



wwPDB EM Validation Summary Report ⓘ

Mar 8, 2026 – 04:08 PM UTC

PDB ID : 8XLP / pdb_00008xlp
EMDB ID : EMD-38455
Title : Structure of inactive Photosystem II associated with CAC antenna from Rhodomonas Salina
Authors : Si, L.; Li, M.
Deposited on : 2023-12-26
Resolution : 2.57 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:

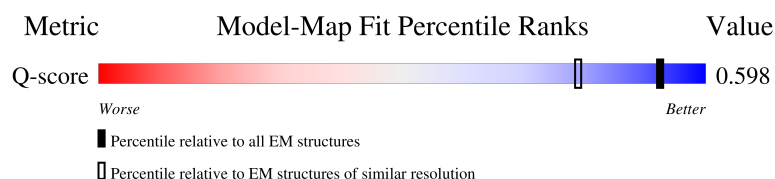
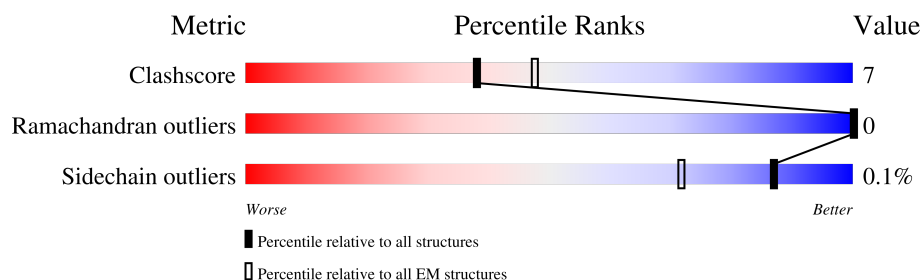
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 2.57 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	7615 (2.07 - 3.07)

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	A	328	
1	a	328	
2	B	509	
2	b	509	

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Mol	Chain	Length	Quality of chain
3	C	487	
3	c	487	
4	D	351	
4	d	351	
5	E	84	
5	e	84	
6	F	42	
6	f	42	
7	H	67	
7	h	67	
8	I	38	
8	i	38	
9	K	45	
9	k	45	
10	L	38	
10	l	38	
11	M	40	
11	m	40	
12	T	32	
12	t	32	
13	W	74	
13	w	74	
14	X	39	
14	x	39	
15	Y	34	

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Mol	Chain	Length	Quality of chain
15	y	34	
16	Z	62	
16	z	62	
17	G	284	
17	g	284	
18	2	217	
18	O	217	
19	3	221	
19	P	221	
20	4	216	
20	Q	216	
21	5	229	
21	R	229	
22	6	227	
22	S	227	
23	1	233	
23	N	233	

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
25	CLA	1	601	X	-	-	-
25	CLA	1	602	X	-	-	-
25	CLA	1	603	X	-	-	-
25	CLA	1	604	X	-	-	-
25	CLA	1	606	X	-	-	-
25	CLA	1	607	X	-	-	-
25	CLA	1	609	X	-	-	-
25	CLA	1	610	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	1	614	X	-	-	-
25	CLA	1	615	X	-	-	-
25	CLA	2	601	X	-	-	-
25	CLA	2	602	X	-	-	-
25	CLA	2	603	X	-	-	-
25	CLA	2	604	X	-	-	-
25	CLA	2	606	X	-	-	-
25	CLA	2	607	X	-	-	-
25	CLA	2	609	X	-	-	-
25	CLA	2	610	X	-	-	-
25	CLA	2	611	X	-	-	-
25	CLA	2	613	X	-	-	-
25	CLA	2	615	X	-	-	-
25	CLA	3	601	X	-	-	-
25	CLA	3	602	X	-	-	-
25	CLA	3	603	X	-	-	-
25	CLA	3	609	X	-	-	-
25	CLA	3	610	X	-	-	-
25	CLA	3	611	X	-	-	-
25	CLA	3	612	X	-	-	-
25	CLA	3	613	X	-	-	-
25	CLA	3	615	X	-	-	-
25	CLA	4	602	X	-	-	-
25	CLA	4	603	X	-	-	-
25	CLA	4	604	X	-	-	-
25	CLA	4	606	X	-	-	-
25	CLA	4	607	X	-	-	-
25	CLA	4	609	X	-	-	-
25	CLA	4	610	X	-	-	-
25	CLA	4	613	X	-	-	-
25	CLA	4	615	X	-	-	-
25	CLA	5	601	X	-	-	-
25	CLA	5	602	X	-	-	-
25	CLA	5	603	X	-	-	-
25	CLA	5	604	X	-	-	-
25	CLA	5	606	X	-	-	-
25	CLA	5	607	X	-	-	-
25	CLA	5	609	X	-	-	-
25	CLA	5	610	X	-	-	-
25	CLA	5	611	X	-	-	-
25	CLA	5	613	X	-	-	-
25	CLA	5	615	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	6	601	X	-	-	-
25	CLA	6	602	X	-	-	-
25	CLA	6	603	X	-	-	-
25	CLA	6	604	X	-	-	-
25	CLA	6	609	X	-	-	-
25	CLA	6	610	X	-	-	-
25	CLA	6	611	X	-	-	-
25	CLA	6	613	X	-	-	-
25	CLA	6	615	X	-	-	-
25	CLA	A	403	X	-	-	-
25	CLA	A	404	X	-	-	-
25	CLA	A	406	X	-	-	-
25	CLA	B	601	X	-	-	-
25	CLA	B	603	X	-	-	-
25	CLA	B	604	X	-	-	-
25	CLA	B	605	X	-	-	-
25	CLA	B	606	X	-	-	-
25	CLA	B	607	X	-	-	-
25	CLA	B	608	X	-	-	-
25	CLA	B	609	X	-	-	-
25	CLA	B	610	X	-	-	-
25	CLA	B	611	X	-	-	-
25	CLA	B	612	X	-	-	-
25	CLA	B	613	X	-	-	-
25	CLA	B	614	X	-	-	-
25	CLA	B	615	X	-	-	-
25	CLA	B	616	X	-	-	-
25	CLA	C	516	X	-	-	-
25	CLA	C	517	X	-	-	-
25	CLA	C	518	X	-	-	-
25	CLA	C	519	X	-	-	-
25	CLA	C	520	X	-	-	-
25	CLA	C	521	X	-	-	-
25	CLA	C	522	X	-	-	-
25	CLA	C	523	X	-	-	-
25	CLA	C	524	X	-	-	-
25	CLA	C	525	X	-	-	-
25	CLA	C	526	X	-	-	-
25	CLA	C	527	X	-	-	-
25	CLA	C	528	X	-	-	-
25	CLA	D	400	X	-	-	-
25	CLA	D	403	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	D	404	X	-	-	-
25	CLA	G	301	X	-	-	-
25	CLA	G	302	X	-	-	-
25	CLA	N	601	X	-	-	-
25	CLA	N	602	X	-	-	-
25	CLA	N	603	X	-	-	-
25	CLA	N	604	X	-	-	-
25	CLA	N	606	X	-	-	-
25	CLA	N	607	X	-	-	-
25	CLA	N	609	X	-	-	-
25	CLA	N	610	X	-	-	-
25	CLA	N	614	X	-	-	-
25	CLA	N	615	X	-	-	-
25	CLA	O	601	X	-	-	-
25	CLA	O	602	X	-	-	-
25	CLA	O	603	X	-	-	-
25	CLA	O	604	X	-	-	-
25	CLA	O	606	X	-	-	-
25	CLA	O	607	X	-	-	-
25	CLA	O	609	X	-	-	-
25	CLA	O	610	X	-	-	-
25	CLA	O	611	X	-	-	-
25	CLA	O	613	X	-	-	-
25	CLA	O	615	X	-	-	-
25	CLA	P	601	X	-	-	-
25	CLA	P	602	X	-	-	-
25	CLA	P	603	X	-	-	-
25	CLA	P	609	X	-	-	-
25	CLA	P	610	X	-	-	-
25	CLA	P	611	X	-	-	-
25	CLA	P	612	X	-	-	-
25	CLA	P	613	X	-	-	-
25	CLA	P	615	X	-	-	-
25	CLA	Q	602	X	-	-	-
25	CLA	Q	603	X	-	-	-
25	CLA	Q	604	X	-	-	-
25	CLA	Q	606	X	-	-	-
25	CLA	Q	607	X	-	-	-
25	CLA	Q	609	X	-	-	-
25	CLA	Q	610	X	-	-	-
25	CLA	Q	613	X	-	-	-
25	CLA	Q	615	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	R	601	X	-	-	-
25	CLA	R	602	X	-	-	-
25	CLA	R	603	X	-	-	-
25	CLA	R	604	X	-	-	-
25	CLA	R	606	X	-	-	-
25	CLA	R	607	X	-	-	-
25	CLA	R	609	X	-	-	-
25	CLA	R	610	X	-	-	-
25	CLA	R	611	X	-	-	-
25	CLA	R	613	X	-	-	-
25	CLA	R	615	X	-	-	-
25	CLA	S	601	X	-	-	-
25	CLA	S	602	X	-	-	-
25	CLA	S	603	X	-	-	-
25	CLA	S	604	X	-	-	-
25	CLA	S	609	X	-	-	-
25	CLA	S	610	X	-	-	-
25	CLA	S	611	X	-	-	-
25	CLA	S	613	X	-	-	-
25	CLA	S	615	X	-	-	-
25	CLA	a	403	X	-	-	-
25	CLA	a	404	X	-	-	-
25	CLA	a	406	X	-	-	-
25	CLA	b	601	X	-	-	-
25	CLA	b	603	X	-	-	-
25	CLA	b	604	X	-	-	-
25	CLA	b	605	X	-	-	-
25	CLA	b	606	X	-	-	-
25	CLA	b	607	X	-	-	-
25	CLA	b	608	X	-	-	-
25	CLA	b	609	X	-	-	-
25	CLA	b	610	X	-	-	-
25	CLA	b	611	X	-	-	-
25	CLA	b	612	X	-	-	-
25	CLA	b	613	X	-	-	-
25	CLA	b	614	X	-	-	-
25	CLA	b	615	X	-	-	-
25	CLA	b	616	X	-	-	-
25	CLA	c	516	X	-	-	-
25	CLA	c	517	X	-	-	-
25	CLA	c	518	X	-	-	-
25	CLA	c	519	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	c	520	X	-	-	-
25	CLA	c	521	X	-	-	-
25	CLA	c	522	X	-	-	-
25	CLA	c	523	X	-	-	-
25	CLA	c	524	X	-	-	-
25	CLA	c	525	X	-	-	-
25	CLA	c	526	X	-	-	-
25	CLA	c	527	X	-	-	-
25	CLA	c	528	X	-	-	-
25	CLA	d	400	X	-	-	-
25	CLA	d	403	X	-	-	-
25	CLA	d	404	X	-	-	-
25	CLA	g	301	X	-	-	-
25	CLA	g	302	X	-	-	-

2 Entry composition

There are 40 unique types of molecules in this entry. The entry contains 70547 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 protein D1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	a	327	Total	C	N	O	S	0	0
			2563	1677	420	454	12		
1	A	327	Total	C	N	O	S	0	0
			2563	1677	420	454	12		

- Molecule 2 is a protein called Photosystem II CP47 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	b	503	Total	C	N	O	S	0	0
			3950	2575	674	689	12		
2	B	503	Total	C	N	O	S	0	0
			3950	2575	674	689	12		

- Molecule 3 is a protein called Photosystem II CP43 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	c	434	Total	C	N	O	S	0	0
			3379	2213	569	587	10		
3	C	434	Total	C	N	O	S	0	0
			3379	2213	569	587	10		

- Molecule 4 is a protein called Photosystem II D2 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	d	341	Total	C	N	O	S	0	0
			2708	1790	443	462	13		
4	D	341	Total	C	N	O	S	0	0
			2708	1790	443	462	13		

- Molecule 5 is a protein called Cytochrome b559 subunit alpha.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	e	64	Total	C	N	O	0	0
			525	345	85	95		
5	E	64	Total	C	N	O	0	0
			525	345	85	95		

- Molecule 6 is a protein called Cytochrome b559 subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	f	32	Total	C	N	O	S	0	0
			261	179	43	38	1		
6	F	32	Total	C	N	O	S	0	0
			261	179	43	38	1		

- Molecule 7 is a protein called Photosystem II reaction center protein H.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	h	65	Total	C	N	O	S	0	0
			508	337	81	88	2		
7	H	65	Total	C	N	O	S	0	0
			508	337	81	88	2		

- Molecule 8 is a protein called Photosystem II reaction center protein I.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	i	35	Total	C	N	O	S	0	0
			284	188	46	49	1		
8	I	35	Total	C	N	O	S	0	0
			284	188	46	49	1		

- Molecule 9 is a protein called Photosystem II reaction center protein K.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	k	37	Total	C	N	O	0	0
			296	209	44	43		
9	K	37	Total	C	N	O	0	0
			296	209	44	43		

- Molecule 10 is a protein called Photosystem II reaction center protein L.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	l	37	Total	C	N	O	0	0
			301	204	47	50		

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Mol	Chain	Residues	Atoms				AltConf	Trace
10	L	37	Total	C	N	O	0	0
			301	204	47	50		

- Molecule 11 is a protein called Photosystem II protein M.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	m	38	Total	C	N	O	0	0
			285	189	45	51		
11	M	38	Total	C	N	O	0	0
			285	189	45	51		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	t	30	Total	C	N	O	S	0	0
			244	169	36	38	1		
12	T	30	Total	C	N	O	S	0	0
			244	169	36	38	1		

- Molecule 13 is a protein called Photosystem II protein W.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	w	45	Total	C	N	O	0	0
			363	235	58	70		
13	W	45	Total	C	N	O	0	0
			363	235	58	70		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	x	36	Total	C	N	O	S	0	0
			268	179	41	47	1		
14	X	36	Total	C	N	O	S	0	0
			268	179	41	47	1		

- Molecule 15 is a protein called Photosystem II reaction center protein Psb30.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	y	32	Total	C	N	O	0	0
			241	159	42	40		
15	Y	32	Total	C	N	O	0	0
			241	159	42	40		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	z	61	Total	C	N	O	S	0	0
			460	314	67	76	3		
16	Z	61	Total	C	N	O	S	0	0
			460	314	67	76	3		

- Molecule 17 is a protein called NCP.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	g	147	Total	C	N	O	S	0	0
			1163	757	190	215	1		
17	G	147	Total	C	N	O	S	0	0
			1163	757	190	215	1		

- Molecule 18 is a protein called CAC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	2	173	Total	C	N	O	S	0	0
			1380	912	225	240	3		
18	O	173	Total	C	N	O	S	0	0
			1380	912	225	240	3		

- Molecule 19 is a protein called CAC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	3	180	Total	C	N	O	S	0	0
			1392	902	232	249	9		
19	P	180	Total	C	N	O	S	0	0
			1392	902	232	249	9		

- Molecule 20 is a protein called CAC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	4	163	Total	C	N	O	S	0	0
			1253	806	216	221	10		
20	Q	163	Total	C	N	O	S	0	0
			1253	806	216	221	10		

- Molecule 21 is a protein called CAC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	5	183	Total	C	N	O	S	0	0
			1430	936	234	257	3		
21	R	183	Total	C	N	O	S	0	0
			1430	936	234	257	3		

- Molecule 22 is a protein called CAC6.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	6	173	Total	C	N	O	S	0	0
			1337	865	228	238	6		
22	S	173	Total	C	N	O	S	0	0
			1337	865	228	238	6		

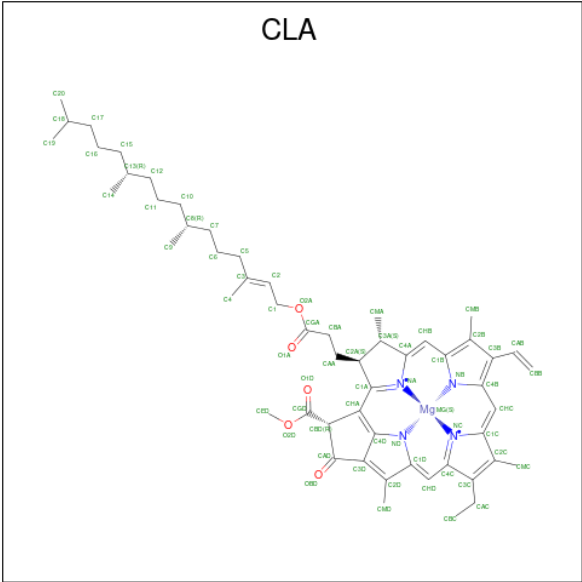
- Molecule 23 is a protein called CAC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	1	190	Total	C	N	O	S	0	0
			1458	933	256	261	8		
23	N	190	Total	C	N	O	S	0	0
			1458	933	256	261	8		

- Molecule 24 is FE (II) ION (CCD ID: FE2) (formula: Fe).

Mol	Chain	Residues	Atoms		AltConf
24	a	1	Total	Fe	0
			1	1	
24	A	1	Total	Fe	0
			1	1	

- Molecule 25 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅).



Mol	Chain	Residues	Atoms					AltConf
25	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	a	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
25	a	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
25	b	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
25	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	b	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
25	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	b	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	c	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	c	1	Total 53	C 43	Mg 1	N 4	O 5	0
25	d	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	d	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	d	1	Total 61	C 51	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
25	g	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	g	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	A	1	Total 49	C 39	Mg 1	N 4	O 5	0
25	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	B	1	Total 50	C 40	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 59	C 49	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	C	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	C	1	Total 52	C 42	Mg 1	N 4	O 5	0
25	D	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	D	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	D	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	2	1	Total 49	C 39	Mg 1	N 4	O 5	0
25	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	2	1	Total 51	C 41	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
25	2	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	2	1	Total 48	C 38	Mg 1	N 4	O 5	0
25	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	2	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	2	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	2	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	3	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	3	1	Total 62	C 52	Mg 1	N 4	O 5	0
25	3	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	3	1	Total 63	C 53	Mg 1	N 4	O 5	0
25	3	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	3	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	3	1	Total 52	C 42	Mg 1	N 4	O 5	0
25	3	1	Total 53	C 43	Mg 1	N 4	O 5	0
25	3	1	Total 55	C 45	Mg 1	N 4	O 5	0
25	3	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	4	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	4	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	4	1	Total 61	C 51	Mg 1	N 4	O 5	0
25	4	1	Total 55	C 45	Mg 1	N 4	O 5	0
25	4	1	Total 43	C 35	Mg 1	N 4	O 3	0

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Mol	Chain	Residues	Atoms					AltConf
25	4	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
25	4	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
25	4	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
25	4	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
25	5	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
25	5	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
25	5	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
25	5	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
25	5	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	5	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
25	5	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	5	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
25	5	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	5	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
25	5	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
25	6	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
25	6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	6	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
25	6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	6	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
25	6	1	Total	C	Mg	N	O	0
			57	47	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
25	6	1	Total 55	C 45	Mg 1	N 4	O 5	0
25	6	1	Total 53	C 43	Mg 1	N 4	O 5	0
25	6	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	G	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	1	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	1	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	1	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	1	1	Total 59	C 49	Mg 1	N 4	O 5	0
25	1	1	Total 50	C 40	Mg 1	N 4	O 5	0
25	1	1	Total 43	C 35	Mg 1	N 4	O 3	0
25	1	1	Total 46	C 36	Mg 1	N 4	O 5	0
25	1	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	1	1	Total 48	C 38	Mg 1	N 4	O 5	0
25	1	1	Total 47	C 37	Mg 1	N 4	O 5	0
25	O	1	Total 49	C 39	Mg 1	N 4	O 5	0
25	O	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	O	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	O	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	O	1	Total 51	C 41	Mg 1	N 4	O 5	0
25	O	1	Total 60	C 50	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
25	O	1	Total 48	C 38	Mg 1	N 4	O 5	0
25	O	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	O	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	O	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	O	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	P	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	P	1	Total 62	C 52	Mg 1	N 4	O 5	0
25	P	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	P	1	Total 63	C 53	Mg 1	N 4	O 5	0
25	P	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	P	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	P	1	Total 52	C 42	Mg 1	N 4	O 5	0
25	P	1	Total 53	C 43	Mg 1	N 4	O 5	0
25	P	1	Total 55	C 45	Mg 1	N 4	O 5	0
25	P	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	Q	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	Q	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	Q	1	Total 61	C 51	Mg 1	N 4	O 5	0
25	Q	1	Total 55	C 45	Mg 1	N 4	O 5	0
25	Q	1	Total 43	C 35	Mg 1	N 4	O 3	0
25	Q	1	Total 56	C 46	Mg 1	N 4	O 5	0

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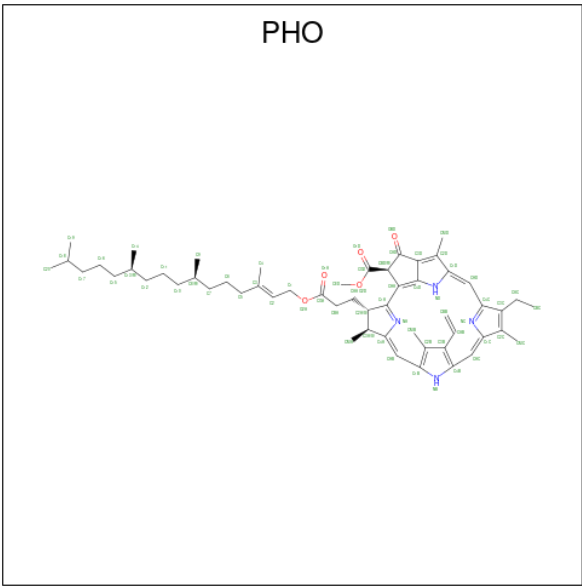
Mol	Chain	Residues	Atoms					AltConf
25	Q	1	Total 51	C 41	Mg 1	N 4	O 5	0
25	Q	1	Total 43	C 35	Mg 1	N 4	O 3	0
25	Q	1	Total 43	C 35	Mg 1	N 4	O 3	0
25	R	1	Total 55	C 45	Mg 1	N 4	O 5	0
25	R	1	Total 55	C 45	Mg 1	N 4	O 5	0
25	R	1	Total 52	C 42	Mg 1	N 4	O 5	0
25	R	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	R	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	R	1	Total 43	C 35	Mg 1	N 4	O 3	0
25	R	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	R	1	Total 59	C 49	Mg 1	N 4	O 5	0
25	R	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	R	1	Total 55	C 45	Mg 1	N 4	O 5	0
25	R	1	Total 46	C 36	Mg 1	N 4	O 5	0
25	S	1	Total 55	C 45	Mg 1	N 4	O 5	0
25	S	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	S	1	Total 55	C 45	Mg 1	N 4	O 5	0
25	S	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	S	1	Total 55	C 45	Mg 1	N 4	O 5	0
25	S	1	Total 57	C 47	Mg 1	N 4	O 5	0
25	S	1	Total 55	C 45	Mg 1	N 4	O 5	0

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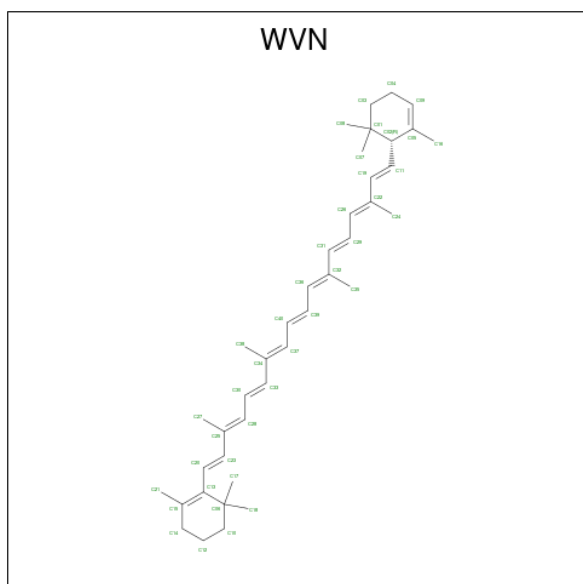
Mol	Chain	Residues	Atoms					AltConf
25	S	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
25	S	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	N	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	N	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
25	N	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
25	N	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
25	N	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
25	N	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
25	N	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
25	N	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
25	N	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
25	N	1	Total	C	Mg	N	O	0
			47	37	1	4	5	

- Molecule 26 is PHEOPHYTIN A (CCD ID: PHO) (formula: C₅₅H₇₄N₄O₅).



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

- Molecule 27 is 1,3,3-trimethyl-2-[(1E,3E,5E,7E,9E,11E,13E,15E,17E)-3,7,12,16-tetramethyl-18-[(1R)-2,6,6-trimethylcyclohex-2-en-1-yl]octadeca-1,3,5,7,9,11,13,15,17-nonaenyl]cyclohexene (CCD ID: WVN) (formula: C₄₀H₅₆).



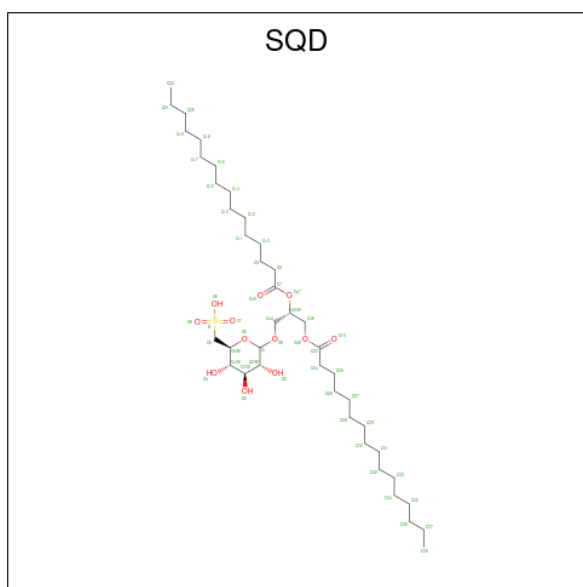
Mol	Chain	Residues	Atoms		AltConf
27	a	1	Total	C	0
			40	40	
27	b	1	Total	C	0
			40	40	
27	b	1	Total	C	0
			40	40	
27	b	1	Total	C	0
			40	40	
27	c	1	Total	C	0
			40	40	
27	c	1	Total	C	0
			40	40	
27	c	1	Total	C	0
			40	40	

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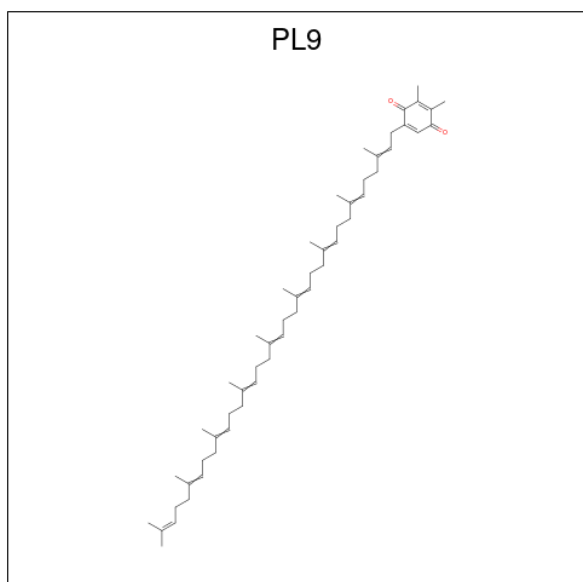
Mol	Chain	Residues	Atoms	AltConf
27	d	1	Total C 40 40	0
27	h	1	Total C 40 40	0
27	y	1	Total C 40 40	0
27	A	1	Total C 40 40	0
27	B	1	Total C 40 40	0
27	B	1	Total C 40 40	0
27	B	1	Total C 40 40	0
27	C	1	Total C 40 40	0
27	C	1	Total C 40 40	0
27	C	1	Total C 40 40	0
27	D	1	Total C 40 40	0
27	H	1	Total C 40 40	0
27	Y	1	Total C 40 40	0
27	3	1	Total C 40 40	0
27	6	1	Total C 40 40	0
27	P	1	Total C 40 40	0
27	S	1	Total C 40 40	0

- Molecule 28 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: C₄₁H₇₈O₁₂S).



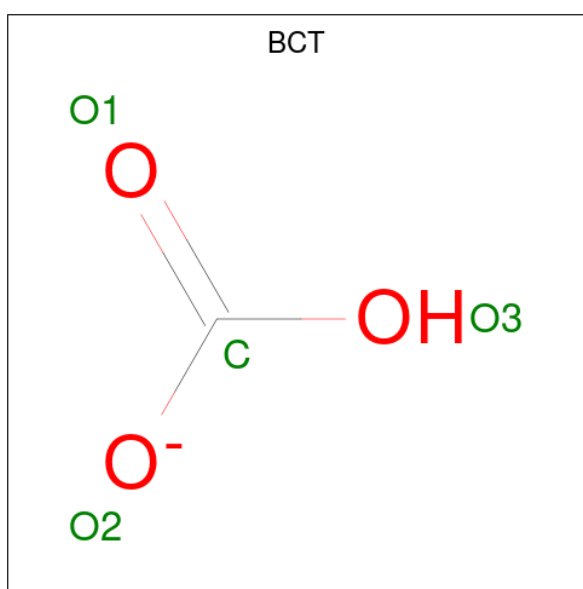
Mol	Chain	Residues	Atoms				AltConf
28	a	1	Total	C	O	S	0
			45	32	12	1	
28	a	1	Total	C	O	S	0
			40	27	12	1	
28	A	1	Total	C	O	S	0
			54	41	12	1	
28	A	1	Total	C	O	S	0
			40	27	12	1	

- Molecule 29 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: $C_{53}H_{80}O_2$).



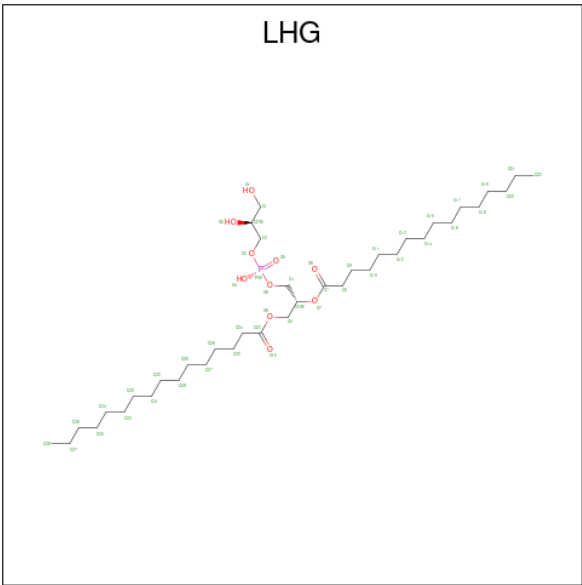
Mol	Chain	Residues	Atoms			AltConf
29	a	1	Total	C	O	0
			33	31	2	
29	d	1	Total	C	O	0
			55	53	2	
29	A	1	Total	C	O	0
			33	31	2	
29	D	1	Total	C	O	0
			55	53	2	

- Molecule 30 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 31 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $\text{C}_{38}\text{H}_{75}\text{O}_{10}\text{P}$).



Mol	Chain	Residues	Atoms				AltConf
31	a	1	Total	C	O	P	0
			42	31	10	1	
31	b	1	Total	C	O	P	0
			43	32	10	1	
31	c	1	Total	C	O	P	0
			40	29	10	1	
31	d	1	Total	C	O	P	0
			49	38	10	1	
31	l	1	Total	C	O	P	0
			49	38	10	1	
31	z	1	Total	C	O	P	0
			25	14	10	1	
31	A	1	Total	C	O	P	0
			42	31	10	1	
31	B	1	Total	C	O	P	0
			43	32	10	1	
31	C	1	Total	C	O	P	0
			40	29	10	1	
31	D	1	Total	C	O	P	0
			49	38	10	1	
31	L	1	Total	C	O	P	0
			49	38	10	1	
31	Z	1	Total	C	O	P	0
			25	14	10	1	
31	2	1	Total	C	O	P	0
			46	35	10	1	
31	3	1	Total	C	O	P	0
			49	38	10	1	

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Mol	Chain	Residues	Atoms				AltConf
31	5	1	Total	C	O	P	0
			46	35	10	1	
31	6	1	Total	C	O	P	0
			40	29	10	1	
31	O	1	Total	C	O	P	0
			46	35	10	1	
31	P	1	Total	C	O	P	0
			49	38	10	1	
31	R	1	Total	C	O	P	0
			46	35	10	1	
31	S	1	Total	C	O	P	0
			40	29	10	1	

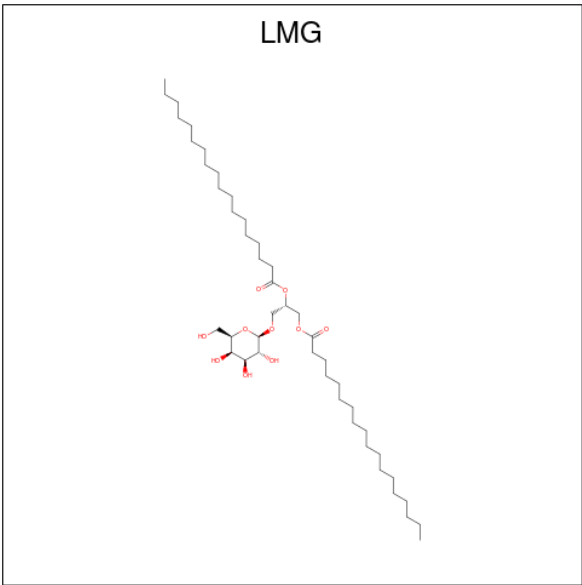
- Molecule 32 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		AltConf
32	a	1	Total	Cl	0
			1	1	
32	c	1	Total	Cl	0
			1	1	
32	A	1	Total	Cl	0
			1	1	
32	C	1	Total	Cl	0
			1	1	

- Molecule 33 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		AltConf
33	a	2	Total	Mn	0
			2	2	
33	A	2	Total	Mn	0
			2	2	

- Molecule 34 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: C₄₅H₈₆O₁₀).



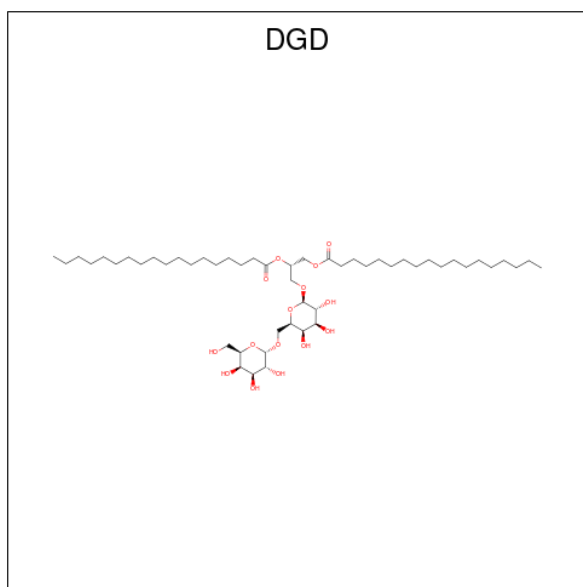
Mol	Chain	Residues	Atoms			AltConf
34	b	1	Total	C	O	0
			51	41	10	
34	c	1	Total	C	O	0
			51	41	10	
34	d	1	Total	C	O	0
			40	30	10	
34	d	1	Total	C	O	0
			37	27	10	
34	f	1	Total	C	O	0
			46	36	10	
34	m	1	Total	C	O	0
			40	30	10	
34	w	1	Total	C	O	0
			48	38	10	
34	z	1	Total	C	O	0
			31	21	10	
34	g	1	Total	C	O	0
			40	30	10	
34	B	1	Total	C	O	0
			51	41	10	
34	C	1	Total	C	O	0
			47	37	10	
34	D	1	Total	C	O	0
			40	30	10	
34	D	1	Total	C	O	0
			37	27	10	
34	F	1	Total	C	O	0
			46	36	10	

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Mol	Chain	Residues	Atoms			AltConf
34	M	1	Total	C	O	0
			40	30	10	
34	W	1	Total	C	O	0
			48	38	10	
34	Z	1	Total	C	O	0
			31	21	10	
34	2	1	Total	C	O	0
			40	30	10	
34	4	1	Total	C	O	0
			43	33	10	
34	G	1	Total	C	O	0
			40	30	10	
34	O	1	Total	C	O	0
			40	30	10	
34	Q	1	Total	C	O	0
			43	33	10	

- Molecule 35 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



Mol	Chain	Residues	Atoms			AltConf
35	c	1	Total	C	O	0
			54	39	15	
35	h	1	Total	C	O	0
			62	47	15	
35	C	1	Total	C	O	0
			54	39	15	

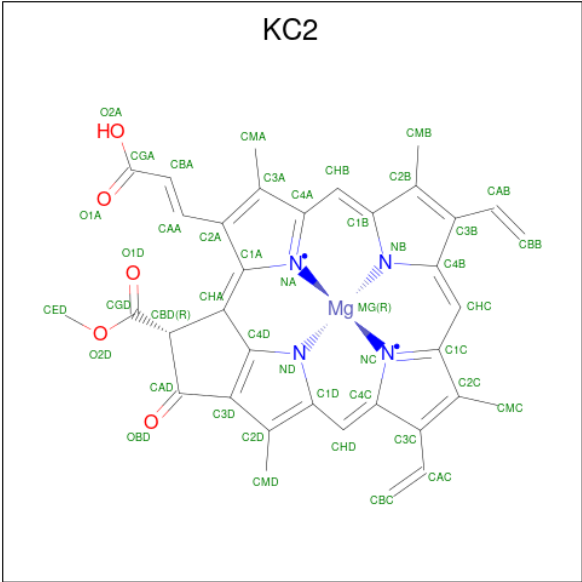
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Mol	Chain	Residues	Atoms			AltConf
35	H	1	Total	C	O	0
			62	47	15	

- # HEM

Mol	Chain	Residues	Atoms					AltConf
36	e	1	Total 43	C 34	Fe 1	N 4	O 4	0
36	E	1	Total 43	C 34	Fe 1	N 4	O 4	0

- 



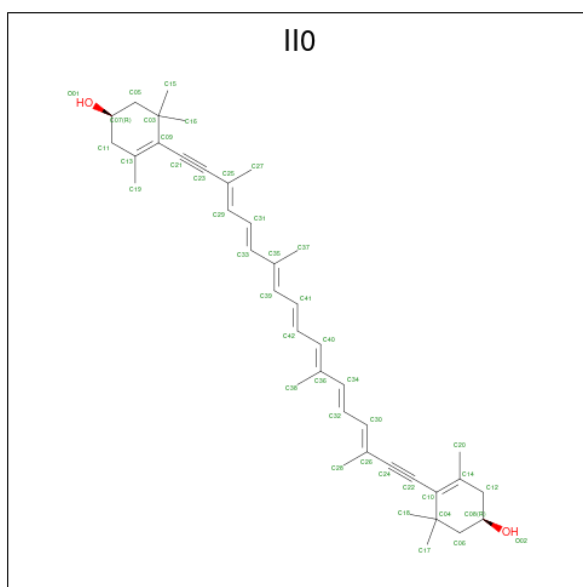
Mol	Chain	Residues	Atoms					AltConf
37	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
37	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
37	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
37	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
37	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
37	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
37	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
37	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
37	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
37	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
37	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
37	O	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
37	P	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
37	Q	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
37	Q	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
37	Q	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
37	R	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
37	S	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
37	S	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
37	N	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
37	N	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
37	N	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
37	N	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

- Molecule 38 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).



Mol	Chain	Residues	Atoms			AltConf
38	2	1	Total	C	O	0
			42	40	2	
38	2	1	Total	C	O	0
			42	40	2	
38	2	1	Total	C	O	0
			42	40	2	
38	2	1	Total	C	O	0
			42	40	2	
38	3	1	Total	C	O	0
			42	40	2	
38	3	1	Total	C	O	0
			42	40	2	
38	3	1	Total	C	O	0
			42	40	2	
38	3	1	Total	C	O	0
			42	40	2	
38	4	1	Total	C	O	0
			42	40	2	
38	4	1	Total	C	O	0
			42	40	2	
38	4	1	Total	C	O	0
			42	40	2	
38	4	1	Total	C	O	0
			42	40	2	
38	5	1	Total	C	O	0
			42	40	2	
38	5	1	Total	C	O	0
			42	40	2	
38	5	1	Total	C	O	0
			42	40	2	
38	5	1	Total	C	O	0
			42	40	2	
38	6	1	Total	C	O	0
			42	40	2	
38	6	1	Total	C	O	0
			42	40	2	
38	6	1	Total	C	O	0
			42	40	2	
38	6	1	Total	C	O	0
			42	40	2	
38	1	1	Total	C	O	0
			42	40	2	
38	1	1	Total	C	O	0
			42	40	2	

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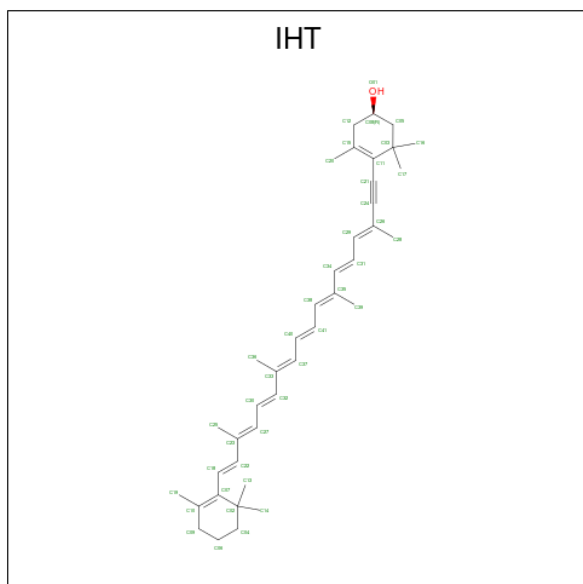
Mol	Chain	Residues	Atoms			AltConf
38	1	1	Total 42	C 40	O 2	0
38	1	1	Total 42	C 40	O 2	0
38	O	1	Total 42	C 40	O 2	0
38	O	1	Total 42	C 40	O 2	0
38	O	1	Total 42	C 40	O 2	0
38	O	1	Total 42	C 40	O 2	0
38	P	1	Total 42	C 40	O 2	0
38	P	1	Total 42	C 40	O 2	0
38	P	1	Total 42	C 40	O 2	0
38	P	1	Total 42	C 40	O 2	0
38	Q	1	Total 42	C 40	O 2	0
38	Q	1	Total 42	C 40	O 2	0
38	Q	1	Total 42	C 40	O 2	0
38	Q	1	Total 42	C 40	O 2	0
38	R	1	Total 42	C 40	O 2	0
38	R	1	Total 42	C 40	O 2	0
38	R	1	Total 42	C 40	O 2	0
38	R	1	Total 42	C 40	O 2	0
38	S	1	Total 42	C 40	O 2	0
38	S	1	Total 42	C 40	O 2	0
38	S	1	Total 42	C 40	O 2	0

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Mol	Chain	Residues	Atoms			AltConf
38	S	1	Total	C	O	0
			42	40	2	
38	N	1	Total	C	O	0
			42	40	2	
38	N	1	Total	C	O	0
			42	40	2	
38	N	1	Total	C	O	0
			42	40	2	
38	N	1	Total	C	O	0
			42	40	2	

- Molecule 39 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).



Mol	Chain	Residues	Atoms			AltConf
39	2	1	Total	C	O	0
			41	40	1	
39	4	1	Total	C	O	0
			41	40	1	
39	5	1	Total	C	O	0
			41	40	1	
39	1	1	Total	C	O	0
			41	40	1	
39	O	1	Total	C	O	0
			41	40	1	

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Mol	Chain	Residues	Atoms			AltConf
39	Q	1	Total	C	O	0
			41	40	1	
39	R	1	Total	C	O	0
			41	40	1	
39	N	1	Total	C	O	0
			41	40	1	

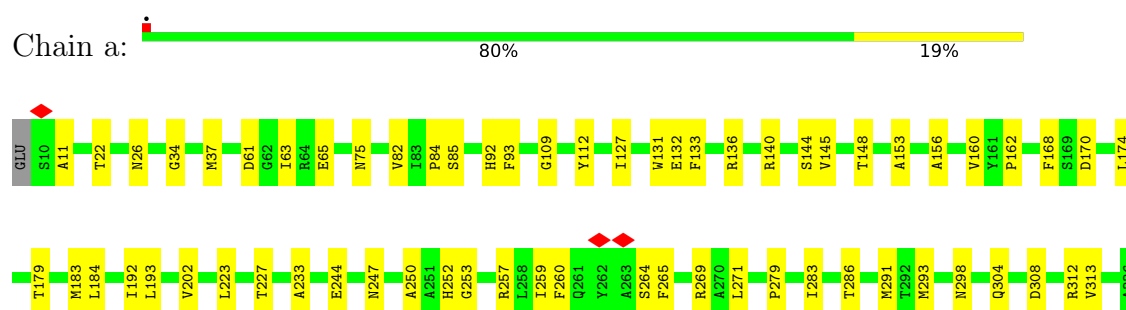
- Molecule 40 is water.

Mol	Chain	Residues	Atoms		AltConf
40	c	1	Total	O	0
			1	1	
40	C	1	Total	O	0
			1	1	

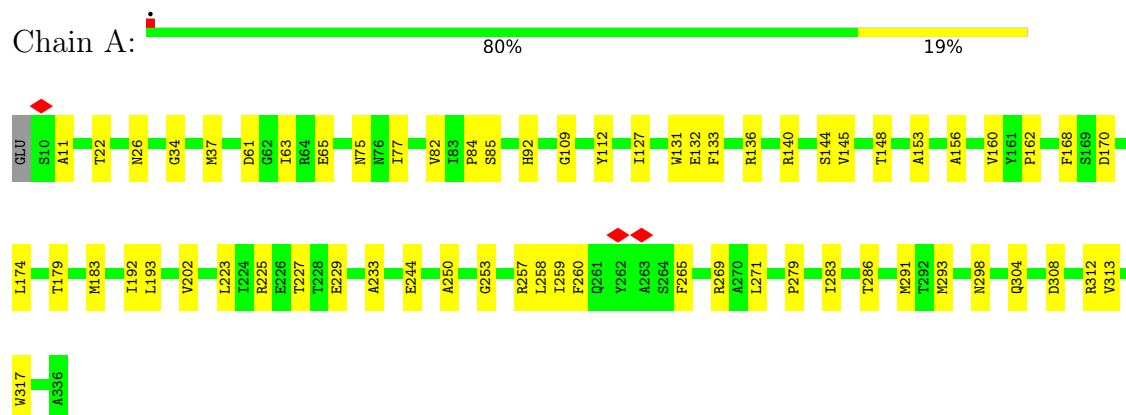
3 Residue-property plots

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.

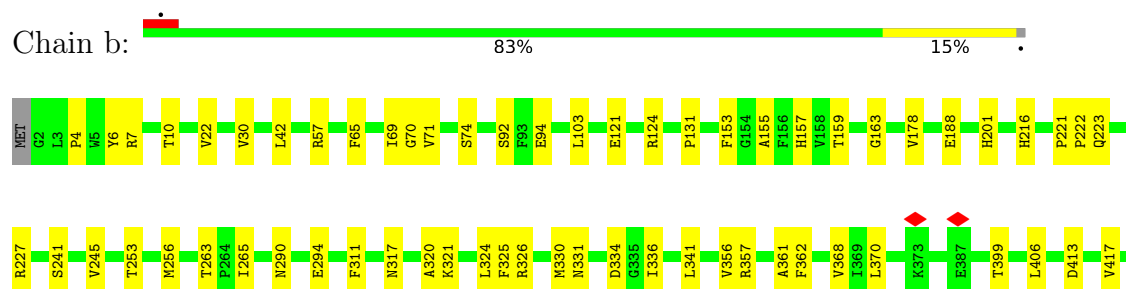
- Molecule 1: Photosystem II protein D1

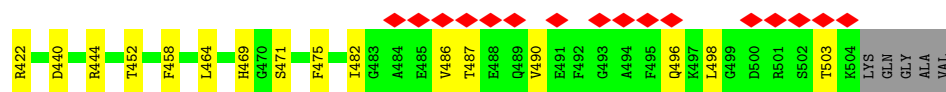


- Molecule 1: Photosystem II protein D1



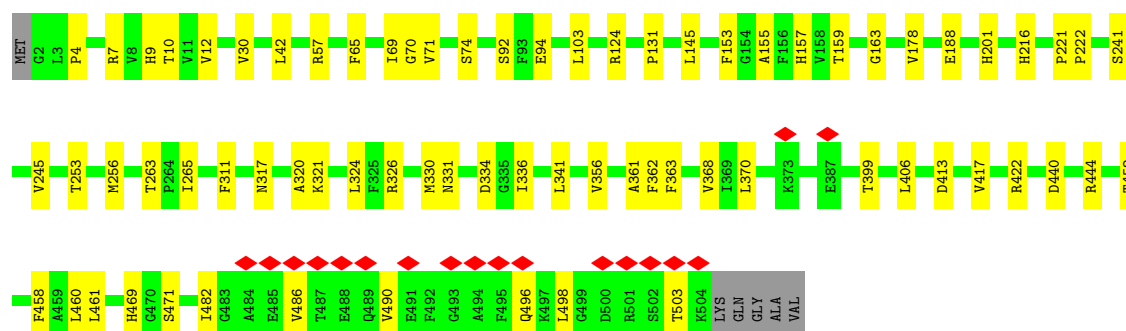
- Molecule 2: Photosystem II CP47 reaction center protein





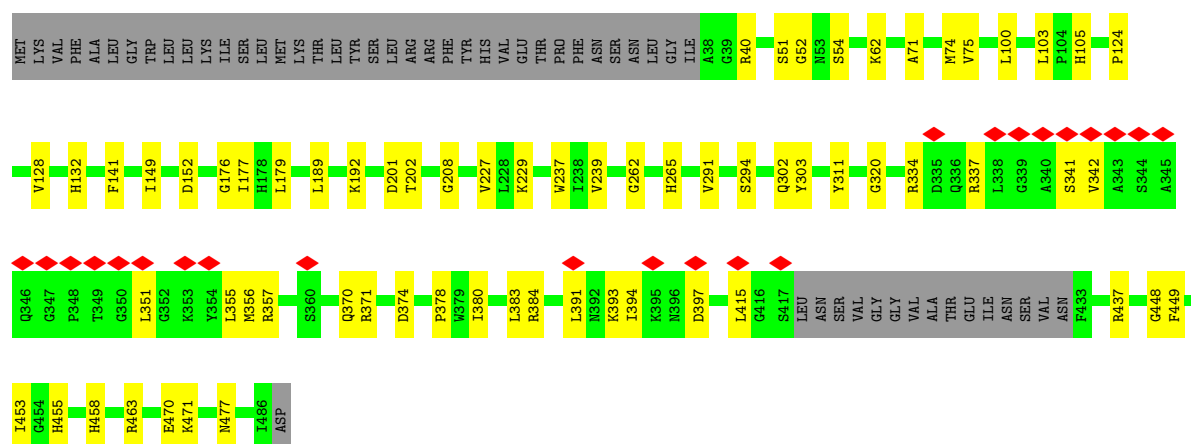
• Molecule 2: Photosystem II CP47 reaction center protein

Chain B: 85% 14%



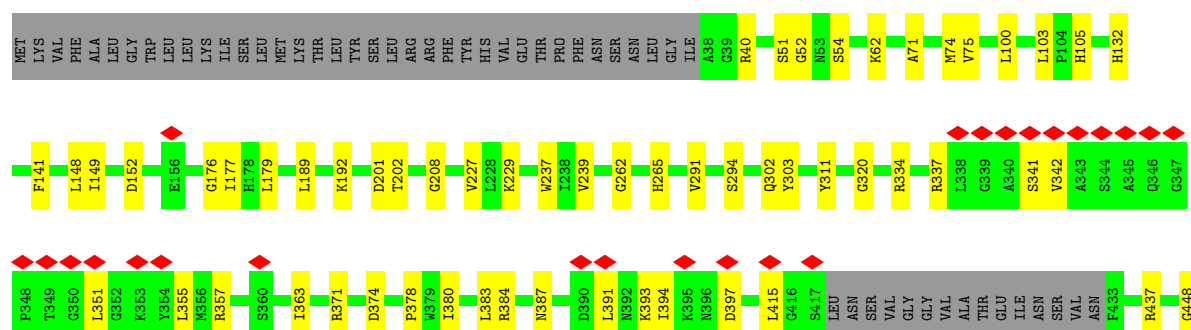
• Molecule 3: Photosystem II CP43 reaction center protein

Chain c: 5% 75% 14% 11%



• Molecule 3: Photosystem II CP43 reaction center protein

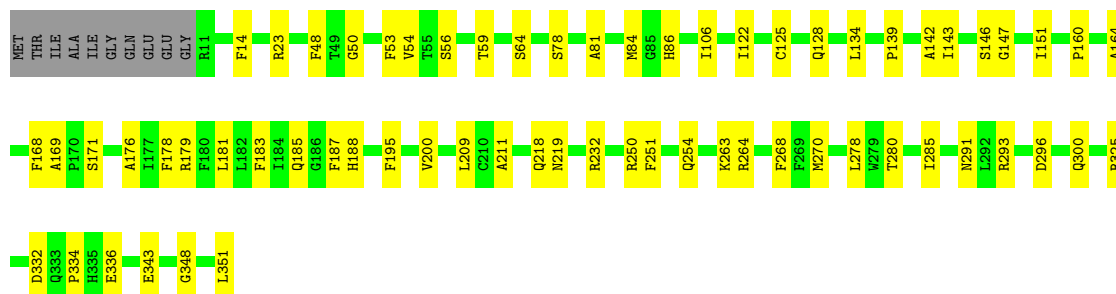
Chain C: 5% 75% 14% 11%





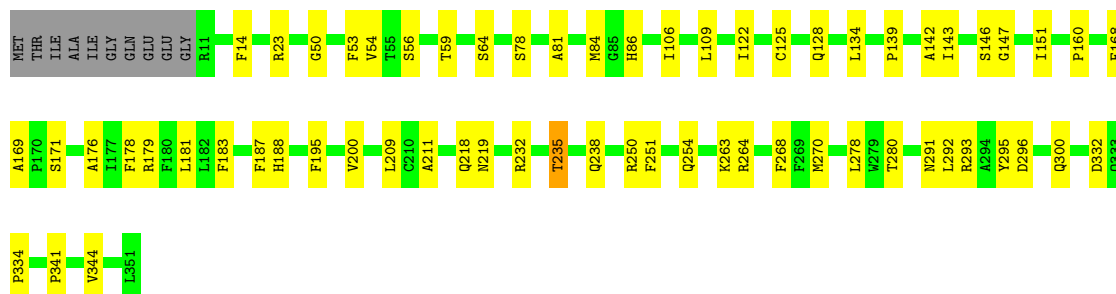
- Molecule 4: Photosystem II D2 protein

Chain d: 79% 19%



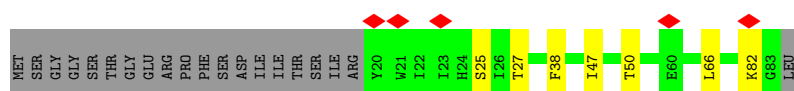
- Molecule 4: Photosystem II D2 protein

Chain D: 79% 18%



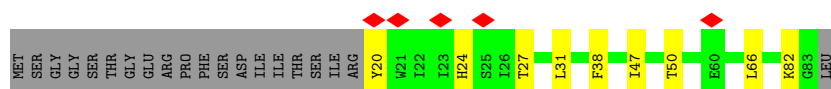
- Molecule 5: Cytochrome b559 subunit alpha

Chain e: 6% 68% 8% 24%



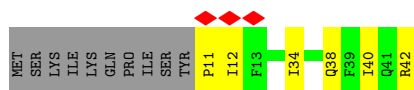
- Molecule 5: Cytochrome b559 subunit alpha

Chain E: 6% 65% 11% 24%



- Molecule 6: Cytochrome b559 subunit beta

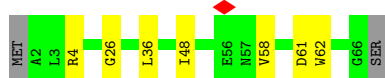
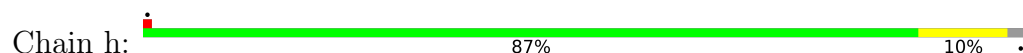
Chain f: 7% 62% 14% 24%



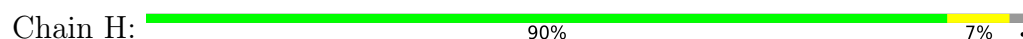
- Molecule 6: Cytochrome b559 subunit beta



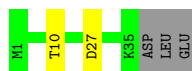
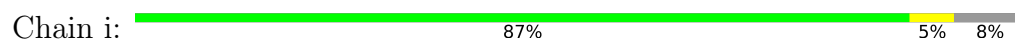
- Molecule 7: Photosystem II reaction center protein H



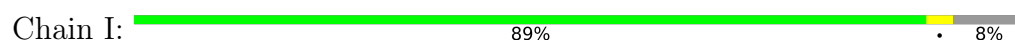
- Molecule 7: Photosystem II reaction center protein H



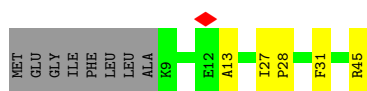
- Molecule 8: Photosystem II reaction center protein I



- Molecule 8: Photosystem II reaction center protein I

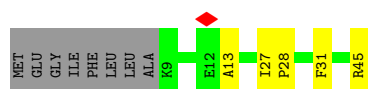


- Molecule 9: Photosystem II reaction center protein K



- Molecule 9: Photosystem II reaction center protein K

Chain K:  71% 11% 18%



- Molecule 10: Photosystem II reaction center protein L

Chain l:  82% 16% .



- Molecule 10: Photosystem II reaction center protein L

Chain L:  87% 11% .



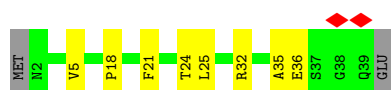
- Molecule 11: Photosystem II protein M

Chain m:  10% 72% 22% 5%



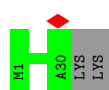
- Molecule 11: Photosystem II protein M

Chain M:  5% 75% 20% 5%



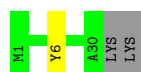
- Molecule 12: Photosystem II reaction center protein T

Chain t:  94% 6%

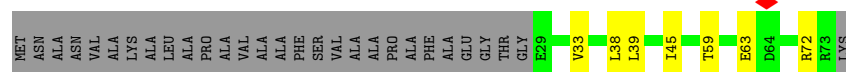


- Molecule 12: Photosystem II reaction center protein T

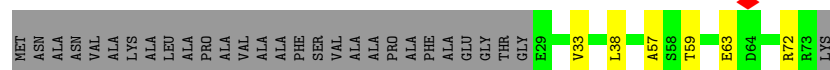
Chain T:  91% . 6%



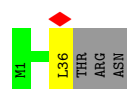
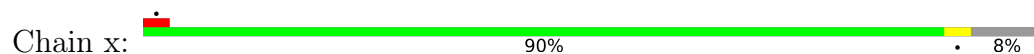
- Molecule 13: Photosystem II protein W



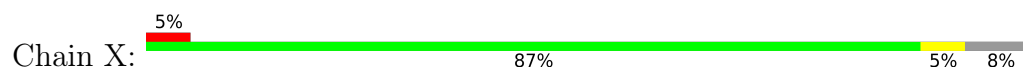
• Molecule 13: Photosystem II protein W



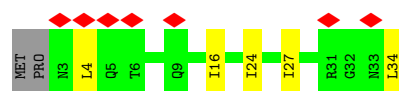
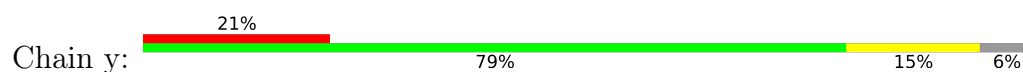
• Molecule 14: Photosystem II reaction center X protein



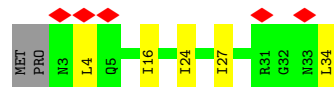
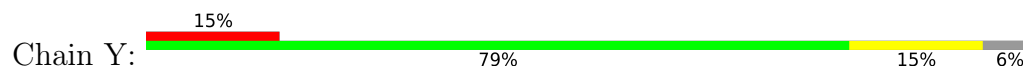
• Molecule 14: Photosystem II reaction center X protein



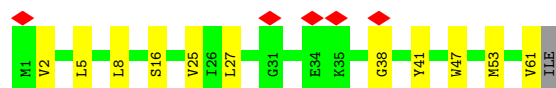
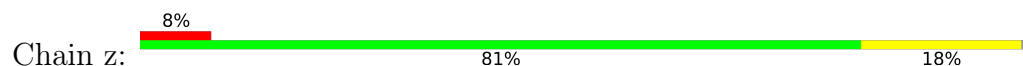
• Molecule 15: Photosystem II reaction center protein Psb30



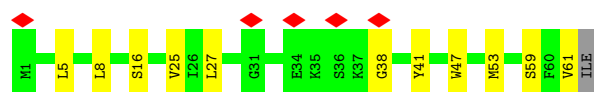
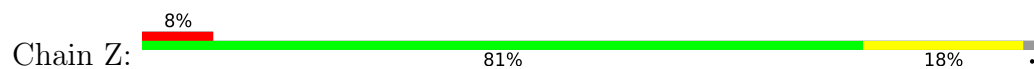
• Molecule 15: Photosystem II reaction center protein Psb30



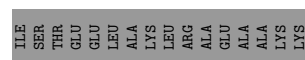
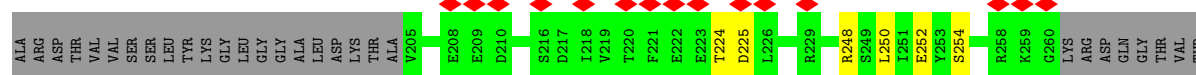
• Molecule 16: Photosystem II reaction center protein Z



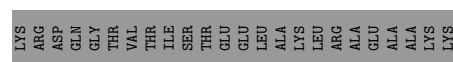
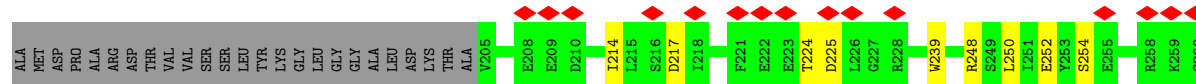
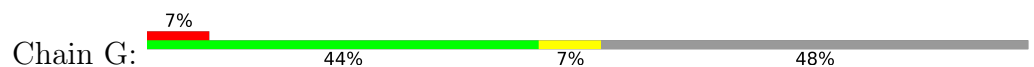
- Molecule 16: Photosystem II reaction center protein Z



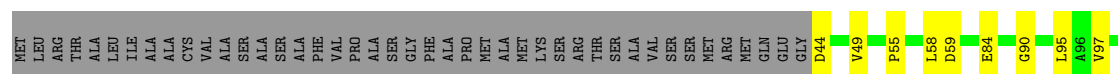
- Molecule 17: NCP



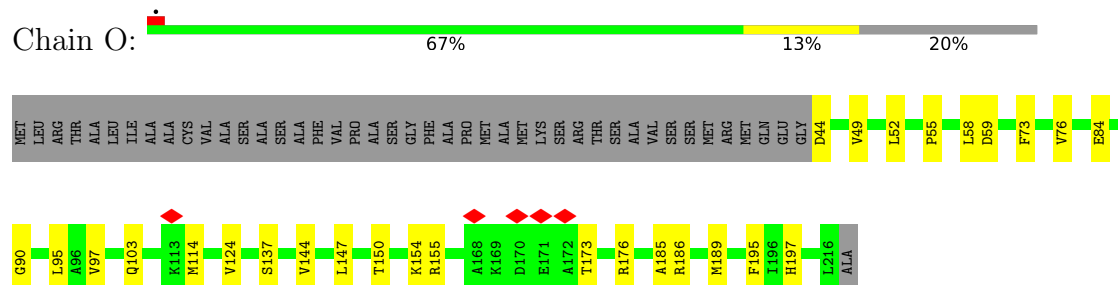
- Molecule 17: NCP



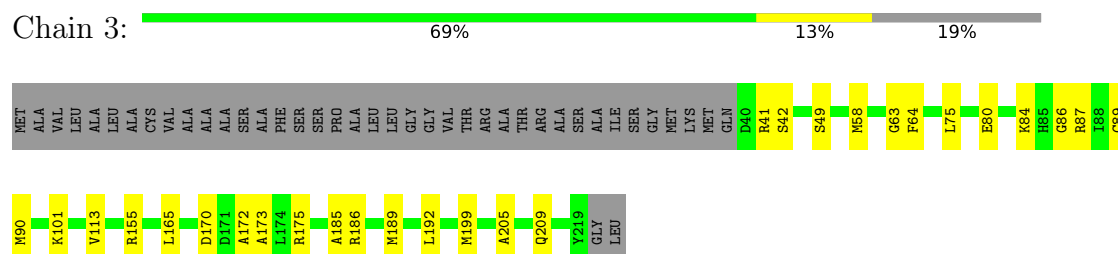
- Molecule 18: CAC2



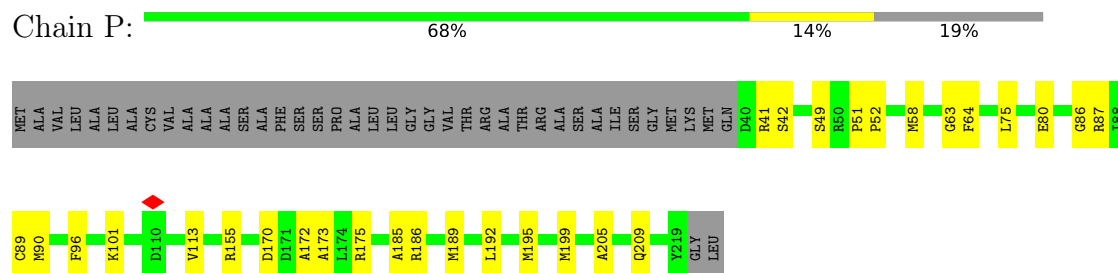
- Molecule 18: CAC2



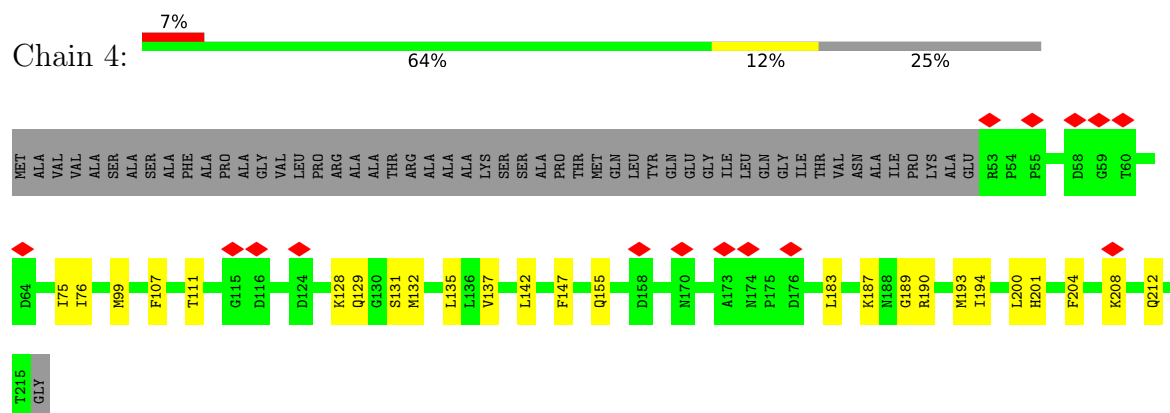
- Molecule 19: CAC3



- Molecule 19: CAC3

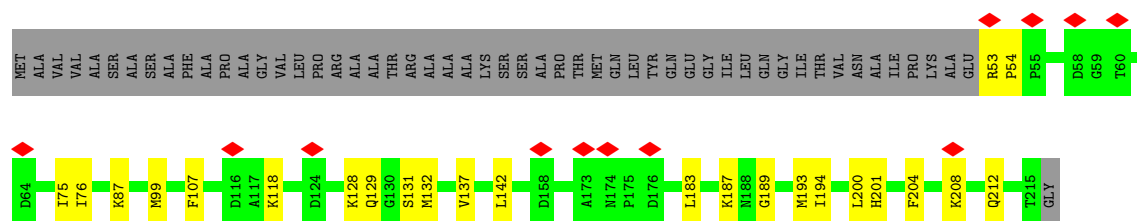


- Molecule 20: CAC4

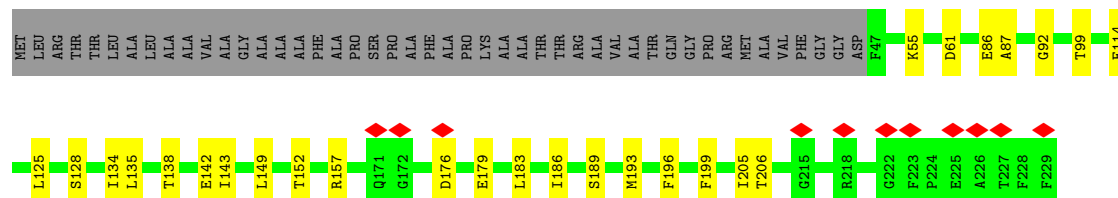


- Molecule 20: CAC4

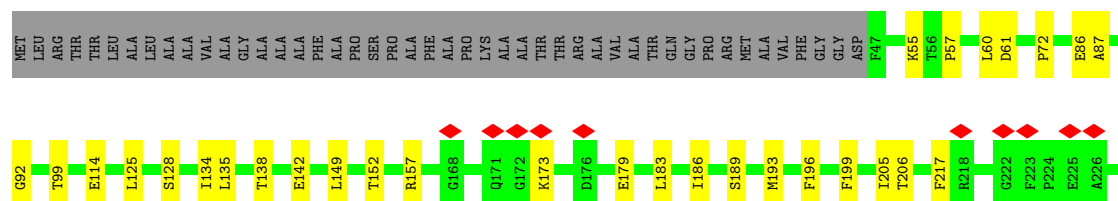




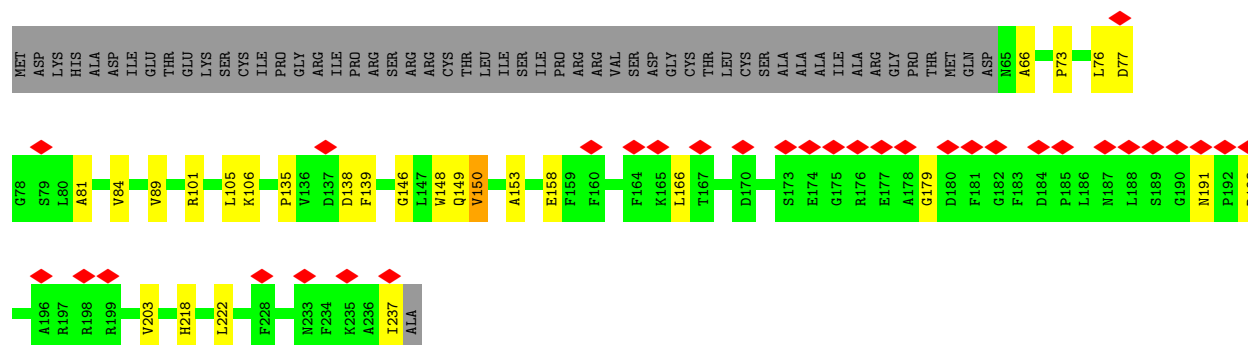
• Molecule 21: CAC5



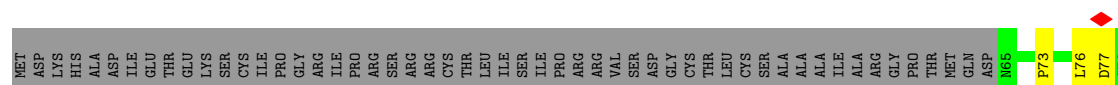
• Molecule 21: CAC5

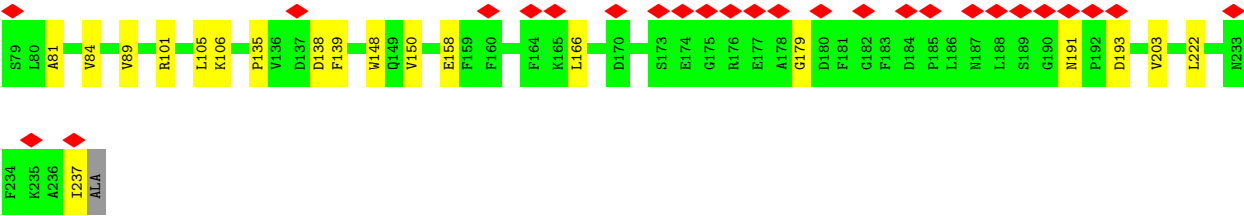


• Molecule 22: CAC6

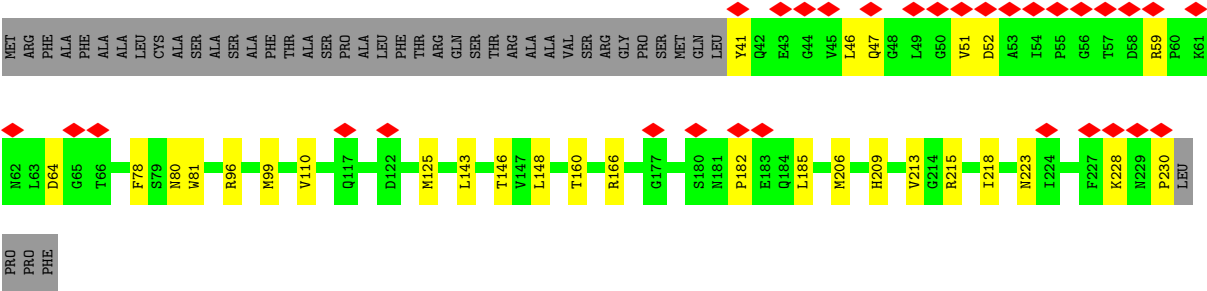


• Molecule 22: CAC6

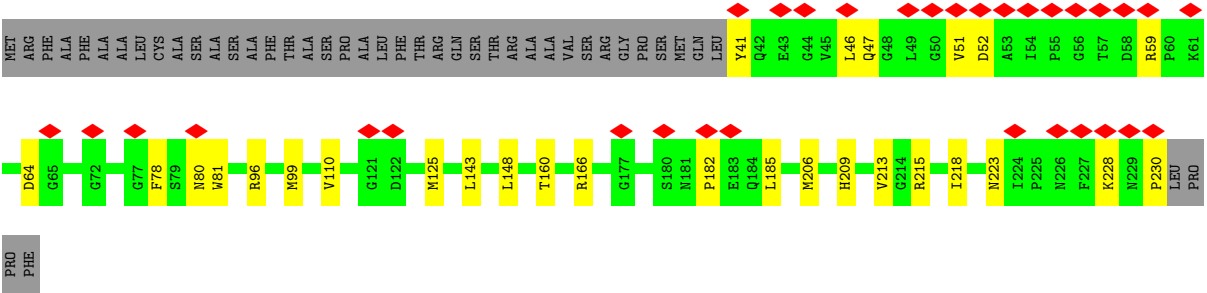




• Molecule 23: CAC1



• Molecule 23: CAC1



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	112613	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	DIRECT ELECTRON DE-16 (4k x 4k)	Depositor
Maximum map value	0.253	Depositor
Minimum map value	0.000	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.024	Depositor
Map size (Å)	432.65326, 432.65326, 432.65326	wwPDB
Map dimensions	416, 416, 416	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0400319, 1.0400319, 1.0400319	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PHO, CL, FE2, DGD, BCT, LMG, WVN, IHT, SQD, LHG, MN, PL9, CLA, II0, HEM, 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	A	0.19	0/2644	0.33	0/3607
1	a	0.13	0/2644	0.28	0/3607
2	B	0.17	0/4082	0.33	1/5557 (0.0%)
2	b	0.13	0/4082	0.30	0/5557
3	C	0.11	0/3491	0.28	0/4763
3	c	0.15	0/3491	0.32	0/4763
4	D	0.17	0/2801	0.32	0/3815
4	d	0.13	0/2801	0.31	0/3815
5	E	0.10	0/541	0.26	0/738
5	e	0.22	0/541	0.47	1/738 (0.1%)
6	F	0.54	0/270	0.85	0/366
6	f	0.49	0/270	0.62	0/366
7	H	0.19	0/519	0.42	0/707
7	h	0.25	0/519	0.58	1/707 (0.1%)
8	I	0.10	0/290	0.27	0/392
8	i	0.11	0/290	0.26	0/392
9	K	0.18	0/307	0.35	0/421
9	k	0.19	0/307	0.38	0/421
10	L	0.26	0/311	0.42	0/424
10	l	0.26	0/311	0.43	0/424
11	M	0.13	0/289	0.31	0/393
11	m	0.14	0/289	0.28	0/393
12	T	0.09	0/251	0.21	0/341
12	t	0.09	0/251	0.21	0/341
13	W	0.12	0/370	0.30	0/503
13	w	0.13	0/370	0.30	0/503
14	X	0.12	0/272	0.25	0/370
14	x	0.12	0/272	0.25	0/370
15	Y	0.08	0/242	0.23	0/329
15	y	0.09	0/242	0.24	0/329
16	Z	0.26	0/470	0.40	0/641
16	z	0.18	0/470	0.33	0/641

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	G	0.16	0/1200	0.35	0/1635
17	g	0.12	0/1200	0.31	0/1635
18	2	0.22	0/1419	0.41	0/1919
18	O	0.16	0/1419	0.35	0/1919
19	3	0.14	0/1428	0.32	0/1930
19	P	0.14	0/1428	0.32	0/1930
20	4	0.23	0/1281	0.43	1/1731 (0.1%)
20	Q	0.22	0/1281	0.41	0/1731
21	5	0.22	0/1469	0.40	0/1988
21	R	0.23	0/1469	0.44	0/1988
22	6	0.22	0/1372	0.61	5/1855 (0.3%)
22	S	0.24	0/1372	0.54	3/1855 (0.2%)
23	1	0.16	0/1490	0.38	0/2017
23	N	0.16	0/1490	0.38	0/2017
All	All	0.18	0/53618	0.36	12/72884 (0.0%)

There are no bond length outliers.

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	6	89	VAL	CB-CA-C	13.16	132.88	111.29
22	S	150	VAL	N-CA-C	-8.88	101.89	110.42
7	h	48	ILE	N-CA-C	8.25	118.34	110.42
22	6	150	VAL	N-CA-C	-8.22	102.53	110.42
22	S	148	TRP	N-CA-C	7.98	120.06	111.36

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	A	2563	0	2469	52	0
1	a	2563	0	2469	51	0
2	B	3950	0	3830	63	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	b	3950	0	3830	73	0
3	C	3379	0	3307	53	0
3	c	3379	0	3307	51	0
4	D	2708	0	2606	54	0
4	d	2708	0	2606	62	0
5	E	525	0	510	8	0
5	e	525	0	510	5	0
6	F	261	0	269	3	0
6	f	261	0	269	3	0
7	H	508	0	529	6	0
7	h	508	0	529	7	0
8	I	284	0	295	1	0
8	i	284	0	295	2	0
9	K	296	0	312	7	0
9	k	296	0	312	5	0
10	L	301	0	301	4	0
10	l	301	0	301	6	0
11	M	285	0	300	12	0
11	m	285	0	300	10	0
12	T	244	0	256	1	0
12	t	244	0	256	0	0
13	W	363	0	350	4	0
13	w	363	0	350	5	0
14	X	268	0	293	2	0
14	x	268	0	293	1	0
15	Y	241	0	275	5	0
15	y	241	0	275	5	0
16	Z	460	0	499	8	0
16	z	460	0	499	8	0
17	G	1163	0	1118	22	0
17	g	1163	0	1118	11	0
18	2	1380	0	1366	21	0
18	O	1380	0	1366	26	0
19	3	1392	0	1377	17	0
19	P	1392	0	1377	19	0
20	4	1253	0	1259	20	0
20	Q	1253	0	1259	19	0
21	5	1430	0	1418	25	0
21	R	1430	0	1418	35	0
22	6	1337	0	1307	28	0
22	S	1337	0	1307	19	0
23	1	1458	0	1468	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	N	1458	0	1468	18	0
24	A	1	0	0	0	0
24	a	1	0	0	0	0
25	1	518	0	444	7	0
25	2	633	0	611	14	0
25	3	570	0	547	10	0
25	4	482	0	445	20	0
25	5	620	0	589	19	0
25	6	525	0	507	14	0
25	A	174	0	170	14	0
25	B	1014	0	1092	42	0
25	C	827	0	894	31	0
25	D	190	0	203	9	0
25	G	110	0	105	3	0
25	N	518	0	444	8	0
25	O	633	0	611	17	0
25	P	570	0	547	11	0
25	Q	482	0	445	17	0
25	R	620	0	589	19	0
25	S	525	0	510	11	0
25	a	174	0	170	15	0
25	b	1014	0	1092	40	0
25	c	828	0	896	26	0
25	d	191	0	205	10	0
25	g	110	0	105	5	0
26	A	64	0	74	2	0
26	D	64	0	74	5	0
26	a	64	0	74	3	0
26	d	64	0	74	5	0
27	3	40	0	0	0	0
27	6	40	0	0	0	0
27	A	40	0	0	0	0
27	B	120	0	0	1	0
27	C	120	0	0	0	0
27	D	40	0	0	0	0
27	H	40	0	0	0	0
27	P	40	0	0	0	0
27	S	40	0	0	0	0
27	Y	40	0	0	0	0
27	a	40	0	0	0	0
27	b	120	0	0	1	0
27	c	120	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	d	40	0	0	0	0
27	h	40	0	0	0	0
27	y	40	0	0	0	0
28	A	94	0	122	2	0
28	a	85	0	101	2	0
29	A	33	0	42	0	0
29	D	55	0	80	3	0
29	a	33	0	42	2	0
29	d	55	0	80	4	0
30	A	4	0	0	0	0
30	a	4	0	0	0	0
31	2	46	0	65	1	0
31	3	49	0	74	2	0
31	5	46	0	65	4	0
31	6	40	0	53	2	0
31	A	42	0	57	0	0
31	B	43	0	59	3	0
31	C	40	0	50	1	0
31	D	49	0	74	4	0
31	L	49	0	74	6	0
31	O	46	0	65	1	0
31	P	49	0	74	3	0
31	R	46	0	65	4	0
31	S	40	0	53	2	0
31	Z	25	0	20	0	0
31	a	42	0	57	0	0
31	b	43	0	59	2	0
31	c	40	0	50	2	0
31	d	49	0	74	4	0
31	l	49	0	74	8	0
31	z	25	0	20	0	0
32	A	1	0	0	0	0
32	C	1	0	0	0	0
32	a	1	0	0	0	0
32	c	1	0	0	0	0
33	A	2	0	0	0	0
33	a	2	0	0	0	0
34	2	40	0	50	0	0
34	4	43	0	56	2	0
34	B	51	0	72	1	0
34	C	47	0	64	0	0
34	D	77	0	94	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	F	46	0	62	0	0
34	G	40	0	50	5	0
34	M	40	0	50	1	0
34	O	40	0	50	1	0
34	Q	43	0	56	2	0
34	W	48	0	66	2	0
34	Z	31	0	32	2	0
34	b	51	0	72	1	0
34	c	51	0	72	4	0
34	d	77	0	94	3	0
34	f	46	0	62	3	0
34	g	40	0	50	3	0
34	m	40	0	50	1	0
34	w	48	0	66	1	0
34	z	31	0	32	2	0
35	C	54	0	66	1	0
35	H	62	0	82	5	0
35	c	54	0	66	1	0
35	h	62	0	82	4	0
36	E	43	0	30	1	0
36	e	43	0	30	1	0
37	1	180	0	0	1	0
37	2	45	0	0	0	0
37	3	45	0	0	0	0
37	4	135	0	0	0	0
37	5	45	0	0	0	0
37	6	90	0	0	10	0
37	N	180	0	0	2	0
37	O	45	0	0	0	0
37	P	45	0	0	0	0
37	Q	135	0	0	0	0
37	R	45	0	0	0	0
37	S	90	0	0	0	0
38	1	168	0	0	0	0
38	2	168	0	0	1	0
38	3	168	0	0	0	0
38	4	168	0	0	1	0
38	5	168	0	0	0	0
38	6	168	0	0	2	0
38	N	168	0	0	0	0
38	O	168	0	0	1	0
38	P	168	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	Q	168	0	0	0	0
38	R	168	0	0	0	0
38	S	168	0	0	2	0
39	1	41	0	0	0	0
39	2	41	0	0	0	0
39	4	41	0	0	0	0
39	5	41	0	0	0	0
39	N	41	0	0	0	0
39	O	41	0	0	0	0
39	Q	41	0	0	0	0
39	R	41	0	0	0	0
40	C	1	0	0	0	0
40	c	1	0	0	0	0
All	All	70547	0	66150	1008	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 7.

