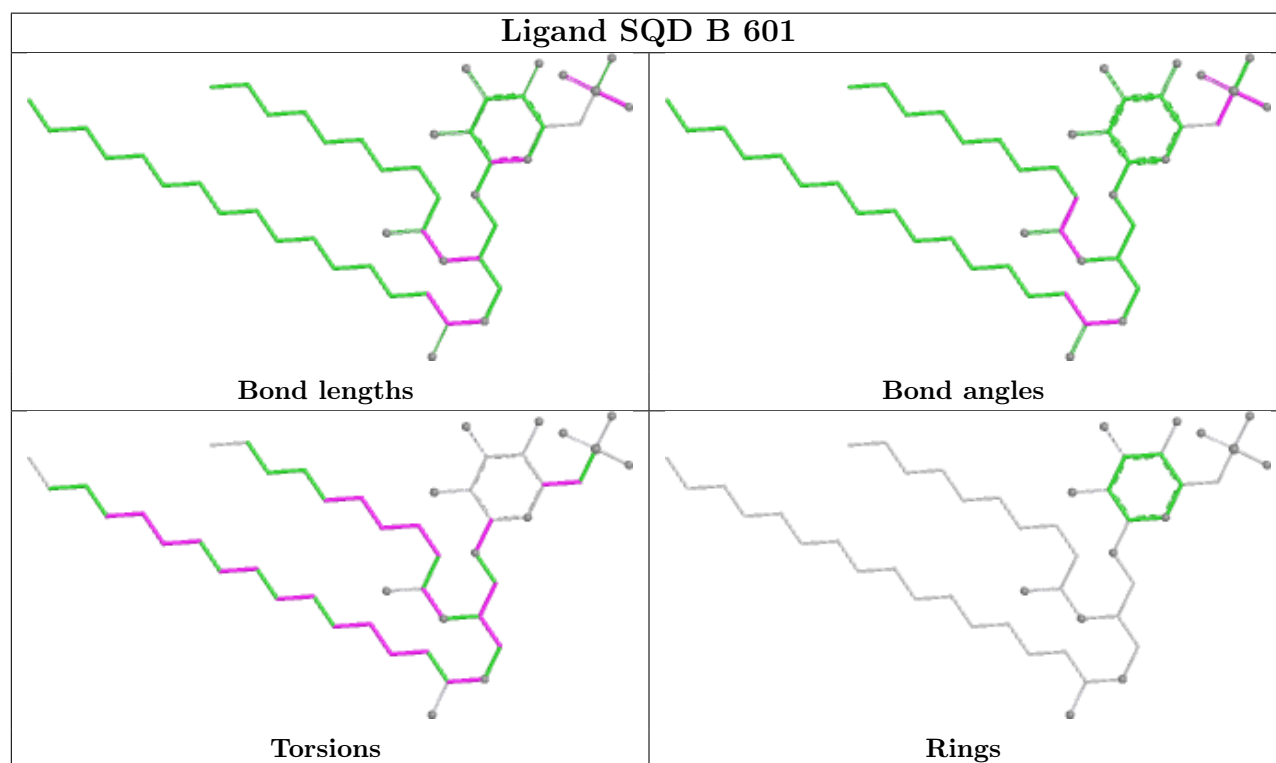
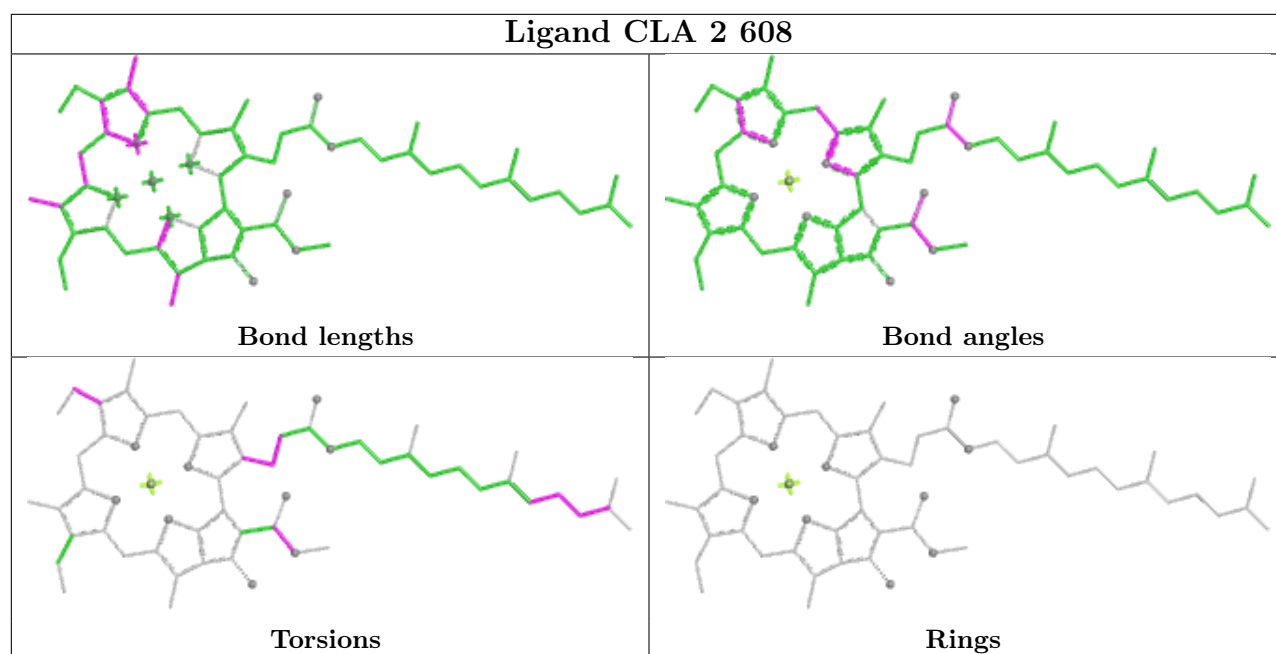