The worst 5 of 1008 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:362:PHE:HE2	4:d:183:PHE:CZ	1.36	1.43
2:b:362:PHE:CE2	4:d:183:PHE:CZ	2.08	1.41
2:b:362:PHE:CE2	4:d:183:PHE:HZ	1.47	1.22
1:a:257:ARG:HH11	2:b:498:LEU:HD13	1.16	1.10
1:A:257:ARG:HH11	2:B:498:LEU:HD13	1.15	1.09

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	325/328 (99%)	320 (98%)	5 (2%)	0	100	100
1	a	325/328 (99%)	319 (98%)	6 (2%)	0	100	100
2	B	501/509 (98%)	495 (99%)	6 (1%)	0	100	100
2	b	501/509 (98%)	495 (99%)	6 (1%)	0	100	100
3	C	430/487 (88%)	421 (98%)	9 (2%)	0	100	100
3	c	430/487 (88%)	420 (98%)	10 (2%)	0	100	100
4	D	339/351 (97%)	329 (97%)	10 (3%)	0	100	100
4	d	339/351 (97%)	330 (97%)	9 (3%)	0	100	100
5	E	62/84 (74%)	62 (100%)	0	0	100	100
5	e	62/84 (74%)	62 (100%)	0	0	100	100
6	F	30/42 (71%)	30 (100%)	0	0	100	100
6	f	30/42 (71%)	30 (100%)	0	0	100	100
7	H	63/67 (94%)	56 (89%)	7 (11%)	0	100	100
7	h	63/67 (94%)	55 (87%)	8 (13%)	0	100	100
8	I	33/38 (87%)	32 (97%)	1 (3%)	0	100	100
8	i	33/38 (87%)	32 (97%)	1 (3%)	0	100	100
9	K	35/45 (78%)	35 (100%)	0	0	100	100
9	k	35/45 (78%)	35 (100%)	0	0	100	100
10	L	35/38 (92%)	35 (100%)	0	0	100	100
10	l	35/38 (92%)	35 (100%)	0	0	100	100
11	M	36/40 (90%)	35 (97%)	1 (3%)	0	100	100
11	m	36/40 (90%)	36 (100%)	0	0	100	100
12	T	28/32 (88%)	28 (100%)	0	0	100	100
12	t	28/32 (88%)	28 (100%)	0	0	100	100
13	W	43/74 (58%)	40 (93%)	3 (7%)	0	100	100
13	w	43/74 (58%)	40 (93%)	3 (7%)	0	100	100
14	X	34/39 (87%)	34 (100%)	0	0	100	100
14	x	34/39 (87%)	34 (100%)	0	0	100	100
15	Y	30/34 (88%)	29 (97%)	1 (3%)	0	100	100
15	y	30/34 (88%)	30 (100%)	0	0	100	100
16	Z	59/62 (95%)	59 (100%)	0	0	100	100
16	z	59/62 (95%)	59 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	G	143/284 (50%)	137 (96%)	6 (4%)	0	100	100
17	g	143/284 (50%)	137 (96%)	6 (4%)	0	100	100
18	2	171/217 (79%)	164 (96%)	7 (4%)	0	100	100
18	O	171/217 (79%)	162 (95%)	9 (5%)	0	100	100
19	3	178/221 (80%)	168 (94%)	10 (6%)	0	100	100
19	P	178/221 (80%)	168 (94%)	10 (6%)	0	100	100
20	4	161/216 (74%)	153 (95%)	8 (5%)	0	100	100
20	Q	161/216 (74%)	153 (95%)	8 (5%)	0	100	100
21	5	181/229 (79%)	172 (95%)	9 (5%)	0	100	100
21	R	181/229 (79%)	171 (94%)	10 (6%)	0	100	100
22	6	171/227 (75%)	163 (95%)	8 (5%)	0	100	100
22	S	171/227 (75%)	165 (96%)	6 (4%)	0	100	100
23	1	188/233 (81%)	174 (93%)	14 (7%)	0	100	100
23	N	188/233 (81%)	174 (93%)	14 (7%)	0	100	100
All	All	6552/7794 (84%)	6341 (97%)	211 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	265/266 (100%)	265 (100%)	0	100	100
1	a	265/266 (100%)	265 (100%)	0	100	100
2	B	400/404 (99%)	399 (100%)	1 (0%)	86	94
2	b	400/404 (99%)	399 (100%)	1 (0%)	86	94
3	C	342/389 (88%)	342 (100%)	0	100	100
3	c	342/389 (88%)	342 (100%)	0	100	100
4	D	274/281 (98%)	273 (100%)	1 (0%)	84	92

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	d	274/281 (98%)	274 (100%)	0	100	100
5	E	56/73 (77%)	56 (100%)	0	100	100
5	e	56/73 (77%)	56 (100%)	0	100	100
6	F	27/37 (73%)	27 (100%)	0	100	100
6	f	27/37 (73%)	27 (100%)	0	100	100
7	H	55/57 (96%)	55 (100%)	0	100	100
7	h	55/57 (96%)	55 (100%)	0	100	100
8	I	33/36 (92%)	33 (100%)	0	100	100
8	i	33/36 (92%)	33 (100%)	0	100	100
9	K	30/36 (83%)	30 (100%)	0	100	100
9	k	30/36 (83%)	30 (100%)	0	100	100
10	L	34/35 (97%)	34 (100%)	0	100	100
10	l	34/35 (97%)	34 (100%)	0	100	100
11	M	30/32 (94%)	30 (100%)	0	100	100
11	m	30/32 (94%)	30 (100%)	0	100	100
12	T	26/28 (93%)	26 (100%)	0	100	100
12	t	26/28 (93%)	26 (100%)	0	100	100
13	W	40/56 (71%)	40 (100%)	0	100	100
13	w	40/56 (71%)	40 (100%)	0	100	100
14	X	31/34 (91%)	31 (100%)	0	100	100
14	x	31/34 (91%)	31 (100%)	0	100	100
15	Y	27/29 (93%)	27 (100%)	0	100	100
15	y	27/29 (93%)	27 (100%)	0	100	100
16	Z	51/52 (98%)	51 (100%)	0	100	100
16	z	51/52 (98%)	51 (100%)	0	100	100
17	G	120/227 (53%)	120 (100%)	0	100	100
17	g	120/227 (53%)	120 (100%)	0	100	100
18	2	141/172 (82%)	140 (99%)	1 (1%)	76	88
18	O	141/172 (82%)	141 (100%)	0	100	100
19	3	142/168 (84%)	142 (100%)	0	100	100
19	P	142/168 (84%)	142 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	4	131/166 (79%)	131 (100%)	0	100	100
20	Q	131/166 (79%)	131 (100%)	0	100	100
21	5	151/179 (84%)	151 (100%)	0	100	100
21	R	151/179 (84%)	151 (100%)	0	100	100
22	6	138/183 (75%)	138 (100%)	0	100	100
22	S	138/183 (75%)	137 (99%)	1 (1%)	76	88
23	1	152/184 (83%)	152 (100%)	0	100	100
23	N	152/184 (83%)	152 (100%)	0	100	100
All	All	5392/6248 (86%)	5387 (100%)	5 (0%)	87	96

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

Mol	Chain	Res	Type
2	b	440	ASP
2	B	440	ASP
4	D	235	THR
18	2	49	VAL
22	S	89	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 54 such sidechains are listed below:

Mol	Chain	Res	Type
3	C	325	GLN
18	2	212	ASN
20	Q	182	GLN
4	D	238	GLN
5	E	24	HIS

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 370 ligands modelled in this entry, 10 are monoatomic - leaving 360 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
25	CLA	B	613	-	69,73,73	1.18	7 (10%)	82,113,113	1.15	4 (4%)
25	CLA	4	602	20	69,73,73	1.16	6 (8%)	82,113,113	1.16	4 (4%)
25	CLA	1	602	23	64,68,73	1.22	6 (9%)	76,107,113	1.18	6 (7%)
25	CLA	b	615	-	69,73,73	1.17	6 (8%)	82,113,113	1.21	5 (6%)
31	LHG	L	101	-	48,48,48	0.94	2 (4%)	51,54,54	1.05	3 (5%)
39	IHT	2	620	-	40,42,42	1.93	10 (25%)	52,58,58	2.65	19 (36%)
25	CLA	5	609	21	69,73,73	1.17	7 (10%)	82,113,113	1.23	6 (7%)
34	LMG	G	303	-	40,40,55	1.05	2 (5%)	48,48,63	1.02	3 (6%)
38	II0	N	618	-	39,43,43	2.58	10 (25%)	48,60,60	2.74	16 (33%)
25	CLA	B	615	-	69,73,73	1.18	6 (8%)	82,113,113	1.23	3 (3%)
25	CLA	2	606	18	55,59,73	1.32	7 (12%)	64,96,113	1.23	6 (9%)
36	HEM	E	102	5,6	50,50,50	1.60	9 (18%)	67,82,82	1.57	10 (14%)
25	CLA	b	604	-	63,67,73	1.25	6 (9%)	74,105,113	1.27	6 (8%)
25	CLA	C	517	-	69,73,73	1.17	7 (10%)	82,113,113	1.16	4 (4%)
34	LMG	W	134	-	48,48,55	0.97	2 (4%)	56,56,63	1.10	4 (7%)
34	LMG	D	402	-	40,40,55	1.05	2 (5%)	48,48,63	1.04	3 (6%)
25	CLA	G	302	17	49,53,73	1.37	6 (12%)	58,89,113	1.24	4 (6%)
30	BCT	a	412	24	3,3,3	1.09	0	2,3,3	4.23	1 (50%)
25	CLA	c	528	-	57,61,73	1.29	7 (12%)	67,98,113	1.22	5 (7%)
37	KC2	R	612	-	49,53,53	2.79	20 (40%)	60,89,89	3.73	33 (55%)
39	IHT	Q	620	-	40,42,42	1.87	10 (25%)	52,58,58	2.74	22 (42%)
25	CLA	R	615	-	50,54,73	1.37	7 (14%)	59,90,113	1.20	4 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	R	602	21	59,63,73	1.26	7 (11%)	70,101,113	1.22	6 (8%)
37	KC2	5	612	-	49,53,53	2.79	20 (40%)	60,89,89	3.72	32 (53%)
34	LMG	f	99	-	46,46,55	0.99	2 (4%)	54,54,63	1.05	3 (5%)
31	LHG	R	621	25	45,45,48	0.97	2 (4%)	48,51,54	1.11	4 (8%)
25	CLA	B	611	-	69,73,73	1.16	7 (10%)	82,113,113	1.13	7 (8%)
25	CLA	B	602	-	69,73,73	1.17	7 (10%)	82,113,113	1.20	6 (7%)
38	II0	O	619	-	39,43,43	2.61	10 (25%)	48,60,60	2.65	17 (35%)
38	II0	N	619	-	39,43,43	2.64	11 (28%)	48,60,60	2.86	15 (31%)
25	CLA	2	604	18	69,73,73	1.18	7 (10%)	82,113,113	1.14	3 (3%)
25	CLA	P	603	-	69,73,73	1.19	7 (10%)	82,113,113	1.17	7 (8%)
37	KC2	4	612	-	49,53,53	2.79	20 (40%)	60,89,89	3.79	34 (56%)
38	II0	Q	619	-	39,43,43	2.64	12 (30%)	48,60,60	2.73	17 (35%)
27	WVN	A	407	-	40,41,41	1.70	10 (25%)	51,56,56	2.44	18 (35%)
25	CLA	b	606	-	69,73,73	1.18	6 (8%)	82,113,113	1.14	7 (8%)
25	CLA	a	403	-	69,73,73	1.18	8 (11%)	82,113,113	1.10	4 (4%)
25	CLA	5	613	21	59,63,73	1.26	6 (10%)	70,101,113	1.36	5 (7%)
25	CLA	S	601	22	59,63,73	1.28	6 (10%)	70,101,113	1.17	4 (5%)
27	WVN	c	530	-	40,41,41	1.71	10 (25%)	51,56,56	1.96	15 (29%)
34	LMG	C	536	-	47,47,55	0.98	2 (4%)	55,55,63	1.19	6 (10%)
25	CLA	N	603	-	64,68,73	1.23	6 (9%)	76,107,113	1.18	6 (7%)
38	II0	R	616	-	39,43,43	2.52	10 (25%)	48,60,60	2.74	13 (27%)
25	CLA	P	604	-	67,71,73	1.18	6 (8%)	79,110,113	1.24	7 (8%)
25	CLA	O	609	18	52,56,73	1.35	6 (11%)	61,92,113	1.18	5 (8%)
39	IHT	4	620	-	40,42,42	1.73	11 (27%)	52,58,58	2.70	21 (40%)
25	CLA	c	519	-	64,68,73	1.22	6 (9%)	76,107,113	1.17	7 (9%)
25	CLA	P	610	19	69,73,73	1.18	5 (7%)	82,113,113	1.14	3 (3%)
27	WVN	P	620	-	40,41,41	1.70	10 (25%)	51,56,56	2.44	21 (41%)
25	CLA	c	522	-	69,73,73	1.17	5 (7%)	82,113,113	1.22	4 (4%)
25	CLA	1	601	23	49,53,73	1.41	7 (14%)	58,89,113	1.32	5 (8%)
27	WVN	b	619	-	40,41,41	1.74	10 (25%)	51,56,56	2.41	19 (37%)
27	WVN	b	618	-	40,41,41	1.75	10 (25%)	51,56,56	2.60	19 (37%)
25	CLA	B	608	-	69,73,73	1.17	7 (10%)	82,113,113	1.11	6 (7%)
34	LMG	b	620	-	51,51,55	0.94	2 (3%)	59,59,63	1.01	3 (5%)
25	CLA	B	612	-	69,73,73	1.16	7 (10%)	82,113,113	1.29	9 (10%)
25	CLA	R	611	31	69,73,73	1.17	6 (8%)	82,113,113	1.10	3 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
38	II0	P	619	-	39,43,43	2.56	10 (25%)	48,60,60	2.75	14 (29%)
25	CLA	6	604	-	69,73,73	1.16	6 (8%)	82,113,113	1.21	8 (9%)
38	II0	P	617	-	39,43,43	2.47	9 (23%)	48,60,60	2.75	12 (25%)
34	LMG	d	402	-	40,40,55	1.05	2 (5%)	48,48,63	1.05	3 (6%)
27	WVN	H	89	-	40,41,41	1.73	10 (25%)	51,56,56	2.67	15 (29%)
27	WVN	Y	89	-	40,41,41	1.78	10 (25%)	51,56,56	2.32	15 (29%)
25	CLA	C	526	-	69,73,73	1.19	7 (10%)	82,113,113	1.19	4 (4%)
34	LMG	M	101	-	40,40,55	1.04	2 (5%)	48,48,63	1.09	4 (8%)
25	CLA	O	615	-	49,53,73	1.38	6 (12%)	58,89,113	1.28	5 (8%)
25	CLA	C	523	-	69,73,73	1.17	7 (10%)	82,113,113	1.15	7 (8%)
37	KC2	1	605	-	49,53,53	2.79	20 (40%)	60,89,89	3.73	32 (53%)
28	SQD	A	408	-	52,54,54	1.11	3 (5%)	62,65,65	1.12	3 (4%)
27	WVN	C	531	-	40,41,41	1.75	10 (25%)	51,56,56	2.40	18 (35%)
37	KC2	1	611	-	49,53,53	2.80	20 (40%)	60,89,89	3.69	32 (53%)
38	II0	5	618	-	39,43,43	2.56	10 (25%)	48,60,60	2.76	13 (27%)
37	KC2	N	613	-	49,53,53	2.86	20 (40%)	60,89,89	3.69	33 (55%)
25	CLA	5	603	-	56,60,73	1.31	8 (14%)	65,97,113	1.37	6 (9%)
25	CLA	O	606	18	55,59,73	1.32	8 (14%)	64,96,113	1.22	6 (9%)
38	II0	4	619	-	39,43,43	2.58	10 (25%)	48,60,60	2.72	16 (33%)
25	CLA	D	404	-	64,68,73	1.22	6 (9%)	76,107,113	1.18	5 (6%)
25	CLA	G	301	-	69,73,73	1.14	6 (8%)	82,113,113	1.12	6 (7%)
25	CLA	P	611	31	56,60,73	1.30	6 (10%)	65,97,113	1.19	6 (9%)
27	WVN	B	619	-	40,41,41	1.71	10 (25%)	51,56,56	2.43	16 (31%)
37	KC2	Q	611	-	49,53,53	2.80	20 (40%)	60,89,89	3.77	32 (53%)
31	LHG	z	103	-	24,24,48	1.33	2 (8%)	27,30,54	1.16	2 (7%)
31	LHG	S	621	25	39,39,48	1.04	2 (5%)	42,45,54	1.05	2 (4%)
26	PHO	a	405	-	58,69,69	2.18	9 (15%)	55,99,99	1.47	7 (12%)
38	II0	R	618	-	39,43,43	2.55	9 (23%)	48,60,60	2.76	13 (27%)
25	CLA	O	611	-	64,68,73	1.23	5 (7%)	76,107,113	1.19	5 (6%)
25	CLA	Q	604	20	65,69,73	1.20	6 (9%)	77,108,113	1.14	6 (7%)
25	CLA	1	615	-	51,55,73	1.35	7 (13%)	60,91,113	1.26	4 (6%)
25	CLA	4	613	-	47,51,73	1.38	6 (12%)	55,86,113	1.30	7 (12%)
31	LHG	3	621	25	48,48,48	0.94	2 (4%)	51,54,54	1.08	4 (7%)
37	KC2	1	612	23	49,53,53	2.77	20 (40%)	60,89,89	3.80	33 (55%)
25	CLA	b	614	-	64,68,73	1.21	5 (7%)	76,107,113	1.10	5 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	3	603	-	69,73,73	1.19	6 (8%)	82,113,113	1.17	7 (8%)
25	CLA	R	607	-	47,51,73	1.38	6 (12%)	55,86,113	1.28	5 (9%)
25	CLA	d	403	-	69,73,73	1.20	8 (11%)	82,113,113	1.14	4 (4%)
34	LMG	O	622	-	40,40,55	1.06	2 (5%)	48,48,63	1.02	3 (6%)
35	DGD	C	532	-	55,55,67	0.93	2 (3%)	69,69,81	0.98	3 (4%)
35	DGD	h	90	-	63,63,67	0.88	2 (3%)	77,77,81	0.87	3 (3%)
25	CLA	1	606	23	54,58,73	1.32	6 (11%)	64,95,113	1.21	6 (9%)
25	CLA	S	602	22	69,73,73	1.16	5 (7%)	82,113,113	1.16	6 (7%)
38	II0	3	618	-	39,43,43	2.55	10 (25%)	48,60,60	2.75	14 (29%)
34	LMG	B	620	-	51,51,55	0.94	2 (3%)	59,59,63	1.03	3 (5%)
25	CLA	S	604	-	69,73,73	1.16	6 (8%)	82,113,113	1.21	8 (9%)
25	CLA	1	607	-	47,51,73	1.42	6 (12%)	55,86,113	1.17	5 (9%)
25	CLA	c	517	-	69,73,73	1.17	7 (10%)	82,113,113	1.16	4 (4%)
25	CLA	g	301	-	69,73,73	1.18	7 (10%)	82,113,113	1.15	6 (7%)
25	CLA	Q	606	20	59,63,73	1.28	7 (11%)	70,101,113	1.16	5 (7%)
25	CLA	3	610	19	69,73,73	1.18	5 (7%)	82,113,113	1.13	3 (3%)
37	KC2	6	606	-	49,53,53	2.82	21 (42%)	60,89,89	3.64	34 (56%)
27	WVN	3	620	-	40,41,41	1.70	10 (25%)	51,56,56	2.45	21 (41%)
37	KC2	N	612	23	49,53,53	2.77	20 (40%)	60,89,89	3.80	33 (55%)
25	CLA	C	516	-	69,73,73	1.18	6 (8%)	82,113,113	1.12	6 (7%)
25	CLA	C	522	-	69,73,73	1.17	5 (7%)	82,113,113	1.22	4 (4%)
25	CLA	4	609	-	60,64,73	1.26	7 (11%)	71,102,113	1.32	4 (5%)
25	CLA	S	603	-	59,63,73	1.26	7 (11%)	70,101,113	1.33	5 (7%)
25	CLA	B	614	-	64,68,73	1.22	6 (9%)	76,107,113	1.10	6 (7%)
25	CLA	B	601	-	54,58,73	1.33	6 (11%)	64,95,113	1.31	5 (7%)
25	CLA	c	516	-	69,73,73	1.18	6 (8%)	82,113,113	1.14	6 (7%)
25	CLA	5	602	21	59,63,73	1.26	6 (10%)	70,101,113	1.21	6 (8%)
38	II0	3	617	-	39,43,43	2.59	11 (28%)	48,60,60	2.75	13 (27%)
25	CLA	O	604	18	69,73,73	1.18	7 (10%)	82,113,113	1.14	3 (3%)
38	II0	5	617	-	39,43,43	2.52	11 (28%)	48,60,60	2.71	13 (27%)
29	PL9	d	405	-	55,55,55	1.03	4 (7%)	68,69,69	1.49	10 (14%)
25	CLA	1	609	23	50,54,73	1.35	6 (12%)	59,90,113	1.27	4 (6%)
25	CLA	5	604	21	64,68,73	1.21	6 (9%)	76,107,113	1.14	5 (6%)
34	LMG	2	622	-	40,40,55	1.06	2 (5%)	48,48,63	1.02	3 (6%)
37	KC2	S	606	22	49,53,53	2.83	21 (42%)	60,89,89	3.68	33 (55%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	b	605	-	69,73,73	1.19	6 (8%)	82,113,113	1.15	5 (6%)
34	LMG	c	536	-	51,51,55	0.92	2 (3%)	59,59,63	0.99	3 (5%)
25	CLA	c	520	-	69,73,73	1.16	7 (10%)	82,113,113	1.15	5 (6%)
25	CLA	Q	610	20	55,59,73	1.31	6 (10%)	64,96,113	1.27	7 (10%)
25	CLA	B	607	-	69,73,73	1.17	6 (8%)	82,113,113	1.11	7 (8%)
25	CLA	3	609	19	69,73,73	1.17	6 (8%)	82,113,113	1.16	7 (8%)
25	CLA	N	604	23	63,67,73	1.23	6 (9%)	74,105,113	1.16	3 (4%)
25	CLA	b	616	-	69,73,73	1.18	7 (10%)	82,113,113	1.15	4 (4%)
27	WVN	C	529	-	40,41,41	1.80	10 (25%)	51,56,56	2.38	18 (35%)
25	CLA	Q	607	-	47,51,73	1.42	6 (12%)	55,86,113	1.19	5 (9%)
31	LHG	O	621	-	45,45,48	0.98	2 (4%)	48,51,54	1.00	3 (6%)
38	II0	P	618	-	39,43,43	2.51	10 (25%)	48,60,60	2.79	16 (33%)
25	CLA	c	521	-	69,73,73	1.17	7 (10%)	82,113,113	1.17	7 (8%)
38	II0	P	616	-	39,43,43	2.54	11 (28%)	48,60,60	2.76	12 (25%)
25	CLA	C	527	-	69,73,73	1.18	7 (10%)	82,113,113	1.18	6 (7%)
28	SQD	a	411	-	38,40,54	1.29	3 (7%)	48,51,65	1.09	4 (8%)
27	WVN	D	408	-	40,41,41	1.76	10 (25%)	51,56,56	2.23	18 (35%)
25	CLA	b	610	-	69,73,73	1.19	6 (8%)	82,113,113	1.11	4 (4%)
25	CLA	2	603	-	69,73,73	1.19	7 (10%)	82,113,113	1.13	5 (6%)
25	CLA	4	606	20	59,63,73	1.26	8 (13%)	70,101,113	1.24	7 (10%)
25	CLA	b	608	-	69,73,73	1.18	7 (10%)	82,113,113	1.11	6 (7%)
34	LMG	m	101	-	40,40,55	1.04	2 (5%)	48,48,63	1.10	4 (8%)
29	PL9	a	409	-	33,33,55	1.16	4 (12%)	41,42,69	1.59	9 (21%)
39	IHT	R	620	-	40,42,42	1.76	11 (27%)	52,58,58	2.91	24 (46%)
25	CLA	C	518	-	69,73,73	1.18	6 (8%)	82,113,113	1.09	3 (3%)
25	CLA	S	610	22	61,65,73	1.24	5 (8%)	72,103,113	1.23	6 (8%)
38	II0	R	619	-	39,43,43	2.55	10 (25%)	48,60,60	2.68	12 (25%)
27	WVN	S	620	-	40,41,41	1.78	10 (25%)	51,56,56	1.97	13 (25%)
38	II0	Q	616	-	39,43,43	2.55	10 (25%)	48,60,60	2.70	14 (29%)
27	WVN	y	89	-	40,41,41	1.72	10 (25%)	51,56,56	2.62	17 (33%)
25	CLA	c	525	-	69,73,73	1.17	6 (8%)	82,113,113	1.20	6 (7%)
27	WVN	C	530	-	40,41,41	1.70	10 (25%)	51,56,56	2.05	16 (31%)
38	II0	N	617	-	39,43,43	2.53	10 (25%)	48,60,60	2.72	14 (29%)
25	CLA	R	606	21	69,73,73	1.19	6 (8%)	82,113,113	1.13	4 (4%)
25	CLA	3	601	19	49,53,73	1.40	6 (12%)	58,89,113	1.21	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	2	610	18	69,73,73	1.18	5 (7%)	82,113,113	1.15	4 (4%)
25	CLA	5	606	21	69,73,73	1.19	7 (10%)	82,113,113	1.12	4 (4%)
25	CLA	N	601	23	49,53,73	1.41	7 (14%)	58,89,113	1.32	5 (8%)
25	CLA	1	604	23	63,67,73	1.23	6 (9%)	74,105,113	1.16	3 (4%)
39	IHT	N	620	-	40,42,42	1.87	9 (22%)	52,58,58	2.80	21 (40%)
25	CLA	R	604	21	64,68,73	1.22	6 (9%)	76,107,113	1.14	6 (7%)
34	LMG	D	407	-	37,37,55	1.09	2 (5%)	45,45,63	1.04	3 (6%)
25	CLA	3	613	19	59,63,73	1.26	6 (10%)	70,101,113	1.25	7 (10%)
31	LHG	B	622	-	42,42,48	1.00	2 (4%)	45,48,54	1.08	3 (6%)
25	CLA	3	615	-	49,53,73	1.37	6 (12%)	58,89,113	1.32	6 (10%)
25	CLA	S	611	31	59,63,73	1.26	6 (10%)	70,101,113	1.16	5 (7%)
31	LHG	5	621	25	45,45,48	0.97	2 (4%)	48,51,54	1.11	4 (8%)
38	II0	4	616	-	39,43,43	2.55	10 (25%)	48,60,60	2.70	14 (29%)
38	II0	Q	617	-	39,43,43	2.56	11 (28%)	48,60,60	2.75	14 (29%)
31	LHG	b	622	-	42,42,48	1.00	2 (4%)	45,48,54	1.10	3 (6%)
27	WVN	B	617	-	40,41,41	1.69	9 (22%)	51,56,56	2.63	18 (35%)
25	CLA	3	602	19	66,70,73	1.18	6 (9%)	78,109,113	1.21	6 (7%)
25	CLA	B	604	-	63,67,73	1.24	6 (9%)	74,105,113	1.27	6 (8%)
26	PHO	D	401	-	58,69,69	2.17	9 (15%)	55,99,99	1.48	6 (10%)
39	IHT	5	620	-	40,42,42	1.80	10 (25%)	52,58,58	2.79	19 (36%)
25	CLA	B	606	-	69,73,73	1.18	7 (10%)	82,113,113	1.15	7 (8%)
25	CLA	c	518	-	69,73,73	1.18	6 (8%)	82,113,113	1.09	3 (3%)
31	LHG	P	621	25	48,48,48	0.94	2 (4%)	51,54,54	1.08	4 (7%)
25	CLA	B	605	-	69,73,73	1.18	6 (8%)	82,113,113	1.15	5 (6%)
38	II0	5	616	-	39,43,43	2.52	10 (25%)	48,60,60	2.74	13 (27%)
25	CLA	P	612	-	57,61,73	1.30	7 (12%)	67,98,113	1.28	8 (11%)
25	CLA	2	609	18	52,56,73	1.35	7 (13%)	61,92,113	1.17	5 (8%)
25	CLA	4	607	-	47,51,73	1.42	6 (12%)	55,86,113	1.19	5 (9%)
31	LHG	D	406	-	48,48,48	0.93	2 (4%)	51,54,54	1.08	3 (5%)
39	IHT	O	620	-	40,42,42	1.89	10 (25%)	52,58,58	2.64	18 (34%)
25	CLA	N	615	-	51,55,73	1.35	5 (9%)	60,91,113	1.27	4 (6%)
25	CLA	2	613	18	64,68,73	1.22	6 (9%)	76,107,113	1.19	6 (7%)
25	CLA	5	607	-	47,51,73	1.39	6 (12%)	55,86,113	1.29	5 (9%)
25	CLA	D	403	-	69,73,73	1.19	7 (10%)	82,113,113	1.14	4 (4%)
25	CLA	6	603	-	59,63,73	1.28	6 (10%)	70,101,113	1.21	6 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	c	526	-	69,73,73	1.18	6 (8%)	82,113,113	1.19	4 (4%)
34	LMG	w	134	-	48,48,55	0.97	2 (4%)	56,56,63	1.13	5 (8%)
38	II0	4	618	-	39,43,43	2.59	10 (25%)	48,60,60	2.75	16 (33%)
25	CLA	b	601	-	54,58,73	1.33	7 (12%)	64,95,113	1.29	5 (7%)
25	CLA	D	400	-	69,73,73	1.17	6 (8%)	82,113,113	1.13	5 (6%)
25	CLA	N	614	-	52,56,73	1.34	4 (7%)	61,92,113	1.33	4 (6%)
25	CLA	c	523	-	69,73,73	1.17	7 (10%)	82,113,113	1.14	7 (8%)
25	CLA	A	404	-	53,57,73	1.34	6 (11%)	61,93,113	1.21	5 (8%)
25	CLA	6	610	22	61,65,73	1.24	5 (8%)	72,103,113	1.23	7 (9%)
25	CLA	6	601	22	59,63,73	1.28	7 (11%)	70,101,113	1.17	4 (5%)
27	WVN	6	620	-	40,41,41	1.80	10 (25%)	51,56,56	1.96	14 (27%)
30	BCT	A	412	24	3,3,3	1.09	0	2,3,3	4.22	1 (50%)
25	CLA	P	613	19	59,63,73	1.26	6 (10%)	70,101,113	1.24	7 (10%)
38	II0	S	618	-	39,43,43	2.67	9 (23%)	48,60,60	2.87	18 (37%)
34	LMG	z	102	-	31,31,55	1.20	2 (6%)	39,39,63	1.10	3 (7%)
25	CLA	b	607	-	69,73,73	1.17	6 (8%)	82,113,113	1.12	6 (7%)
35	DGD	H	90	-	63,63,67	0.88	2 (3%)	77,77,81	0.87	3 (3%)
25	CLA	d	404	-	65,69,73	1.20	6 (9%)	77,108,113	1.17	5 (6%)
37	KC2	S	612	22	49,53,53	2.77	20 (40%)	60,89,89	3.83	32 (53%)
38	II0	2	618	-	39,43,43	2.52	10 (25%)	48,60,60	2.69	15 (31%)
37	KC2	2	612	-	49,53,53	2.78	20 (40%)	60,89,89	3.75	33 (55%)
25	CLA	2	615	-	49,53,73	1.37	6 (12%)	58,89,113	1.28	5 (8%)
26	PHO	A	405	-	58,69,69	2.17	10 (17%)	55,99,99	1.46	7 (12%)
25	CLA	N	609	23	50,54,73	1.34	7 (14%)	59,90,113	1.31	5 (8%)
25	CLA	C	520	-	69,73,73	1.17	7 (10%)	82,113,113	1.17	6 (7%)
25	CLA	2	602	18	69,73,73	1.17	5 (7%)	82,113,113	1.18	6 (7%)
31	LHG	Z	103	-	24,24,48	1.34	2 (8%)	27,30,54	1.16	2 (7%)
25	CLA	Q	609	20	60,64,73	1.24	7 (11%)	71,102,113	1.27	5 (7%)
31	LHG	2	621	-	45,45,48	0.98	2 (4%)	48,51,54	1.01	3 (6%)
25	CLA	c	524	-	69,73,73	1.18	6 (8%)	82,113,113	1.20	6 (7%)
25	CLA	R	613	21	59,63,73	1.27	6 (10%)	70,101,113	1.37	5 (7%)
38	II0	5	619	-	39,43,43	2.56	10 (25%)	48,60,60	2.68	12 (25%)
38	II0	3	619	-	39,43,43	2.57	10 (25%)	48,60,60	2.75	14 (29%)
25	CLA	3	611	31	56,60,73	1.29	7 (12%)	65,97,113	1.18	6 (9%)
25	CLA	6	613	-	57,61,73	1.27	5 (8%)	67,98,113	1.24	8 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	WVN	h	89	-	40,41,41	1.73	10 (25%)	51,56,56	2.59	14 (27%)
29	PL9	A	409	-	33,33,55	1.17	4 (12%)	41,42,69	1.60	9 (21%)
37	KC2	Q	612	-	49,53,53	2.79	20 (40%)	60,89,89	3.79	34 (56%)
25	CLA	6	602	22	69,73,73	1.17	6 (8%)	82,113,113	1.15	6 (7%)
37	KC2	Q	605	-	49,53,53	2.80	20 (40%)	60,89,89	3.69	32 (53%)
37	KC2	3	606	19	49,53,53	2.80	20 (40%)	60,89,89	3.72	32 (53%)
25	CLA	P	602	19	66,70,73	1.19	6 (9%)	78,109,113	1.21	6 (7%)
38	II0	N	616	-	39,43,43	2.55	10 (25%)	48,60,60	2.77	13 (27%)
38	II0	4	617	-	39,43,43	2.55	11 (28%)	48,60,60	2.75	14 (29%)
34	LMG	d	407	-	37,37,55	1.09	2 (5%)	45,45,63	1.04	3 (6%)
31	LHG	d	406	-	48,48,48	0.93	2 (4%)	51,54,54	1.08	3 (5%)
25	CLA	P	601	19	49,53,73	1.40	6 (12%)	58,89,113	1.22	3 (5%)
25	CLA	c	527	-	69,73,73	1.18	6 (8%)	82,113,113	1.17	5 (6%)
25	CLA	1	603	-	64,68,73	1.23	5 (7%)	76,107,113	1.18	6 (7%)
25	CLA	5	611	31	69,73,73	1.17	6 (8%)	82,113,113	1.09	3 (3%)
25	CLA	O	607	-	64,68,73	1.24	6 (9%)	76,107,113	1.05	5 (6%)
38	II0	S	617	-	39,43,43	2.51	11 (28%)	48,60,60	2.75	12 (25%)
38	II0	S	616	-	39,43,43	2.52	10 (25%)	48,60,60	2.78	10 (20%)
25	CLA	3	612	-	57,61,73	1.31	8 (14%)	67,98,113	1.28	8 (11%)
38	II0	1	616	-	39,43,43	2.55	10 (25%)	48,60,60	2.78	13 (27%)
37	KC2	4	605	-	49,53,53	2.80	20 (40%)	60,89,89	3.69	32 (53%)
25	CLA	C	524	-	69,73,73	1.18	6 (8%)	82,113,113	1.20	6 (7%)
39	IHT	1	620	-	40,42,42	1.81	10 (25%)	52,58,58	2.82	20 (38%)
25	CLA	N	610	23	64,68,73	1.23	6 (9%)	76,107,113	1.17	4 (5%)
25	CLA	N	606	23	54,58,73	1.32	6 (11%)	64,95,113	1.21	6 (9%)
38	II0	2	617	-	39,43,43	2.53	10 (25%)	48,60,60	2.72	13 (27%)
37	KC2	6	612	22	49,53,53	2.76	20 (40%)	60,89,89	3.83	32 (53%)
25	CLA	O	603	-	69,73,73	1.20	8 (11%)	82,113,113	1.13	6 (7%)
25	CLA	P	609	19	69,73,73	1.18	5 (7%)	82,113,113	1.17	7 (8%)
38	II0	O	616	-	39,43,43	2.54	10 (25%)	48,60,60	2.74	12 (25%)
25	CLA	C	528	-	56,60,73	1.29	7 (12%)	65,97,113	1.21	6 (9%)
27	WVN	c	529	-	40,41,41	1.76	10 (25%)	51,56,56	2.29	16 (31%)
34	LMG	g	303	-	40,40,55	1.05	2 (5%)	48,48,63	1.02	3 (6%)
37	KC2	O	612	-	49,53,53	2.77	20 (40%)	60,89,89	3.75	33 (55%)
38	II0	S	619	-	39,43,43	2.55	10 (25%)	48,60,60	2.71	12 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	4	604	20	65,69,73	1.20	6 (9%)	77,108,113	1.14	5 (6%)
37	KC2	P	606	19	49,53,53	2.80	20 (40%)	60,89,89	3.72	32 (53%)
38	II0	1	618	-	39,43,43	2.58	10 (25%)	48,60,60	2.73	16 (33%)
25	CLA	4	615	-	47,51,73	1.39	6 (12%)	55,86,113	1.23	4 (7%)
25	CLA	4	610	20	55,59,73	1.31	6 (10%)	64,96,113	1.26	6 (9%)
31	LHG	a	413	-	41,41,48	1.01	2 (4%)	44,47,54	0.99	2 (4%)
38	II0	2	619	-	39,43,43	2.61	10 (25%)	48,60,60	2.65	17 (35%)
38	II0	6	618	-	39,43,43	2.67	9 (23%)	48,60,60	2.86	18 (37%)
25	CLA	2	611	-	64,68,73	1.23	6 (9%)	76,107,113	1.19	4 (5%)
28	SQD	A	411	-	38,40,54	1.29	3 (7%)	48,51,65	1.09	4 (8%)
26	PHO	d	401	-	58,69,69	2.17	9 (15%)	55,99,99	1.48	6 (10%)
38	II0	Q	618	-	39,43,43	2.55	10 (25%)	48,60,60	2.75	15 (31%)
27	WVN	B	618	-	40,41,41	1.75	10 (25%)	51,56,56	2.49	14 (27%)
25	CLA	C	525	-	69,73,73	1.17	6 (8%)	82,113,113	1.20	6 (7%)
31	LHG	6	621	25	39,39,48	1.04	2 (5%)	42,45,54	1.05	2 (4%)
25	CLA	1	610	23	64,68,73	1.22	6 (9%)	76,107,113	1.18	4 (5%)
28	SQD	a	408	-	43,45,54	1.22	3 (6%)	53,56,65	1.18	3 (5%)
25	CLA	B	609	-	69,73,73	1.18	7 (10%)	82,113,113	1.14	5 (6%)
38	II0	O	618	-	39,43,43	2.61	11 (28%)	48,60,60	2.70	14 (29%)
25	CLA	5	615	-	50,54,73	1.36	7 (14%)	59,90,113	1.21	4 (6%)
25	CLA	2	601	18	53,57,73	1.33	5 (9%)	61,93,113	1.33	5 (8%)
25	CLA	Q	603	-	69,73,73	1.21	6 (8%)	82,113,113	1.19	8 (9%)
25	CLA	b	612	-	69,73,73	1.17	7 (10%)	82,113,113	1.29	9 (10%)
25	CLA	A	406	-	64,68,73	1.21	6 (9%)	76,107,113	1.15	4 (5%)
25	CLA	O	610	18	69,73,73	1.18	5 (7%)	82,113,113	1.15	4 (4%)
25	CLA	5	610	21	63,67,73	1.24	6 (9%)	74,105,113	1.17	4 (5%)
34	LMG	Q	621	-	43,43,55	1.05	2 (4%)	51,51,63	0.89	2 (3%)
38	II0	R	617	-	39,43,43	2.53	11 (28%)	48,60,60	2.72	13 (27%)
25	CLA	2	607	-	64,68,73	1.24	6 (9%)	76,107,113	1.05	5 (6%)
25	CLA	P	615	-	49,53,73	1.36	6 (12%)	58,89,113	1.32	6 (10%)
25	CLA	R	603	-	56,60,73	1.31	8 (14%)	65,97,113	1.37	6 (9%)
38	II0	6	617	-	39,43,43	2.53	10 (25%)	48,60,60	2.75	12 (25%)
25	CLA	C	521	-	69,73,73	1.17	6 (8%)	82,113,113	1.16	7 (8%)
25	CLA	O	602	18	69,73,73	1.18	6 (8%)	82,113,113	1.19	6 (7%)
38	II0	O	617	-	39,43,43	2.48	8 (20%)	48,60,60	2.71	14 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	R	601	21	59,63,73	1.28	6 (10%)	70,101,113	1.21	5 (7%)
25	CLA	C	519	-	64,68,73	1.21	6 (9%)	76,107,113	1.16	7 (9%)
25	CLA	b	603	-	69,73,73	1.18	7 (10%)	82,113,113	1.08	4 (4%)
38	II0	1	617	-	39,43,43	2.52	10 (25%)	48,60,60	2.72	14 (29%)
37	KC2	N	611	-	49,53,53	2.80	20 (40%)	60,89,89	3.69	32 (53%)
27	WVN	a	407	-	40,41,41	1.82	10 (25%)	51,56,56	2.33	20 (39%)
25	CLA	B	603	-	69,73,73	1.17	7 (10%)	82,113,113	1.09	4 (4%)
25	CLA	a	404	-	53,57,73	1.34	6 (11%)	61,93,113	1.22	5 (8%)
25	CLA	b	611	-	69,73,73	1.16	7 (10%)	82,113,113	1.13	7 (8%)
25	CLA	S	609	22	59,63,73	1.26	6 (10%)	70,101,113	1.32	6 (8%)
25	CLA	a	406	-	64,68,73	1.21	6 (9%)	76,107,113	1.15	5 (6%)
25	CLA	Q	613	-	47,51,73	1.38	7 (14%)	55,86,113	1.29	7 (12%)
38	II0	1	619	-	39,43,43	2.58	10 (25%)	48,60,60	2.86	15 (31%)
38	II0	6	619	-	39,43,43	2.52	11 (28%)	48,60,60	2.71	12 (25%)
25	CLA	6	611	31	59,63,73	1.26	7 (11%)	70,101,113	1.16	5 (7%)
25	CLA	d	400	-	69,73,73	1.17	6 (8%)	82,113,113	1.14	5 (6%)
25	CLA	B	616	-	69,73,73	1.18	7 (10%)	82,113,113	1.15	4 (4%)
37	KC2	1	613	-	49,53,53	2.86	20 (40%)	60,89,89	3.70	32 (53%)
31	LHG	l	101	-	48,48,48	0.94	2 (4%)	51,54,54	1.05	3 (5%)
25	CLA	6	615	-	69,73,73	1.16	6 (8%)	82,113,113	1.18	4 (4%)
25	CLA	b	613	-	69,73,73	1.18	6 (8%)	82,113,113	1.14	4 (4%)
29	PL9	D	405	-	55,55,55	1.03	4 (7%)	68,69,69	1.48	10 (14%)
25	CLA	4	603	-	69,73,73	1.21	7 (10%)	82,113,113	1.18	8 (9%)
25	CLA	Q	602	20	69,73,73	1.17	6 (8%)	82,113,113	1.15	5 (6%)
37	KC2	4	611	-	49,53,53	2.80	20 (40%)	60,89,89	3.77	32 (53%)
31	LHG	C	535	-	39,39,48	1.03	2 (5%)	42,45,54	1.12	3 (7%)
25	CLA	S	613	-	57,61,73	1.27	5 (8%)	67,98,113	1.24	8 (11%)
27	WVN	b	617	-	40,41,41	1.69	11 (27%)	51,56,56	2.65	17 (33%)
25	CLA	R	610	21	63,67,73	1.24	5 (7%)	74,105,113	1.18	4 (5%)
25	CLA	O	601	18	53,57,73	1.33	5 (9%)	61,93,113	1.33	5 (8%)
25	CLA	A	403	-	69,73,73	1.18	8 (11%)	82,113,113	1.10	4 (4%)
25	CLA	B	610	-	69,73,73	1.18	5 (7%)	82,113,113	1.11	4 (4%)
25	CLA	5	601	21	59,63,73	1.27	6 (10%)	70,101,113	1.20	5 (7%)
31	LHG	c	535	-	39,39,48	1.04	2 (5%)	42,45,54	1.14	3 (7%)
34	LMG	Z	102	-	31,31,55	1.20	2 (6%)	39,39,63	1.09	3 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
35	DGD	c	532	-	55,55,67	0.94	2 (3%)	69,69,81	0.98	4 (5%)
25	CLA	3	604	-	67,71,73	1.18	6 (8%)	79,110,113	1.24	6 (7%)
25	CLA	b	602	-	69,73,73	1.17	5 (7%)	82,113,113	1.20	6 (7%)
25	CLA	N	602	23	64,68,73	1.21	6 (9%)	76,107,113	1.19	6 (7%)
38	II0	3	616	-	39,43,43	2.54	10 (25%)	48,60,60	2.76	12 (25%)
25	CLA	O	613	18	64,68,73	1.22	6 (9%)	76,107,113	1.20	6 (7%)
25	CLA	S	615	-	69,73,73	1.16	6 (8%)	82,113,113	1.18	4 (4%)
36	HEM	e	102	5,6	50,50,50	1.59	9 (18%)	67,82,82	1.58	10 (14%)
25	CLA	1	614	-	52,56,73	1.34	5 (9%)	61,92,113	1.32	4 (6%)
38	II0	6	616	-	39,43,43	2.52	10 (25%)	48,60,60	2.78	10 (20%)
27	WVN	d	408	-	40,41,41	1.75	10 (25%)	51,56,56	2.31	19 (37%)
31	LHG	A	413	-	41,41,48	1.02	2 (4%)	44,47,54	0.99	2 (4%)
25	CLA	Q	615	-	47,51,73	1.40	6 (12%)	55,86,113	1.23	4 (7%)
25	CLA	b	609	-	69,73,73	1.18	6 (8%)	82,113,113	1.13	5 (6%)
25	CLA	g	302	17	49,53,73	1.38	7 (14%)	58,89,113	1.50	7 (12%)
25	CLA	R	609	21	69,73,73	1.17	8 (11%)	82,113,113	1.23	6 (7%)
34	LMG	F	99	-	46,46,55	0.99	2 (4%)	54,54,63	1.04	3 (5%)
37	KC2	N	605	-	49,53,53	2.79	20 (40%)	60,89,89	3.73	32 (53%)
25	CLA	N	607	-	47,51,73	1.42	6 (12%)	55,86,113	1.18	5 (9%)
27	WVN	c	531	-	40,41,41	1.72	10 (25%)	51,56,56	2.42	16 (31%)
34	LMG	4	621	-	43,43,55	1.05	2 (4%)	51,51,63	0.90	2 (3%)
25	CLA	6	609	22	59,63,73	1.25	6 (10%)	70,101,113	1.26	6 (8%)
38	II0	2	616	-	39,43,43	2.54	10 (25%)	48,60,60	2.75	12 (25%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	B	613	-	1/1/15/20	14/39/115/115	-
25	CLA	4	602	20	1/1/15/20	6/39/115/115	-
25	CLA	1	602	23	1/1/14/20	5/33/109/115	-
25	CLA	b	615	-	1/1/15/20	9/39/115/115	-
31	LHG	L	101	-	-	5/53/53/53	-
39	IHT	2	620	-	-	5/25/65/65	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	5	609	21	1/1/15/20	9/39/115/115	-
34	LMG	G	303	-	-	8/35/55/70	0/1/1/1
38	II0	N	618	-	-	3/21/67/67	0/2/2/2
25	CLA	B	615	-	1/1/15/20	9/39/115/115	-
25	CLA	2	606	18	1/1/12/20	7/23/99/115	-
36	HEM	E	102	5,6	-	8/14/54/54	-
25	CLA	b	604	-	1/1/13/20	9/32/108/115	-
25	CLA	C	517	-	1/1/15/20	13/39/115/115	-
34	LMG	W	134	-	-	9/43/63/70	0/1/1/1
34	LMG	D	402	-	-	9/35/55/70	0/1/1/1
25	CLA	G	302	17	1/1/11/20	6/15/91/115	-
25	CLA	c	528	-	1/1/12/20	9/25/101/115	-
37	KC2	R	612	-	-	8/15/71/71	-
39	IHT	Q	620	-	-	8/25/65/65	0/2/2/2
25	CLA	R	615	-	1/1/11/20	7/17/93/115	-
25	CLA	R	602	21	1/1/13/20	12/27/103/115	-
37	KC2	5	612	-	-	8/15/71/71	-
34	LMG	f	99	-	-	4/41/61/70	0/1/1/1
31	LHG	R	621	25	-	15/50/50/53	-
25	CLA	B	611	-	1/1/15/20	9/39/115/115	-
25	CLA	B	602	-	-	4/39/115/115	-
38	II0	O	619	-	-	5/21/67/67	0/2/2/2
38	II0	N	619	-	-	4/21/67/67	0/2/2/2
25	CLA	2	604	18	1/1/15/20	13/39/115/115	-
25	CLA	P	603	-	1/1/15/20	16/39/115/115	-
37	KC2	4	612	-	-	4/15/71/71	-
38	II0	Q	619	-	-	5/21/67/67	0/2/2/2
27	WVN	A	407	-	-	2/29/63/63	0/2/2/2
25	CLA	b	606	-	1/1/15/20	10/39/115/115	-
25	CLA	a	403	-	1/1/15/20	10/39/115/115	-
25	CLA	5	613	21	1/1/13/20	14/27/103/115	-
25	CLA	S	601	22	1/1/13/20	10/27/103/115	-
27	WVN	c	530	-	-	10/29/63/63	0/2/2/2
34	LMG	C	536	-	-	19/42/62/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	N	603	-	1/1/14/20	9/33/109/115	-
38	II0	R	616	-	-	0/21/67/67	0/2/2/2
25	CLA	P	604	-	-	6/37/113/115	-
25	CLA	O	609	18	1/1/11/20	3/19/95/115	-
39	IHT	4	620	-	-	8/25/65/65	0/2/2/2
25	CLA	c	519	-	1/1/14/20	11/33/109/115	-
25	CLA	P	610	19	1/1/15/20	12/39/115/115	-
27	WVN	P	620	-	-	8/29/63/63	0/2/2/2
25	CLA	c	522	-	1/1/15/20	9/39/115/115	-
25	CLA	1	601	23	1/1/11/20	8/15/91/115	-
27	WVN	b	619	-	-	10/29/63/63	0/2/2/2
27	WVN	b	618	-	-	10/29/63/63	0/2/2/2
25	CLA	B	608	-	1/1/15/20	3/39/115/115	-
34	LMG	b	620	-	-	6/46/66/70	0/1/1/1
25	CLA	B	612	-	1/1/15/20	12/39/115/115	-
25	CLA	R	611	31	1/1/15/20	17/39/115/115	-
38	II0	P	619	-	-	6/21/67/67	0/2/2/2
25	CLA	6	604	-	1/1/15/20	16/39/115/115	-
38	II0	P	617	-	-	0/21/67/67	0/2/2/2
34	LMG	d	402	-	-	9/35/55/70	0/1/1/1
27	WVN	H	89	-	-	7/29/63/63	0/2/2/2
27	WVN	Y	89	-	-	9/29/63/63	0/2/2/2
25	CLA	C	526	-	1/1/15/20	10/39/115/115	-
34	LMG	M	101	-	-	6/35/55/70	0/1/1/1
25	CLA	O	615	-	1/1/11/20	8/15/91/115	-
25	CLA	C	523	-	1/1/15/20	12/39/115/115	-
37	KC2	1	605	-	-	12/15/71/71	-
28	SQD	A	408	-	-	5/49/69/69	0/1/1/1
27	WVN	C	531	-	-	10/29/63/63	0/2/2/2
37	KC2	1	611	-	-	4/15/71/71	-
38	II0	5	618	-	-	0/21/67/67	0/2/2/2
37	KC2	N	613	-	-	10/15/71/71	-
25	CLA	5	603	-	1/1/12/20	11/24/100/115	-
25	CLA	O	606	18	1/1/12/20	6/23/99/115	-
38	II0	4	619	-	-	4/21/67/67	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	D	404	-	1/1/14/20	11/33/109/115	-
25	CLA	G	301	-	1/1/15/20	22/39/115/115	-
25	CLA	P	611	31	1/1/12/20	7/24/100/115	-
27	WVN	B	619	-	-	10/29/63/63	0/2/2/2
37	KC2	Q	611	-	-	7/15/71/71	-
31	LHG	z	103	-	-	6/29/29/53	-
31	LHG	S	621	25	-	9/44/44/53	-
26	PHO	a	405	-	-	13/37/103/103	0/5/6/6
38	II0	R	618	-	-	0/21/67/67	0/2/2/2
25	CLA	O	611	-	1/1/14/20	16/33/109/115	-
25	CLA	Q	604	20	1/1/14/20	15/35/111/115	-
25	CLA	1	615	-	1/1/11/20	10/18/94/115	-
25	CLA	4	613	-	1/1/10/20	6/13/89/115	-
31	LHG	3	621	25	-	15/53/53/53	-
37	KC2	1	612	23	-	4/15/71/71	-
25	CLA	b	614	-	1/1/14/20	9/33/109/115	-
25	CLA	3	603	-	1/1/15/20	16/39/115/115	-
25	CLA	R	607	-	1/1/10/20	5/13/89/115	-
25	CLA	d	403	-	1/1/15/20	6/39/115/115	-
34	LMG	O	622	-	-	2/35/55/70	0/1/1/1
35	DGD	C	532	-	-	8/43/83/95	0/2/2/2
35	DGD	h	90	-	-	14/51/91/95	0/2/2/2
25	CLA	1	606	23	1/1/12/20	5/21/97/115	-
25	CLA	S	602	22	1/1/15/20	15/39/115/115	-
38	II0	3	618	-	-	2/21/67/67	0/2/2/2
34	LMG	B	620	-	-	7/46/66/70	0/1/1/1
25	CLA	S	604	-	1/1/15/20	16/39/115/115	-
25	CLA	1	607	-	1/1/10/20	5/13/89/115	-
25	CLA	c	517	-	1/1/15/20	13/39/115/115	-
25	CLA	g	301	-	1/1/15/20	10/39/115/115	-
25	CLA	Q	606	20	1/1/13/20	9/27/103/115	-
25	CLA	3	610	19	1/1/15/20	12/39/115/115	-
37	KC2	6	606	-	-	8/15/71/71	-
27	WVN	3	620	-	-	8/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
37	KC2	N	612	23	-	4/15/71/71	-
25	CLA	C	516	-	1/1/15/20	6/39/115/115	-
25	CLA	C	522	-	1/1/15/20	8/39/115/115	-
25	CLA	4	609	-	1/1/13/20	9/29/105/115	-
25	CLA	S	603	-	1/1/13/20	11/27/103/115	-
25	CLA	B	614	-	1/1/14/20	8/33/109/115	-
25	CLA	B	601	-	1/1/12/20	8/21/97/115	-
25	CLA	c	516	-	1/1/15/20	6/39/115/115	-
25	CLA	5	602	21	1/1/13/20	12/27/103/115	-
38	II0	3	617	-	-	1/21/67/67	0/2/2/2
25	CLA	O	604	18	1/1/15/20	13/39/115/115	-
38	II0	5	617	-	-	1/21/67/67	0/2/2/2
29	PL9	d	405	-	-	9/53/73/73	0/1/1/1
25	CLA	1	609	23	1/1/11/20	7/17/93/115	-
25	CLA	5	604	21	1/1/14/20	7/33/109/115	-
34	LMG	2	622	-	-	2/35/55/70	0/1/1/1
37	KC2	S	606	22	-	9/15/71/71	-
25	CLA	b	605	-	1/1/15/20	8/39/115/115	-
34	LMG	c	536	-	-	19/46/66/70	0/1/1/1
25	CLA	c	520	-	1/1/15/20	9/39/115/115	-
25	CLA	Q	610	20	1/1/12/20	4/23/99/115	-
25	CLA	B	607	-	1/1/15/20	13/39/115/115	-
25	CLA	3	609	19	1/1/15/20	9/39/115/115	-
25	CLA	N	604	23	1/1/13/20	6/32/108/115	-
25	CLA	b	616	-	1/1/15/20	15/39/115/115	-
27	WVN	C	529	-	-	10/29/63/63	0/2/2/2
25	CLA	Q	607	-	1/1/10/20	2/13/89/115	-
31	LHG	O	621	-	-	7/50/50/53	-
38	II0	P	618	-	-	2/21/67/67	0/2/2/2
25	CLA	c	521	-	1/1/15/20	6/39/115/115	-
38	II0	P	616	-	-	2/21/67/67	0/2/2/2
25	CLA	C	527	-	1/1/15/20	12/39/115/115	-
28	SQD	a	411	-	-	4/35/55/69	0/1/1/1
27	WVN	D	408	-	-	9/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	b	610	-	1/1/15/20	10/39/115/115	-
25	CLA	2	603	-	1/1/15/20	8/39/115/115	-
25	CLA	4	606	20	1/1/13/20	13/27/103/115	-
25	CLA	b	608	-	1/1/15/20	5/39/115/115	-
34	LMG	m	101	-	-	7/35/55/70	0/1/1/1
29	PL9	a	409	-	-	10/27/47/73	0/1/1/1
39	IHT	R	620	-	-	11/25/65/65	0/2/2/2
25	CLA	C	518	-	1/1/15/20	9/39/115/115	-
25	CLA	S	610	22	1/1/13/20	8/30/106/115	-
38	II0	R	619	-	-	3/21/67/67	0/2/2/2
27	WVN	S	620	-	-	8/29/63/63	0/2/2/2
38	II0	Q	616	-	-	2/21/67/67	0/2/2/2
27	WVN	y	89	-	-	7/29/63/63	0/2/2/2
25	CLA	c	525	-	1/1/15/20	13/39/115/115	-
27	WVN	C	530	-	-	9/29/63/63	0/2/2/2
38	II0	N	617	-	-	0/21/67/67	0/2/2/2
25	CLA	R	606	21	1/1/15/20	13/39/115/115	-
25	CLA	3	601	19	1/1/11/20	2/15/91/115	-
25	CLA	2	610	18	1/1/15/20	8/39/115/115	-
25	CLA	5	606	21	1/1/15/20	13/39/115/115	-
25	CLA	N	601	23	1/1/11/20	8/15/91/115	-
25	CLA	1	604	23	1/1/13/20	6/32/108/115	-
39	IHT	N	620	-	-	7/25/65/65	0/2/2/2
25	CLA	R	604	21	1/1/14/20	7/33/109/115	-
34	LMG	D	407	-	-	2/32/52/70	0/1/1/1
25	CLA	3	613	19	1/1/13/20	11/27/103/115	-
31	LHG	B	622	-	-	11/47/47/53	-
25	CLA	3	615	-	1/1/11/20	6/15/91/115	-
25	CLA	S	611	31	1/1/13/20	11/27/103/115	-
31	LHG	5	621	25	-	15/50/50/53	-
38	II0	4	616	-	-	2/21/67/67	0/2/2/2
38	II0	Q	617	-	-	0/21/67/67	0/2/2/2
31	LHG	b	622	-	-	19/47/47/53	-
27	WVN	B	617	-	-	11/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	3	602	19	1/1/14/20	13/36/112/115	-
25	CLA	B	604	-	1/1/13/20	9/32/108/115	-
26	PHO	D	401	-	-	11/37/103/103	0/5/6/6
39	IHT	5	620	-	-	7/25/65/65	0/2/2/2
25	CLA	B	606	-	1/1/15/20	12/39/115/115	-
25	CLA	c	518	-	1/1/15/20	10/39/115/115	-
31	LHG	P	621	25	-	16/53/53/53	-
25	CLA	B	605	-	1/1/15/20	8/39/115/115	-
38	II0	5	616	-	-	0/21/67/67	0/2/2/2
25	CLA	P	612	-	1/1/12/20	7/25/101/115	-
25	CLA	2	609	18	1/1/11/20	2/19/95/115	-
25	CLA	4	607	-	1/1/10/20	2/13/89/115	-
31	LHG	D	406	-	-	11/53/53/53	-
39	IHT	O	620	-	-	6/25/65/65	0/2/2/2
25	CLA	N	615	-	1/1/11/20	10/18/94/115	-
25	CLA	2	613	18	1/1/14/20	11/33/109/115	-
25	CLA	5	607	-	1/1/10/20	6/13/89/115	-
25	CLA	D	403	-	1/1/15/20	6/39/115/115	-
25	CLA	6	603	-	1/1/13/20	8/27/103/115	-
25	CLA	c	526	-	1/1/15/20	9/39/115/115	-
34	LMG	w	134	-	-	9/43/63/70	0/1/1/1
38	II0	4	618	-	-	2/21/67/67	0/2/2/2
25	CLA	b	601	-	1/1/12/20	9/21/97/115	-
25	CLA	D	400	-	1/1/15/20	8/39/115/115	-
25	CLA	N	614	-	1/1/11/20	5/19/95/115	-
25	CLA	c	523	-	1/1/15/20	12/39/115/115	-
25	CLA	A	404	-	1/1/11/20	10/20/96/115	-
25	CLA	6	610	22	1/1/13/20	8/30/106/115	-
25	CLA	6	601	22	1/1/13/20	10/27/103/115	-
27	WVN	6	620	-	-	7/29/63/63	0/2/2/2
25	CLA	P	613	19	1/1/13/20	11/27/103/115	-
38	II0	S	618	-	-	4/21/67/67	0/2/2/2
34	LMG	z	102	-	-	5/26/46/70	0/1/1/1
25	CLA	b	607	-	1/1/15/20	12/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	DGD	H	90	-	-	14/51/91/95	0/2/2/2
25	CLA	d	404	-	1/1/14/20	14/35/111/115	-
37	KC2	S	612	22	-	5/15/71/71	-
38	II0	2	618	-	-	1/21/67/67	0/2/2/2
37	KC2	2	612	-	-	7/15/71/71	-
25	CLA	2	615	-	1/1/11/20	8/15/91/115	-
26	PHO	A	405	-	-	13/37/103/103	0/5/6/6
25	CLA	N	609	23	1/1/11/20	9/17/93/115	-
25	CLA	C	520	-	1/1/15/20	12/39/115/115	-
25	CLA	2	602	18	1/1/15/20	14/39/115/115	-
31	LHG	Z	103	-	-	6/29/29/53	-
25	CLA	Q	609	20	1/1/13/20	8/29/105/115	-
31	LHG	2	621	-	-	7/50/50/53	-
25	CLA	c	524	-	1/1/15/20	12/39/115/115	-
25	CLA	R	613	21	1/1/13/20	14/27/103/115	-
38	II0	5	619	-	-	3/21/67/67	0/2/2/2
38	II0	3	619	-	-	6/21/67/67	0/2/2/2
25	CLA	3	611	31	1/1/12/20	7/24/100/115	-
25	CLA	6	613	-	1/1/12/20	4/25/101/115	-
27	WVN	h	89	-	-	11/29/63/63	0/2/2/2
29	PL9	A	409	-	-	10/27/47/73	0/1/1/1
37	KC2	Q	612	-	-	4/15/71/71	-
25	CLA	6	602	22	1/1/15/20	15/39/115/115	-
37	KC2	Q	605	-	-	7/15/71/71	-
37	KC2	3	606	19	-	10/15/71/71	-
25	CLA	P	602	19	1/1/14/20	13/36/112/115	-
38	II0	N	616	-	-	4/21/67/67	0/2/2/2
38	II0	4	617	-	-	0/21/67/67	0/2/2/2
34	LMG	d	407	-	-	2/32/52/70	0/1/1/1
31	LHG	d	406	-	-	11/53/53/53	-
25	CLA	P	601	19	1/1/11/20	4/15/91/115	-
25	CLA	c	527	-	1/1/15/20	12/39/115/115	-
25	CLA	1	603	-	1/1/14/20	11/33/109/115	-
25	CLA	5	611	31	1/1/15/20	17/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	O	607	-	1/1/14/20	16/33/109/115	-
38	II0	S	617	-	-	1/21/67/67	0/2/2/2
38	II0	S	616	-	-	5/21/67/67	0/2/2/2
25	CLA	3	612	-	1/1/12/20	7/25/101/115	-
38	II0	1	616	-	-	4/21/67/67	0/2/2/2
37	KC2	4	605	-	-	7/15/71/71	-
25	CLA	C	524	-	1/1/15/20	12/39/115/115	-
39	IHT	1	620	-	-	7/25/65/65	0/2/2/2
25	CLA	N	610	23	1/1/14/20	6/33/109/115	-
25	CLA	N	606	23	1/1/12/20	5/21/97/115	-
38	II0	2	617	-	-	0/21/67/67	0/2/2/2
37	KC2	6	612	22	-	5/15/71/71	-
25	CLA	O	603	-	1/1/15/20	8/39/115/115	-
25	CLA	P	609	19	1/1/15/20	9/39/115/115	-
38	II0	O	616	-	-	1/21/67/67	0/2/2/2
25	CLA	C	528	-	1/1/12/20	11/24/100/115	-
27	WVN	c	529	-	-	9/29/63/63	0/2/2/2
34	LMG	g	303	-	-	8/35/55/70	0/1/1/1
37	KC2	O	612	-	-	7/15/71/71	-
38	II0	S	619	-	-	4/21/67/67	0/2/2/2
25	CLA	4	604	20	1/1/14/20	15/35/111/115	-
37	KC2	P	606	19	-	10/15/71/71	-
38	II0	1	618	-	-	3/21/67/67	0/2/2/2
25	CLA	4	615	-	1/1/10/20	4/13/89/115	-
25	CLA	4	610	20	1/1/12/20	4/23/99/115	-
31	LHG	a	413	-	-	26/46/46/53	-
38	II0	2	619	-	-	5/21/67/67	0/2/2/2
38	II0	6	618	-	-	4/21/67/67	0/2/2/2
25	CLA	2	611	-	1/1/14/20	16/33/109/115	-
28	SQD	A	411	-	-	3/35/55/69	0/1/1/1
26	PHO	d	401	-	-	11/37/103/103	0/5/6/6
38	II0	Q	618	-	-	2/21/67/67	0/2/2/2
27	WVN	B	618	-	-	10/29/63/63	0/2/2/2
25	CLA	C	525	-	1/1/15/20	13/39/115/115	-
31	LHG	6	621	25	-	10/44/44/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	1	610	23	1/1/14/20	6/33/109/115	-
28	SQD	a	408	-	-	4/40/60/69	0/1/1/1
25	CLA	B	609	-	1/1/15/20	7/39/115/115	-
38	II0	O	618	-	-	3/21/67/67	0/2/2/2
25	CLA	5	615	-	1/1/11/20	7/17/93/115	-
25	CLA	2	601	18	1/1/11/20	9/20/96/115	-
25	CLA	Q	603	-	1/1/15/20	16/39/115/115	-
25	CLA	b	612	-	1/1/15/20	13/39/115/115	-
25	CLA	A	406	-	1/1/14/20	9/33/109/115	-
25	CLA	O	610	18	1/1/15/20	8/39/115/115	-
25	CLA	5	610	21	1/1/13/20	10/32/108/115	-
34	LMG	Q	621	-	-	4/38/58/70	0/1/1/1
38	II0	R	617	-	-	1/21/67/67	0/2/2/2
25	CLA	2	607	-	1/1/14/20	16/33/109/115	-
25	CLA	P	615	-	1/1/11/20	7/15/91/115	-
25	CLA	R	603	-	1/1/12/20	11/24/100/115	-
38	II0	6	617	-	-	1/21/67/67	0/2/2/2
25	CLA	C	521	-	1/1/15/20	7/39/115/115	-
25	CLA	O	602	18	1/1/15/20	14/39/115/115	-
38	II0	O	617	-	-	1/21/67/67	0/2/2/2
25	CLA	R	601	21	1/1/13/20	6/27/103/115	-
25	CLA	C	519	-	1/1/14/20	11/33/109/115	-
25	CLA	b	603	-	1/1/15/20	7/39/115/115	-
38	II0	1	617	-	-	0/21/67/67	0/2/2/2
37	KC2	N	611	-	-	4/15/71/71	-
27	WVN	a	407	-	-	10/29/63/63	0/2/2/2
25	CLA	B	603	-	1/1/15/20	7/39/115/115	-
25	CLA	a	404	-	1/1/11/20	10/20/96/115	-
25	CLA	b	611	-	1/1/15/20	9/39/115/115	-
25	CLA	S	609	22	1/1/13/20	14/27/103/115	-
25	CLA	a	406	-	1/1/14/20	9/33/109/115	-
25	CLA	Q	613	-	1/1/10/20	6/13/89/115	-
38	II0	1	619	-	-	3/21/67/67	0/2/2/2
38	II0	6	619	-	-	3/21/67/67	0/2/2/2
25	CLA	6	611	31	1/1/13/20	11/27/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	d	400	-	1/1/15/20	8/39/115/115	-
25	CLA	B	616	-	1/1/15/20	15/39/115/115	-
37	KC2	1	613	-	-	9/15/71/71	-
31	LHG	l	101	-	-	5/53/53/53	-
25	CLA	6	615	-	1/1/15/20	10/39/115/115	-
25	CLA	b	613	-	1/1/15/20	17/39/115/115	-
29	PL9	D	405	-	-	9/53/73/73	0/1/1/1
25	CLA	4	603	-	1/1/15/20	16/39/115/115	-
25	CLA	Q	602	20	1/1/15/20	6/39/115/115	-
37	KC2	4	611	-	-	7/15/71/71	-
31	LHG	C	535	-	-	15/44/44/53	-
25	CLA	S	613	-	1/1/12/20	4/25/101/115	-
27	WVN	b	617	-	-	13/29/63/63	0/2/2/2
25	CLA	R	610	21	1/1/13/20	10/32/108/115	-
25	CLA	O	601	18	1/1/11/20	9/20/96/115	-
25	CLA	A	403	-	1/1/15/20	10/39/115/115	-
25	CLA	B	610	-	1/1/15/20	10/39/115/115	-
25	CLA	5	601	21	1/1/13/20	6/27/103/115	-
31	LHG	c	535	-	-	11/44/44/53	-
34	LMG	Z	102	-	-	5/26/46/70	0/1/1/1
35	DGD	c	532	-	-	8/43/83/95	0/2/2/2
25	CLA	3	604	-	-	6/37/113/115	-
25	CLA	b	602	-	-	4/39/115/115	-
25	CLA	N	602	23	1/1/14/20	6/33/109/115	-
38	II0	3	616	-	-	2/21/67/67	0/2/2/2
25	CLA	O	613	18	1/1/14/20	11/33/109/115	-
25	CLA	S	615	-	1/1/15/20	10/39/115/115	-
36	HEM	e	102	5,6	-	8/14/54/54	-
25	CLA	1	614	-	1/1/11/20	5/19/95/115	-
38	II0	6	616	-	-	5/21/67/67	0/2/2/2
27	WVN	d	408	-	-	12/29/63/63	0/2/2/2
31	LHG	A	413	-	-	28/46/46/53	-
25	CLA	Q	615	-	1/1/10/20	4/13/89/115	-
25	CLA	b	609	-	1/1/15/20	7/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	g	302	17	1/1/11/20	8/15/91/115	-
25	CLA	R	609	21	1/1/15/20	10/39/115/115	-
34	LMG	F	99	-	-	4/41/61/70	0/1/1/1
37	KC2	N	605	-	-	12/15/71/71	-
25	CLA	N	607	-	1/1/10/20	5/13/89/115	-
27	WVN	c	531	-	-	11/29/63/63	0/2/2/2
34	LMG	4	621	-	-	4/38/58/70	0/1/1/1
25	CLA	6	609	22	1/1/13/20	8/27/103/115	-
38	II0	2	616	-	-	1/21/67/67	0/2/2/2

The worst 5 of 2677 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	S	618	II0	C13-C09	-10.91	1.22	1.35
38	6	618	II0	C13-C09	-10.87	1.23	1.35
38	2	619	II0	C13-C09	-10.48	1.23	1.35
38	4	619	II0	C13-C09	-10.46	1.23	1.35
38	O	619	II0	C13-C09	-10.45	1.23	1.35

The worst 5 of 3292 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	6	612	KC2	C1A-NA-C4A	-12.23	101.10	106.68
37	4	612	KC2	C1A-NA-C4A	-12.22	101.11	106.68
37	Q	612	KC2	C1A-NA-C4A	-12.21	101.11	106.68
37	S	612	KC2	C1A-NA-C4A	-12.21	101.11	106.68
37	O	612	KC2	C1A-NA-C4A	-12.15	101.14	106.68

5 of 190 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
25	a	403	CLA	ND
25	a	404	CLA	ND
25	a	406	CLA	ND
25	b	601	CLA	ND
25	b	603	CLA	ND

5 of 2948 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
25	a	403	CLA	C4B-C3B-CAB-CBB
25	a	404	CLA	C1A-C2A-CAA-CBA
25	a	404	CLA	C3A-C2A-CAA-CBA
25	a	406	CLA	C1A-C2A-CAA-CBA
25	a	406	CLA	C3A-C2A-CAA-CBA

There are no ring outliers.

217 monomers are involved in 456 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	B	613	CLA	9	0
25	4	602	CLA	1	0
25	1	602	CLA	1	0
25	b	615	CLA	2	0
31	L	101	LHG	6	0
25	5	609	CLA	5	0
34	G	303	LMG	5	0
25	B	615	CLA	3	0
36	E	102	HEM	1	0
25	b	604	CLA	3	0
25	C	517	CLA	4	0
34	W	134	LMG	2	0
34	D	402	LMG	4	0
25	c	528	CLA	1	0
25	R	615	CLA	1	0
25	R	602	CLA	2	0
34	f	99	LMG	3	0
31	R	621	LHG	4	0
25	B	611	CLA	3	0
25	B	602	CLA	2	0
25	2	604	CLA	1	0
25	P	603	CLA	1	0
25	b	606	CLA	4	0
25	a	403	CLA	11	0
25	5	613	CLA	1	0
25	N	603	CLA	3	0
25	O	609	CLA	3	0
25	P	610	CLA	2	0
25	c	522	CLA	3	0
25	B	608	CLA	2	0
34	b	620	LMG	1	0
25	B	612	CLA	6	0
25	R	611	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	6	604	CLA	2	0
34	d	402	LMG	3	0
25	C	526	CLA	2	0
34	M	101	LMG	1	0
25	O	615	CLA	1	0
25	C	523	CLA	3	0
28	A	408	SQD	1	0
37	N	613	KC2	2	0
25	5	603	CLA	1	0
25	D	404	CLA	1	0
25	G	301	CLA	3	0
25	P	611	CLA	5	0
31	S	621	LHG	2	0
26	a	405	PHO	3	0
25	O	611	CLA	1	0
25	Q	604	CLA	3	0
25	4	613	CLA	1	0
31	3	621	LHG	2	0
25	b	614	CLA	2	0
25	d	403	CLA	7	0
34	O	622	LMG	1	0
35	C	532	DGD	1	0
35	h	90	DGD	4	0
34	B	620	LMG	1	0
25	S	604	CLA	3	0
25	l	607	CLA	1	0
25	c	517	CLA	3	0
25	g	301	CLA	5	0
25	Q	606	CLA	1	0
25	3	610	CLA	1	0
37	6	606	KC2	10	0
25	C	516	CLA	2	0
25	C	522	CLA	3	0
25	4	609	CLA	5	0
25	S	603	CLA	2	0
25	B	614	CLA	1	0
25	B	601	CLA	1	0
25	c	516	CLA	2	0
25	5	602	CLA	2	0
25	O	604	CLA	2	0
29	d	405	PL9	4	0
25	1	609	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	5	604	CLA	1	0
25	b	605	CLA	4	0
34	c	536	LMG	4	0
25	c	520	CLA	2	0
25	B	607	CLA	1	0
25	3	609	CLA	1	0
25	N	604	CLA	1	0
25	b	616	CLA	3	0
25	Q	607	CLA	2	0
31	O	621	LHG	1	0
25	c	521	CLA	4	0
25	C	527	CLA	2	0
28	a	411	SQD	1	0
25	b	610	CLA	5	0
25	2	603	CLA	2	0
25	4	606	CLA	1	0
25	b	608	CLA	2	0
34	m	101	LMG	1	0
29	a	409	PL9	2	0
25	C	518	CLA	4	0
25	S	610	CLA	1	0
25	c	525	CLA	5	0
25	R	606	CLA	4	0
25	3	601	CLA	1	0
25	2	610	CLA	1	0
25	5	606	CLA	4	0
25	R	604	CLA	2	0
34	D	407	LMG	2	0
31	B	622	LHG	3	0
25	3	615	CLA	1	0
25	S	611	CLA	1	0
31	5	621	LHG	4	0
31	b	622	LHG	2	0
27	B	617	WVN	1	0
25	B	604	CLA	3	0
26	D	401	PHO	5	0
25	B	606	CLA	5	0
25	c	518	CLA	4	0
31	P	621	LHG	3	0
25	B	605	CLA	6	0
25	2	609	CLA	1	0
25	4	607	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	D	406	LHG	4	0
25	D	403	CLA	7	0
25	6	603	CLA	2	0
25	c	526	CLA	1	0
34	w	134	LMG	1	0
38	4	618	II0	1	0
25	D	400	CLA	1	0
25	c	523	CLA	3	0
25	A	404	CLA	3	0
25	6	610	CLA	1	0
34	z	102	LMG	2	0
25	b	607	CLA	2	0
35	H	90	DGD	5	0
25	d	404	CLA	1	0
38	2	618	II0	1	0
25	2	615	CLA	1	0
26	A	405	PHO	2	0
25	N	609	CLA	1	0
25	C	520	CLA	3	0
25	2	602	CLA	3	0
25	Q	609	CLA	2	0
31	2	621	LHG	1	0
25	R	613	CLA	1	0
25	3	611	CLA	5	0
25	6	613	CLA	2	0
25	6	602	CLA	2	0
34	d	407	LMG	2	0
31	d	406	LHG	4	0
25	P	601	CLA	1	0
25	c	527	CLA	2	0
25	1	603	CLA	3	0
25	5	611	CLA	2	0
25	O	607	CLA	4	0
38	S	617	II0	2	0
25	O	603	CLA	1	0
25	P	609	CLA	1	0
25	C	528	CLA	1	0
34	g	303	LMG	3	0
25	4	604	CLA	3	0
25	4	615	CLA	1	0
25	2	611	CLA	1	0
28	A	411	SQD	1	0

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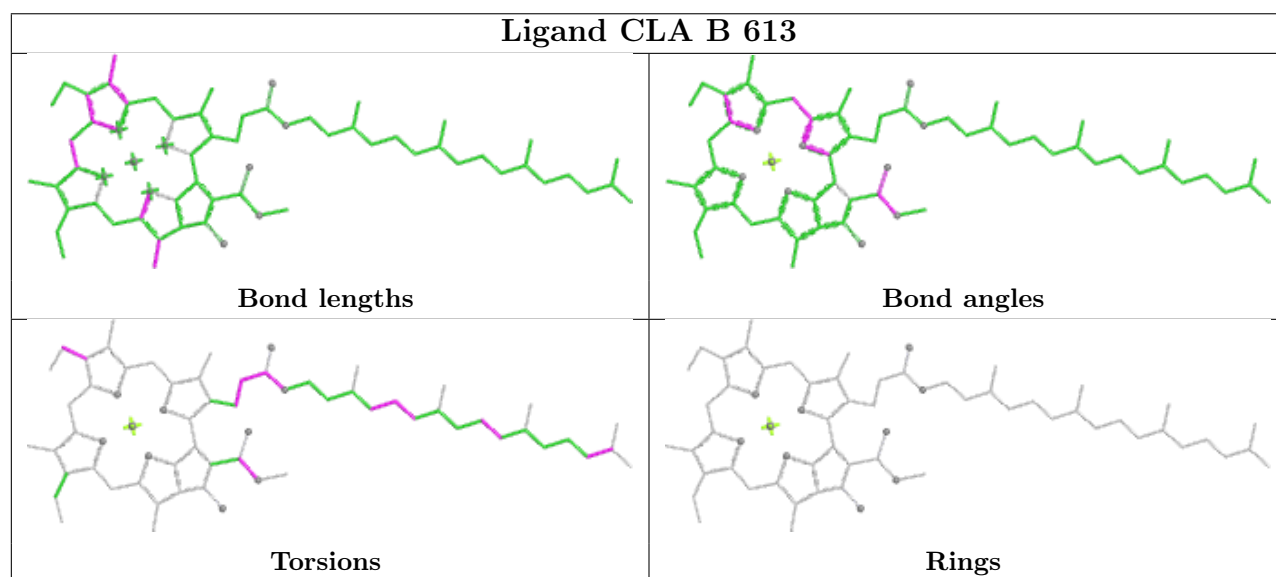
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26	d	401	PHO	5	0
25	C	525	CLA	6	0
31	6	621	LHG	2	0
28	a	408	SQD	1	0
25	B	609	CLA	4	0
38	O	618	II0	1	0
25	5	615	CLA	1	0
25	Q	603	CLA	6	0
25	b	612	CLA	7	0
25	A	406	CLA	2	0
25	O	610	CLA	3	0
25	5	610	CLA	2	0
34	Q	621	LMG	2	0
25	2	607	CLA	4	0
25	P	615	CLA	1	0
25	R	603	CLA	1	0
38	6	617	II0	2	0
25	C	521	CLA	5	0
25	O	602	CLA	2	0
25	R	601	CLA	1	0
25	b	603	CLA	2	0
25	B	603	CLA	1	0
25	a	404	CLA	2	0
25	b	611	CLA	3	0
25	S	609	CLA	4	0
25	a	406	CLA	3	0
25	Q	613	CLA	2	0
25	6	611	CLA	2	0
25	d	400	CLA	2	0
25	B	616	CLA	1	0
37	1	613	KC2	1	0
31	l	101	LHG	8	0
25	6	615	CLA	1	0
25	b	613	CLA	6	0
29	D	405	PL9	3	0
25	4	603	CLA	7	0
25	Q	602	CLA	1	0
31	C	535	LHG	1	0
25	S	613	CLA	1	0
27	b	617	WVN	1	0
25	R	610	CLA	1	0
25	A	403	CLA	10	0

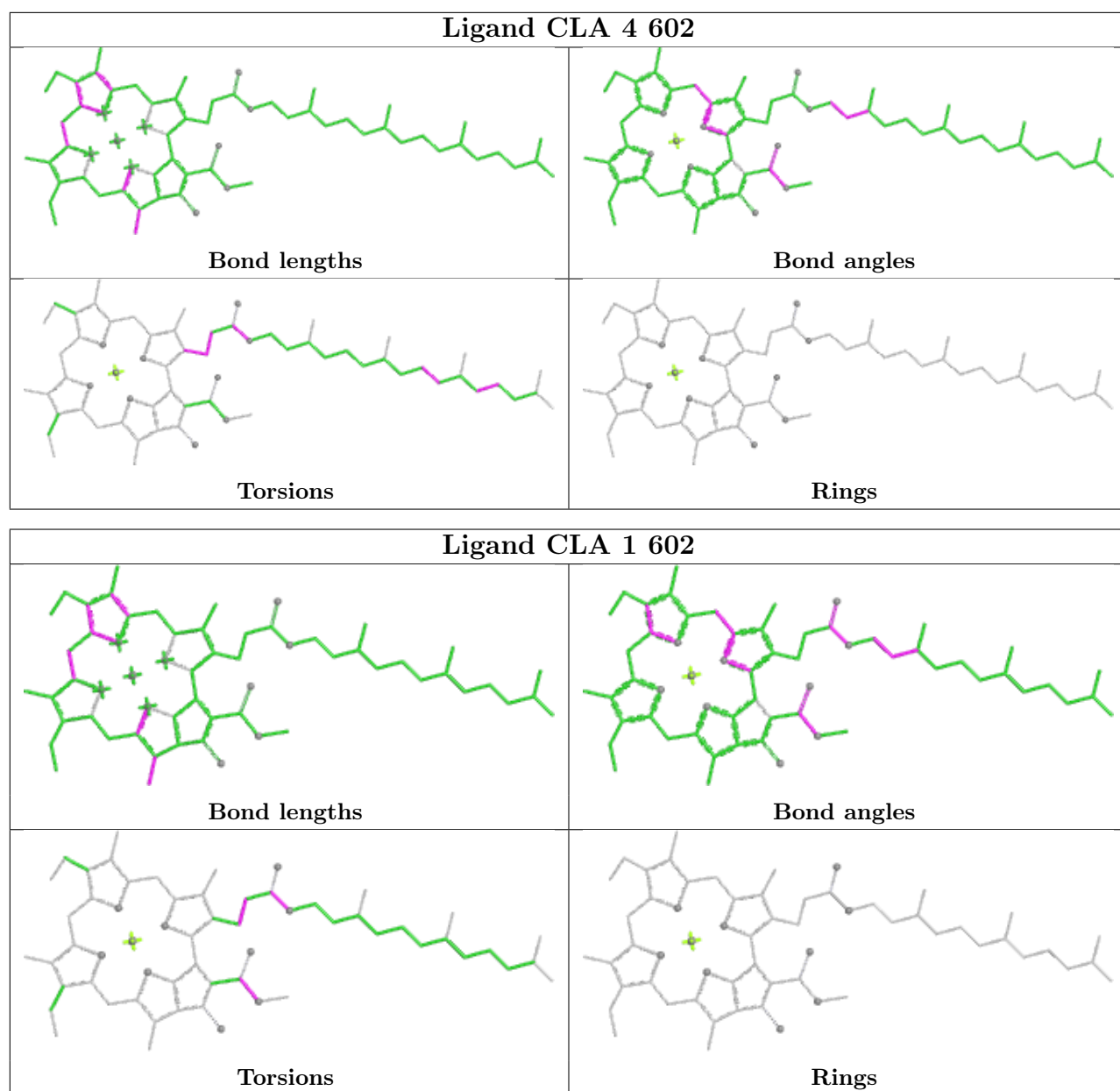
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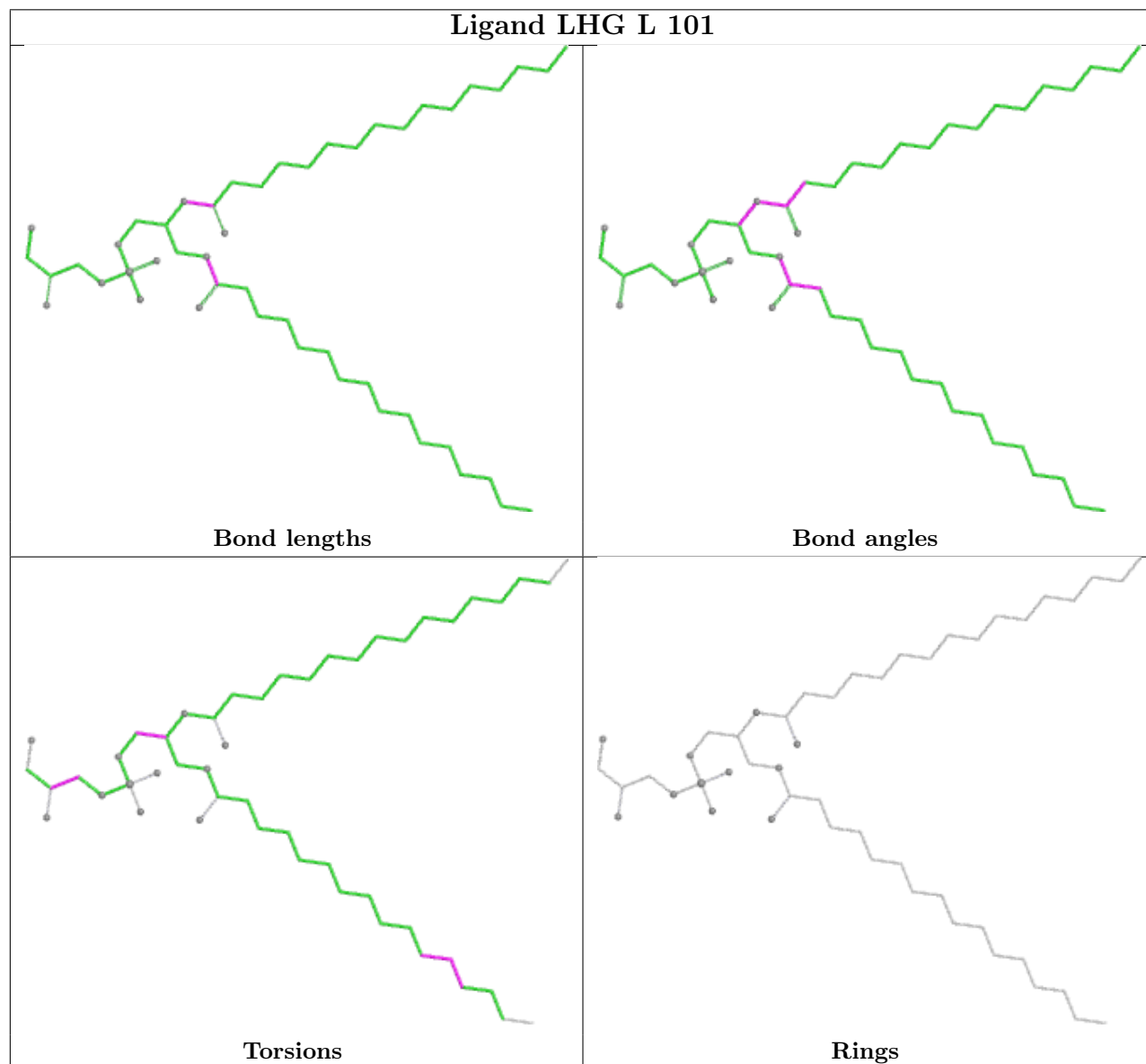
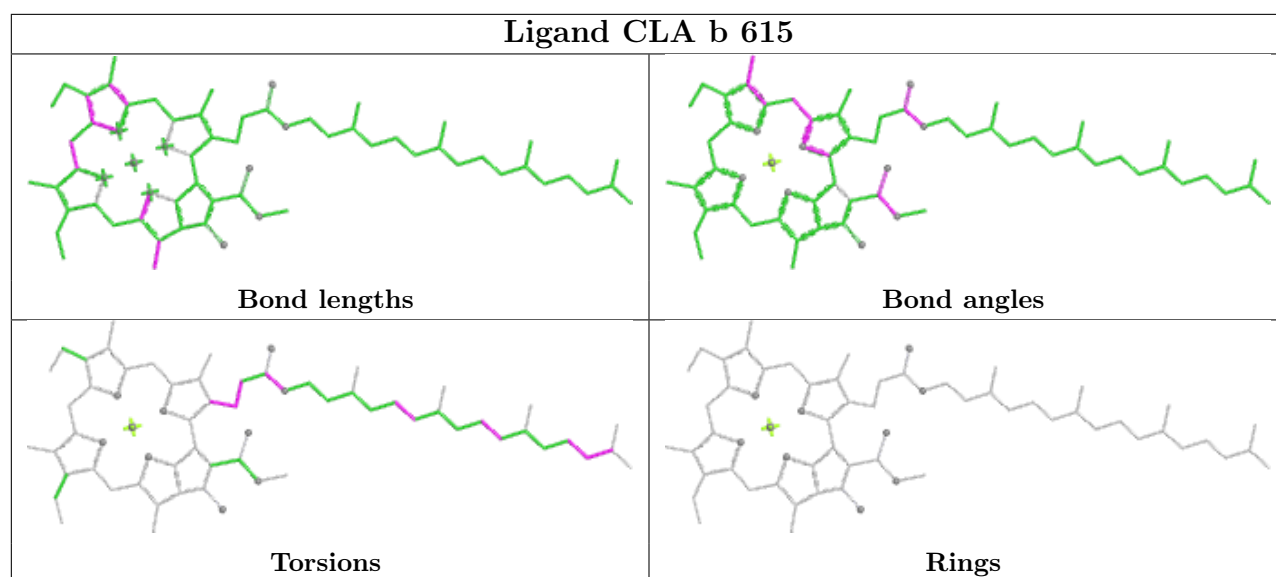
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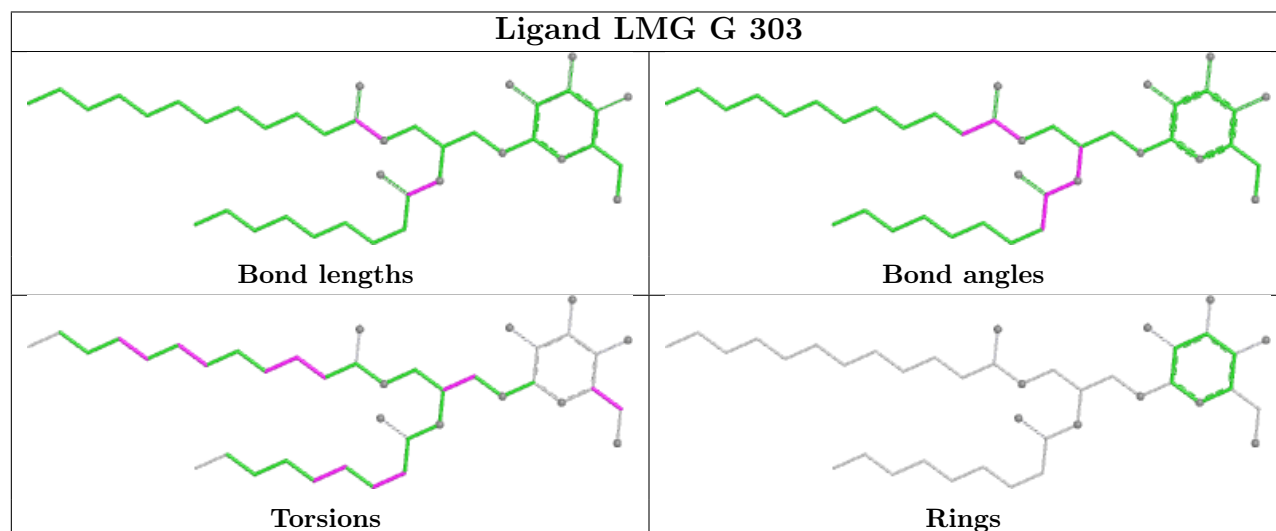
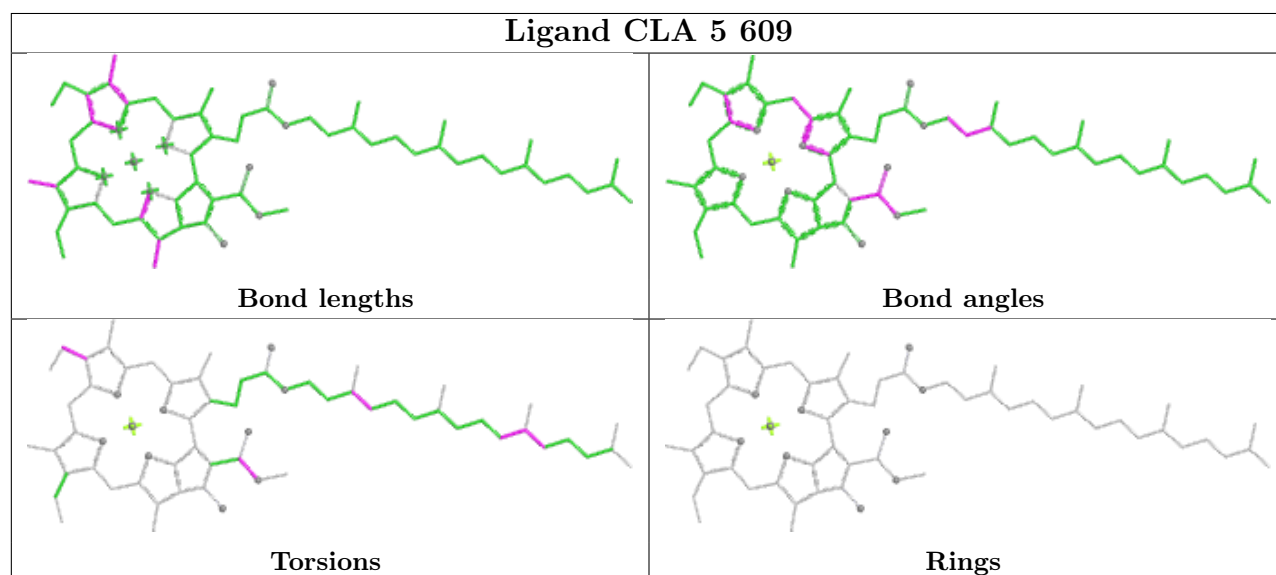
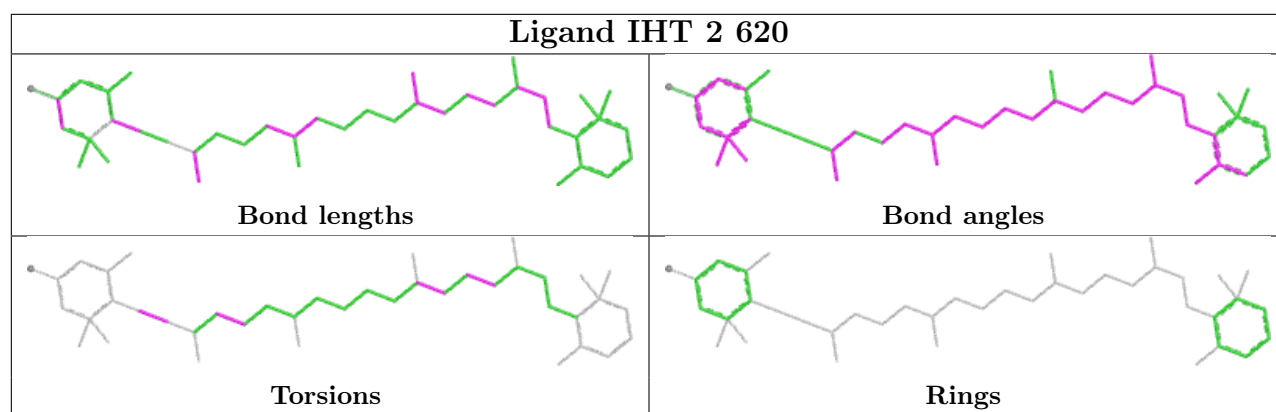
Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	B	610	CLA	5	0
25	5	601	CLA	1	0
31	c	535	LHG	2	0
34	Z	102	LMG	2	0
35	c	532	DGD	1	0
25	3	604	CLA	1	0
25	b	602	CLA	2	0
25	N	602	CLA	1	0
25	S	615	CLA	2	0
36	e	102	HEM	1	0
25	Q	615	CLA	1	0
25	b	609	CLA	4	0
25	R	609	CLA	5	0
25	N	607	CLA	2	0
34	4	621	LMG	2	0
25	6	609	CLA	4	0

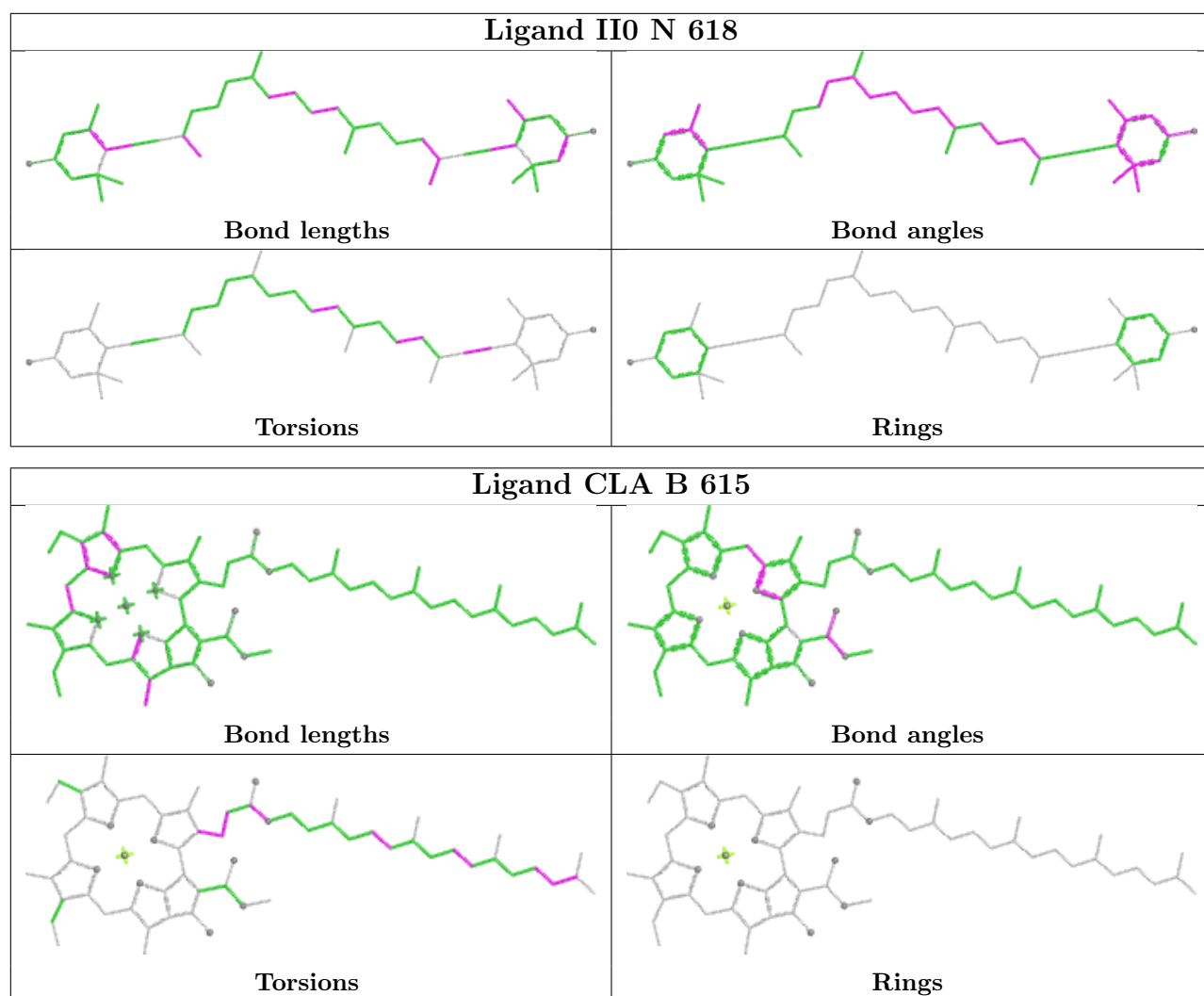
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

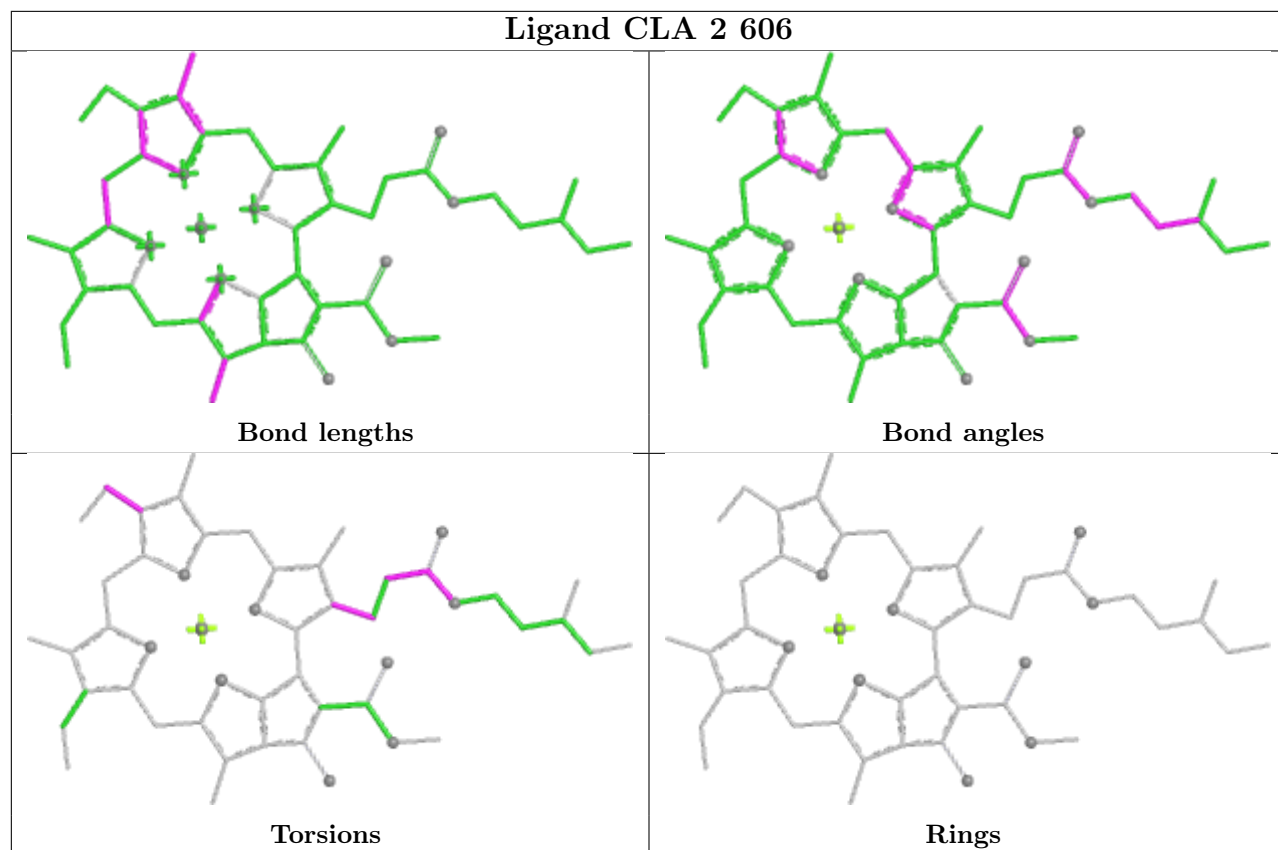


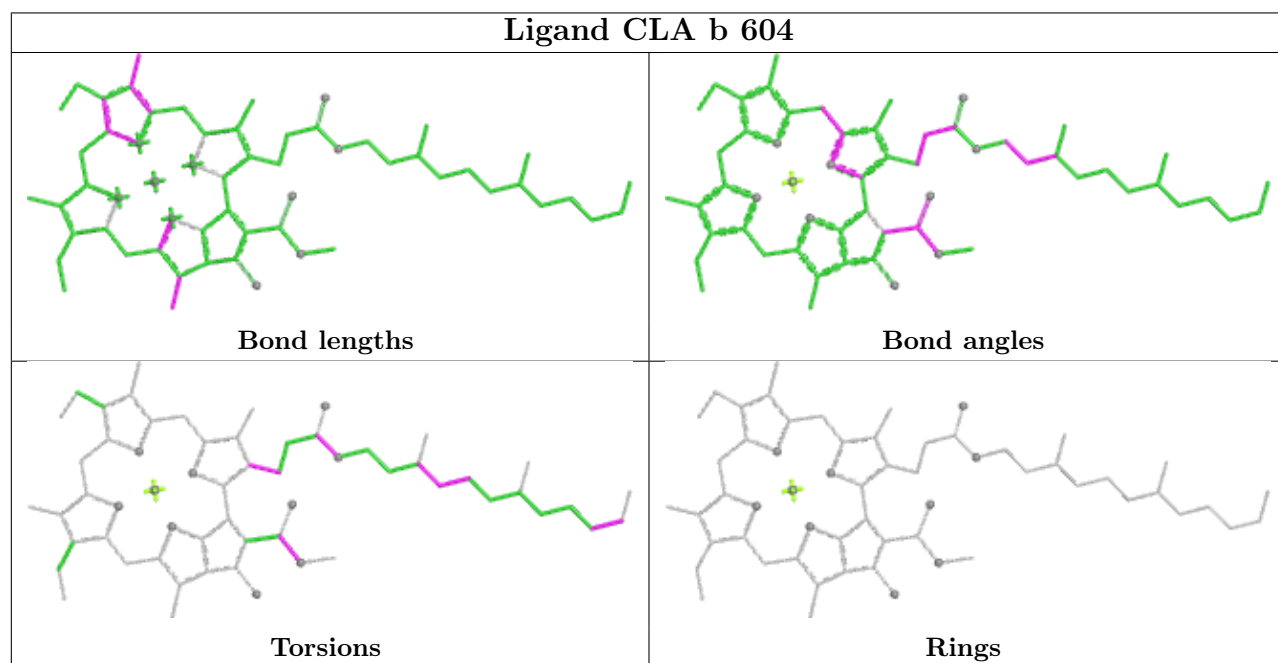
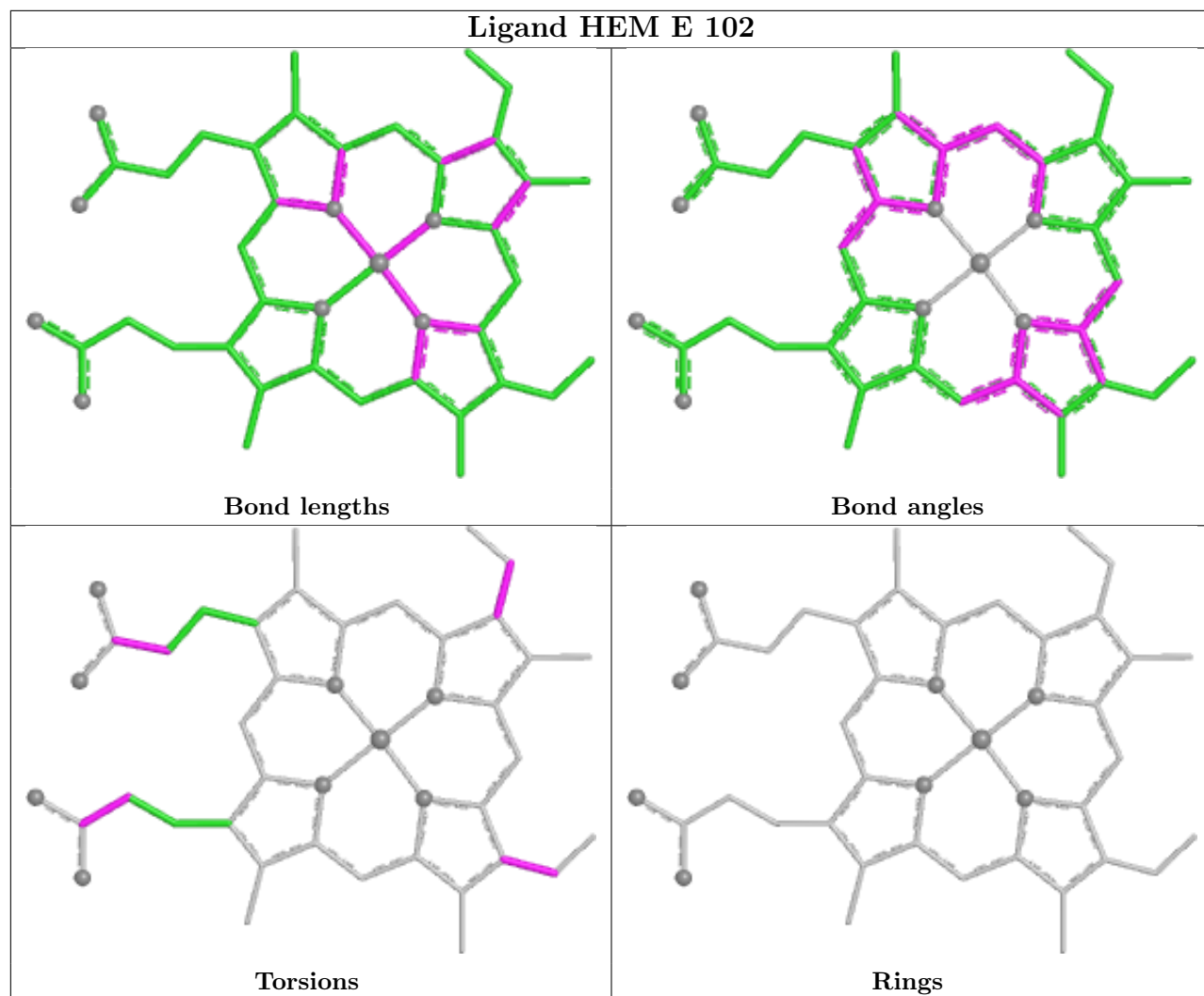


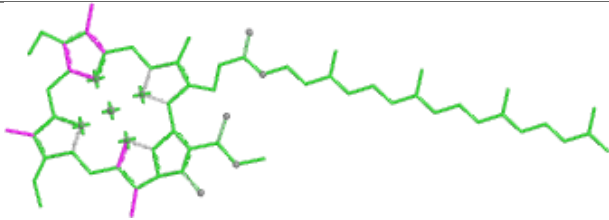
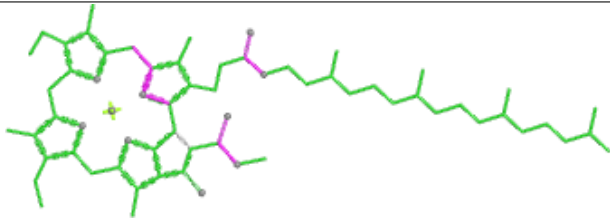
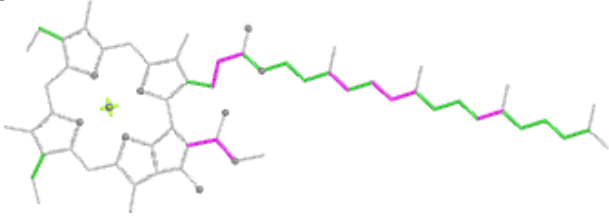
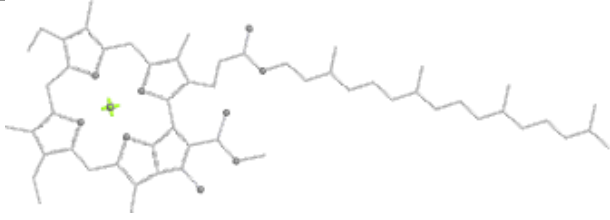


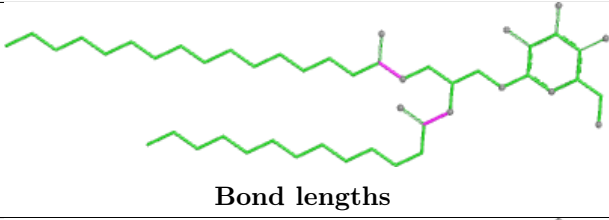
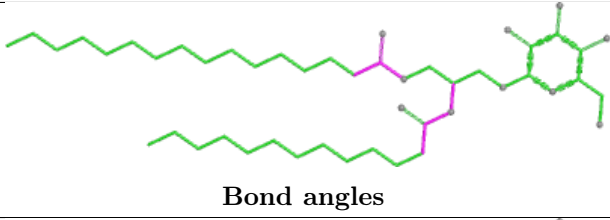
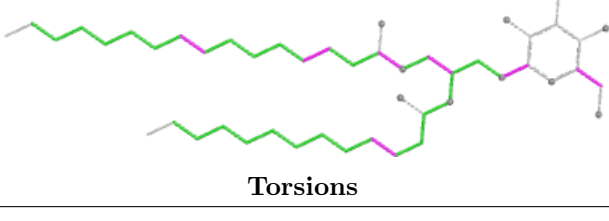
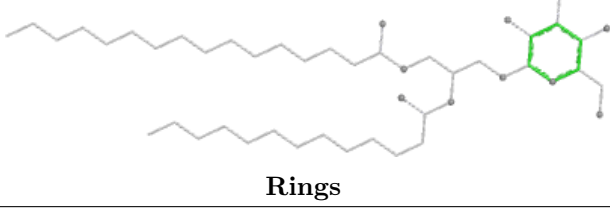


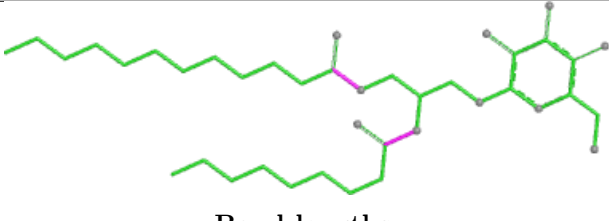
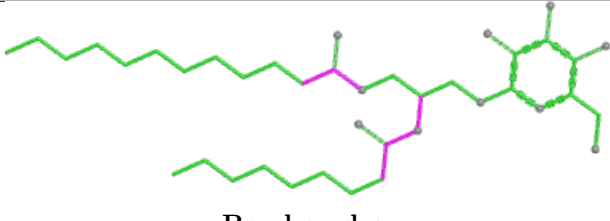
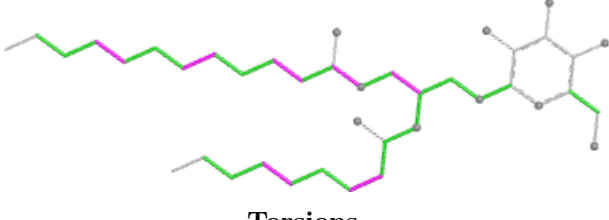
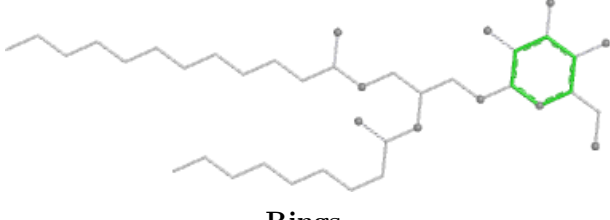




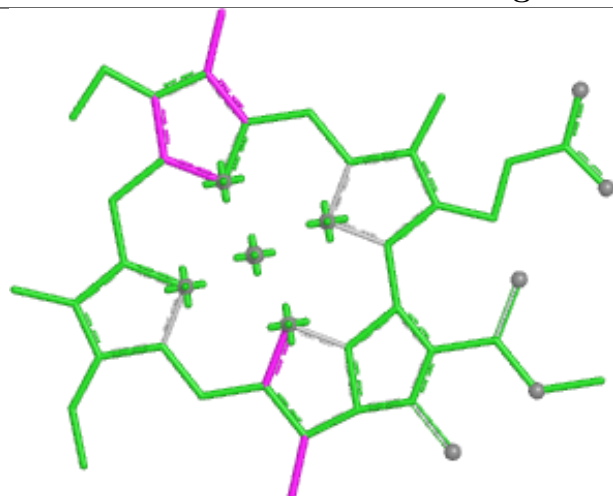


Ligand CLA C 517	
	
Bond lengths	Bond angles
	
Torsions	Rings

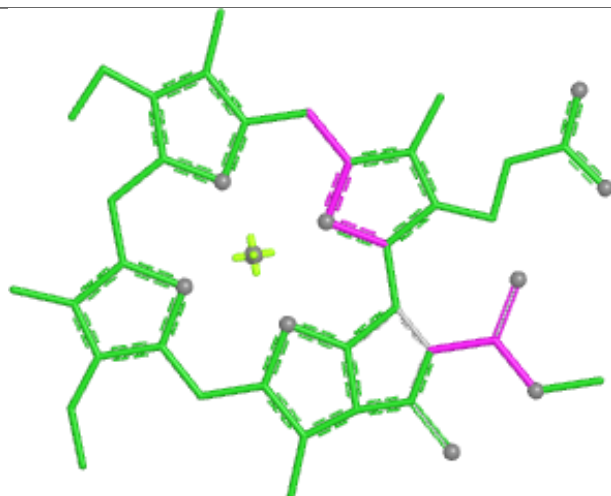
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Bond lengths	Bond angles
	
Torsions	Rings

Ligand LMG D 402	
	
Bond lengths	Bond angles
	
Torsions	Rings

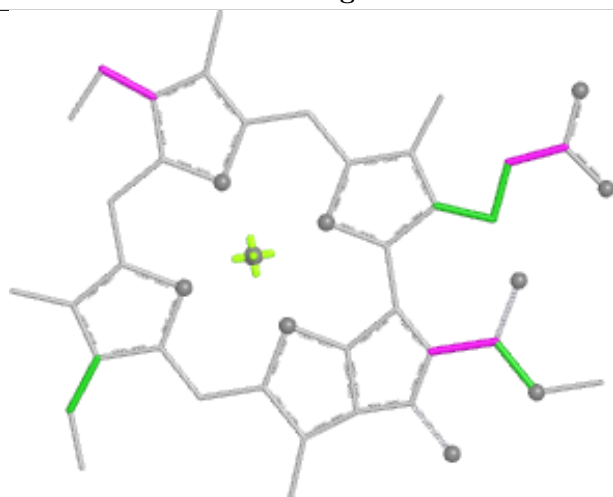
Ligand CLA G 302



Bond lengths



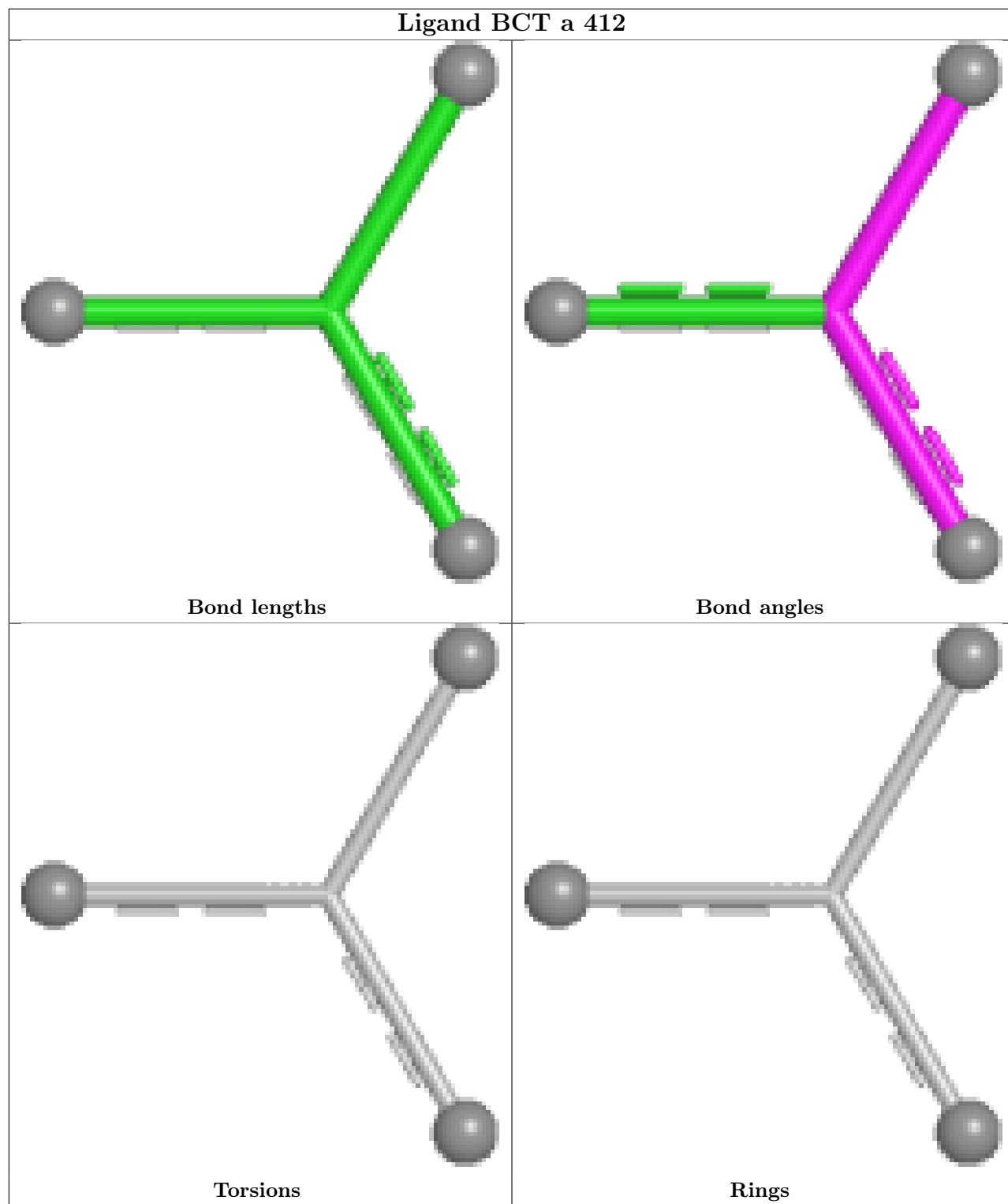
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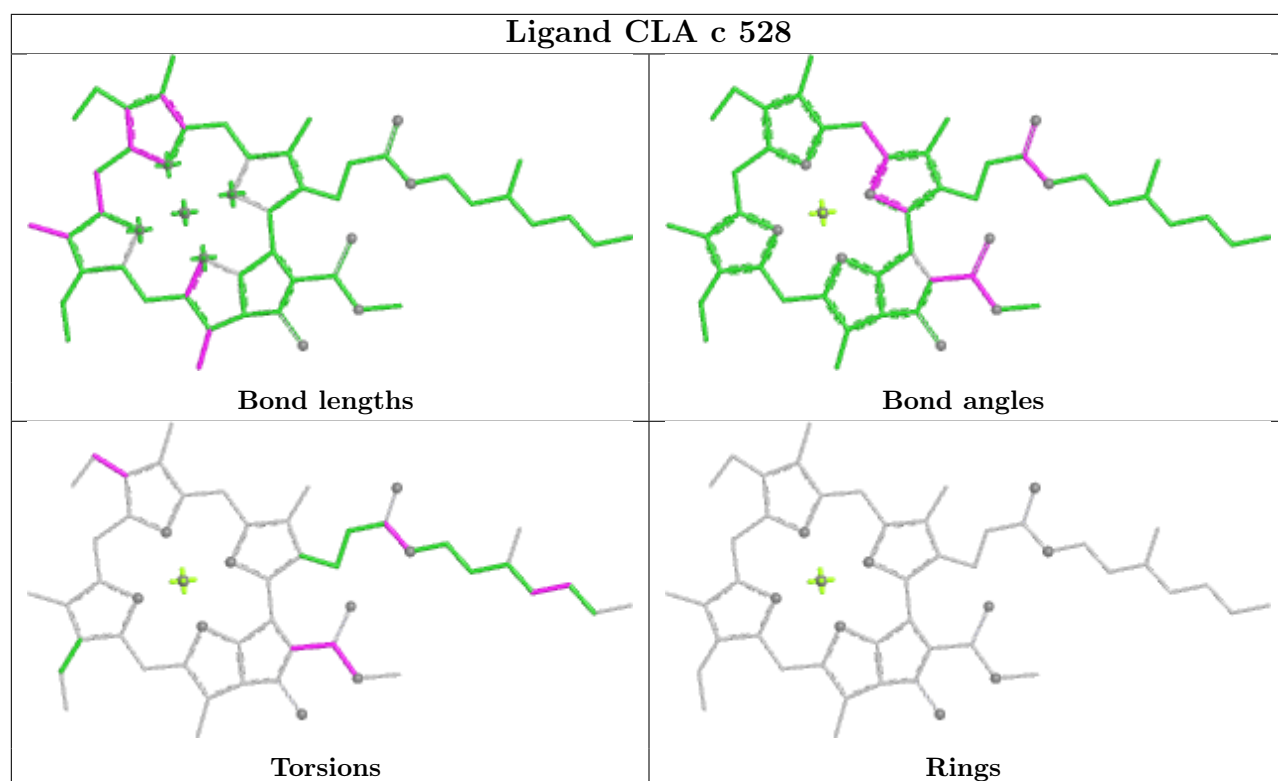


Torsions

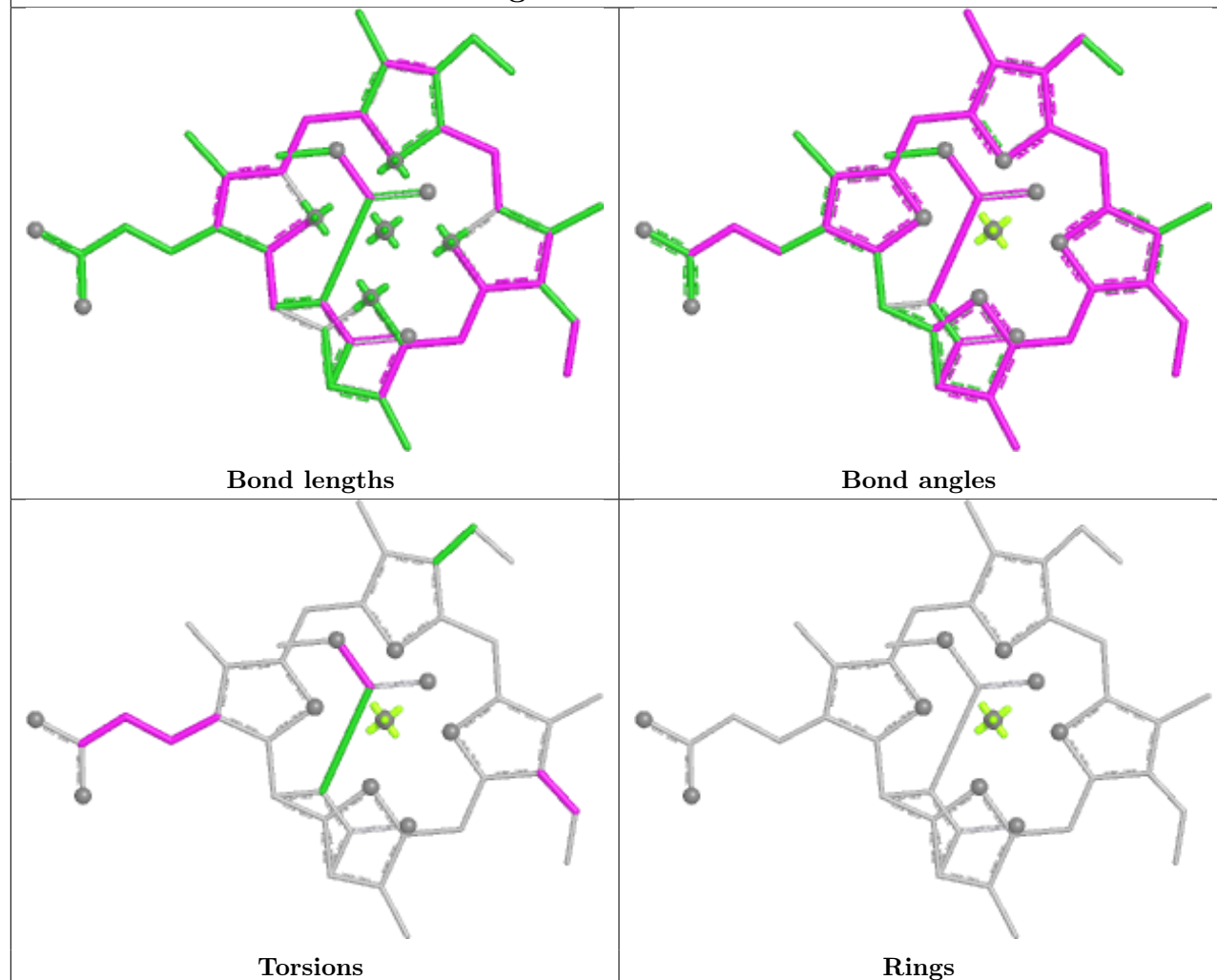


Rings

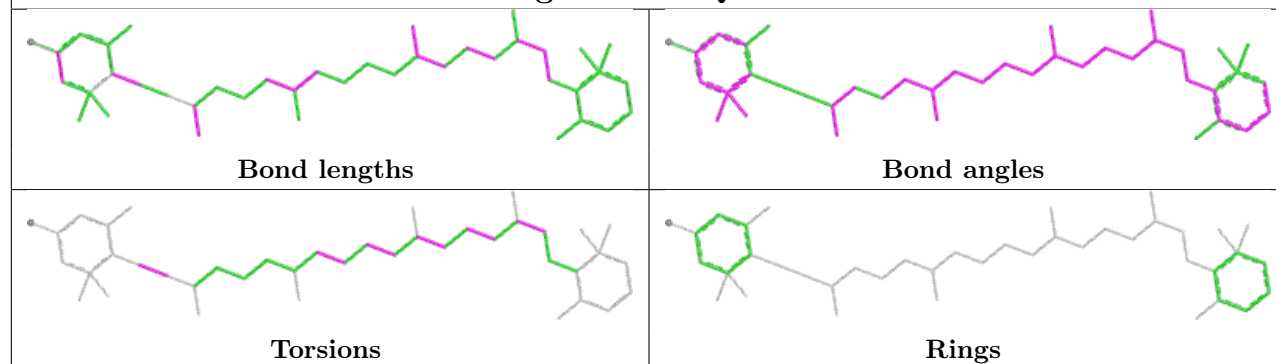




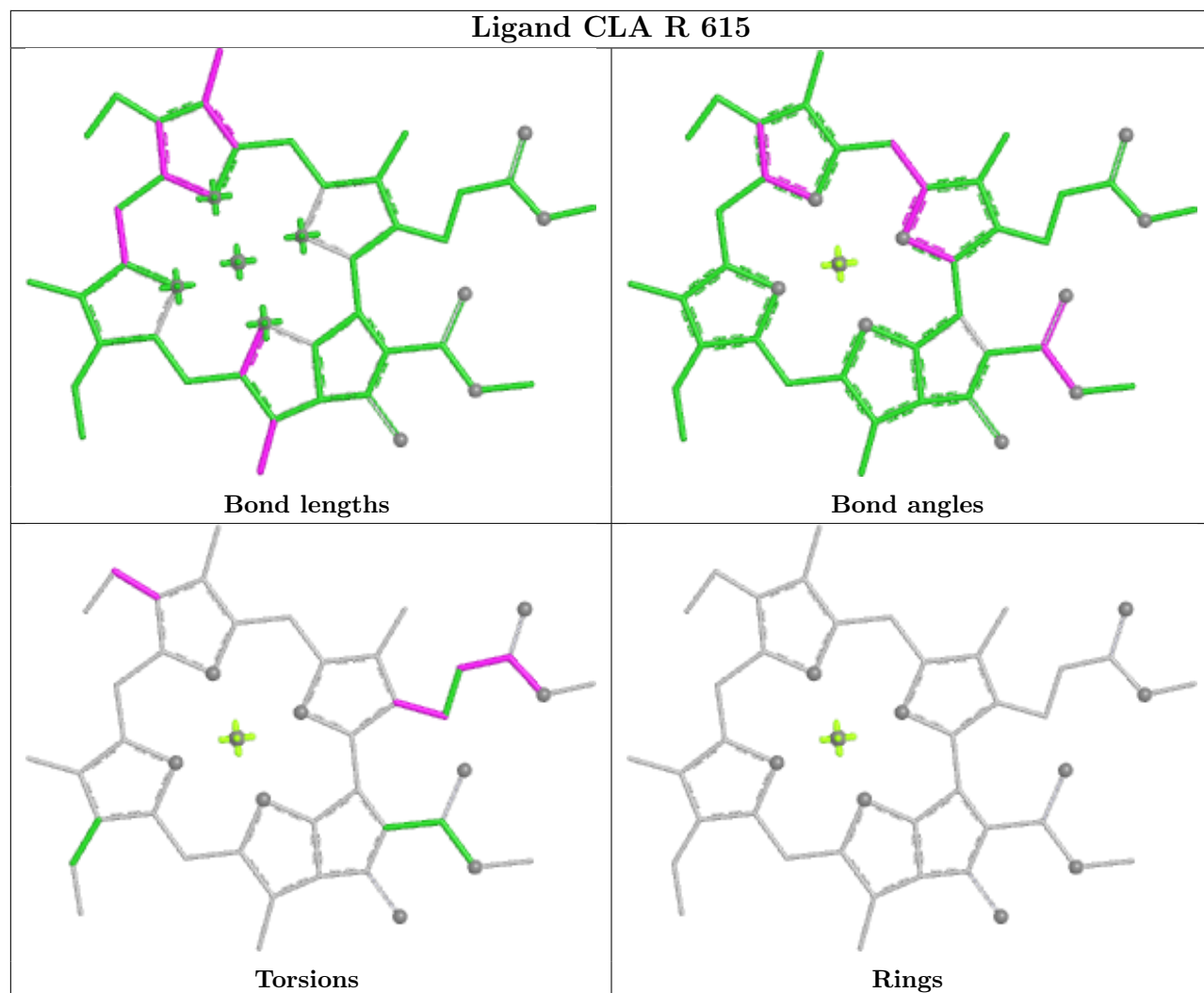
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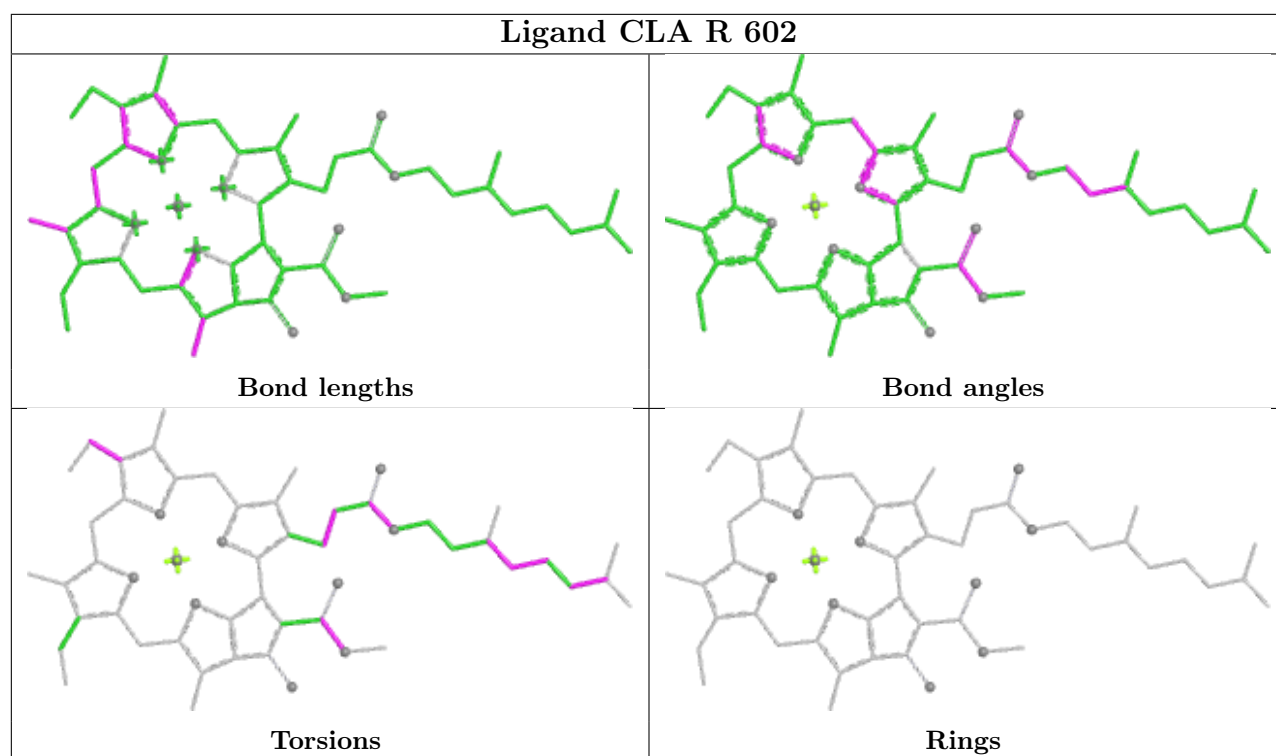


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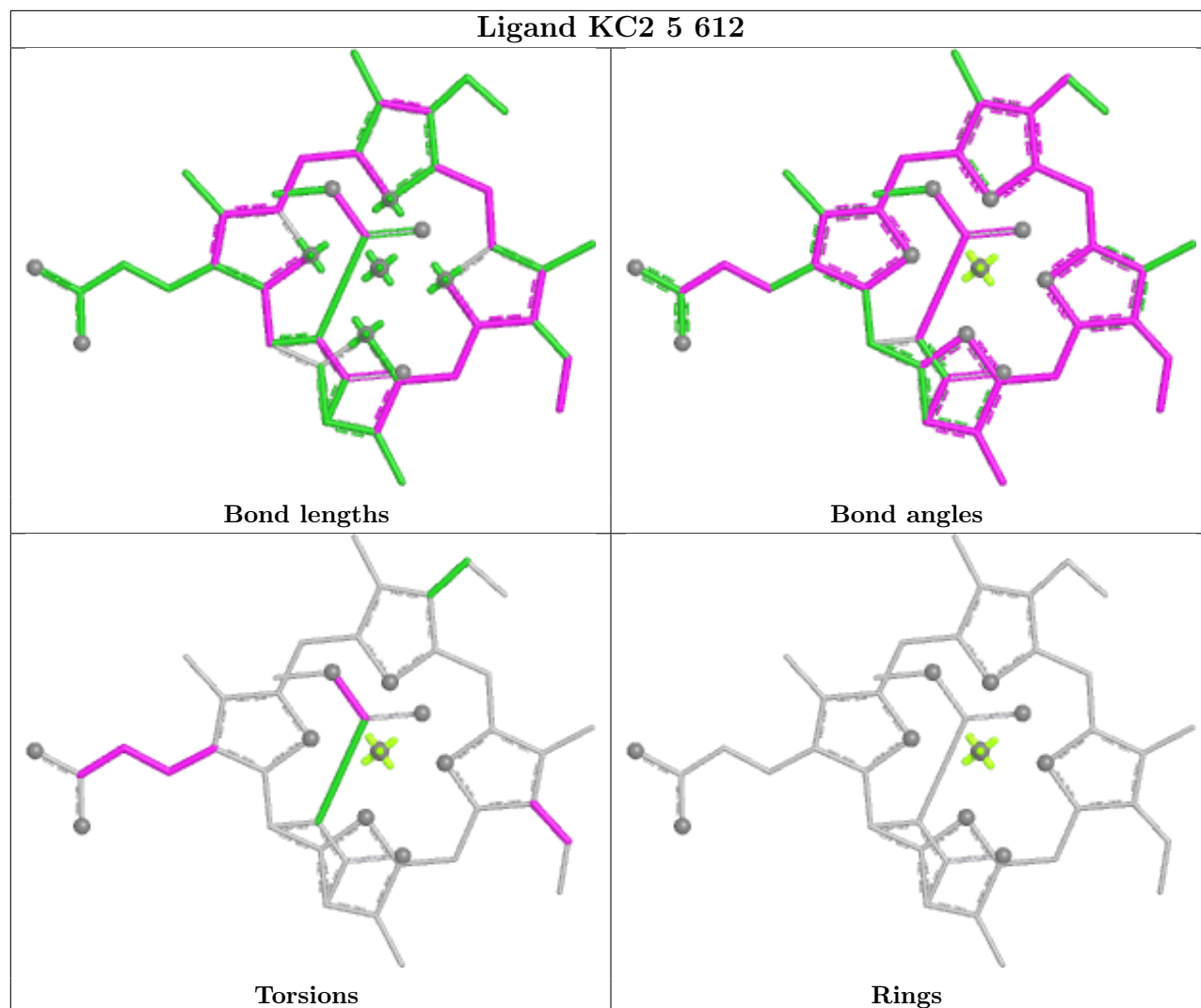


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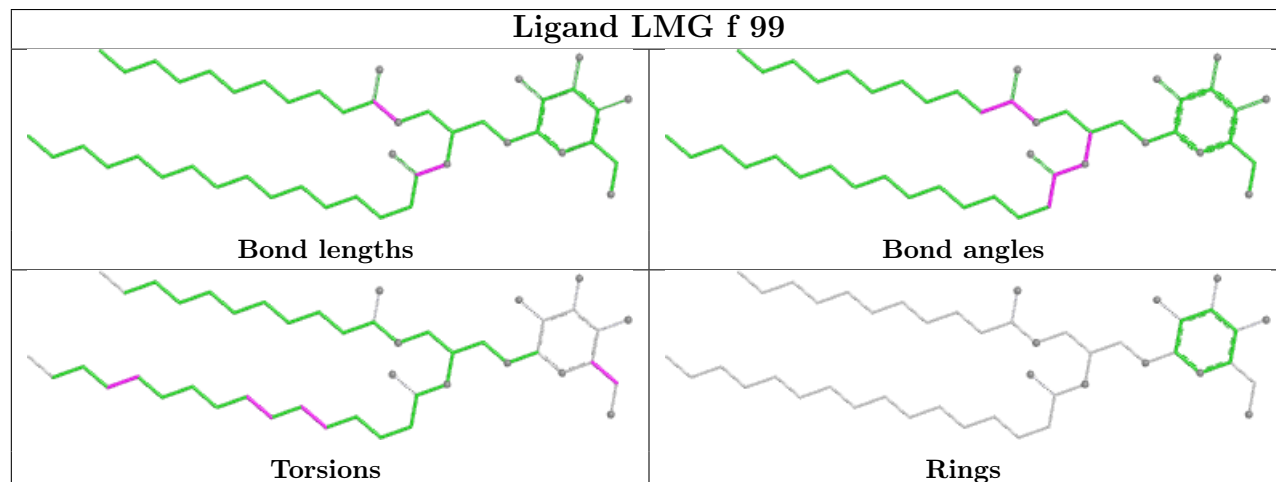


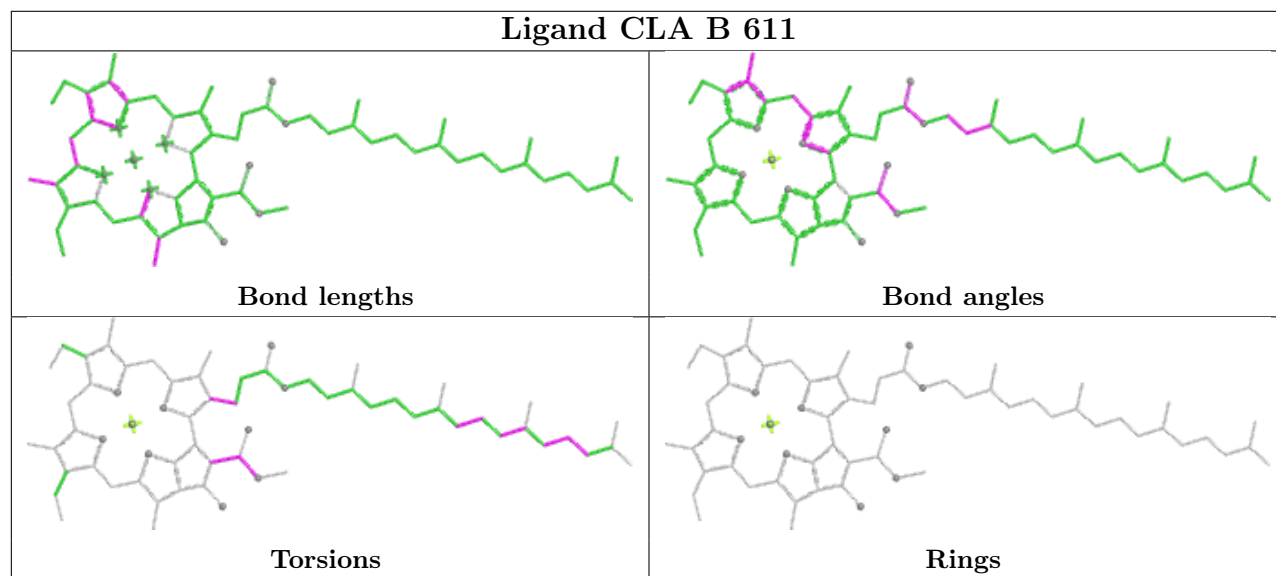
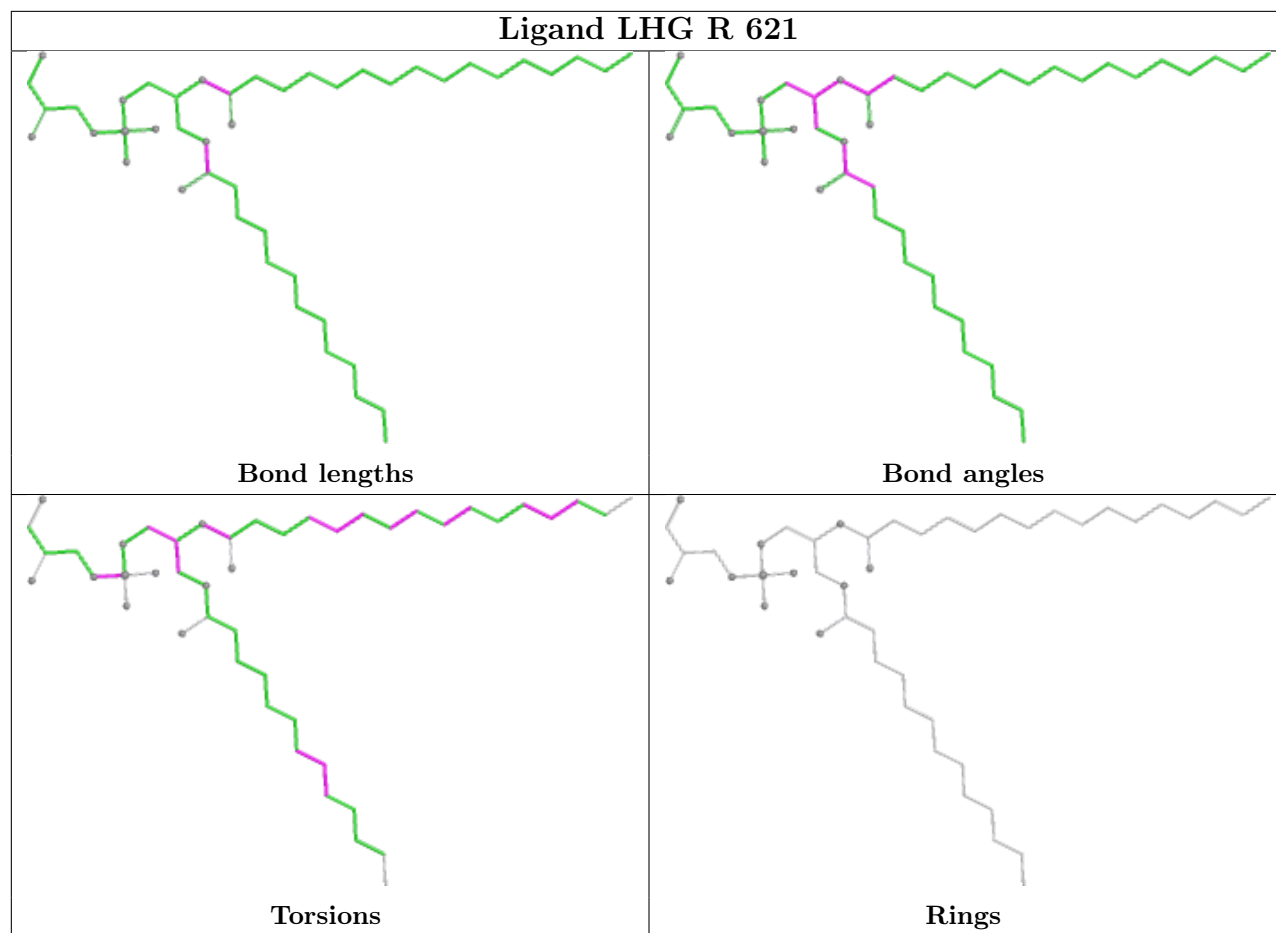


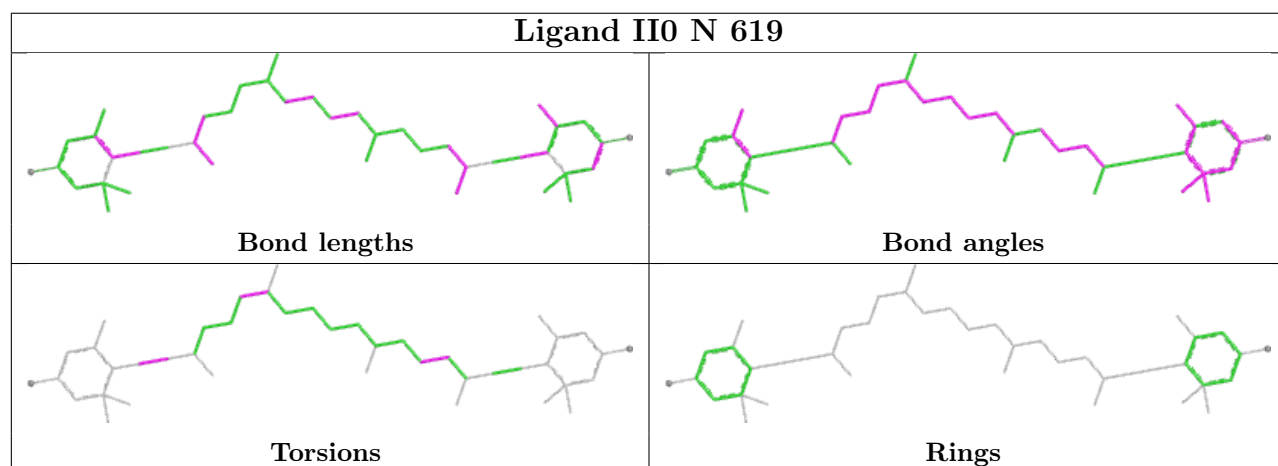
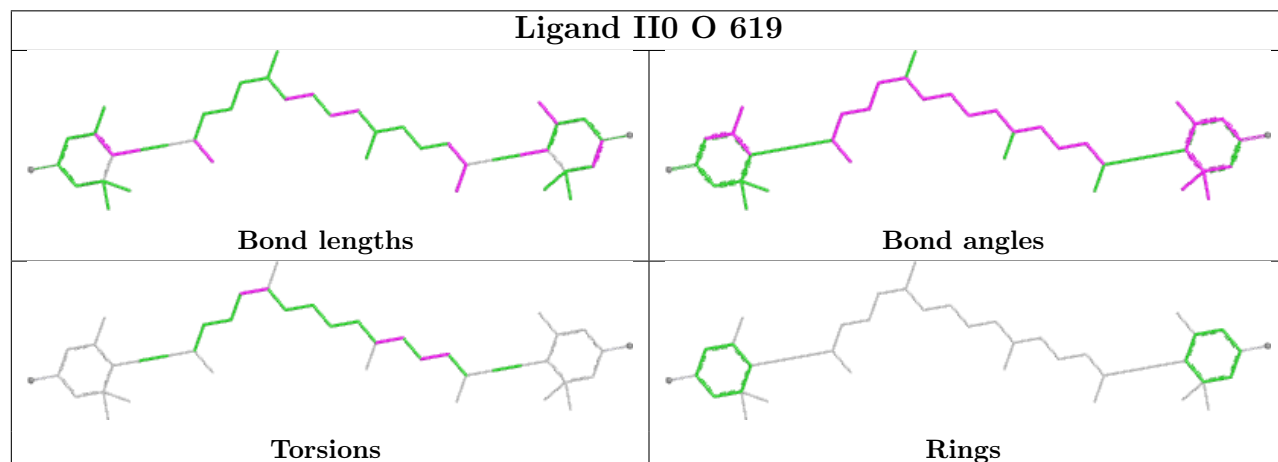
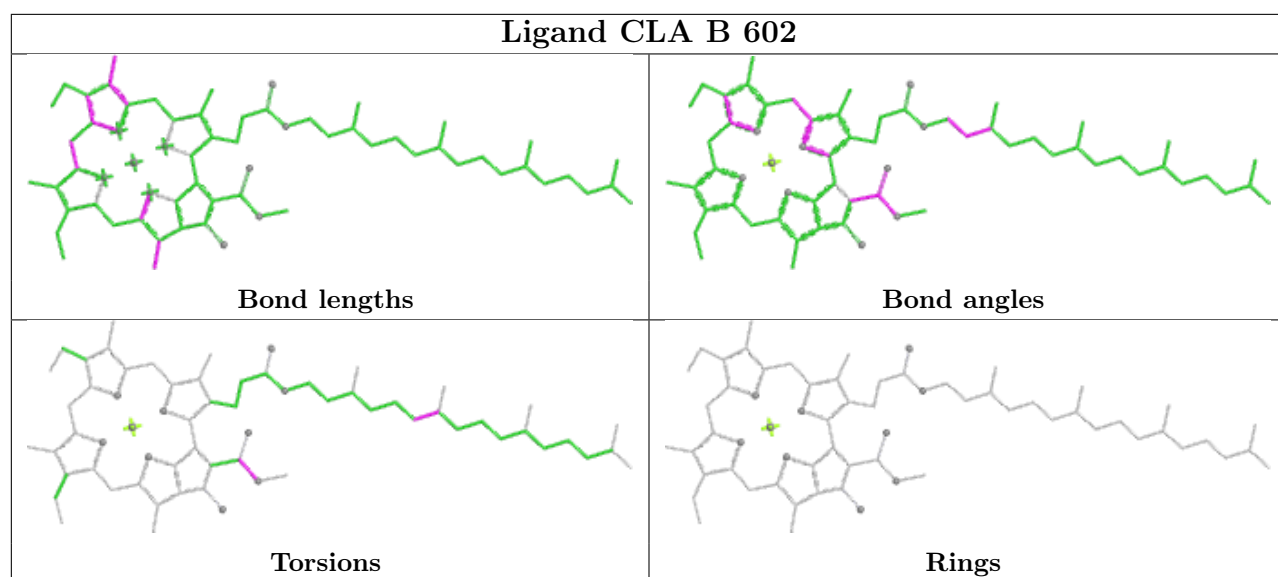
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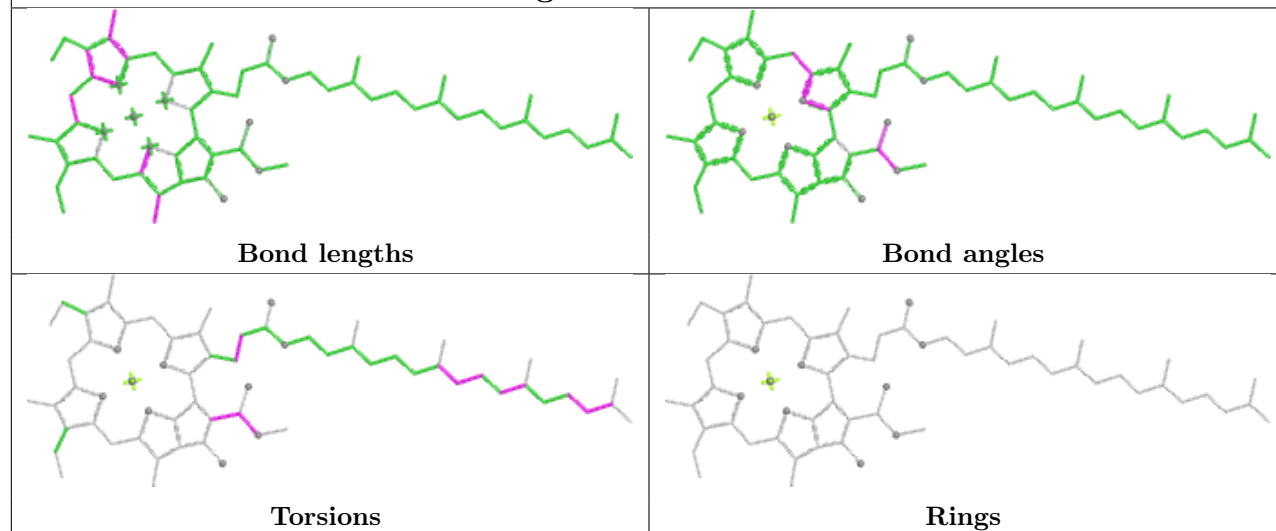
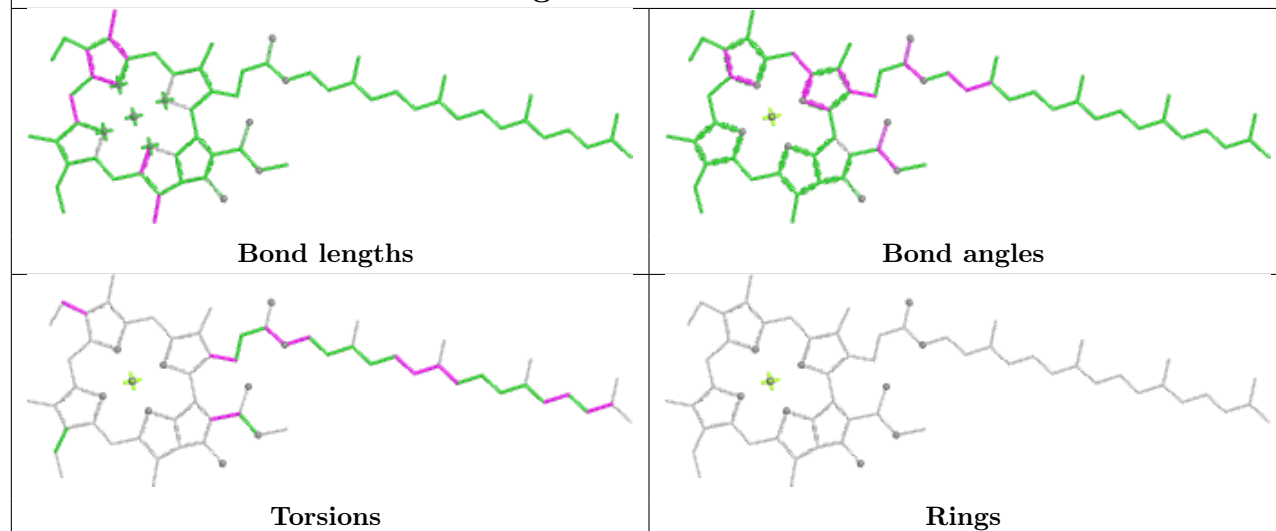


Ligand LMG f 99

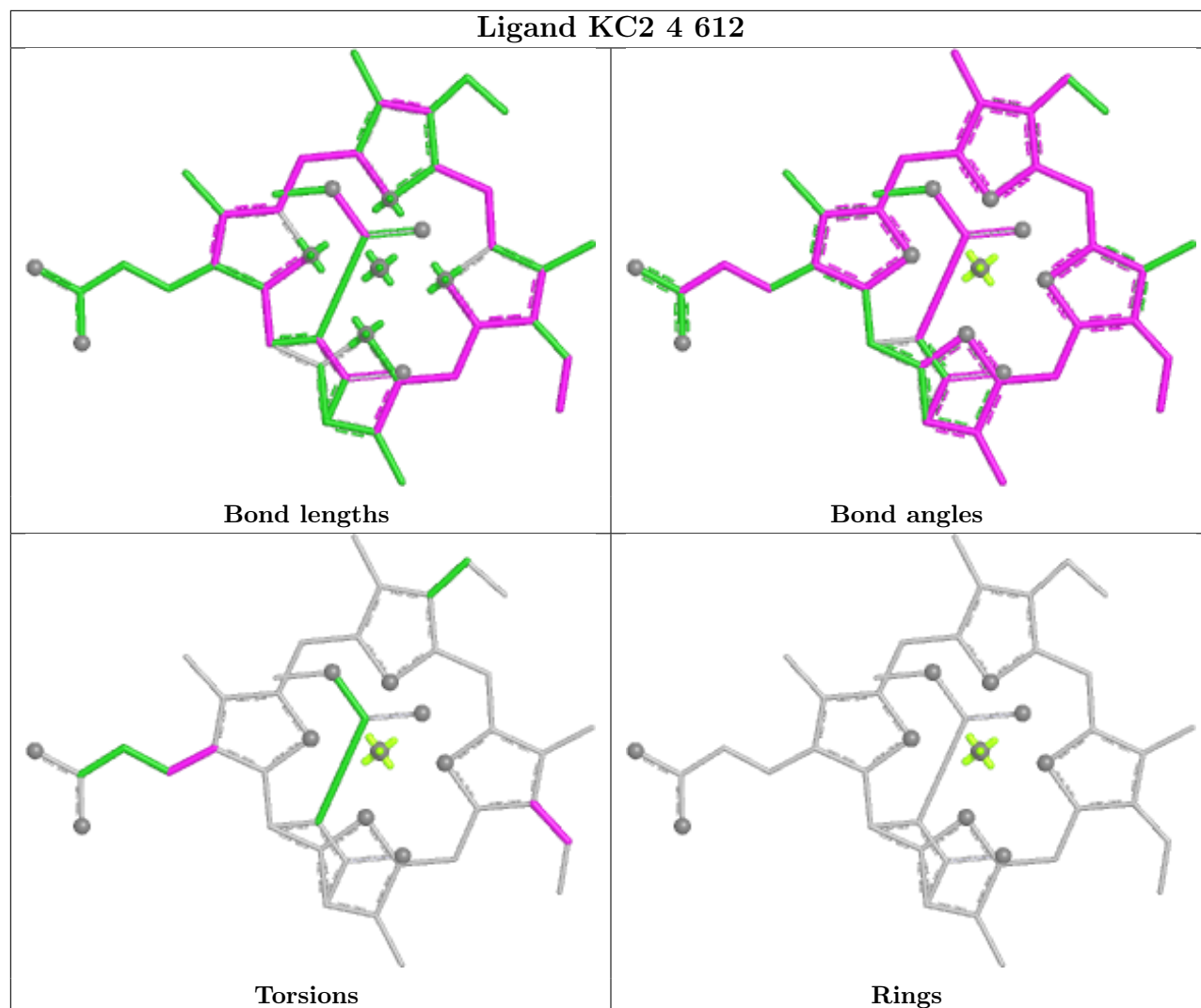




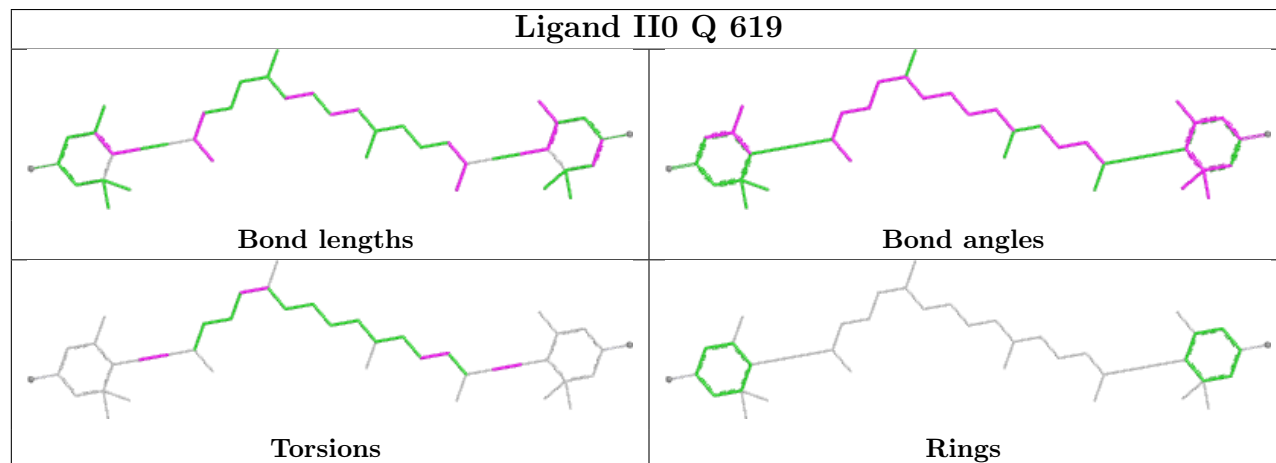


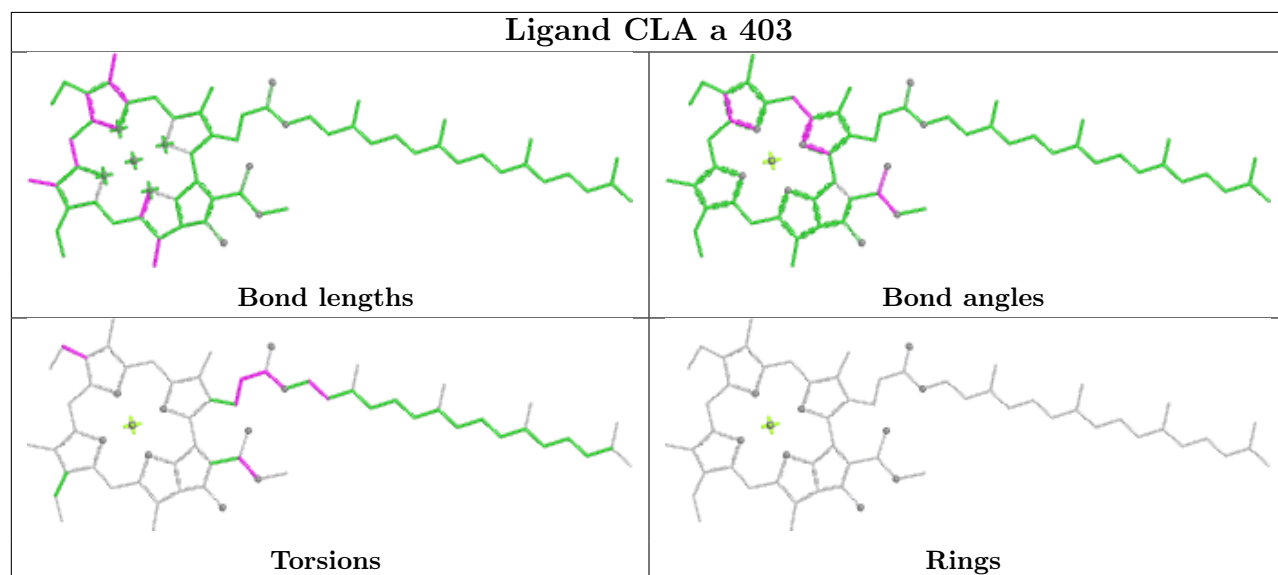
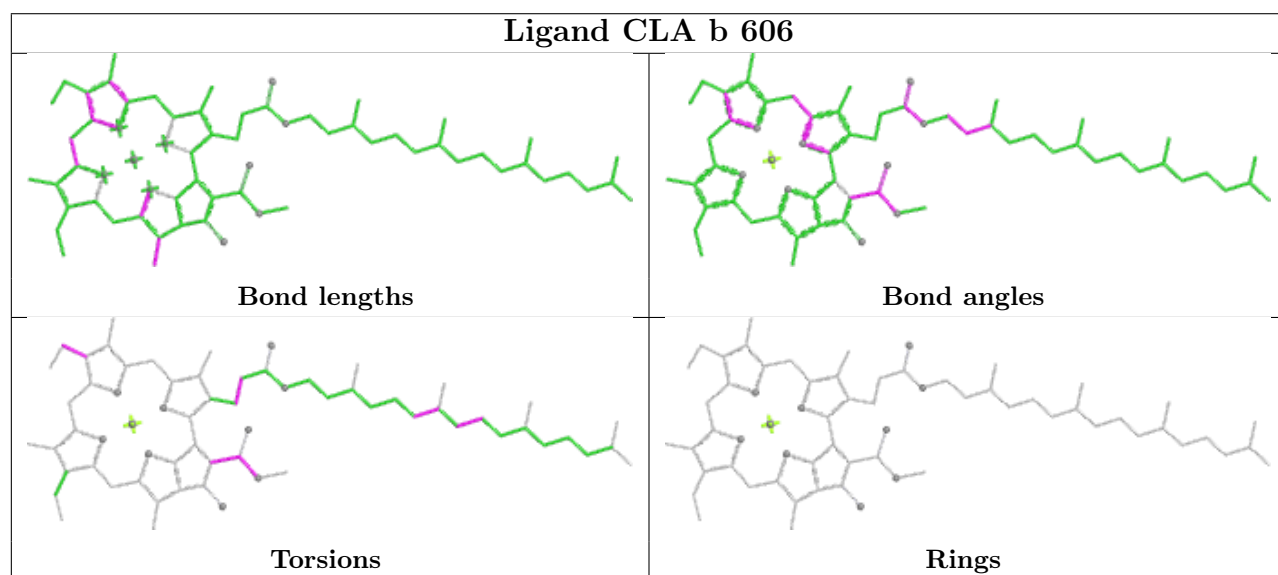
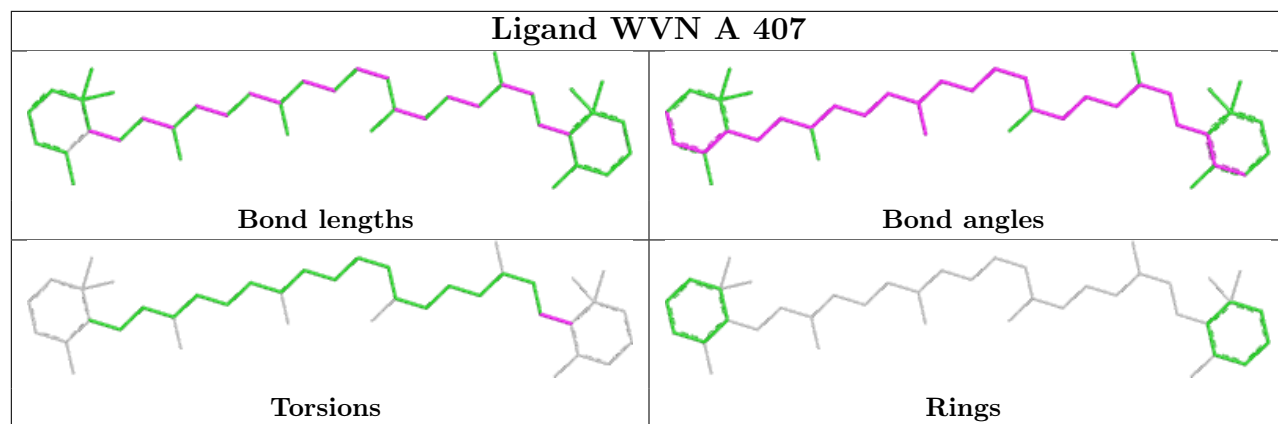
Ligand CLA 2 604**Ligand CLA P 603**

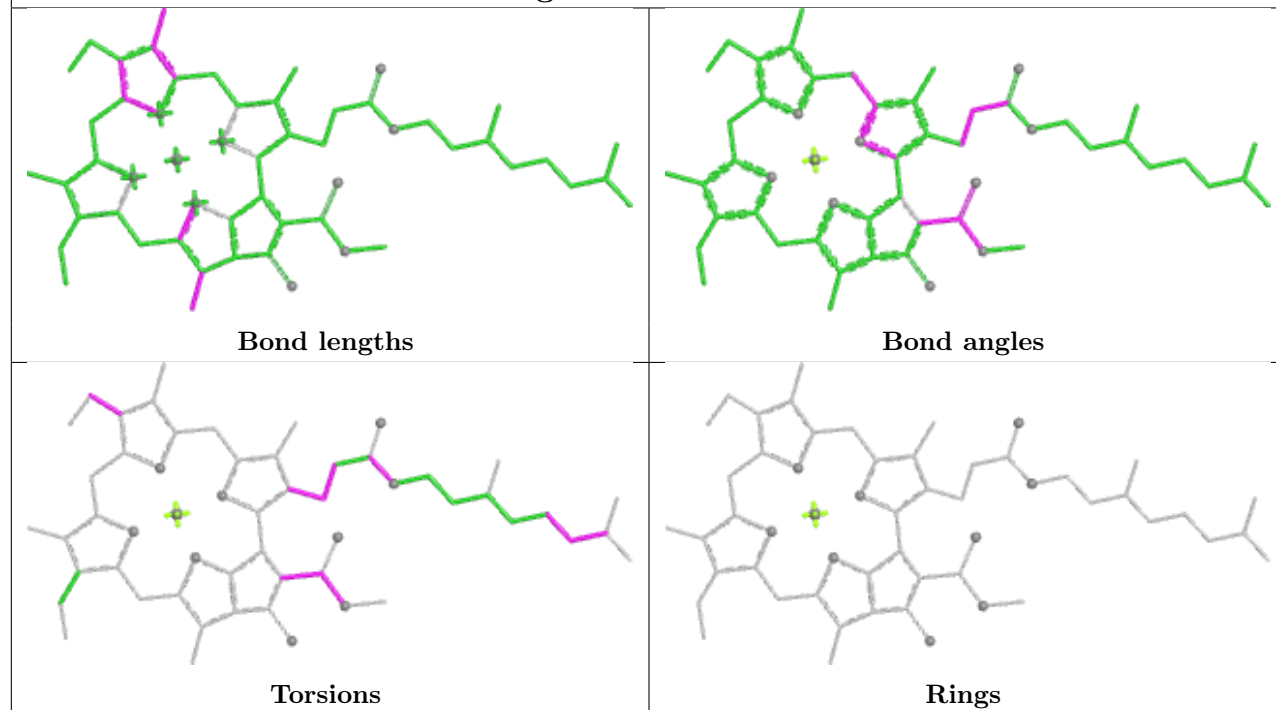
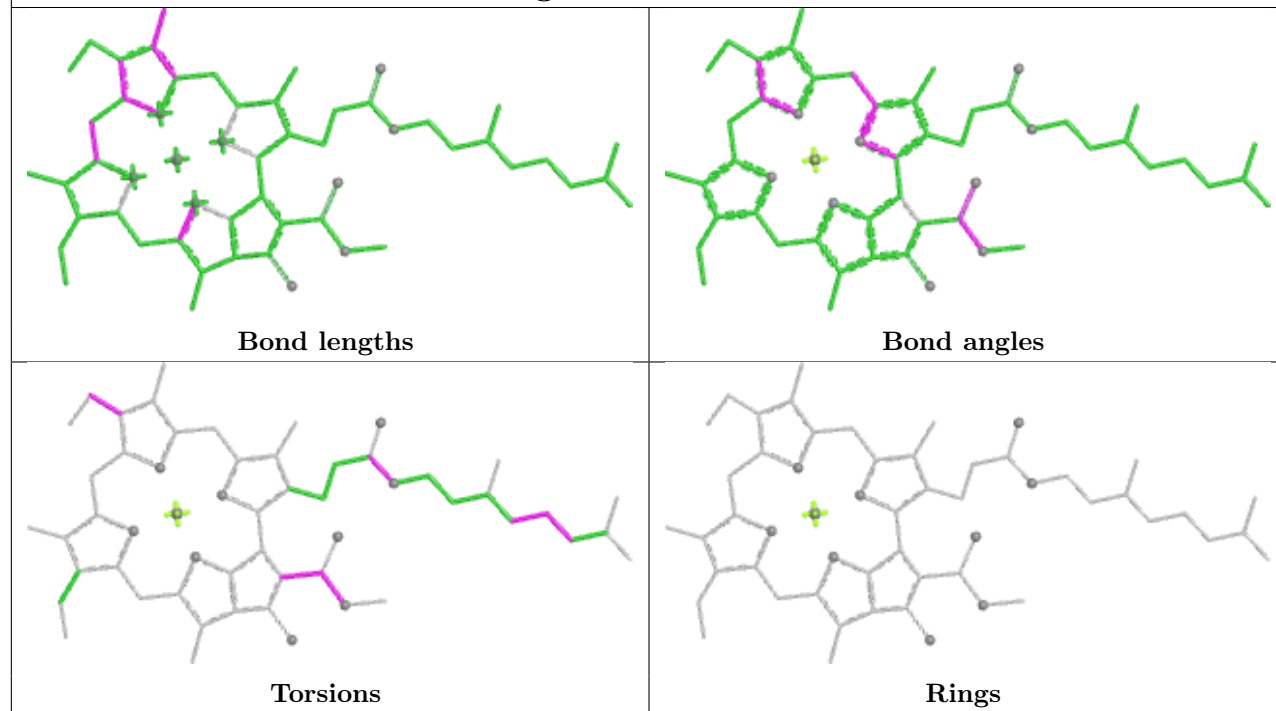
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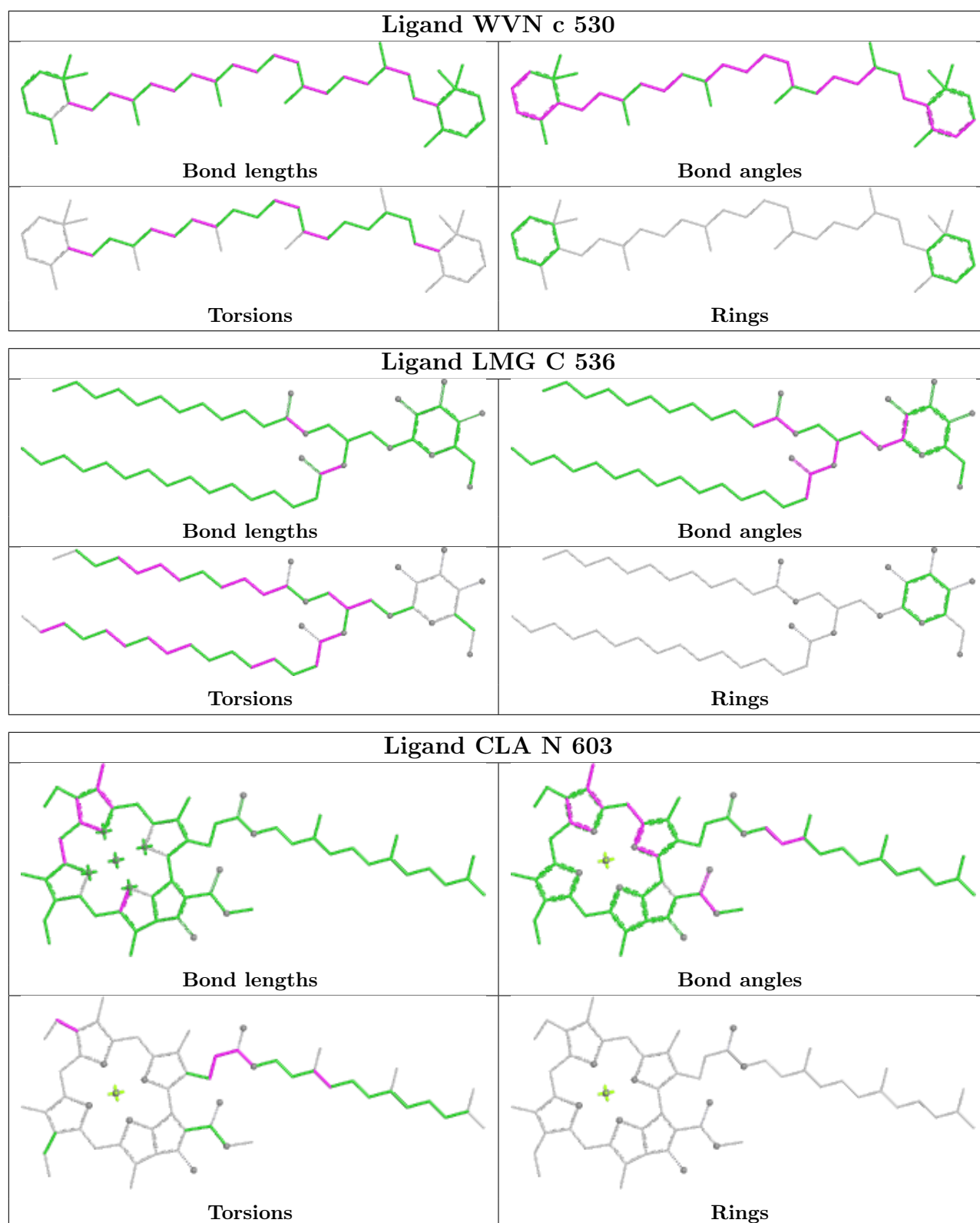


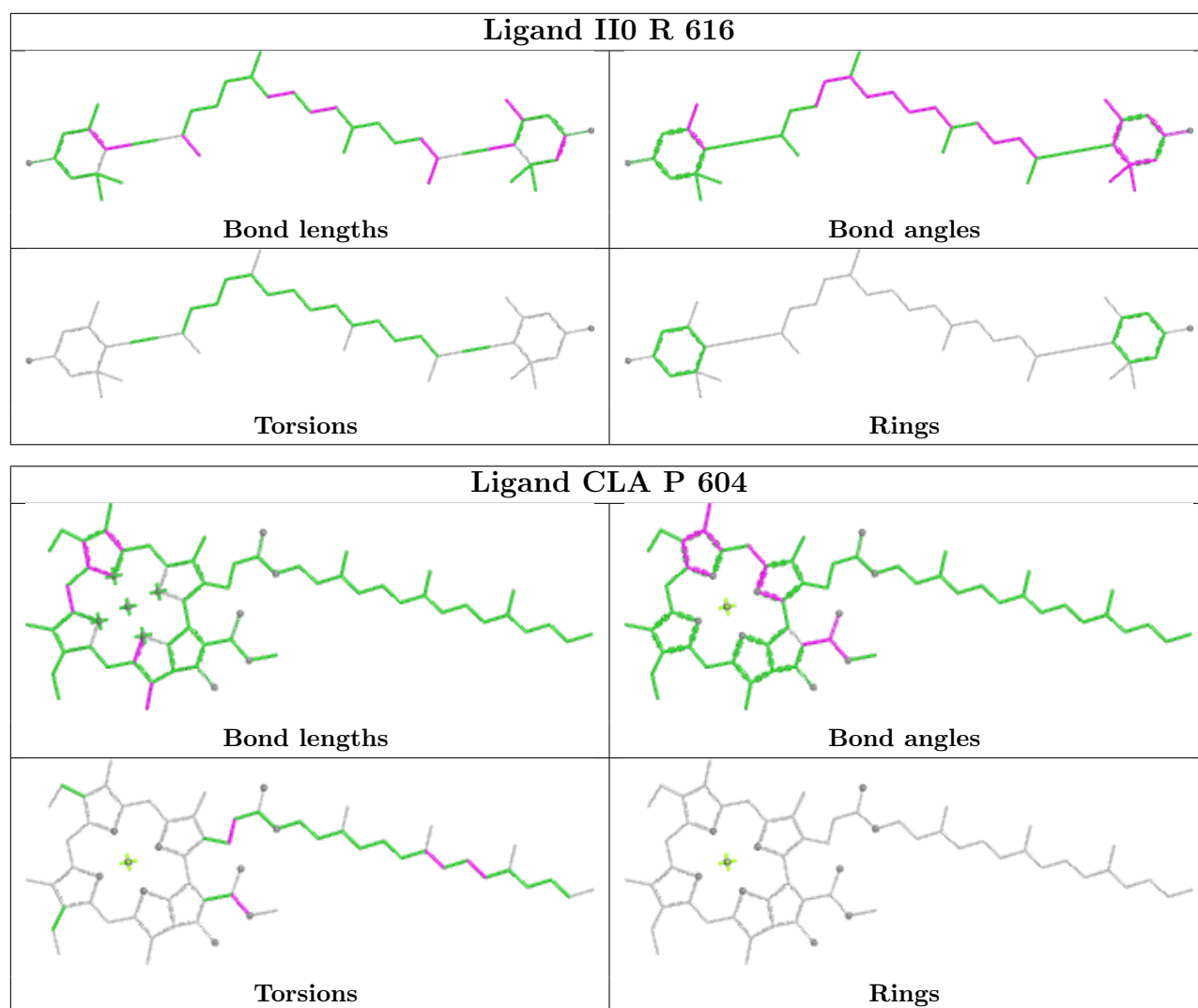
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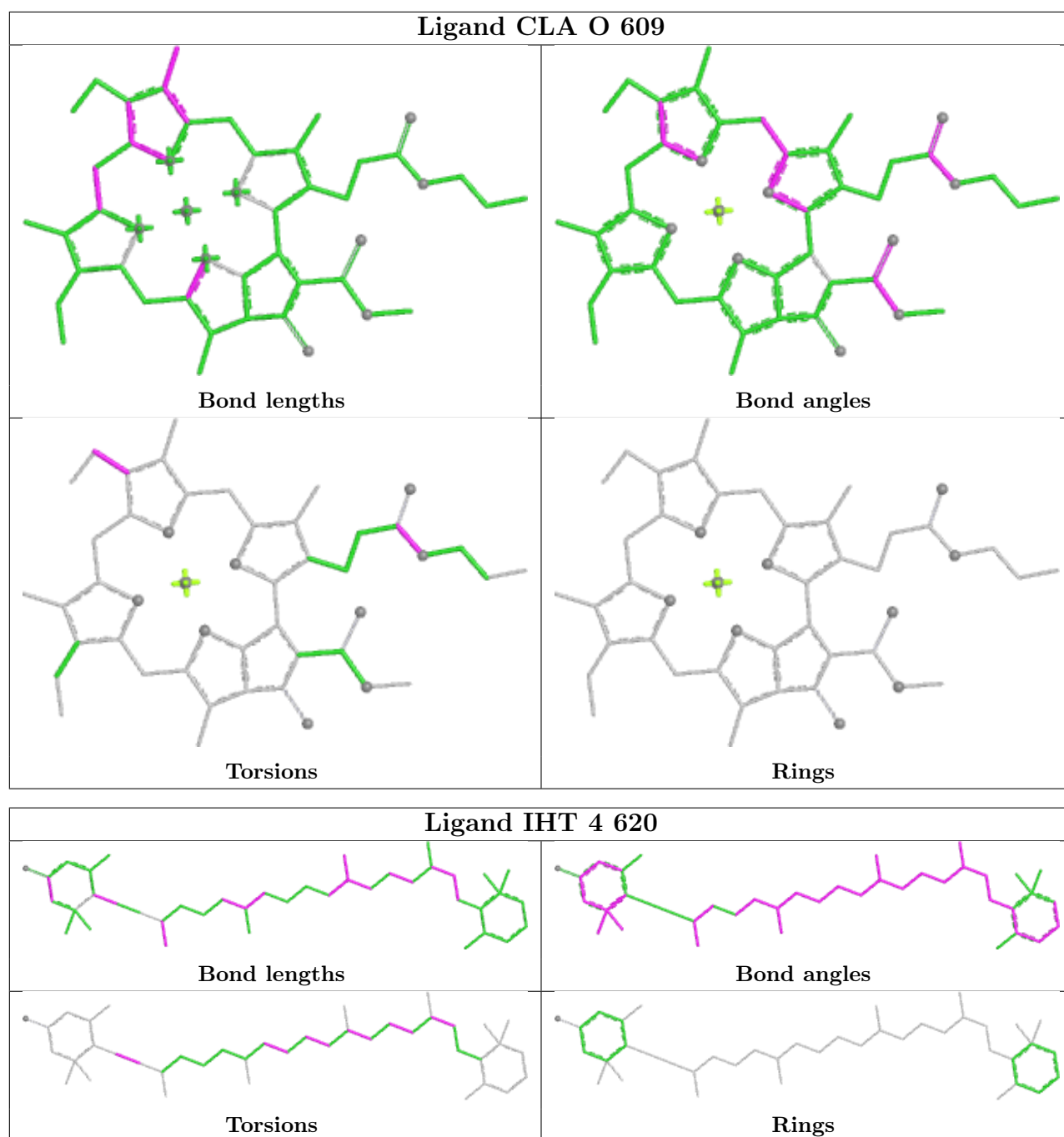




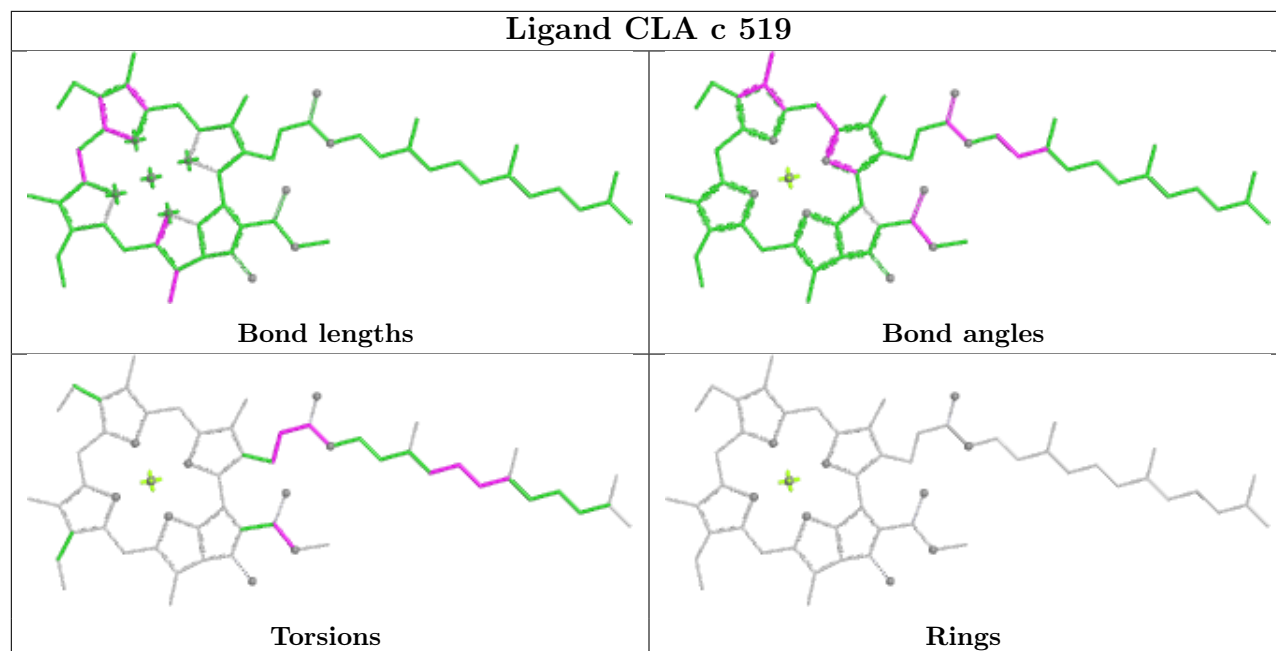
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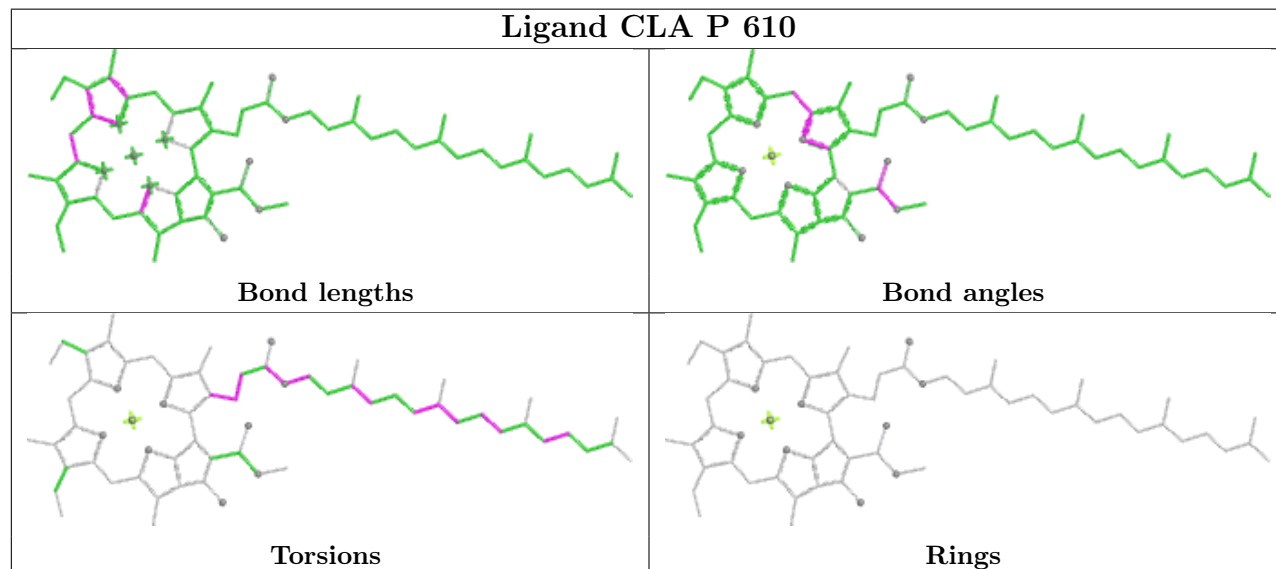




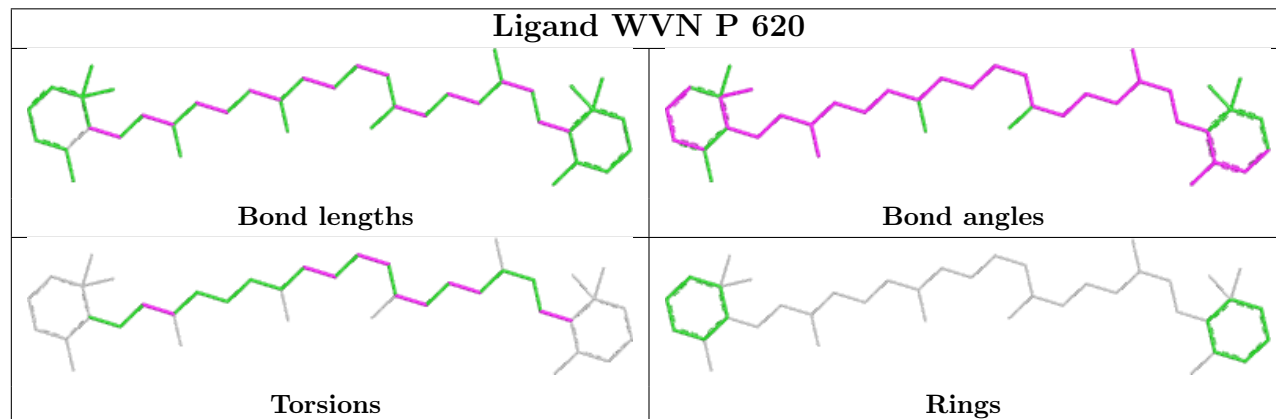
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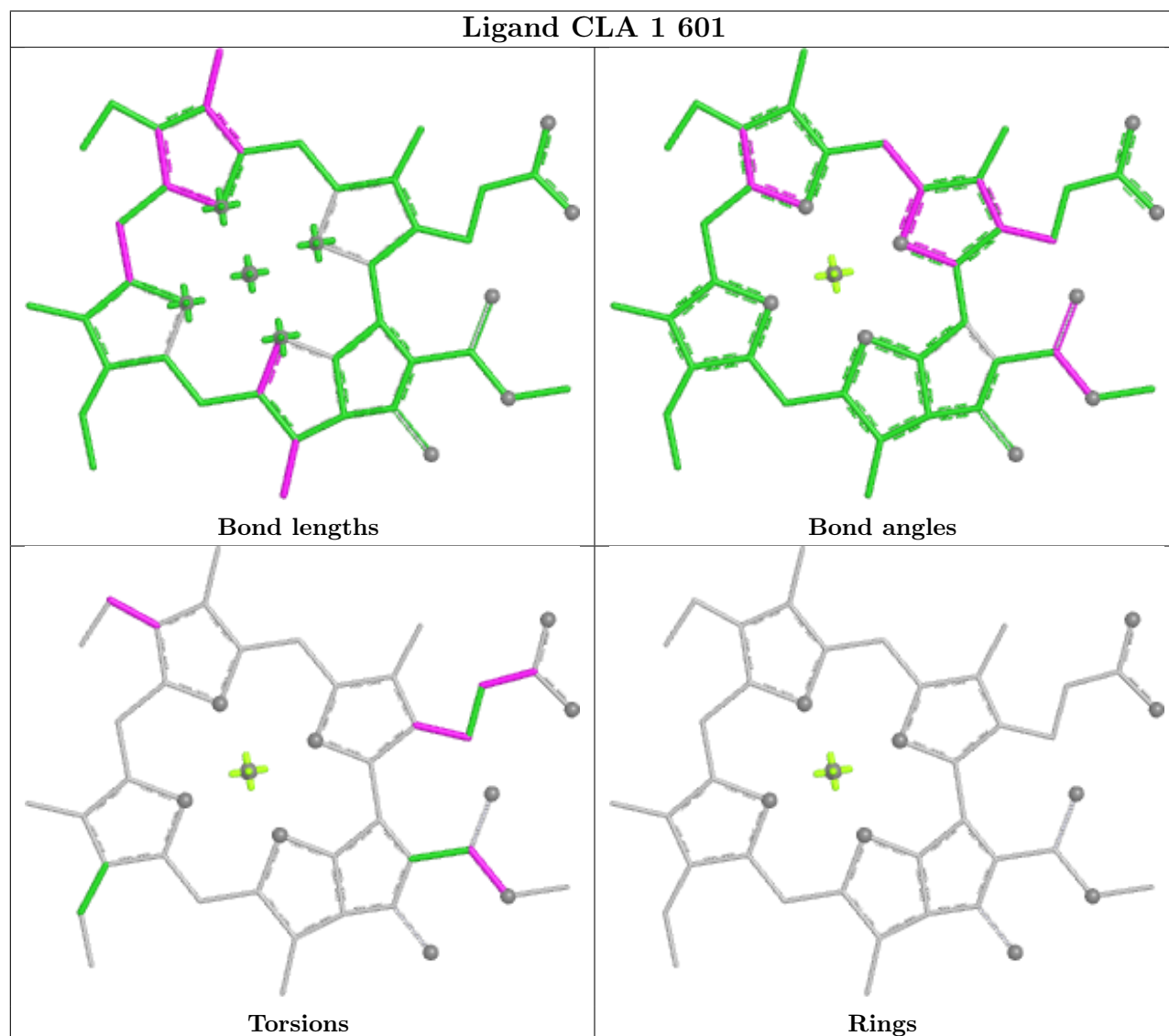
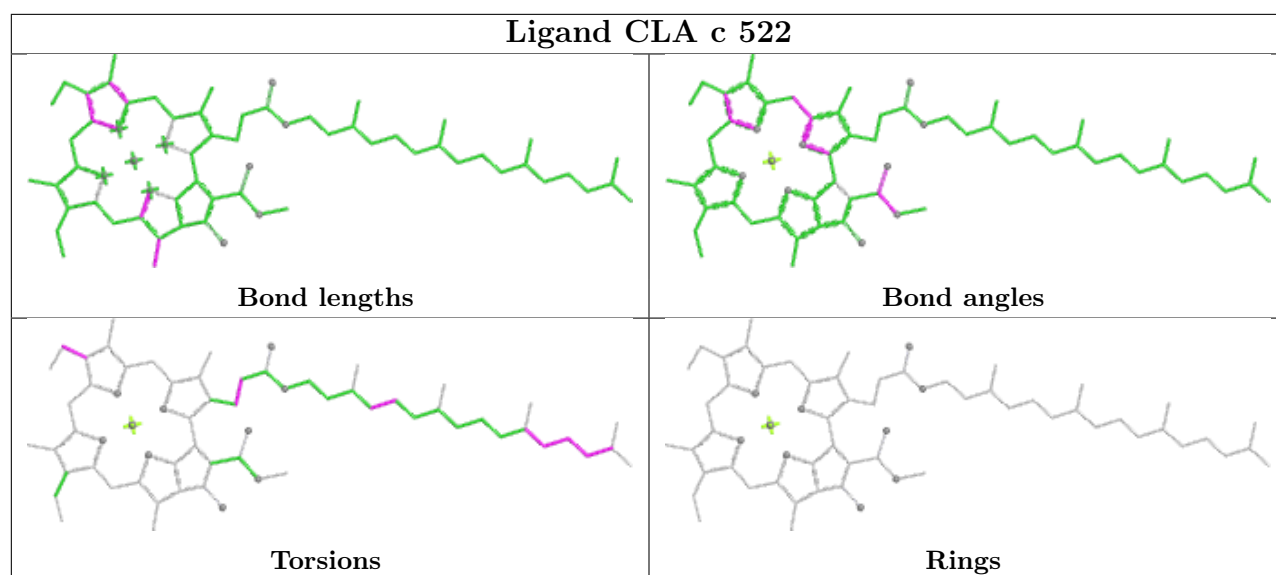


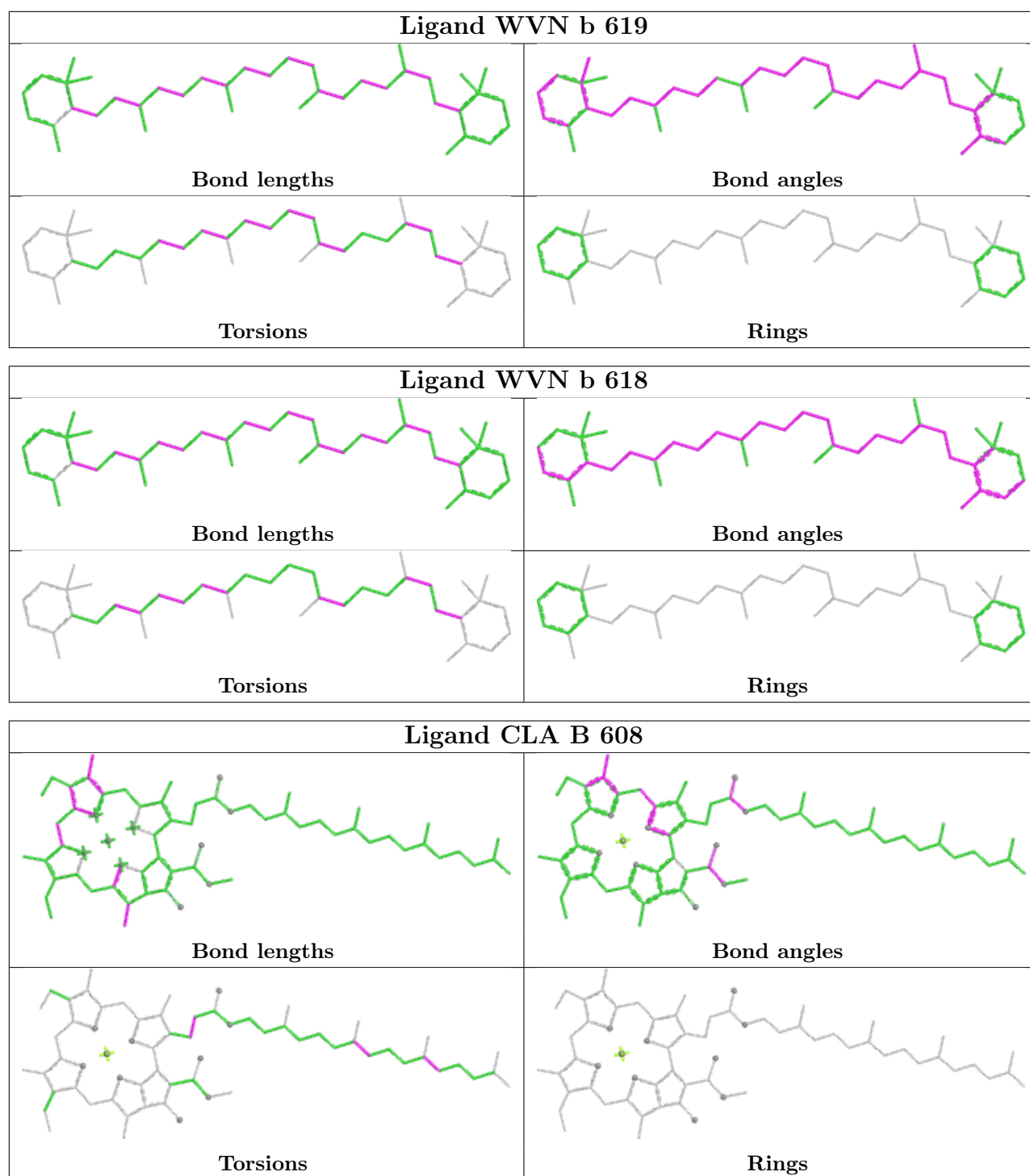
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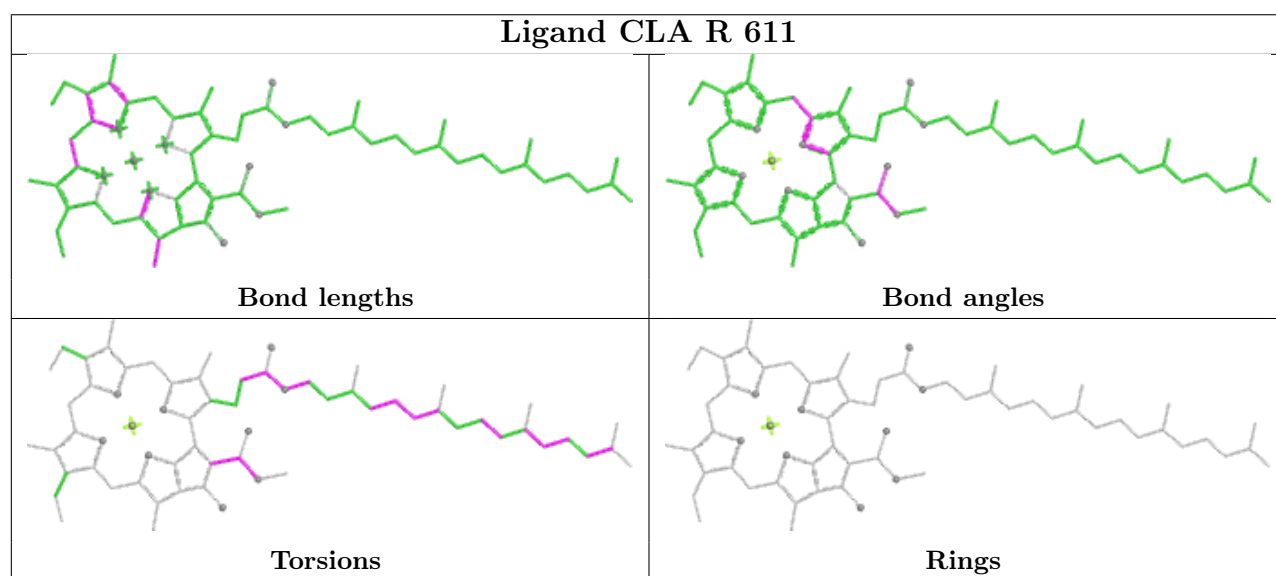
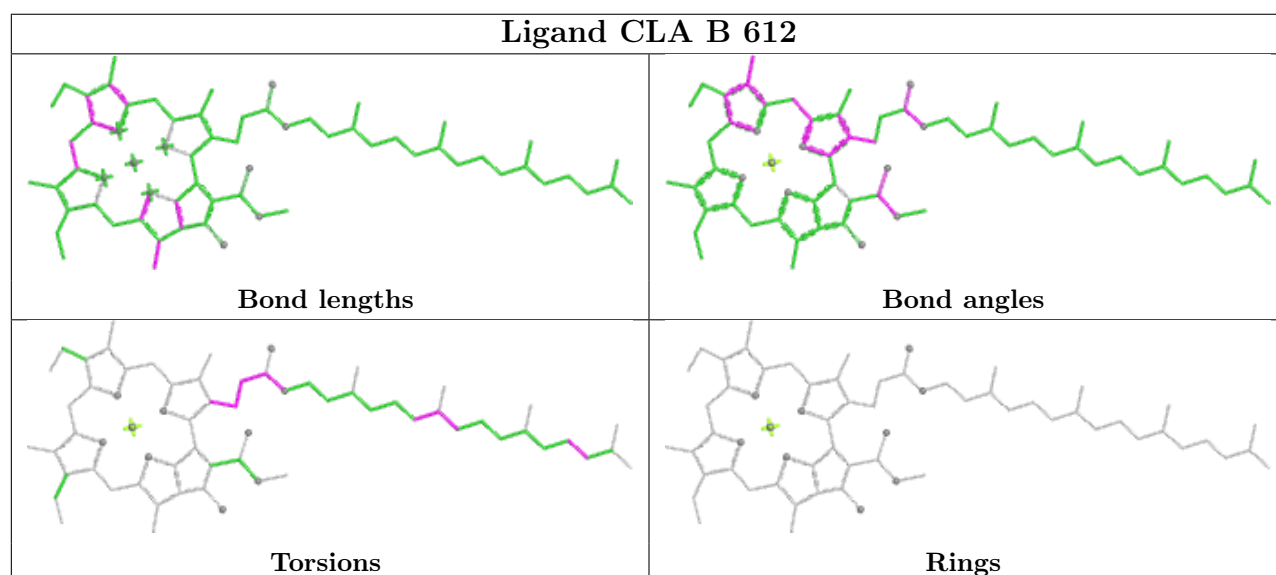
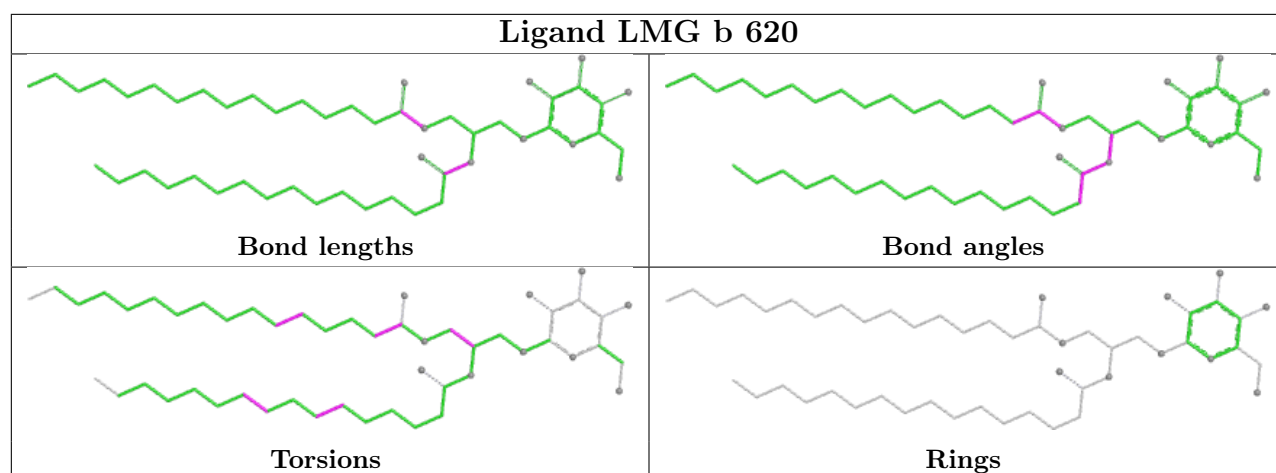