Torsions

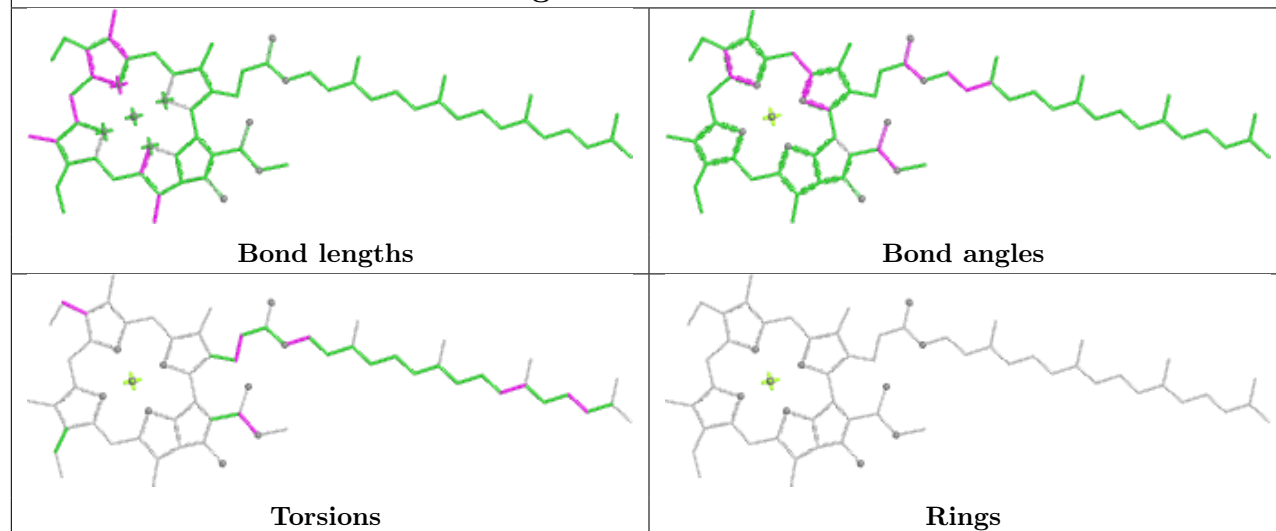


Rings

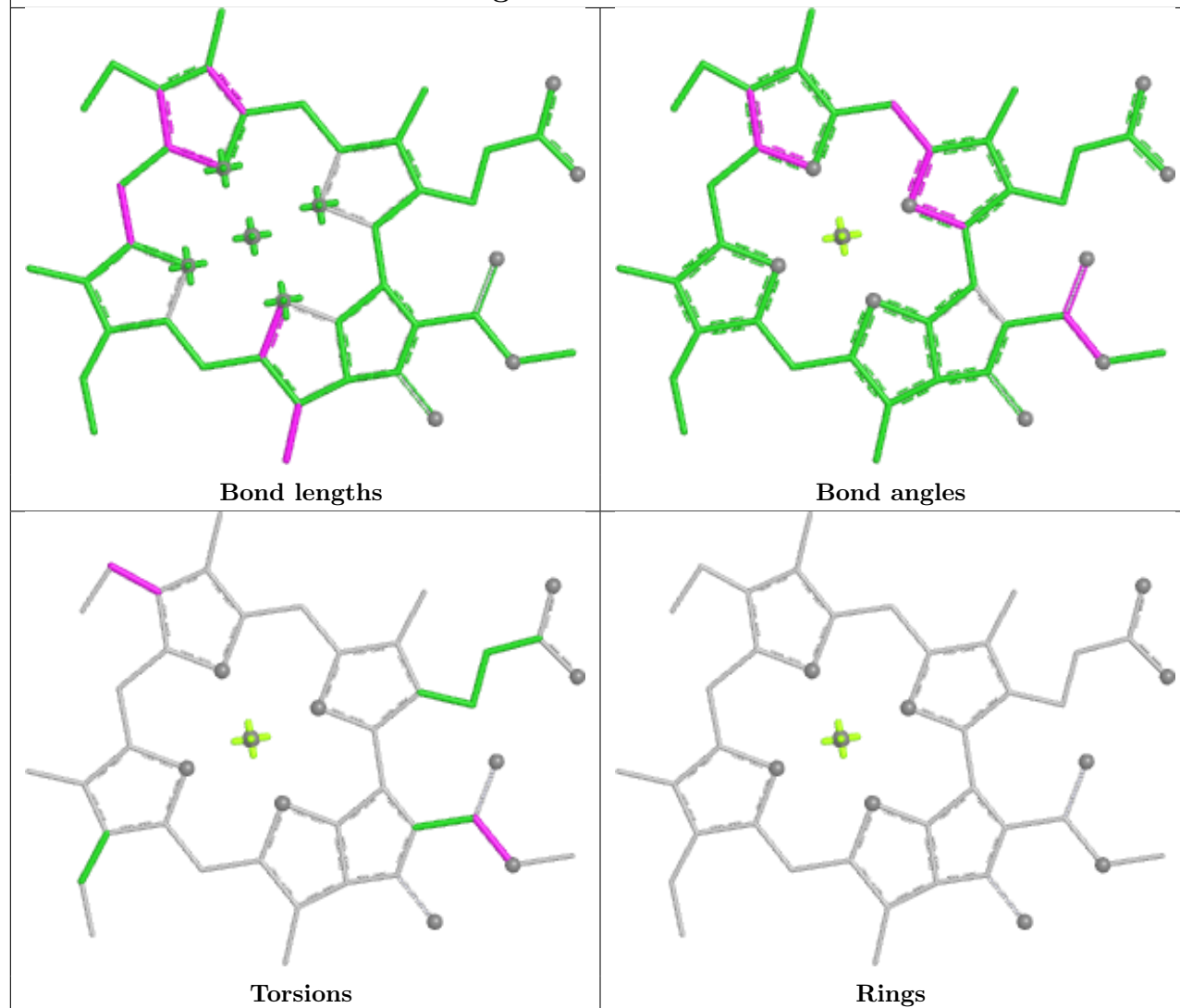


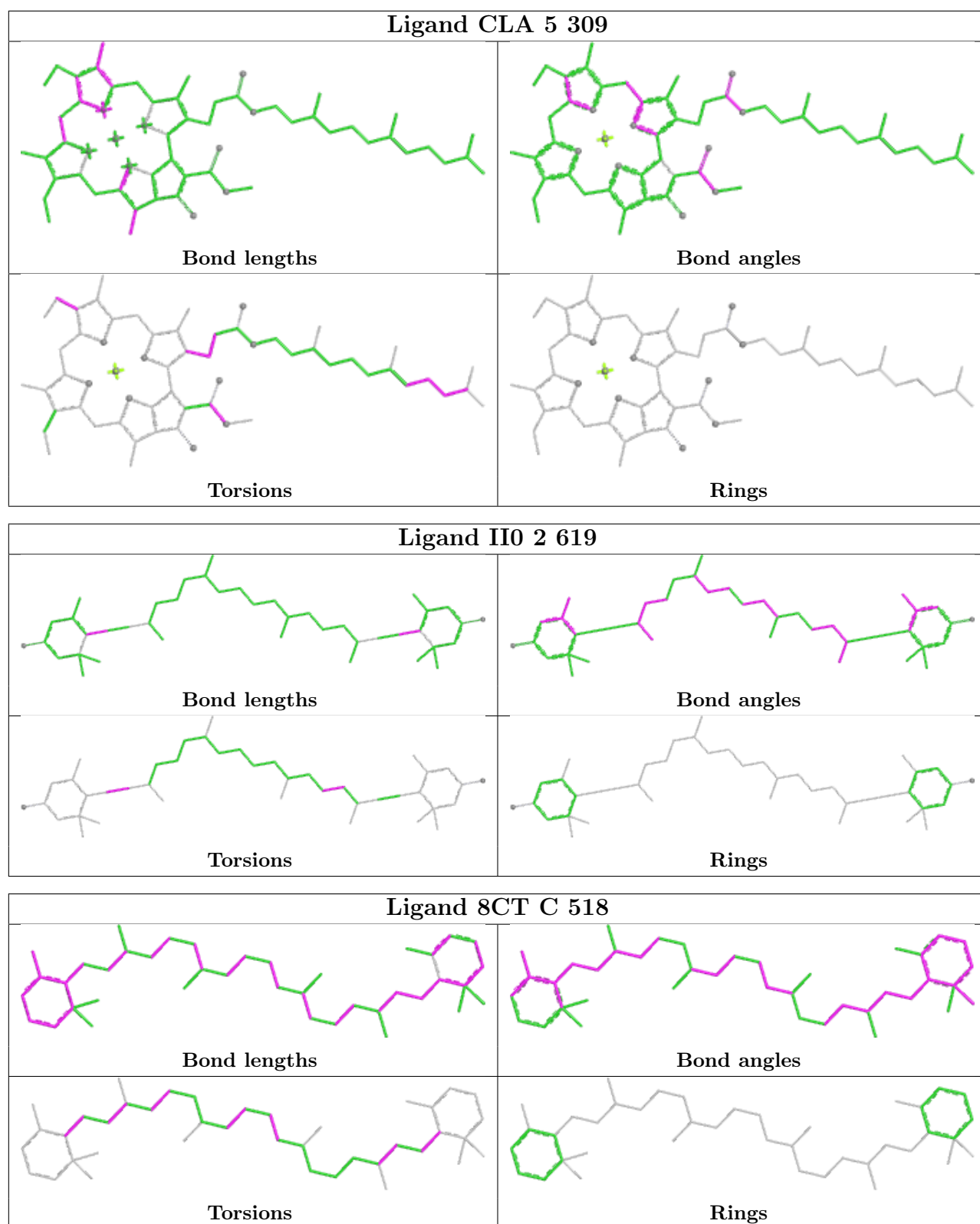


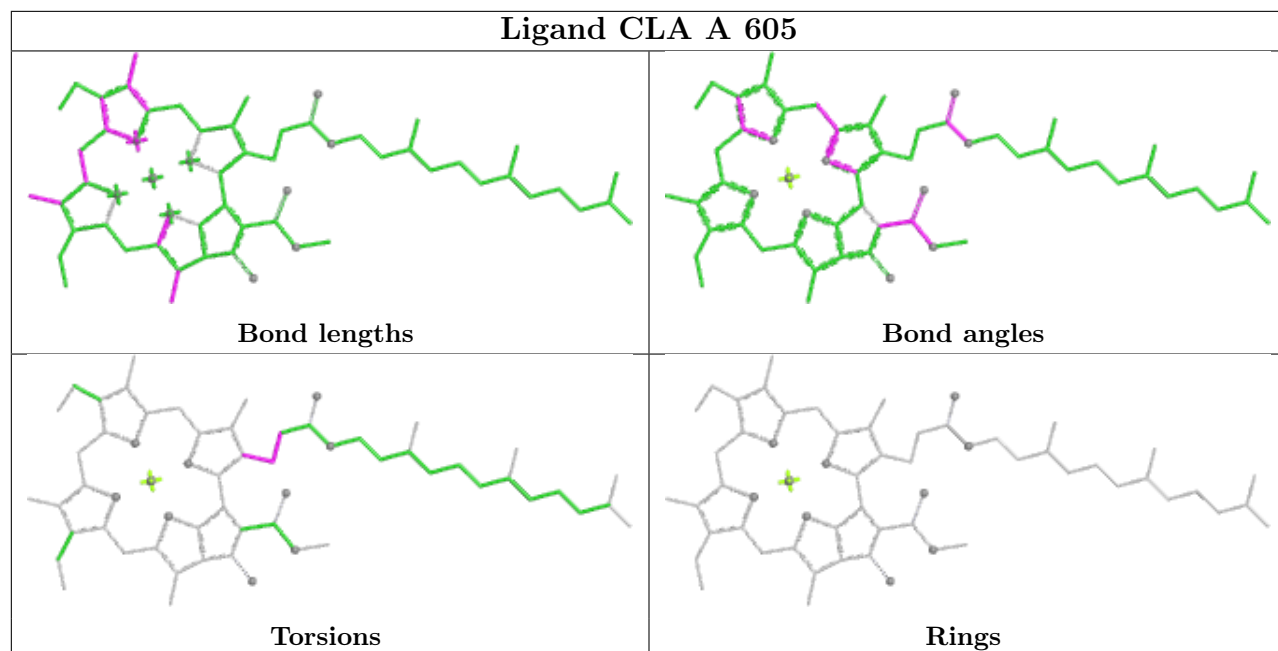
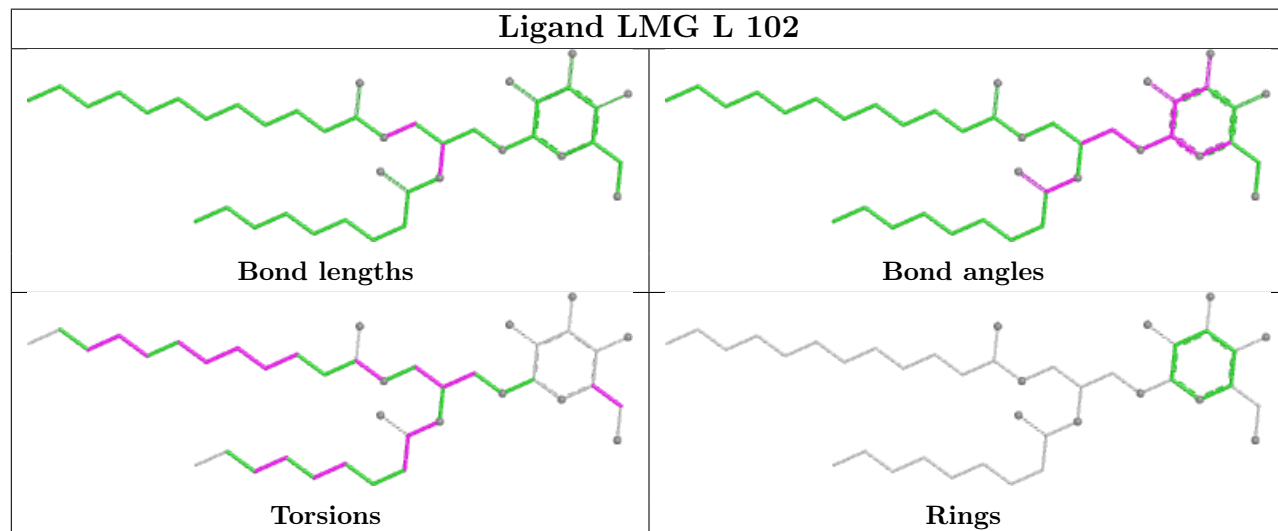
Ligand CLA B 611