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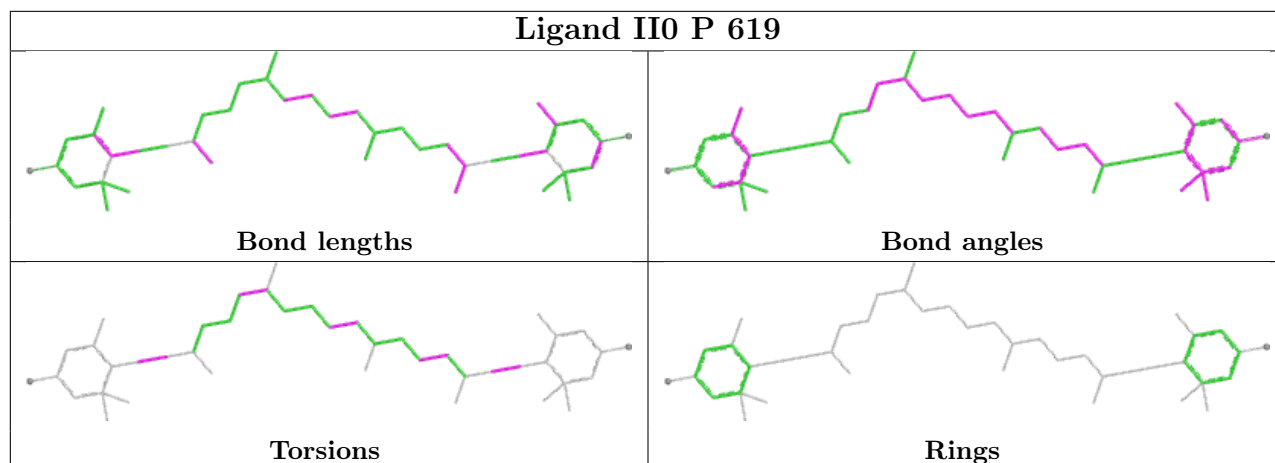




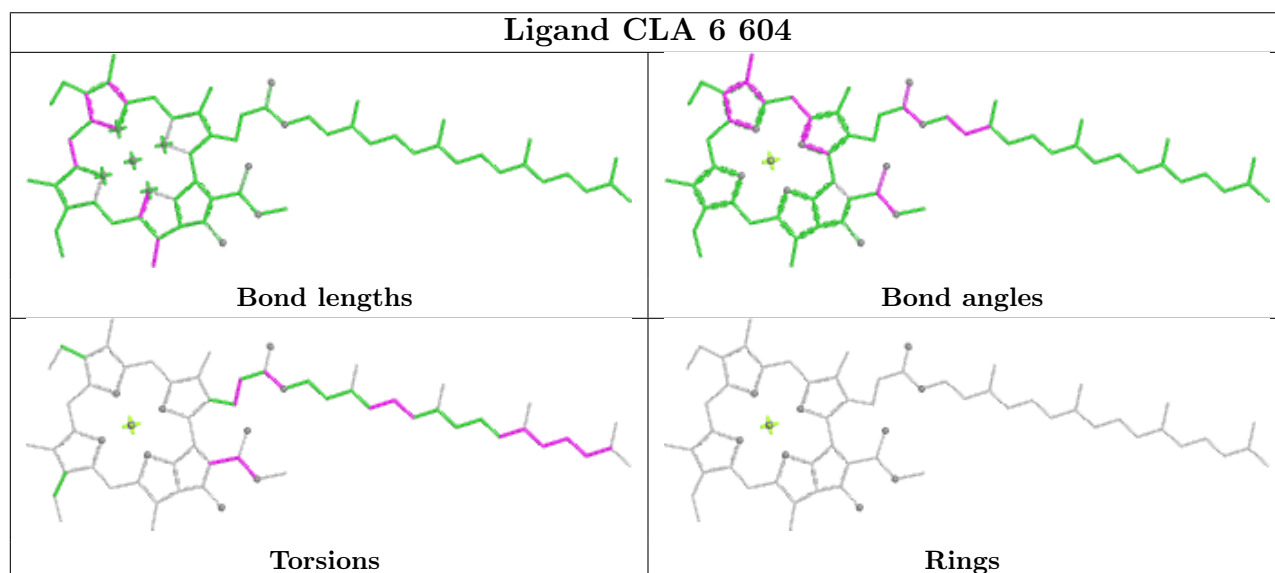




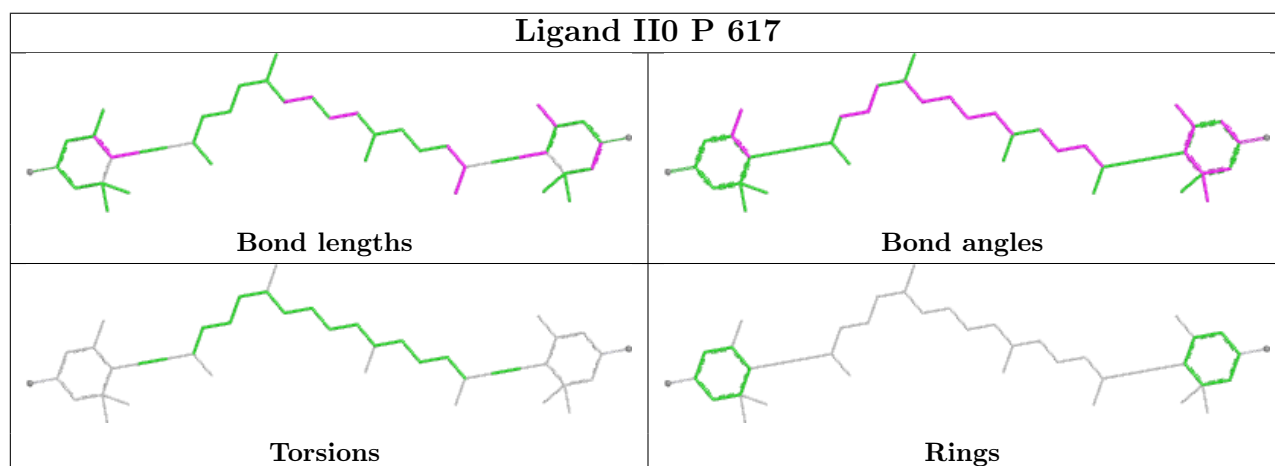
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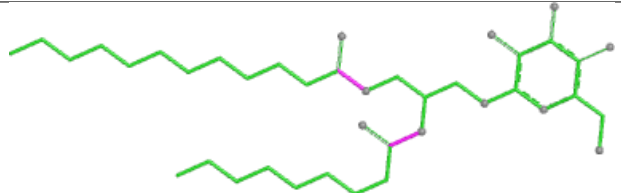
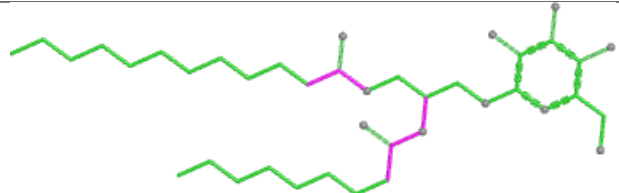
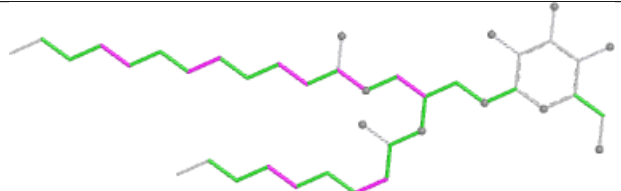
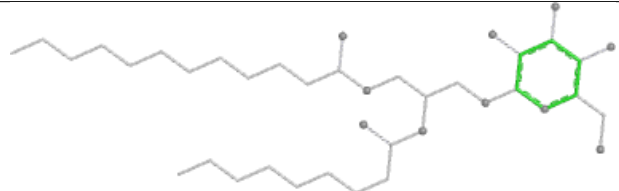


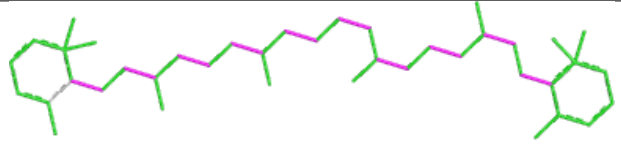
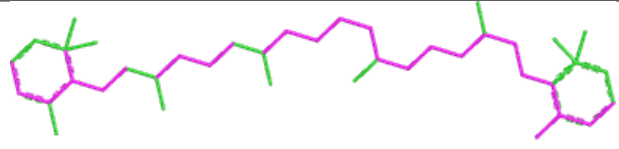
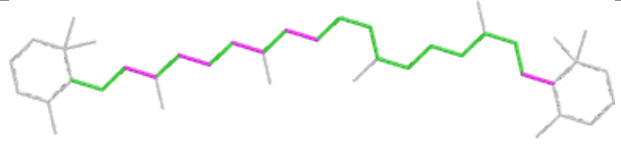
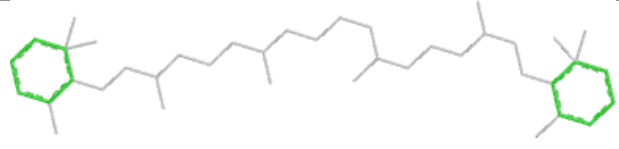
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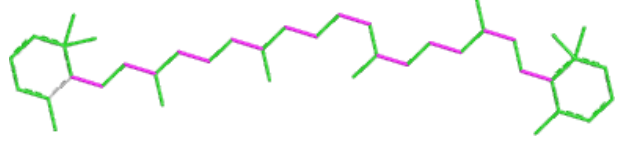
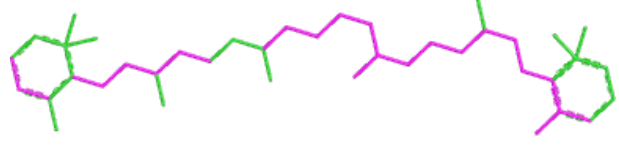
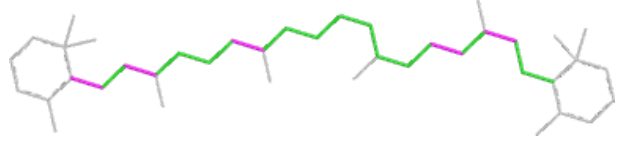
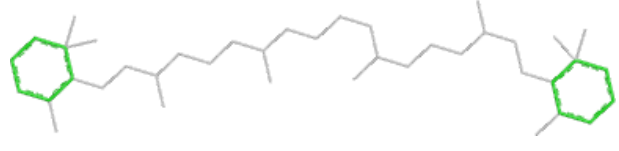


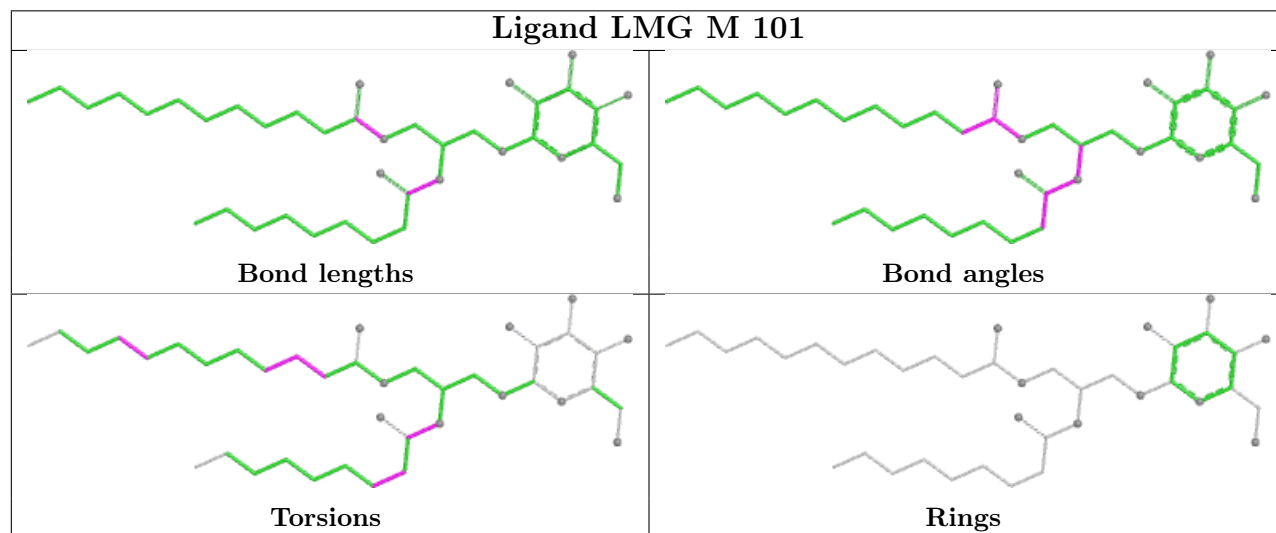
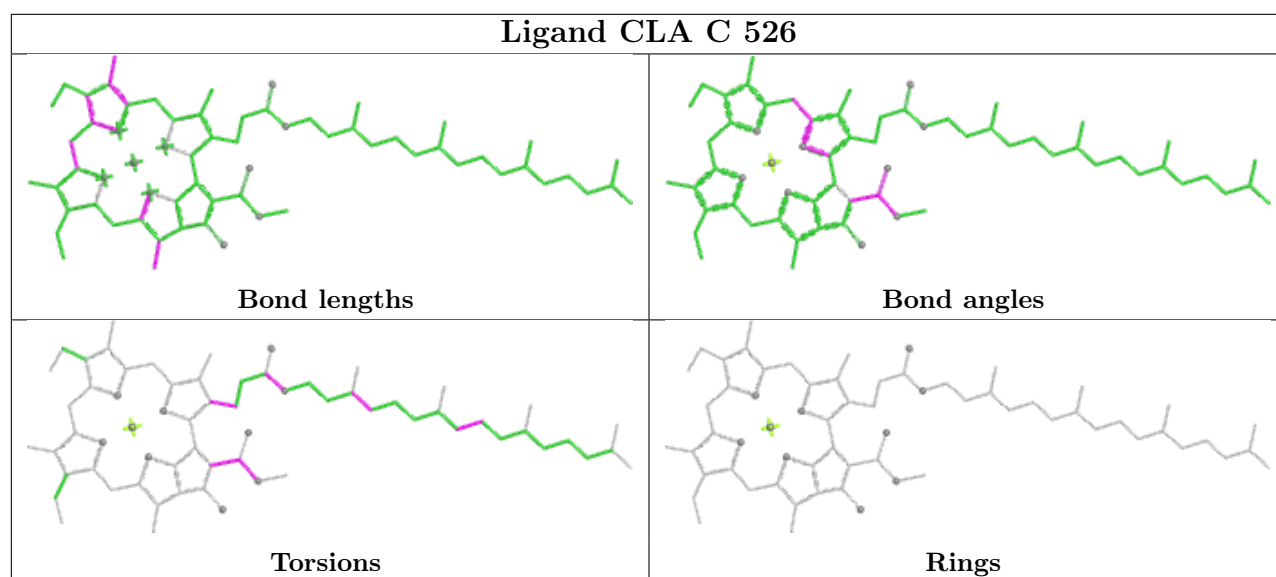
Ligand II0 P 617



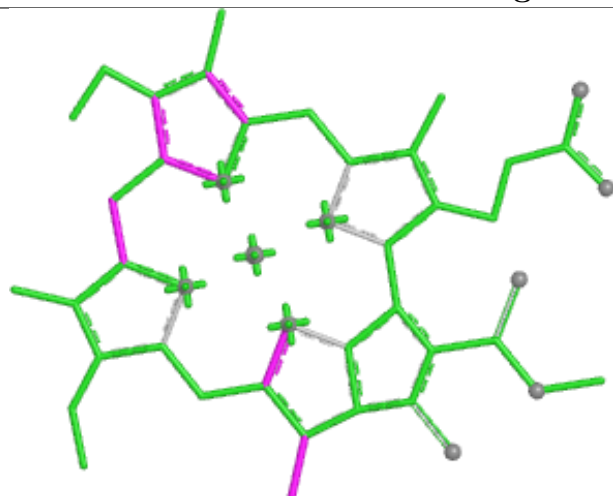
Ligand LMG d 402	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand WVN H 89	
	
Bond lengths	Bond angles
	
Torsions	Rings

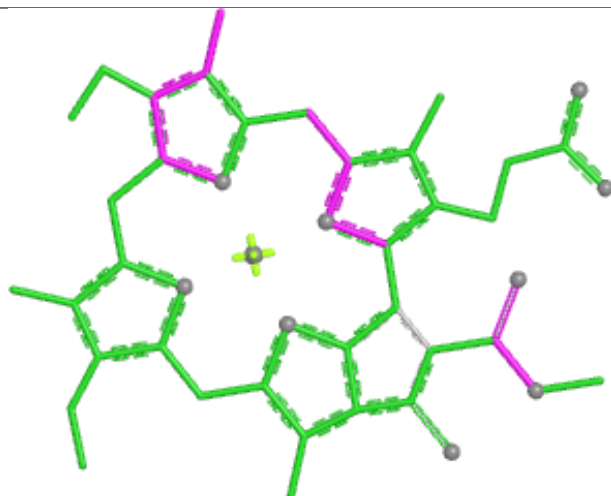
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Bond lengths	Bond angles
	
Torsions	Rings



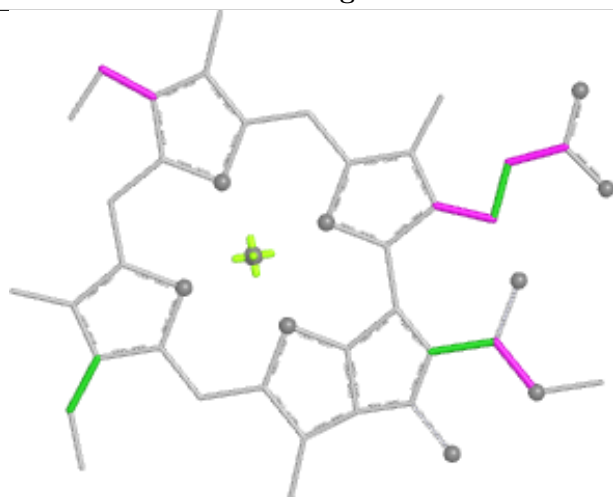
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Bond lengths



Bond angles

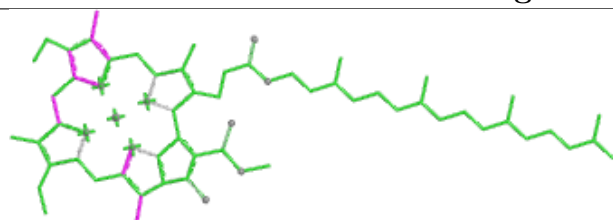


Torsions

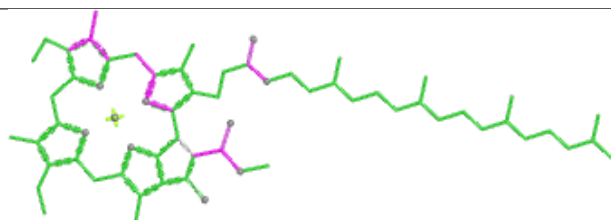


Rings

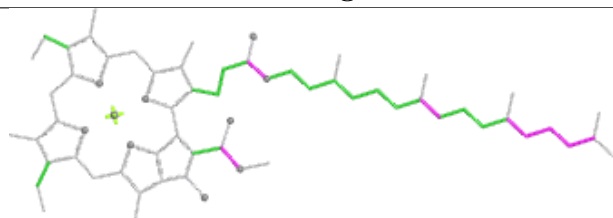
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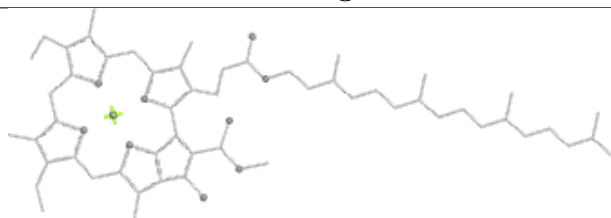
Bond lengths



Bond angles

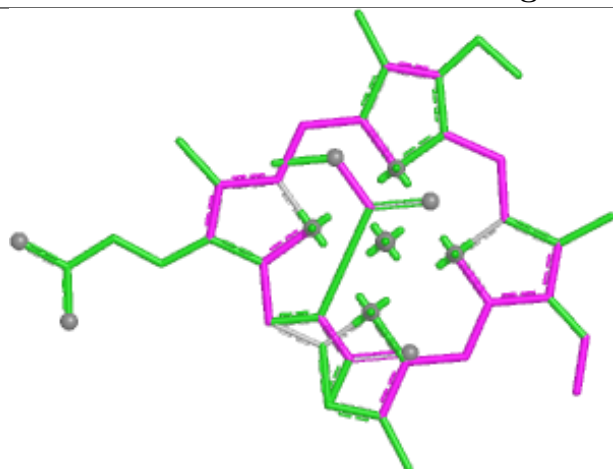


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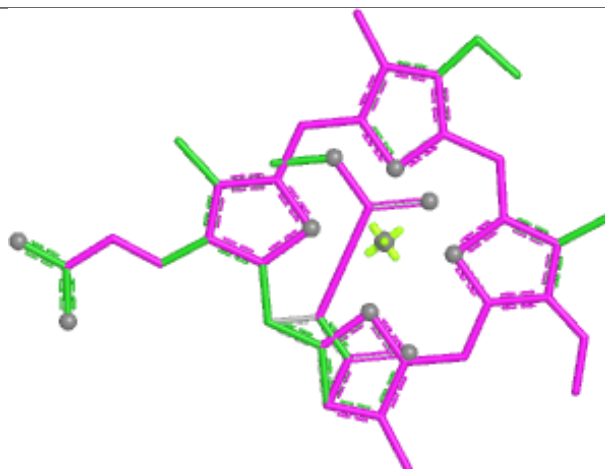


Rings

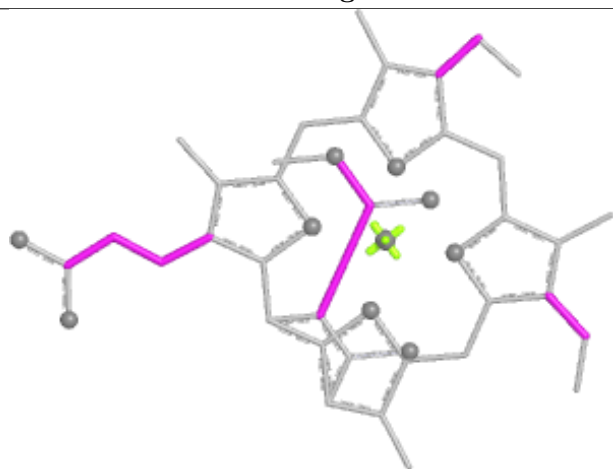
Ligand KC2 1 605



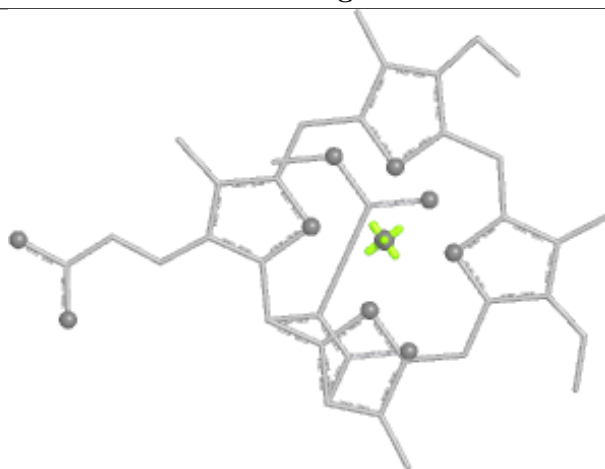
Bond lengths



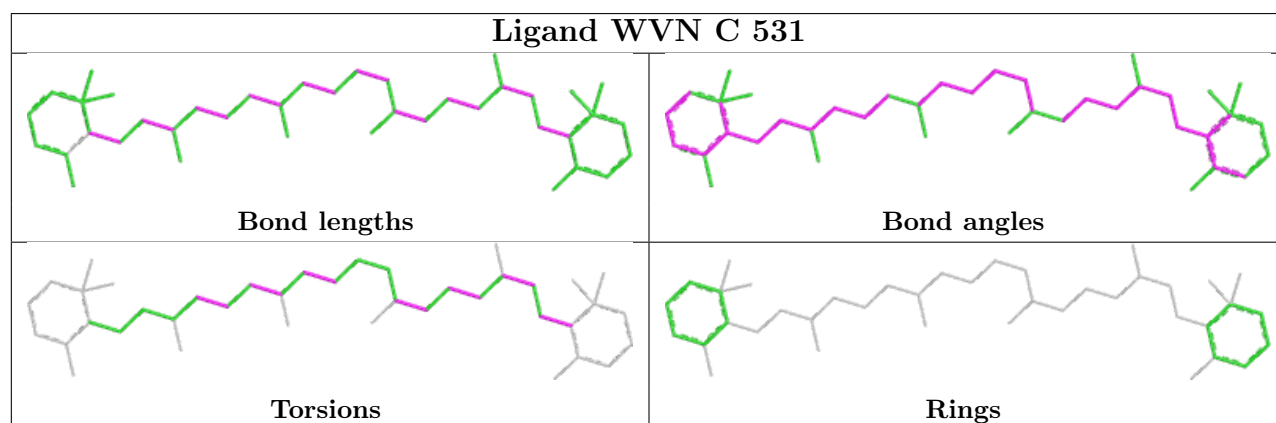
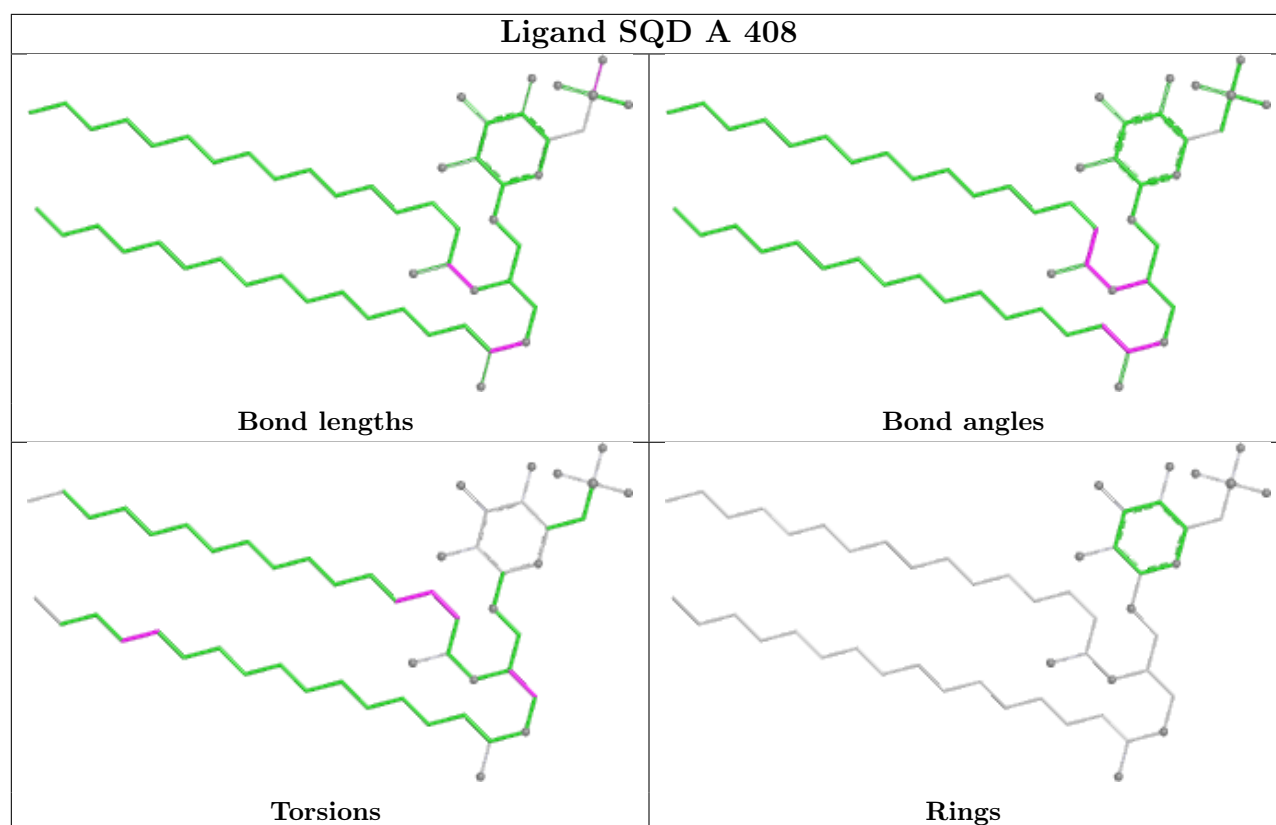
Bond angles



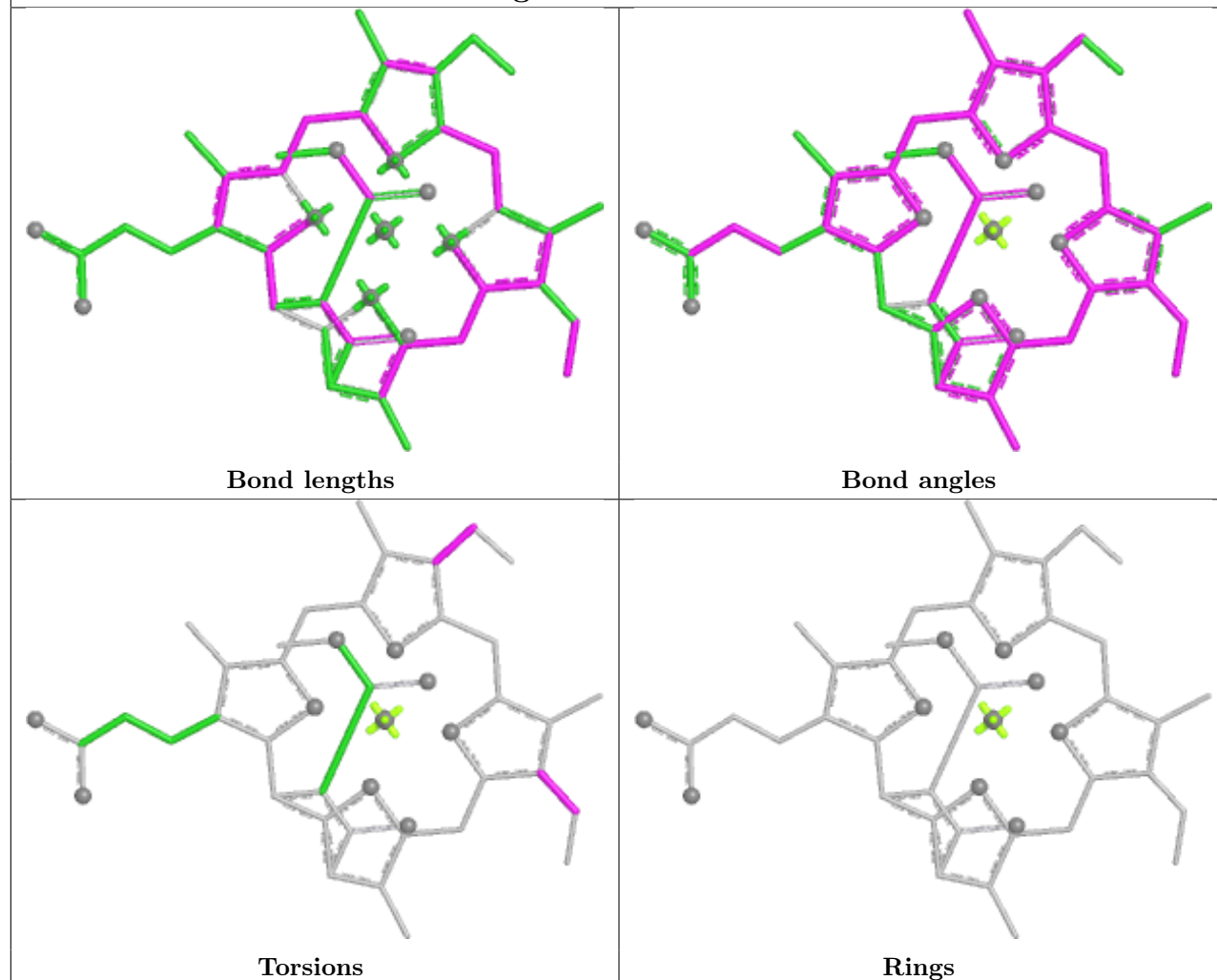
Torsions



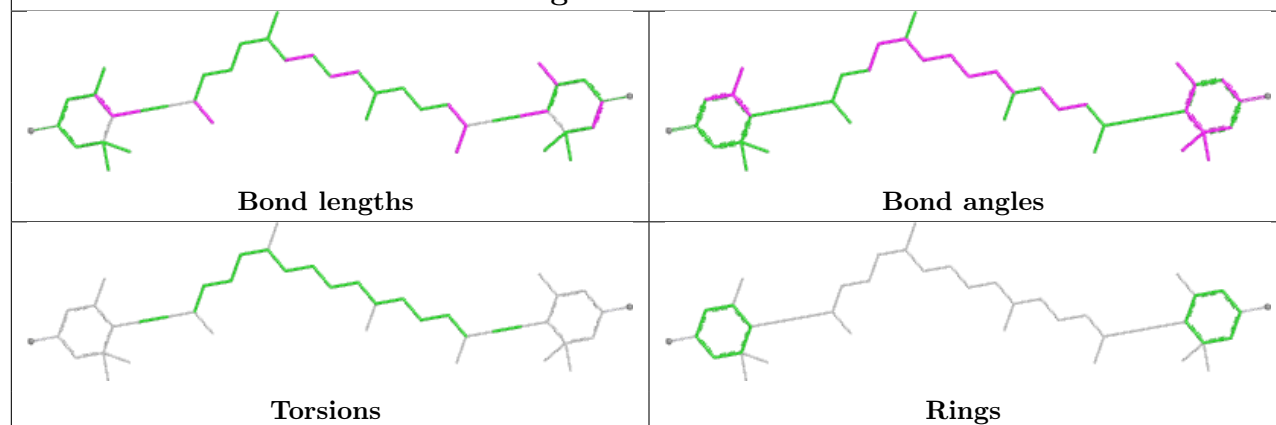
Rings



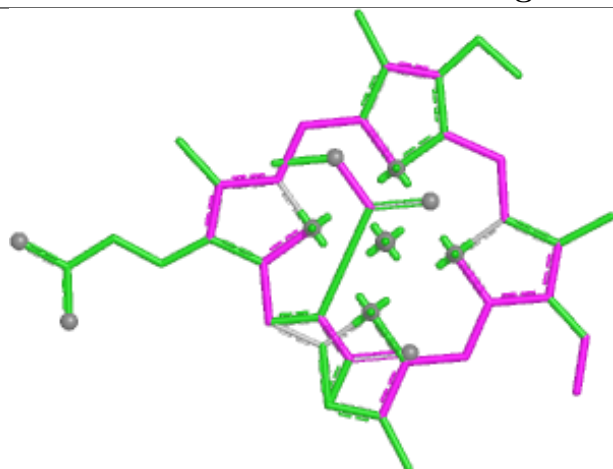
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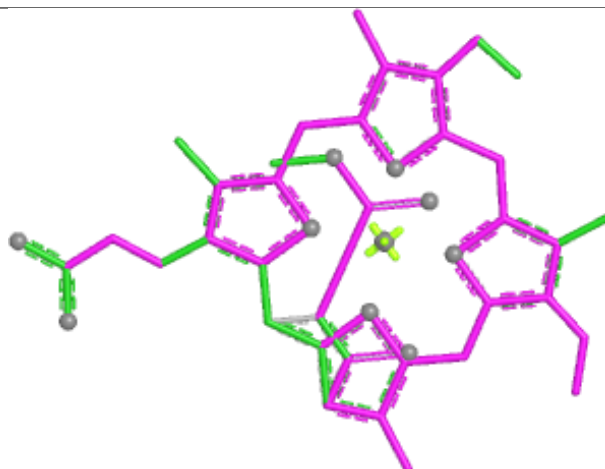
Ligand II0 5 618



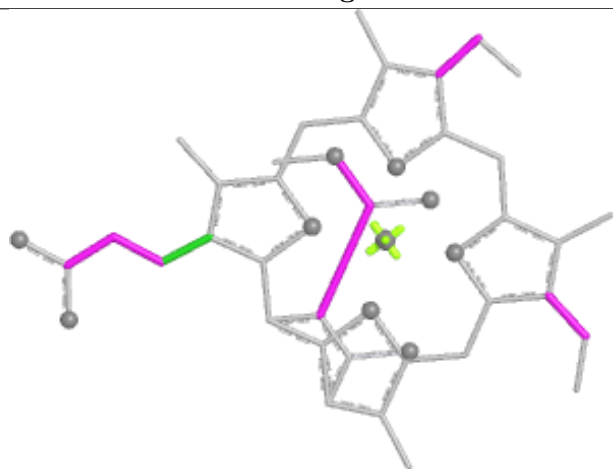
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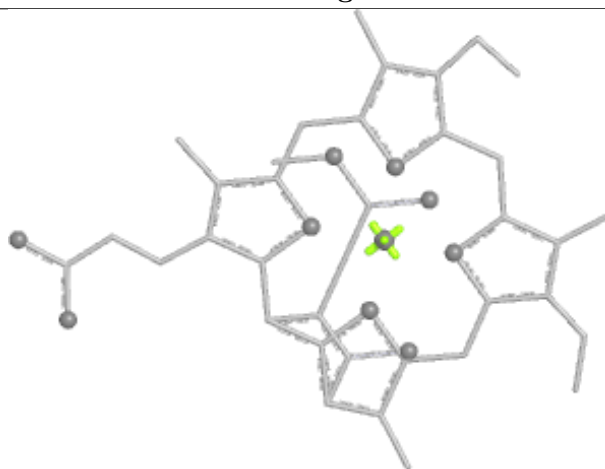
Bond lengths



Bond angles

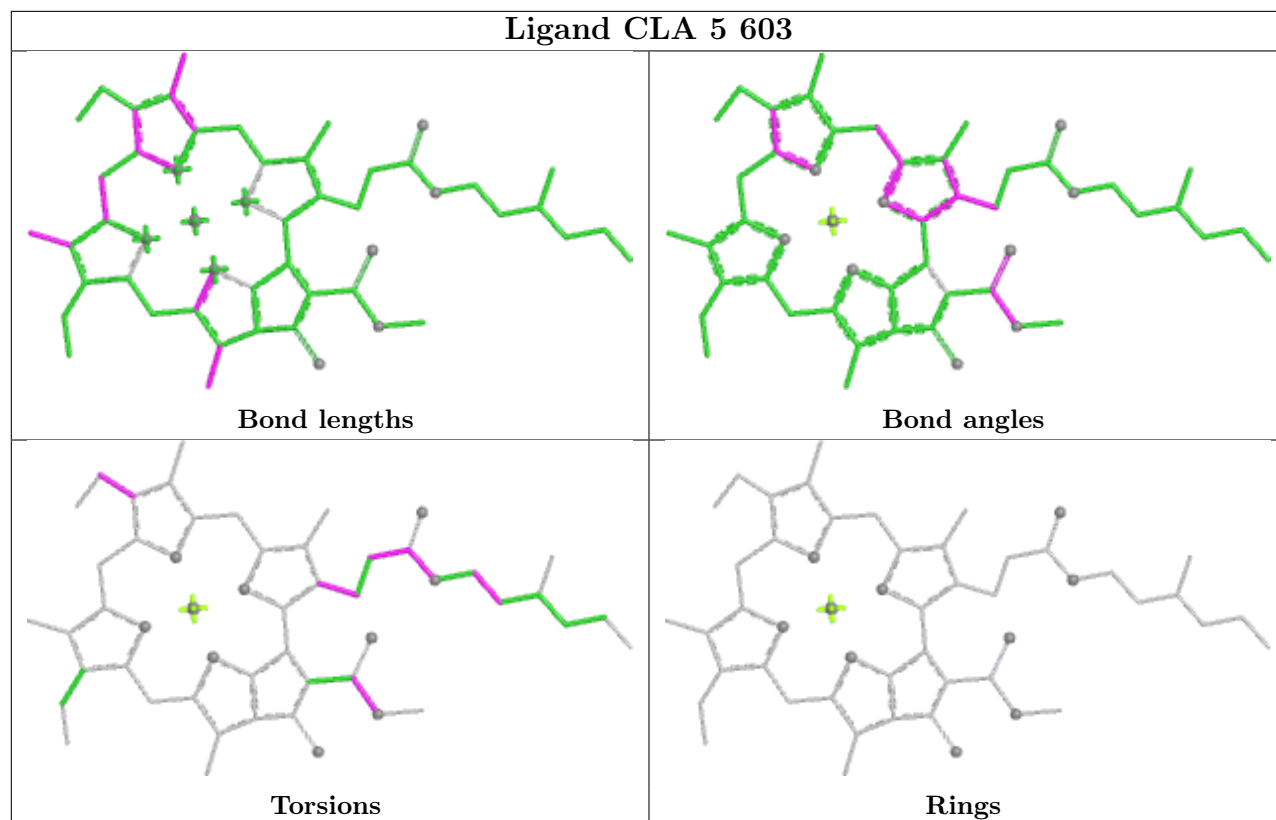


Torsions

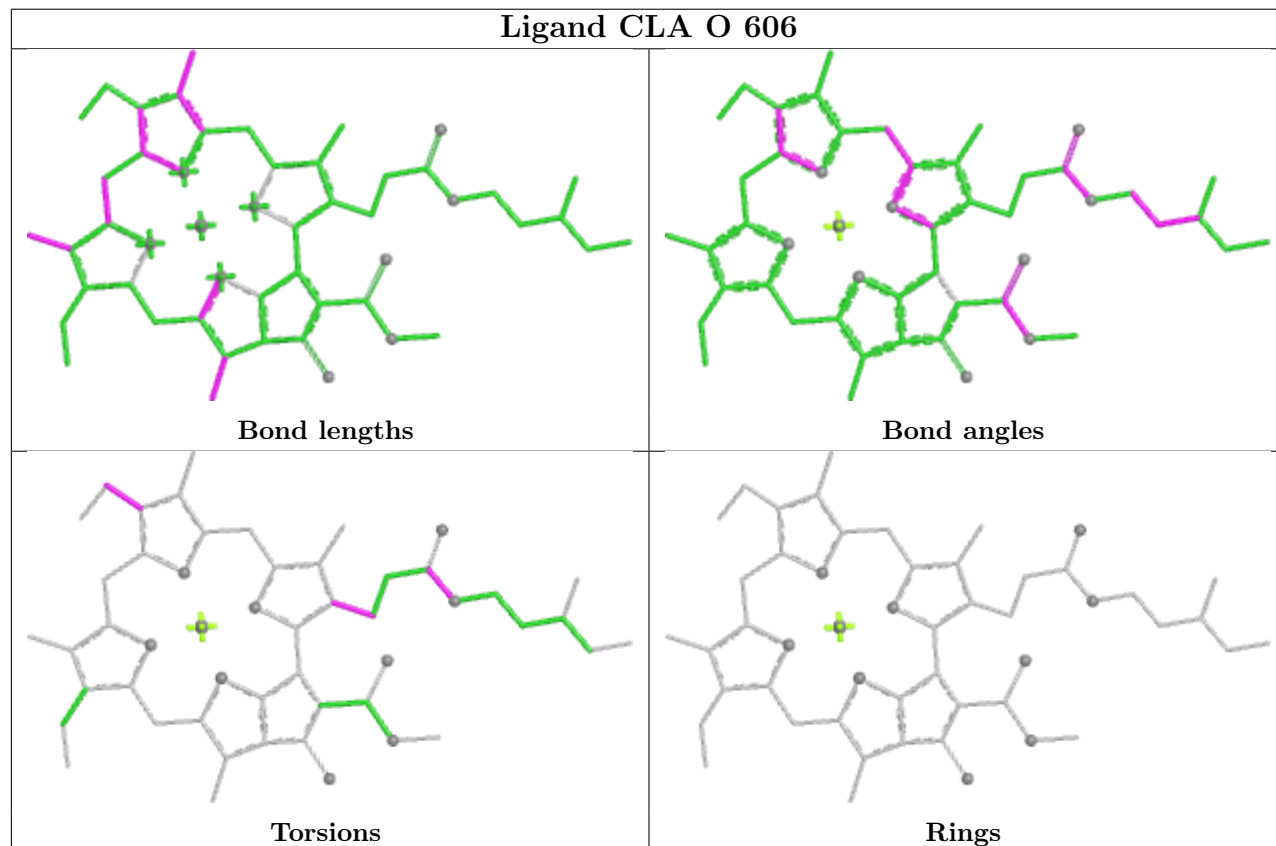


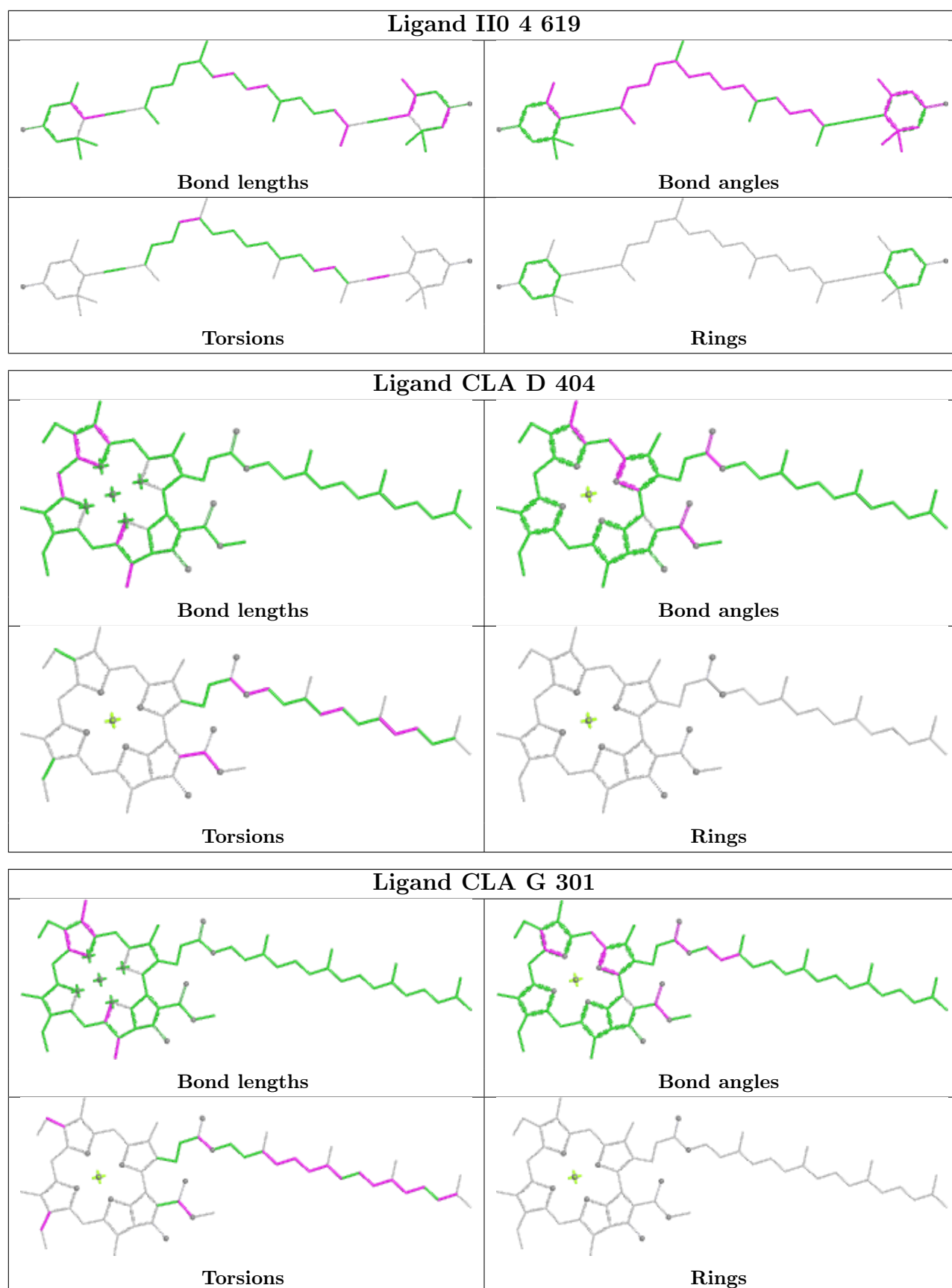
Rings

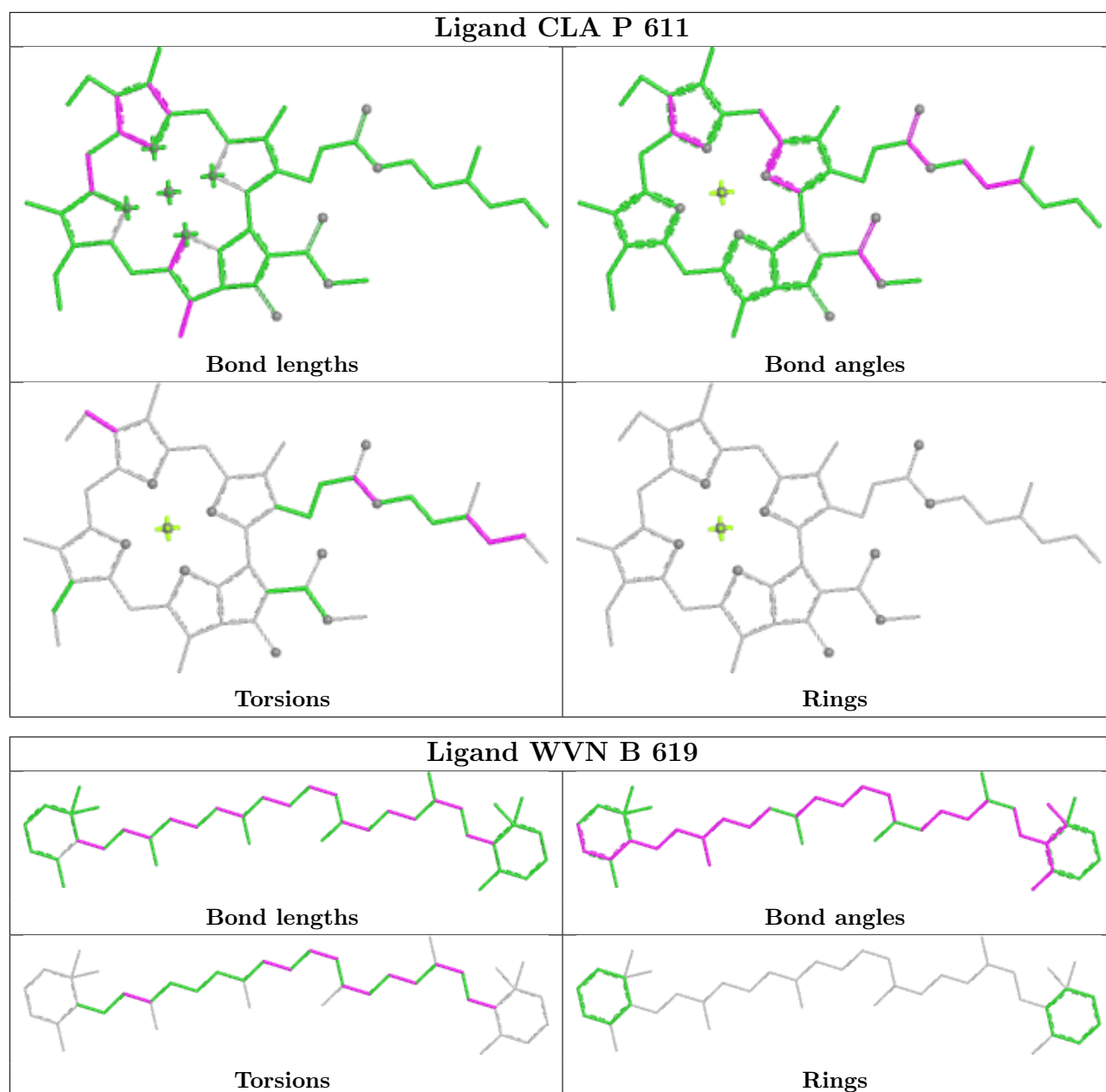
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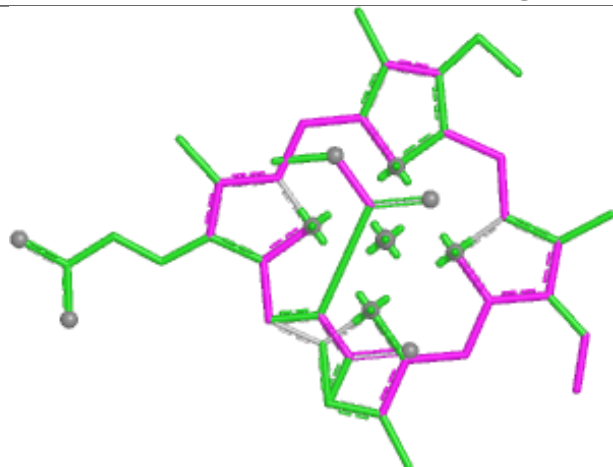
Ligand CLA O 606



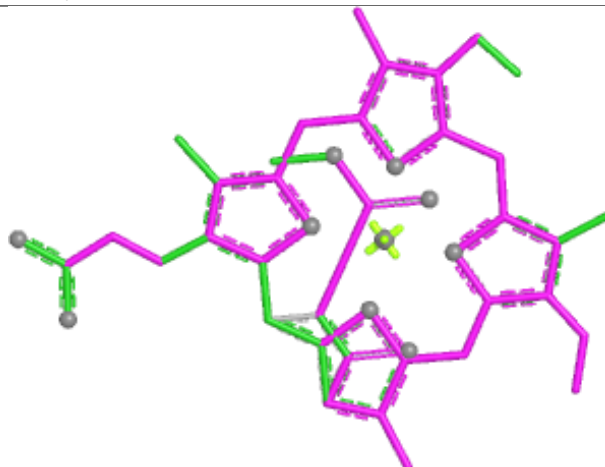




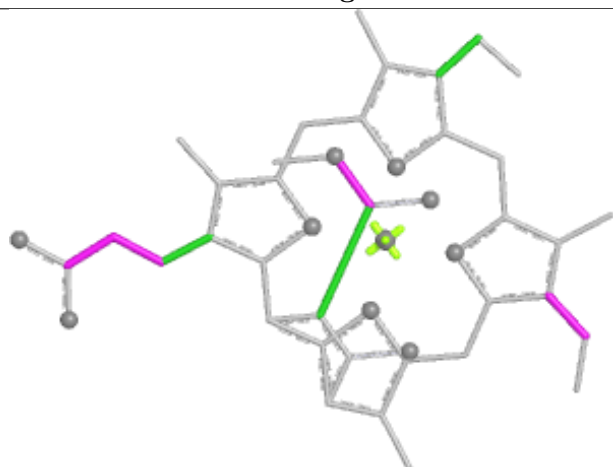
Ligand KC2 Q 611



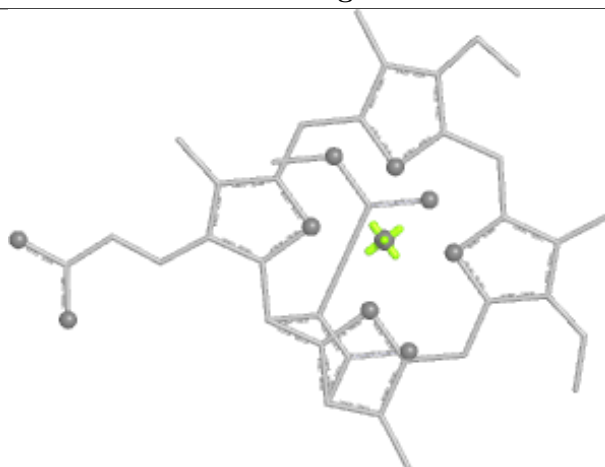
Bond lengths



Bond angles

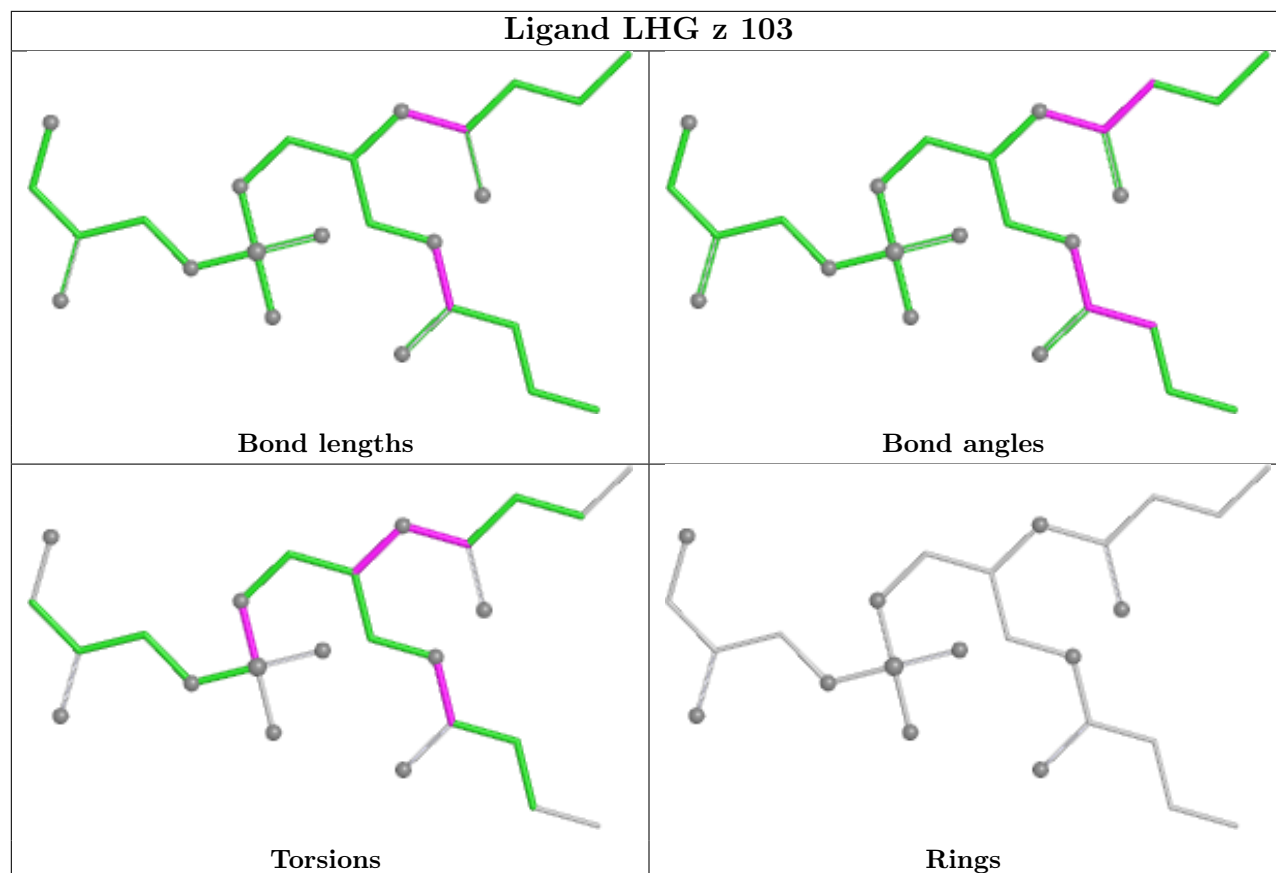


Torsions

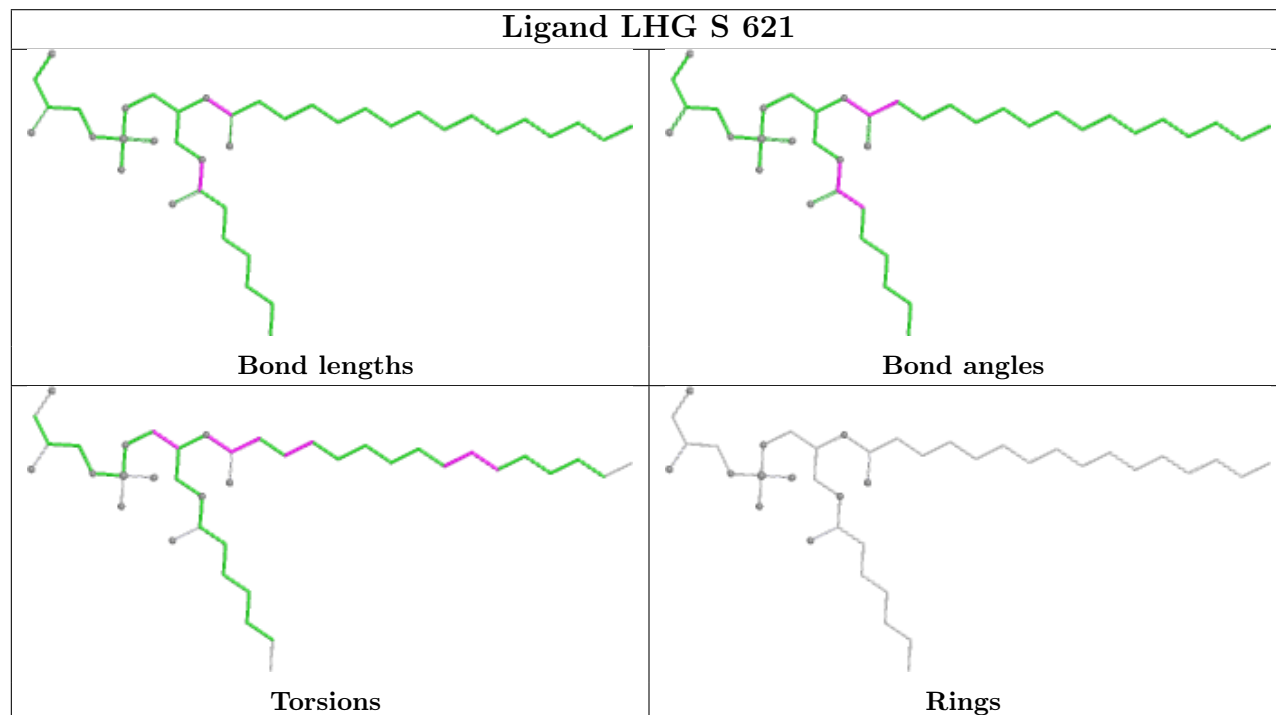


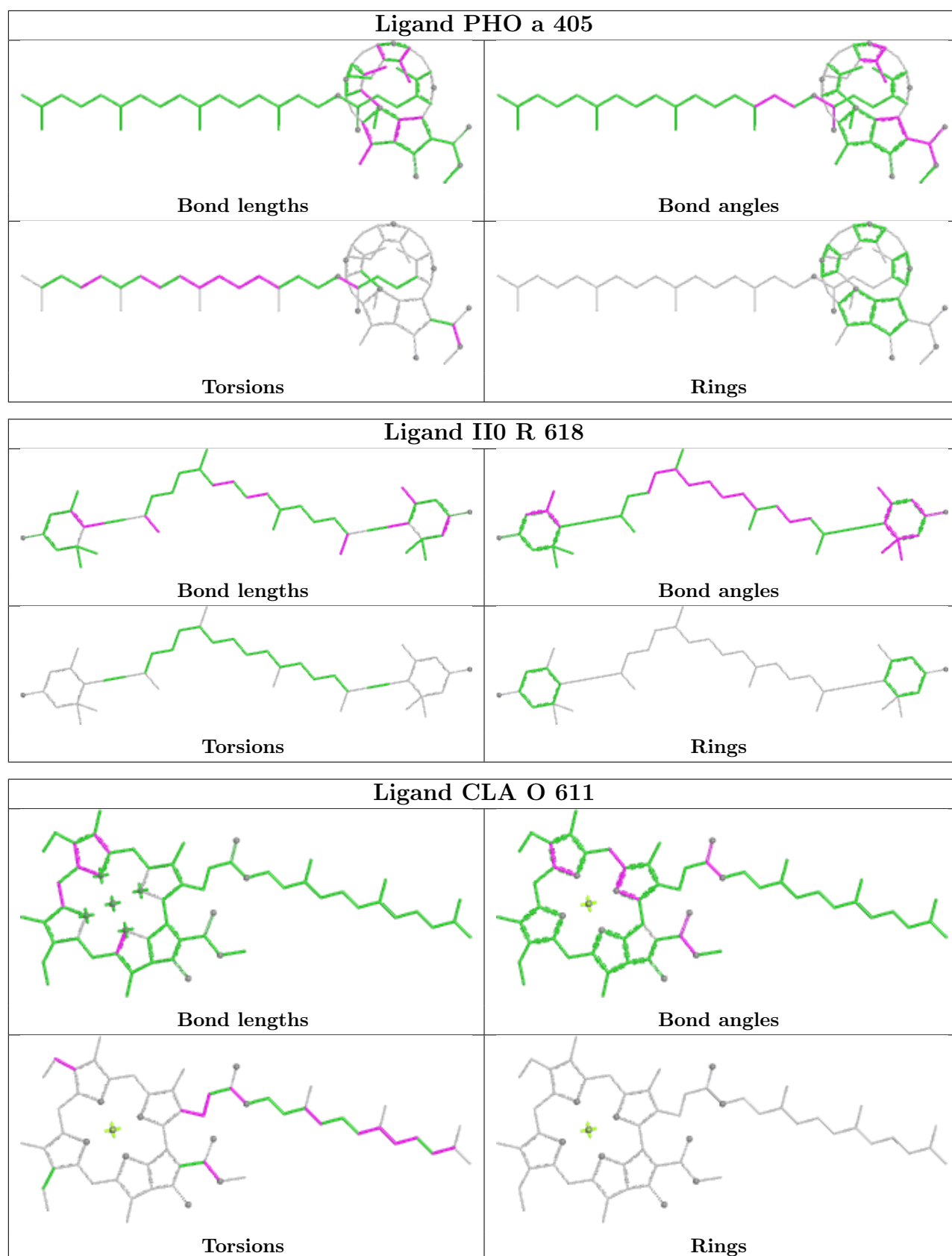
Rings

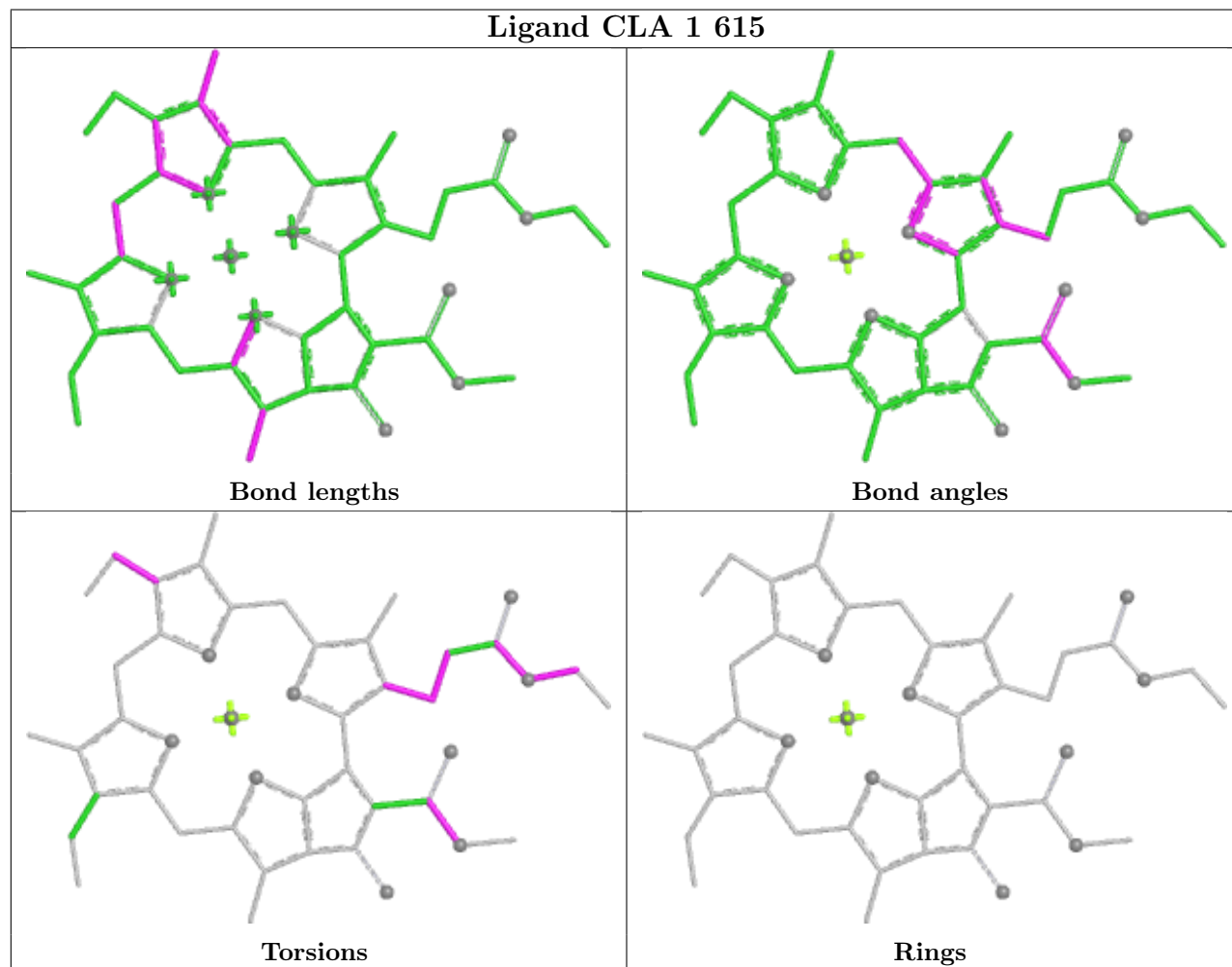
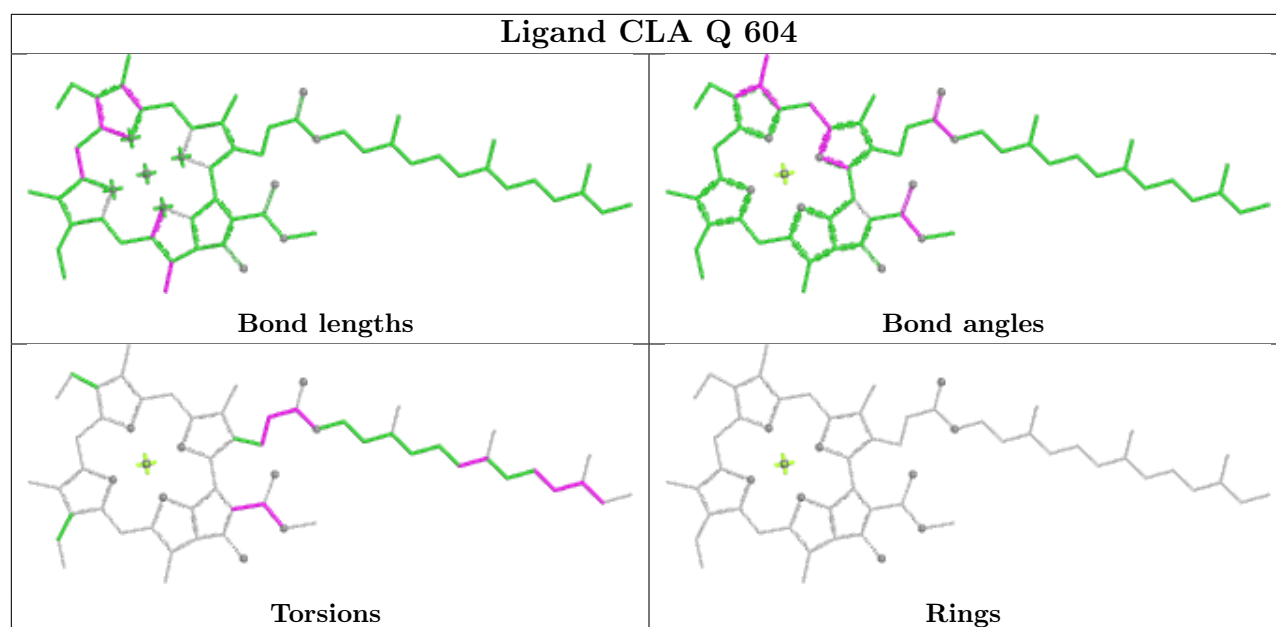
Ligand LHG z 103



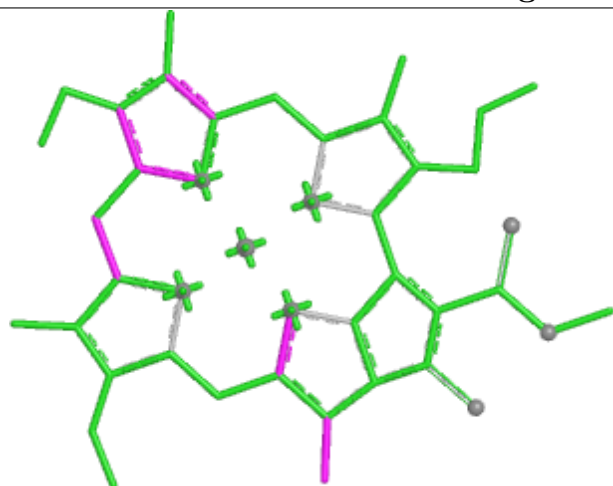
Ligand LHG S 621



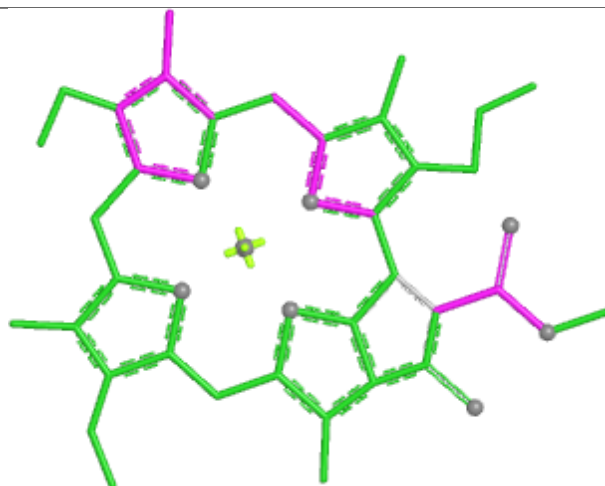




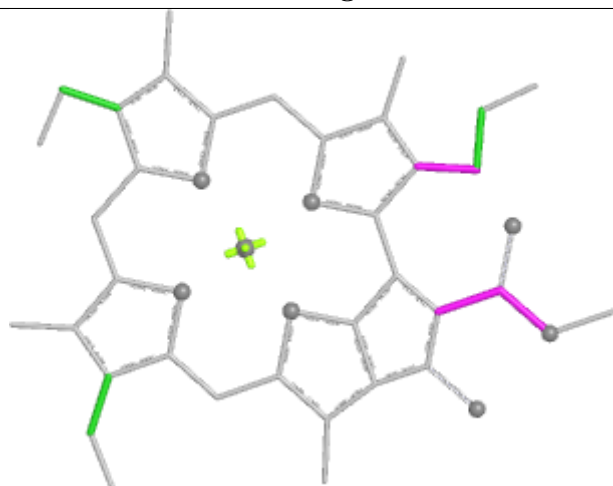
Ligand CLA 4 613



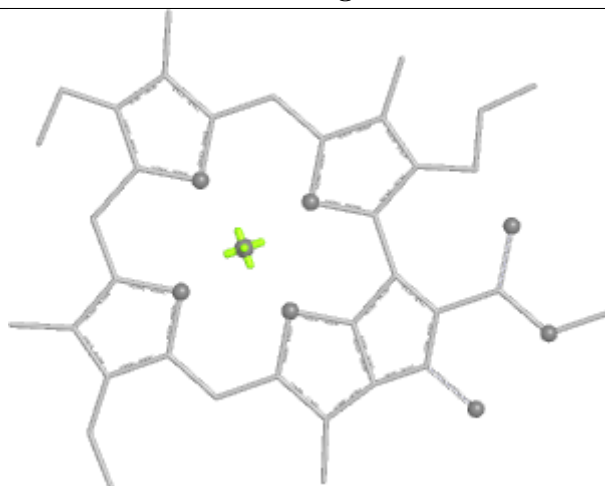
Bond lengths



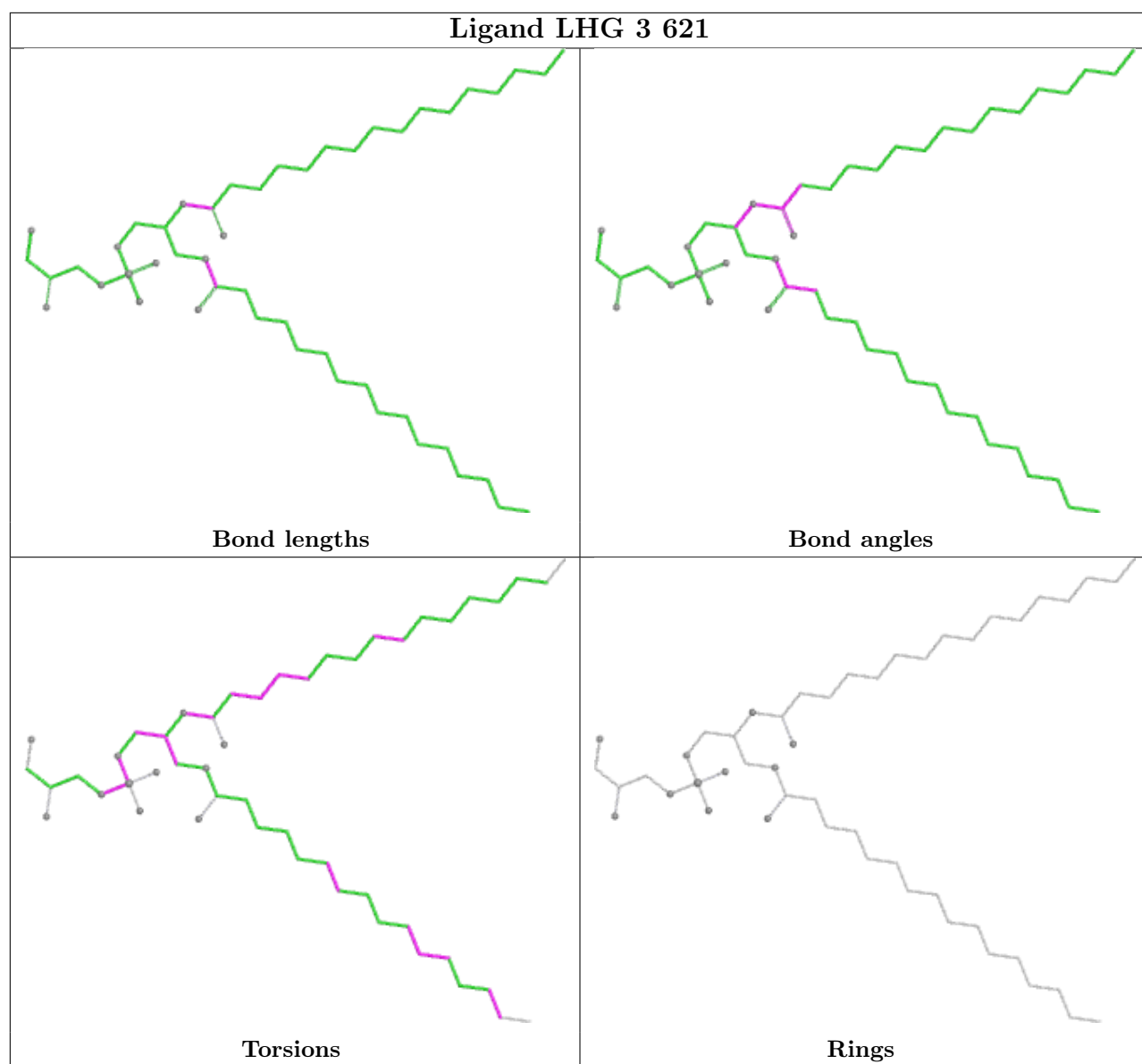
Bond angles



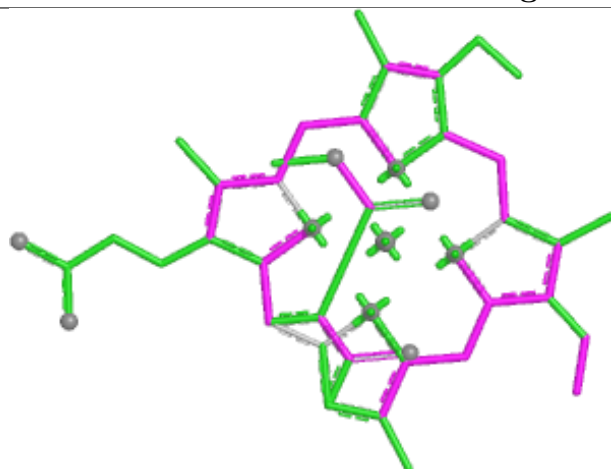
Torsions



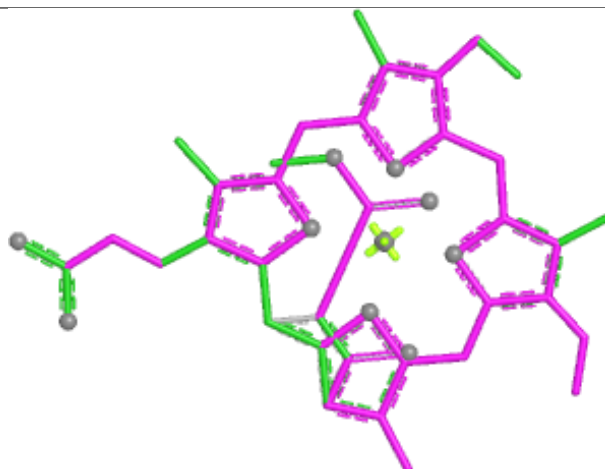
Rings



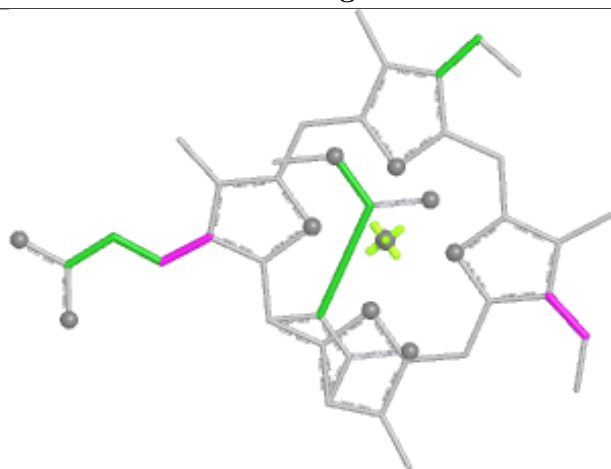
Ligand KC2 1 612



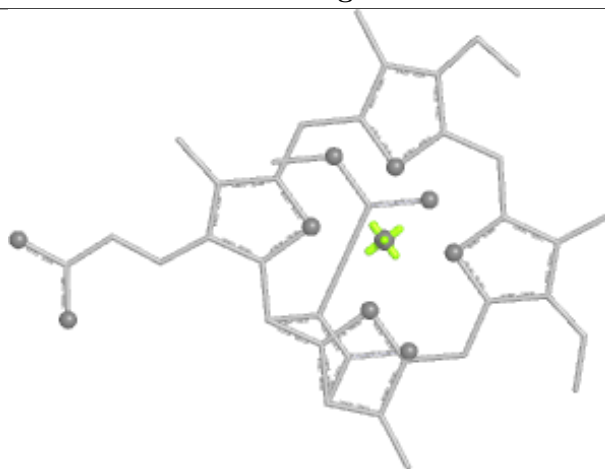
Bond lengths



Bond angles

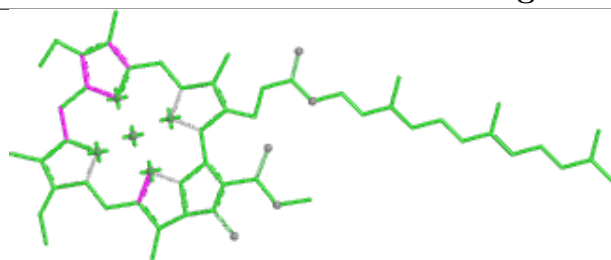


Torsions

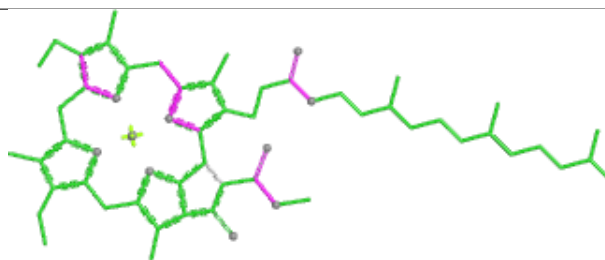


Rings

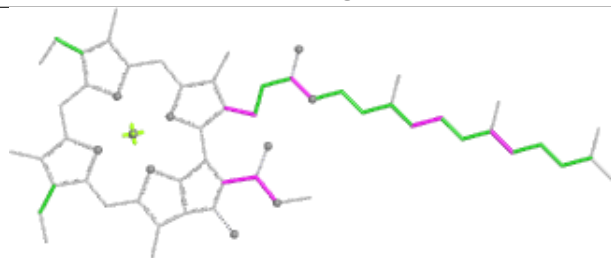
Ligand CLA b 614



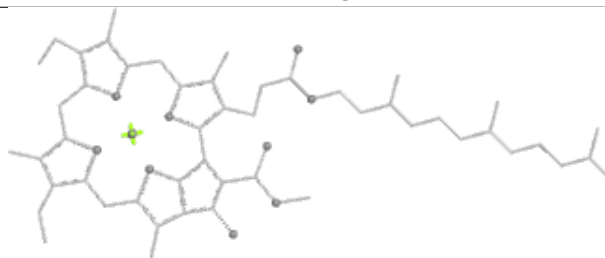
Bond lengths



Bond angles

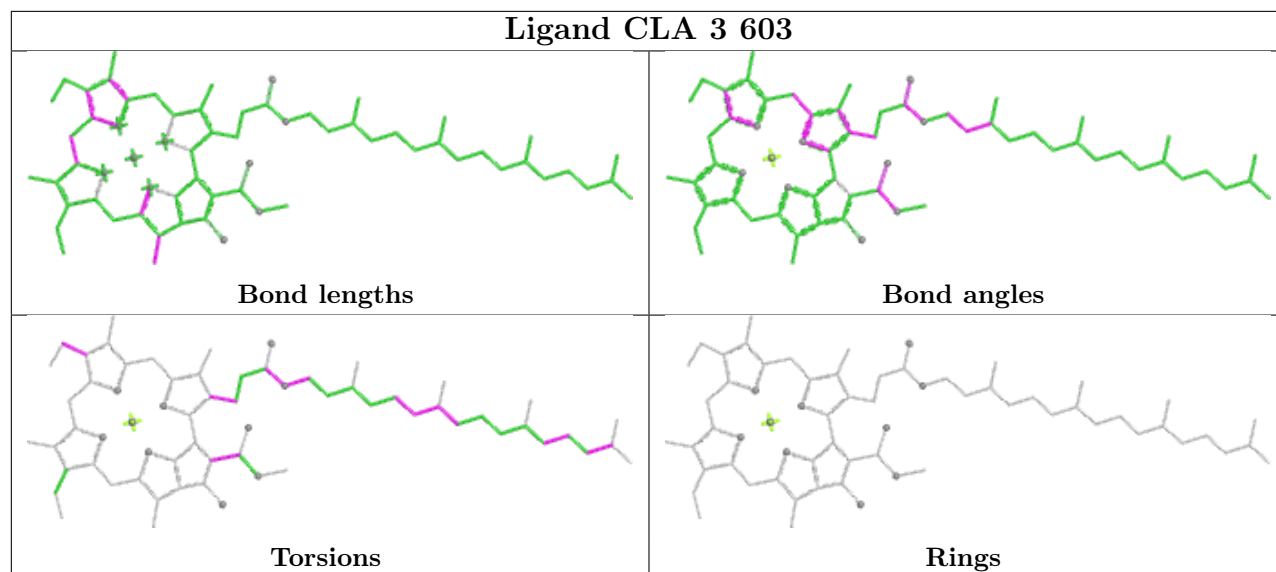


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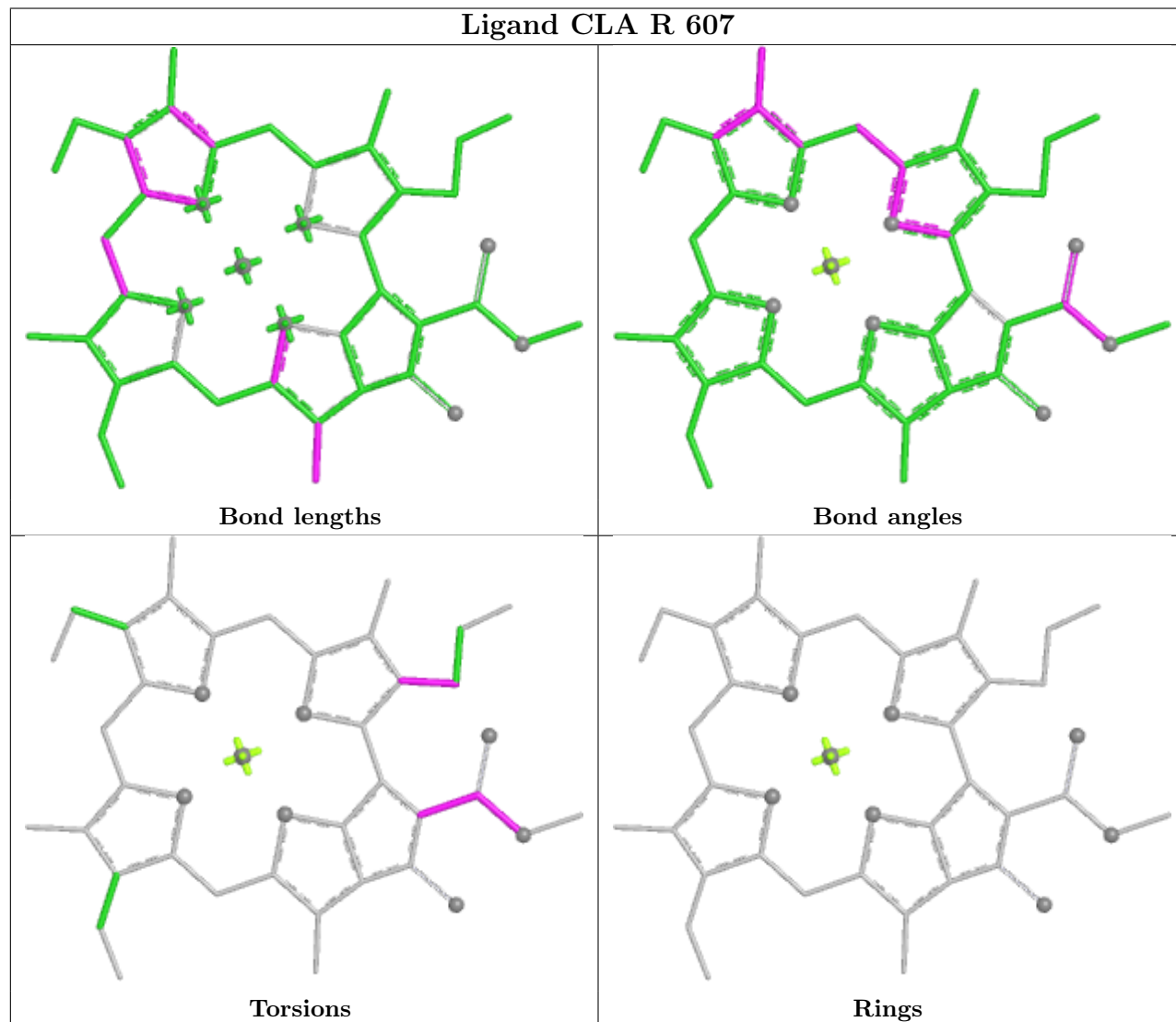


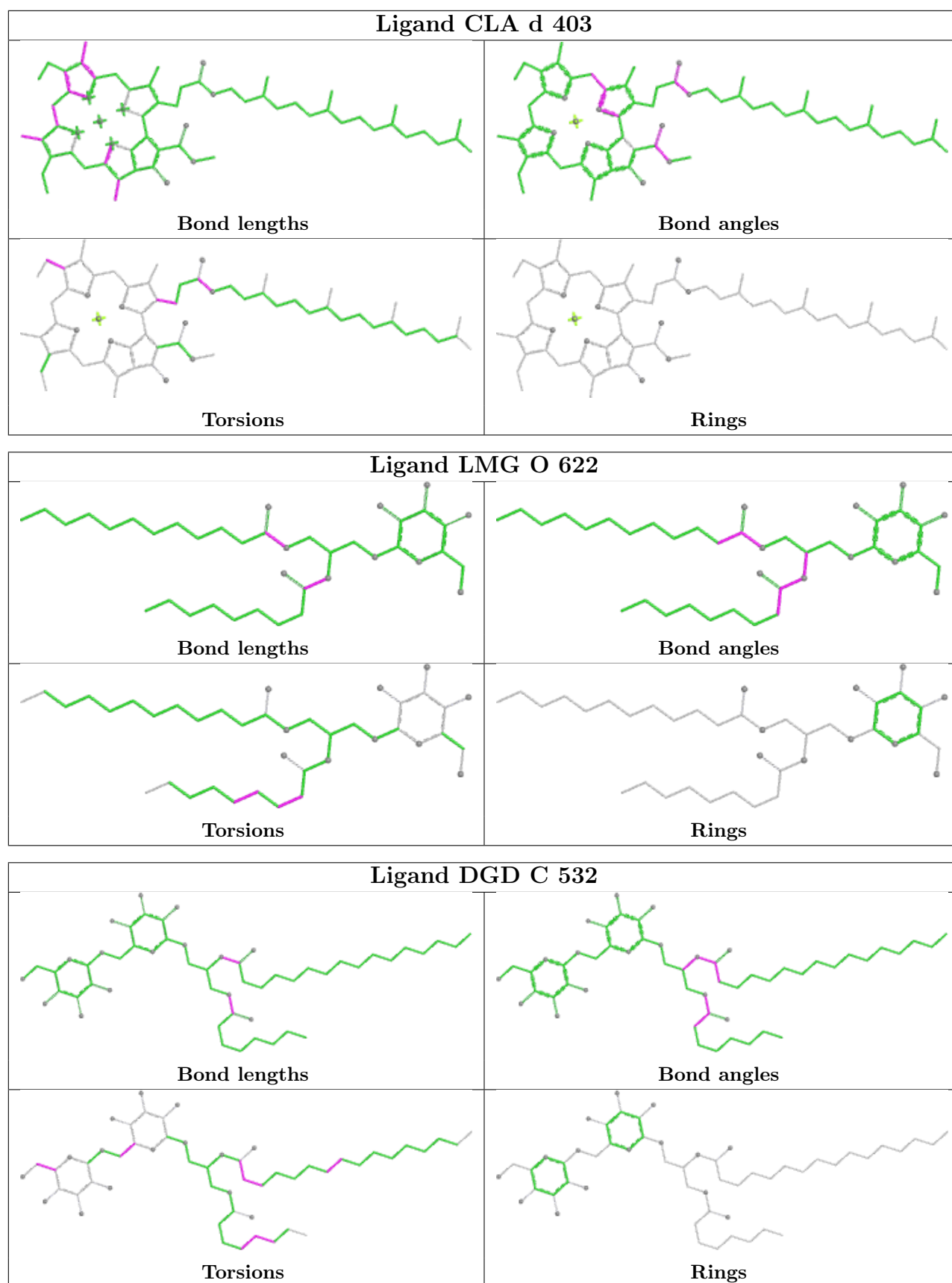
Rings

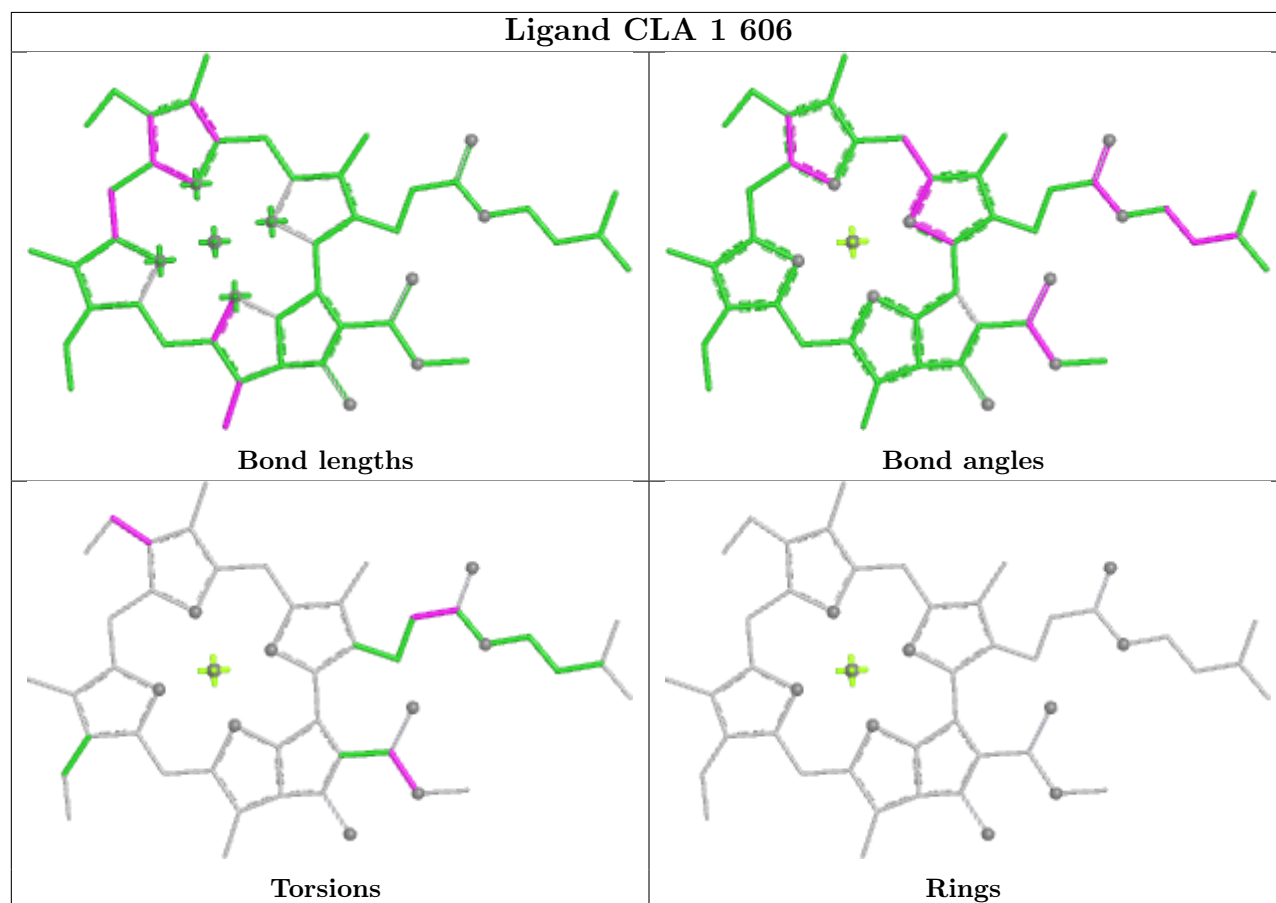
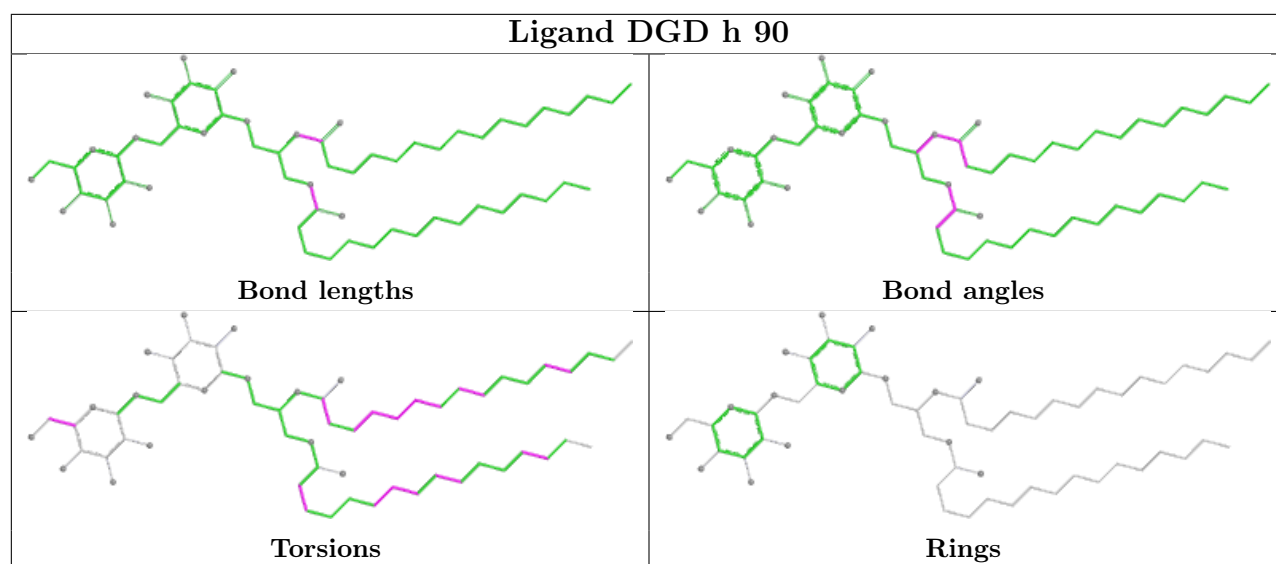
Ligand CLA 3 603

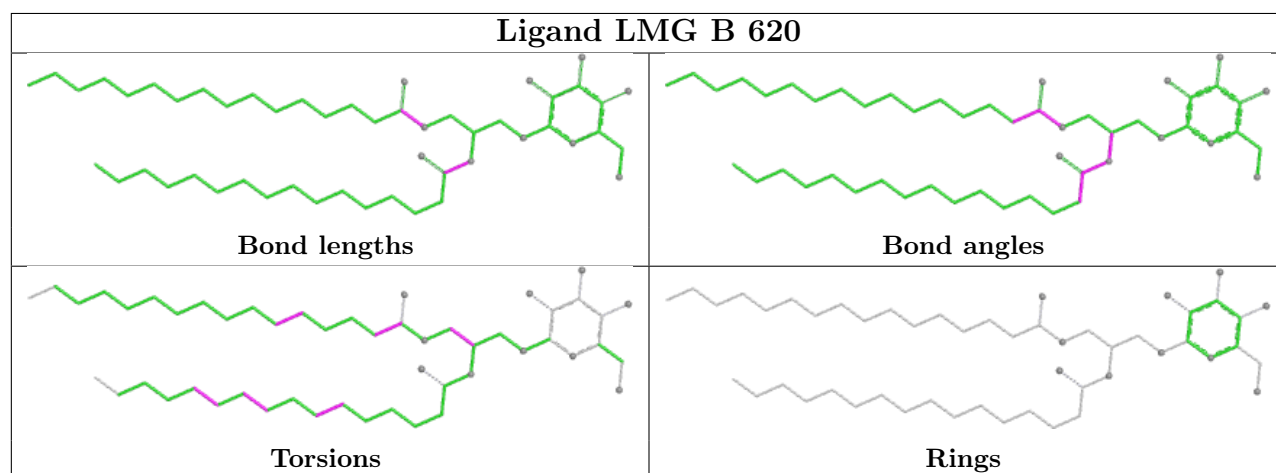
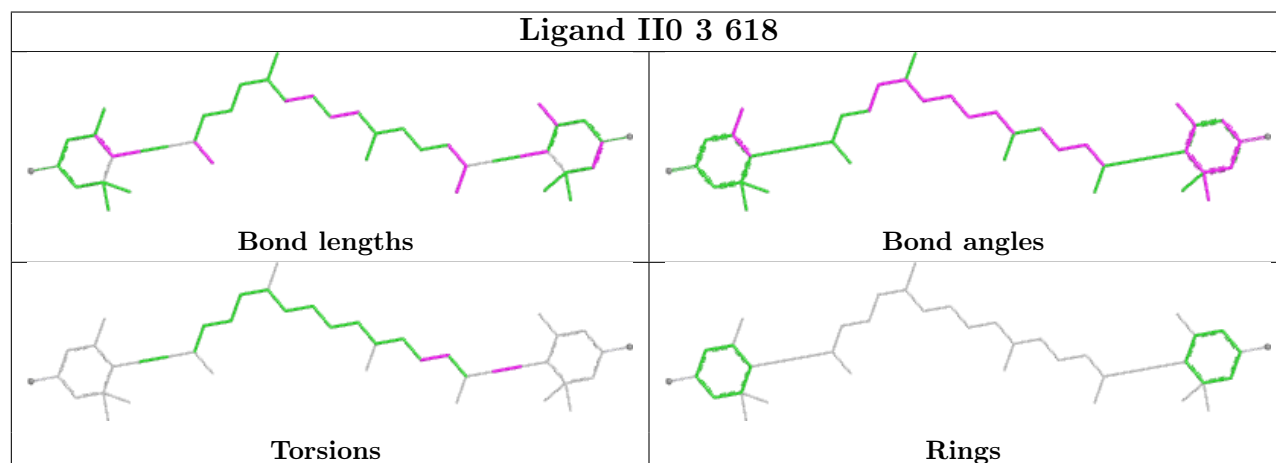
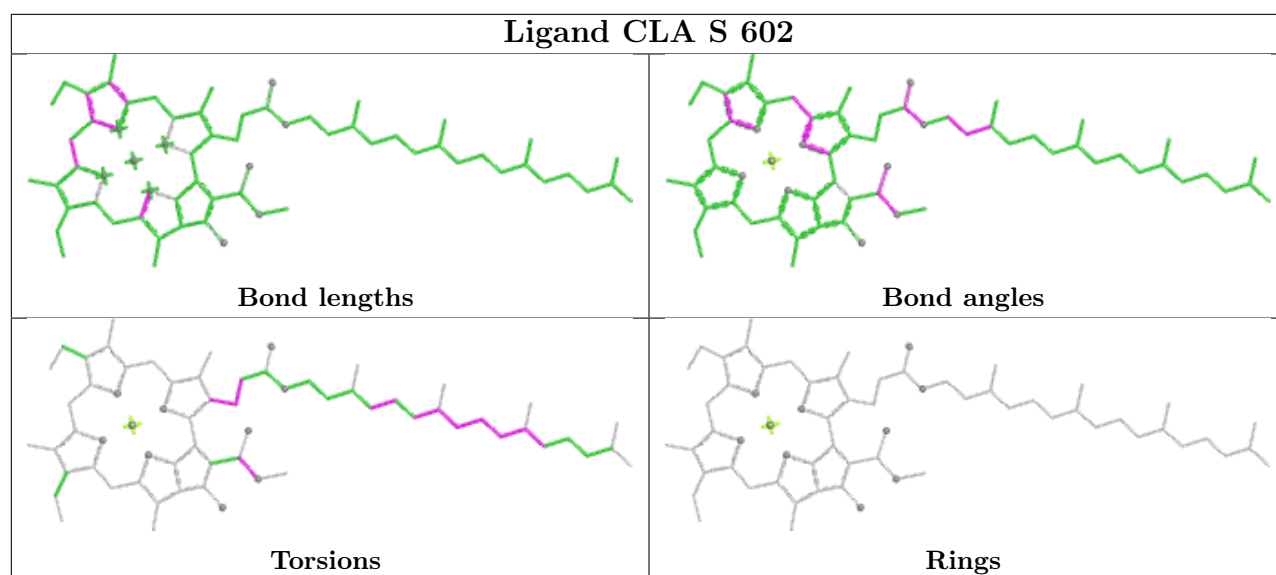


Ligand CLA R 607

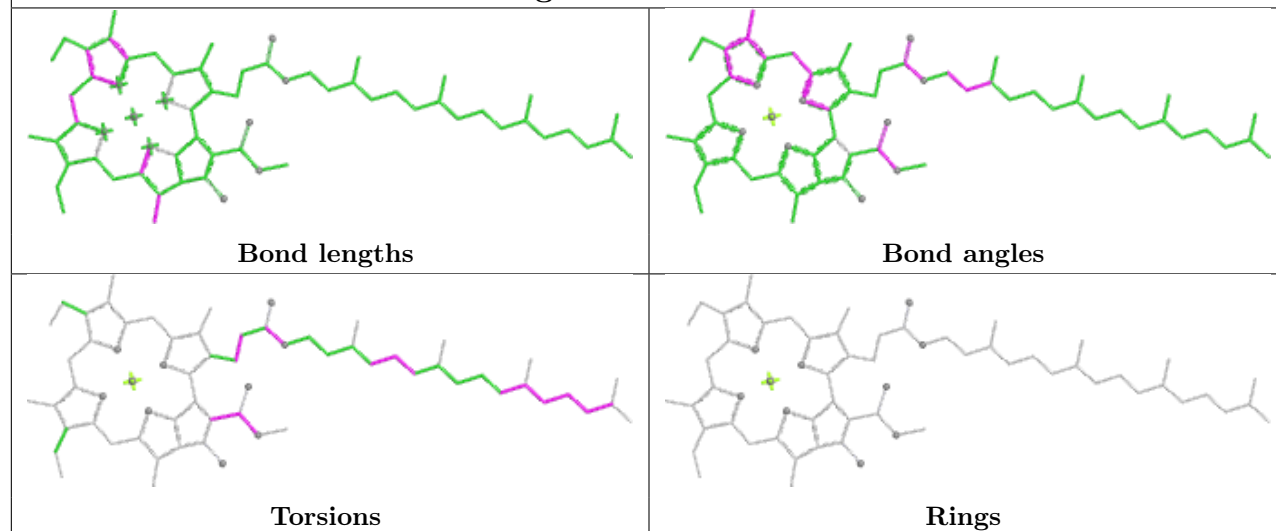




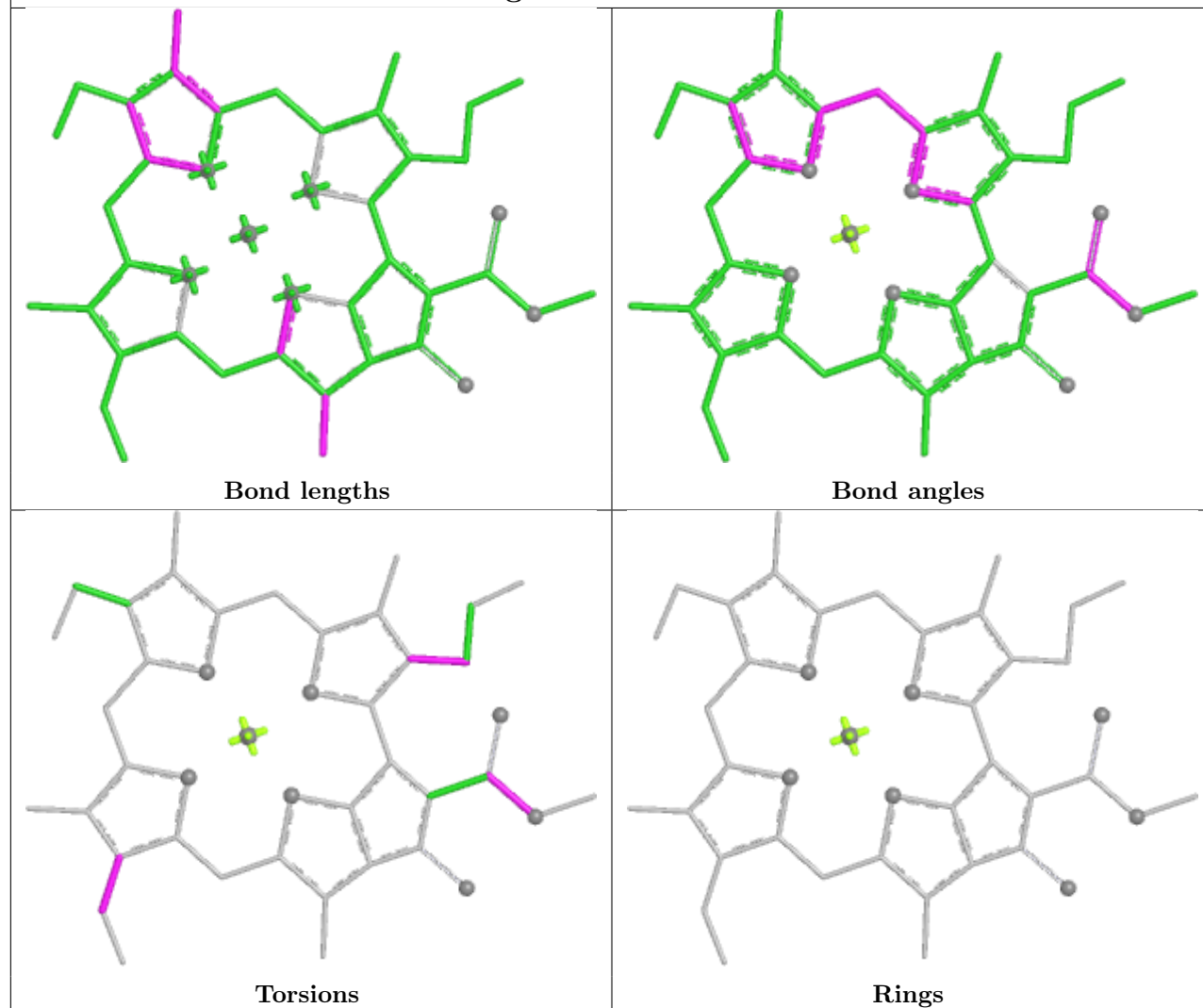


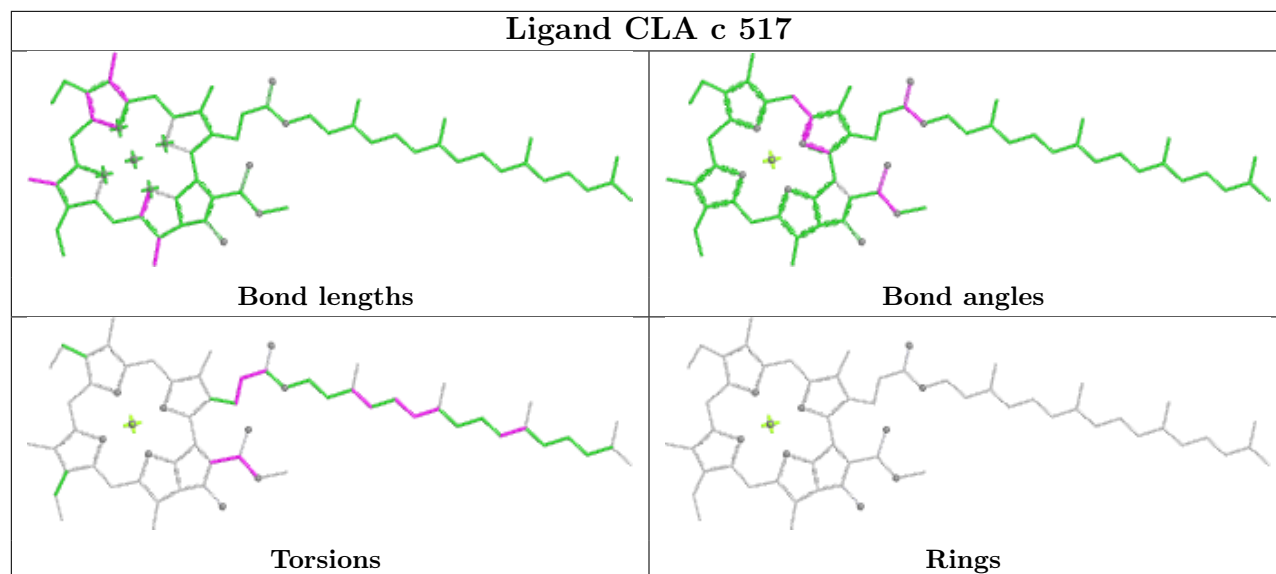
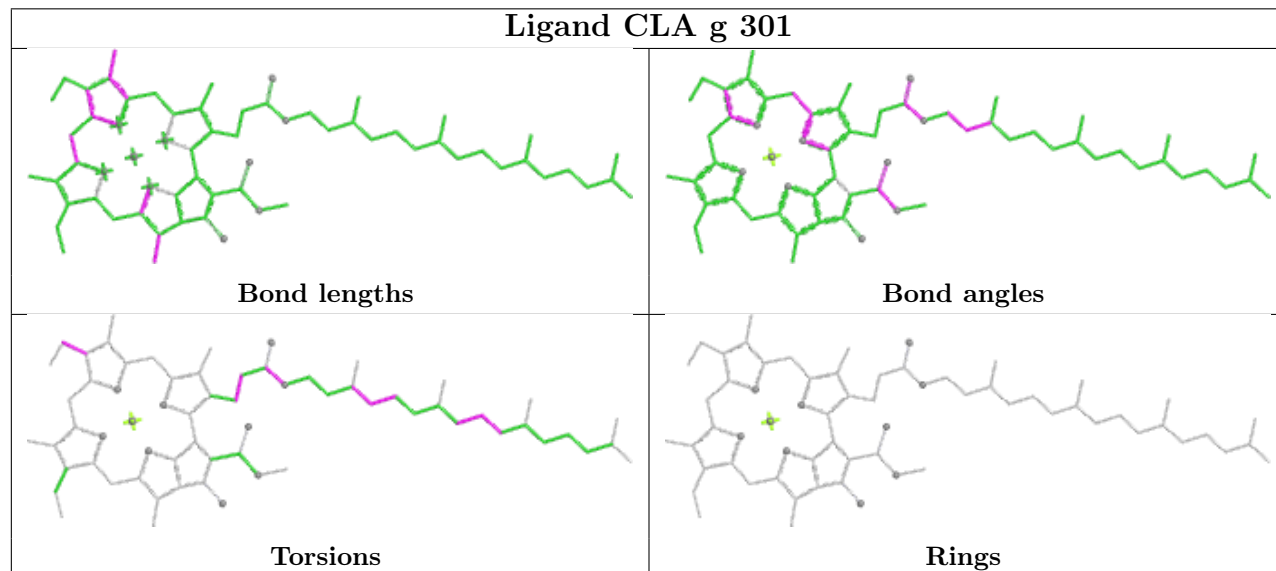


Ligand CLA S 604

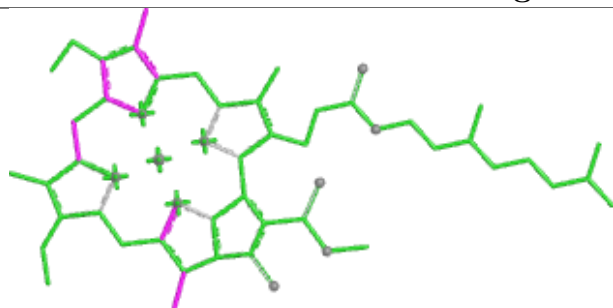


Ligand CLA 1 607

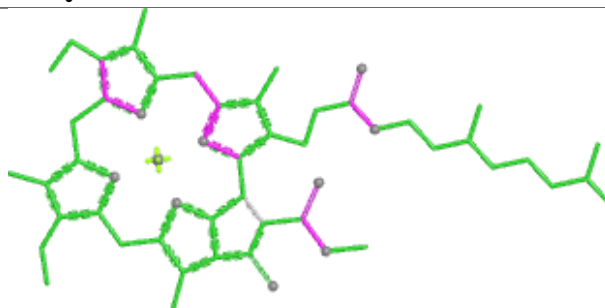


Ligand CLA c 517**Ligand CLA g 301**

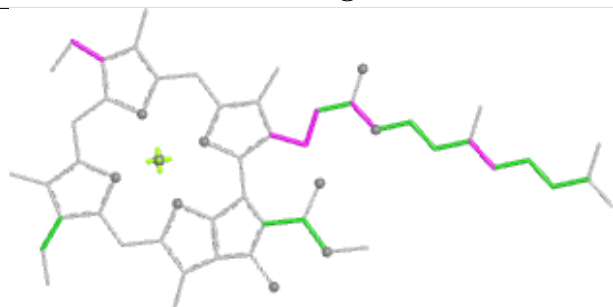
Ligand CLA Q 606



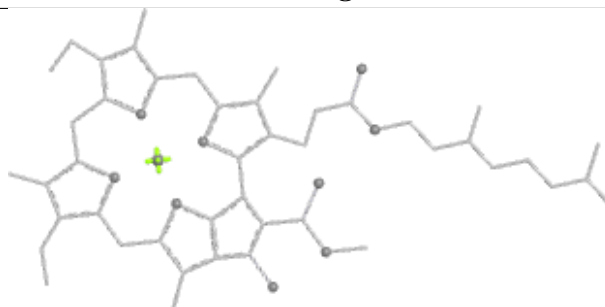
Bond lengths



Bond angles

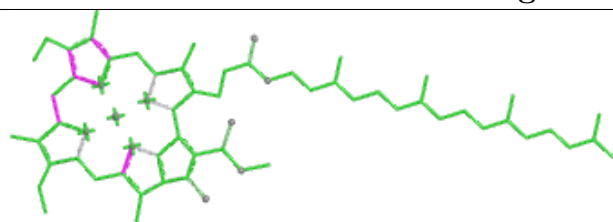


Torsions

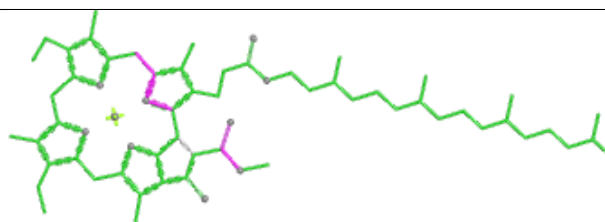


Rings

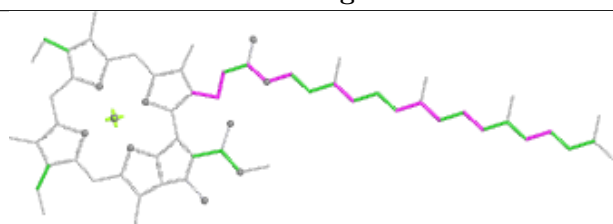
Ligand CLA 3 610



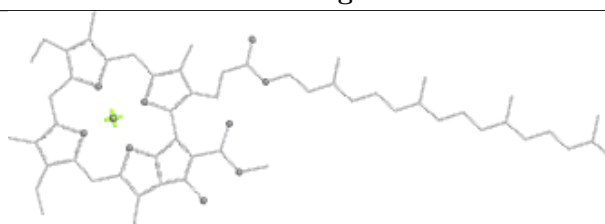
Bond lengths



Bond angles

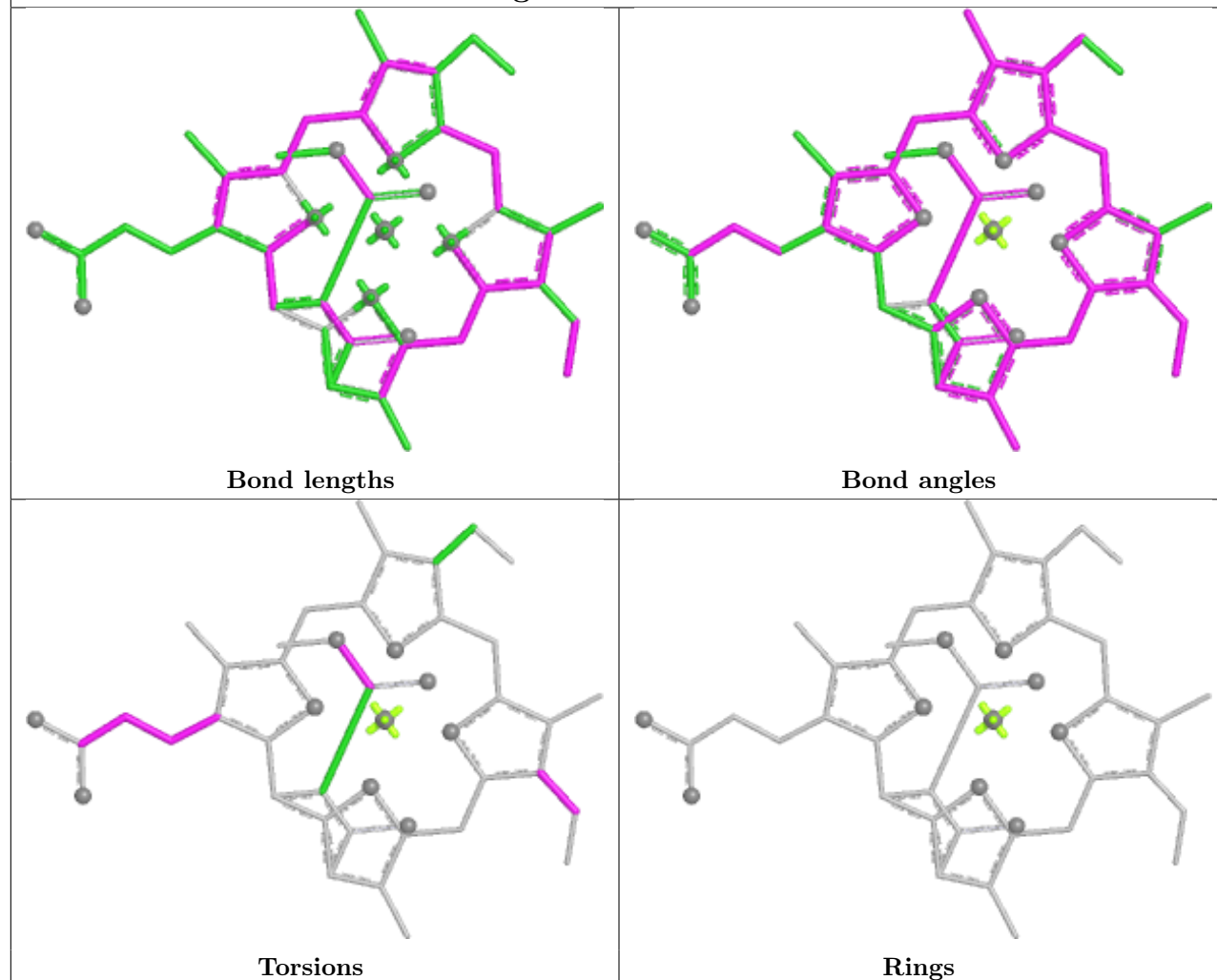


Torsions

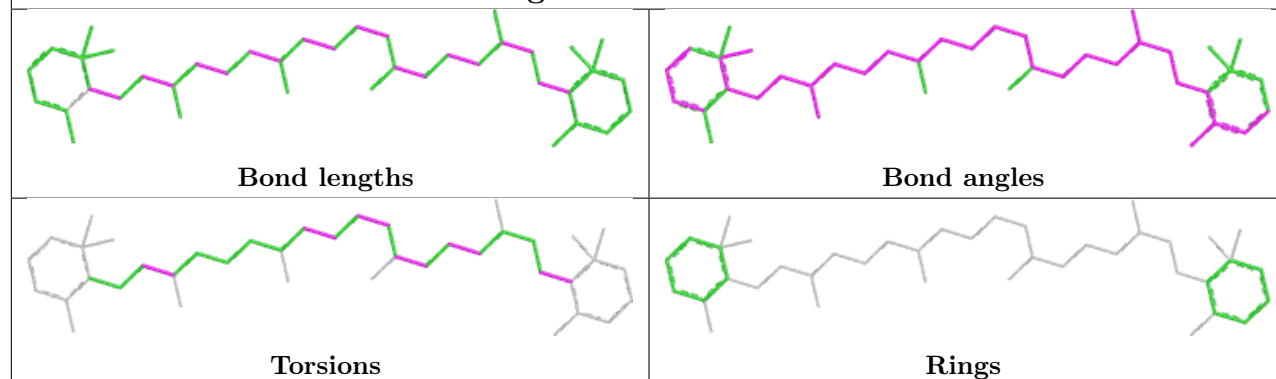


Rings

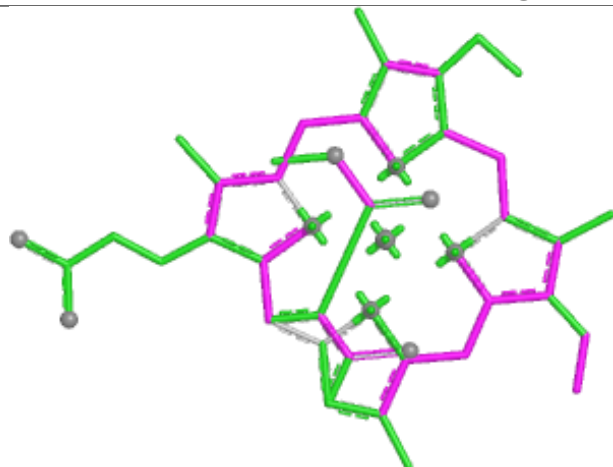
Ligand KC2 6 606



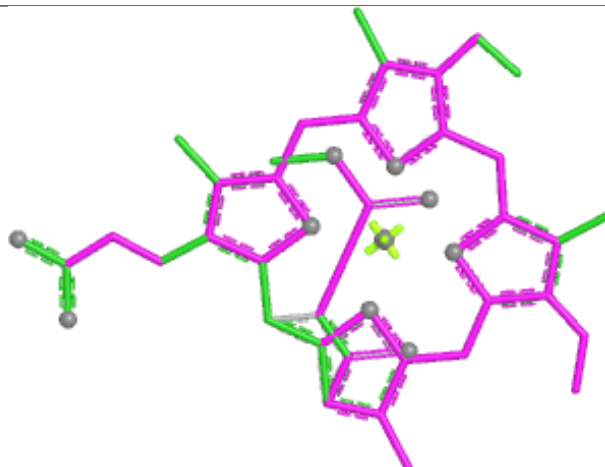
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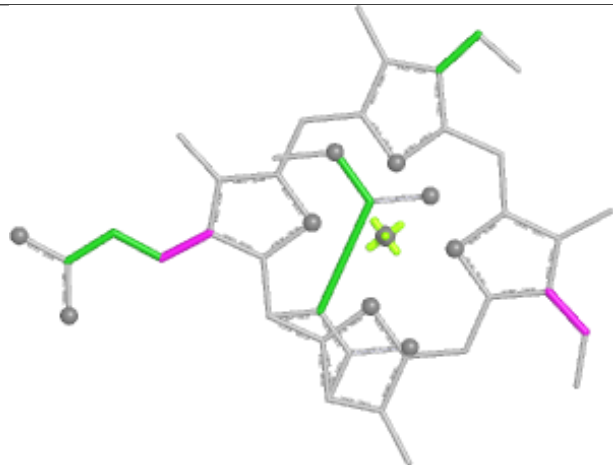
Ligand KC2 N 612



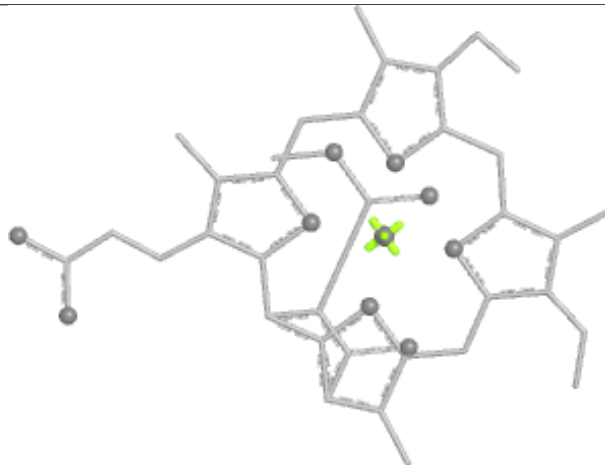
Bond lengths



Bond angles

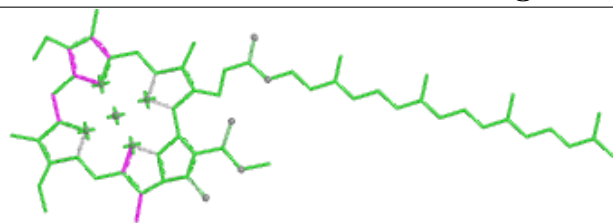


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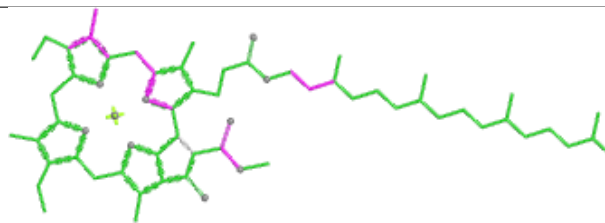


Rings

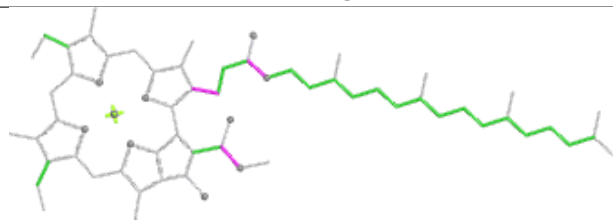
Ligand CLA C 516



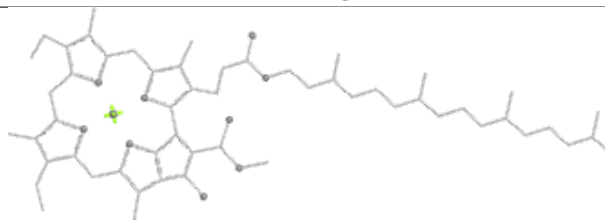
Bond lengths



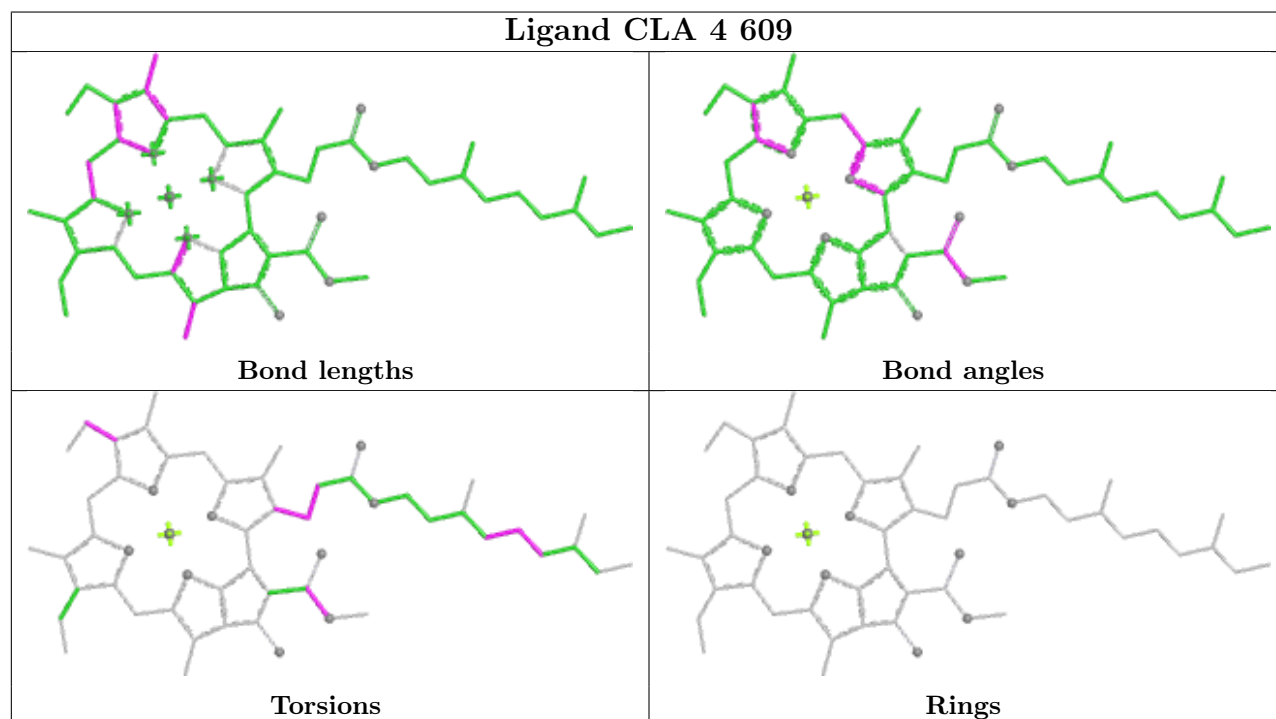
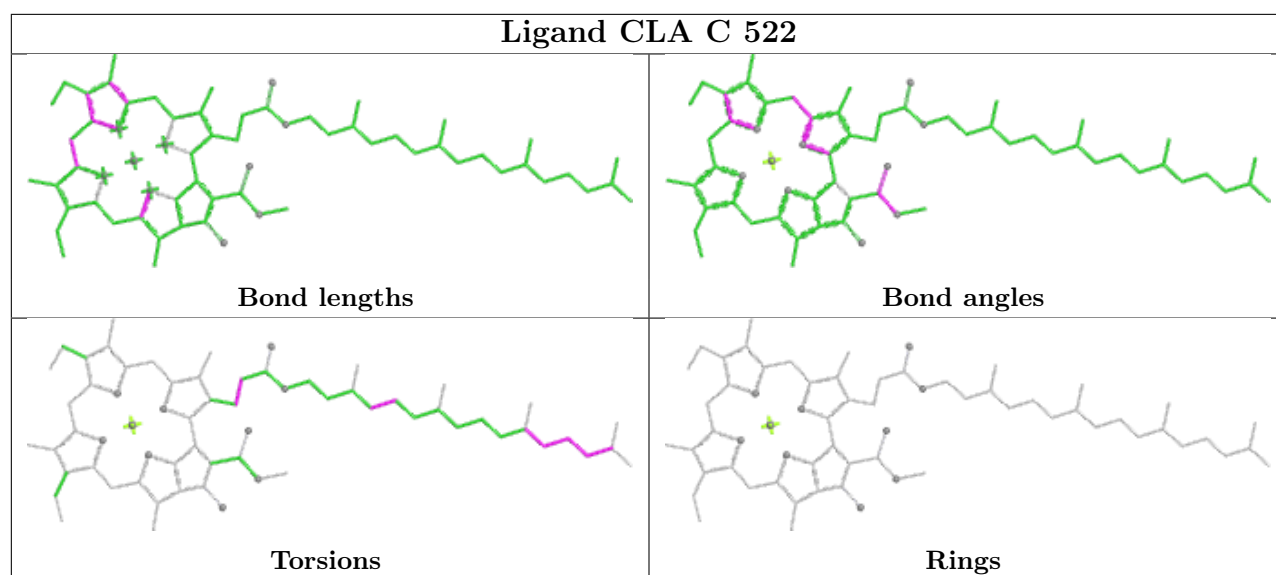
Bond angles



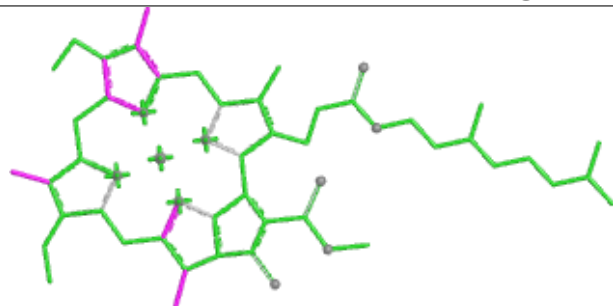
Torsions



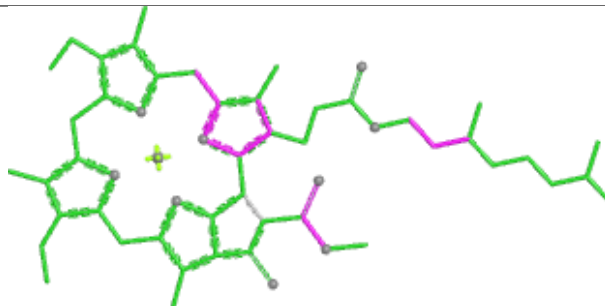
Rings



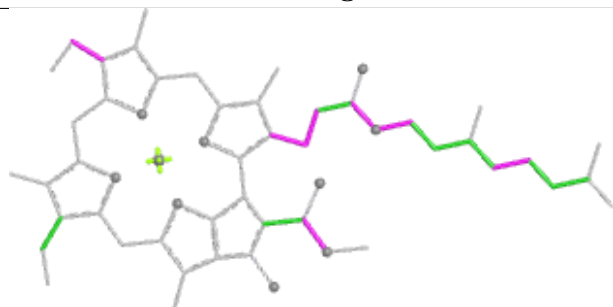
Ligand CLA S 603



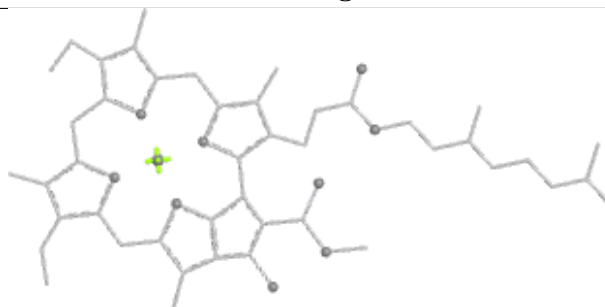
Bond lengths



Bond angles

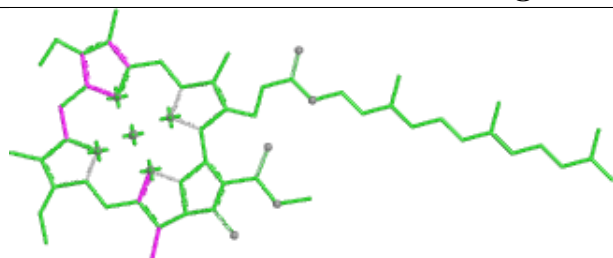


Torsions

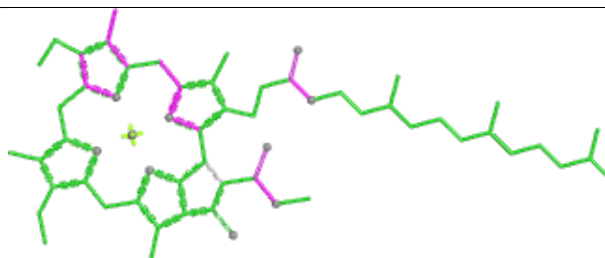


Rings

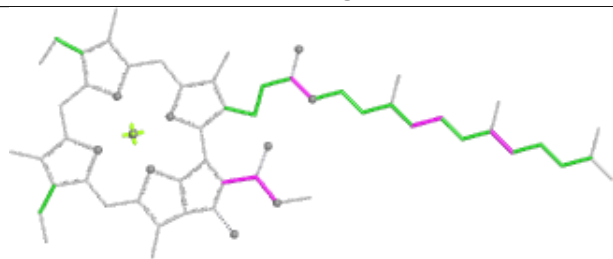
Ligand CLA B 614



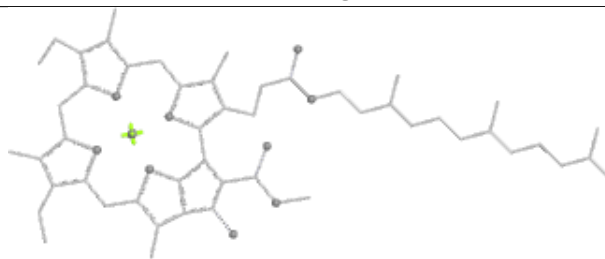
Bond lengths



Bond angles

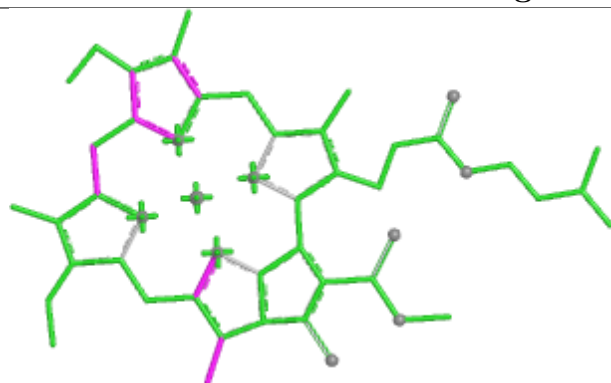


Torsions

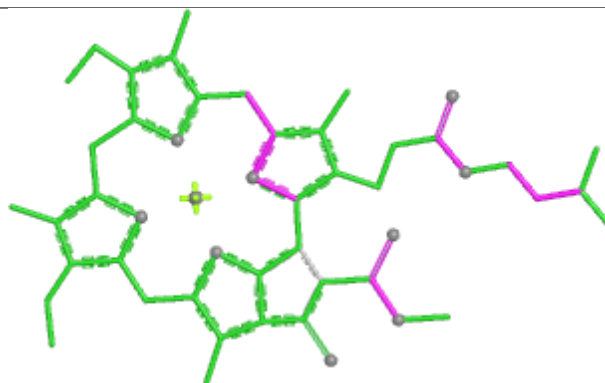


Rings

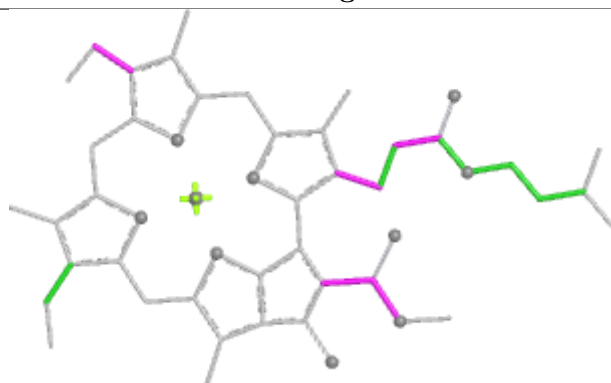
Ligand CLA B 601



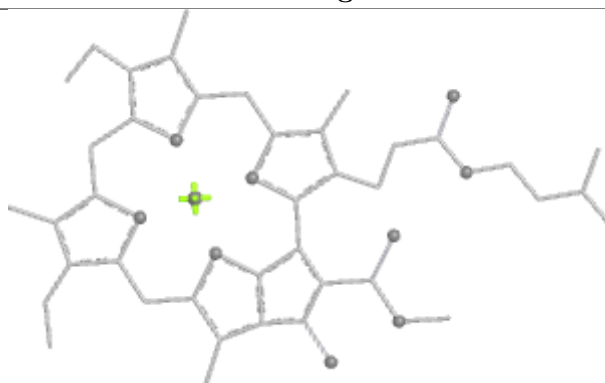
Bond lengths



Bond angles

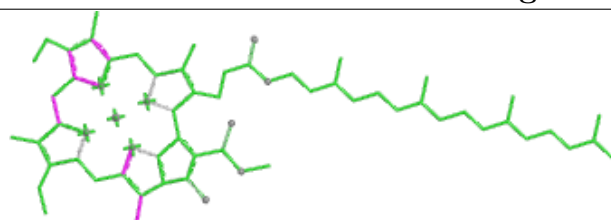


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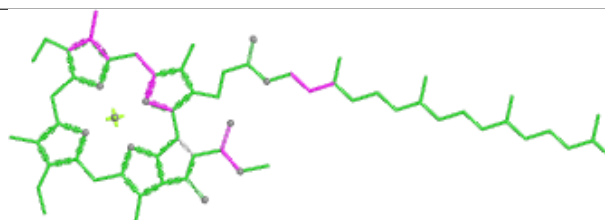


Rings

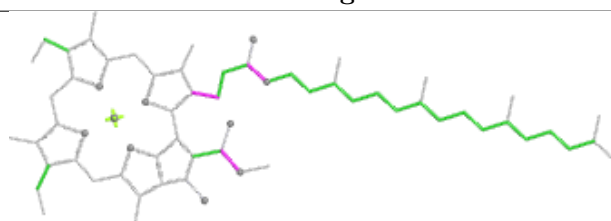
Ligand CLA c 516



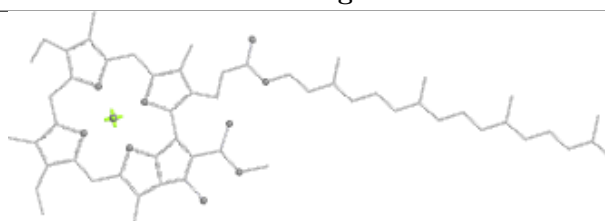
Bond lengths



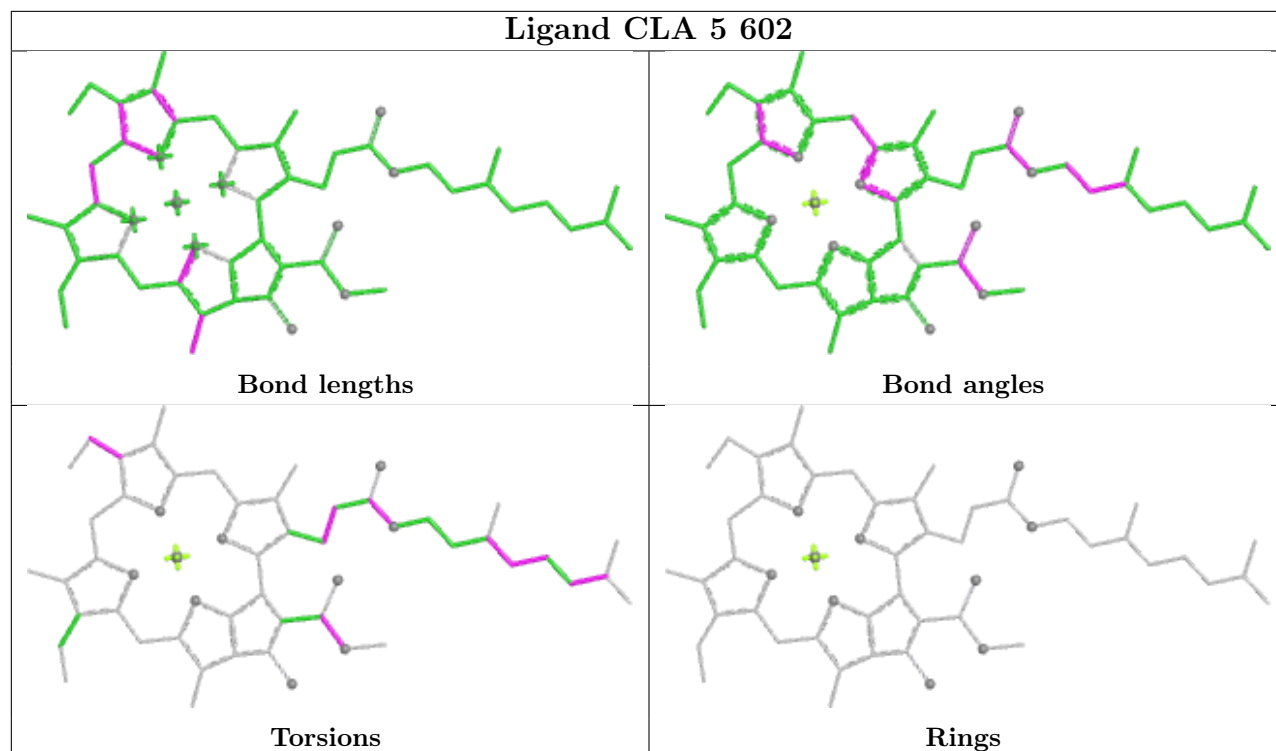
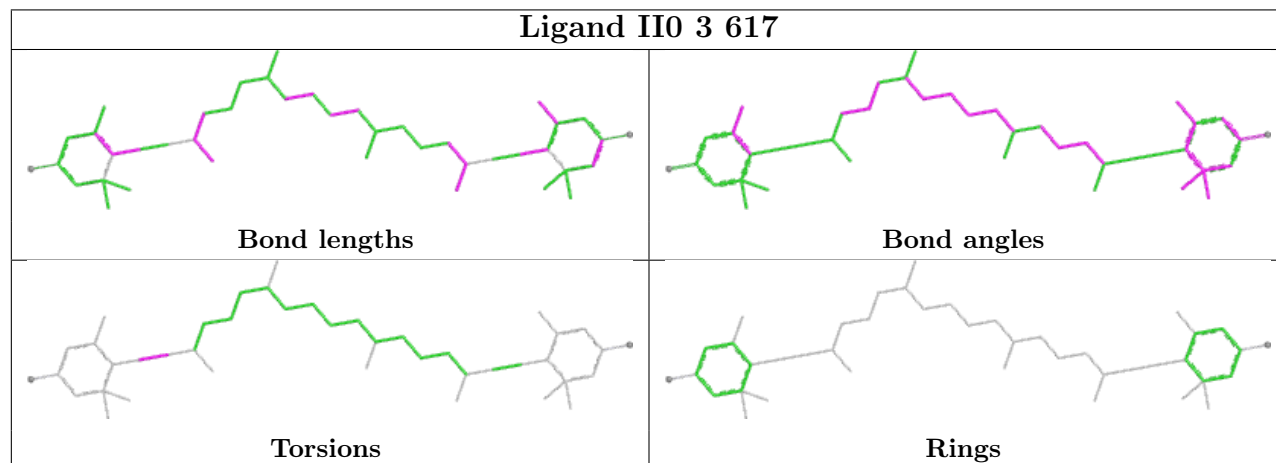
Bond angles

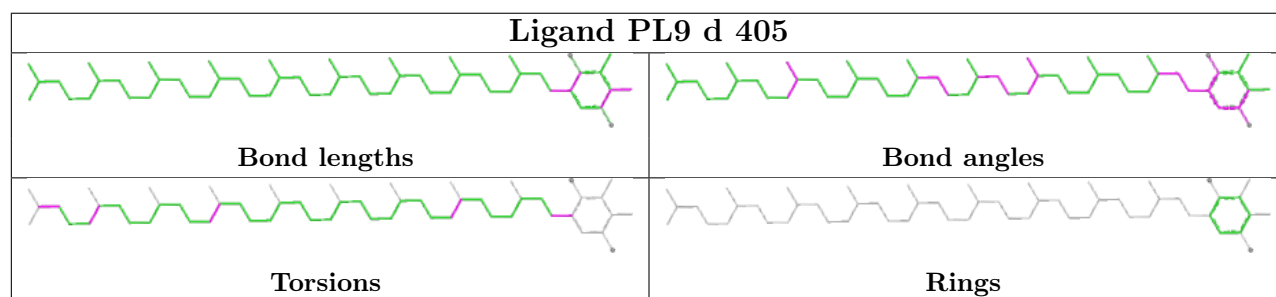
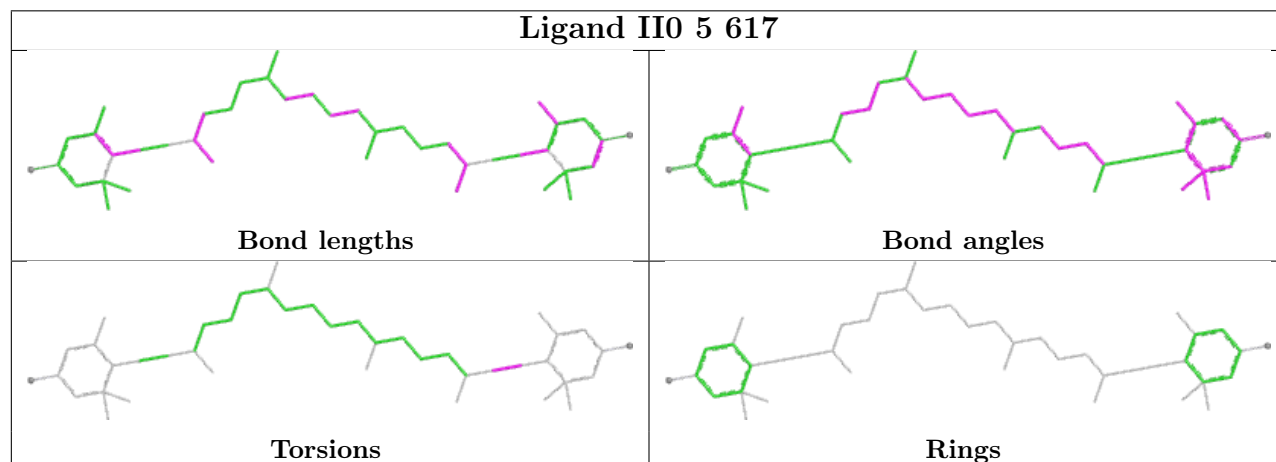
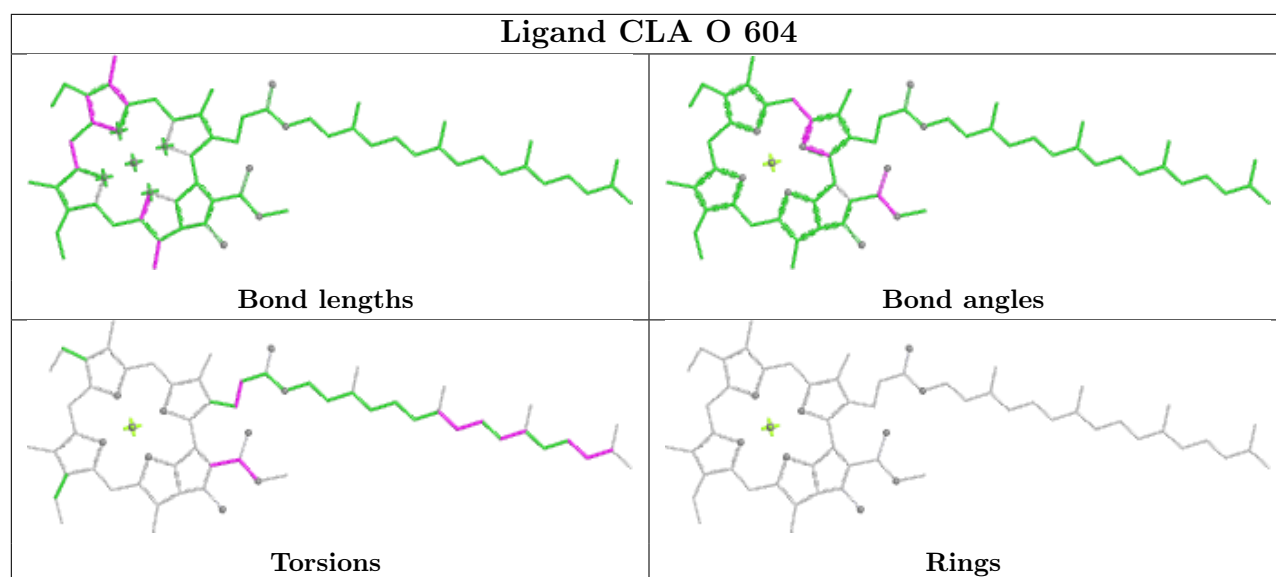


Torsions

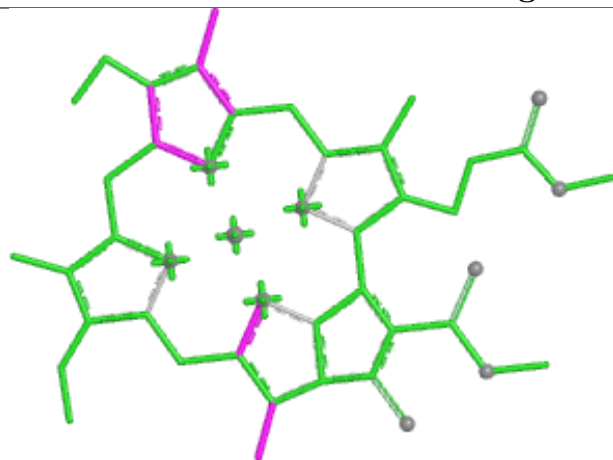


Rings

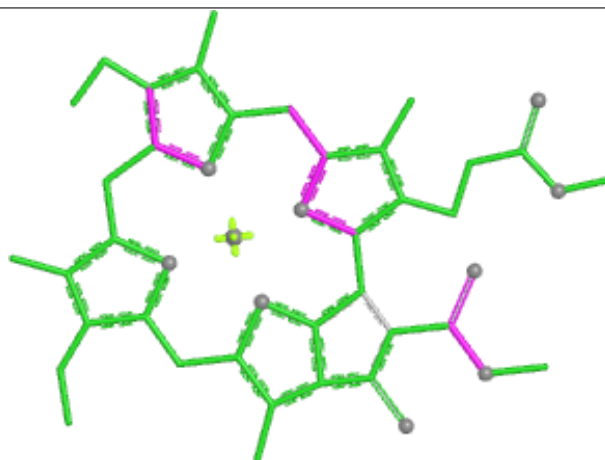
Ligand CLA 5 602**Ligand II0 3 617**



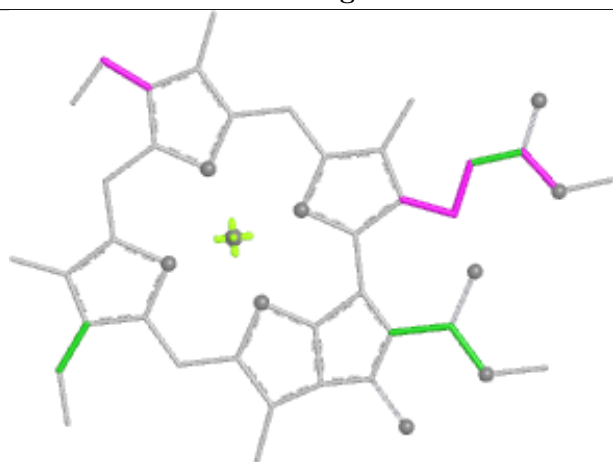
Ligand CLA 1 609



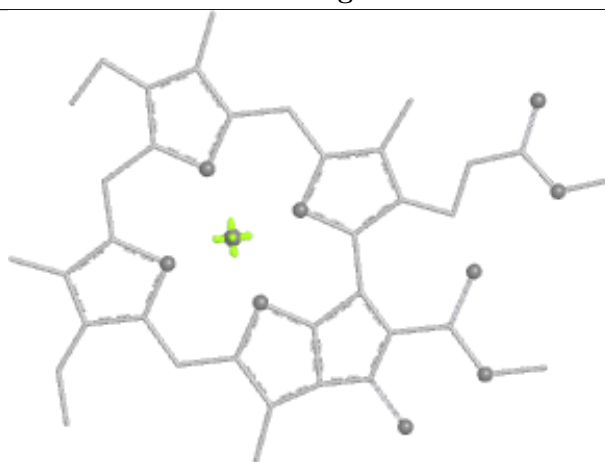
Bond lengths



Bond angles

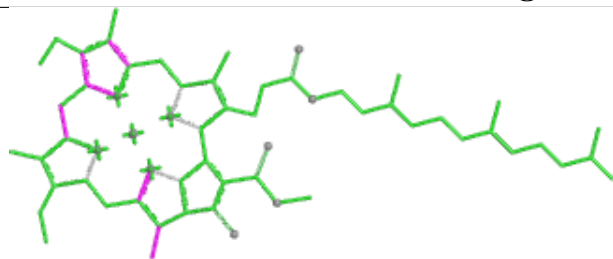


Torsions

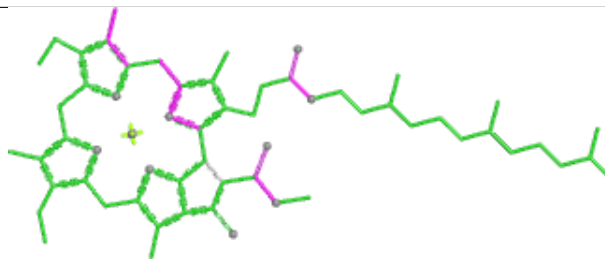


Rings

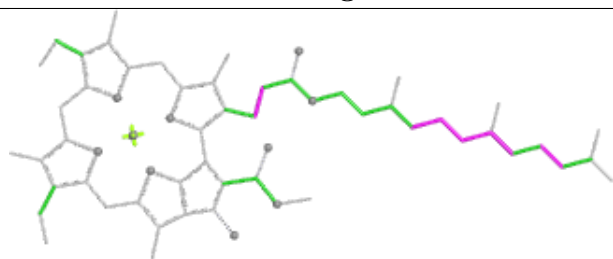
Ligand CLA 5 604



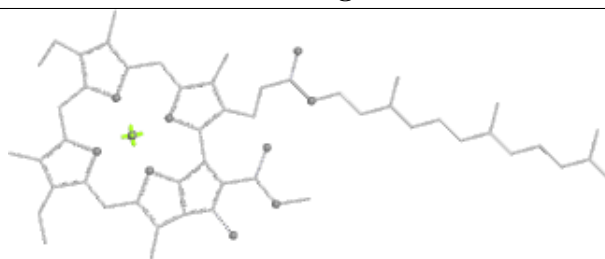
Bond lengths



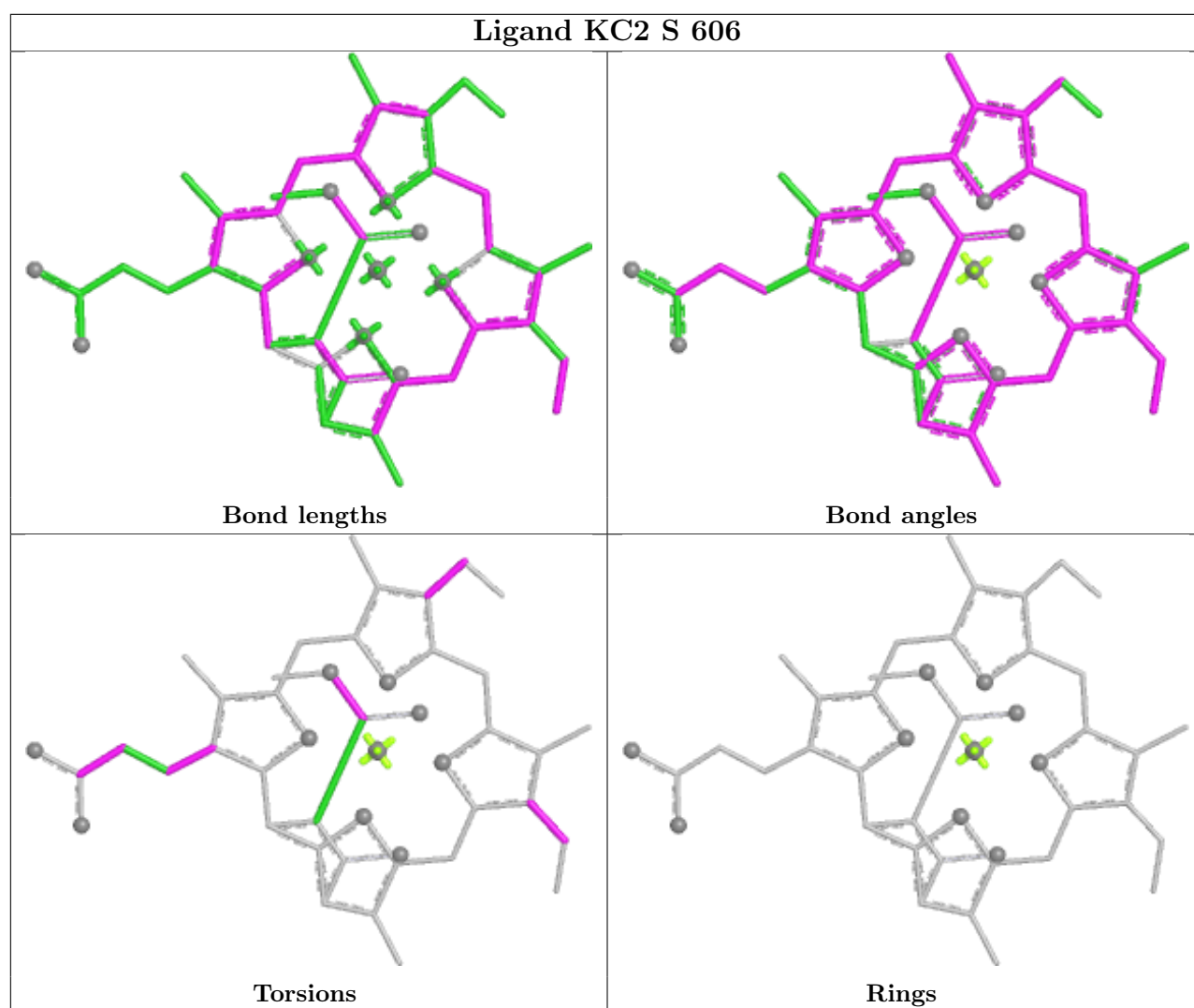
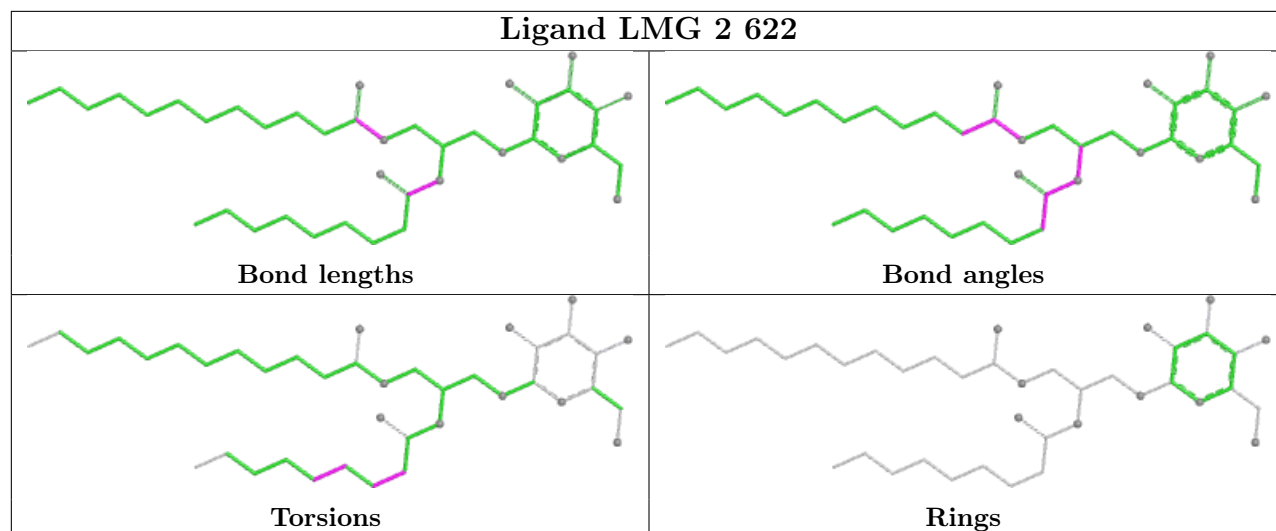
Bond angles

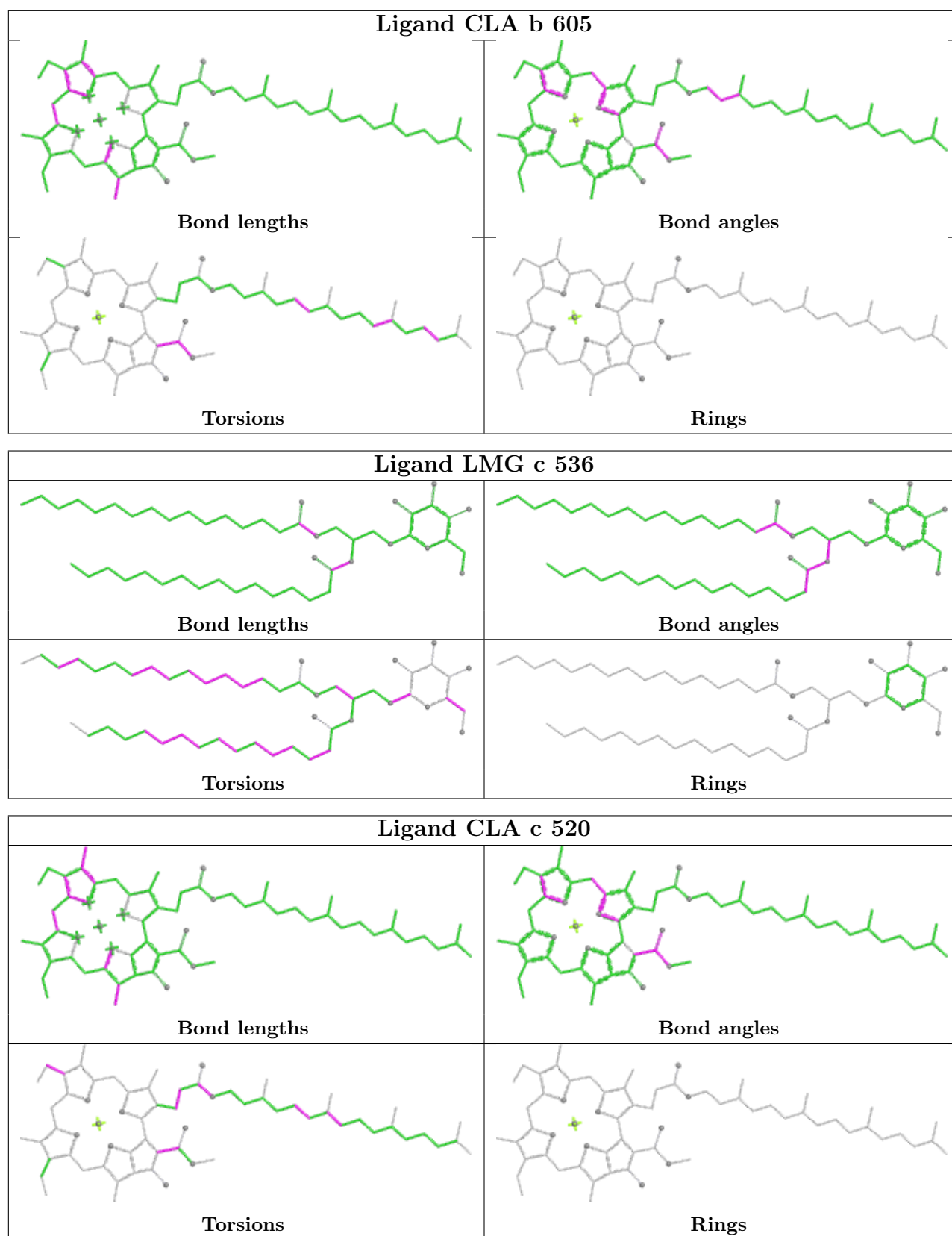


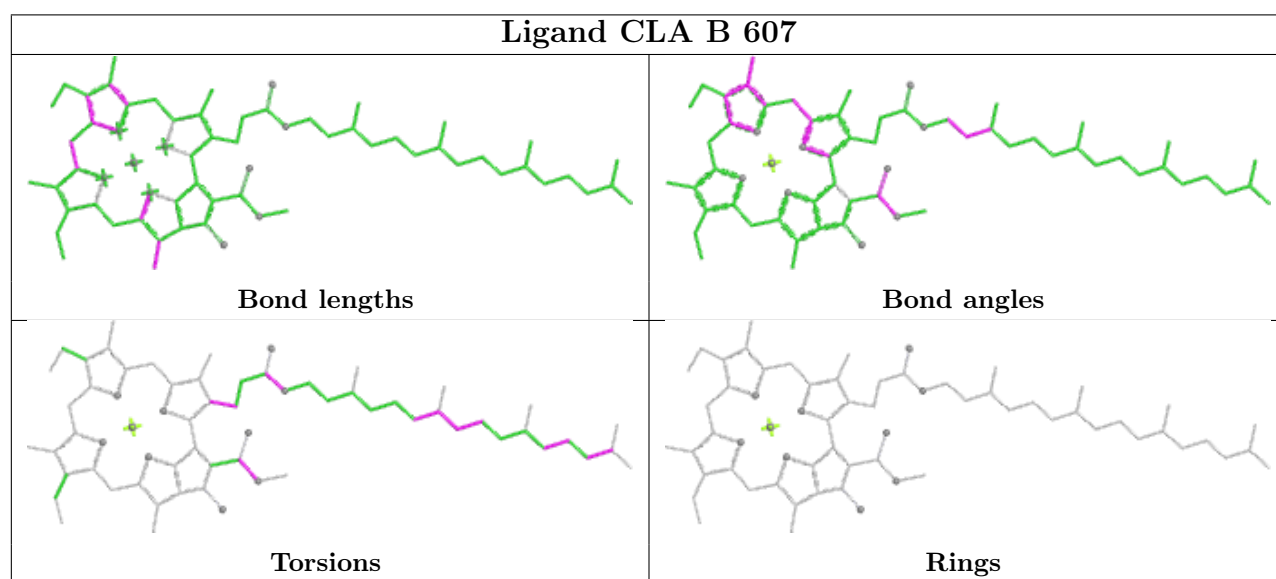
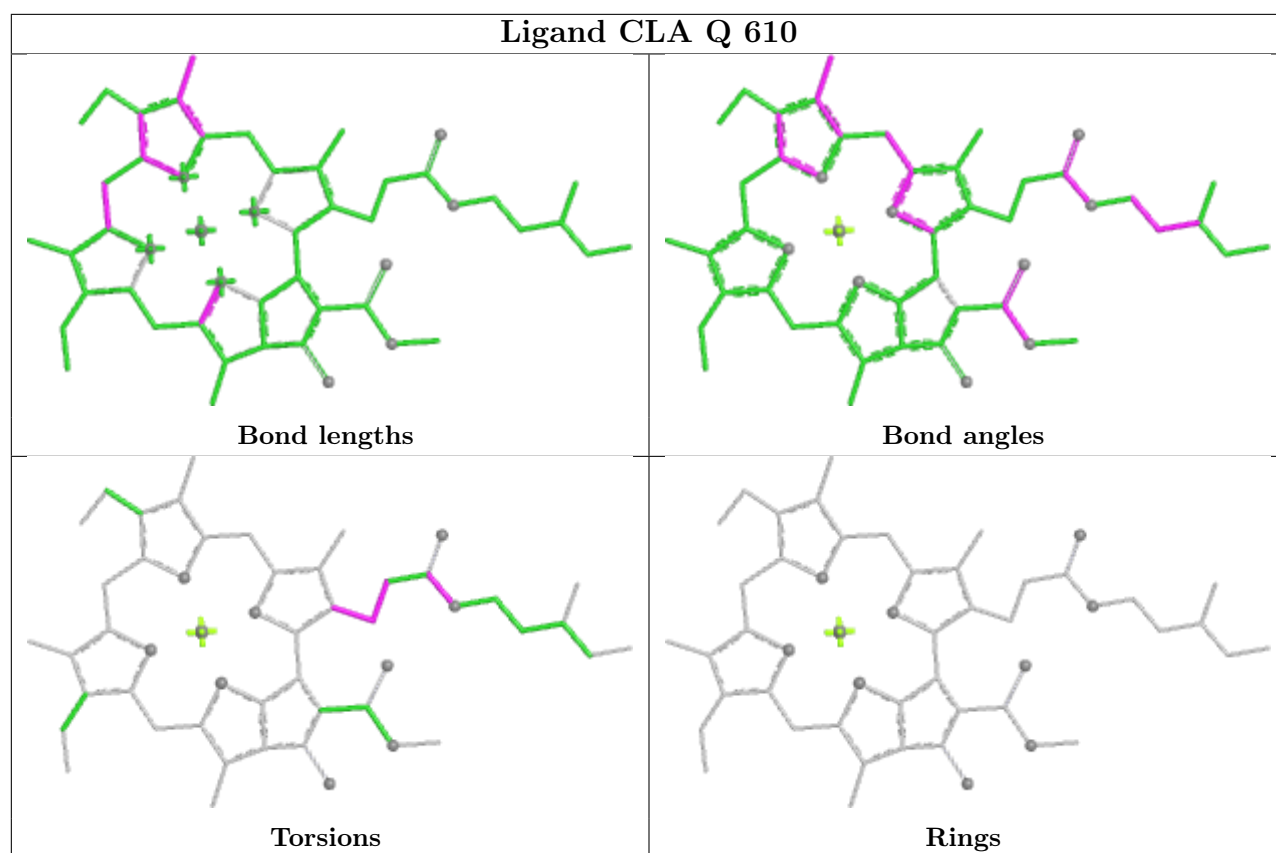
Torsions

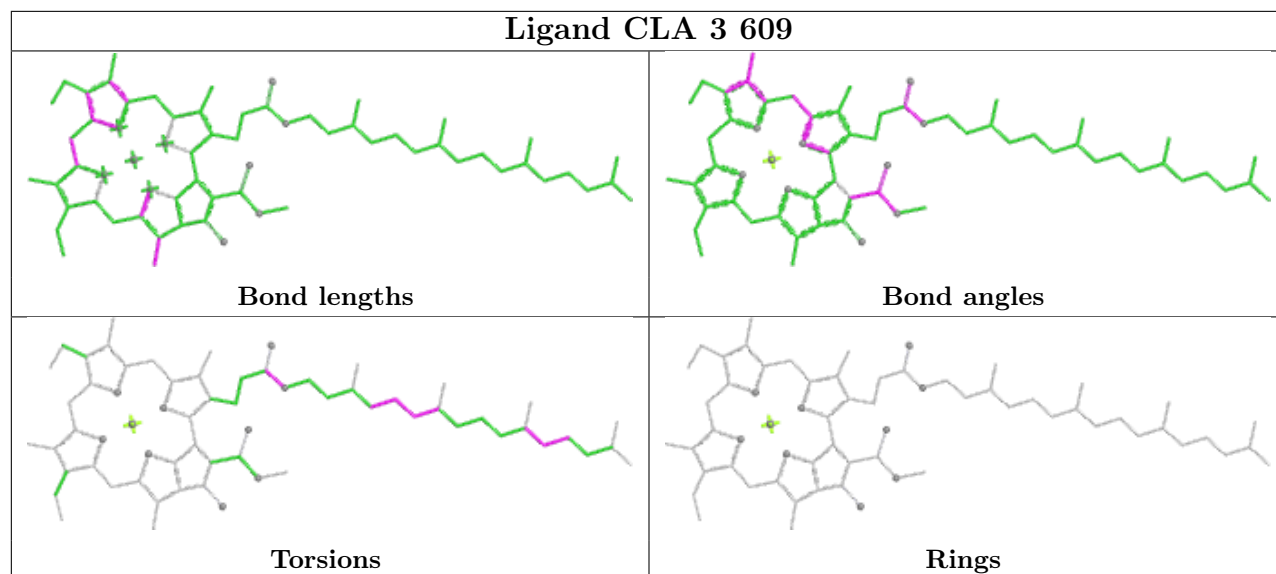
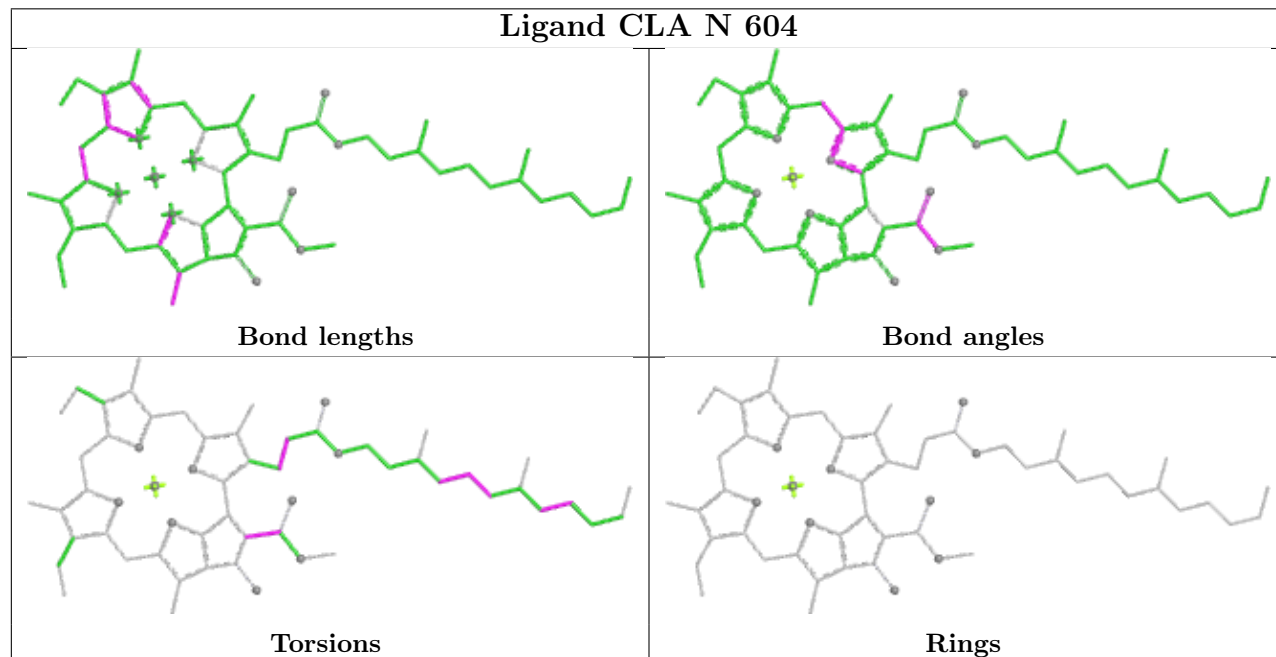


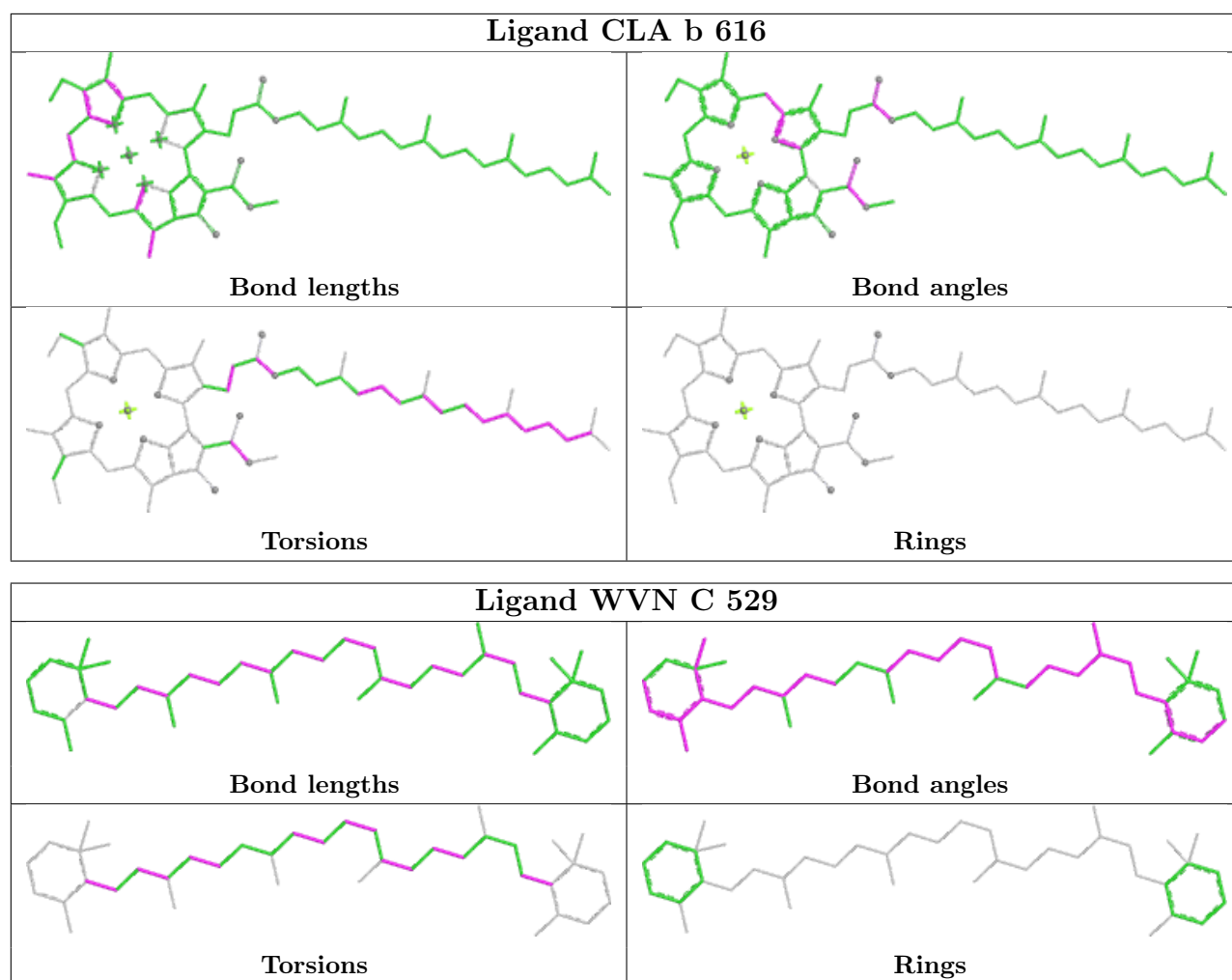
Rings



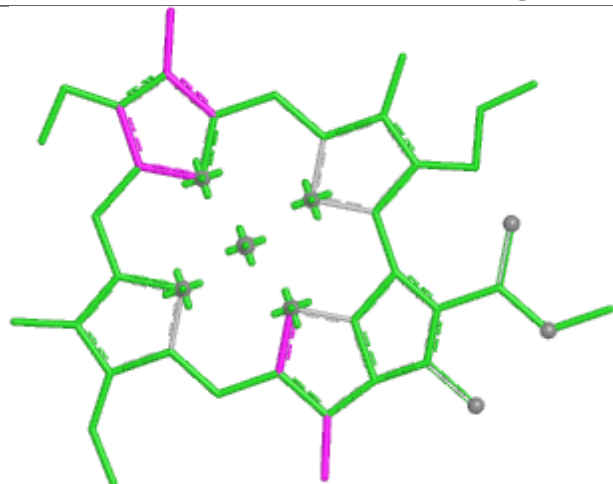




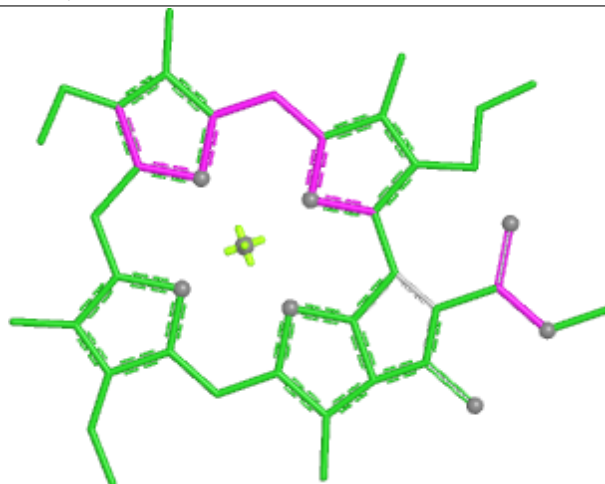
Ligand CLA 3 609**Ligand CLA N 604**



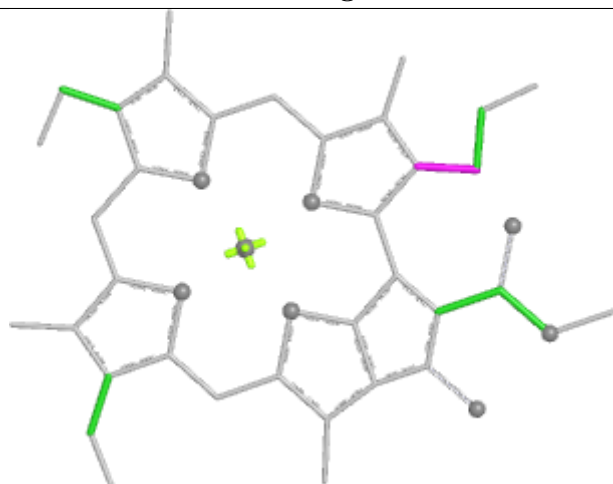
Ligand CLA Q 607



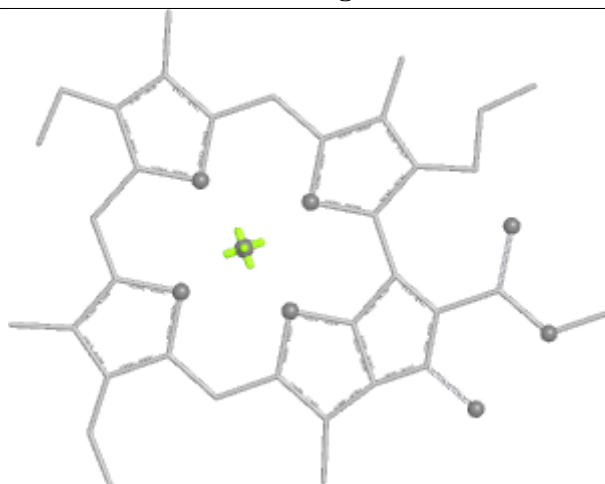
Bond lengths



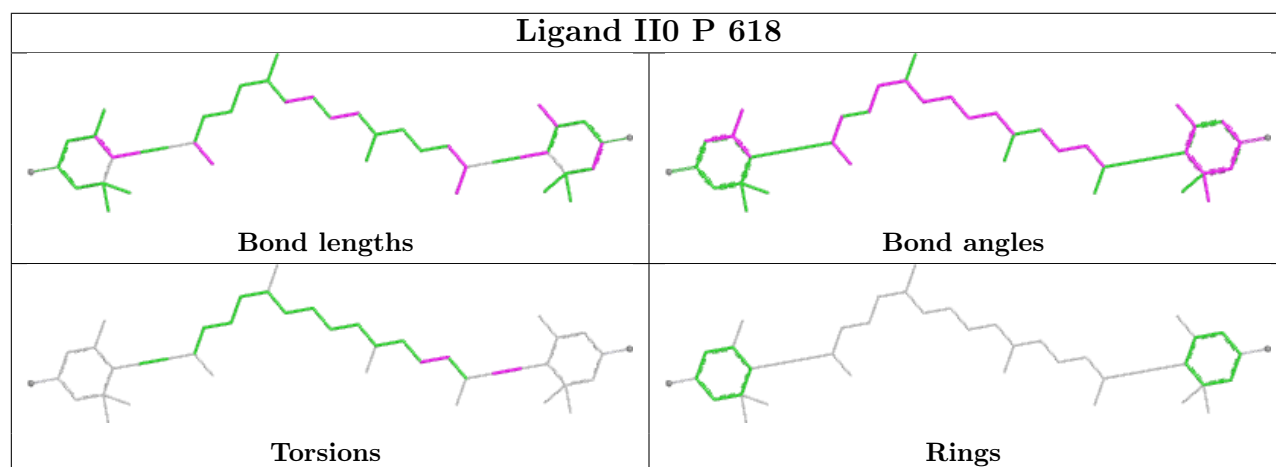
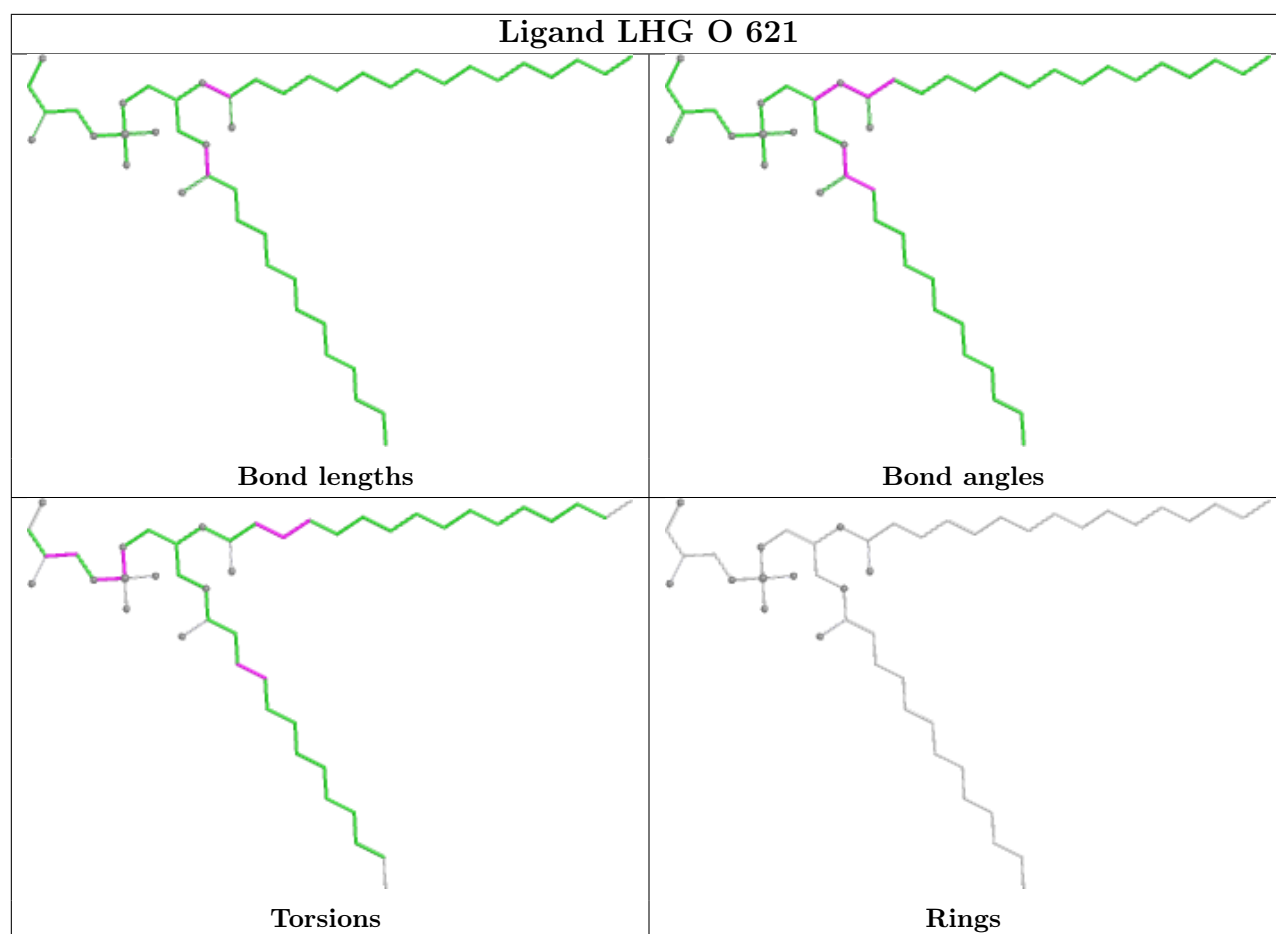
Bond angles