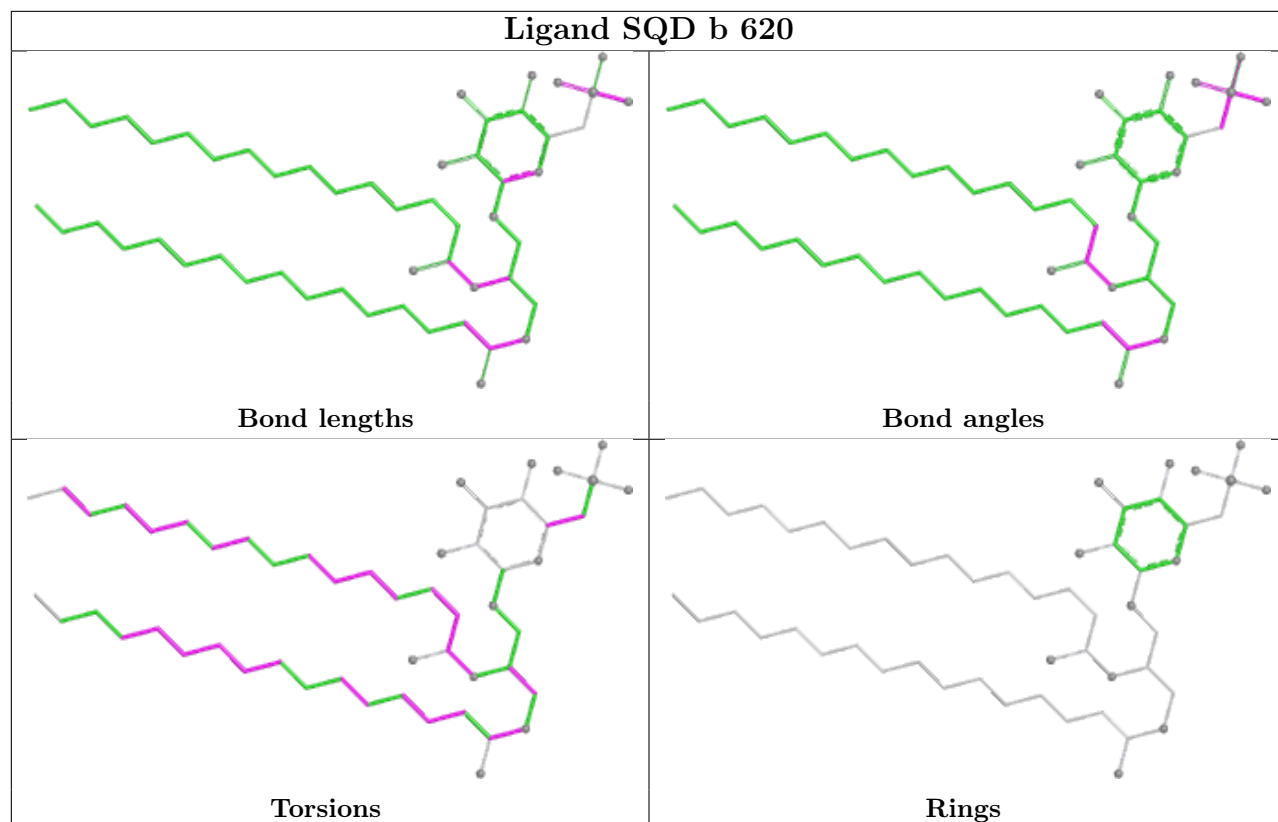


Ligand CLA P 606

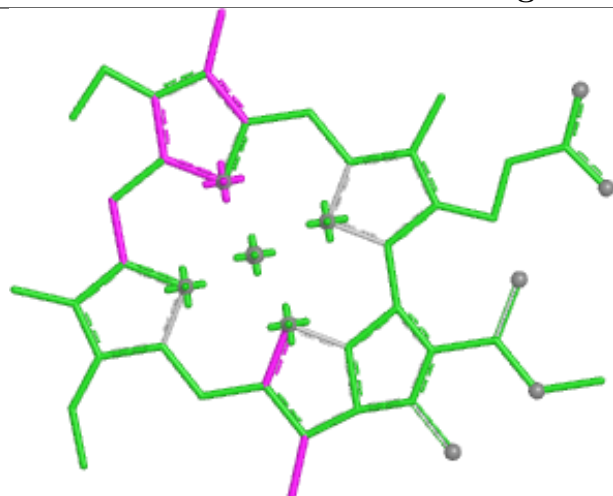




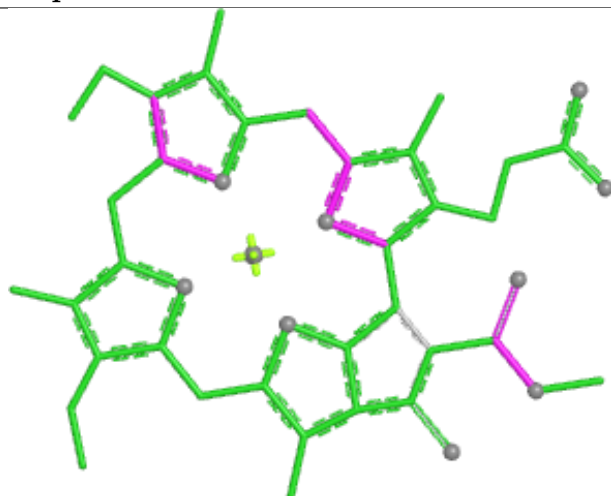
Ligand CLA A 605**Ligand LMG L 102**



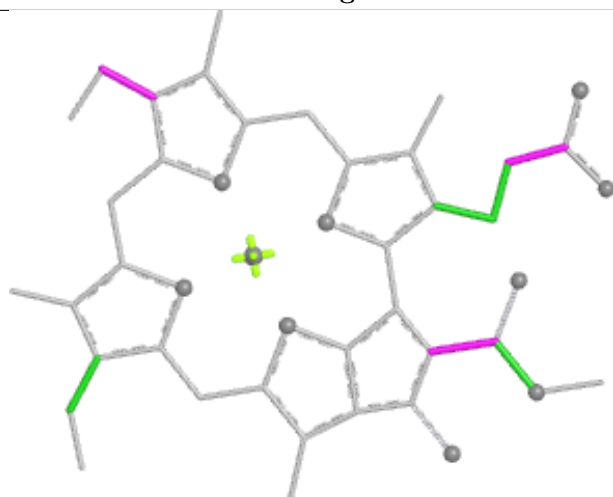
Ligand CLA p 307



Bond lengths



Bond angles

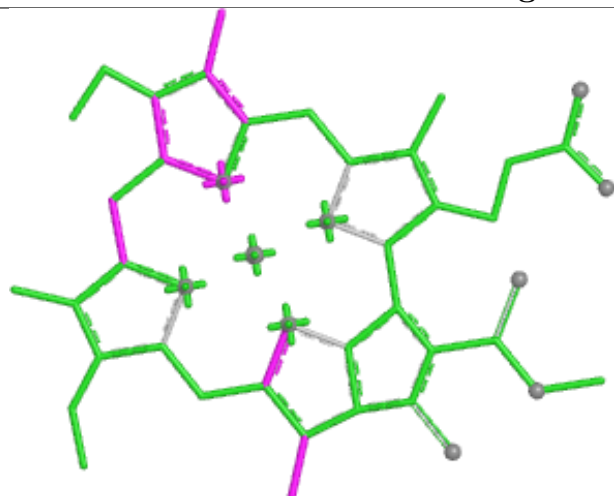


Torsions

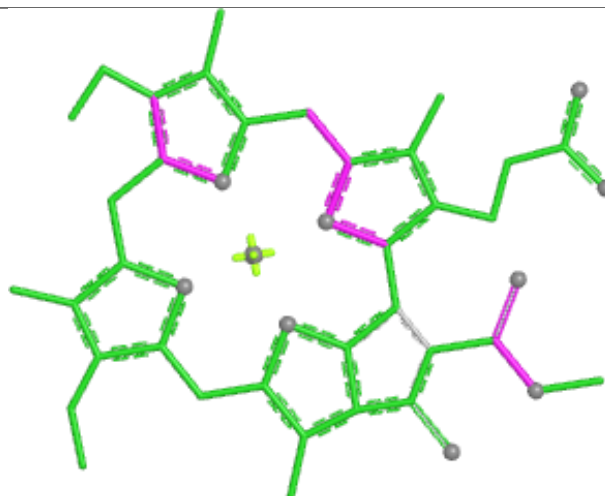


Rings

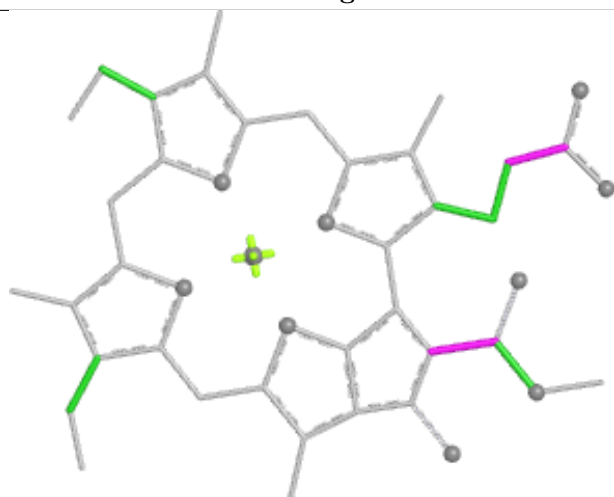
Ligand CLA 2 606



Bond lengths



Bond angles

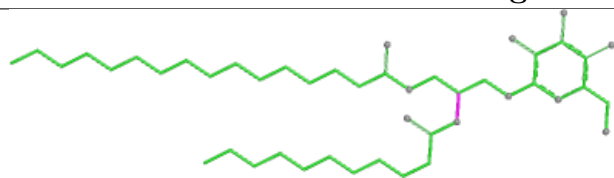


Torsions

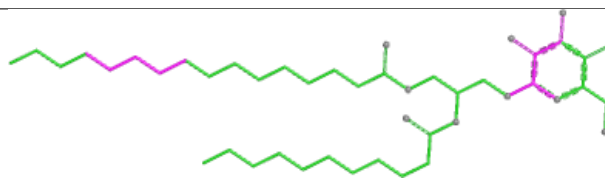


Rings

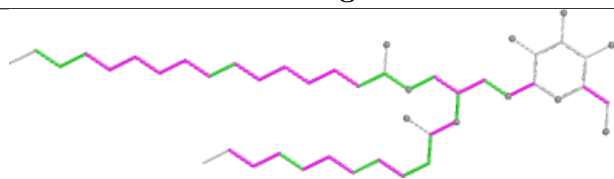
Ligand LMG C 517



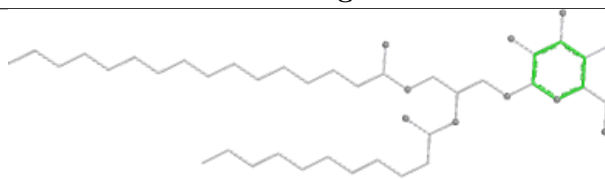
Bond lengths



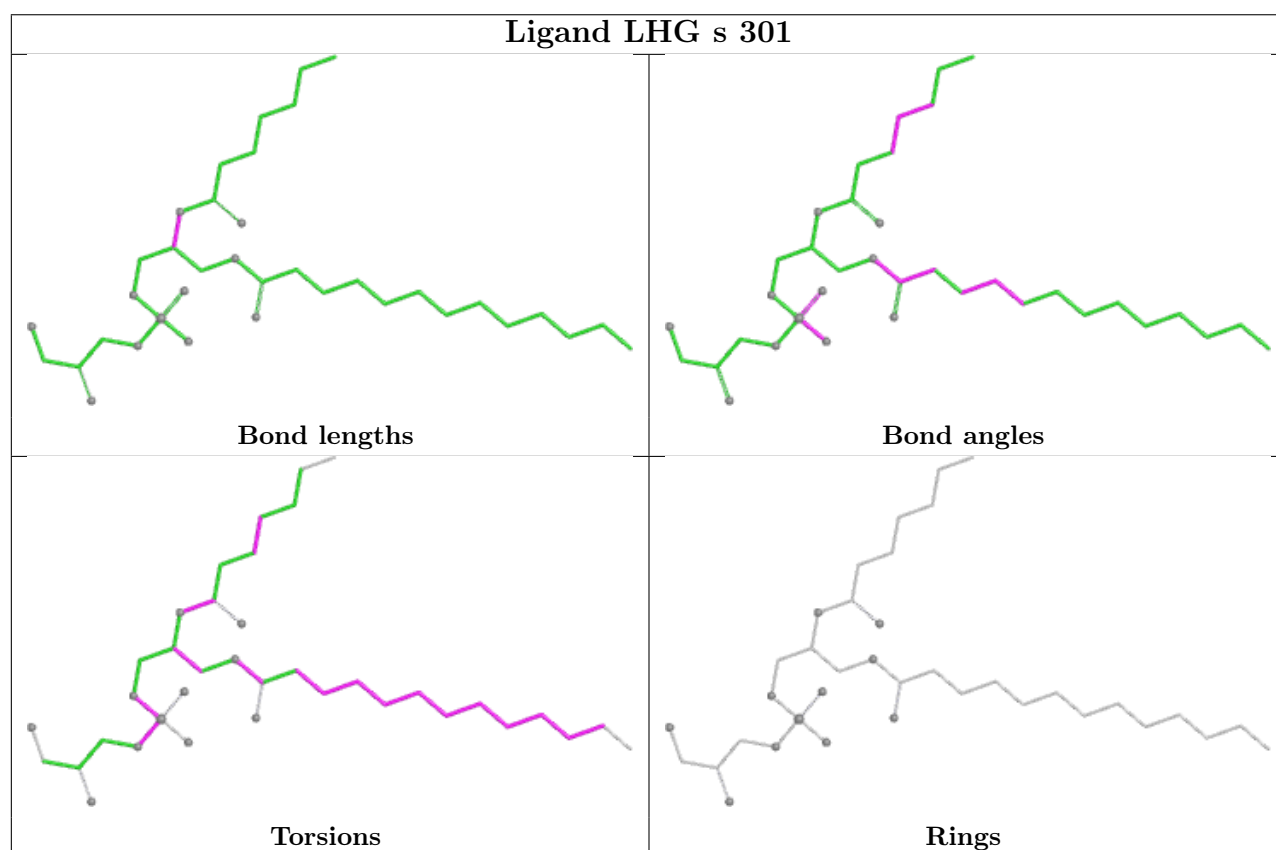
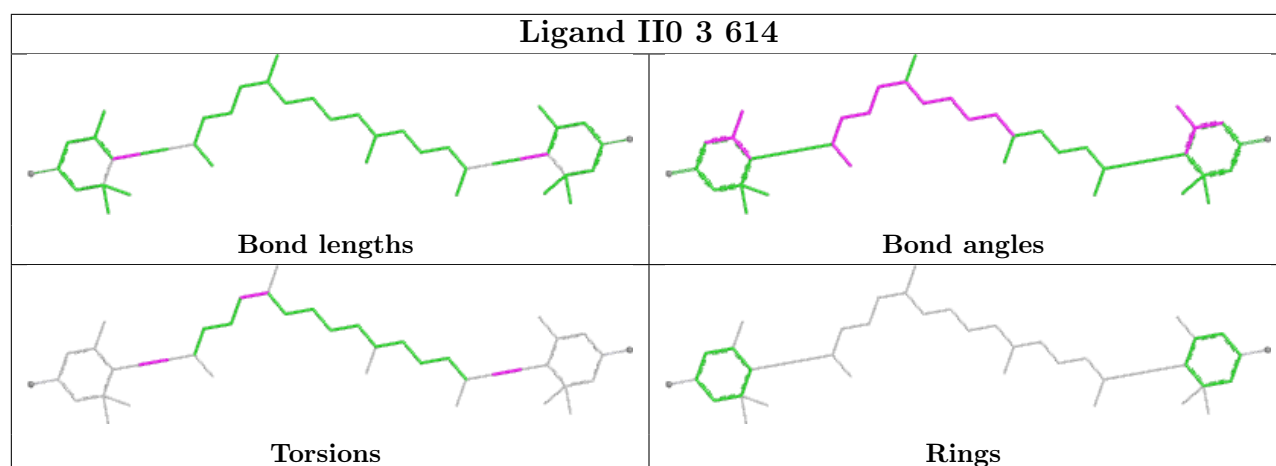
Bond angles