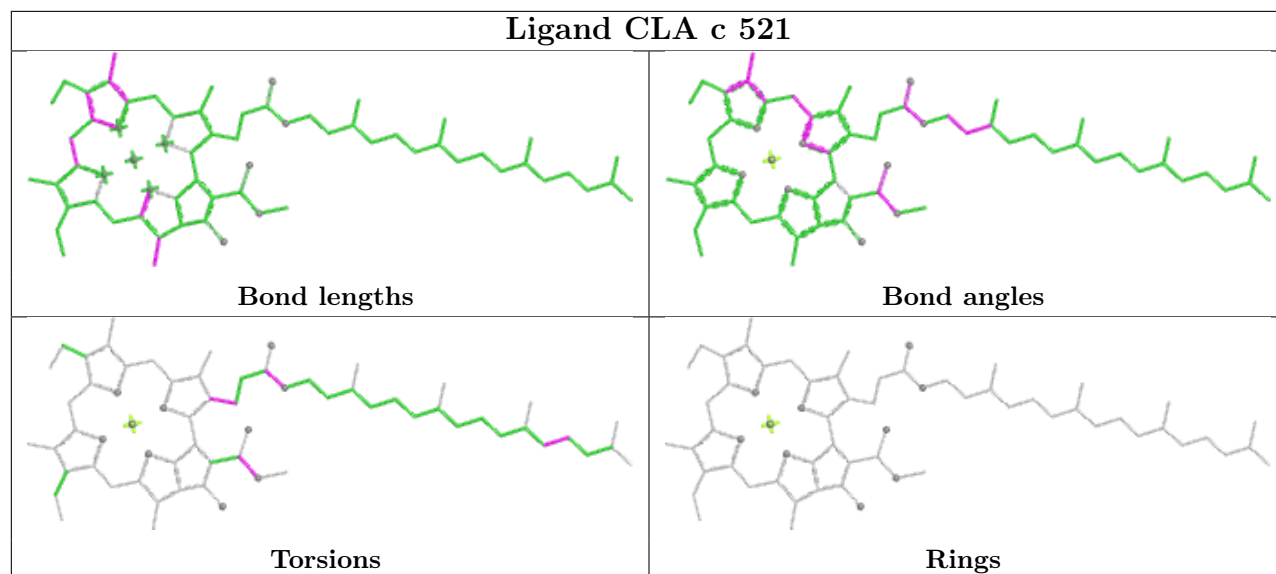
Torsions



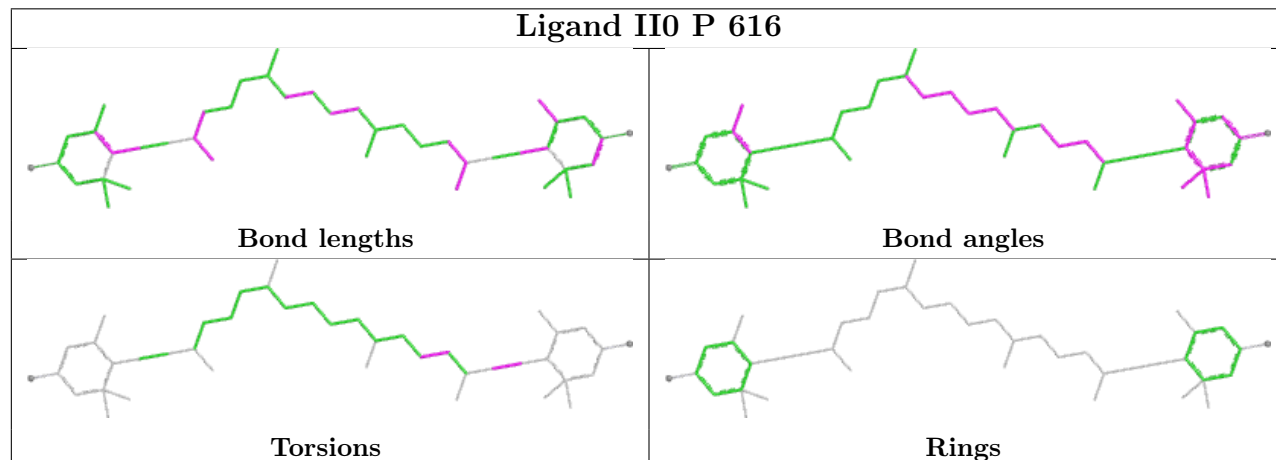
Rings



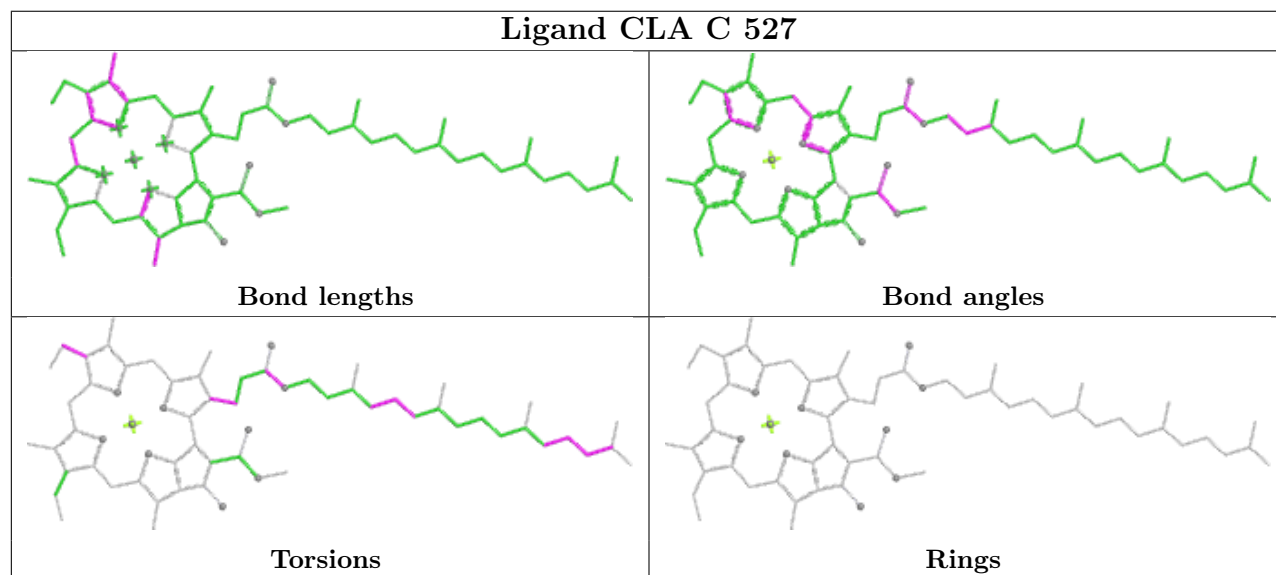
Ligand CLA c 521

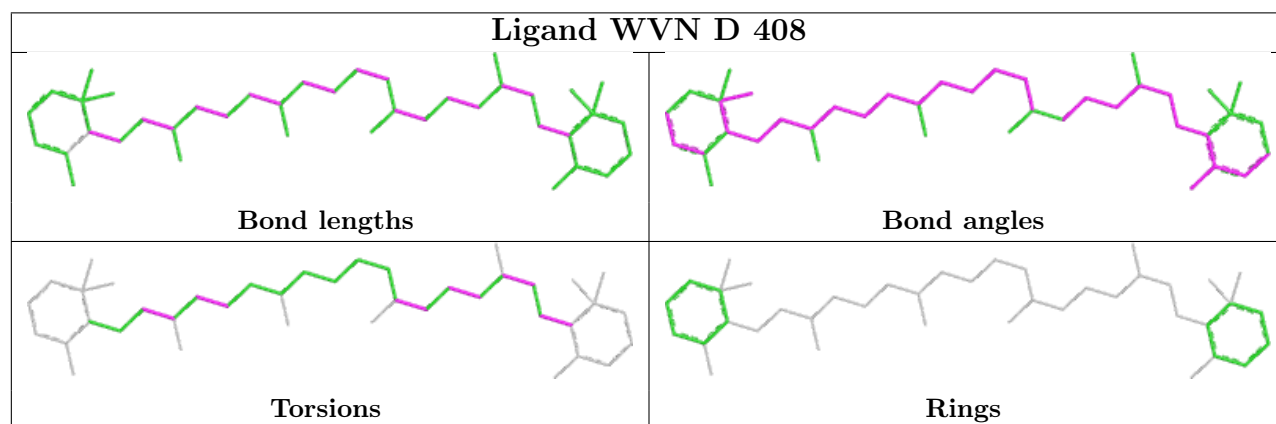
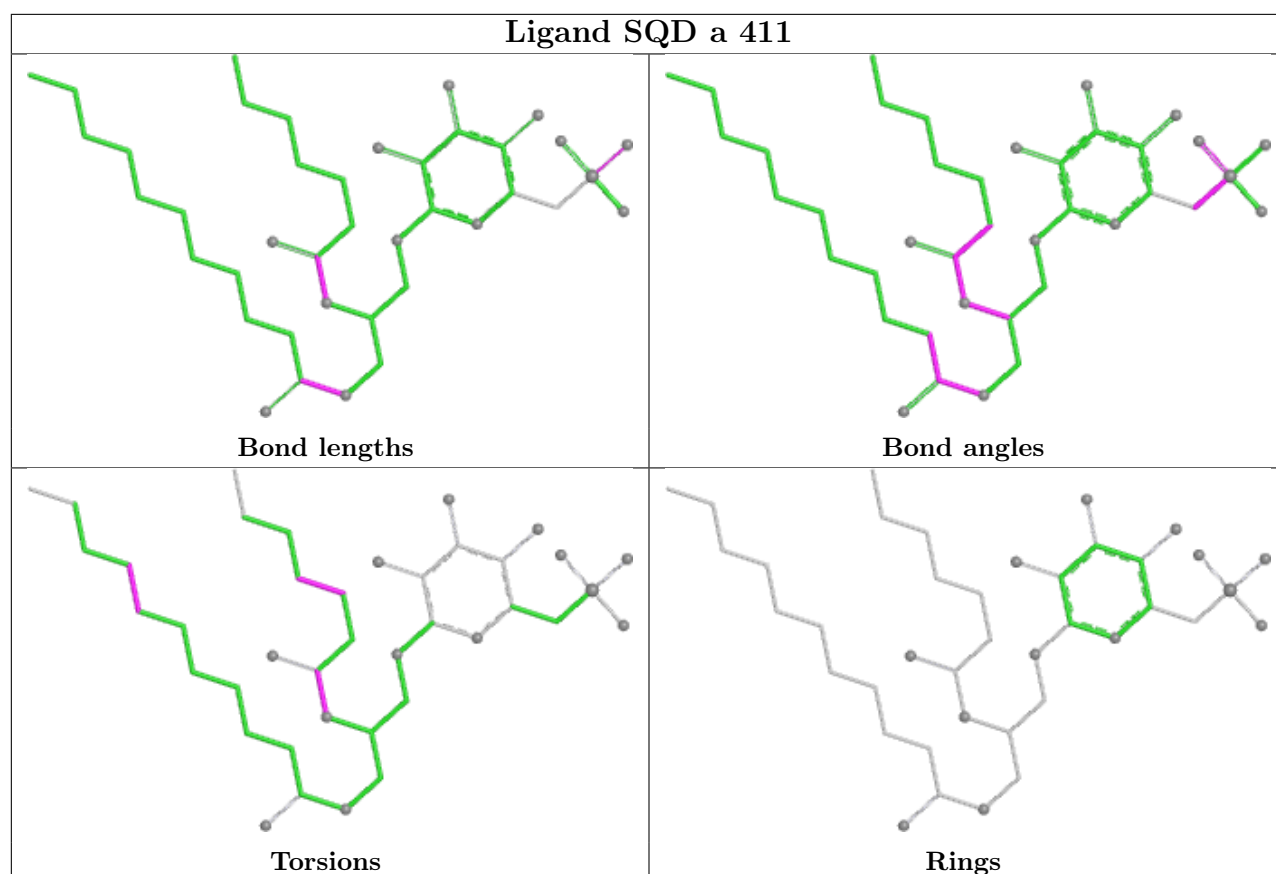


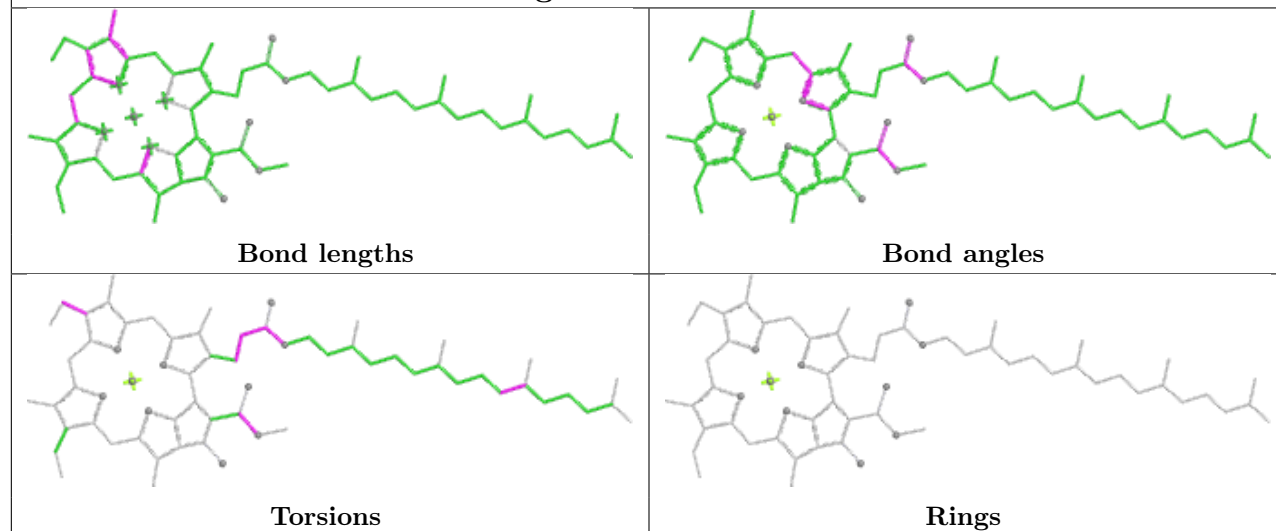
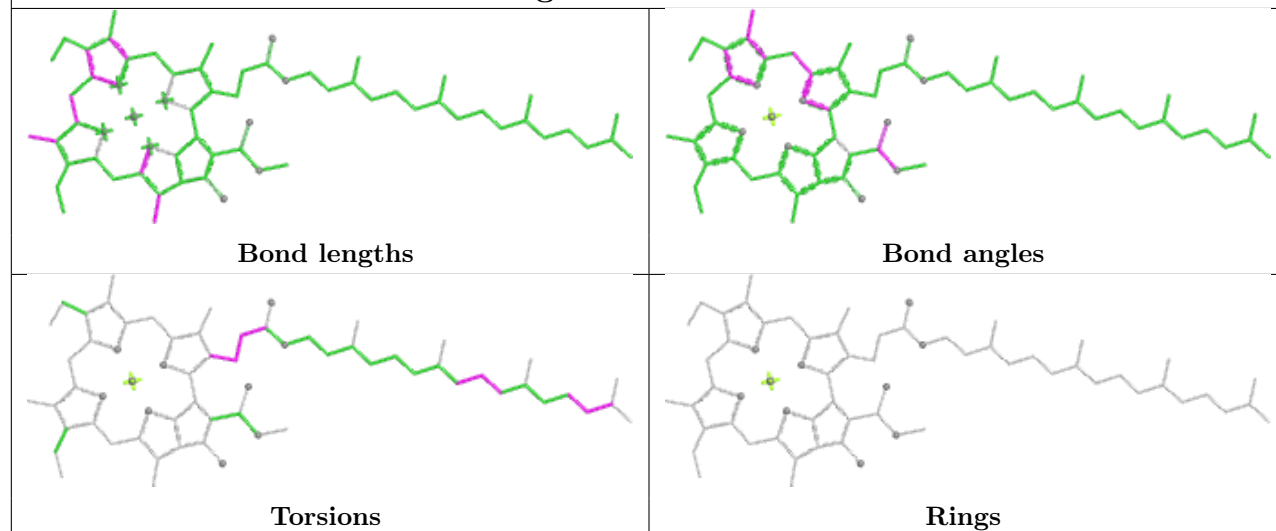
Ligand II0 P 616



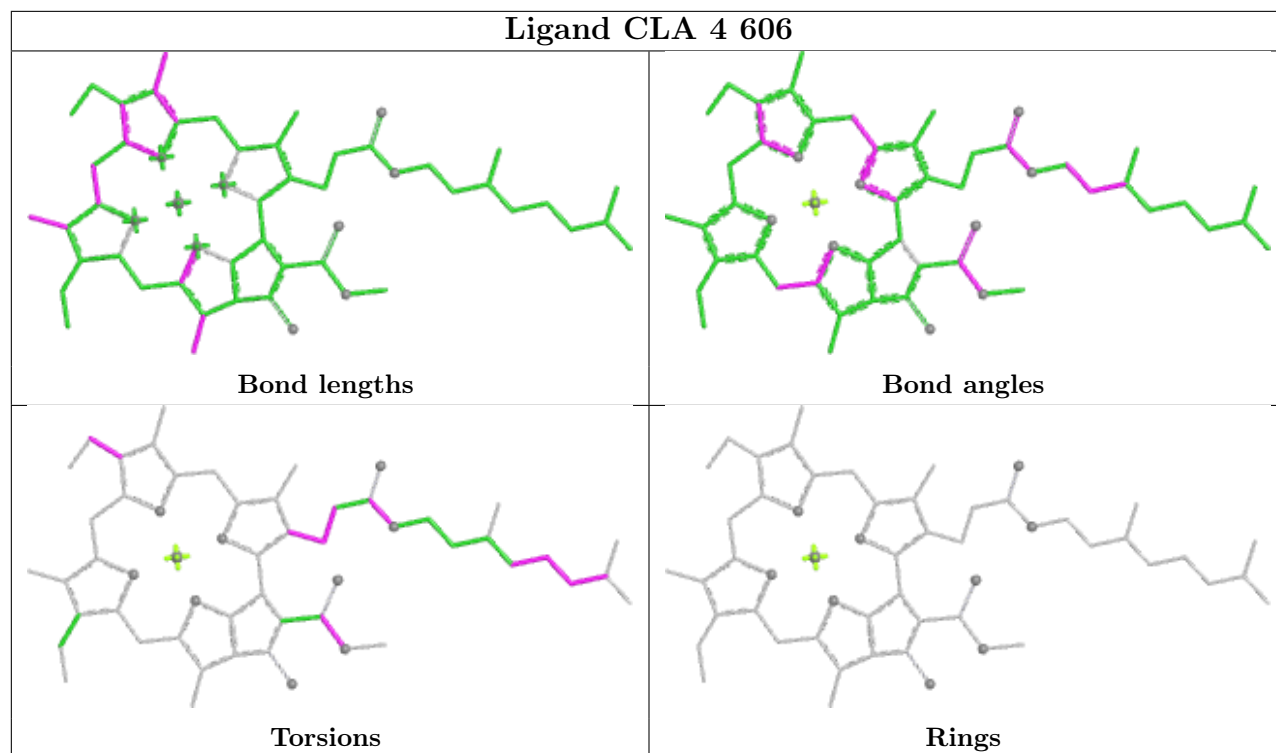
Ligand CLA C 527



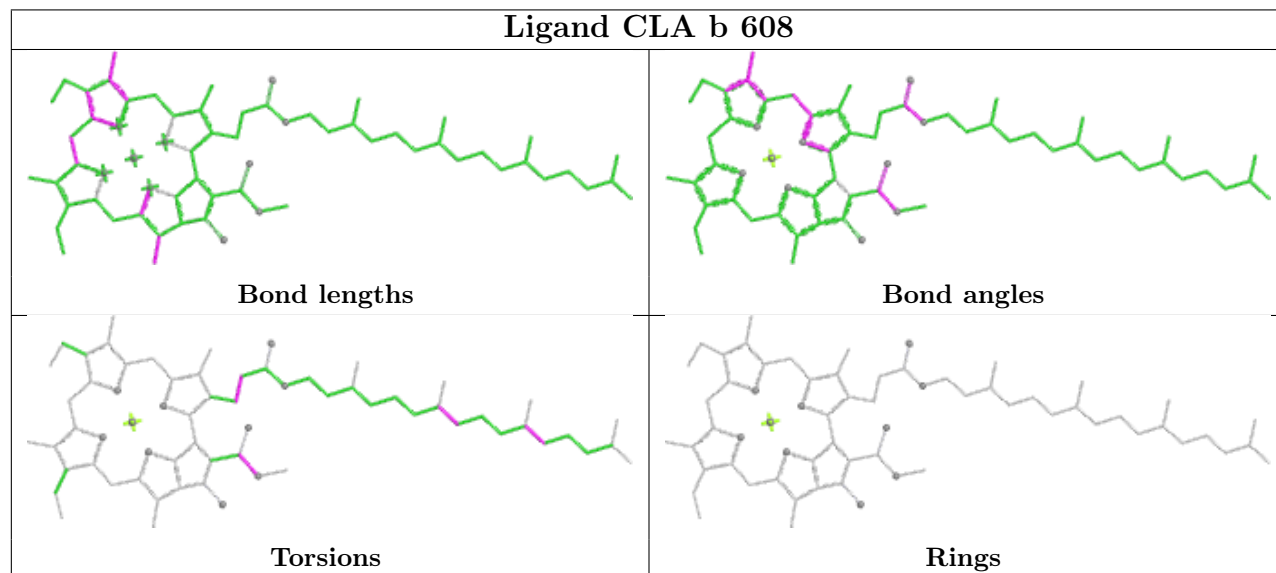


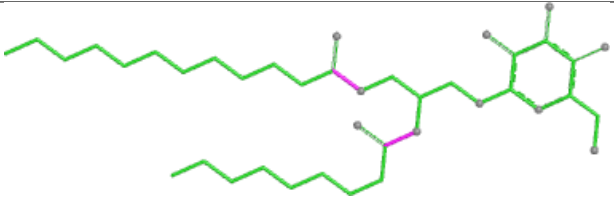
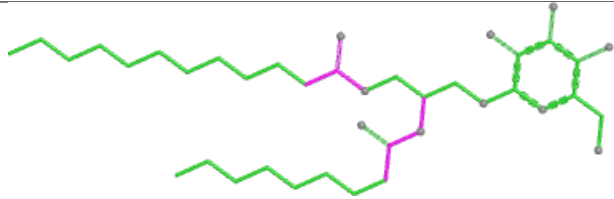
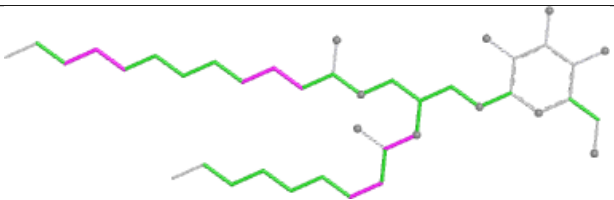
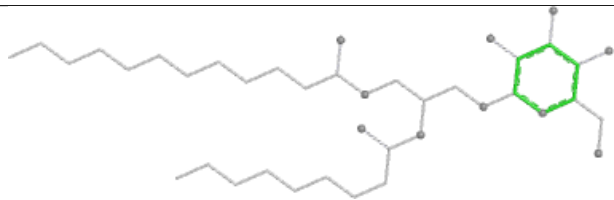
Ligand CLA b 610**Ligand CLA 2 603**

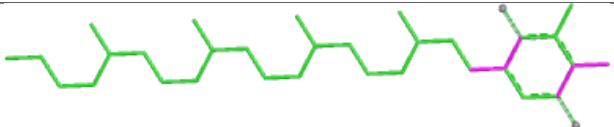
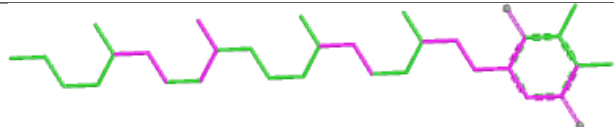
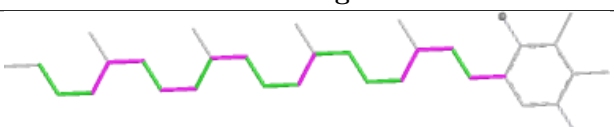
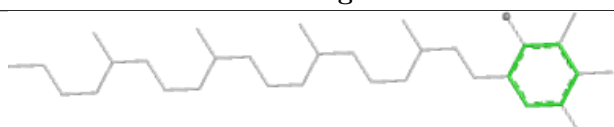
Ligand CLA 4 606

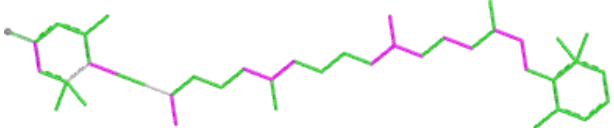
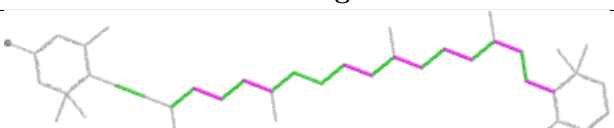


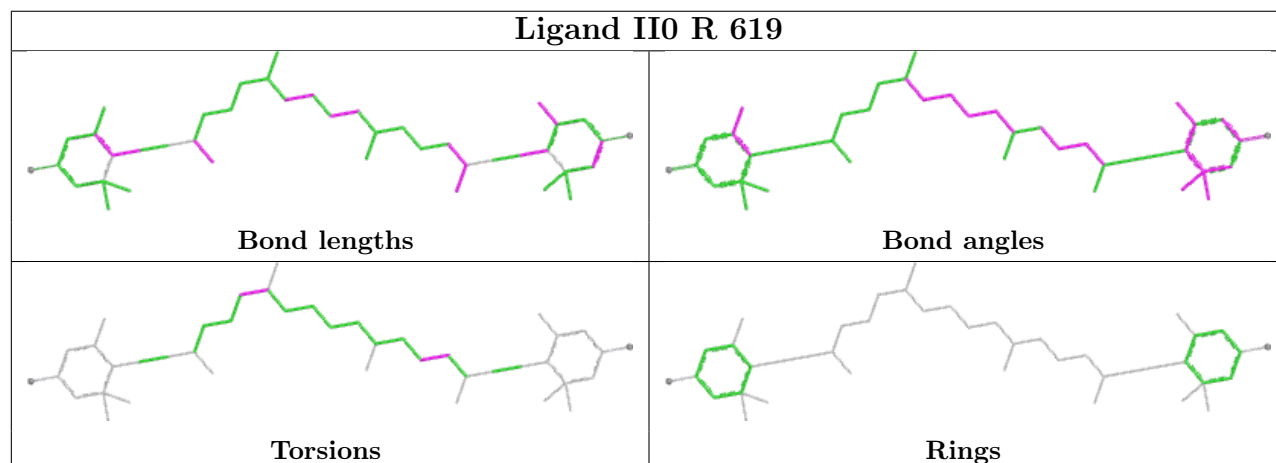
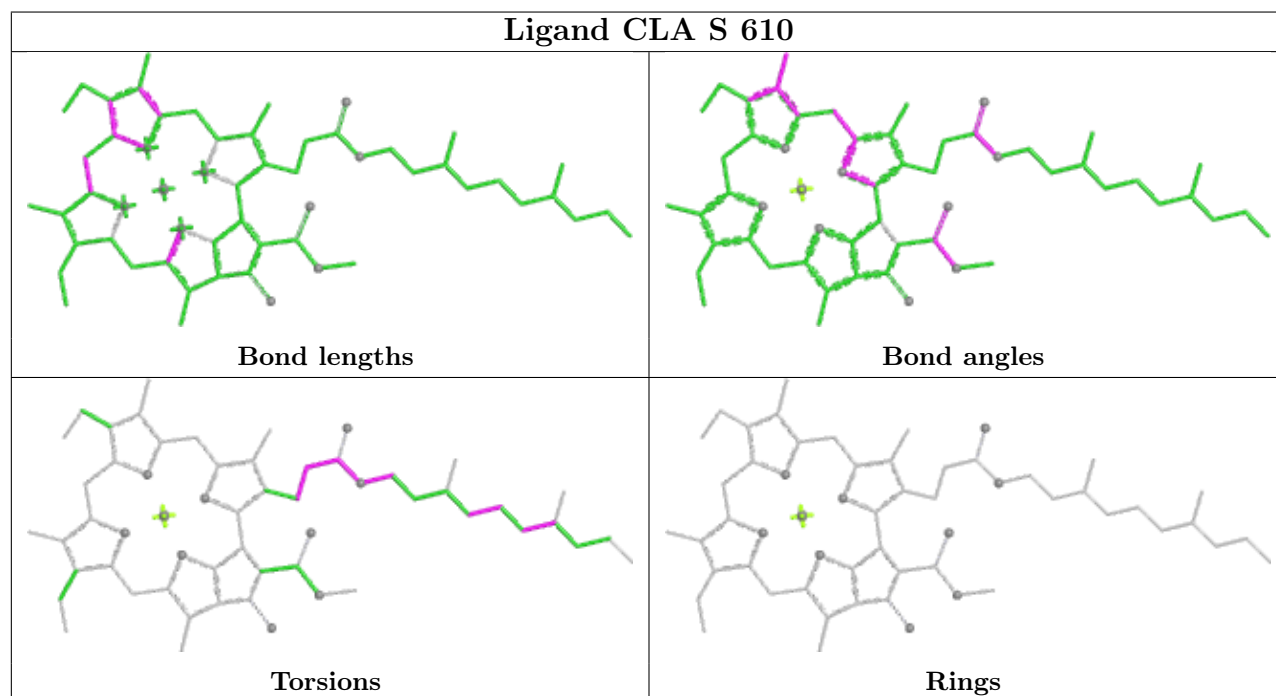
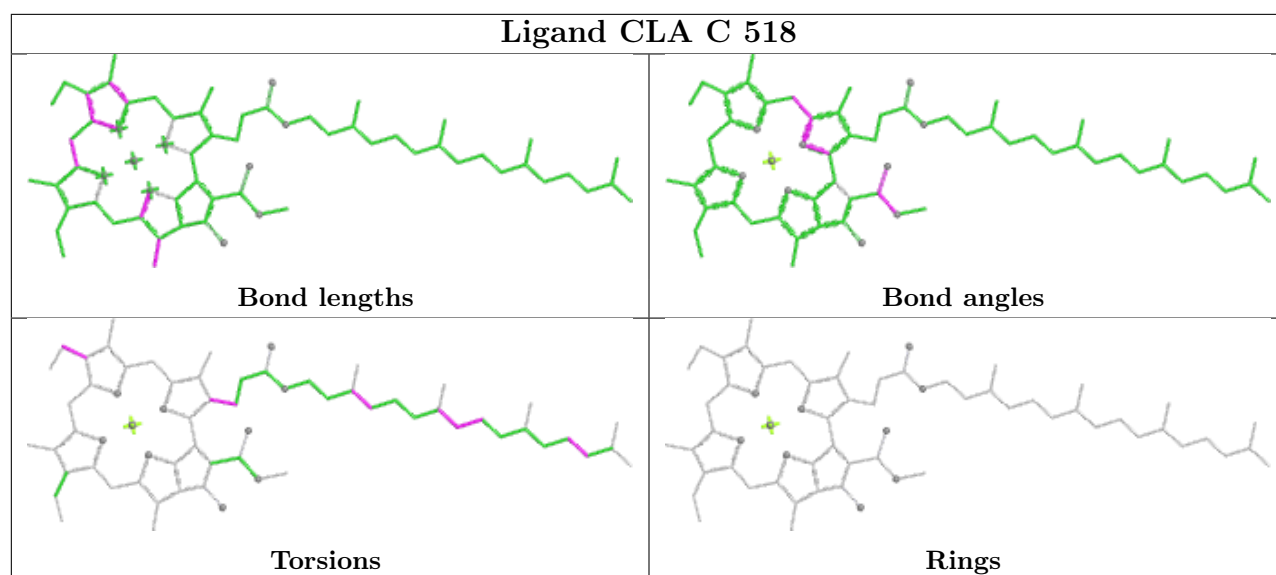
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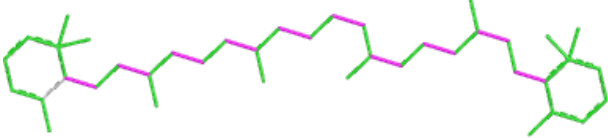
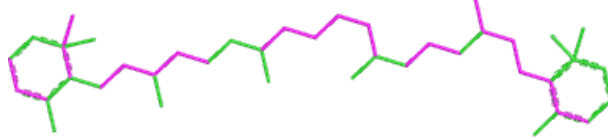
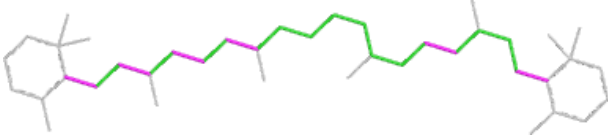
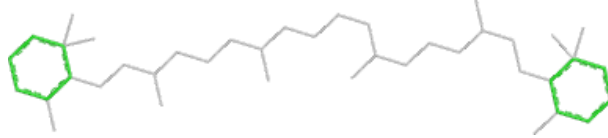
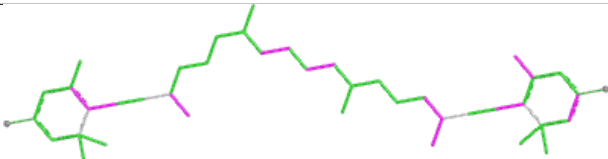
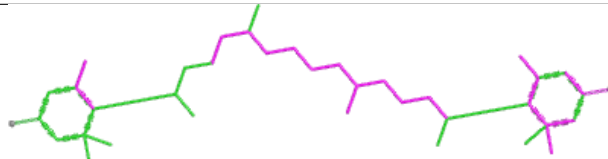
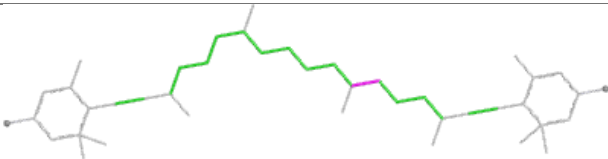
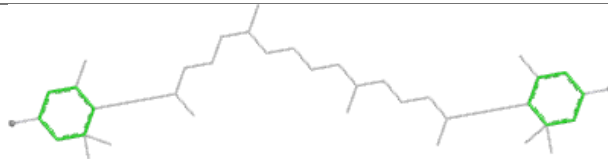
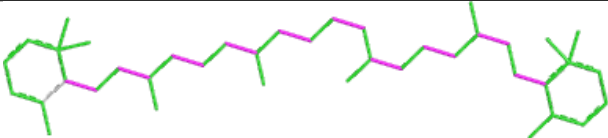
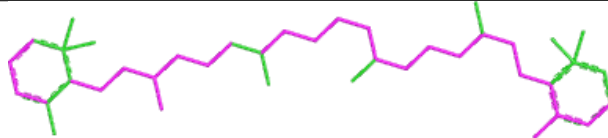
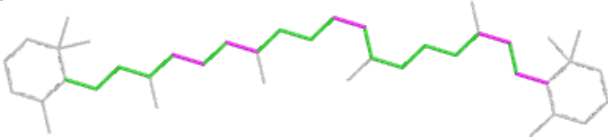
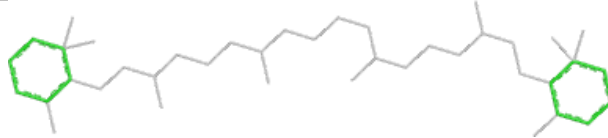


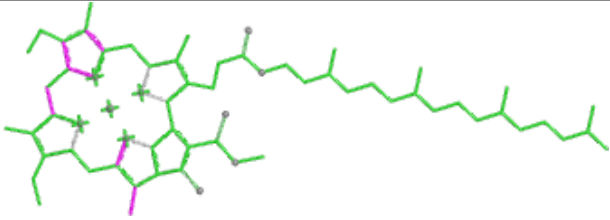
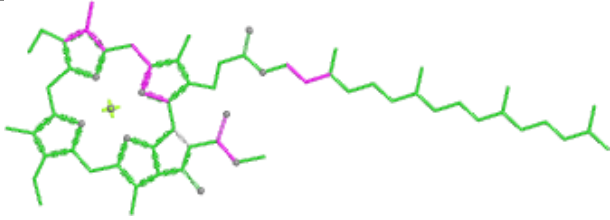
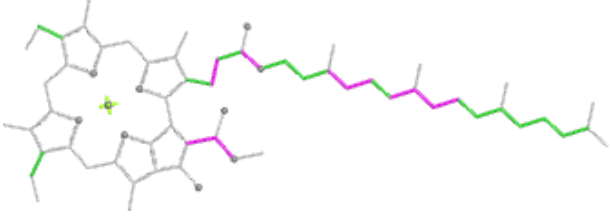
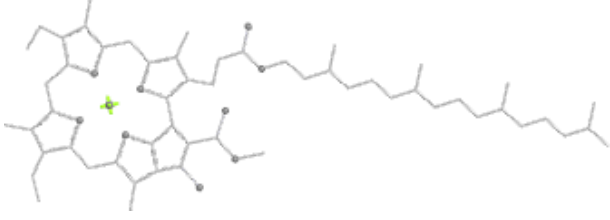
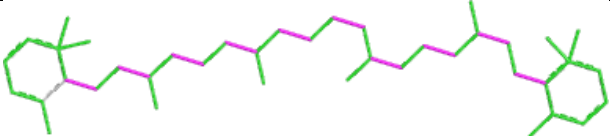
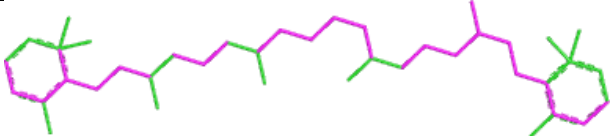
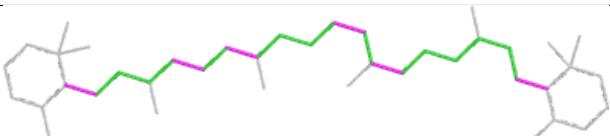
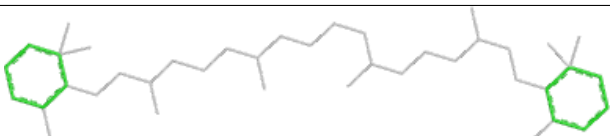
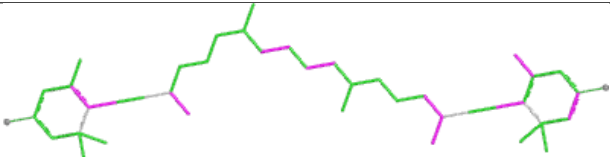
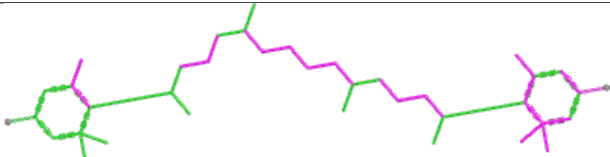
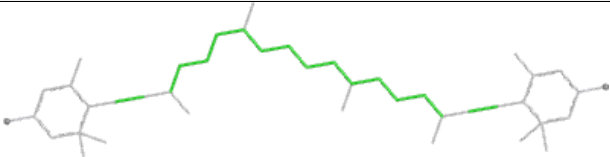
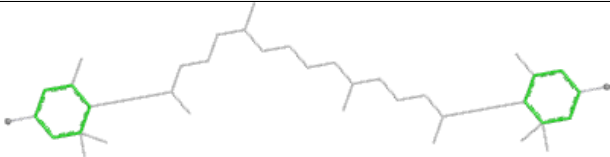
Ligand LMG m 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand PL9 a 409	
	
Bond lengths	Bond angles
	
Torsions	Rings

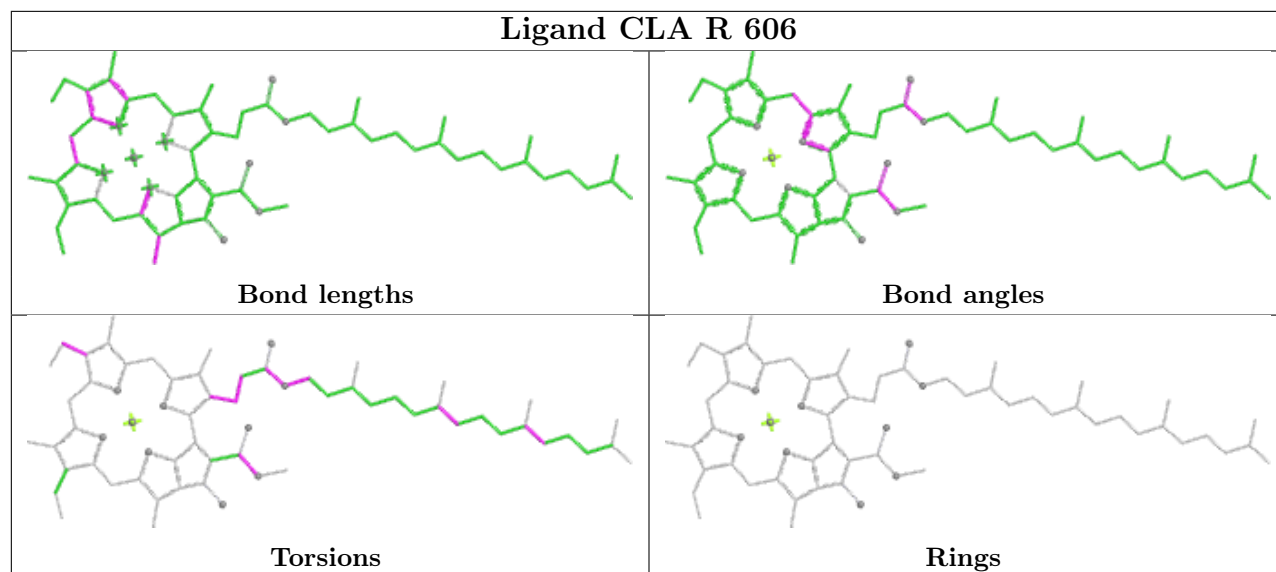
Ligand IHT R 620	
	
Bond lengths	Bond angles
	
Torsions	Rings



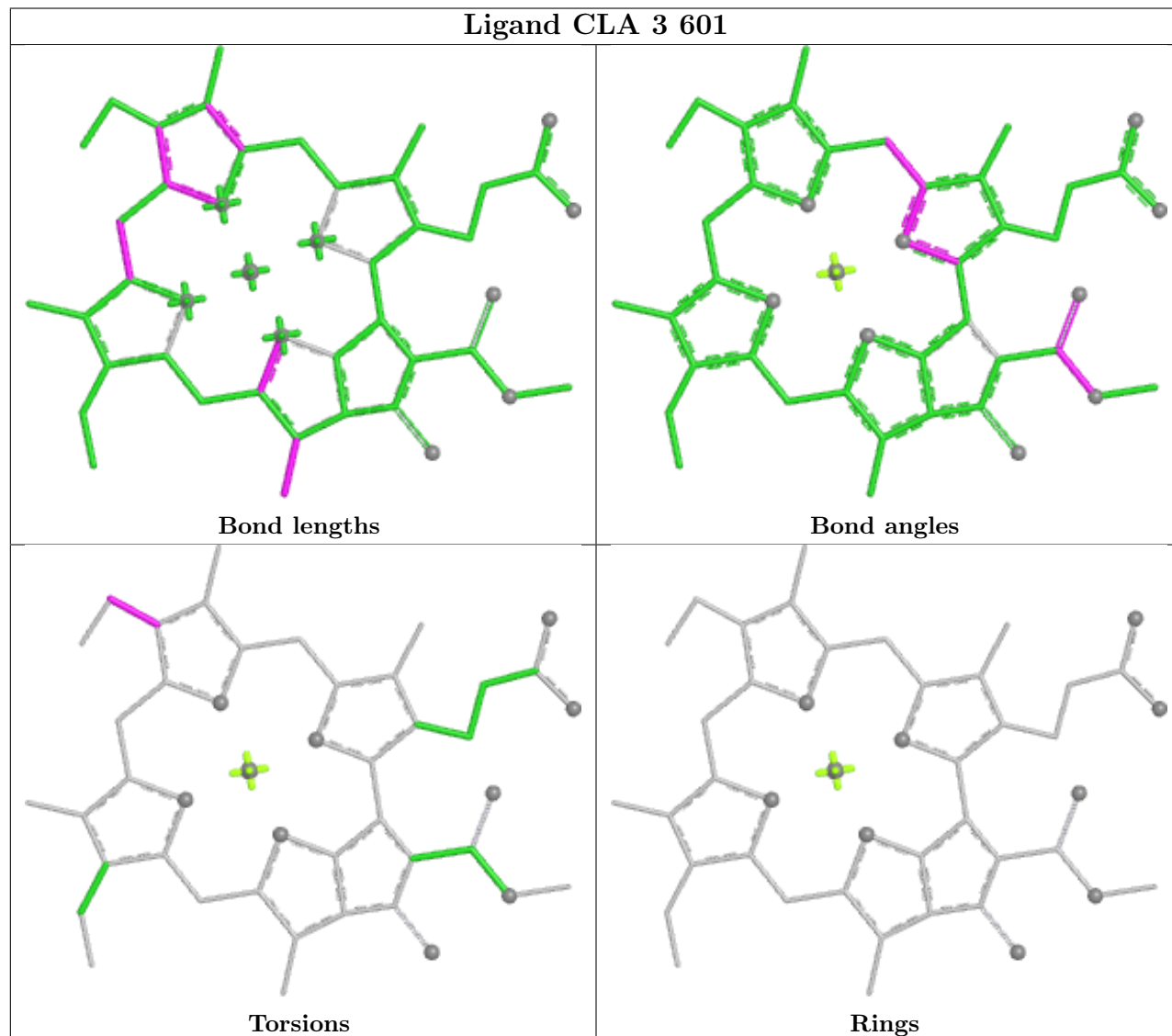
Ligand WVN S 620	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand II0 Q 616	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand WVN y 89	
 Bond lengths	 Bond angles
 Torsions	 Rings

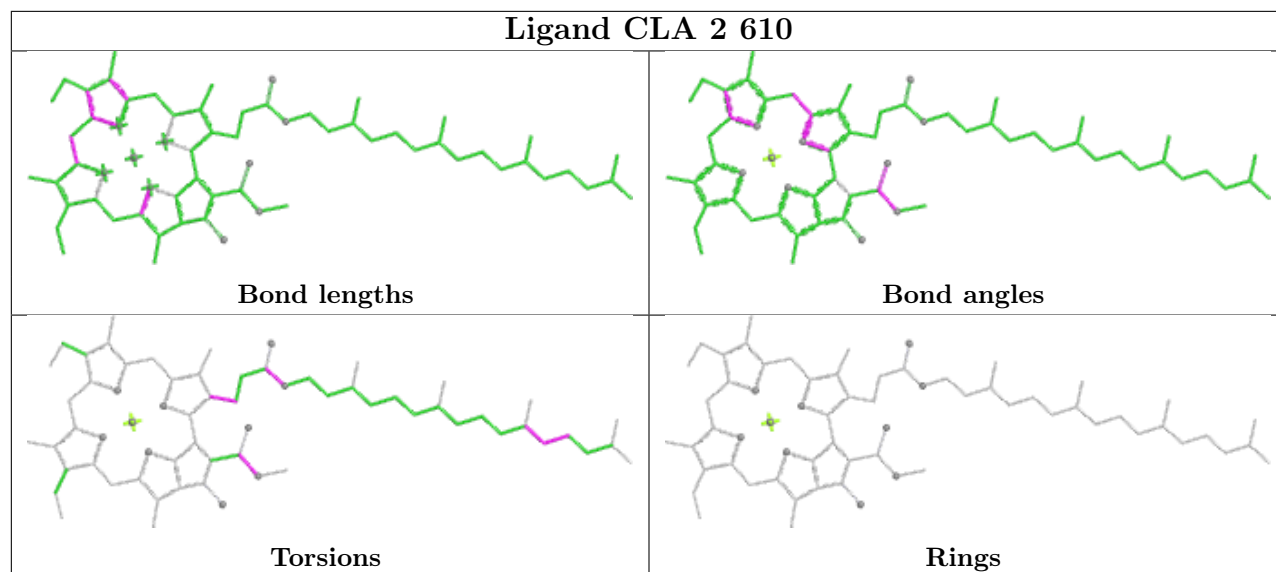
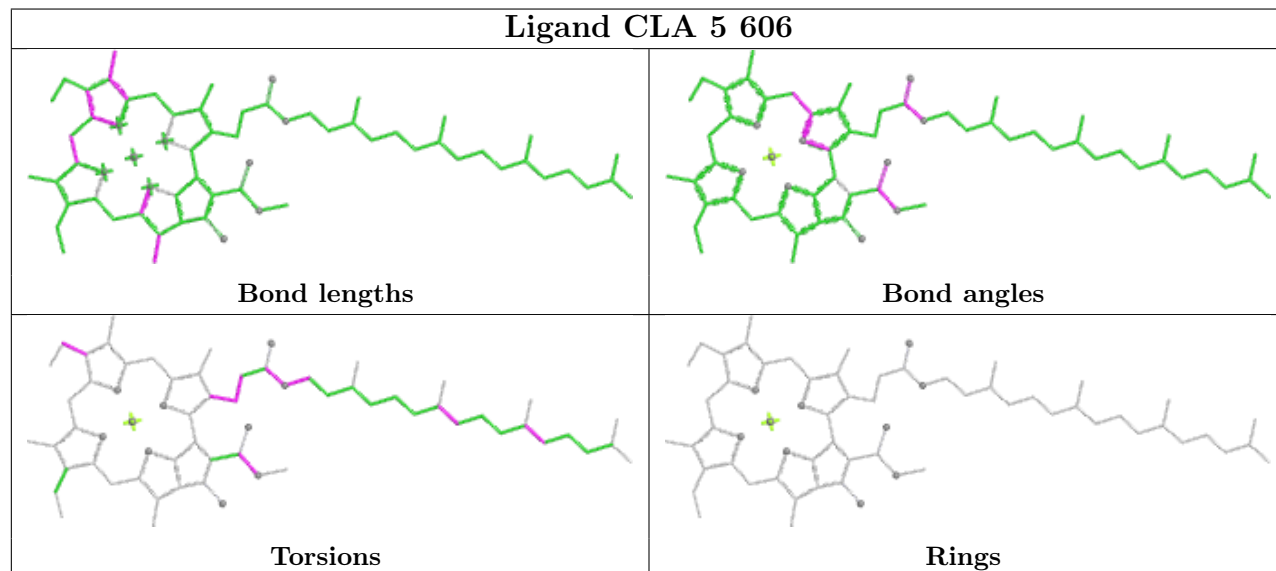
Ligand CLA c 525	
 Bond lengths	 Bond angles
 Torsions	 Rings
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 Torsions	 Rings
Ligand II0 N 617	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA R 606

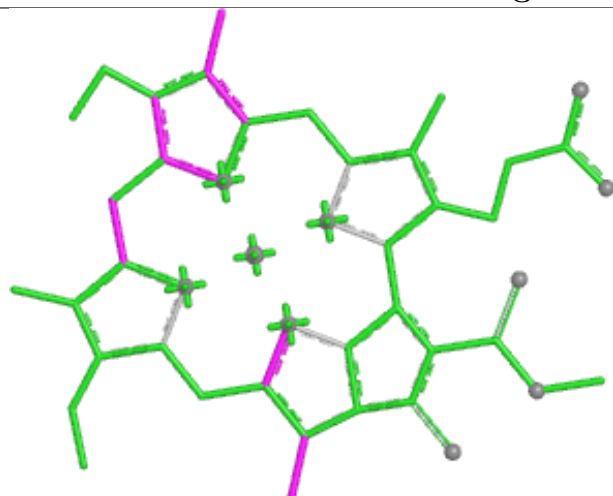


Ligand CLA 3 601

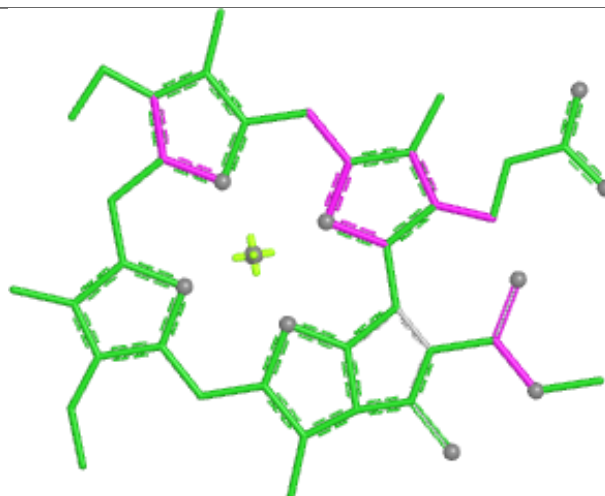


Ligand CLA 2 610**Ligand CLA 5 606**

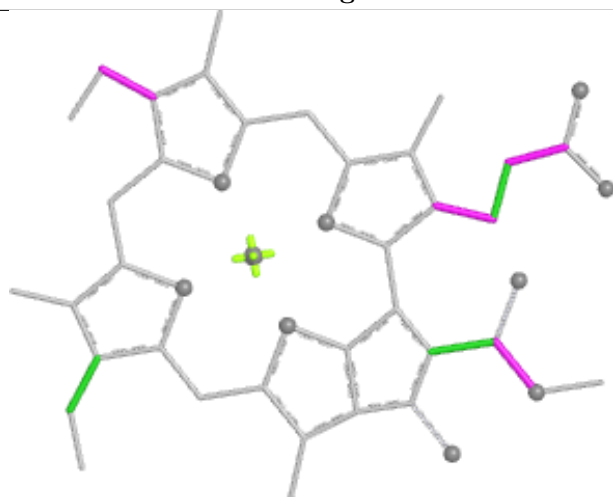
Ligand CLA N 601



Bond lengths



Bond angles

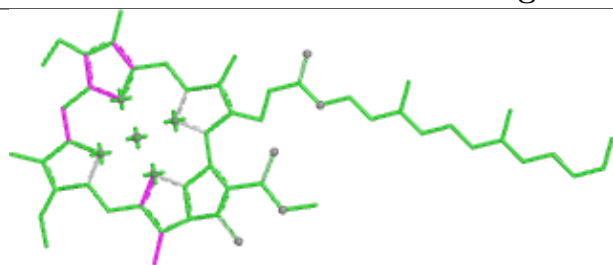


Torsions

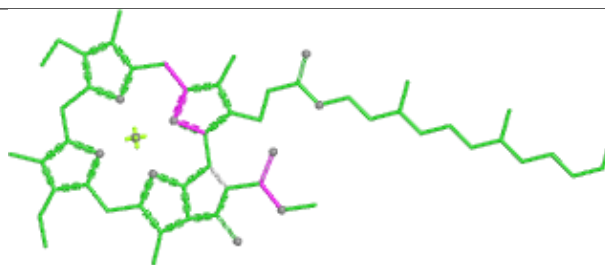


Rings

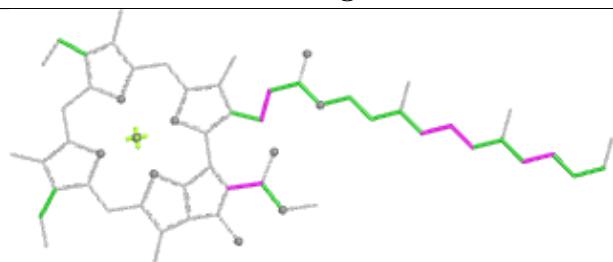
Ligand CLA 1 604



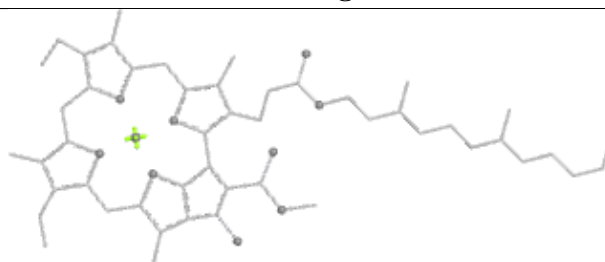
Bond lengths



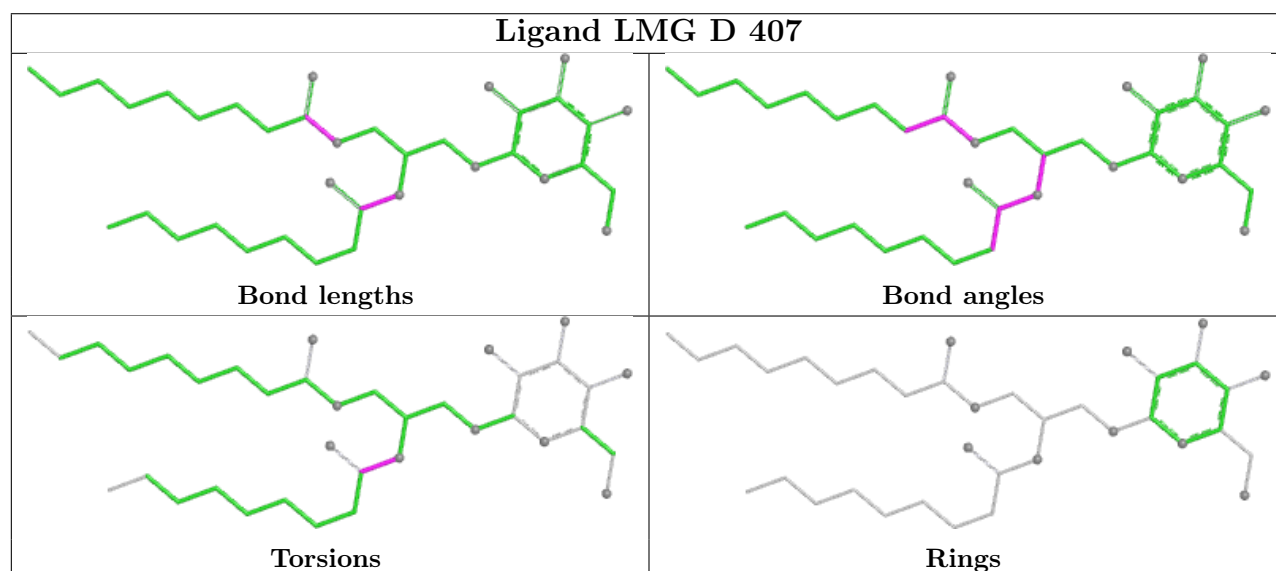
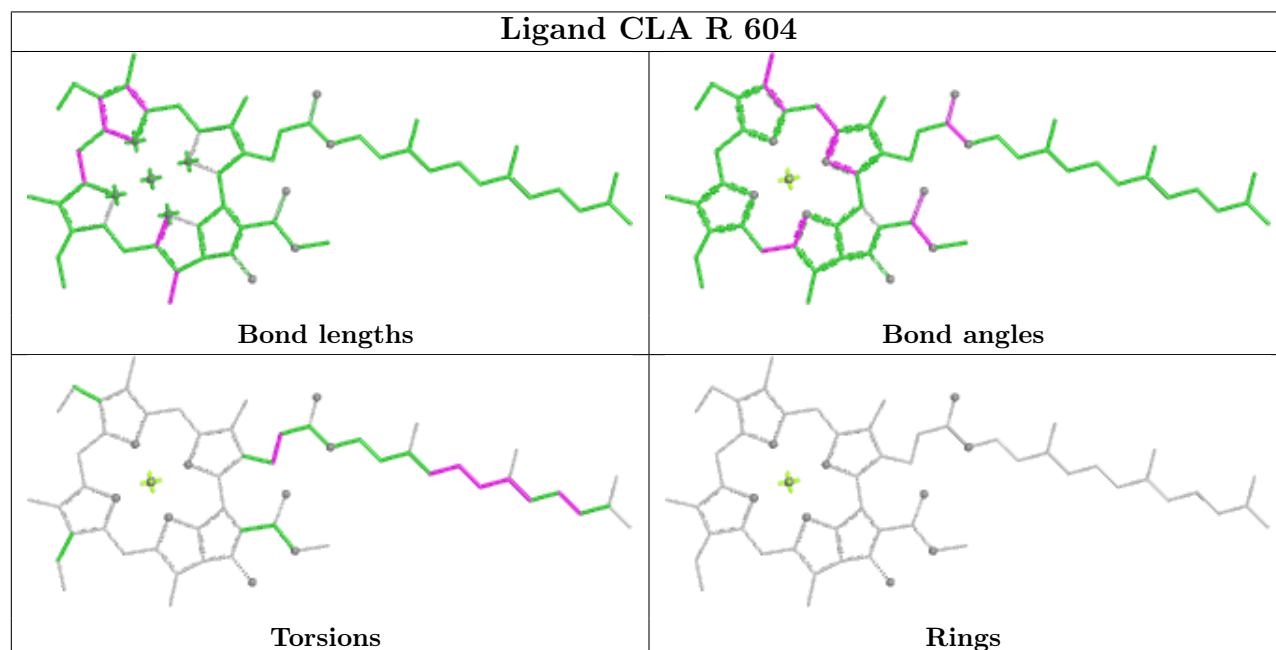
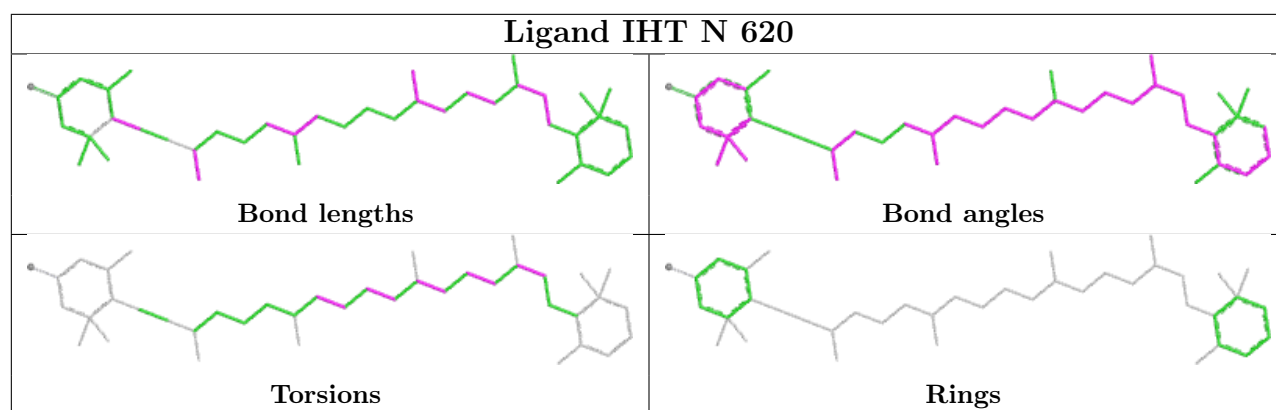
Bond angles

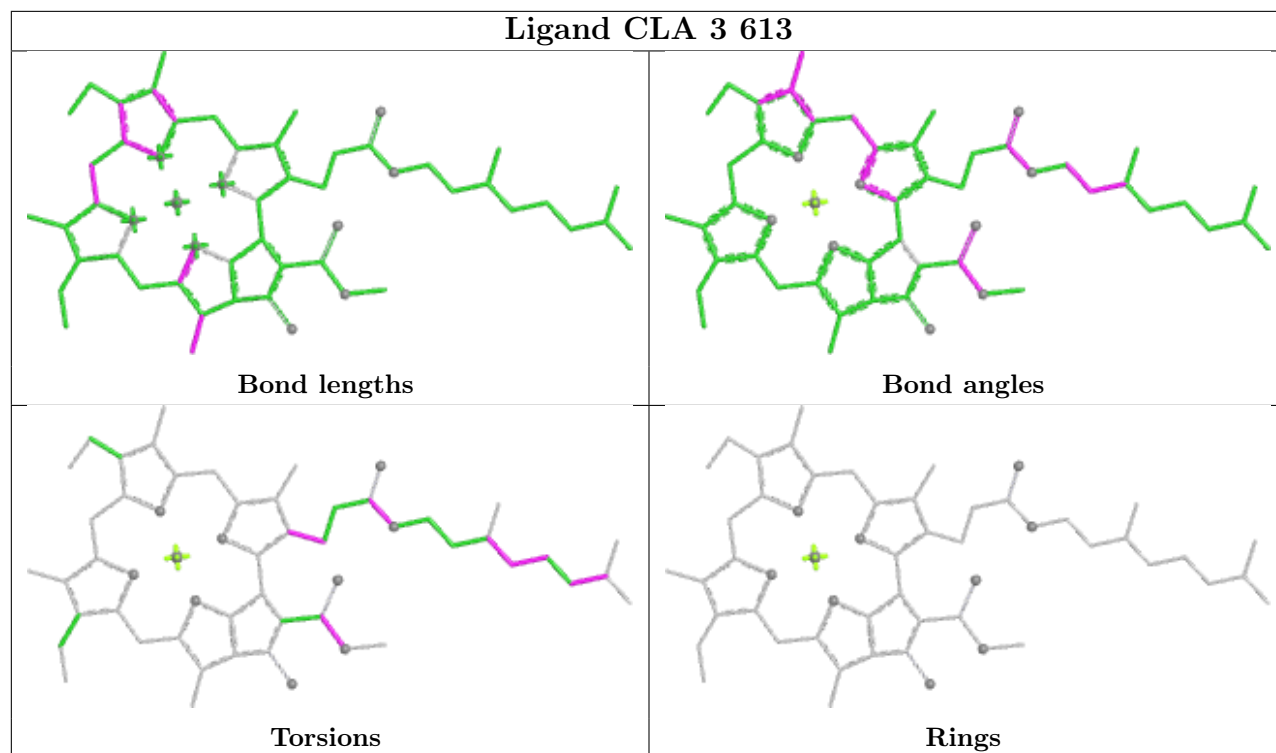
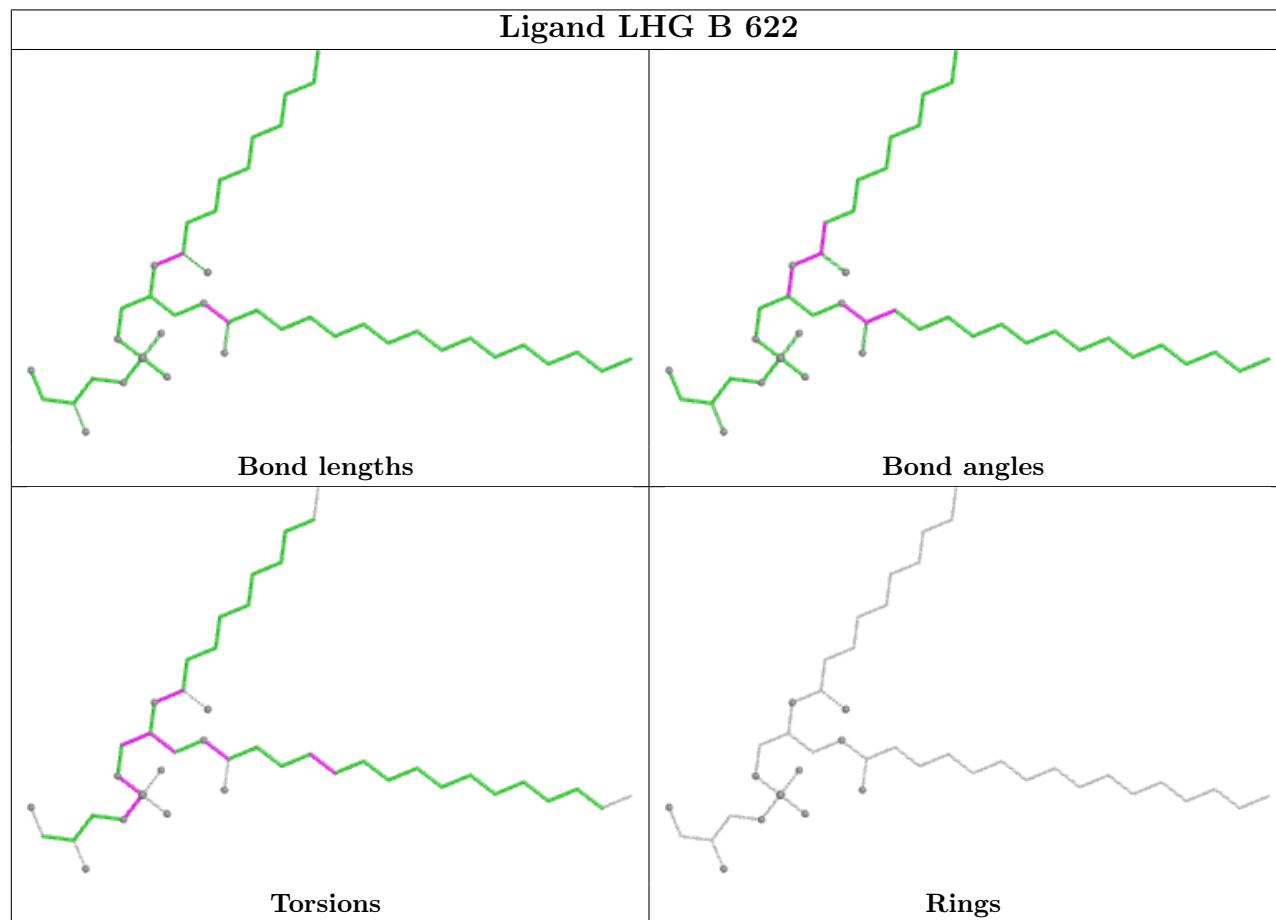


Torsions

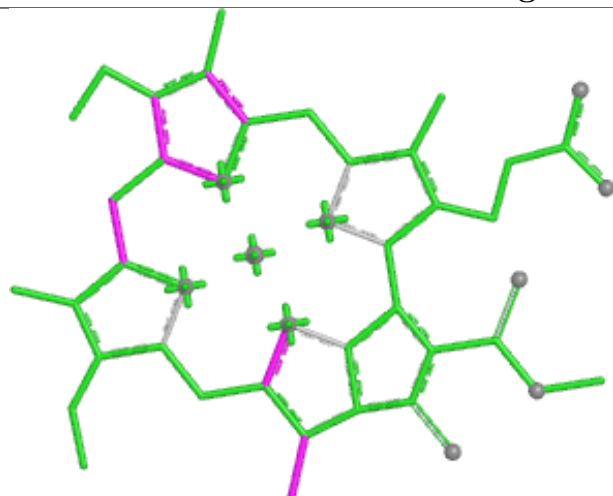


Rings

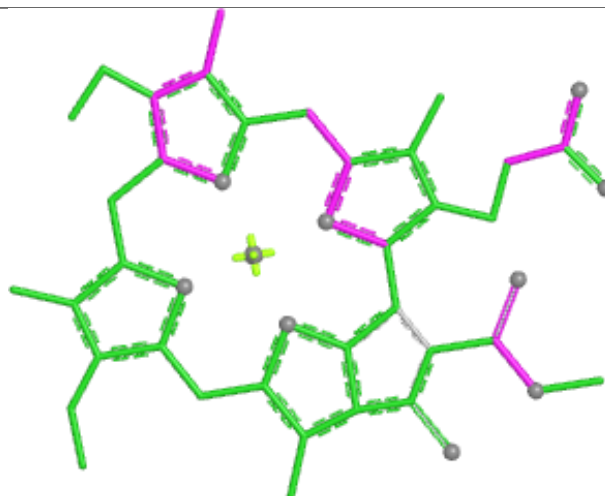


Ligand CLA 3 613**Ligand LHG B 622**

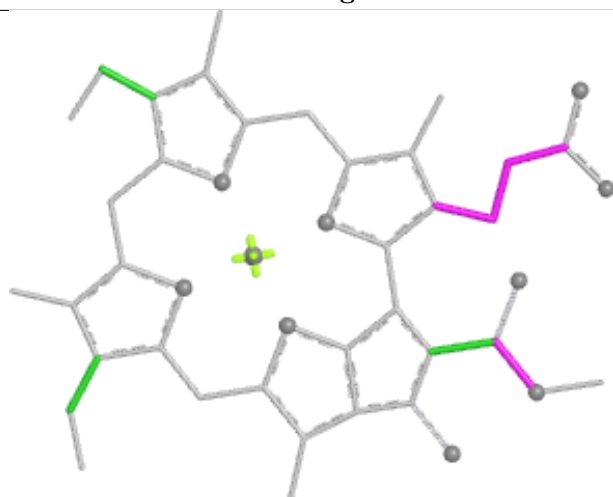
Ligand CLA 3 615



Bond lengths



Bond angles

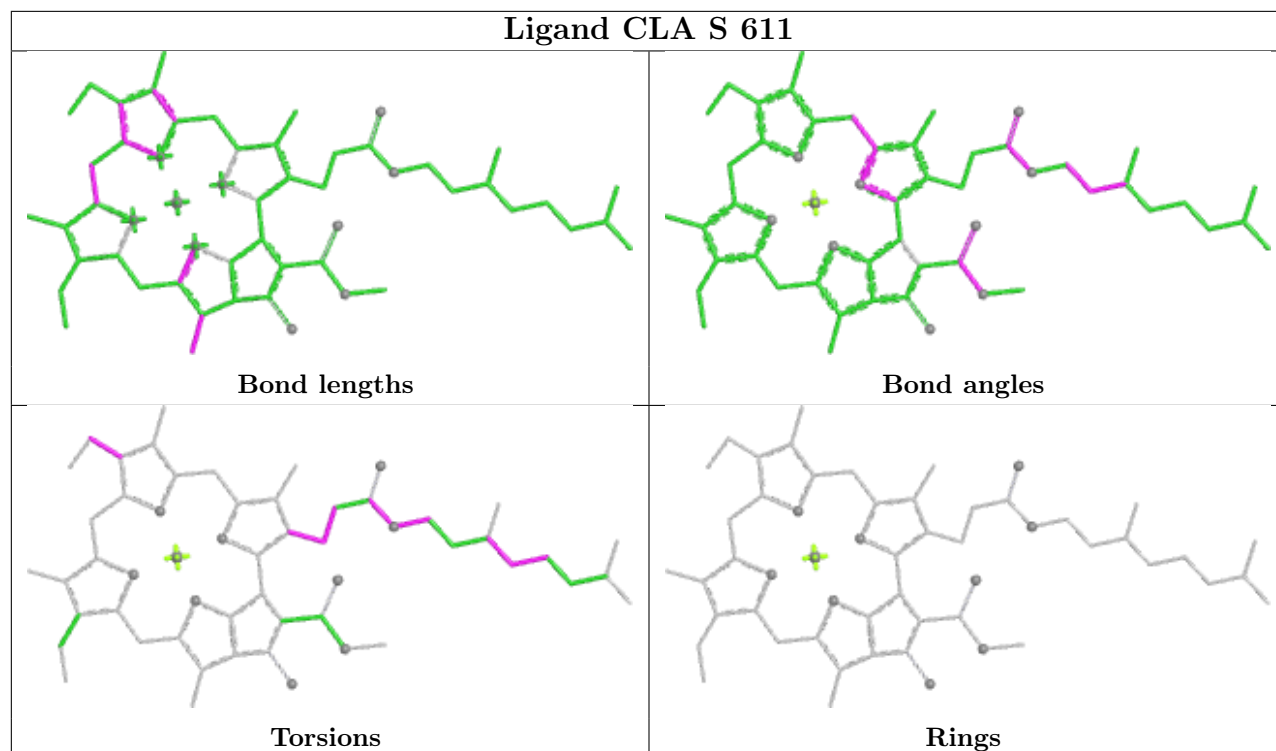


Torsions

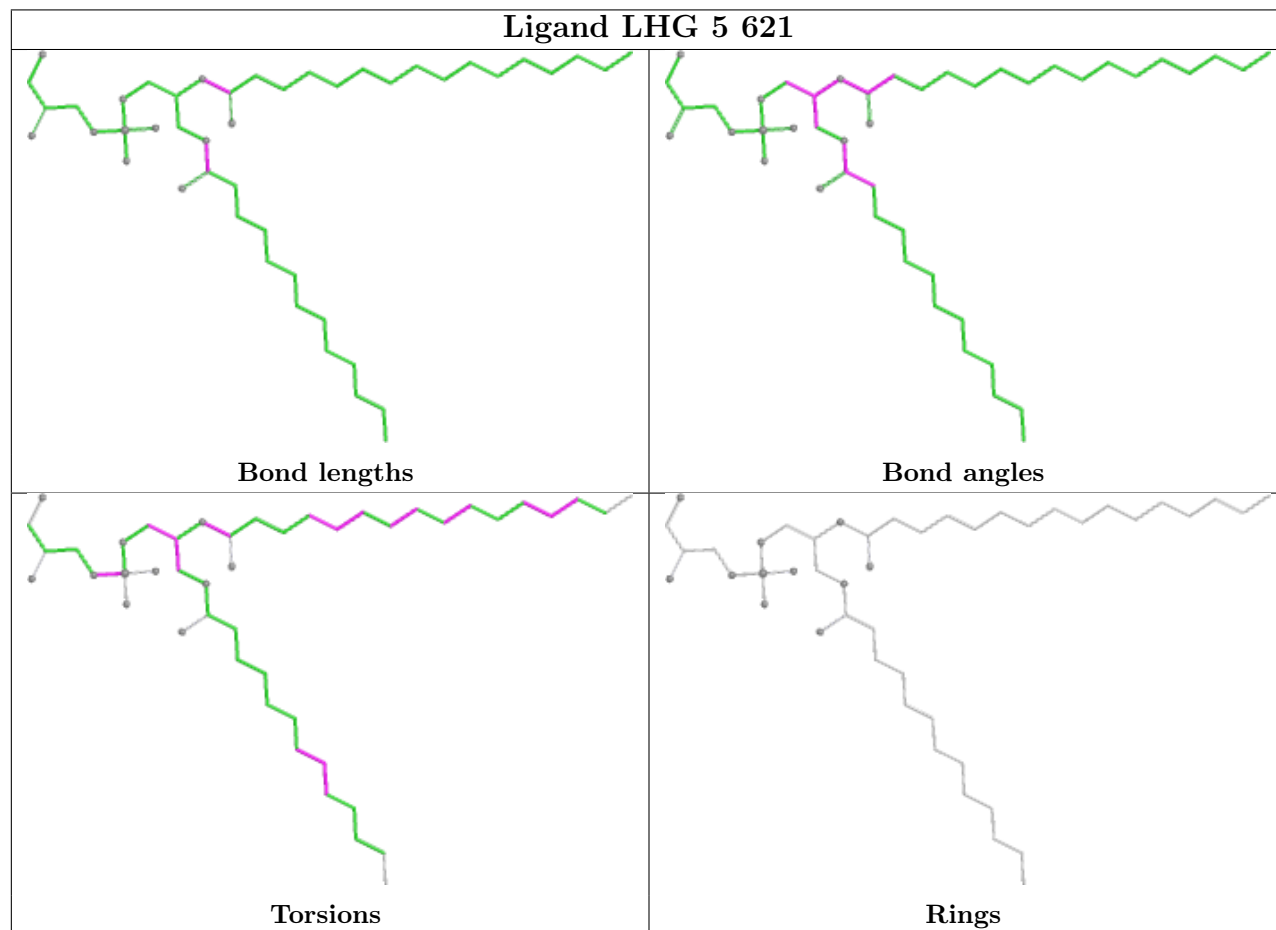


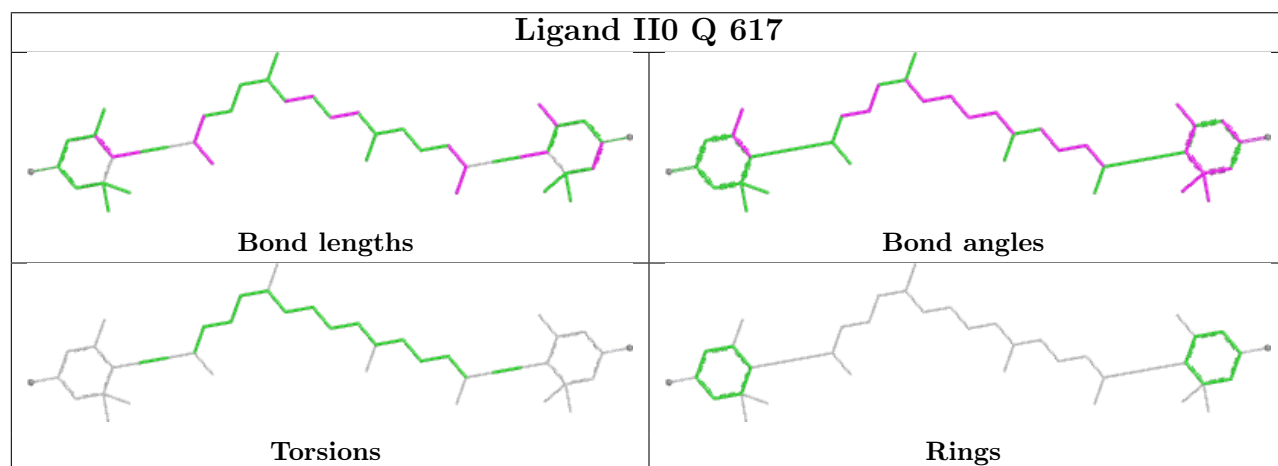
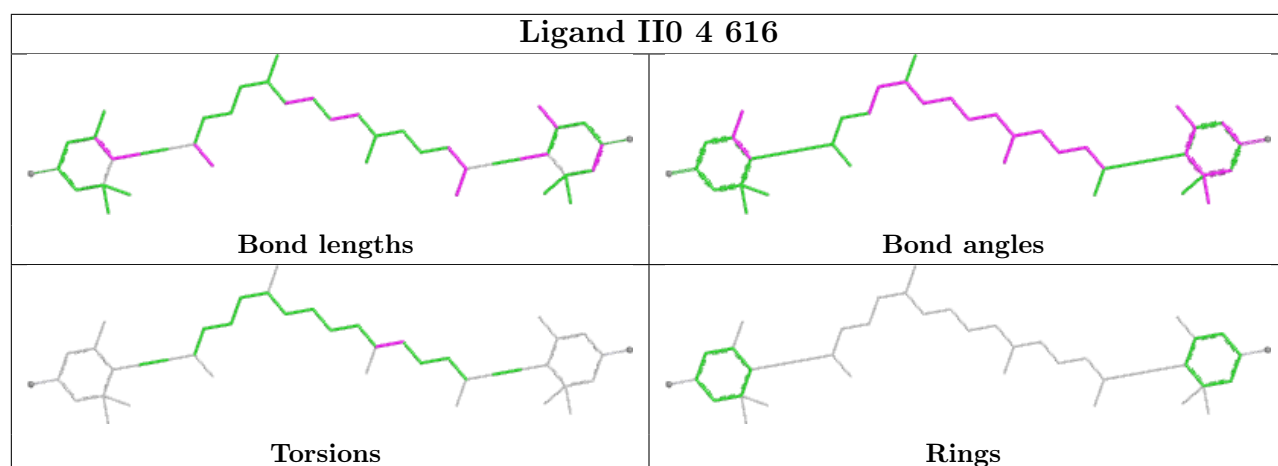
Rings

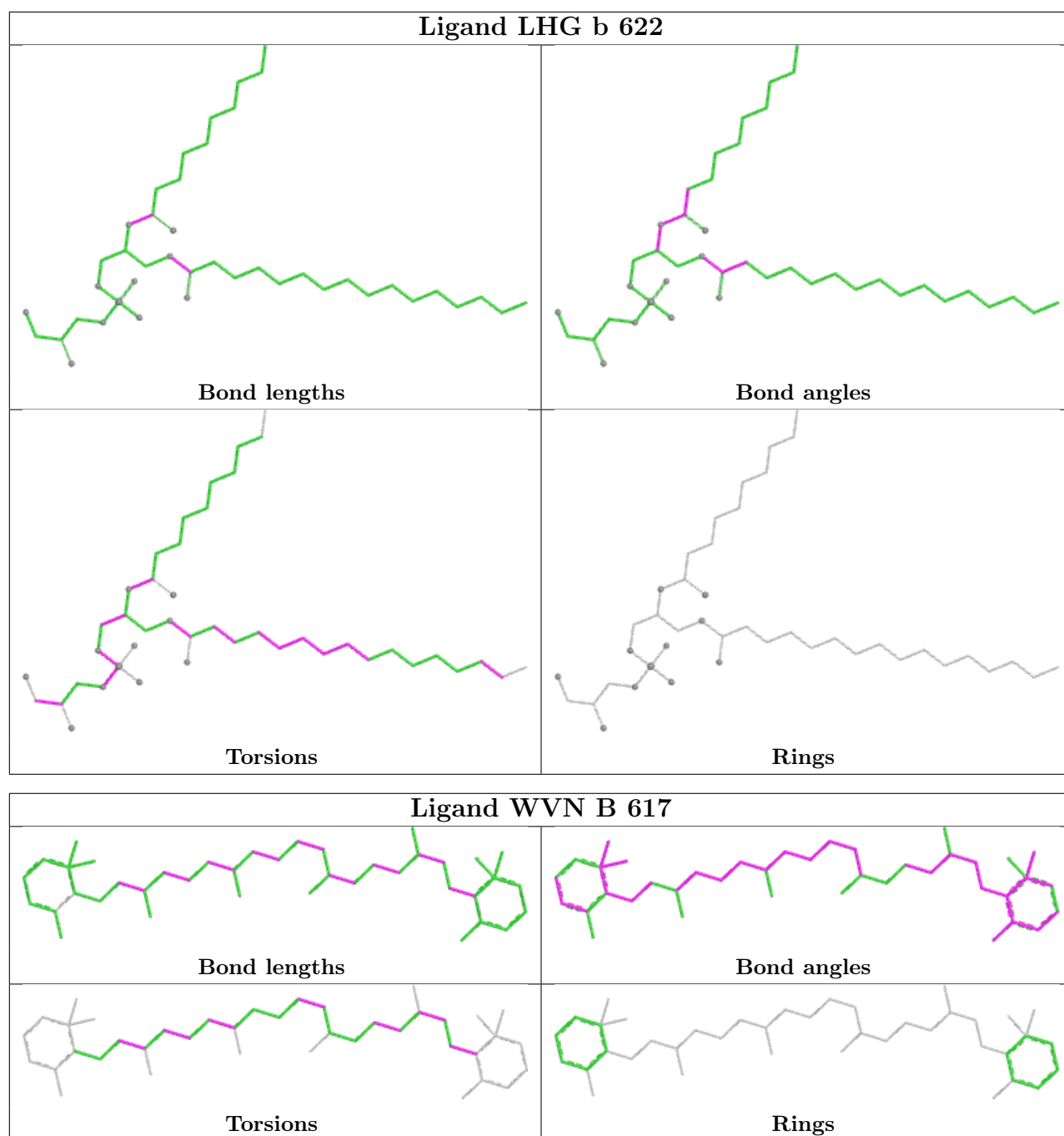
Ligand CLA S 611

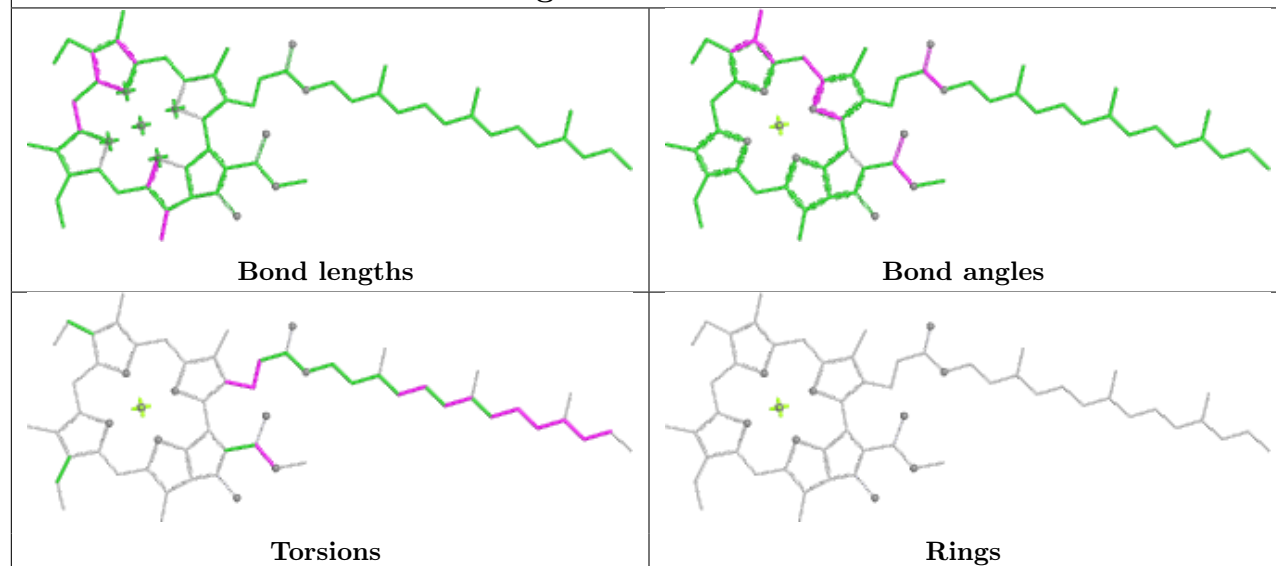
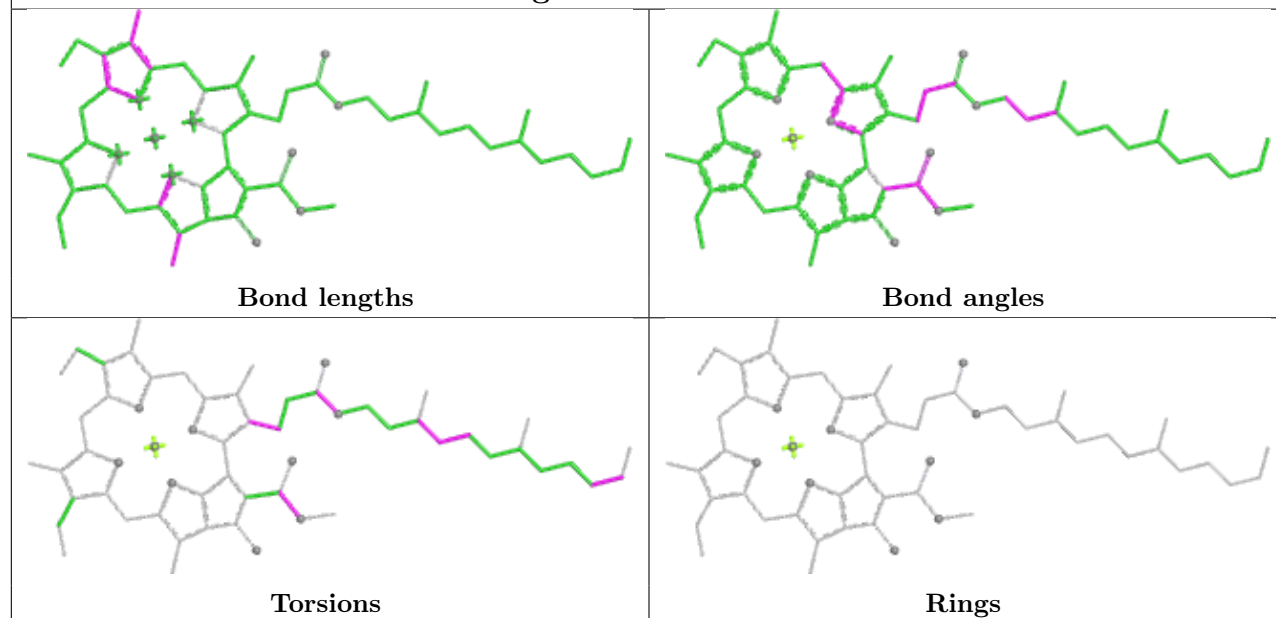


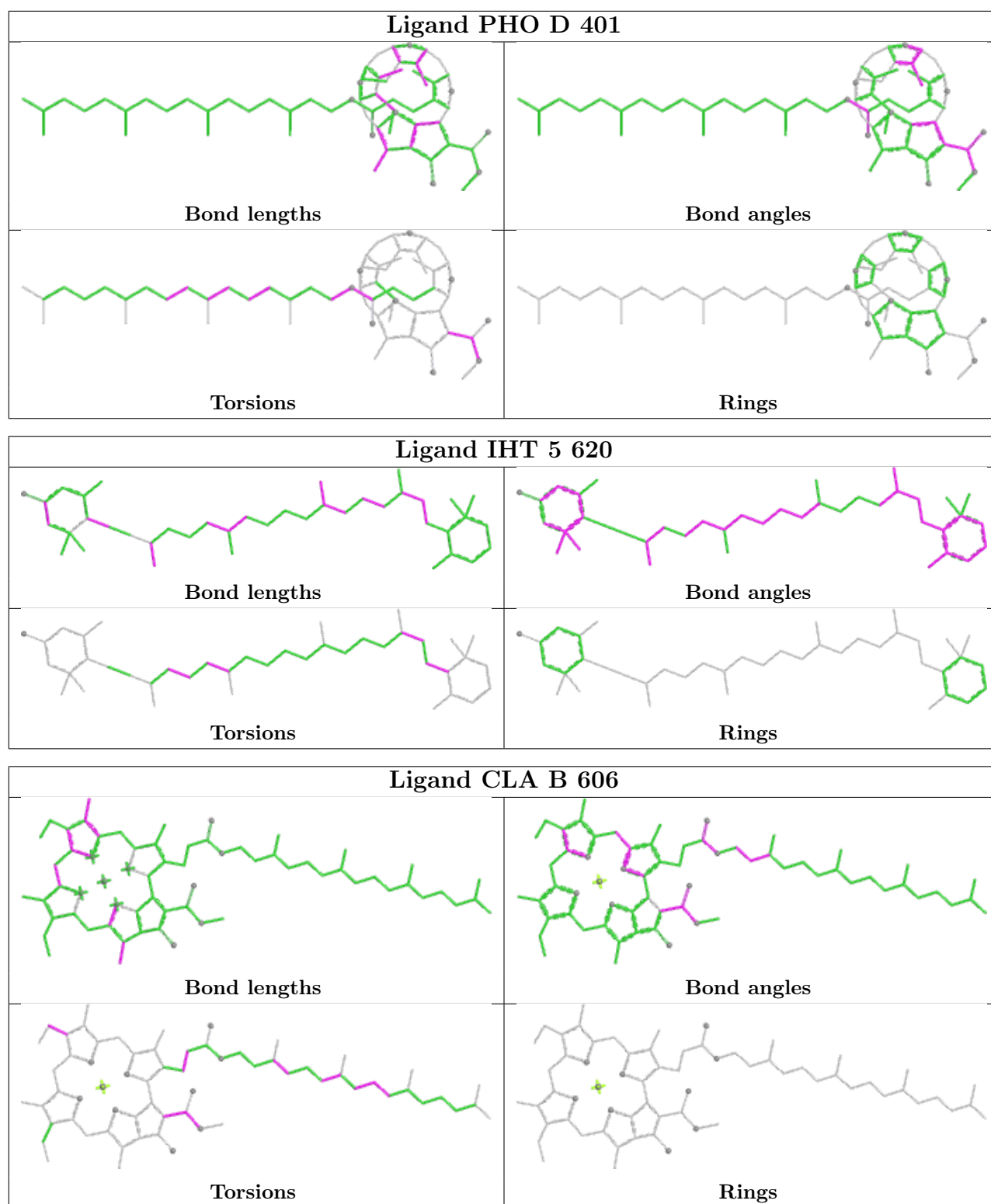
Ligand LHG 5 621

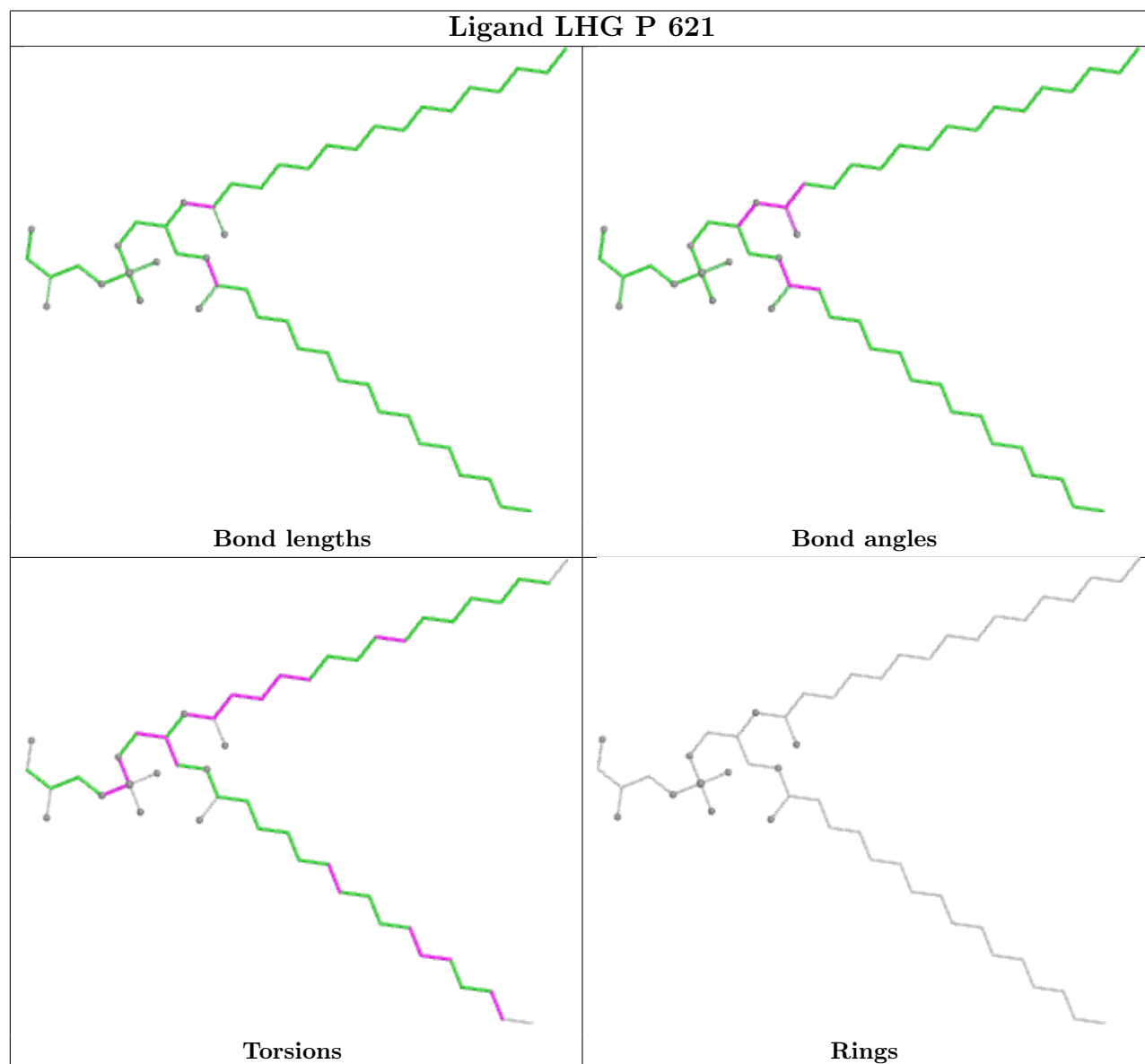
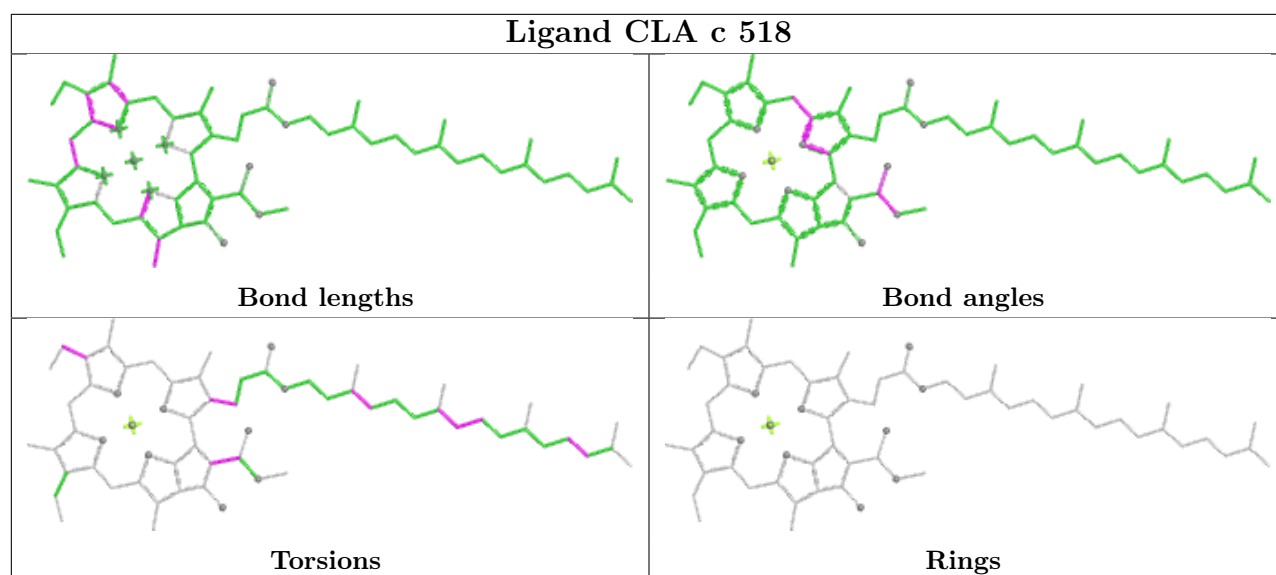


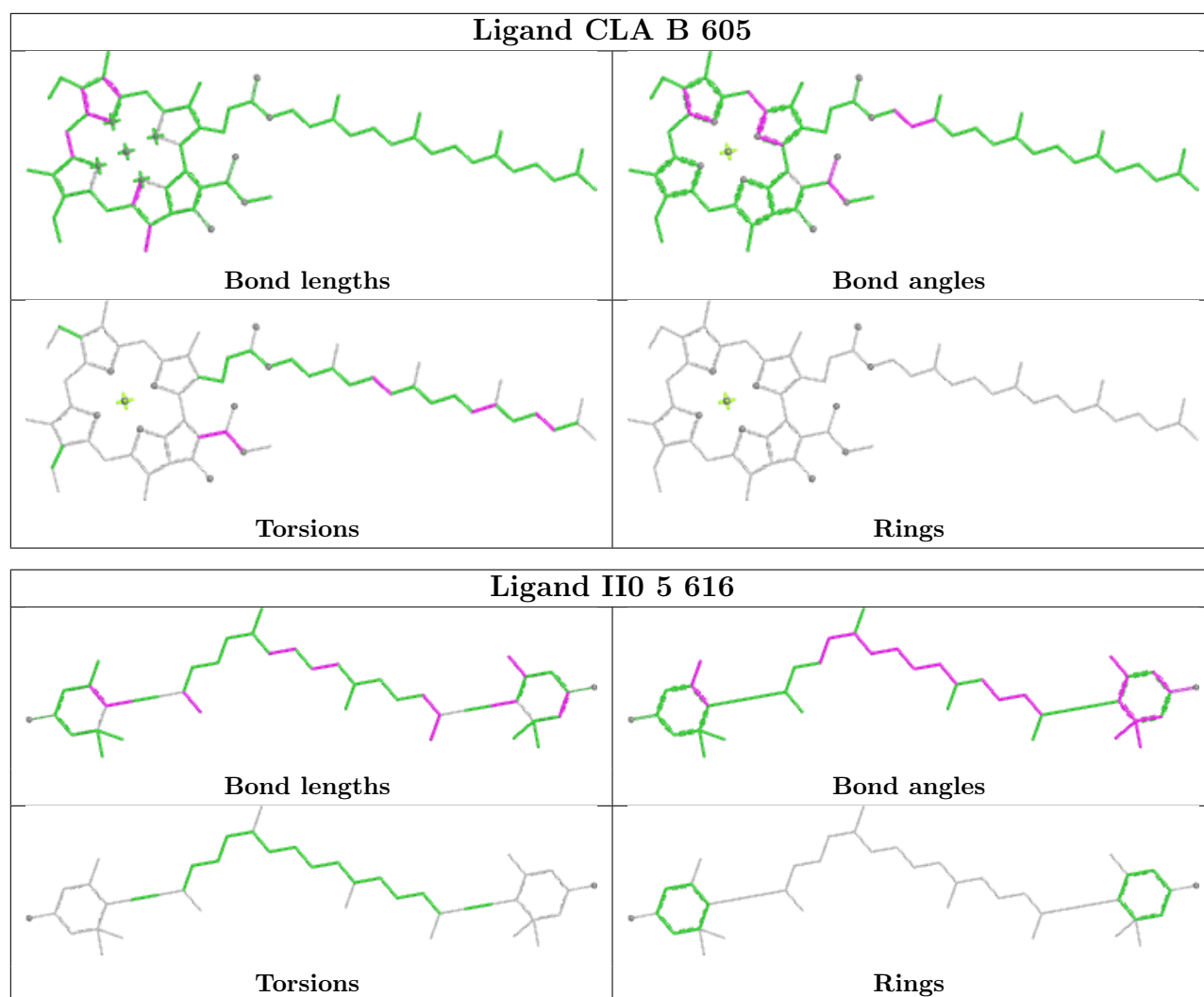




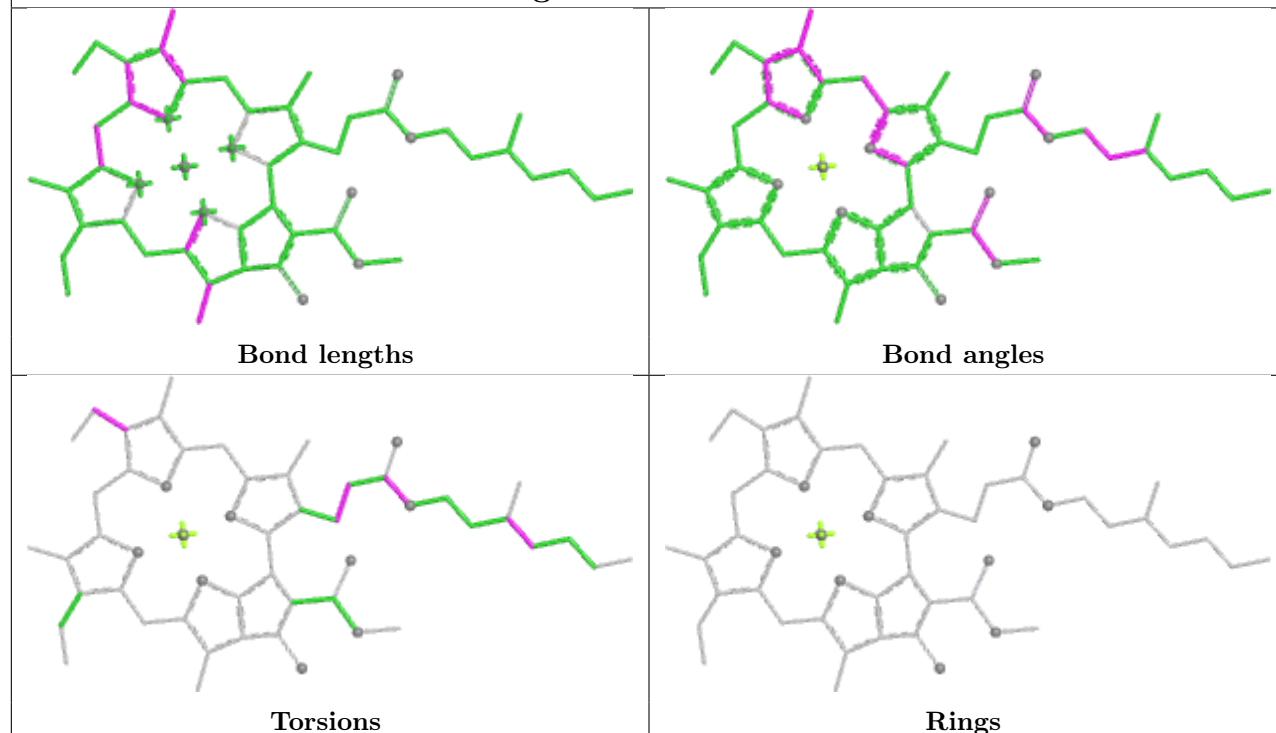
Ligand CLA 3 602**Ligand CLA B 604**



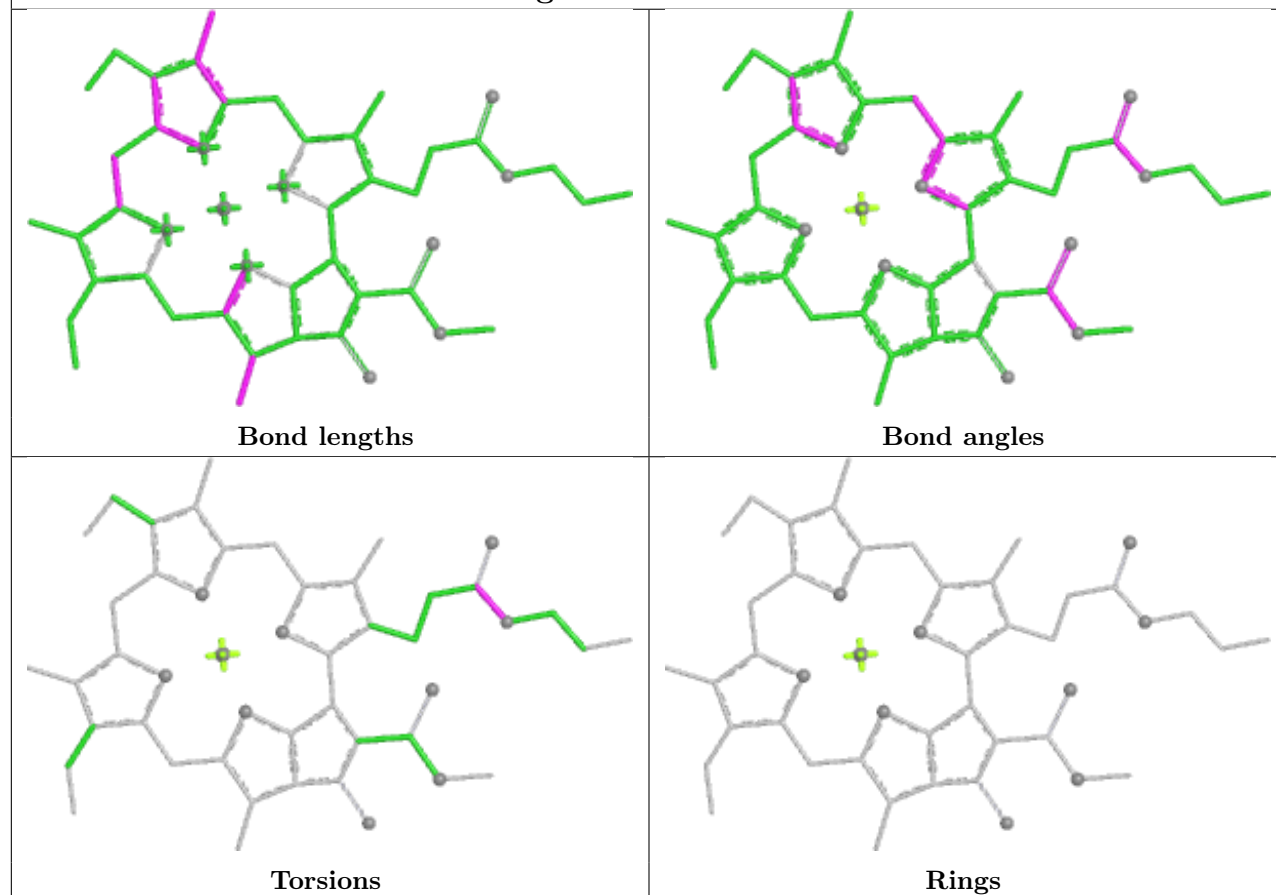




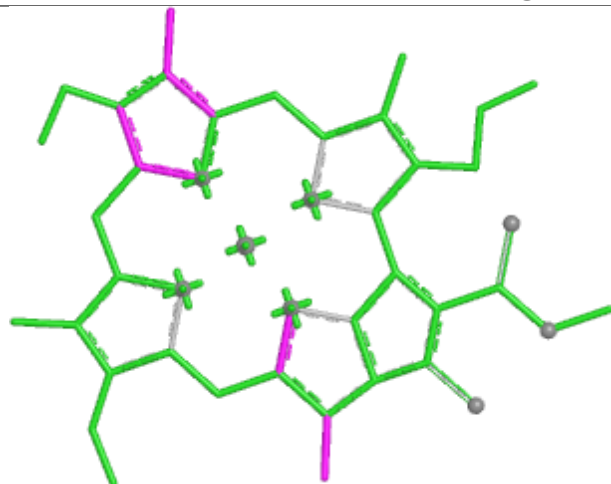
Ligand CLA P 612



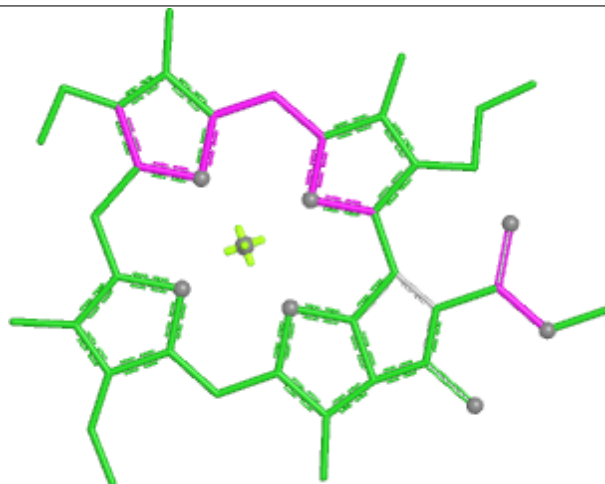
Ligand CLA 2 609



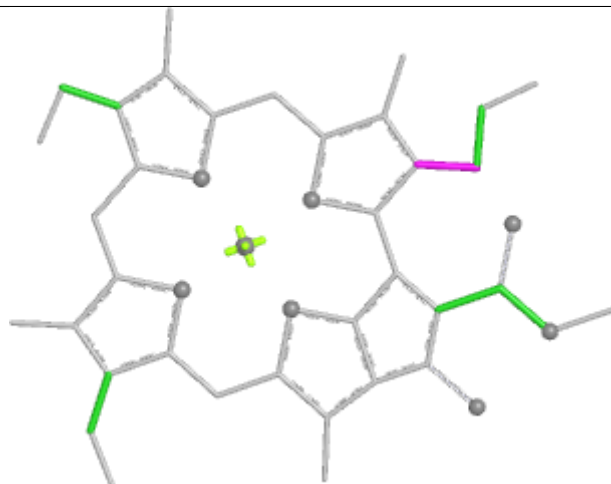
Ligand CLA 4 607



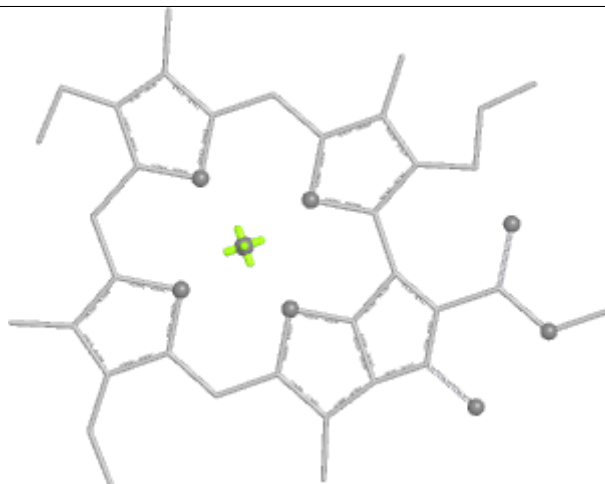
Bond lengths



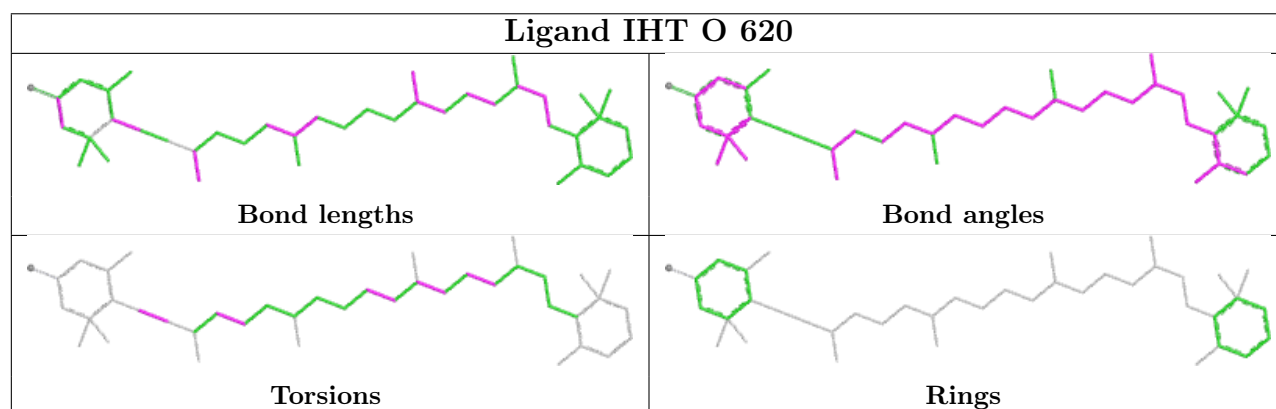
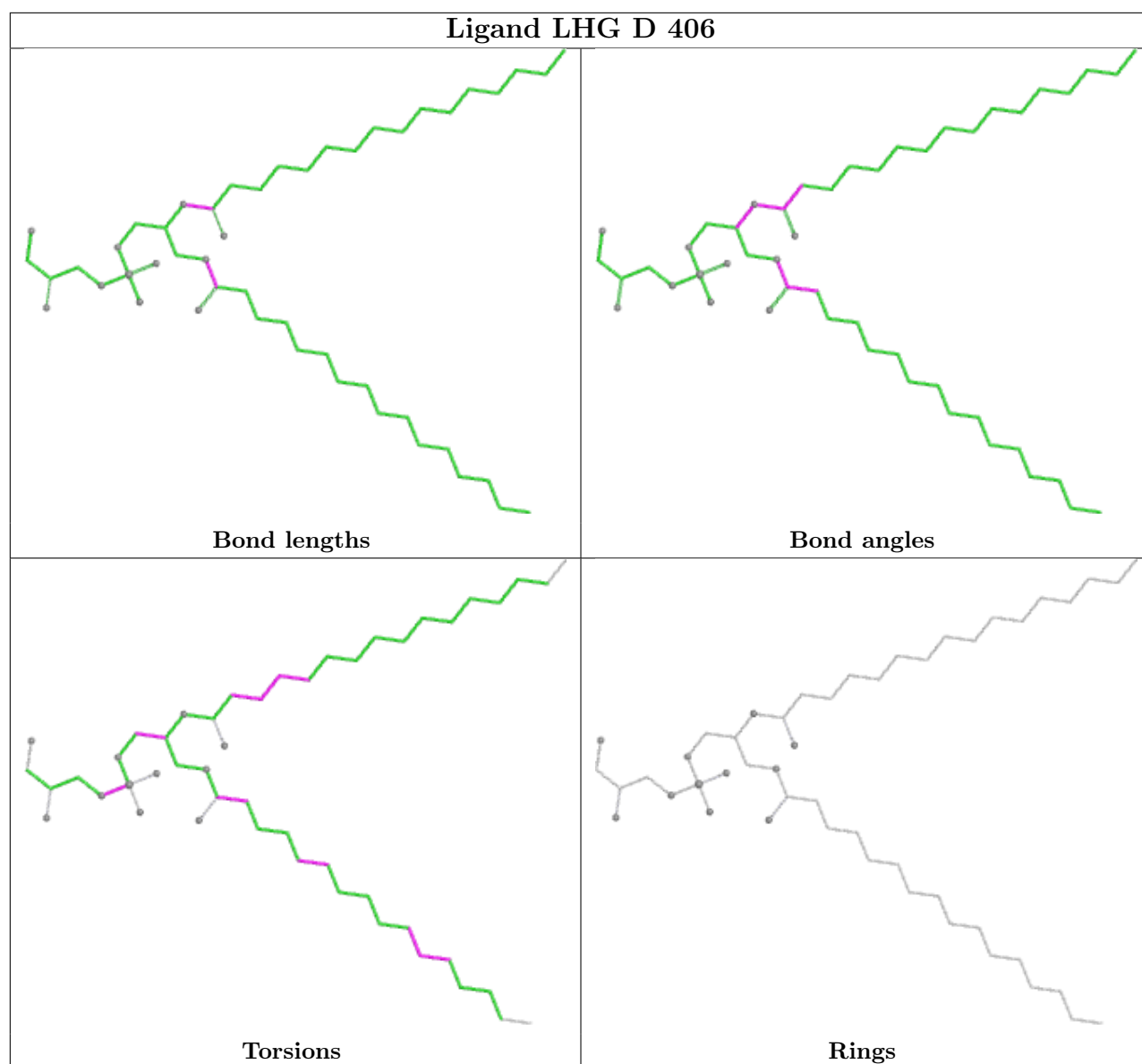
Bond angles



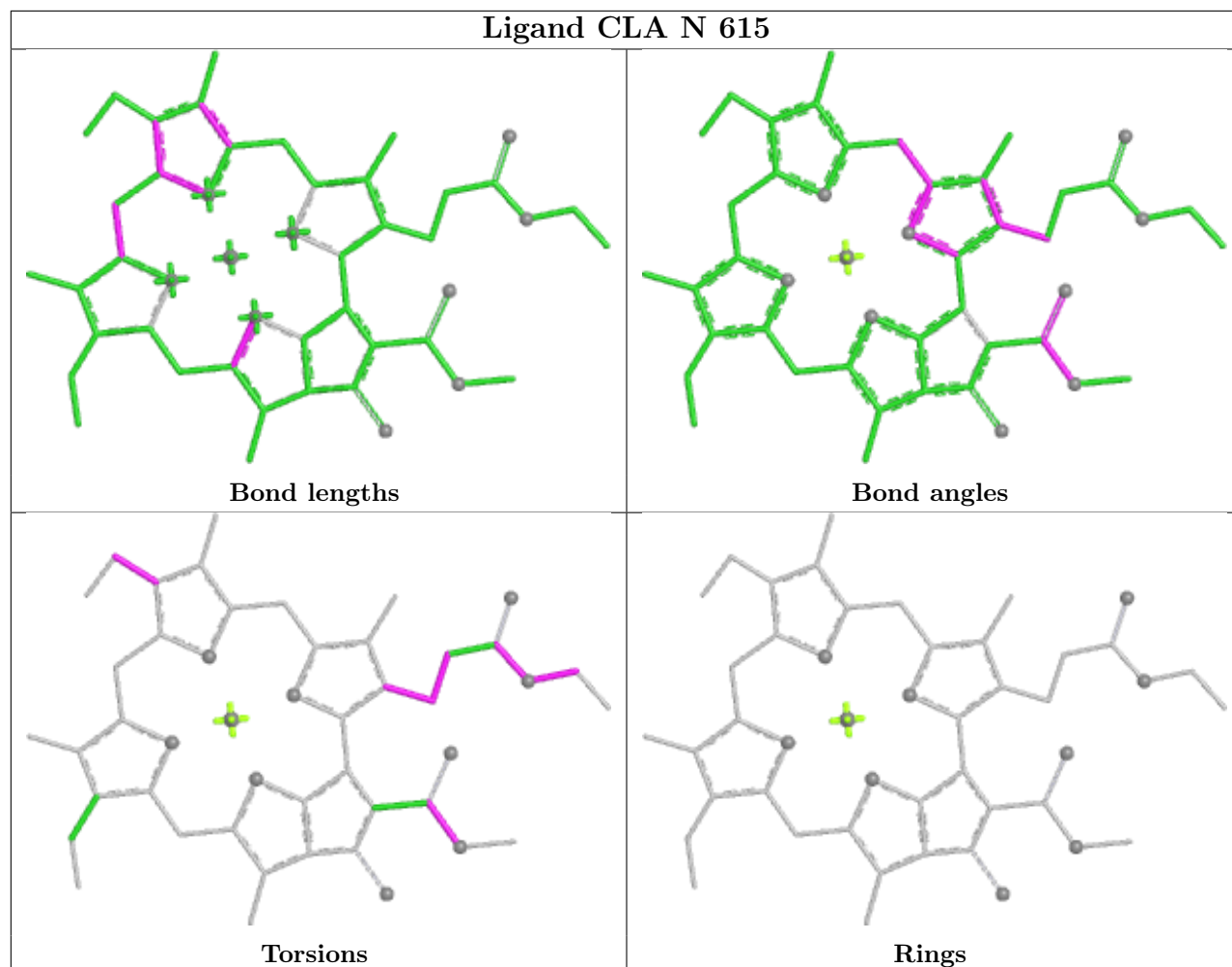
Torsions



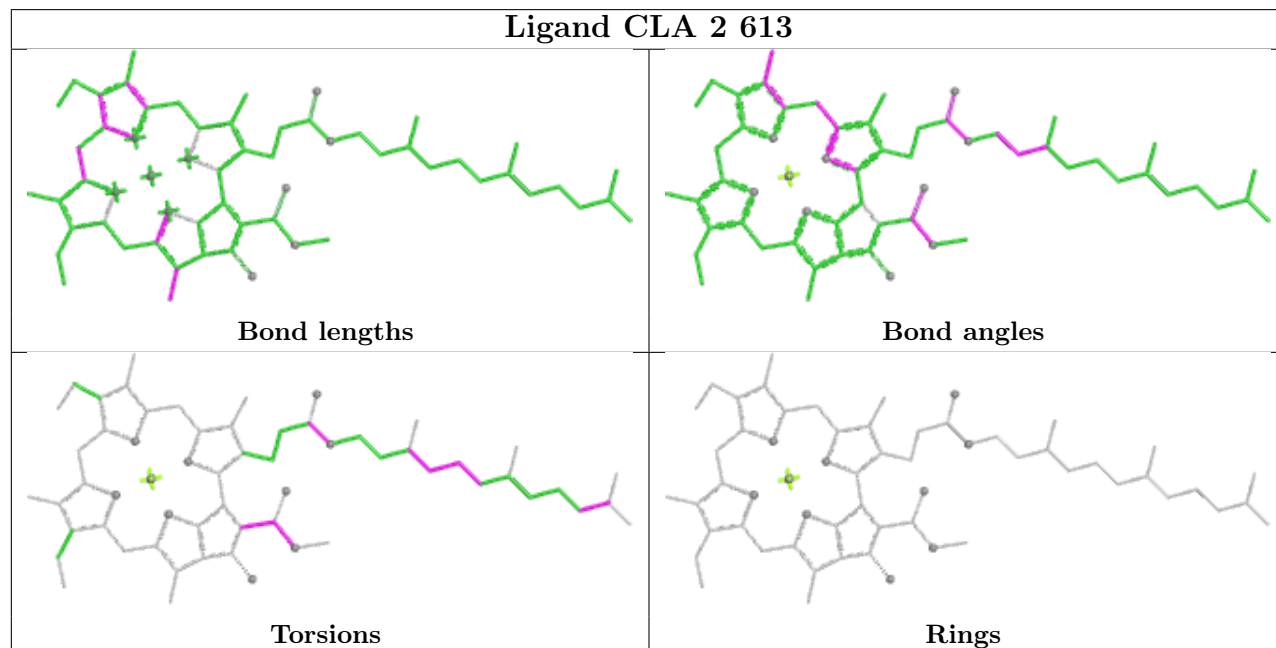
Rings



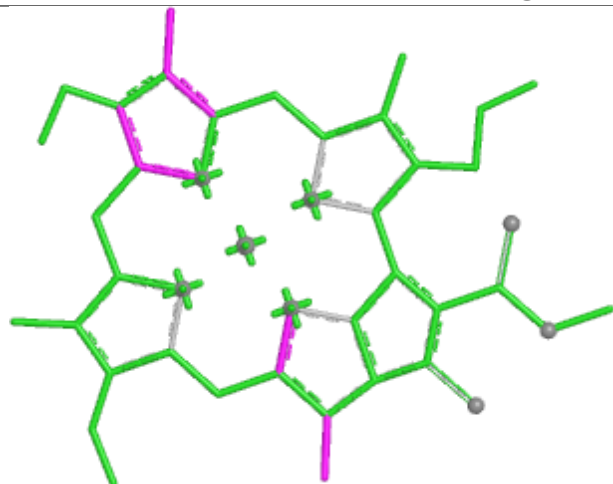
Ligand CLA N 615



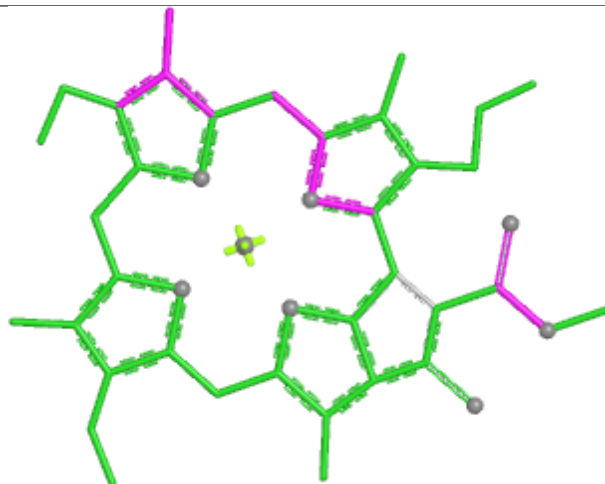
Ligand CLA 2 613



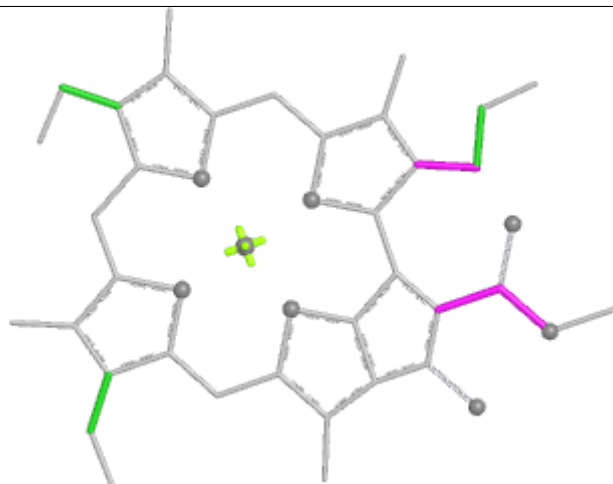
Ligand CLA 5 607



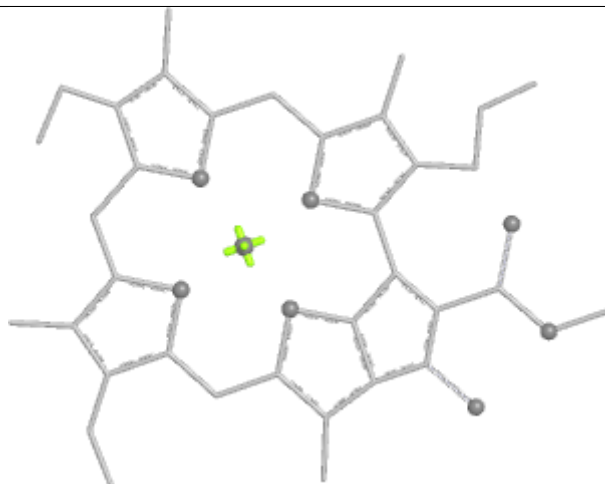
Bond lengths



Bond angles

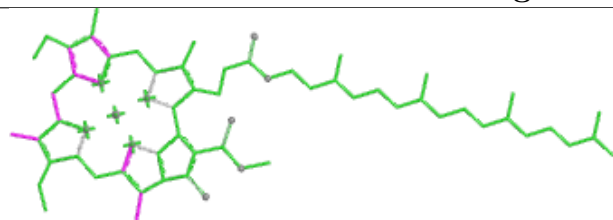


Torsions

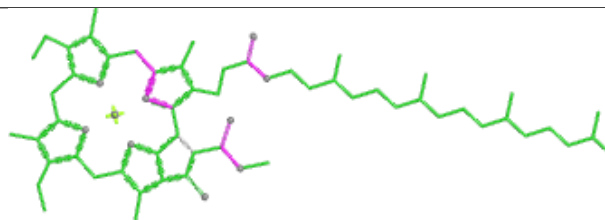


Rings

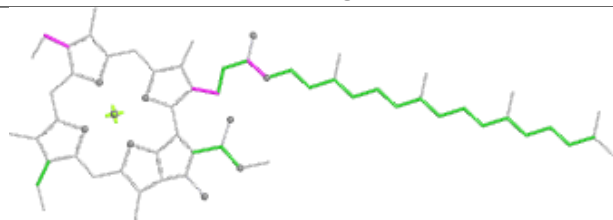
Ligand CLA D 403



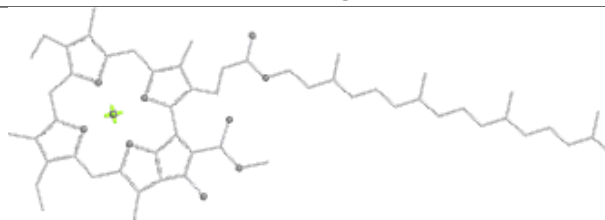
Bond lengths



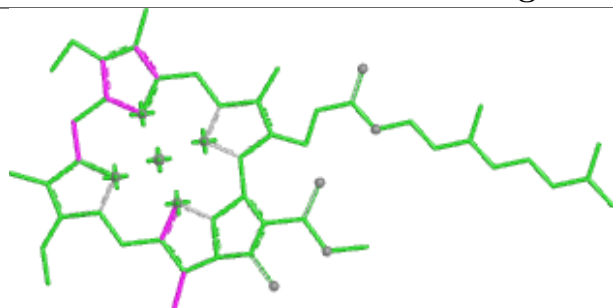
Bond angles



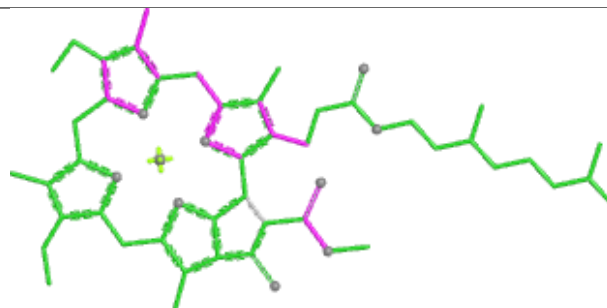
Torsions



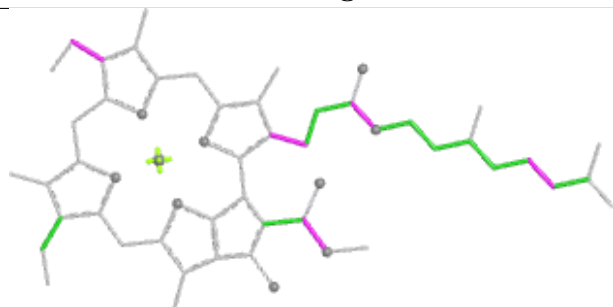
Rings

Ligand CLA 6 603

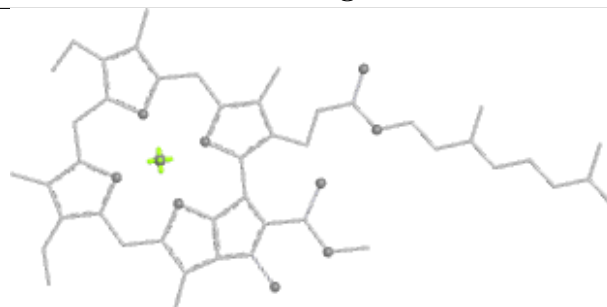
Bond lengths



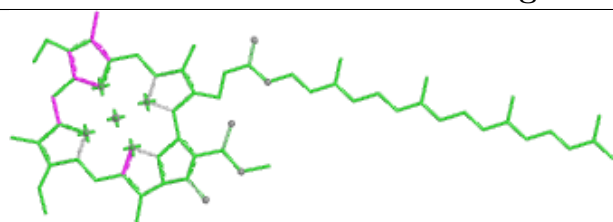
Bond angles



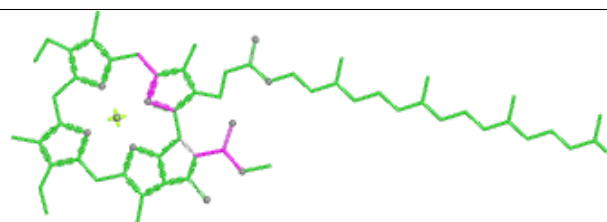
Torsions



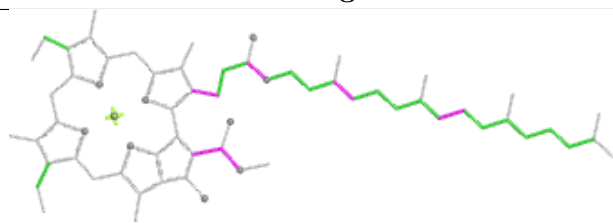
Rings

Ligand CLA c 526

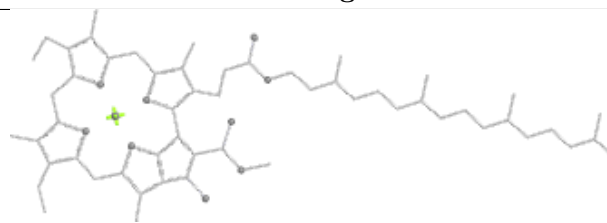
Bond lengths



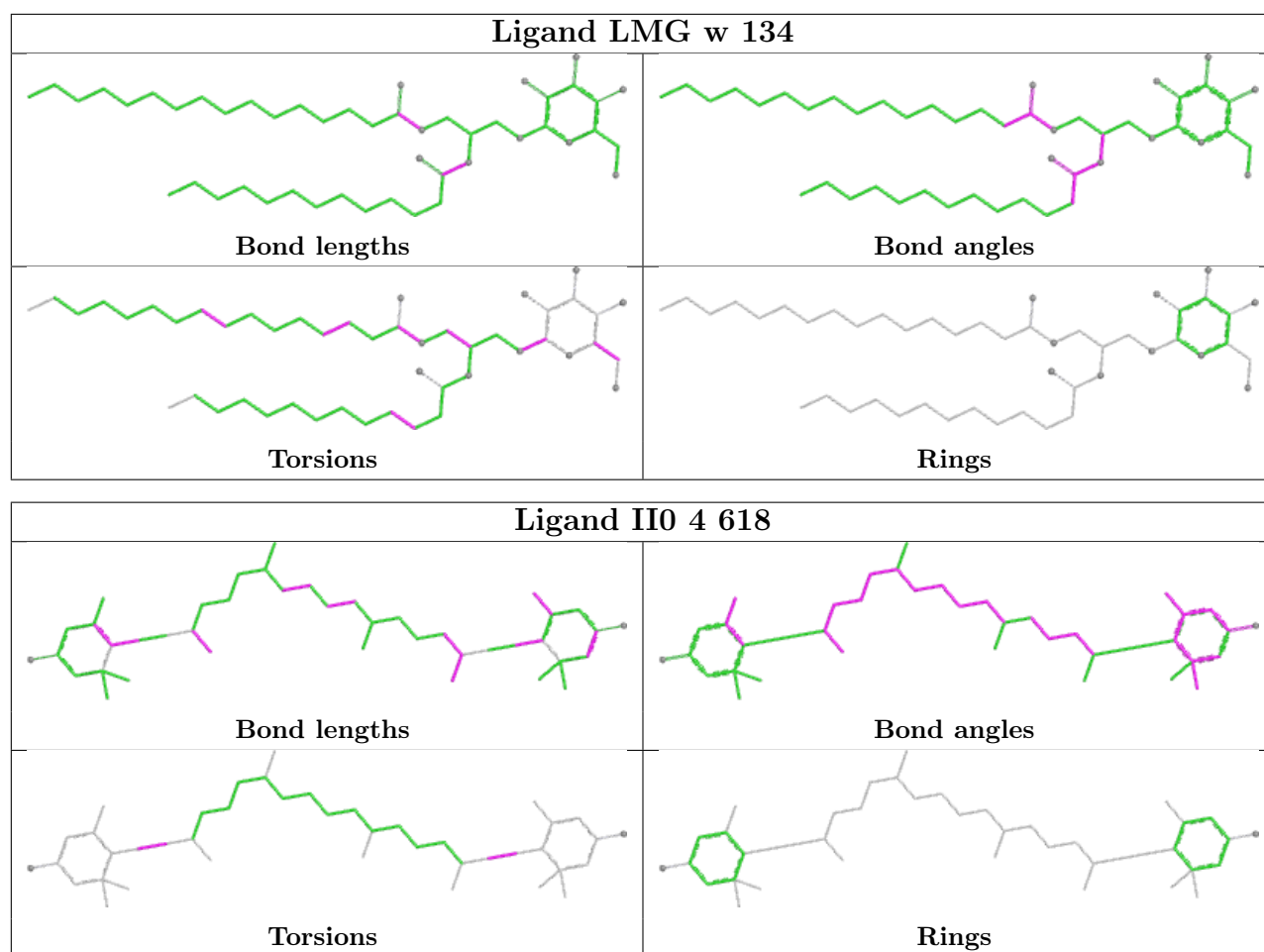
Bond angles



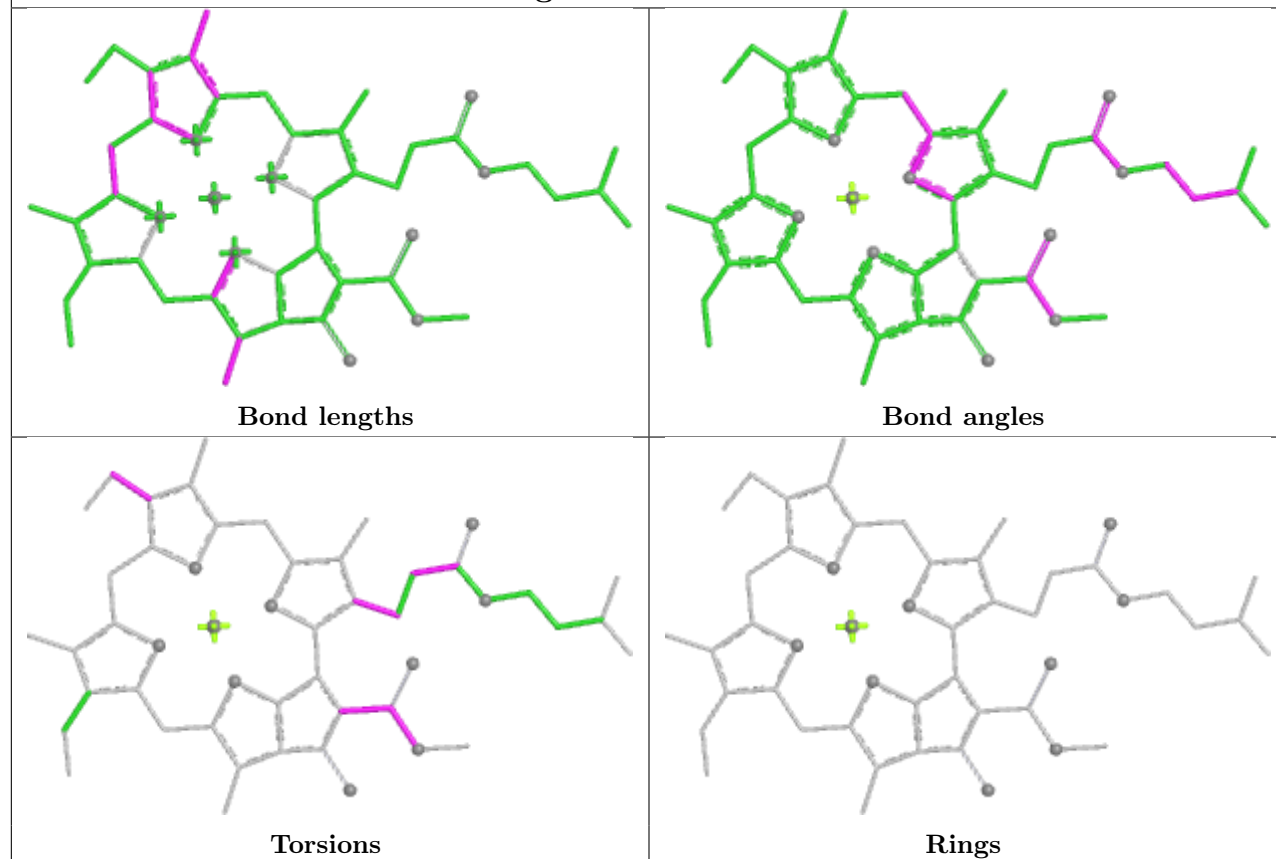
Torsions



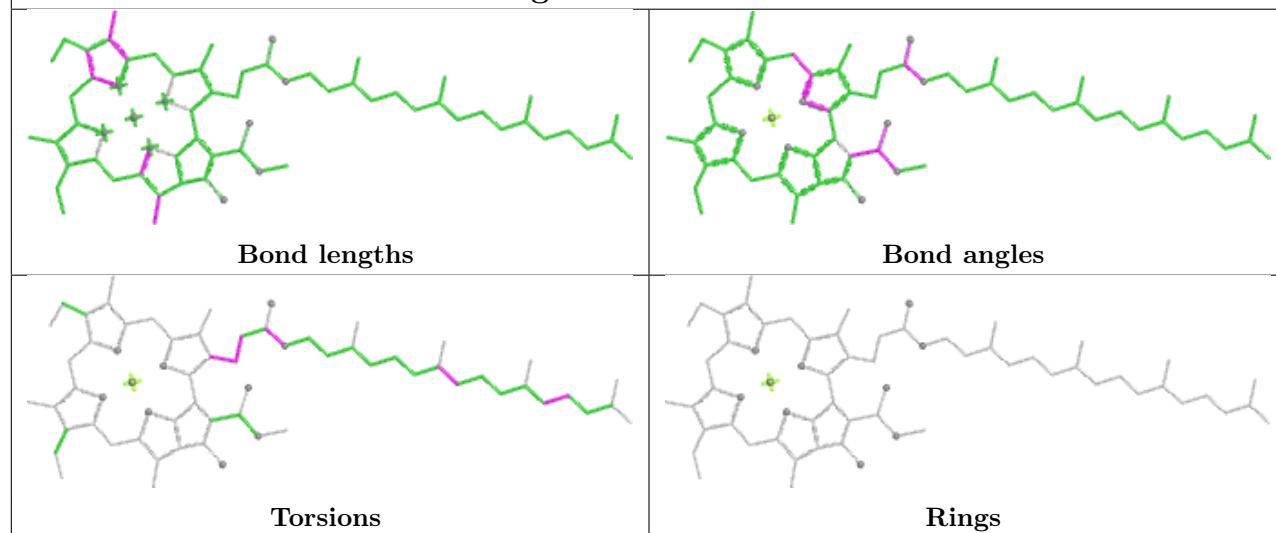
Rings



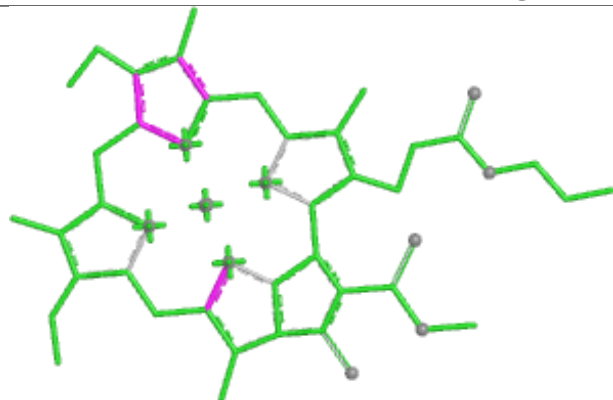
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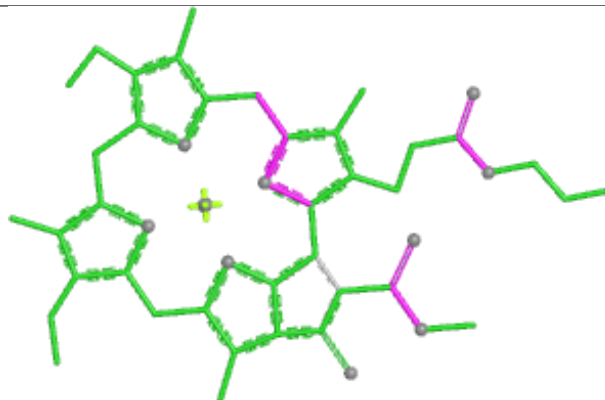
Ligand CLA D 400



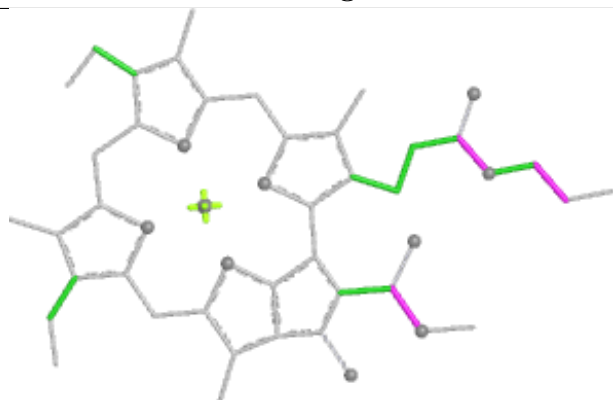
Ligand CLA N 614



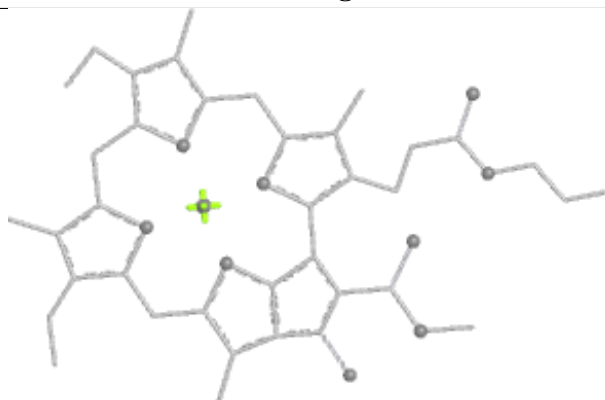
Bond lengths



Bond angles

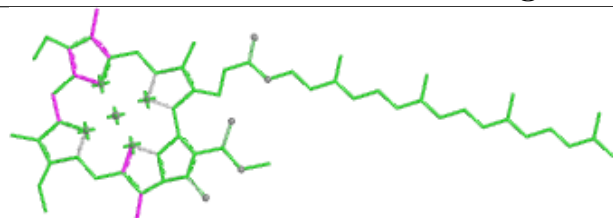


Torsions

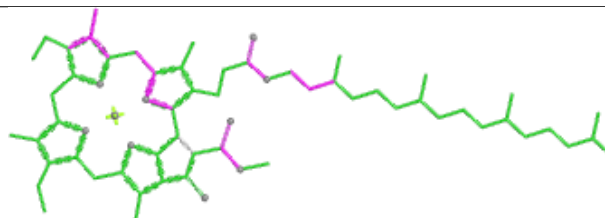


Rings

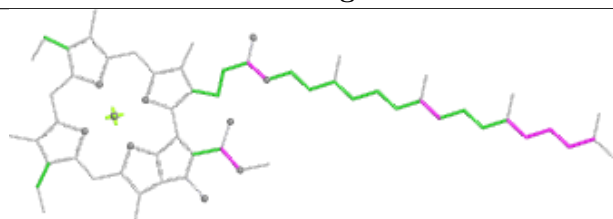
Ligand CLA c 523



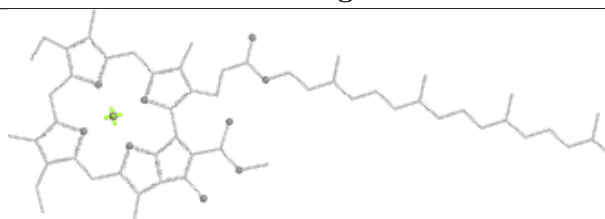
Bond lengths



Bond angles

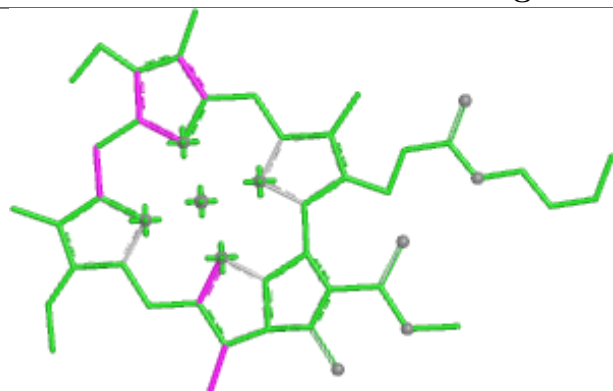


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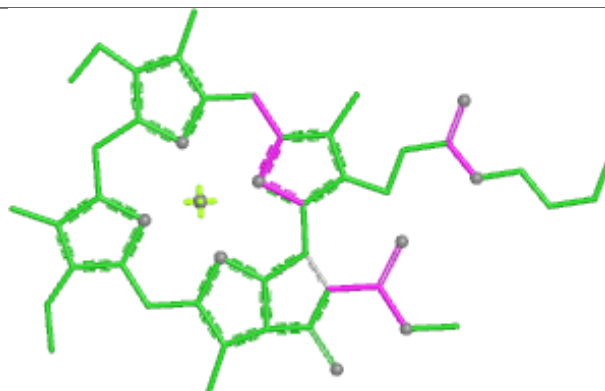


Rings

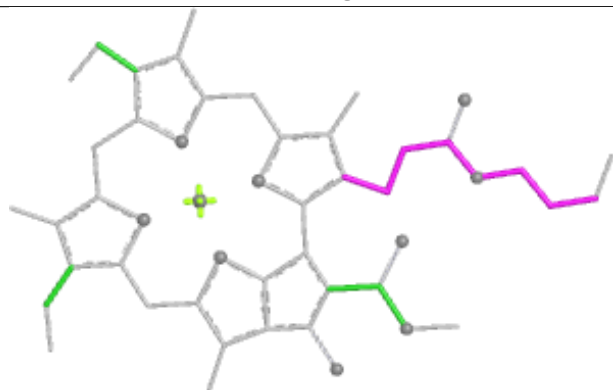
Ligand CLA A 404



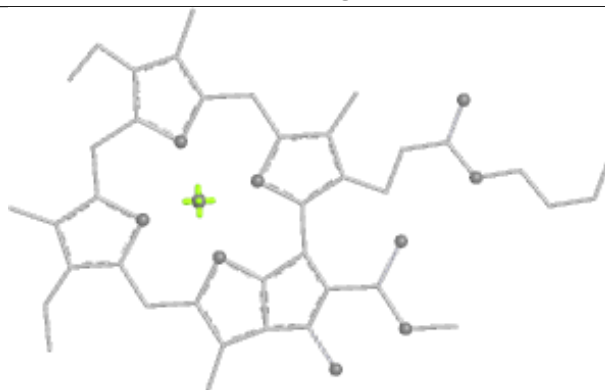
Bond lengths



Bond angles

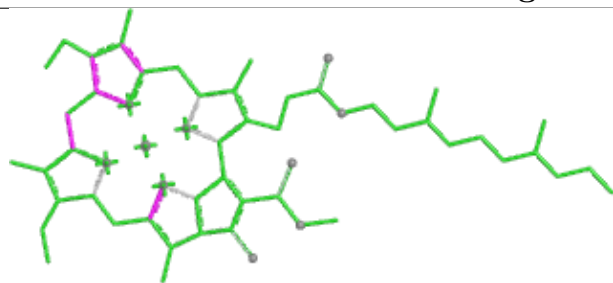


Torsions

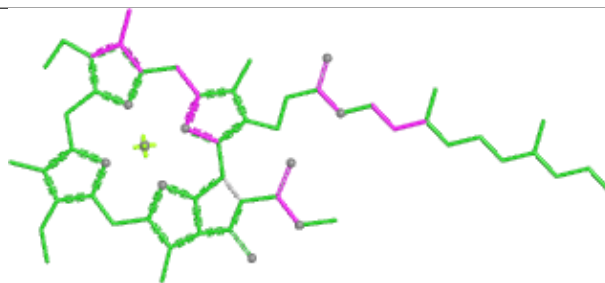


Rings

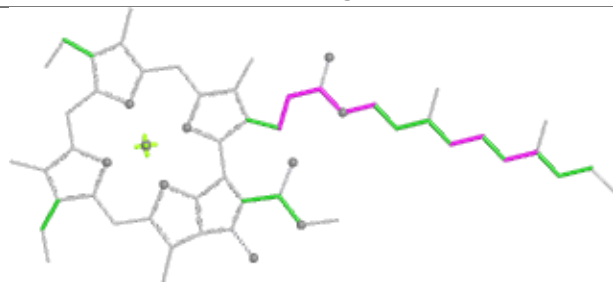
Ligand CLA 6 610



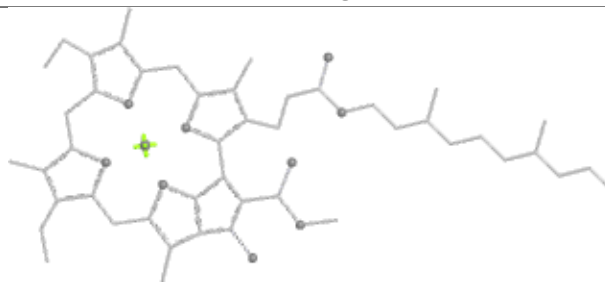
Bond lengths



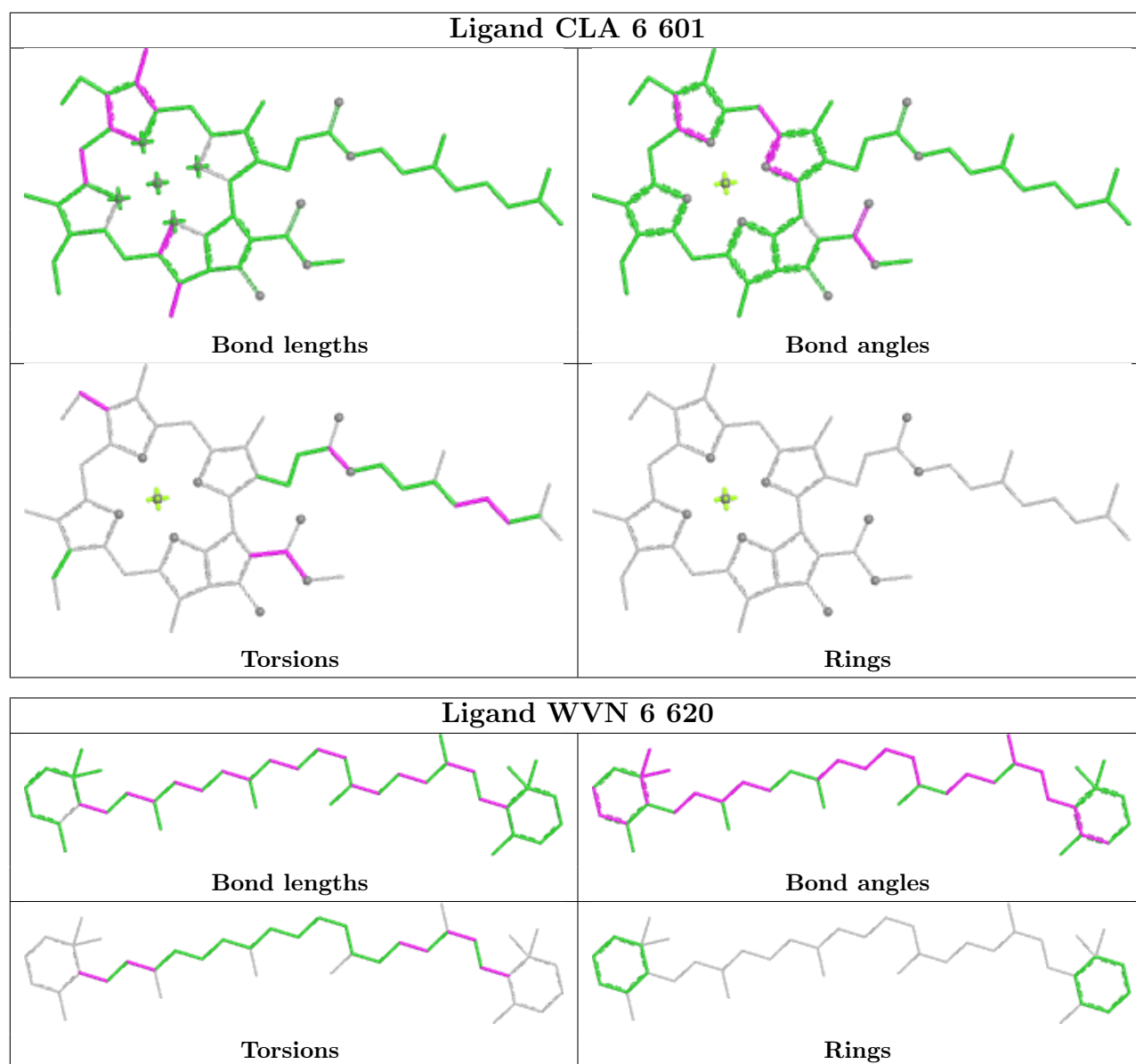
Bond angles

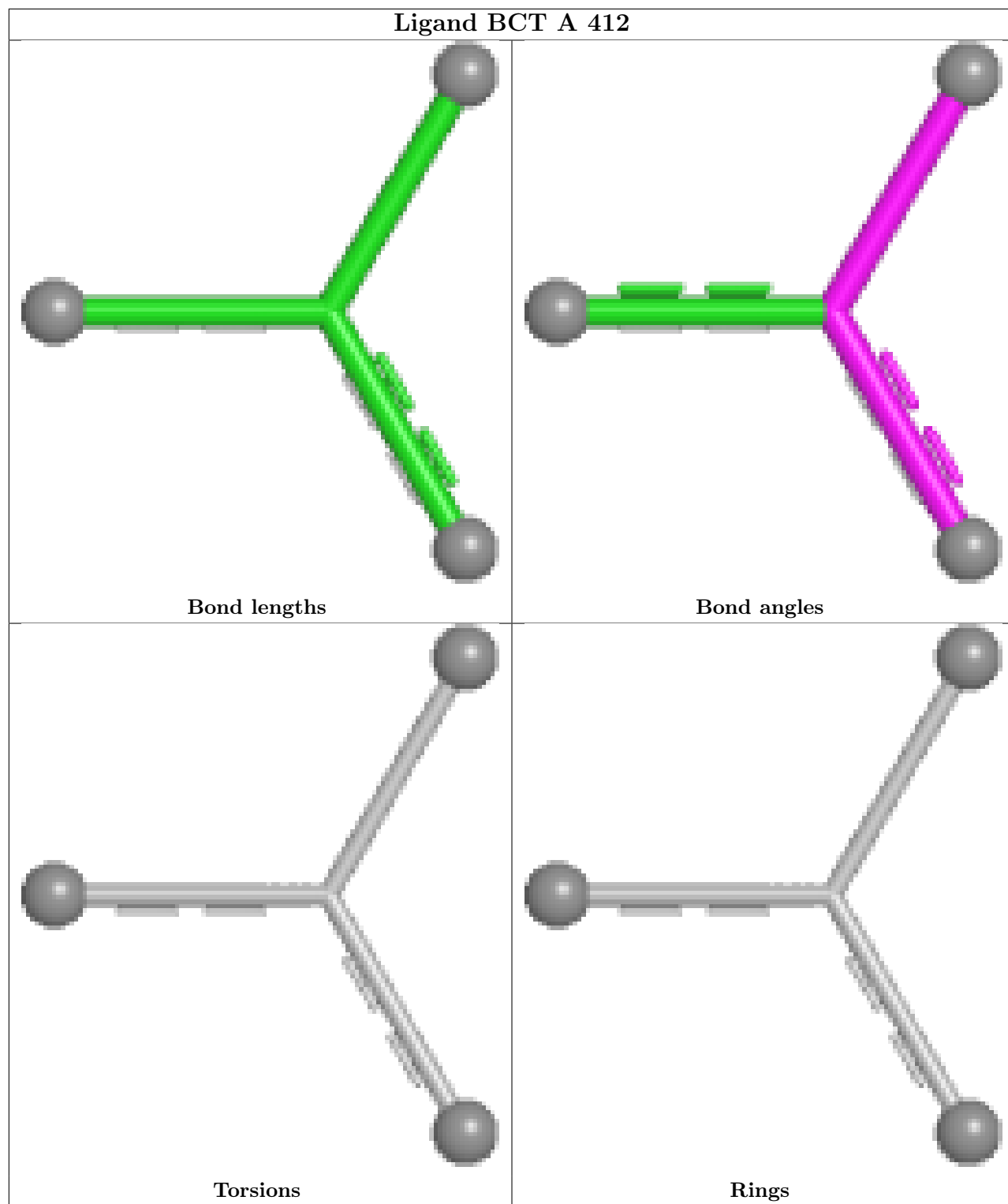


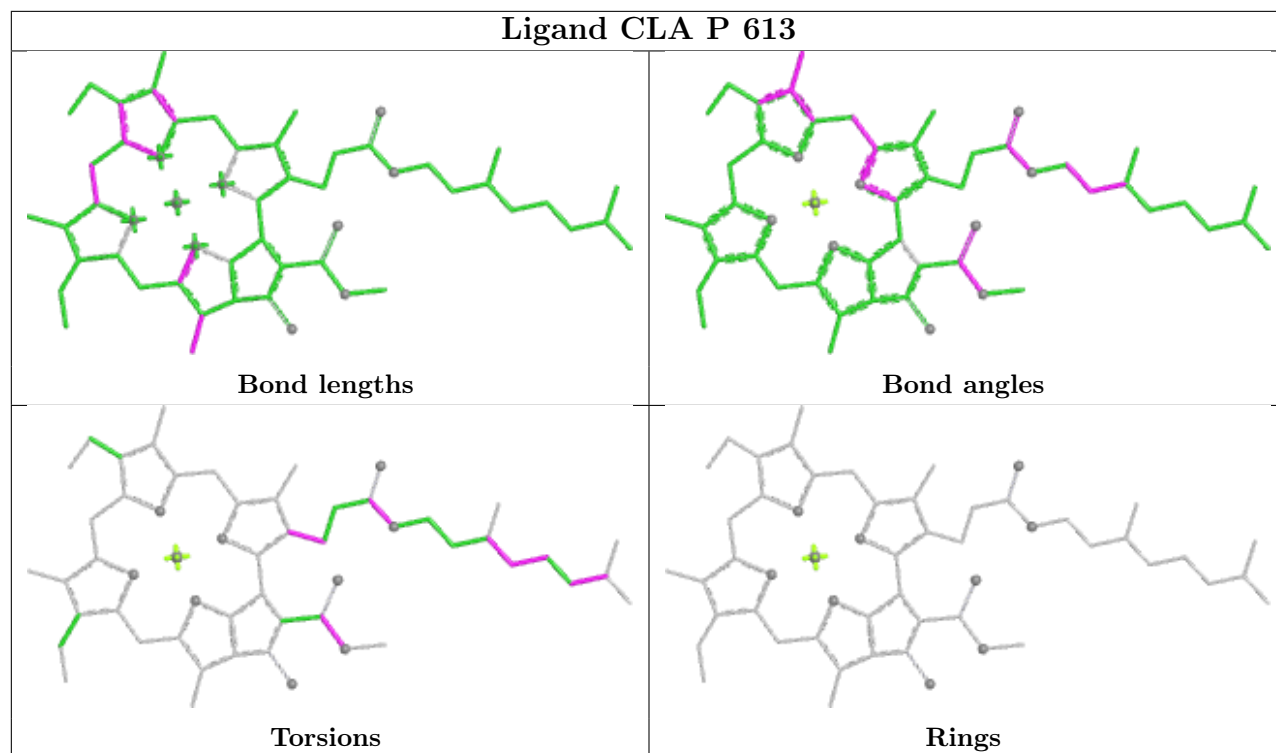
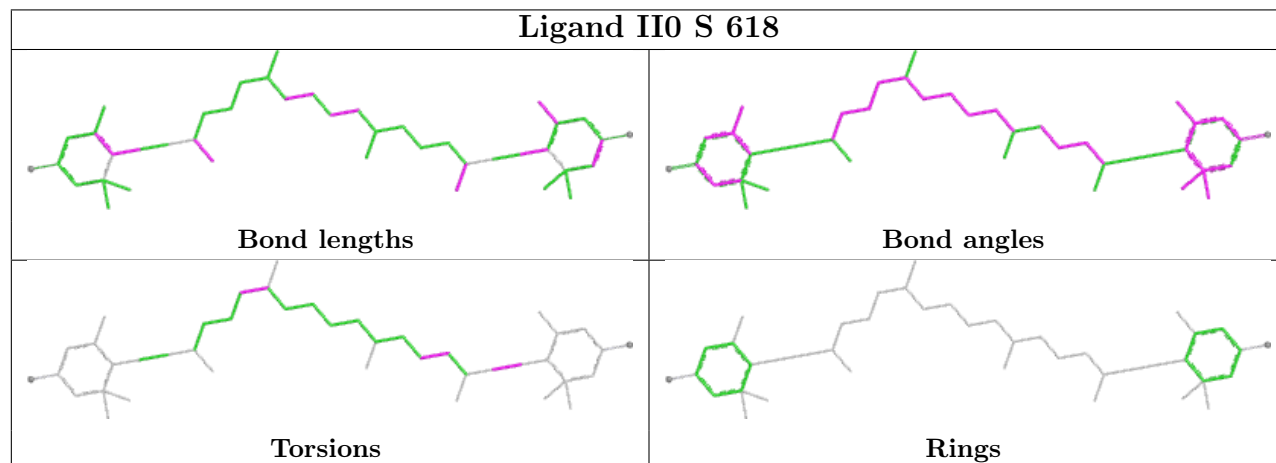
Torsions

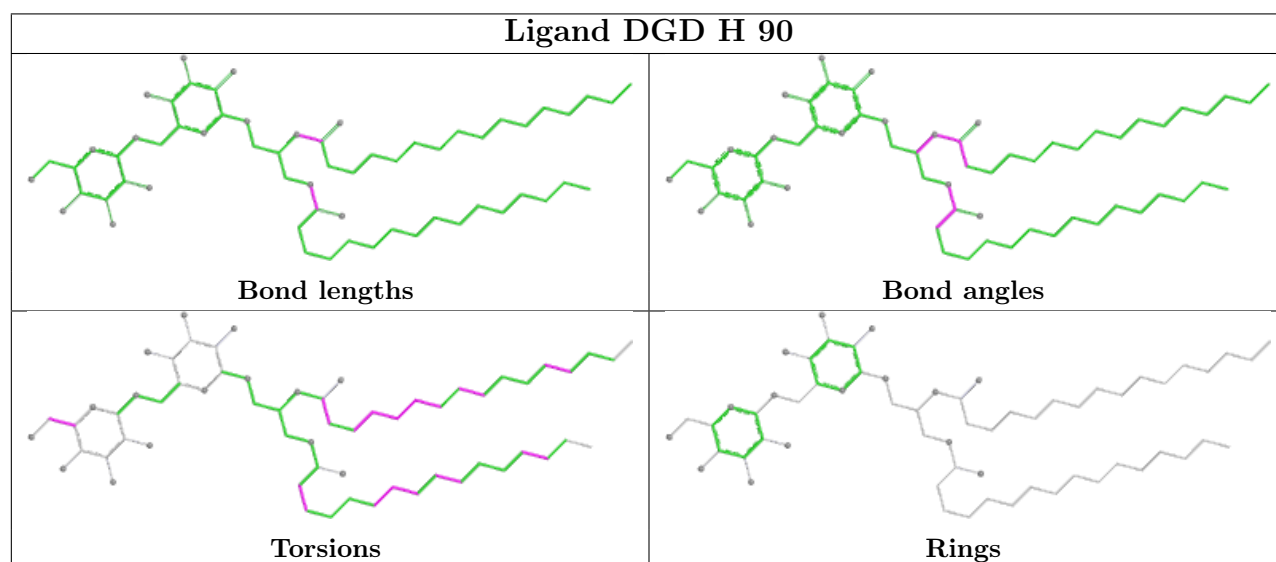
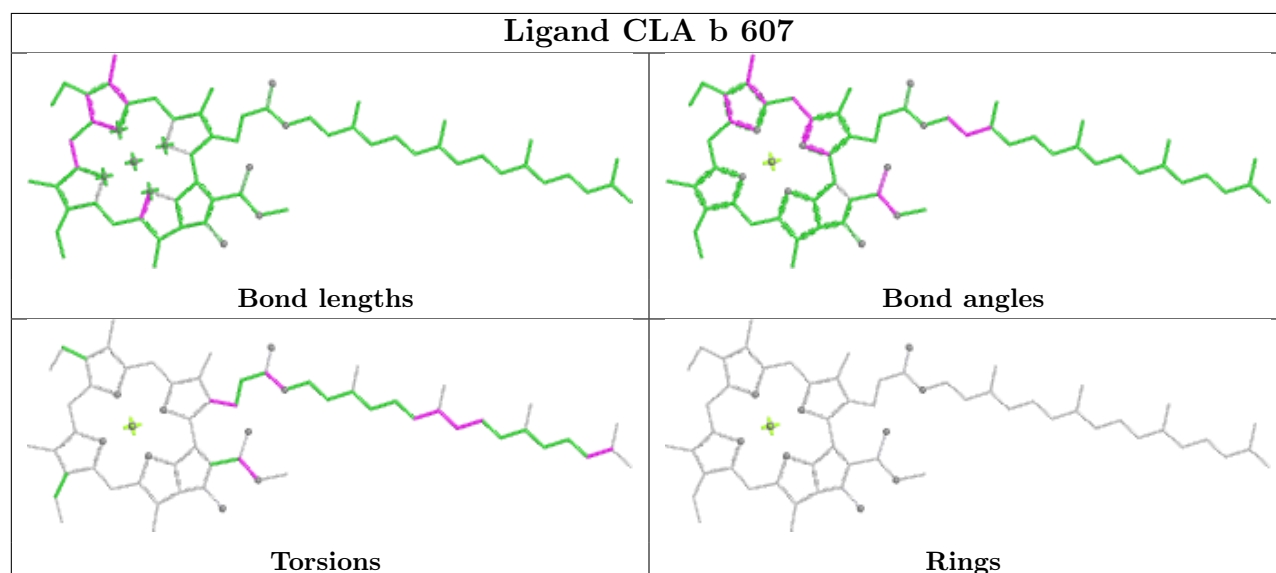
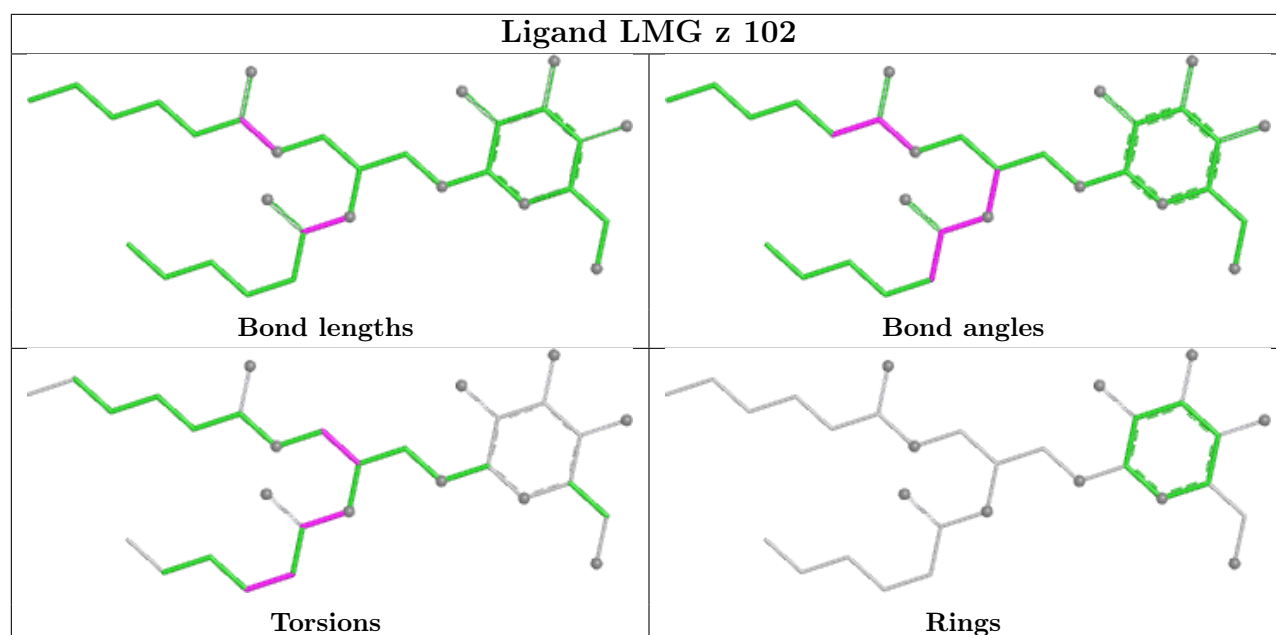


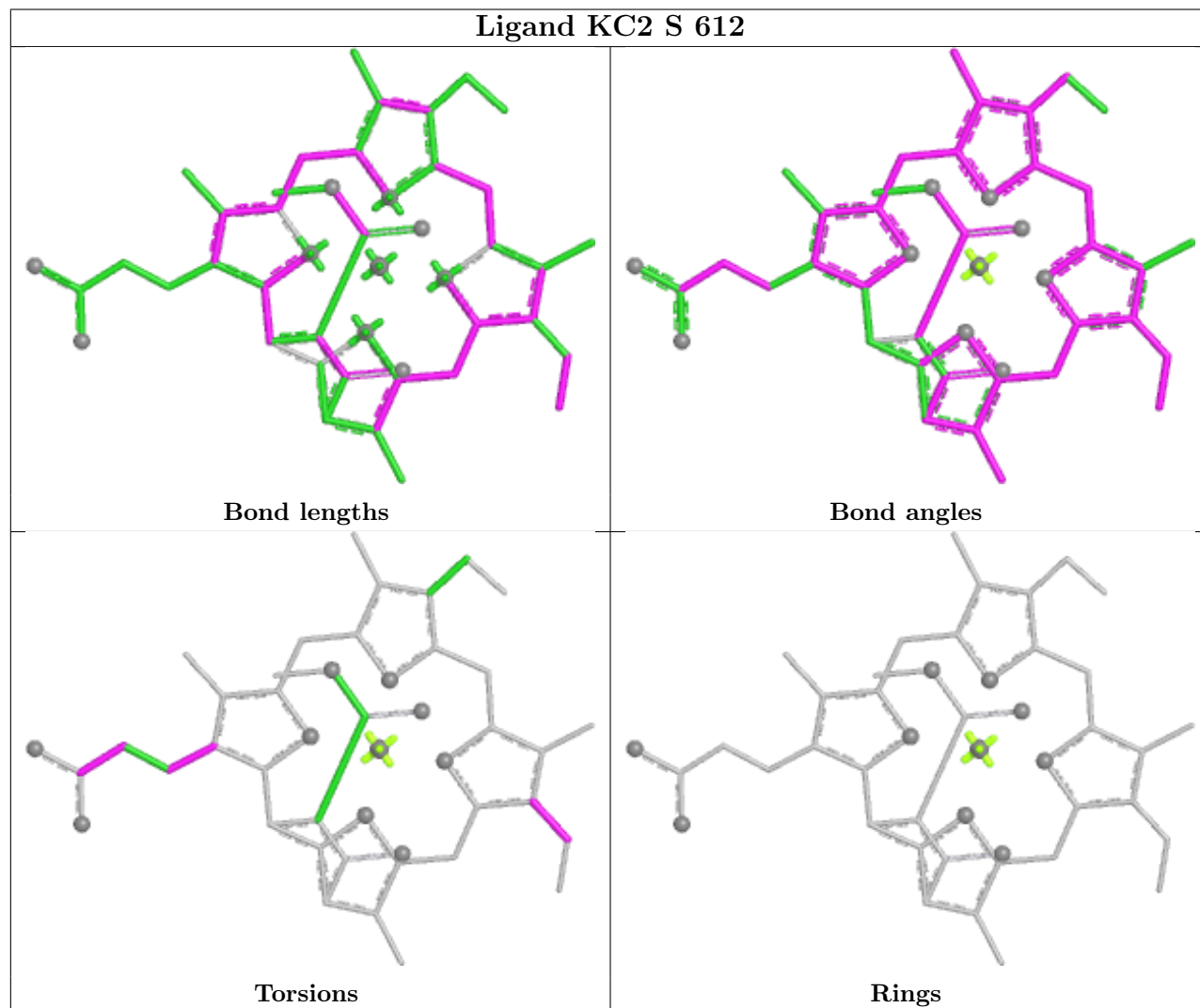
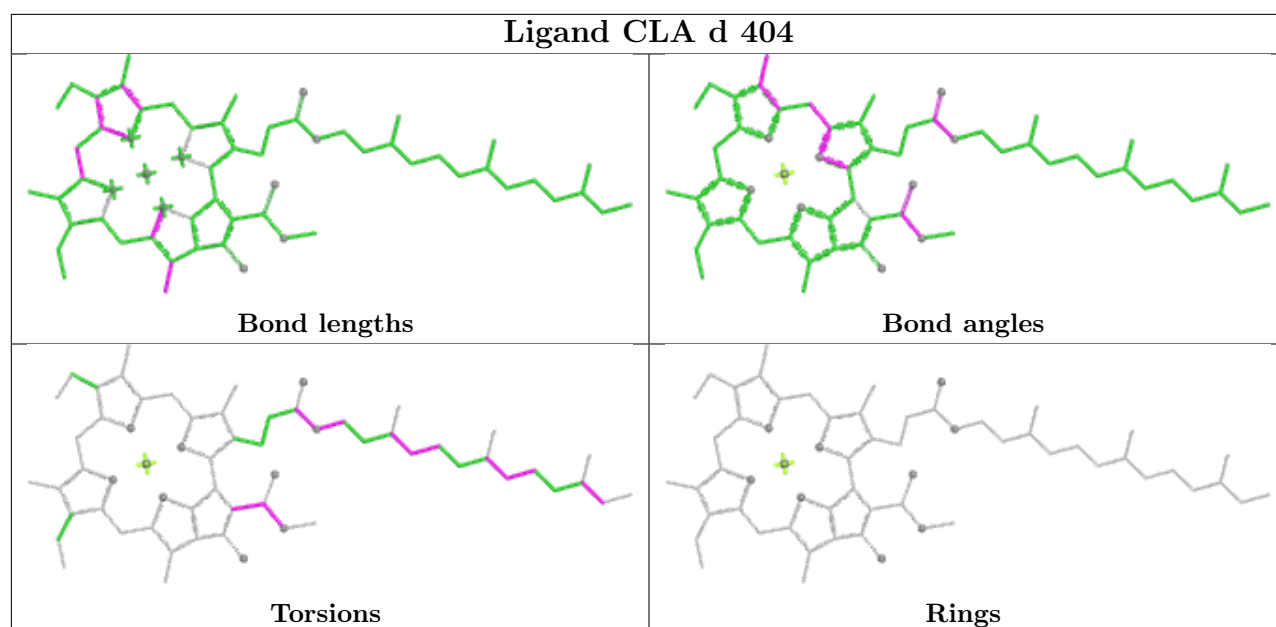
Rings

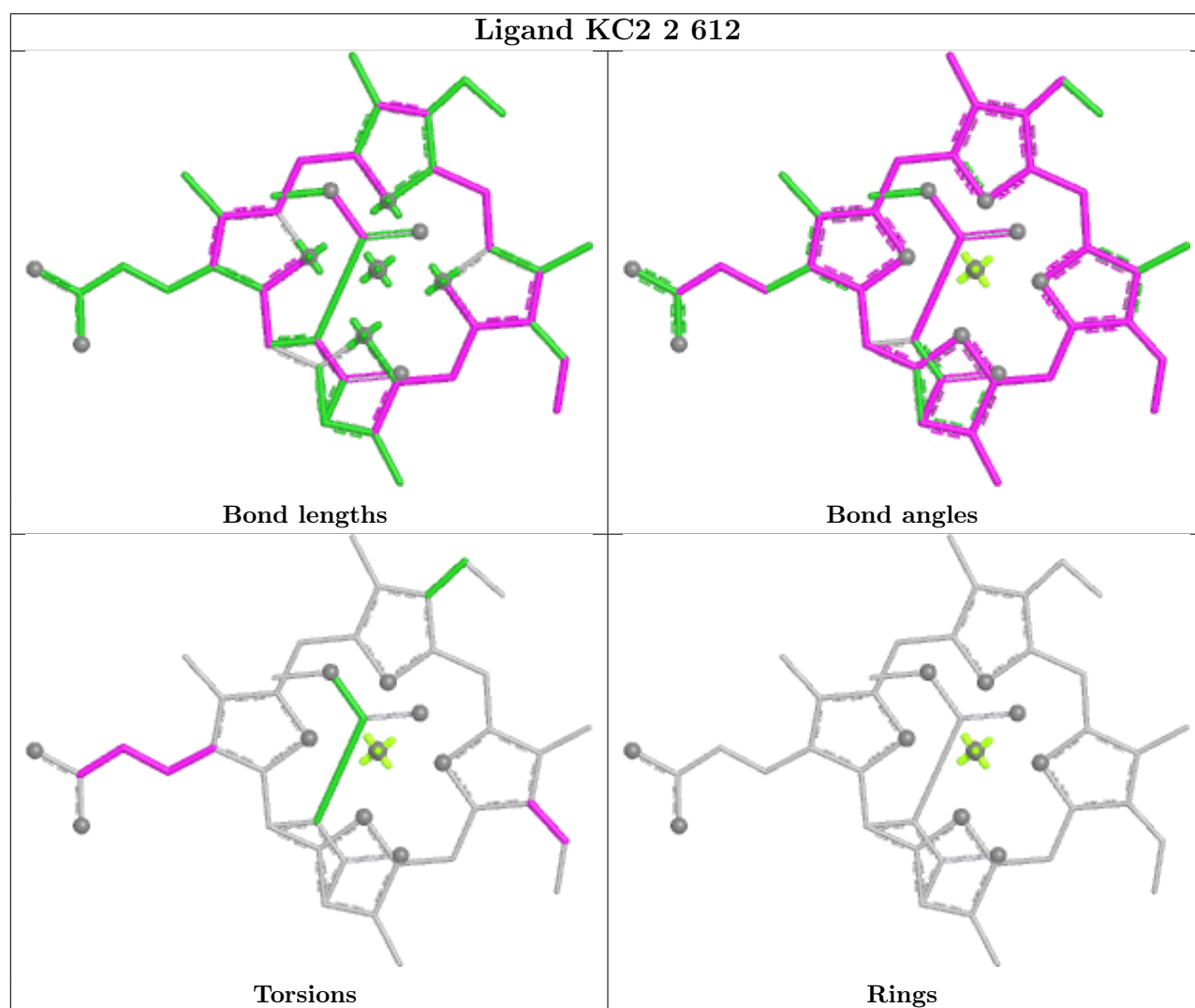
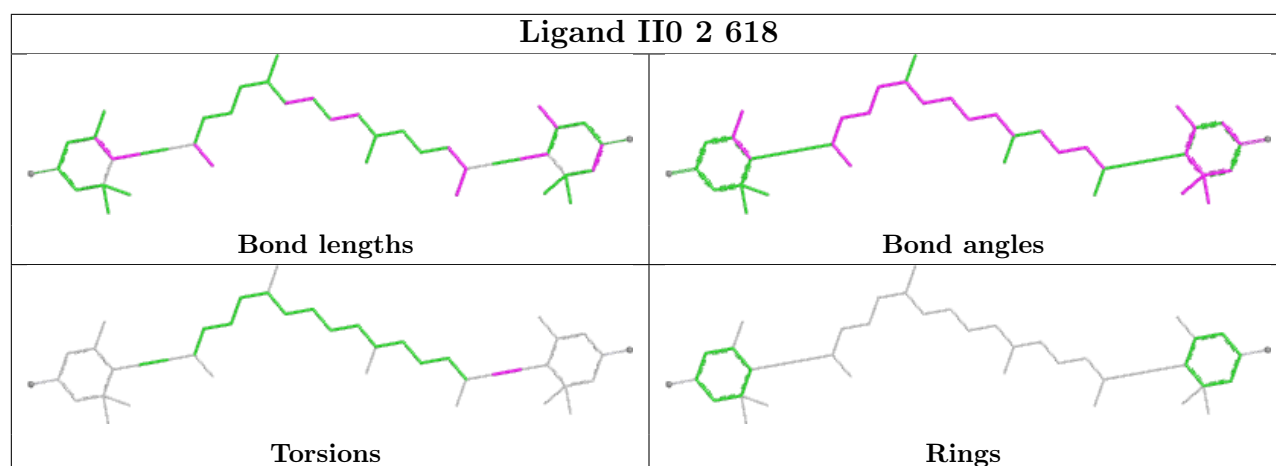