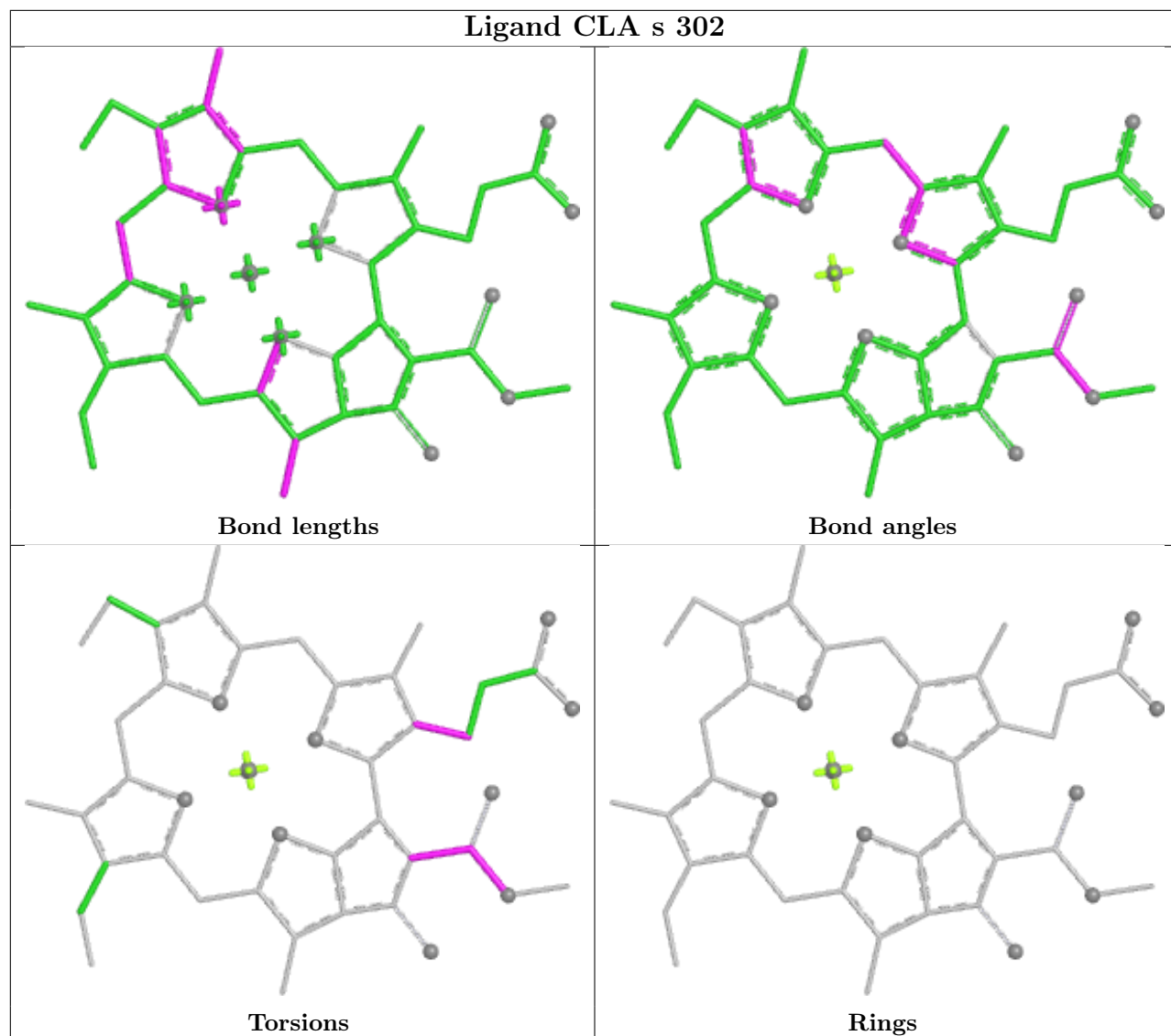
Torsions



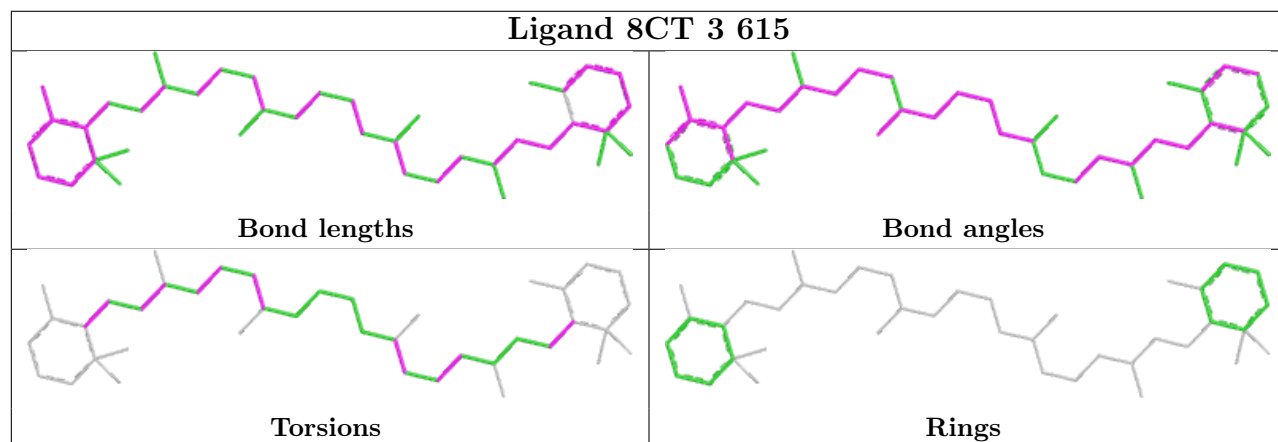
Rings

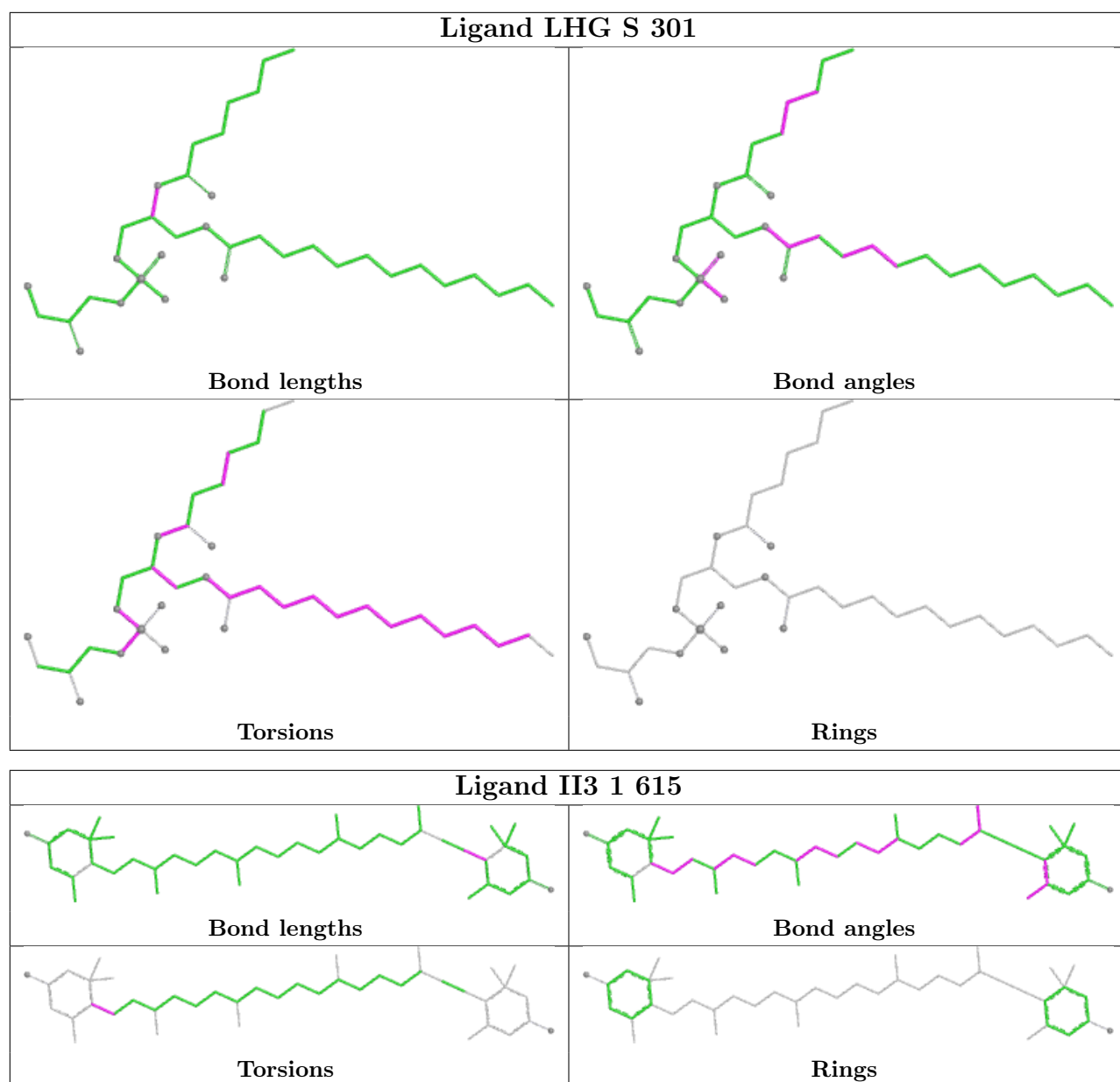


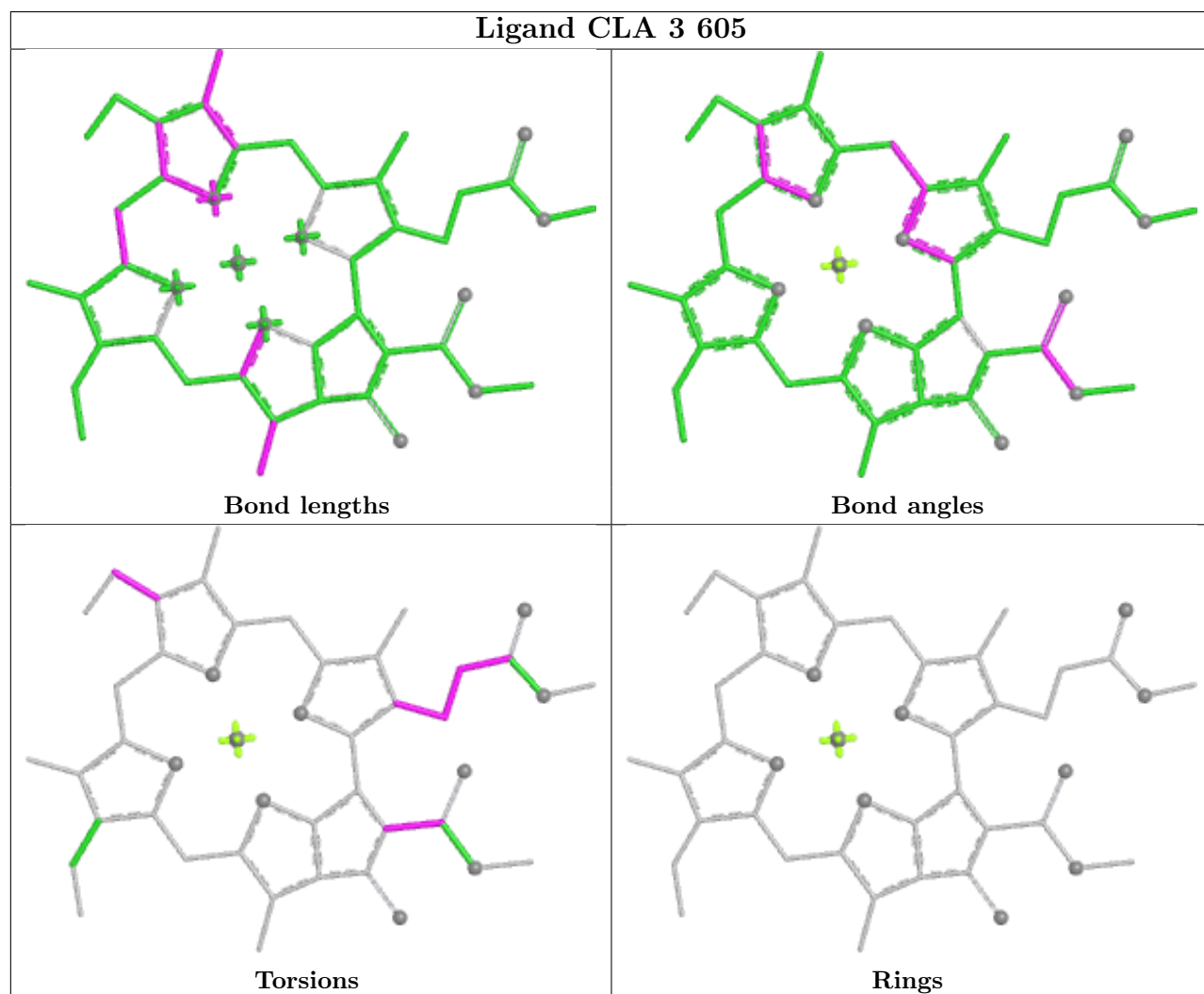
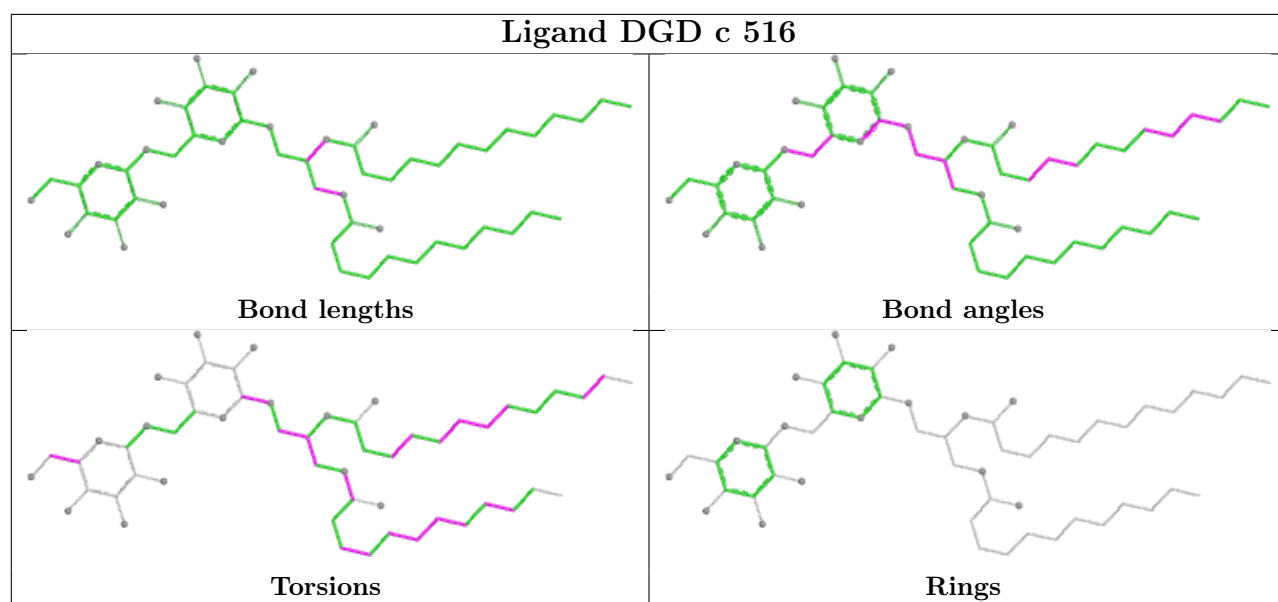
Ligand CLA s 302

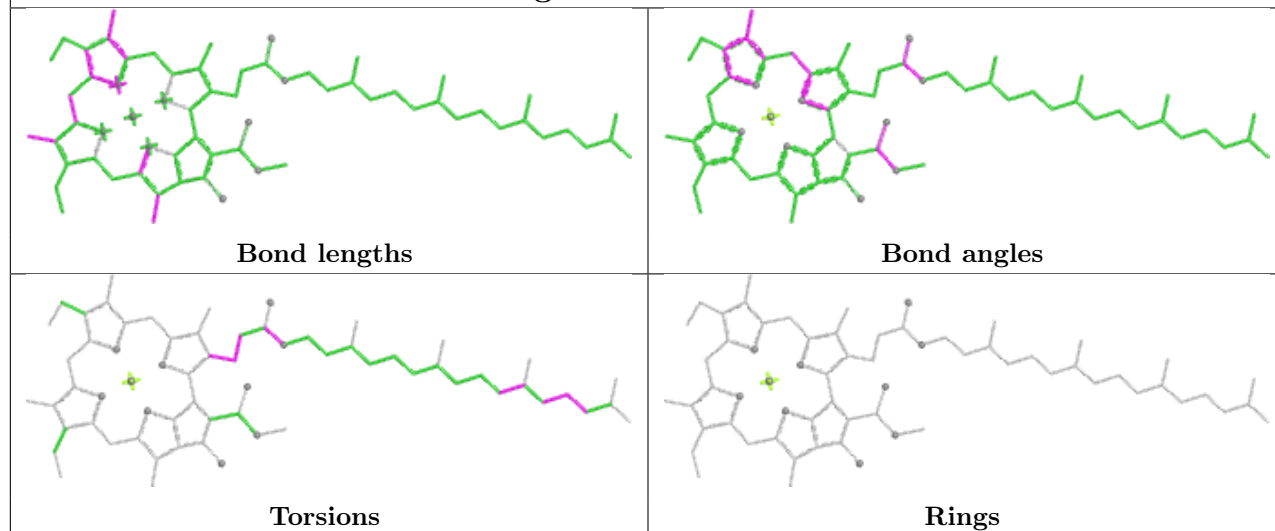
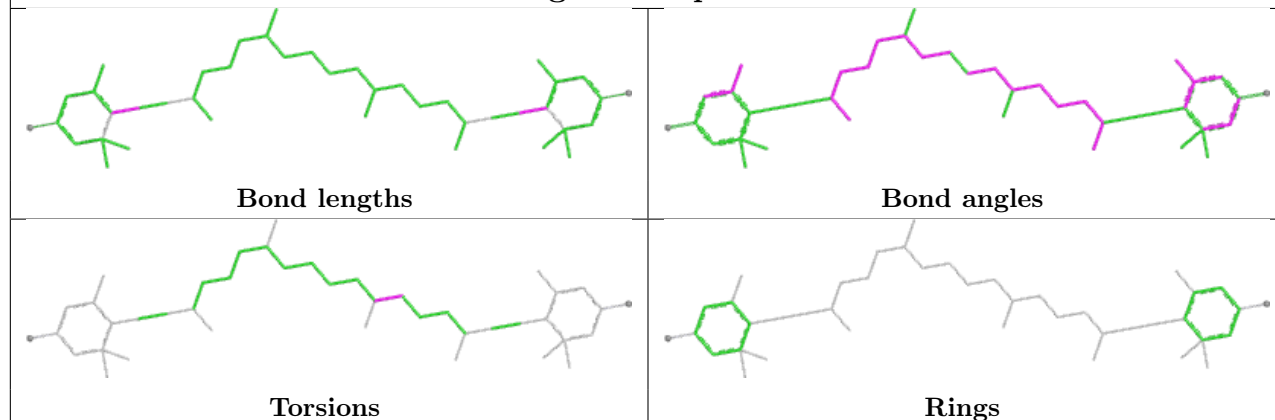
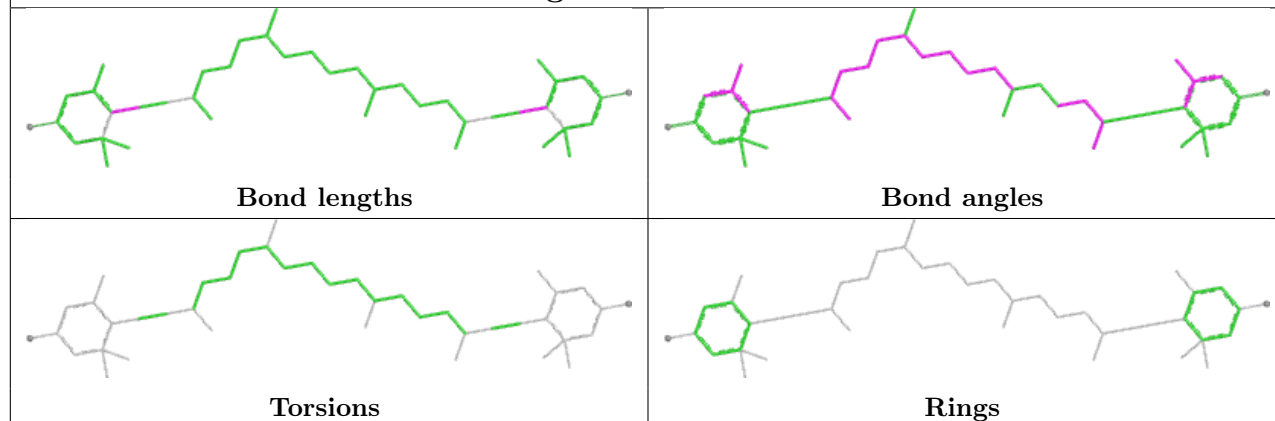


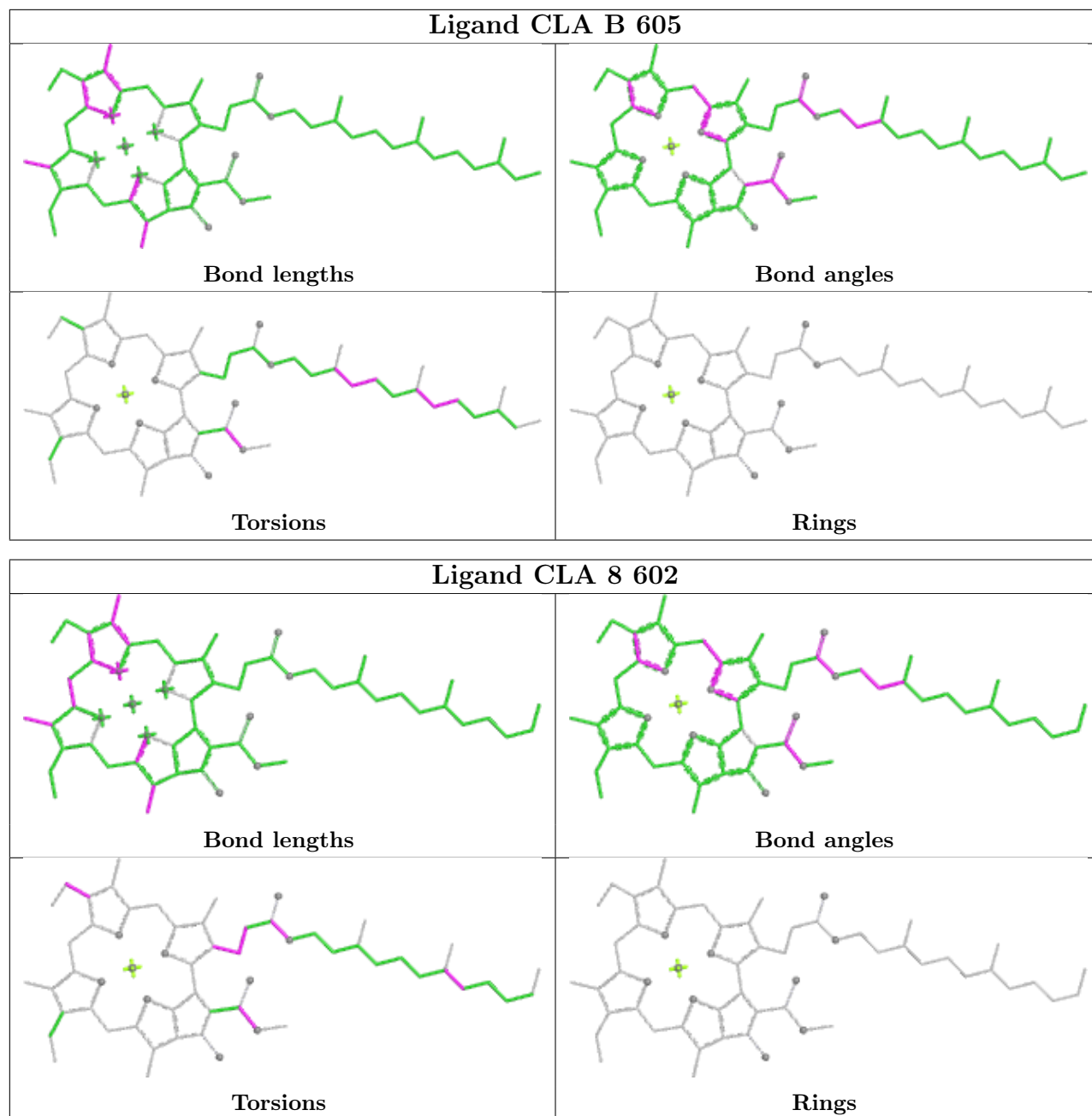
Ligand 8CT 3 615



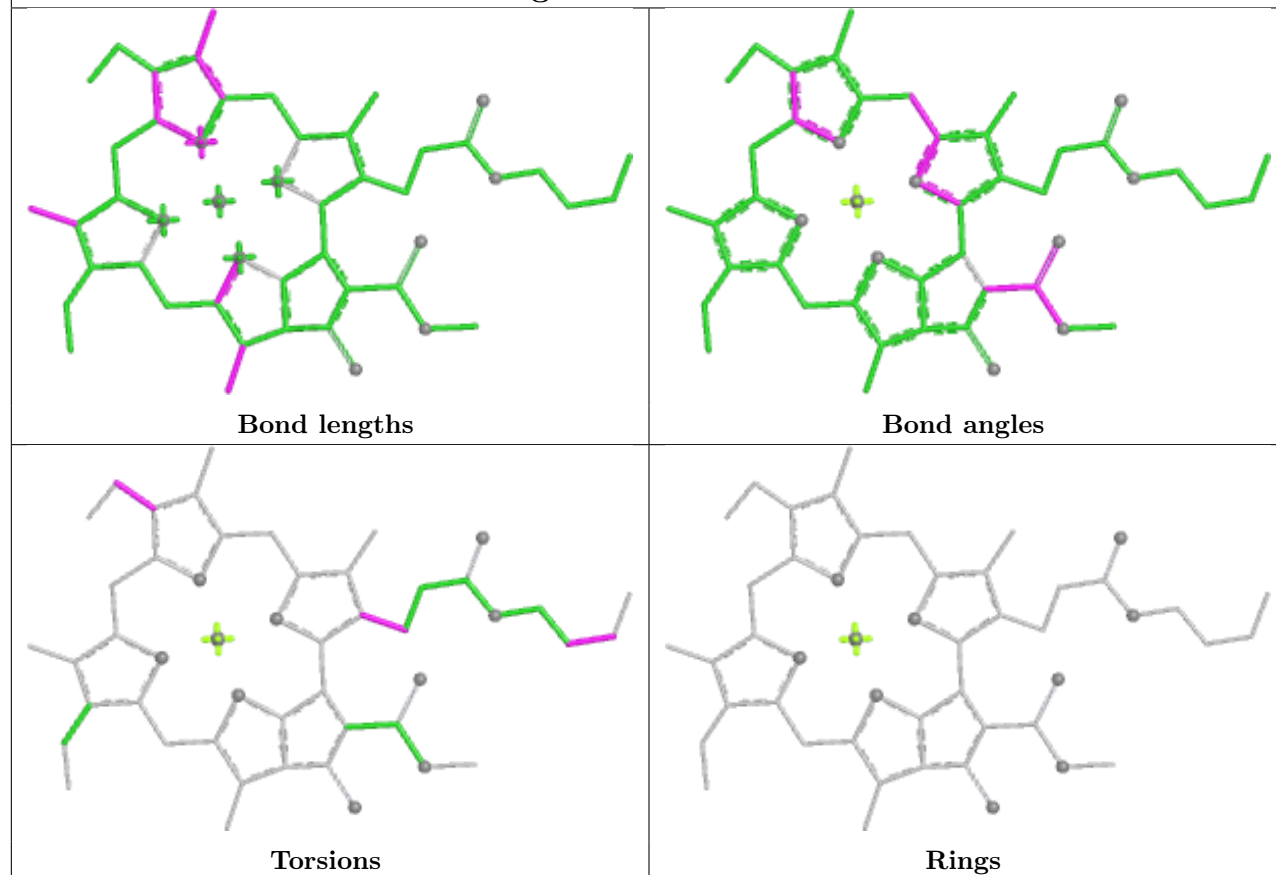




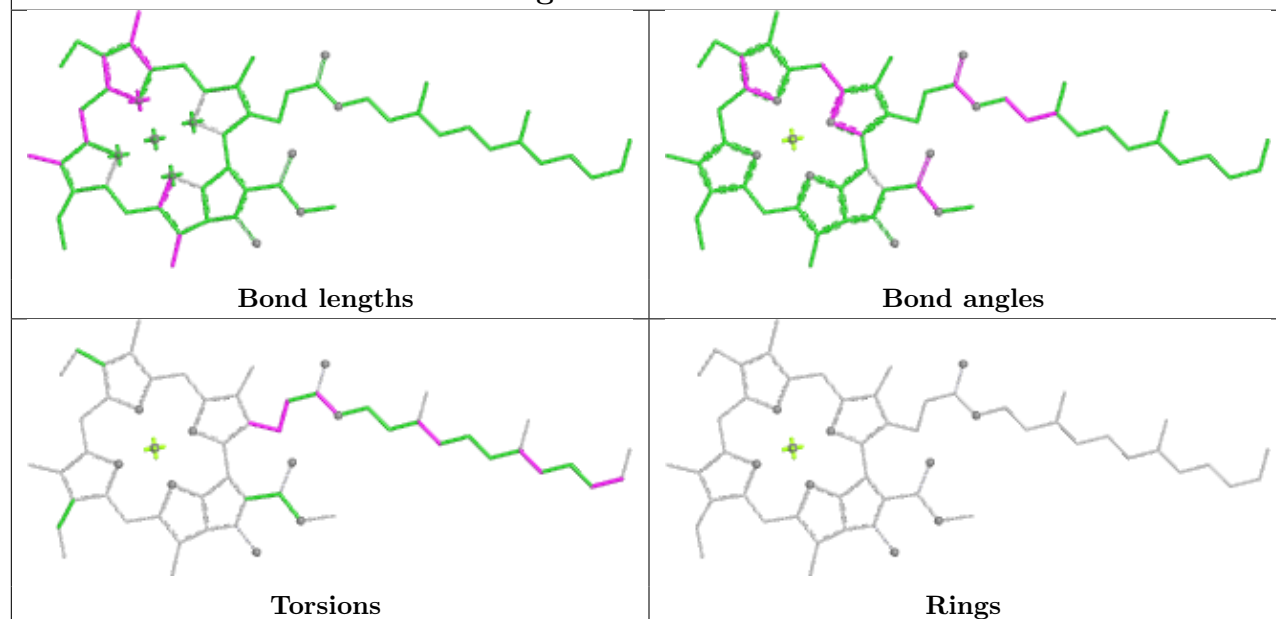
Ligand CLA b 609**Ligand II0 p 301****Ligand II0 P 612**



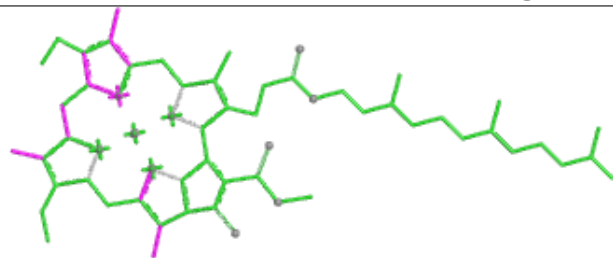
Ligand CLA A 603



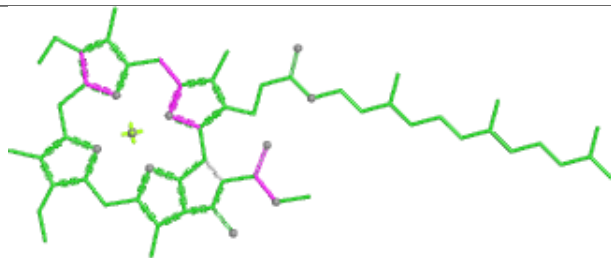
Ligand CLA 3 602



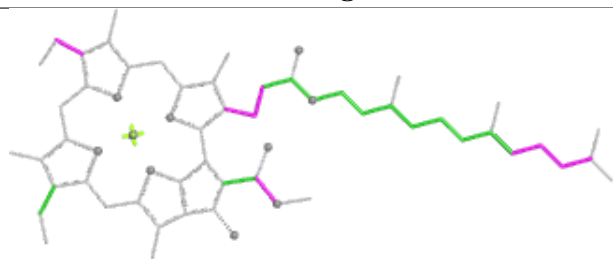
Ligand CLA 1 608



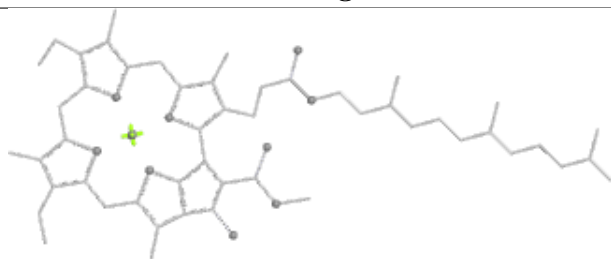
Bond lengths



Bond angles

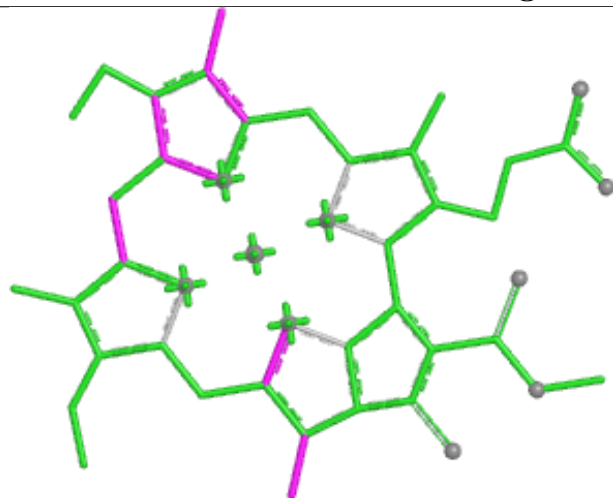


Torsions

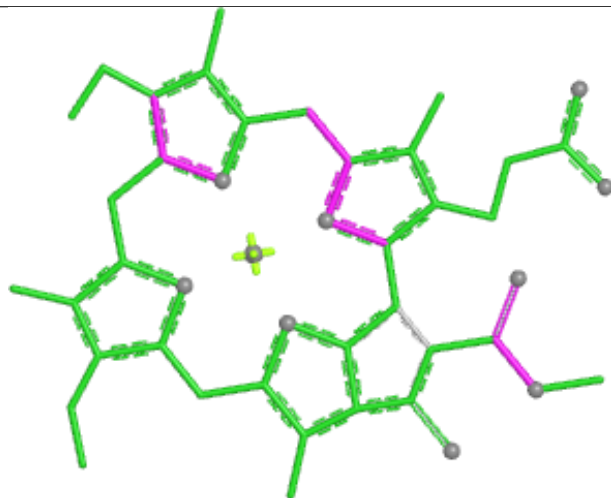


Rings

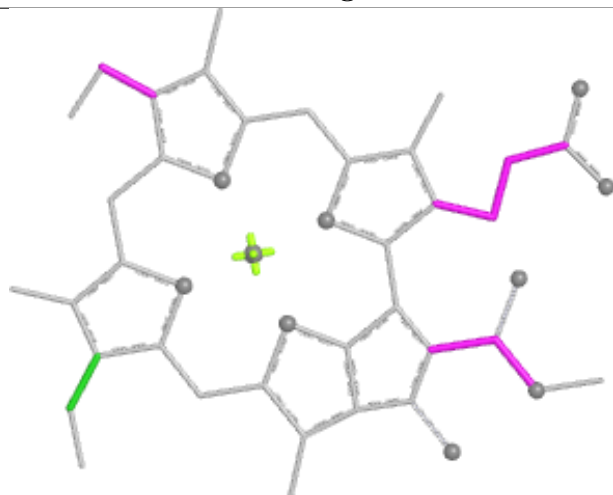
Ligand CLA 5 313



Bond lengths



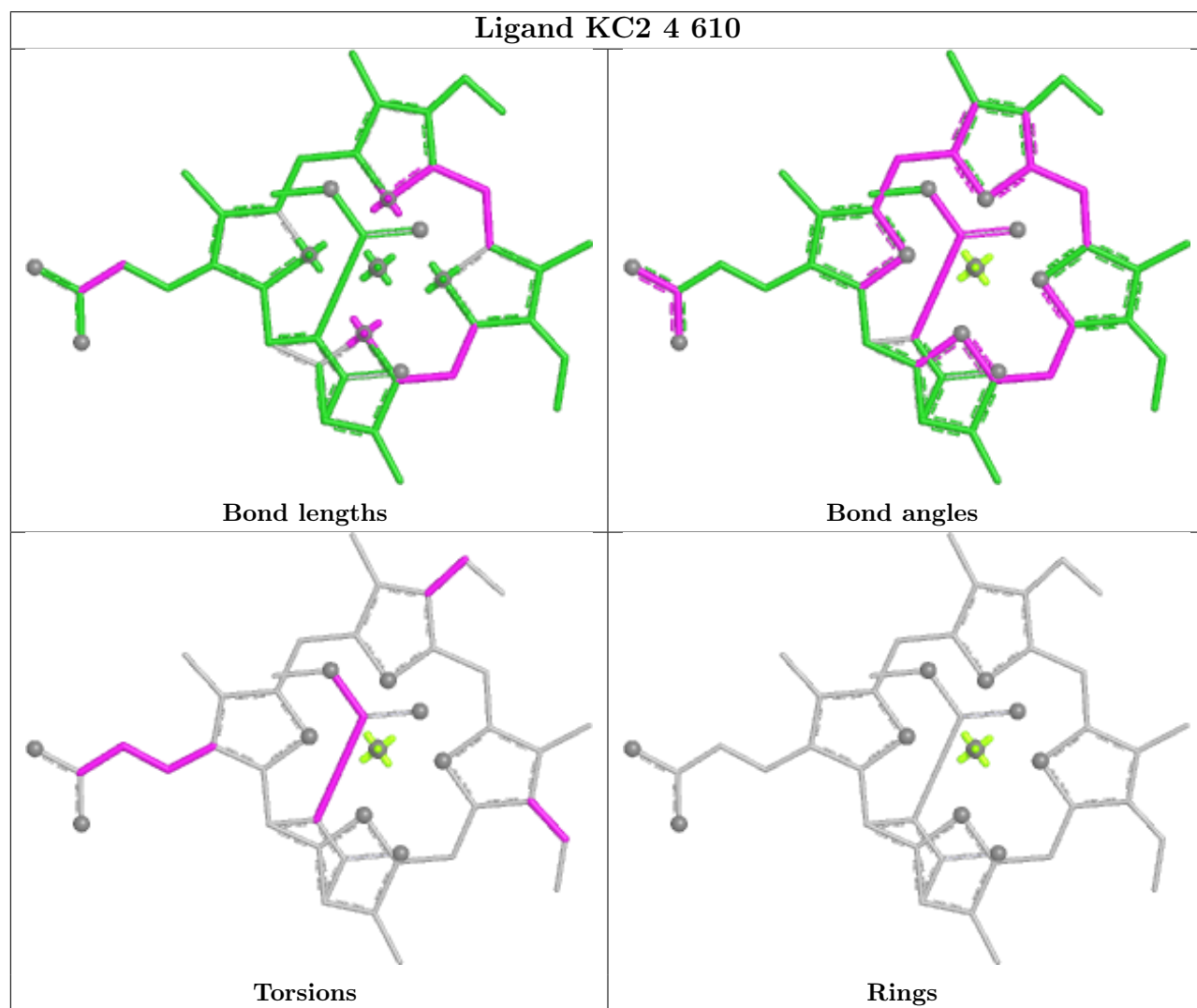
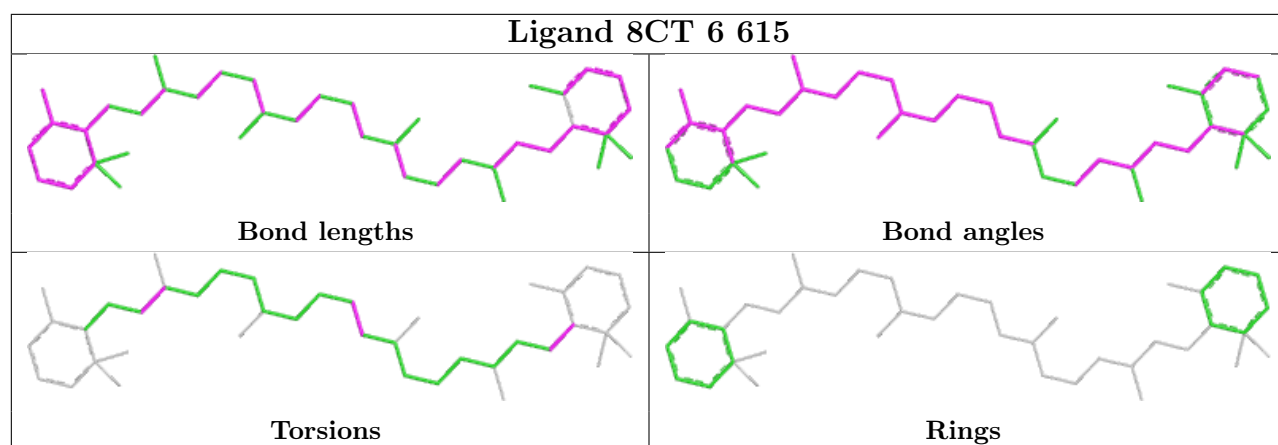
Bond angles

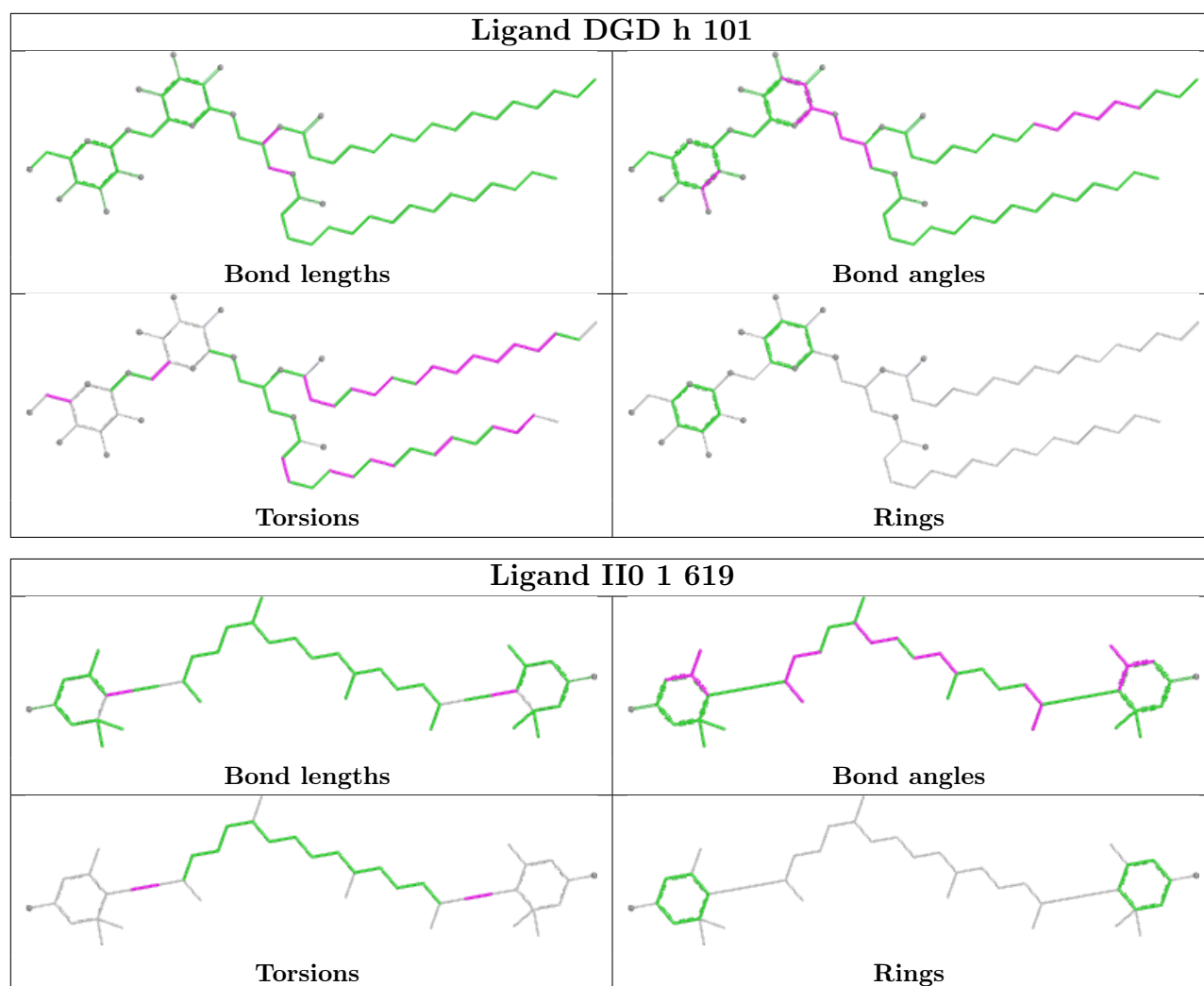


Torsions



Rings





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

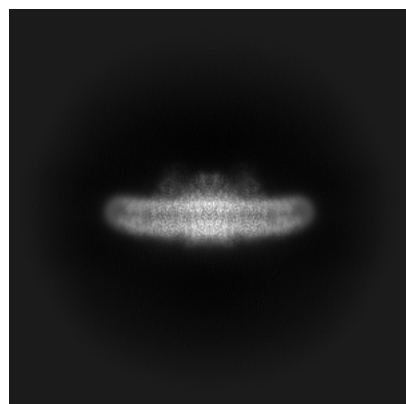
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-37414. These allow visual inspection of the internal detail of the map and identification of artifacts.

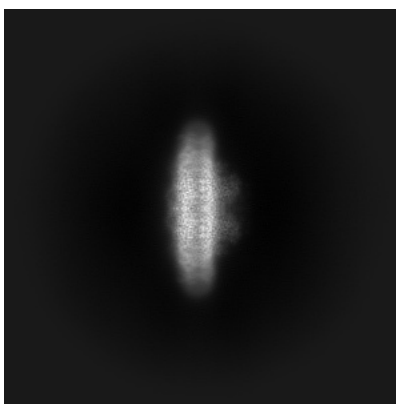
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

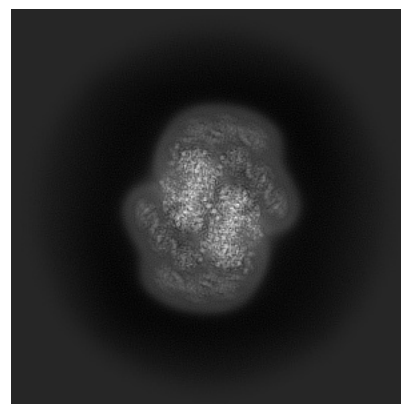
6.1.1 Primary map



X

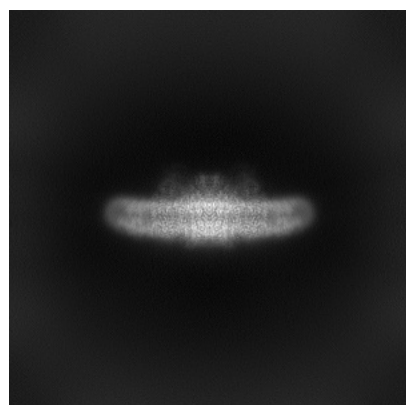


Y

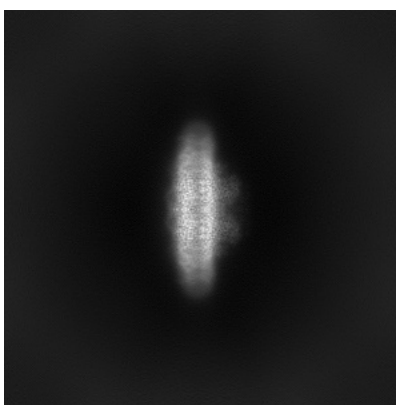


Z

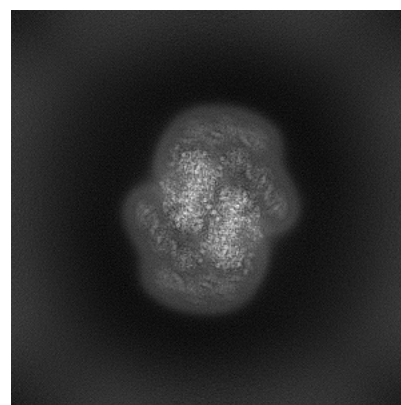
6.1.2 Raw map



X



Y

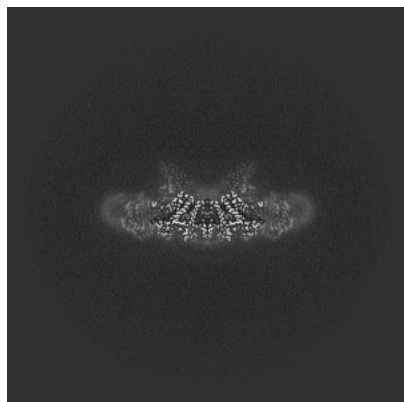


Z

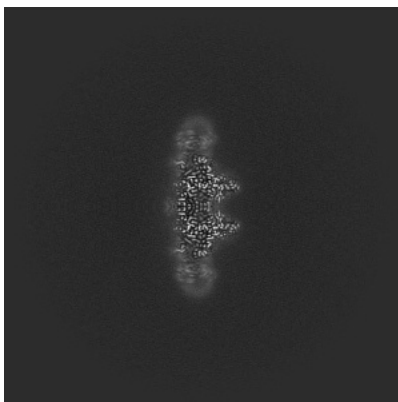
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

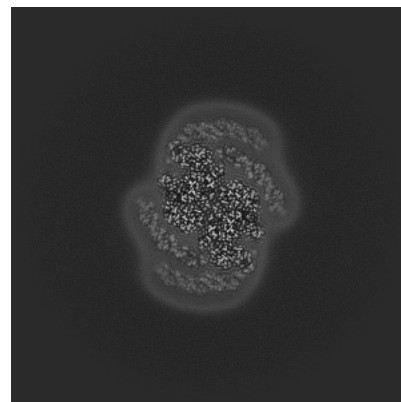
6.2.1 Primary map



X Index: 256

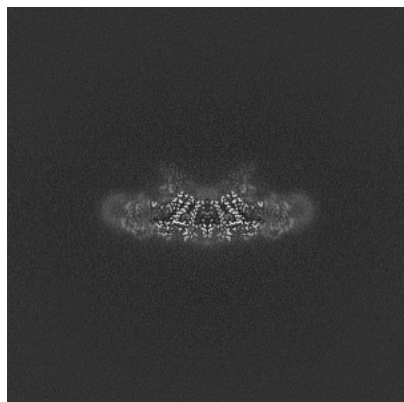


Y Index: 256

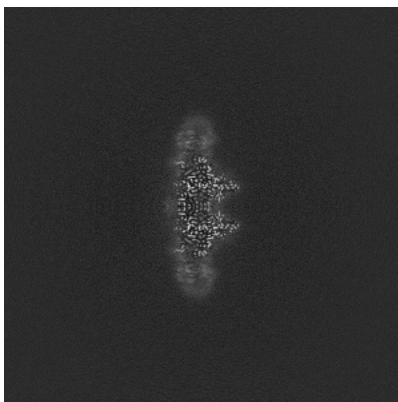


Z Index: 256

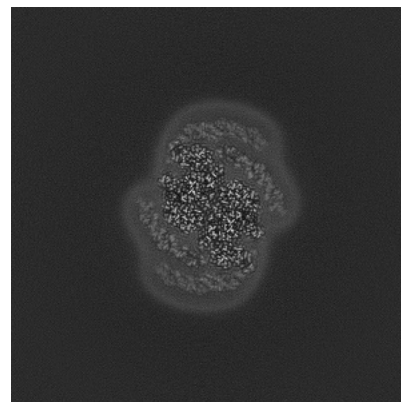
6.2.2 Raw map



X Index: 256



Y Index: 256

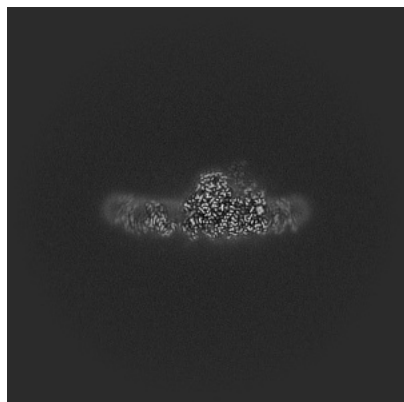


Z Index: 256

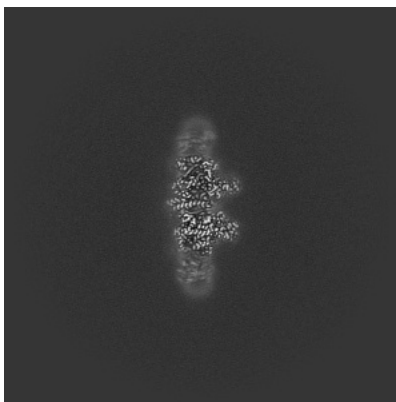
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

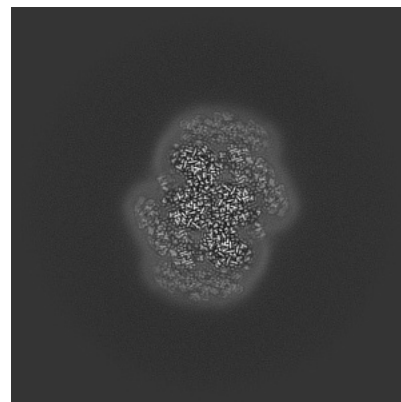
6.3.1 Primary map



X Index: 229

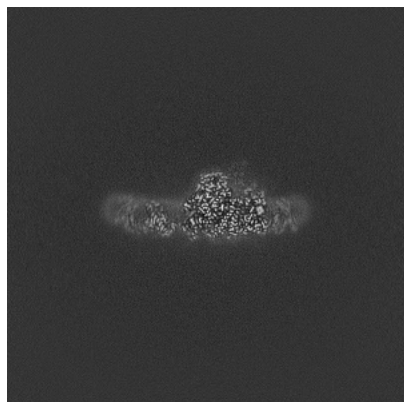


Y Index: 251

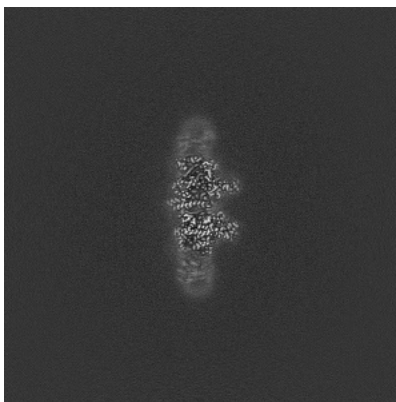


Z Index: 235

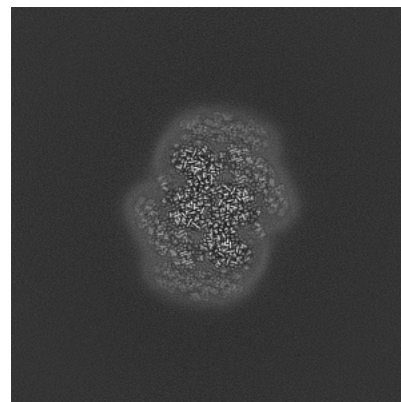
6.3.2 Raw map



X Index: 229



Y Index: 251



Z Index: 235

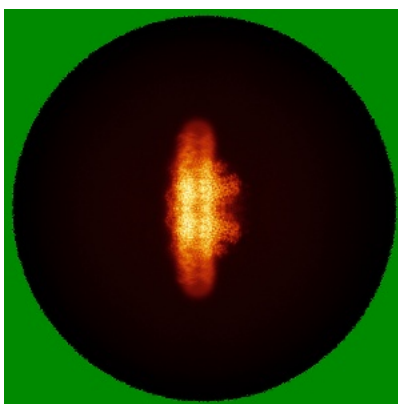
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

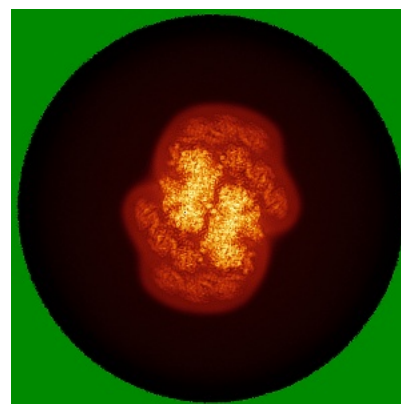
6.4.1 Primary map



X



Y

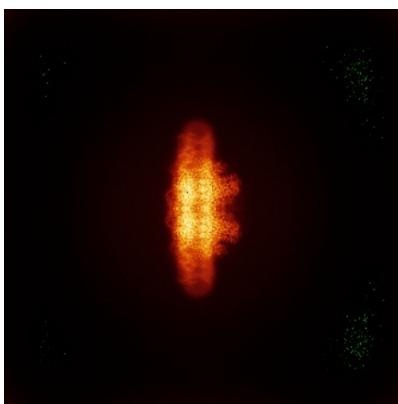


Z

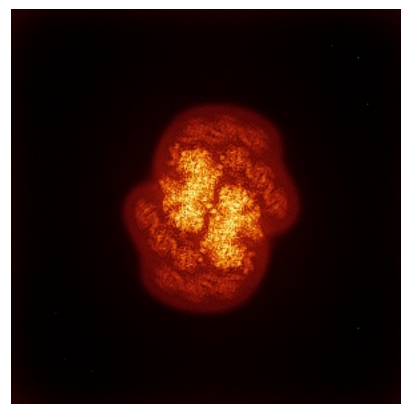
6.4.2 Raw map



X



Y

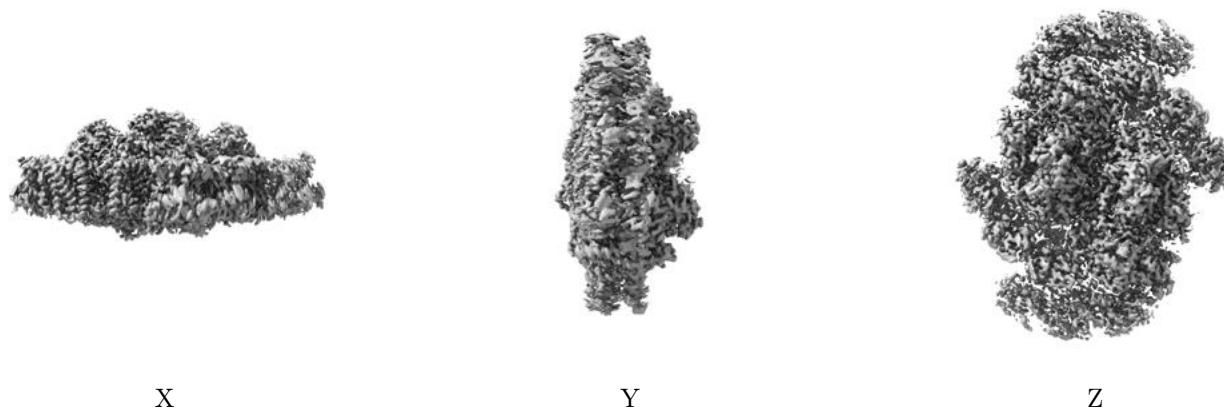


Z

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.

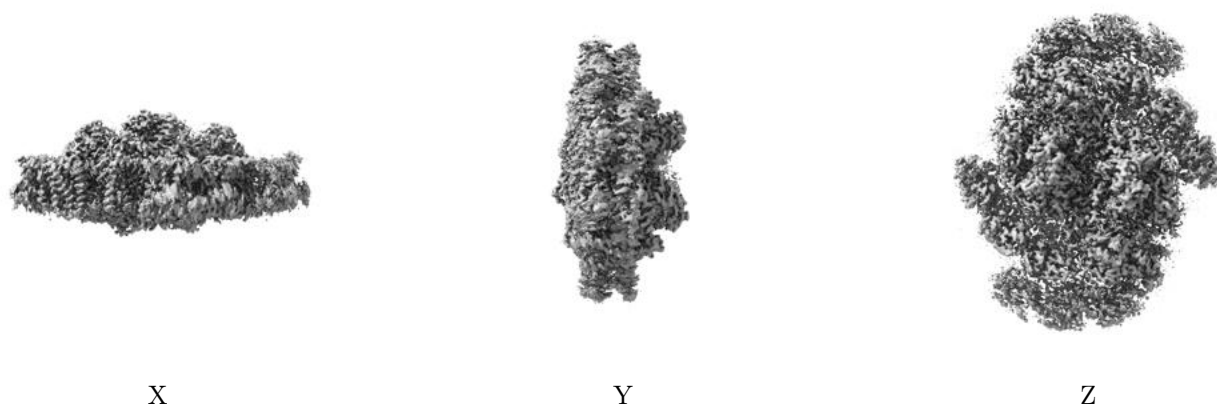
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.253. 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



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.

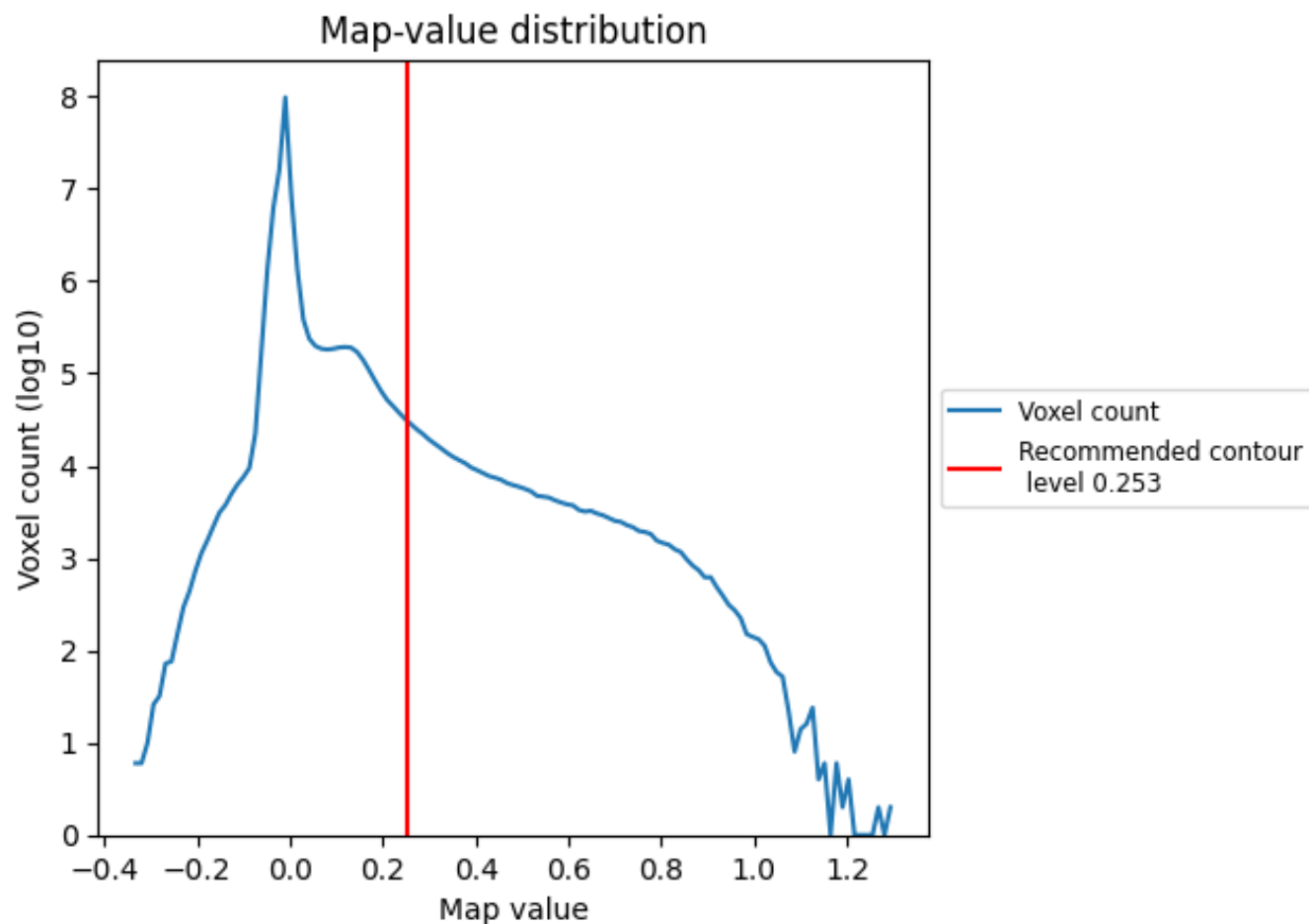
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

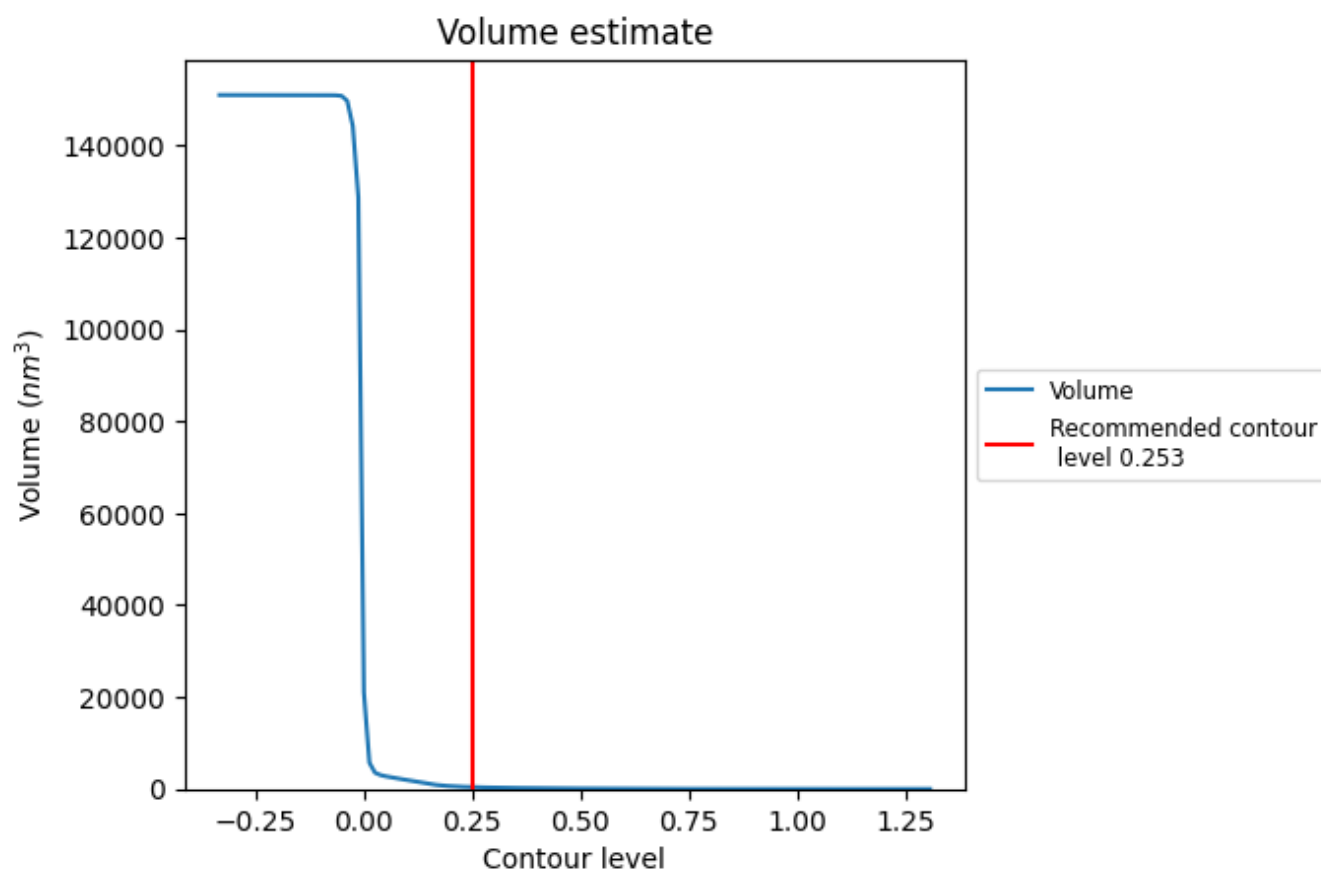
This section contains the results of statistical analysis of the map.

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.

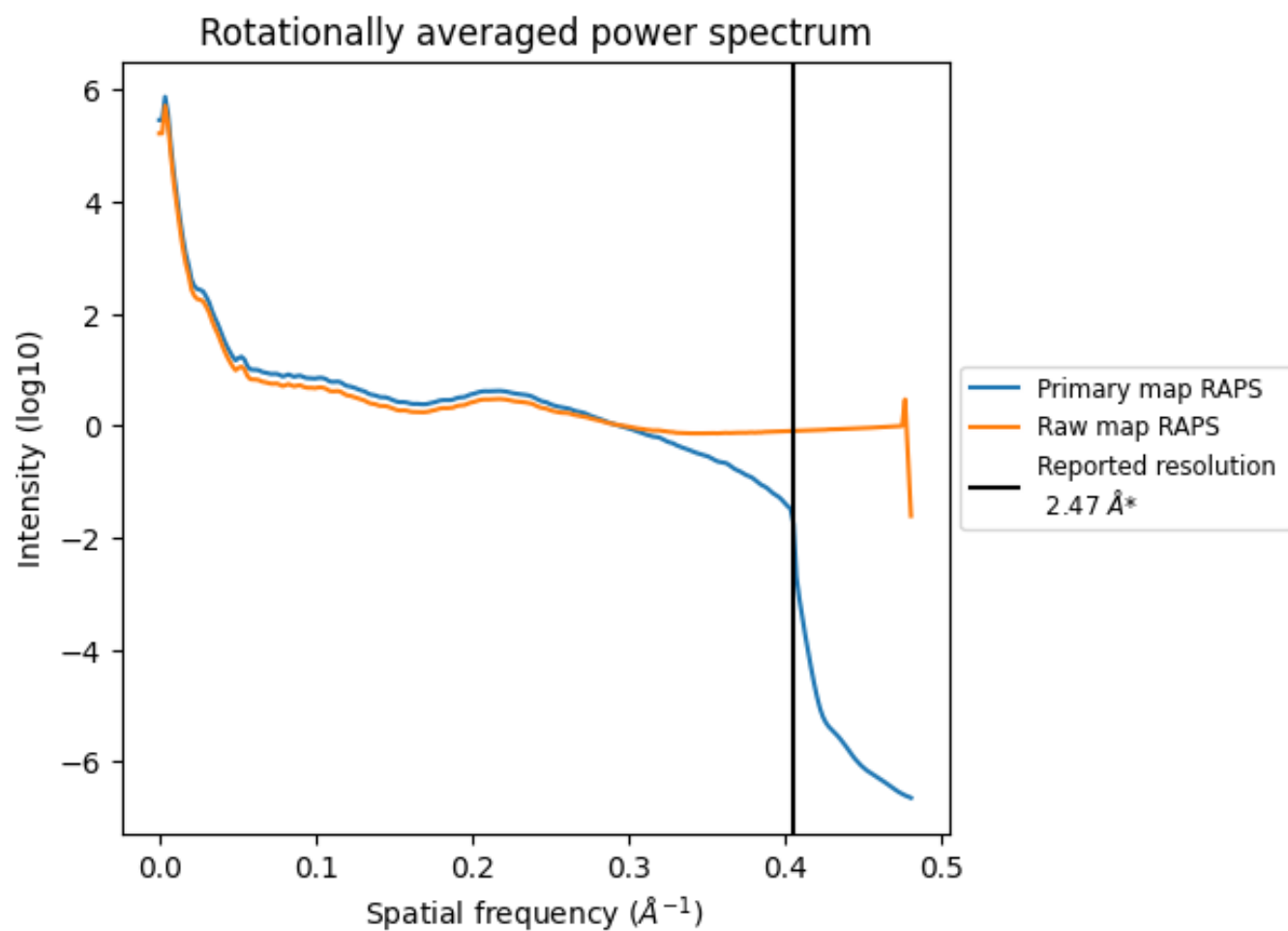
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 394 nm^3 ; this corresponds to an approximate mass of 356 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 ⓘ

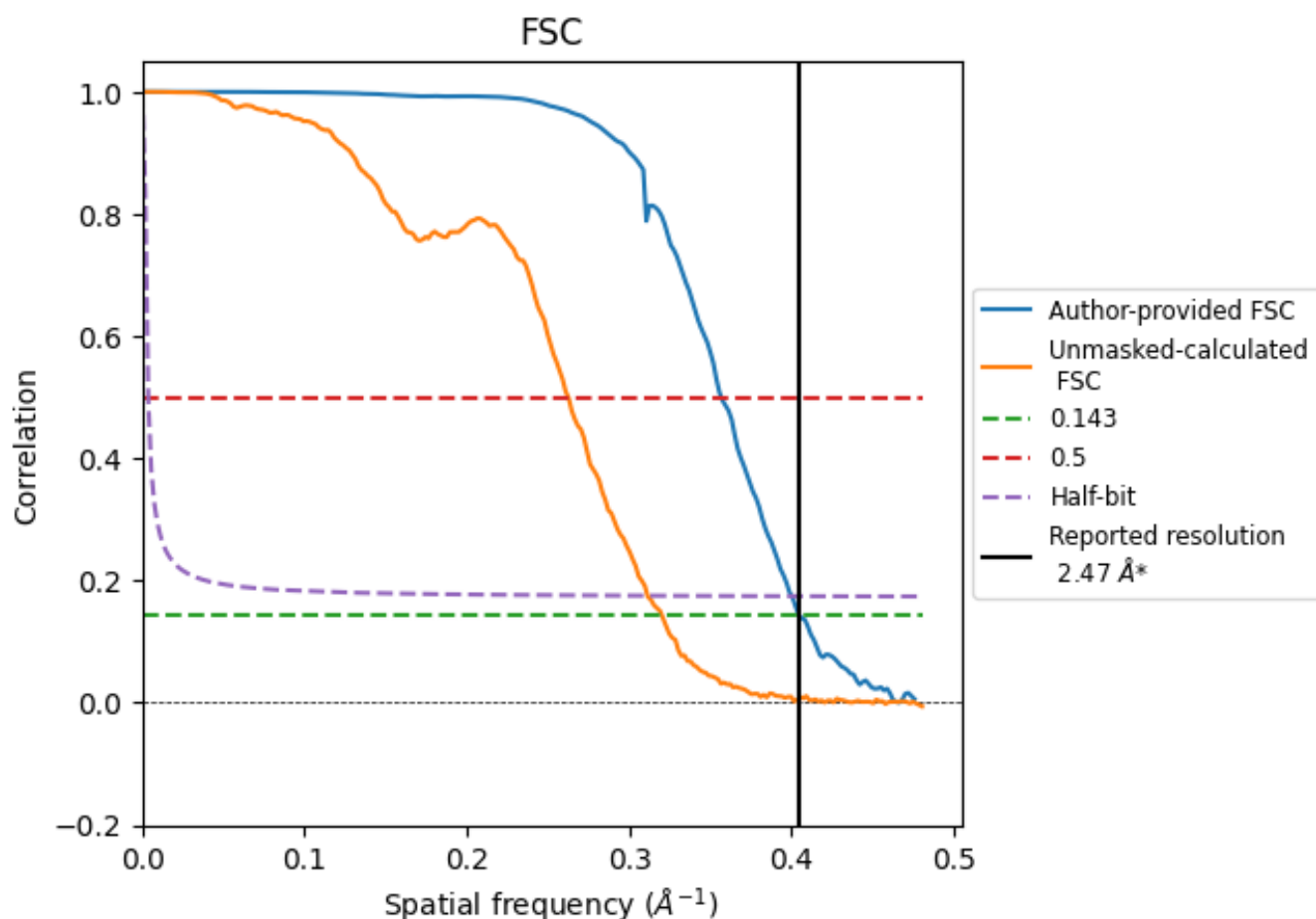


*Reported resolution corresponds to spatial frequency of 0.405 $\text{\AA}^{-1}$

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 0.405 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

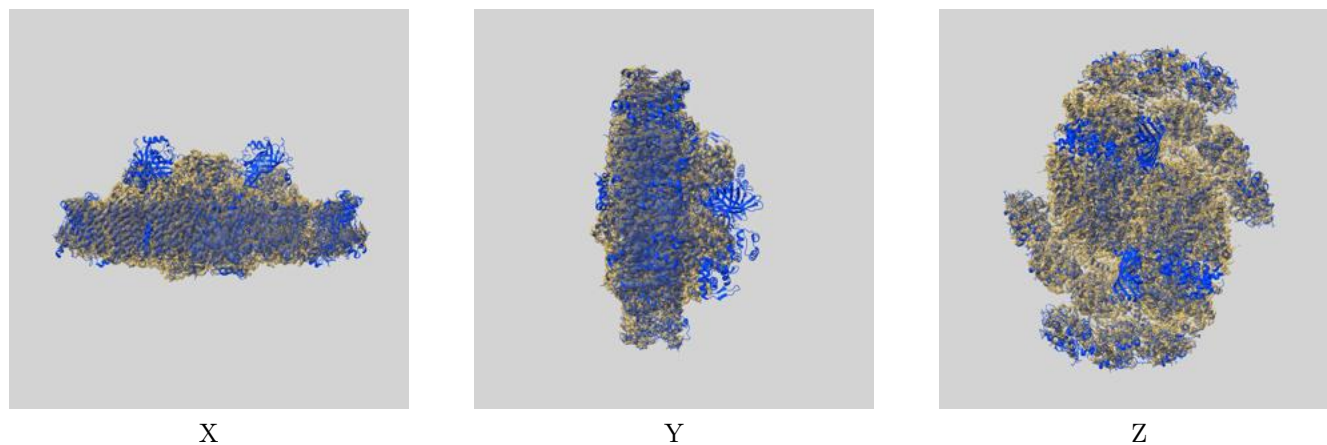
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.47	-	-
Author-provided FSC curve	2.47	2.80	2.50
Unmasked-calculated*	3.12	3.81	3.21

*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 3.12 differs from the reported value 2.47 by more than 10 %

9 Map-model fit [i](#)

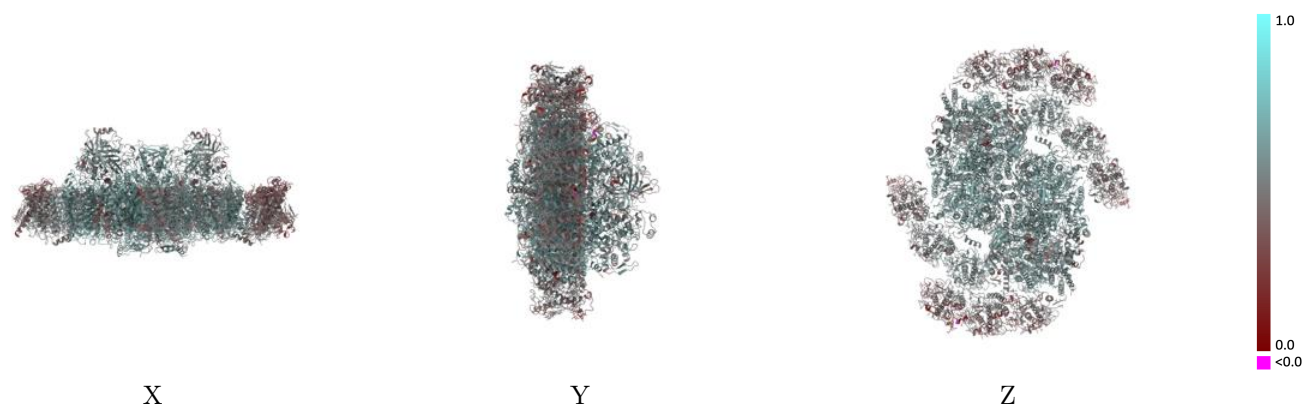
This section contains information regarding the fit between EMDB map EMD-37414 and PDB model 8WB4. Per-residue inclusion information can be found in [section 3](#) on [page 43](#).

9.1 Map-model overlay [i](#)



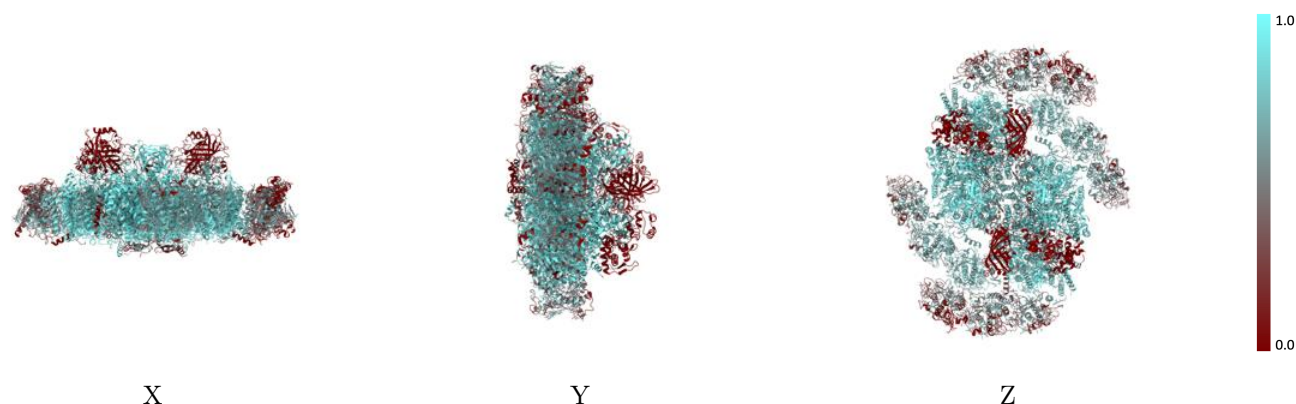
The images above show the 3D surface view of the map at the recommended contour level 0.253 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



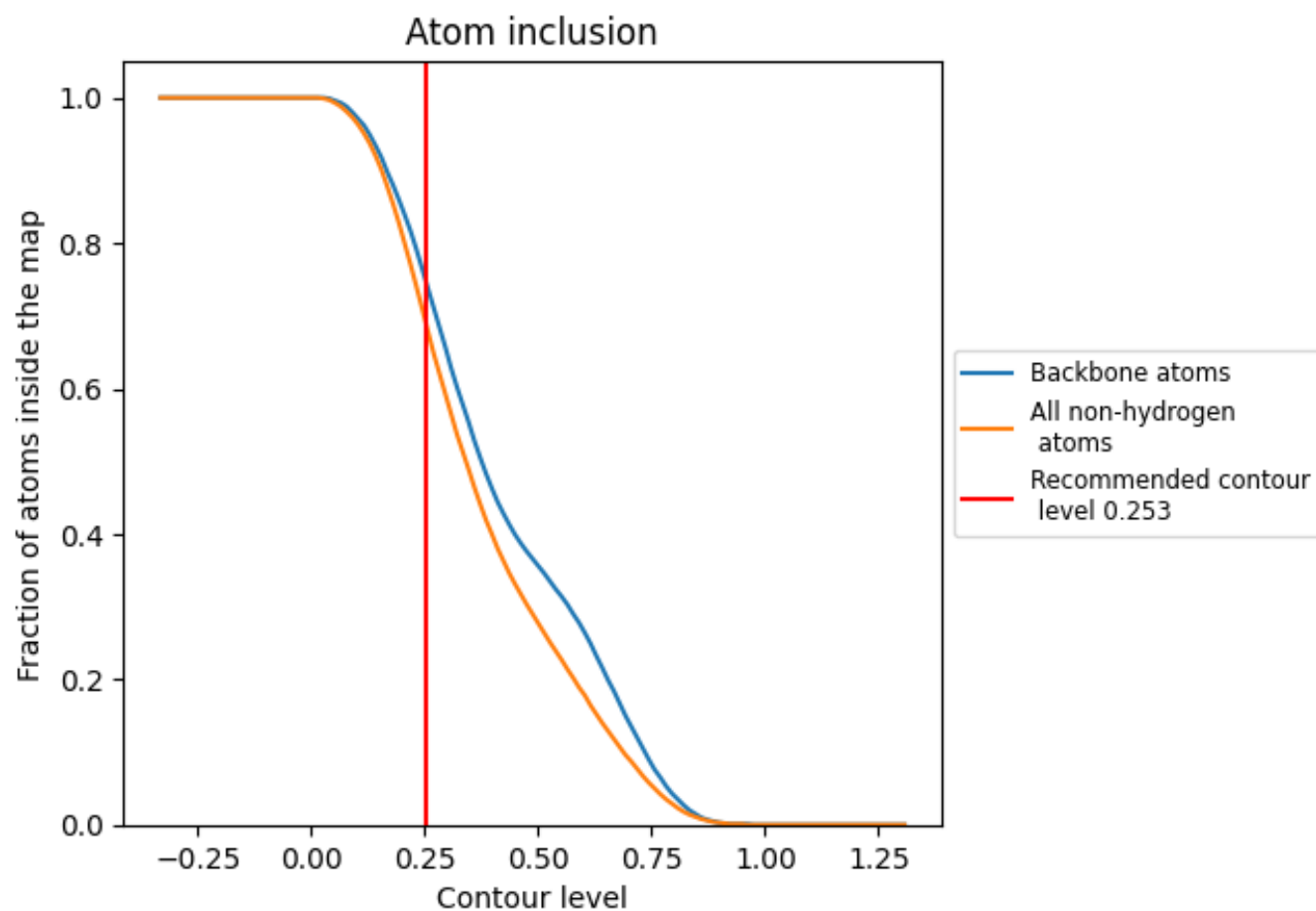
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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](#)



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 (0.253).

9.4 Atom inclusion [i](#)



At the recommended contour level, 75% of all backbone atoms, 69% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.253) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6870	 0.5390
0	 0.3220	 0.3940
1	 0.5160	 0.4300
2	 0.7030	 0.5030
3	 0.8210	 0.5590
4	 0.3280	 0.3940
5	 0.3860	 0.4010
6	 0.4790	 0.4320
7	 0.5140	 0.4320
8	 0.7060	 0.5030
9	 0.8200	 0.5590
A	 0.9490	 0.6200
B	 0.9280	 0.6140
C	 0.9050	 0.6000
D	 0.9620	 0.6290
E	 0.7590	 0.5330
F	 0.8680	 0.5520
G	 0.4320	 0.5120
H	 0.9650	 0.6130
I	 0.9890	 0.6320
J	 0.2870	 0.4670
K	 0.9140	 0.5930
L	 0.9340	 0.6010
M	 0.9440	 0.6050
O	 0.0060	 0.4920
P	 0.4830	 0.4330
Q	 0.0570	 0.5560
R	 0.4620	 0.4100
S	 0.6270	 0.5060
T	 0.9250	 0.6230
U	 0.0110	 0.4830
V	 0.0170	 0.5160
W	 0.8750	 0.5900
X	 0.8780	 0.5930
Y	 0.6150	 0.4860



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Chain	Atom inclusion	Q-score
Z	 0.7650	 0.5140
a	 0.9470	 0.6180
b	 0.9290	 0.6150
c	 0.9040	 0.6010
d	 0.9620	 0.6310
e	 0.7600	 0.5390
f	 0.8430	 0.5560
g	 0.4160	 0.4930
h	 0.9650	 0.6160
i	 0.9890	 0.6260
j	 0.2870	 0.4630
k	 0.9110	 0.5940
l	 0.9340	 0.5980
m	 0.9350	 0.6030
o	 0.0070	 0.4880
p	 0.3940	 0.4020
q	 0.0570	 0.5540
r	 0.4620	 0.4120
s	 0.6270	 0.5080
t	 0.9250	 0.6230
u	 0.0110	 0.4850
v	 0.0160	 0.5190
w	 0.8750	 0.5860
x	 0.8780	 0.5880
y	 0.6110	 0.4880
z	 0.7570	 0.5180