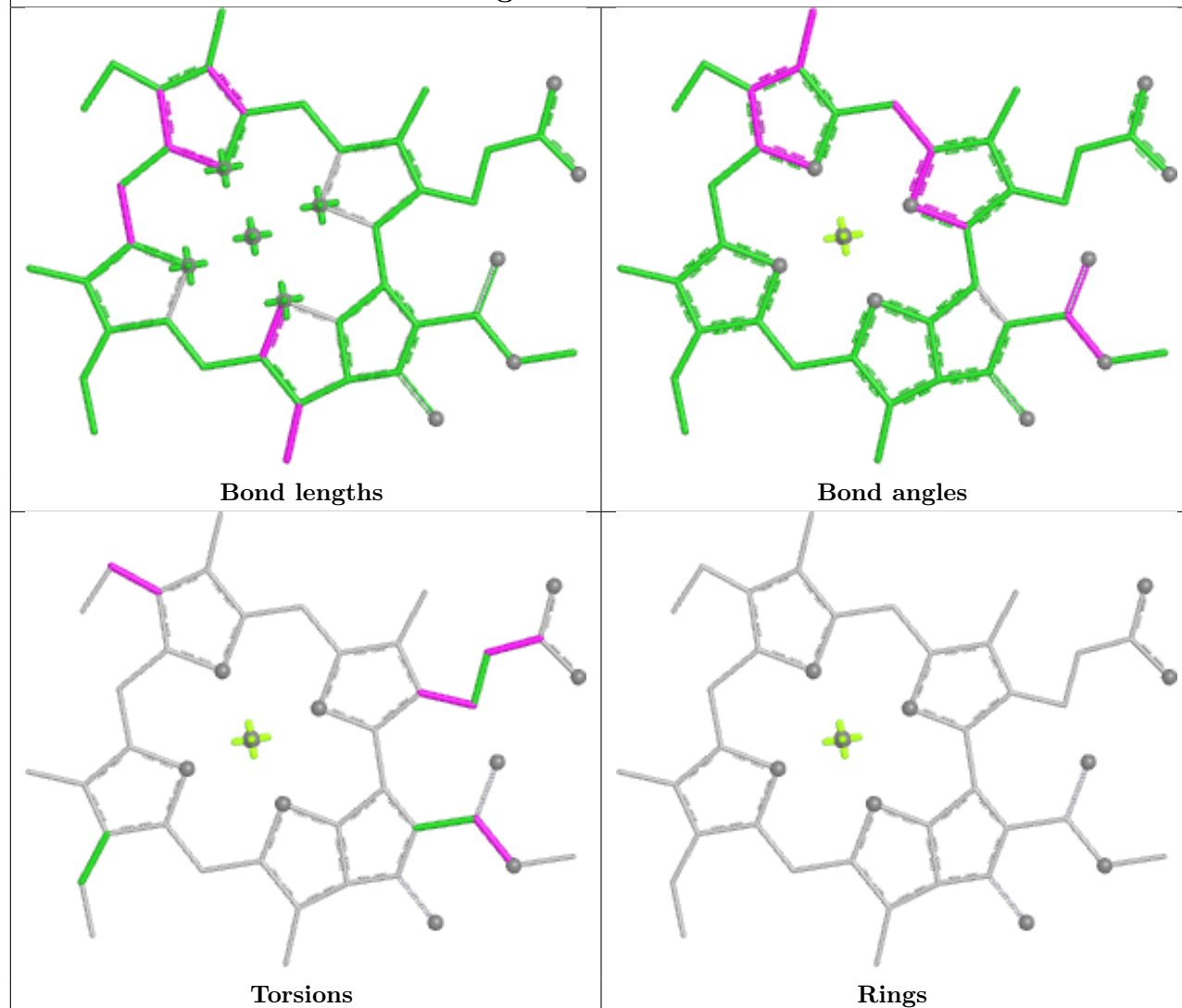
Ligand CLA P 613**Ligand II0 S 618**



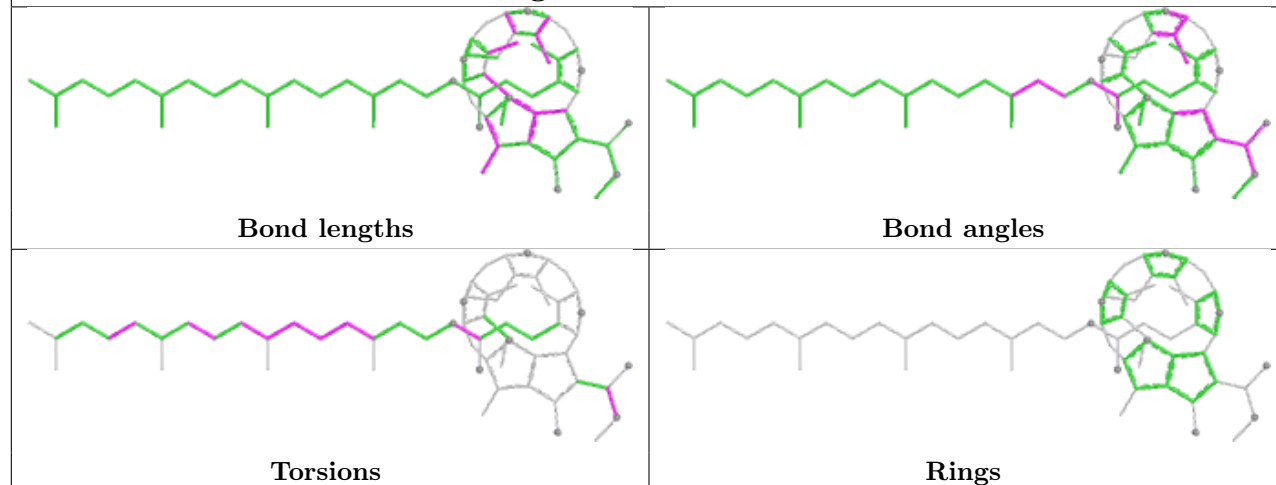




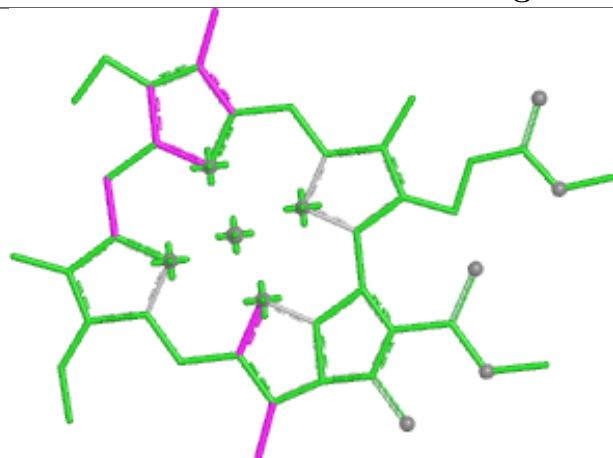
Ligand CLA 2 615



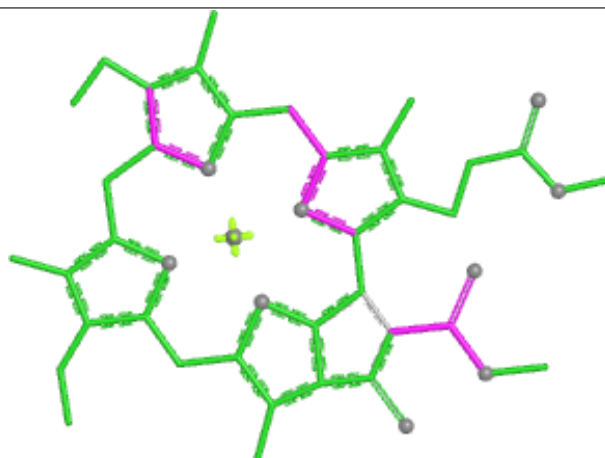
Ligand PHO A 405



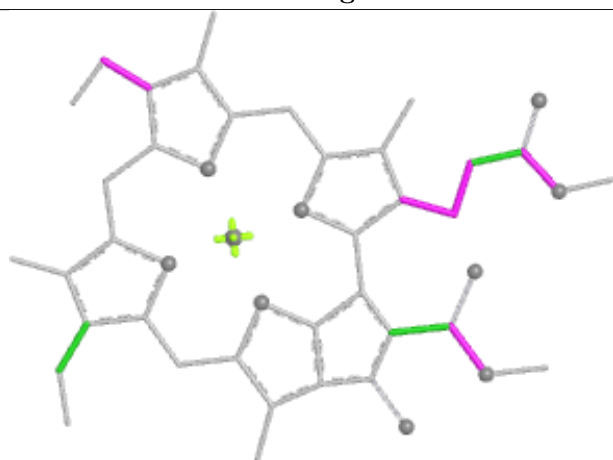
Ligand CLA N 609



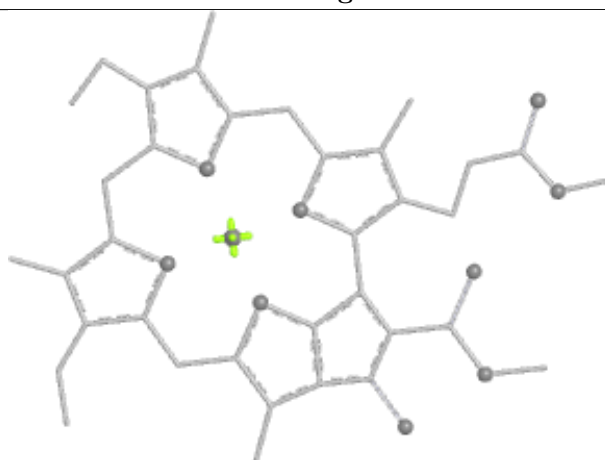
Bond lengths



Bond angles

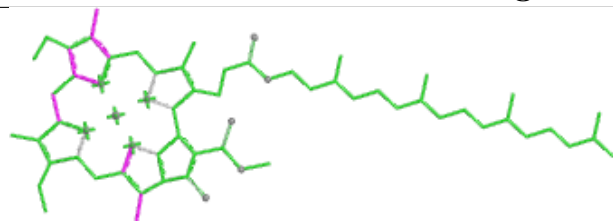


Torsions

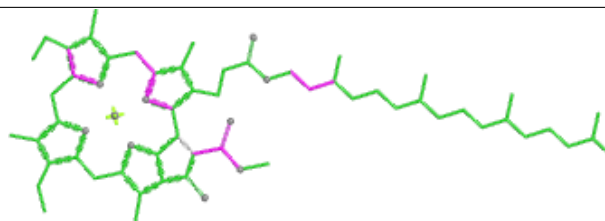


Rings

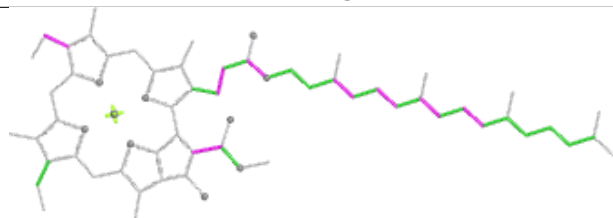
Ligand CLA C 520



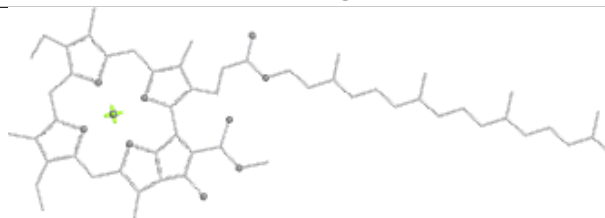
Bond lengths



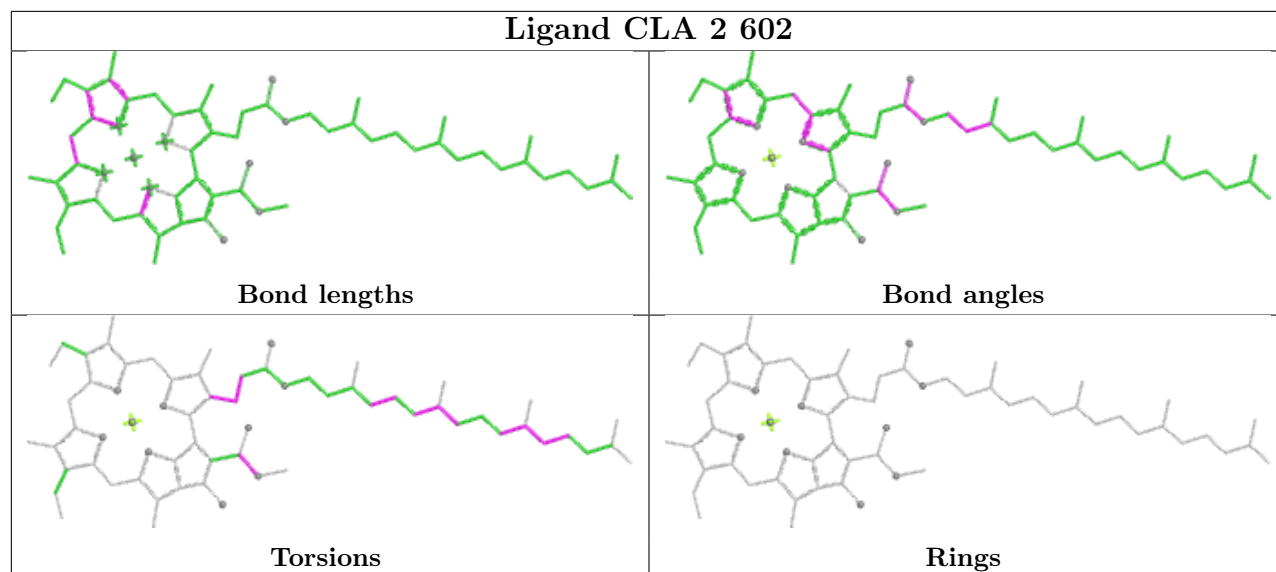
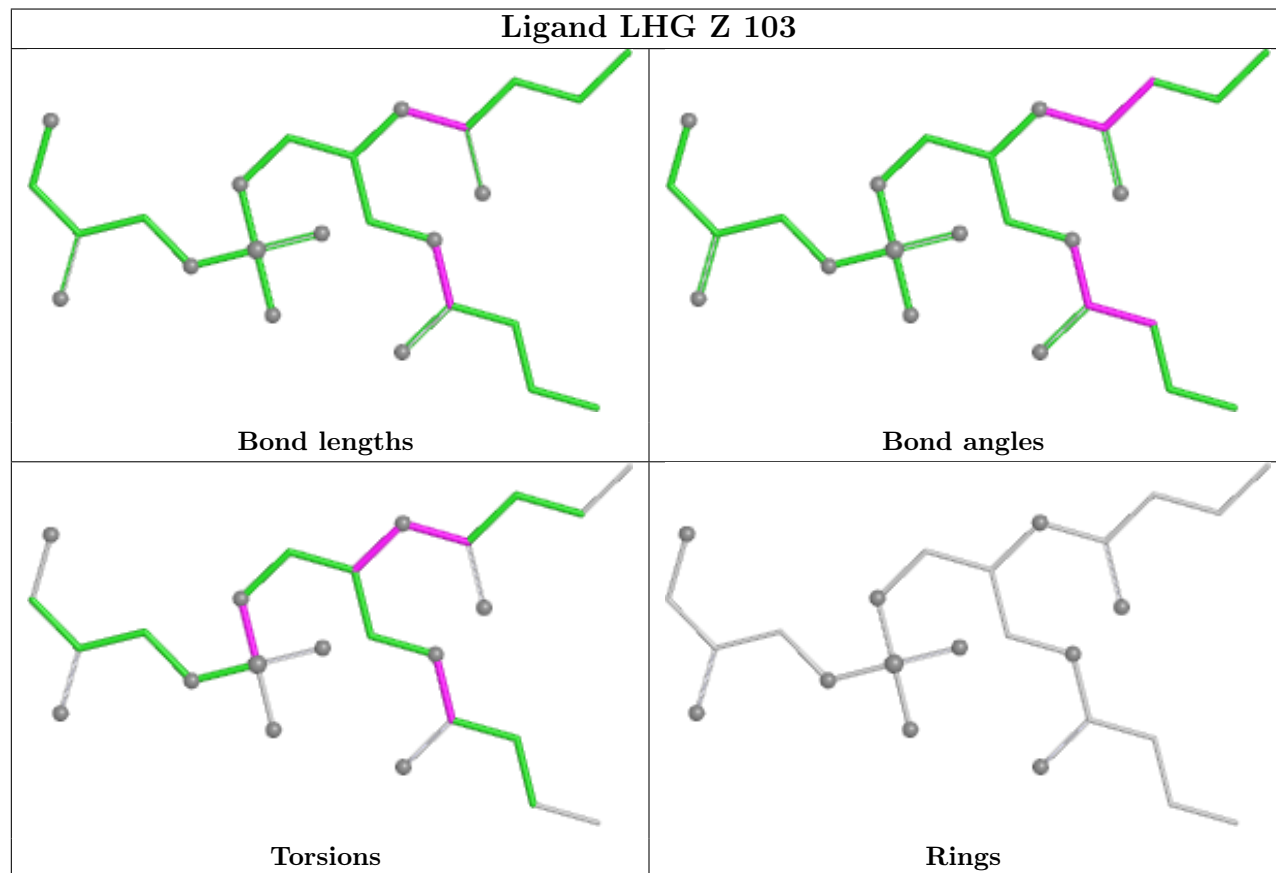
Bond angles

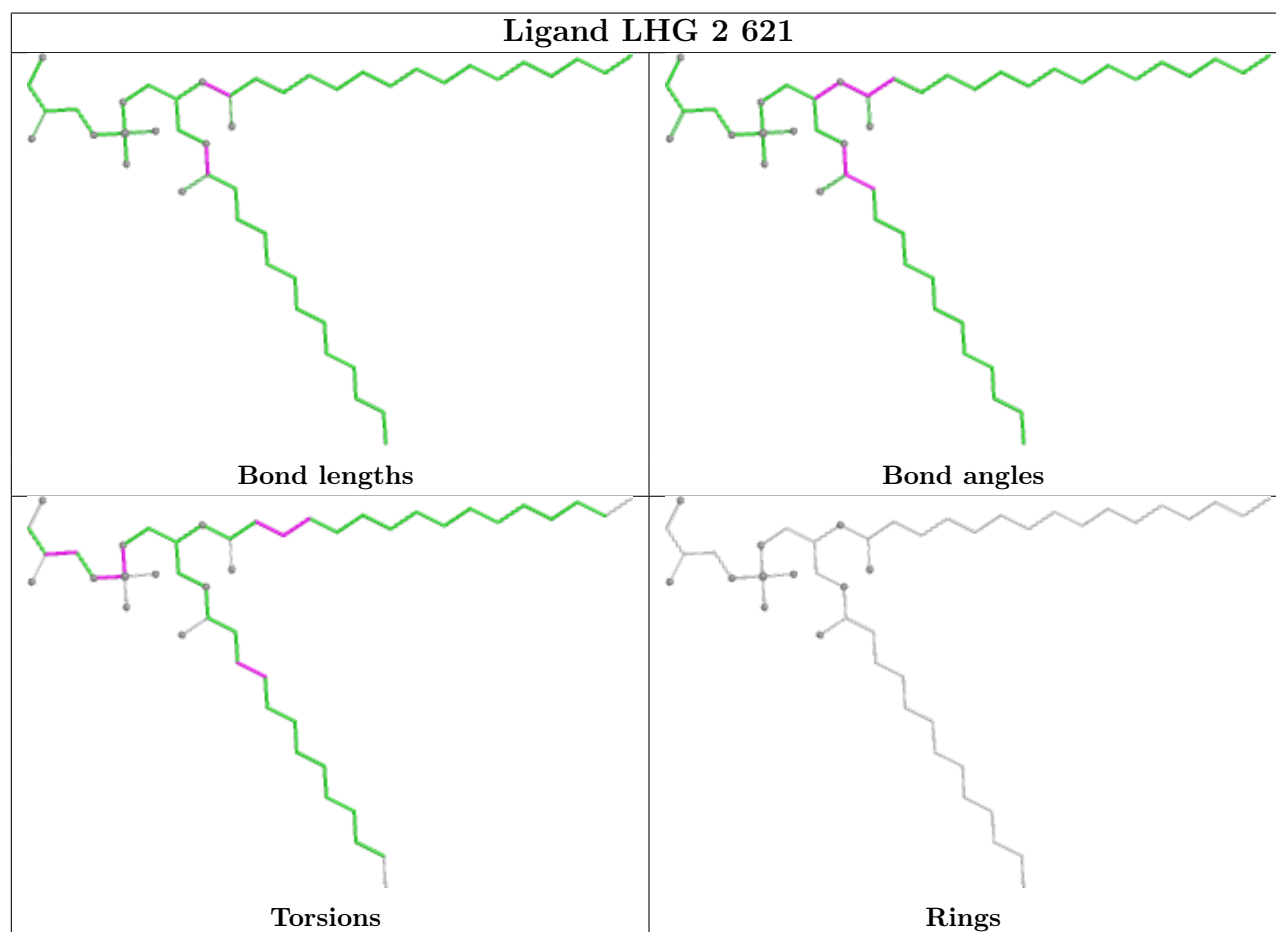
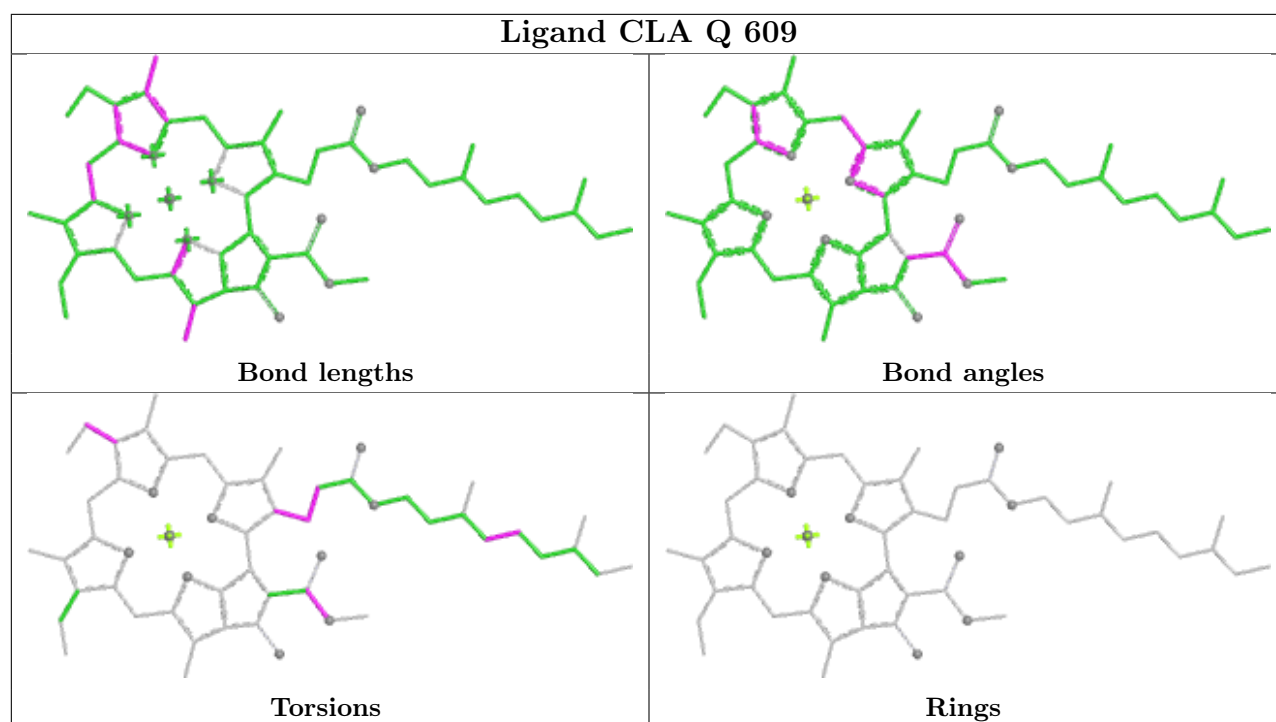


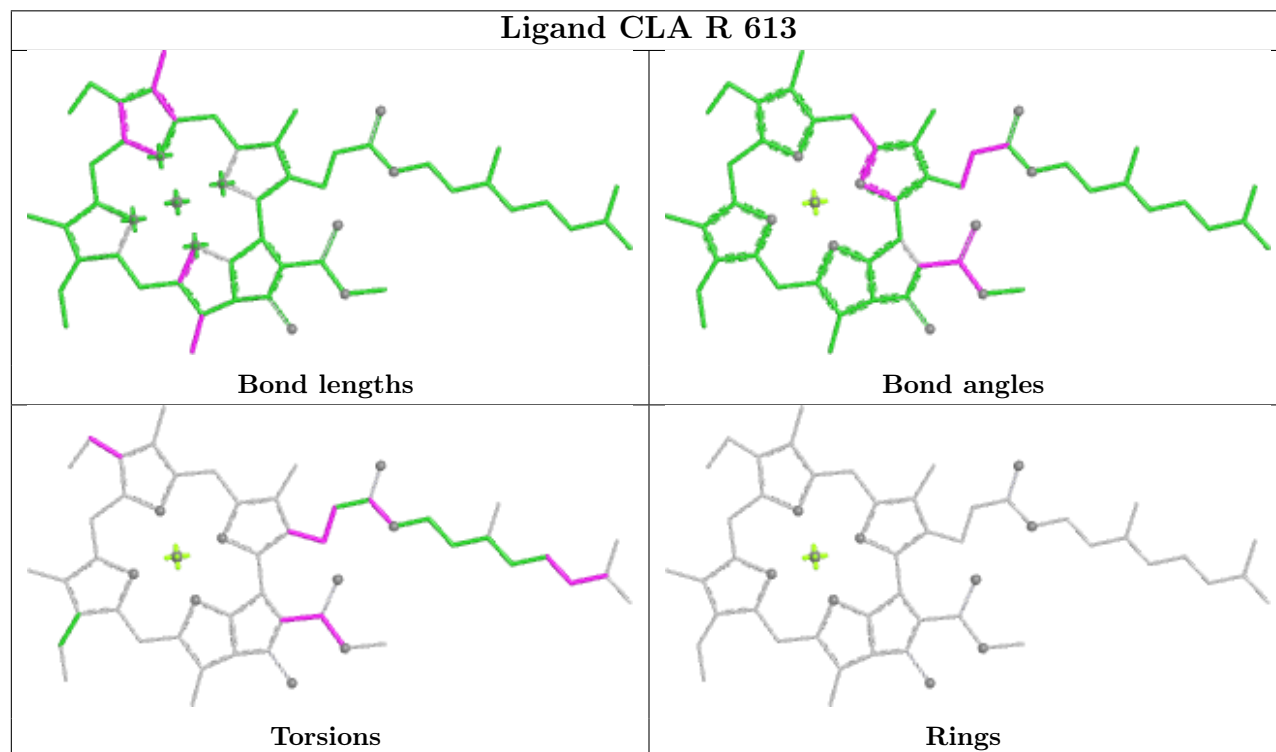
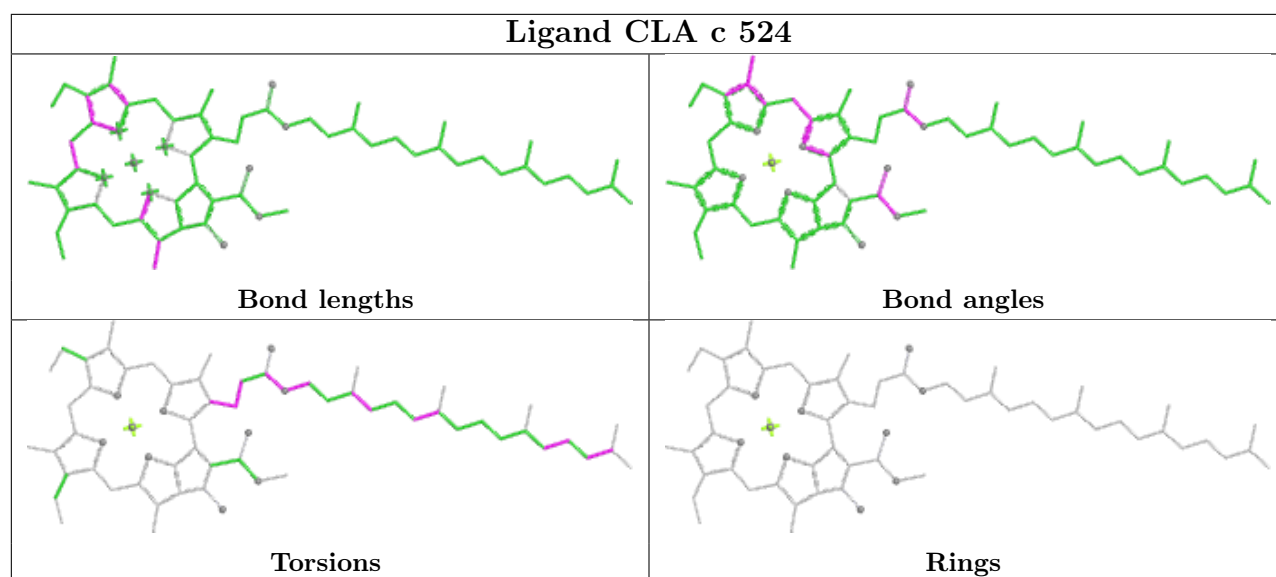
Torsions



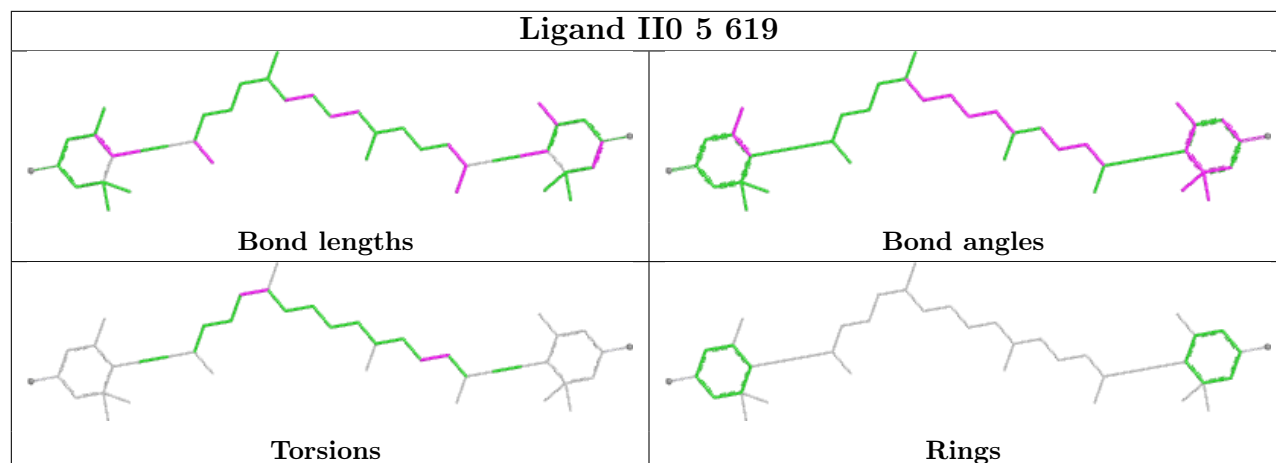
Rings

Ligand CLA 2 602**Ligand LHG Z 103**

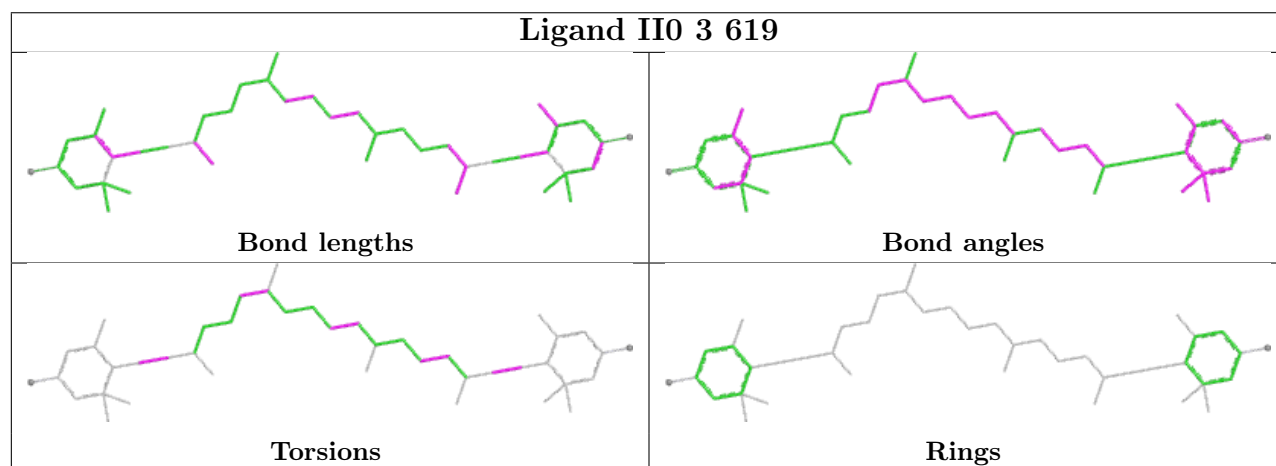




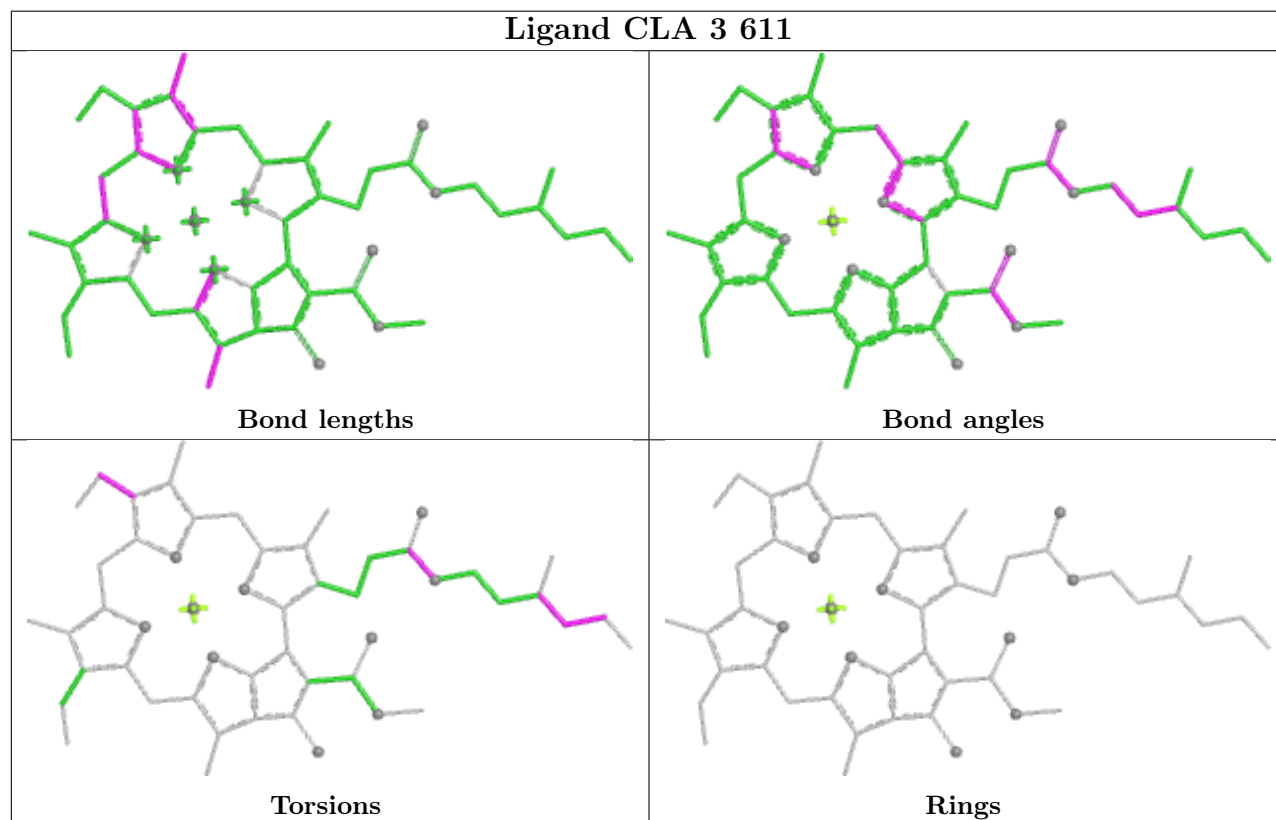
Ligand II0 5 619

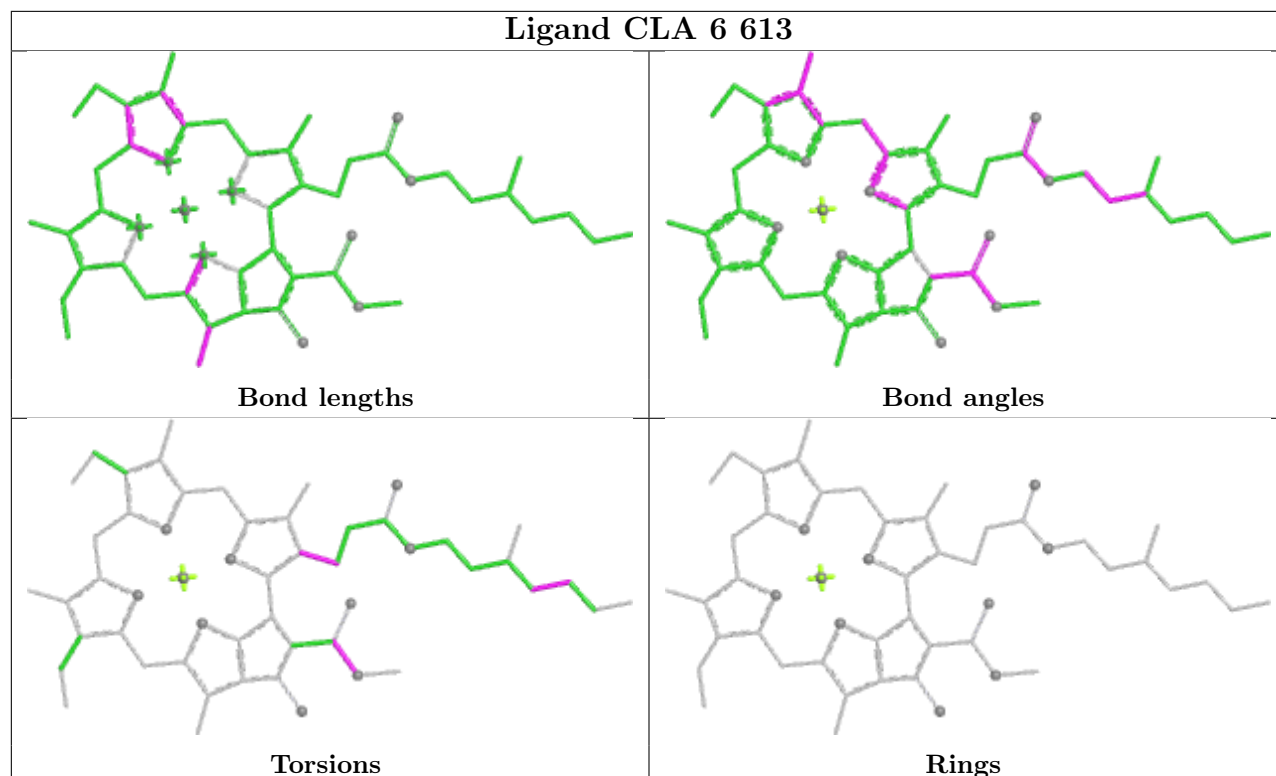
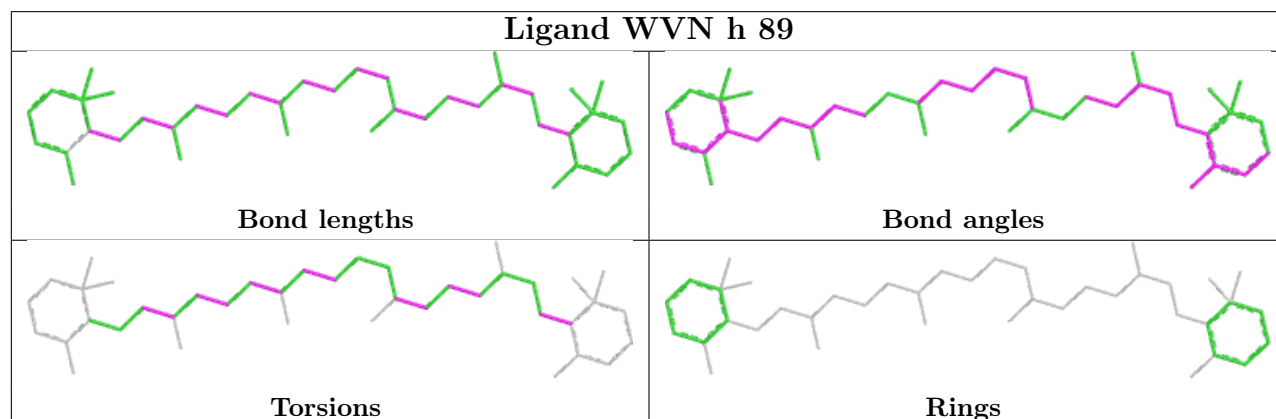
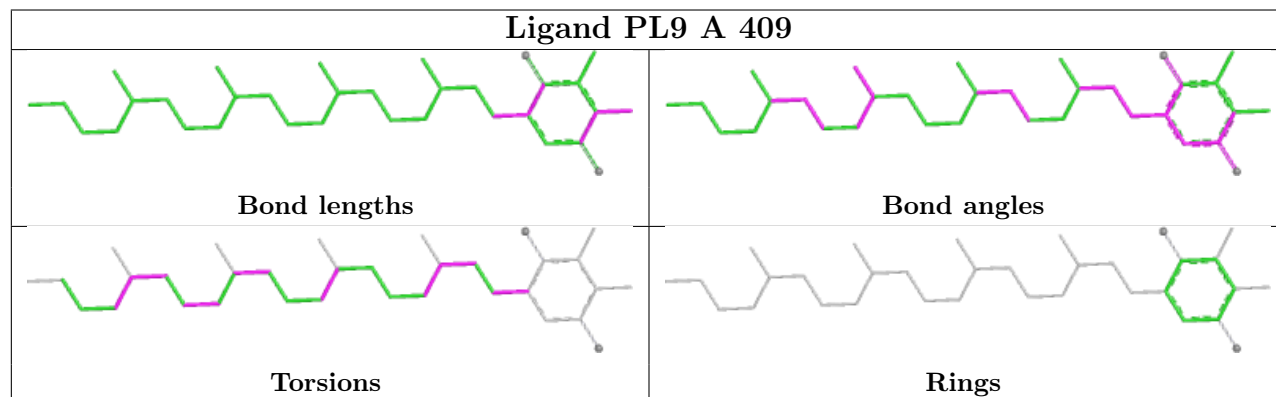


Ligand II0 3 619

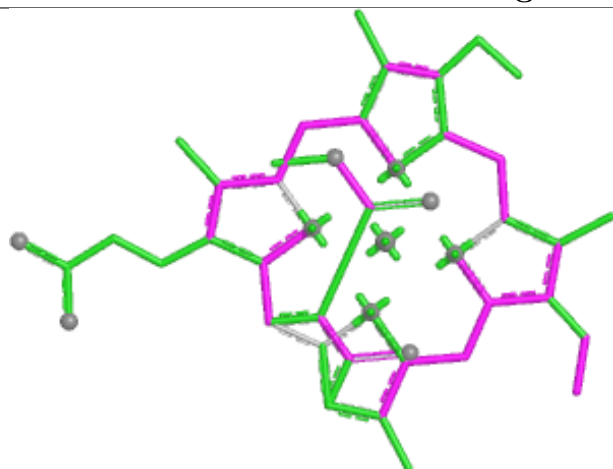


Ligand CLA 3 611

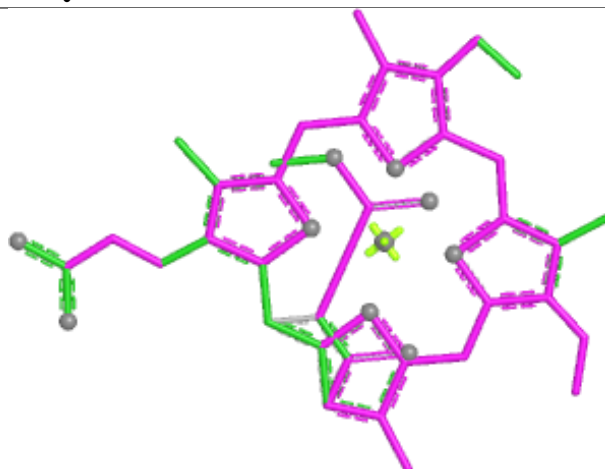


Ligand CLA 6 613**Ligand WVN h 89****Ligand PL9 A 409**

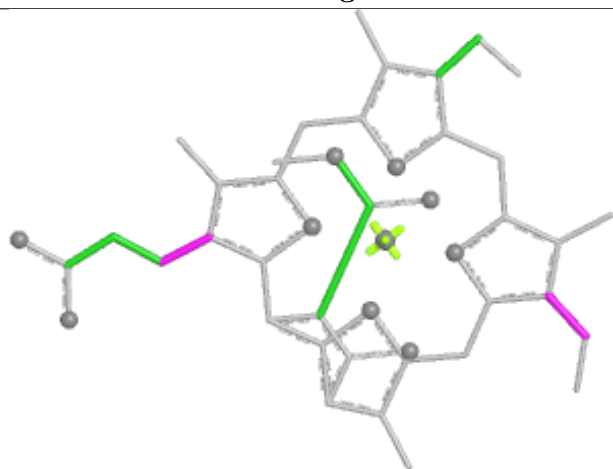
Ligand KC2 Q 612



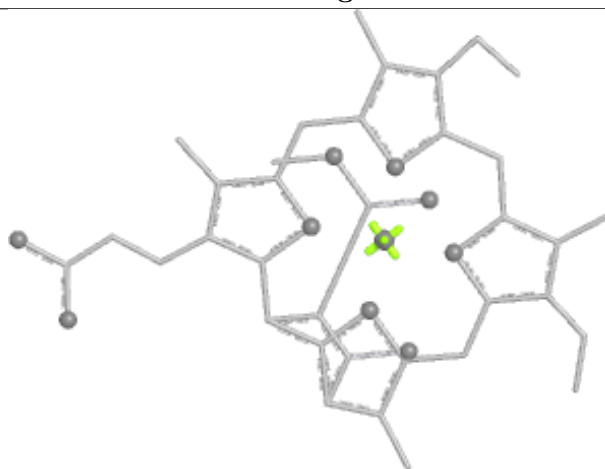
Bond lengths



Bond angles

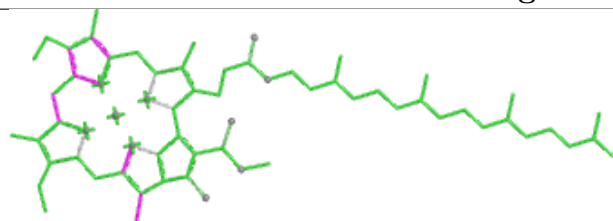


Torsions

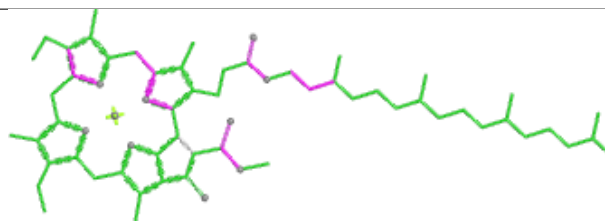


Rings

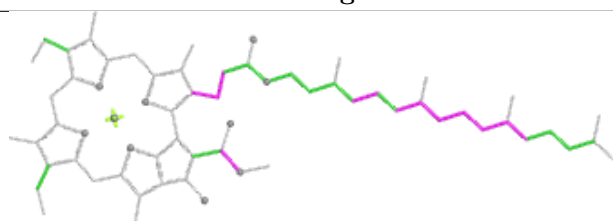
Ligand CLA 6 602



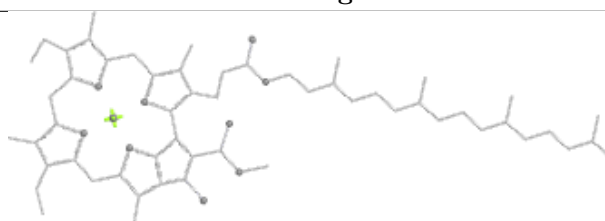
Bond lengths



Bond angles

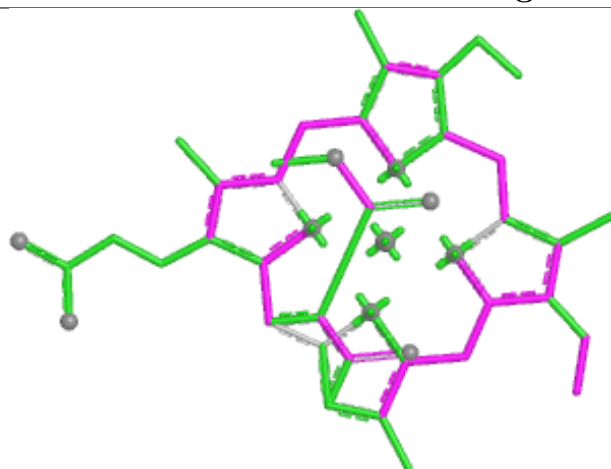


Torsions

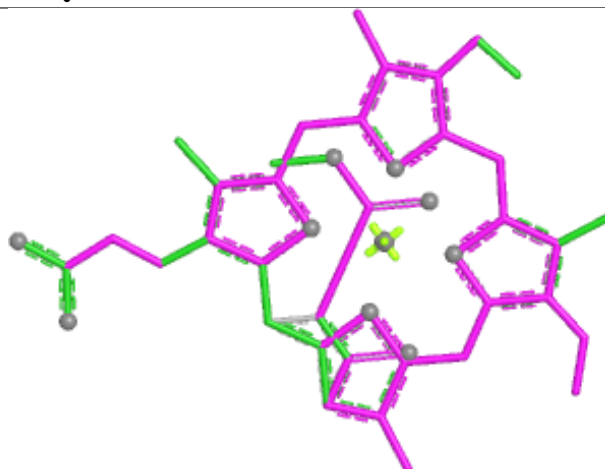


Rings

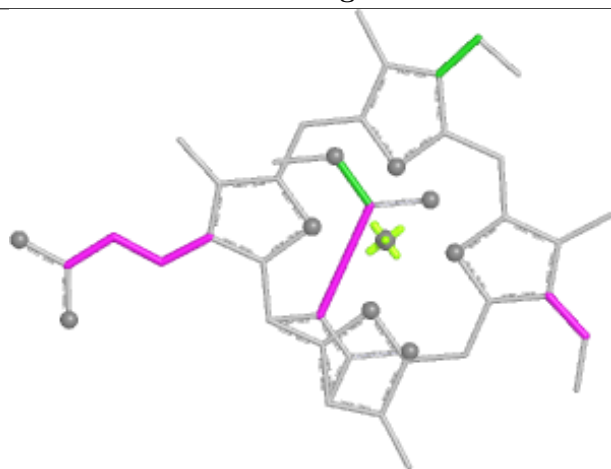
Ligand KC2 Q 605



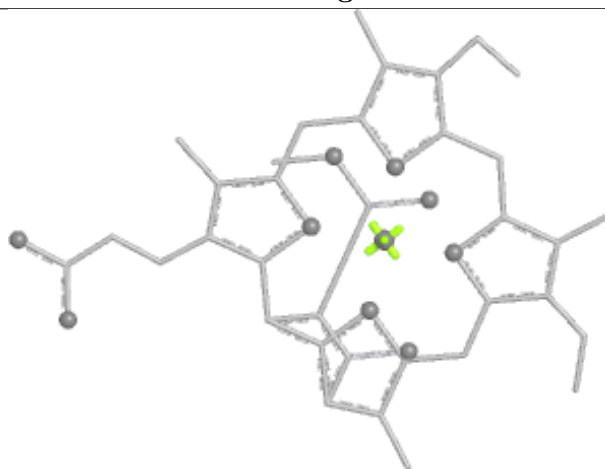
Bond lengths



Bond angles

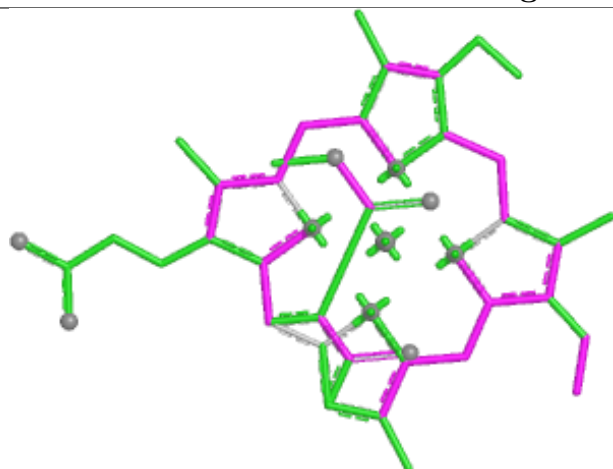


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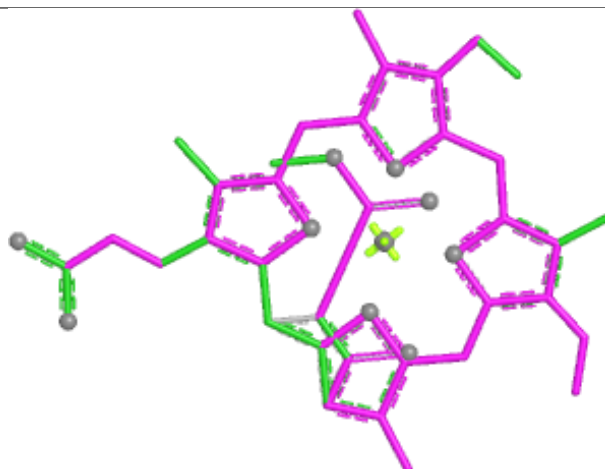


Rings

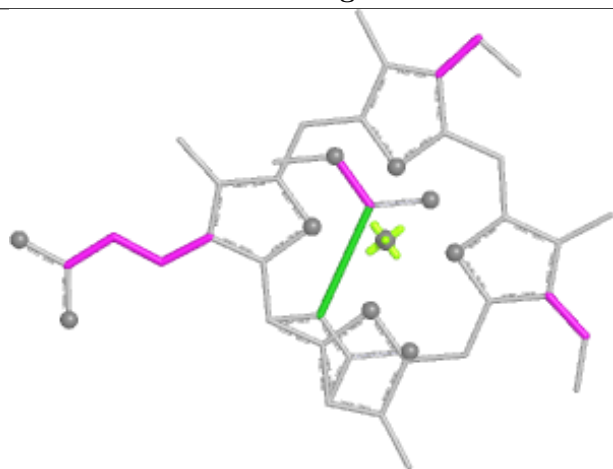
Ligand KC2 3 606



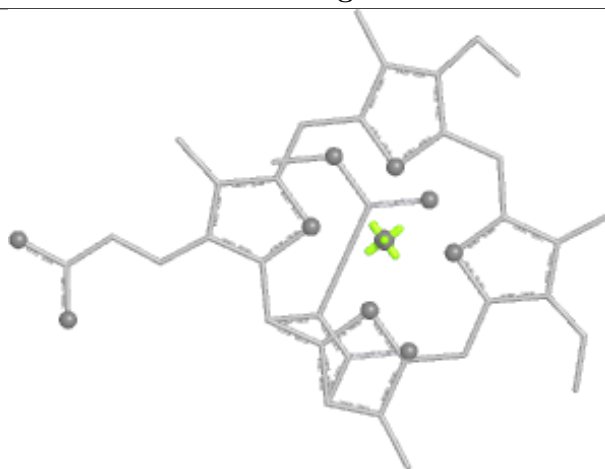
Bond lengths



Bond angles

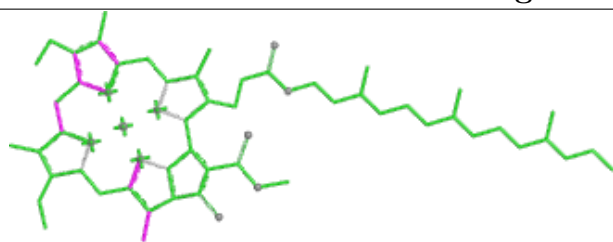


Torsions

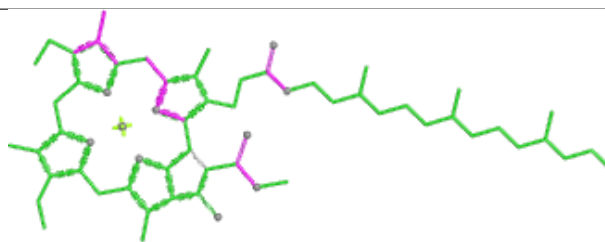


Rings

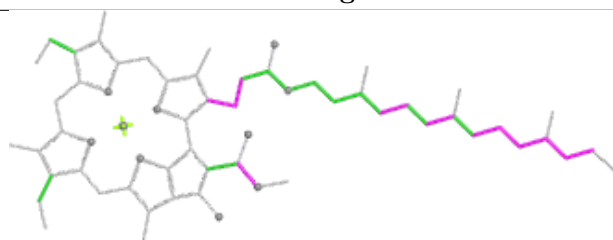
Ligand CLA P 602



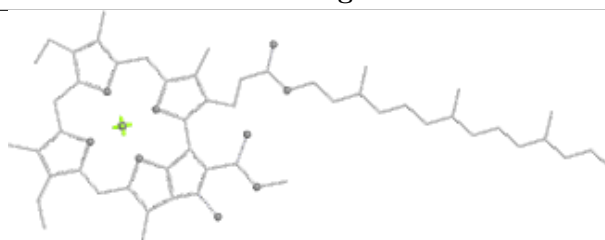
Bond lengths



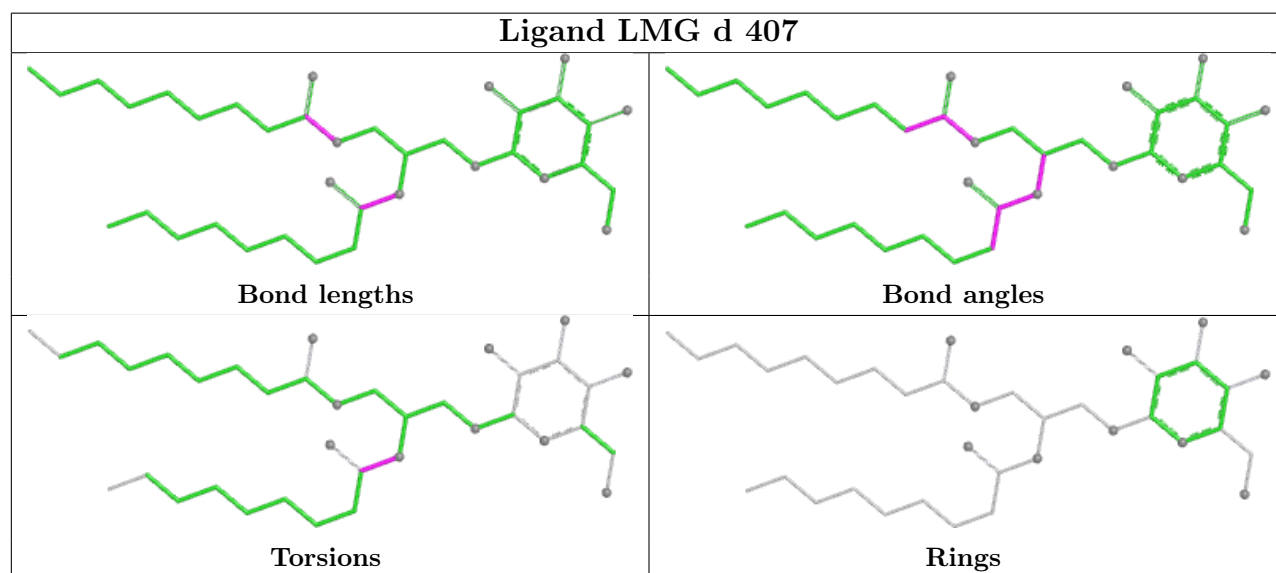
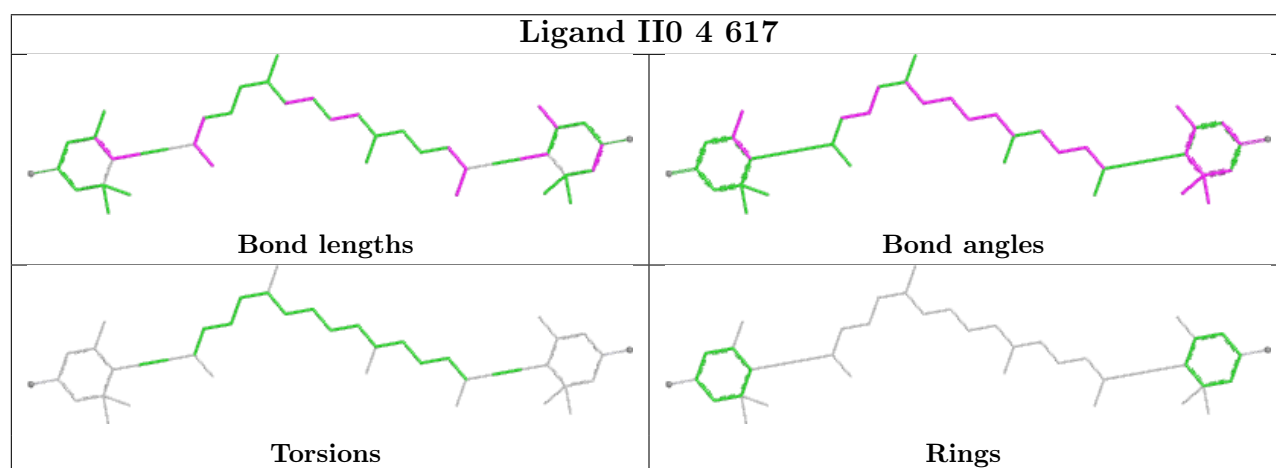
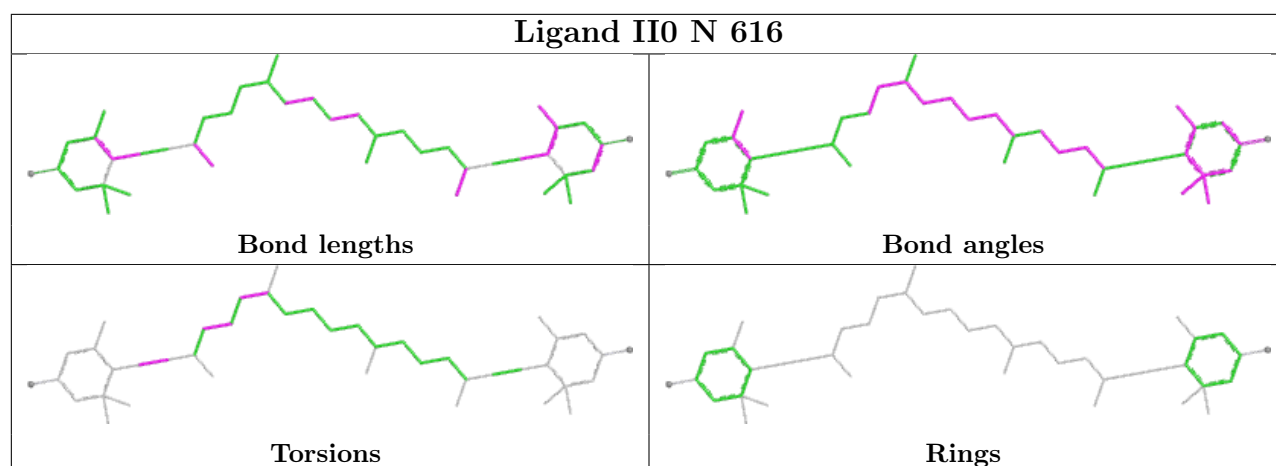
Bond angles

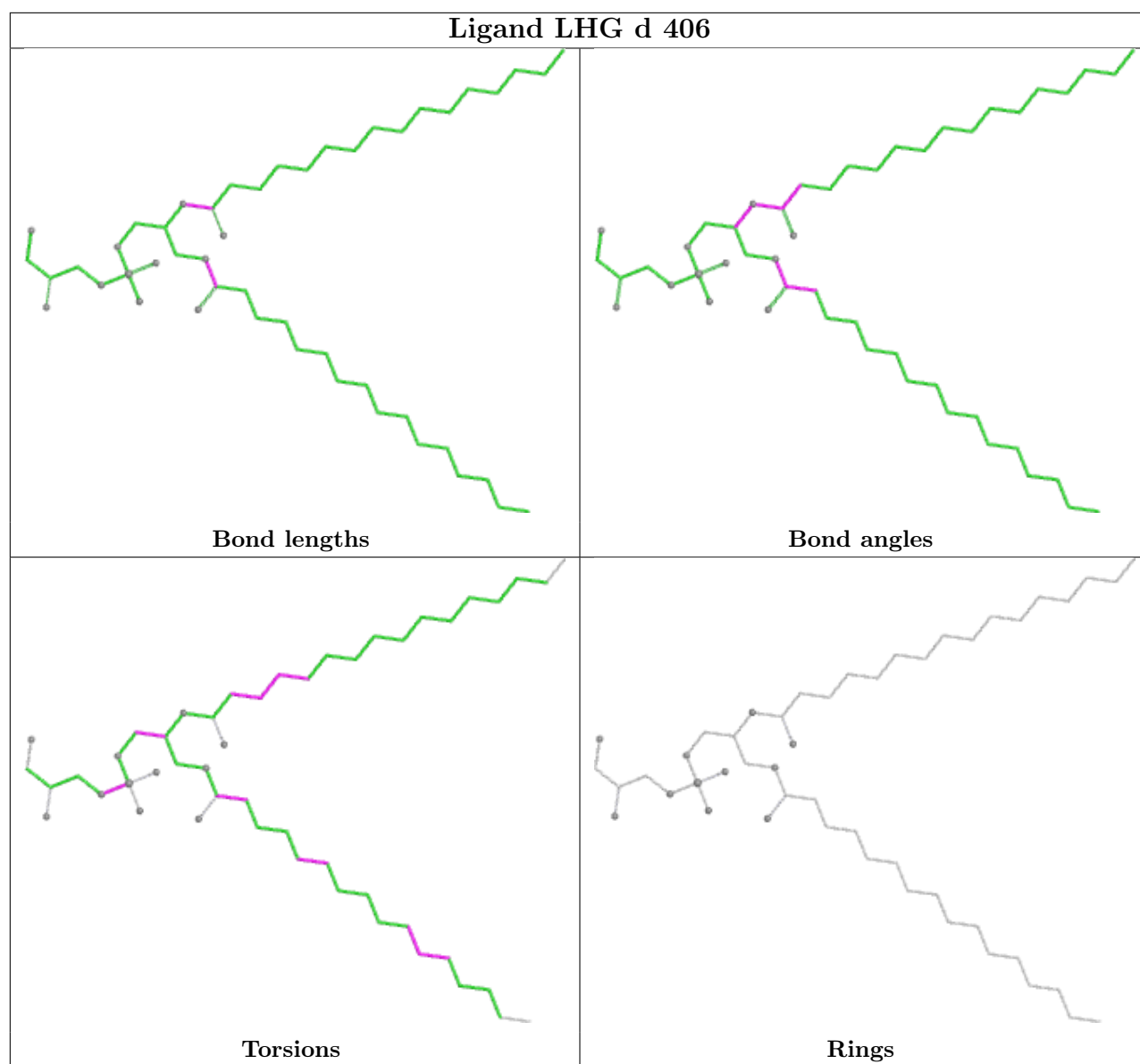


Torsions

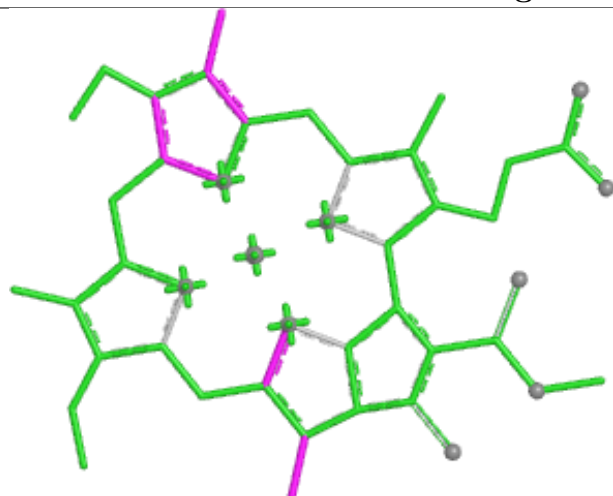


Rings

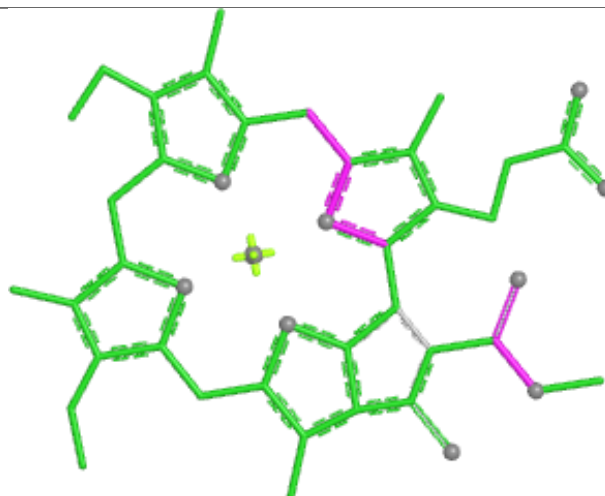




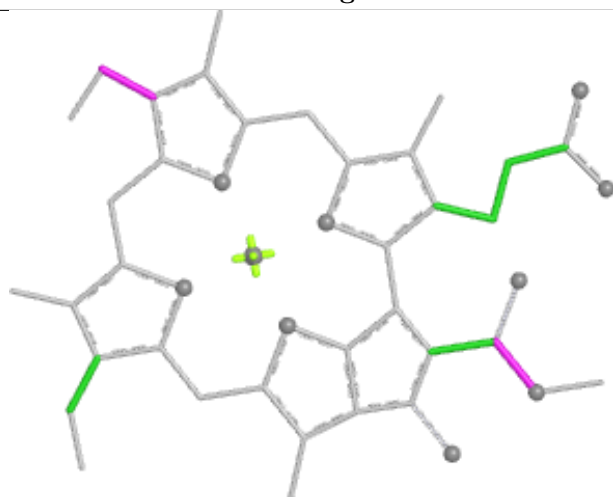
Ligand CLA P 601



Bond lengths



Bond angles

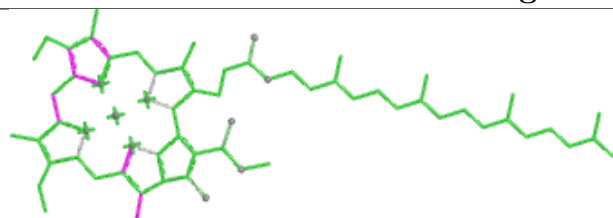


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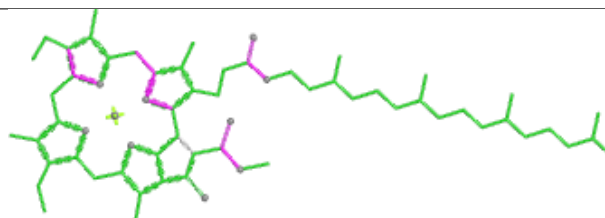


Rings

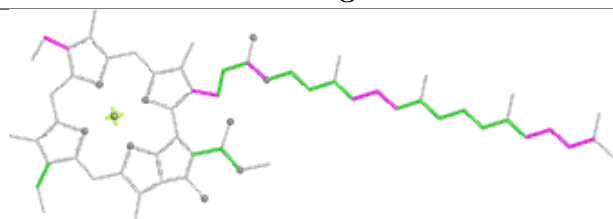
Ligand CLA c 527



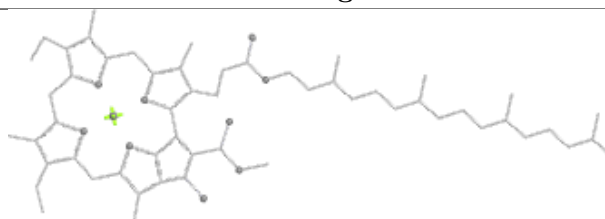
Bond lengths



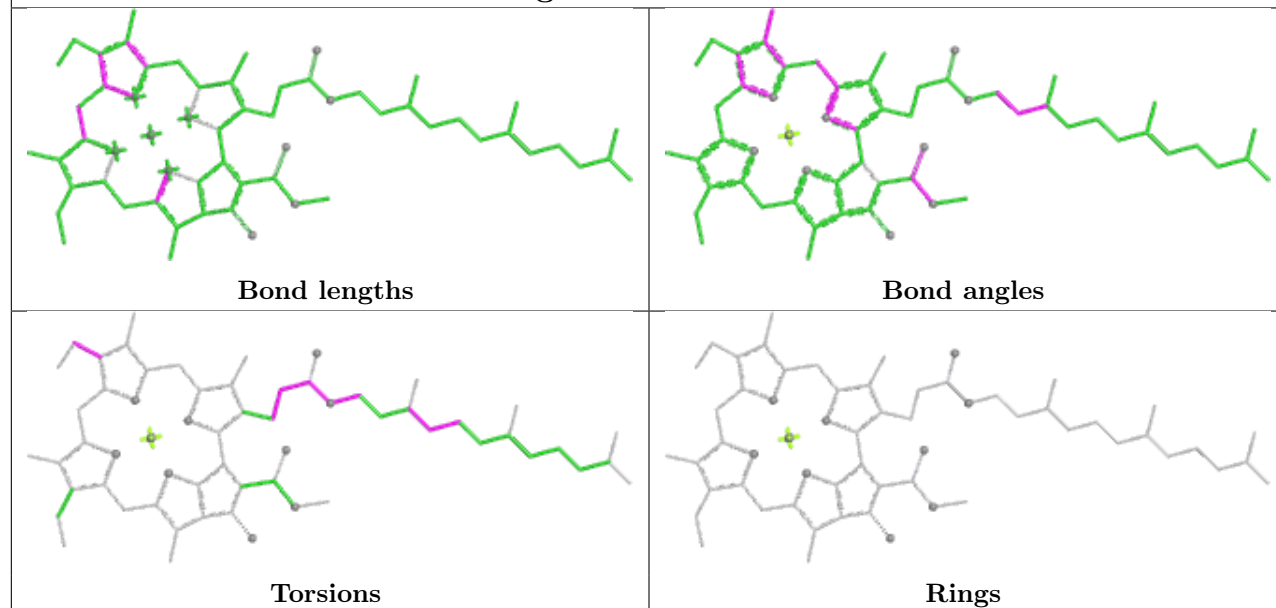
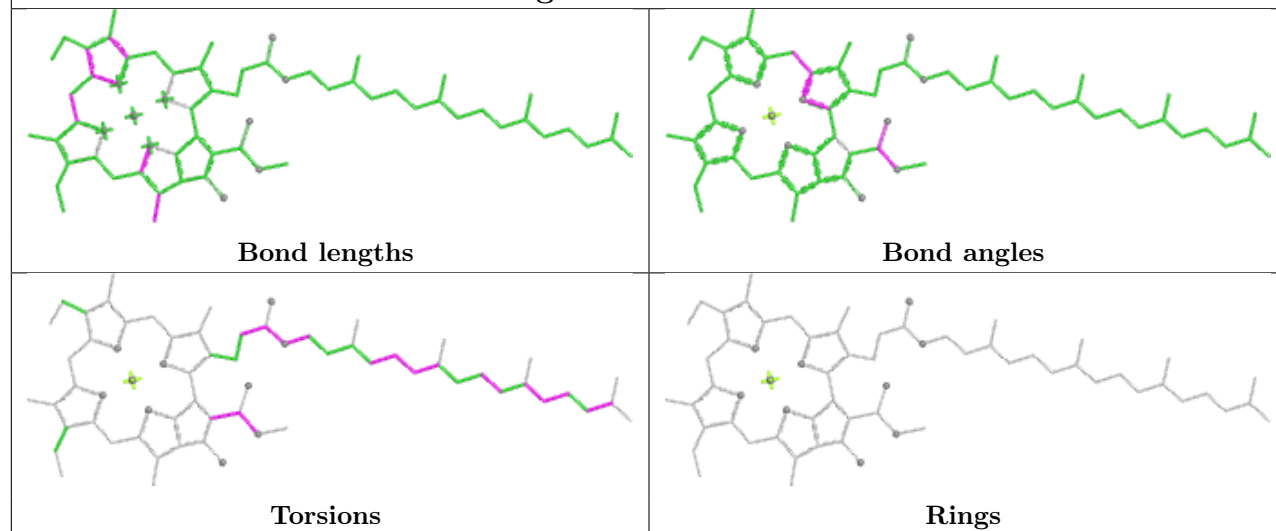
Bond angles

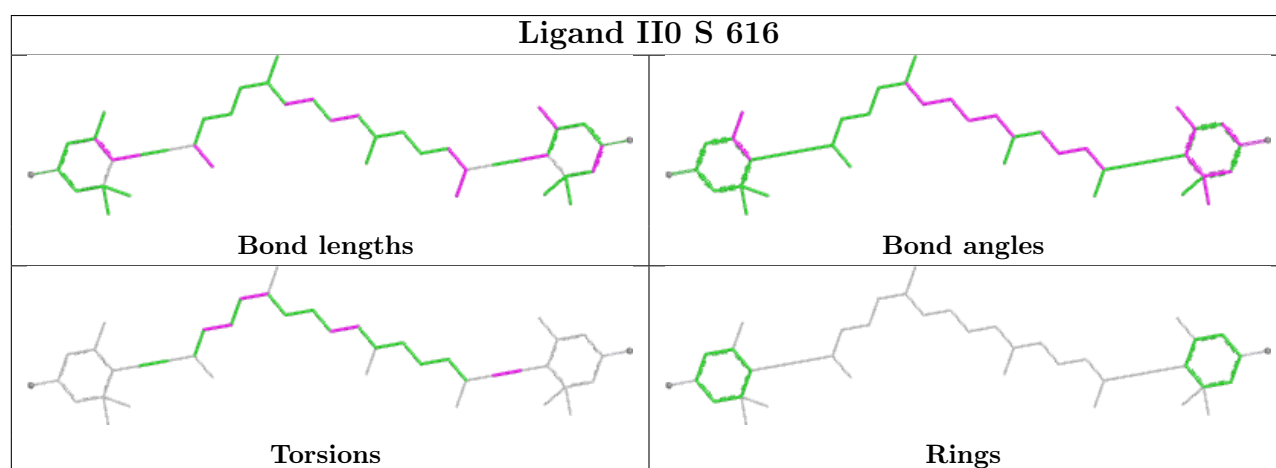
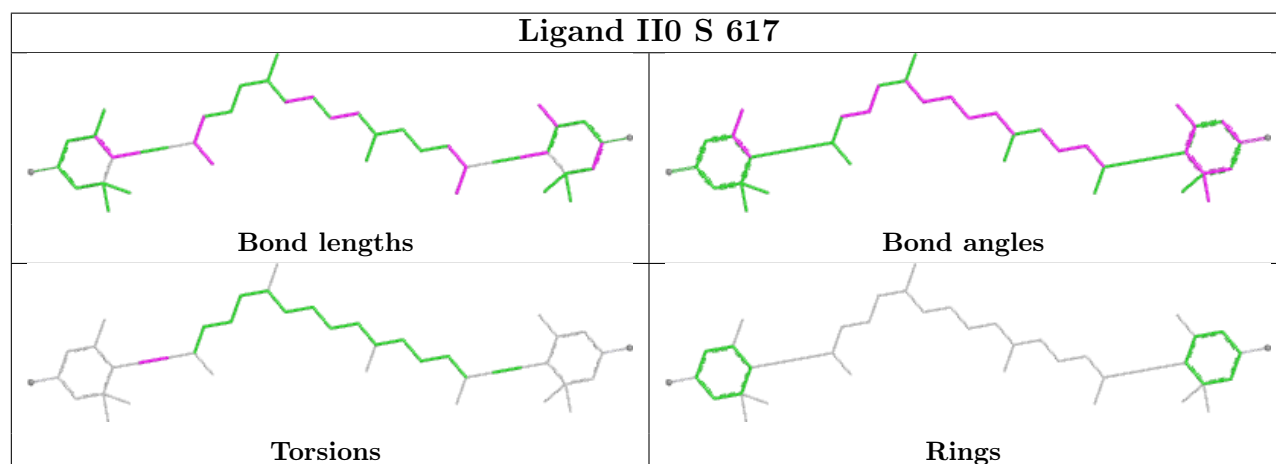
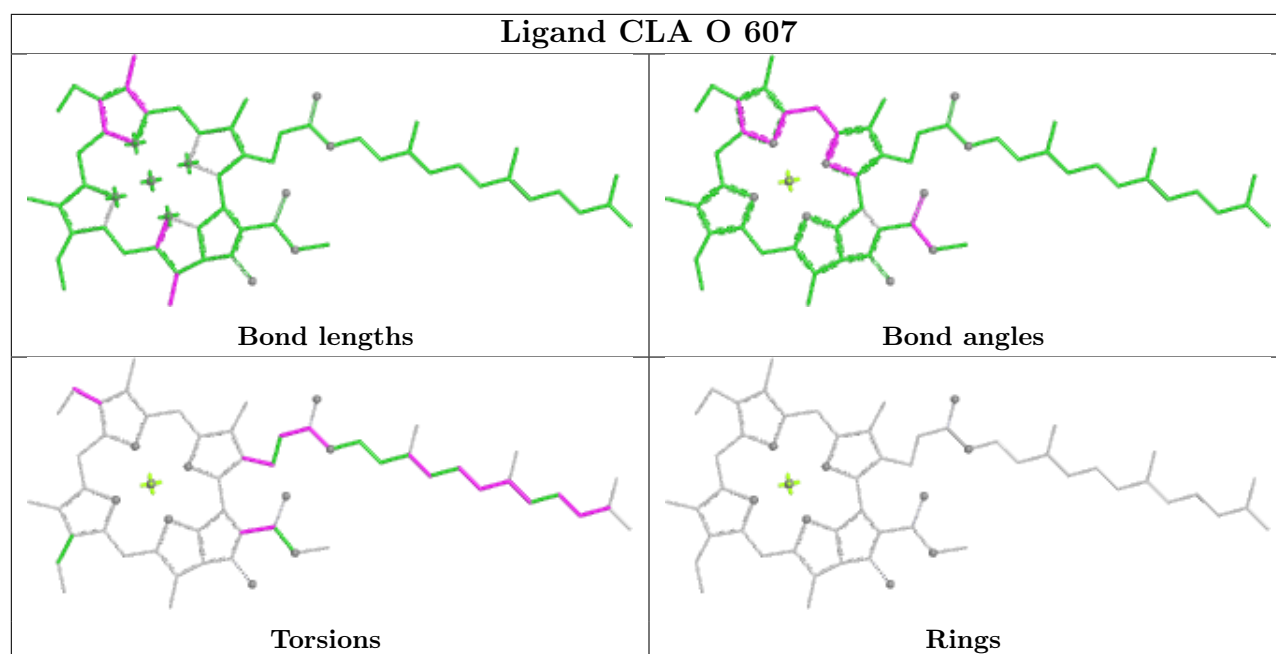


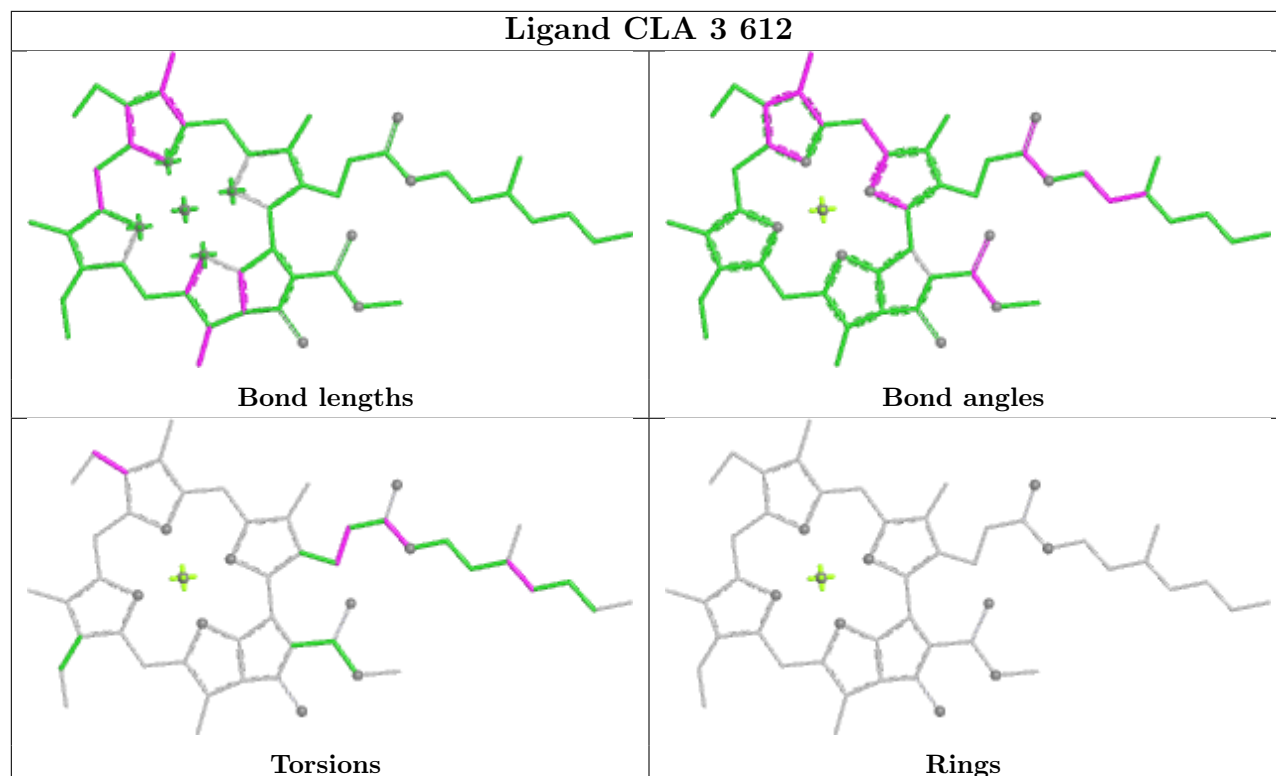
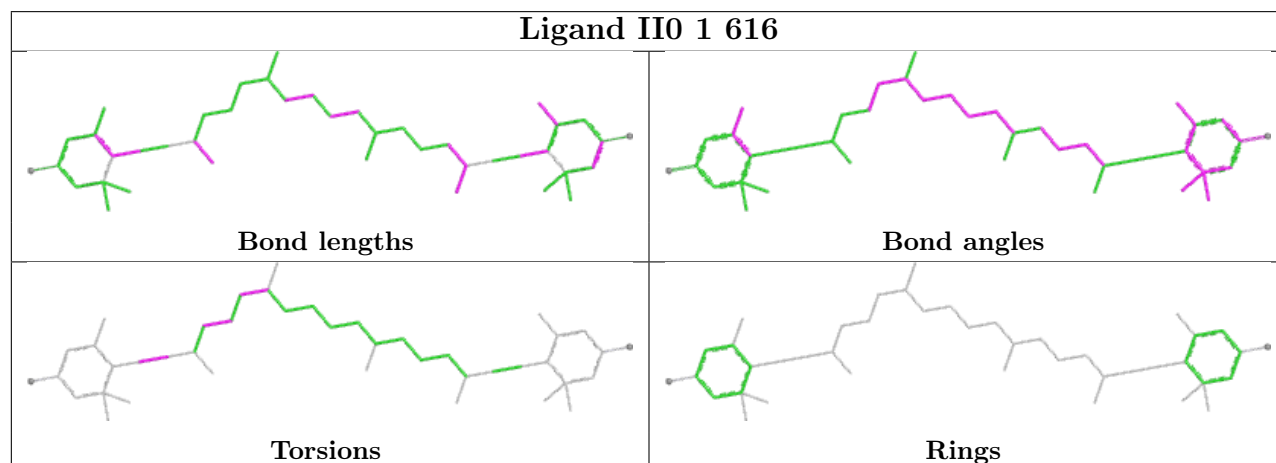
Torsions



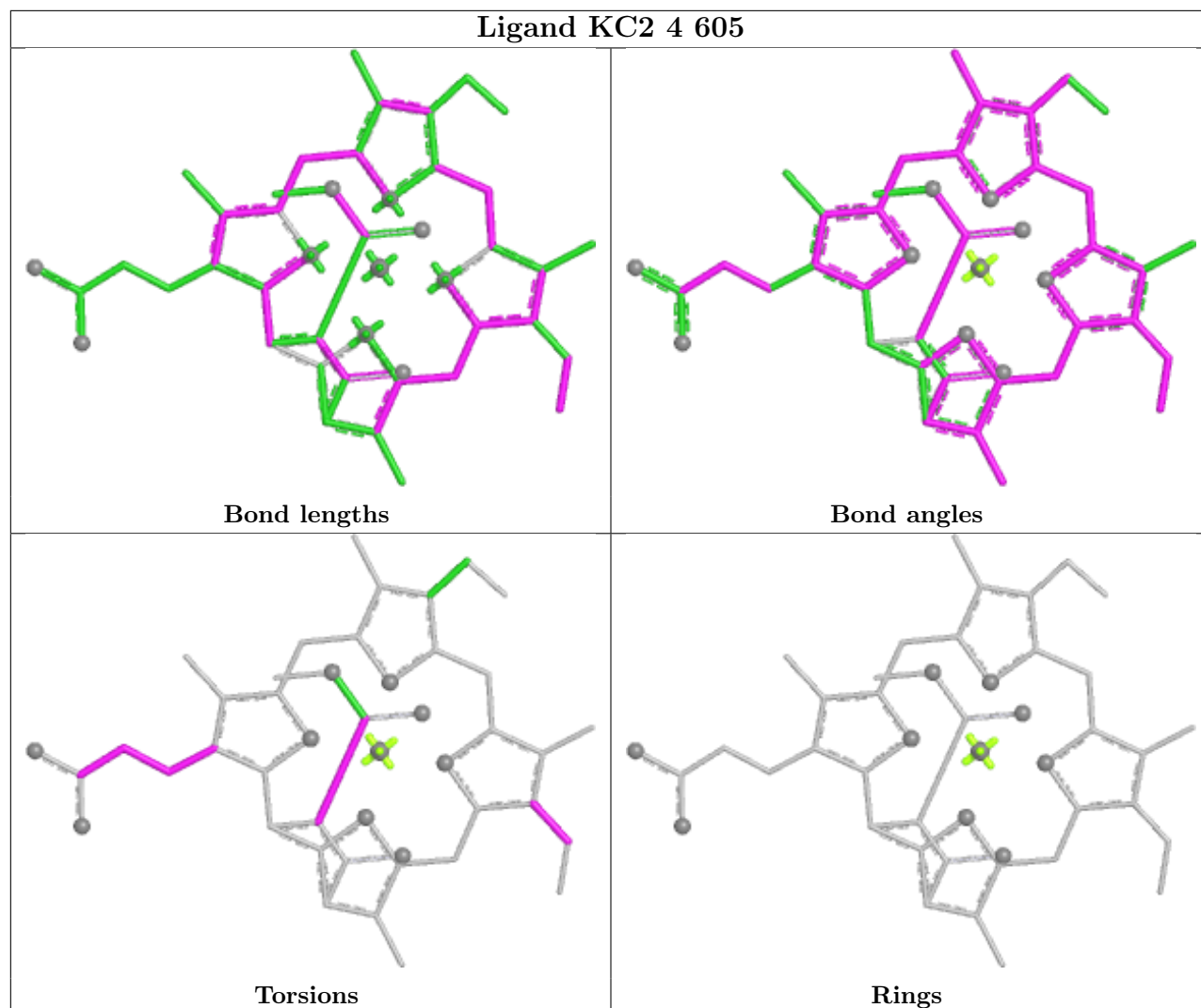
Rings

Ligand CLA 1 603**Ligand CLA 5 611**

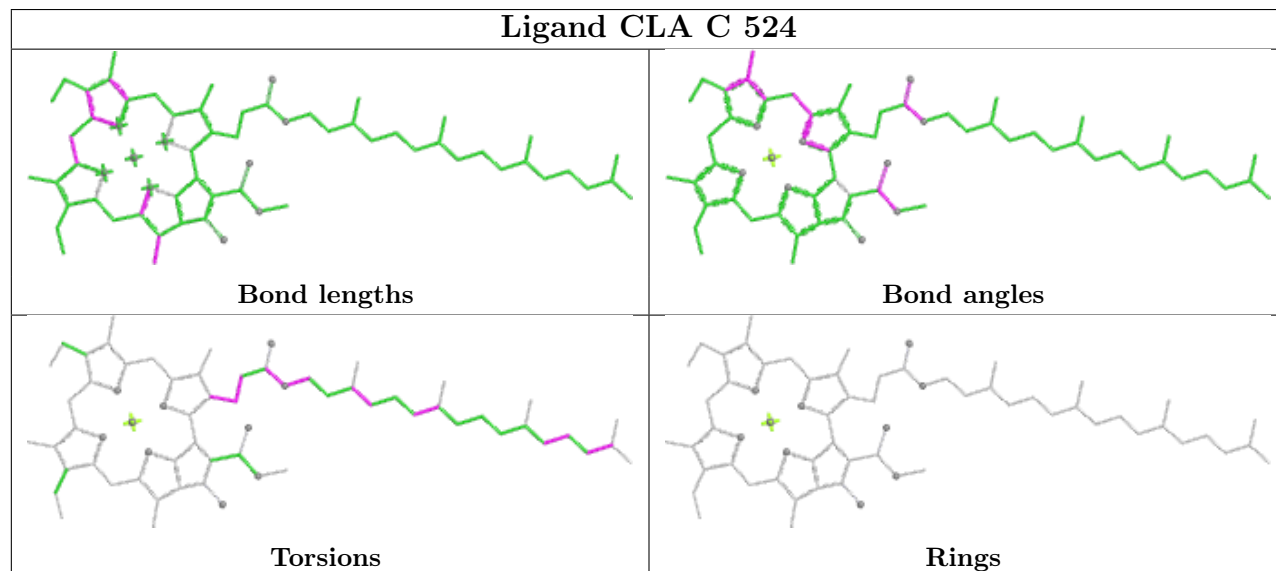


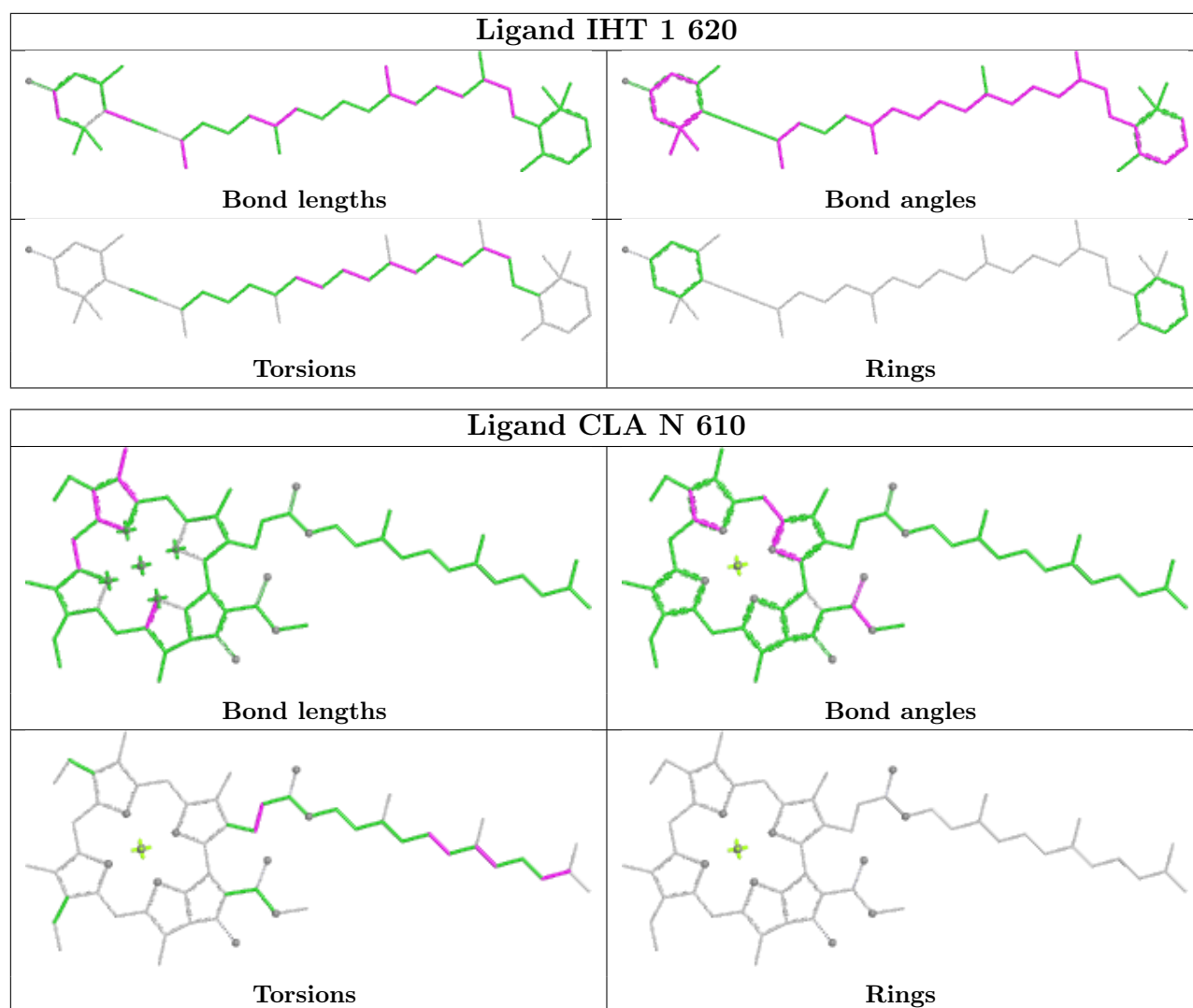
Ligand CLA 3 612**Ligand II0 1 616**

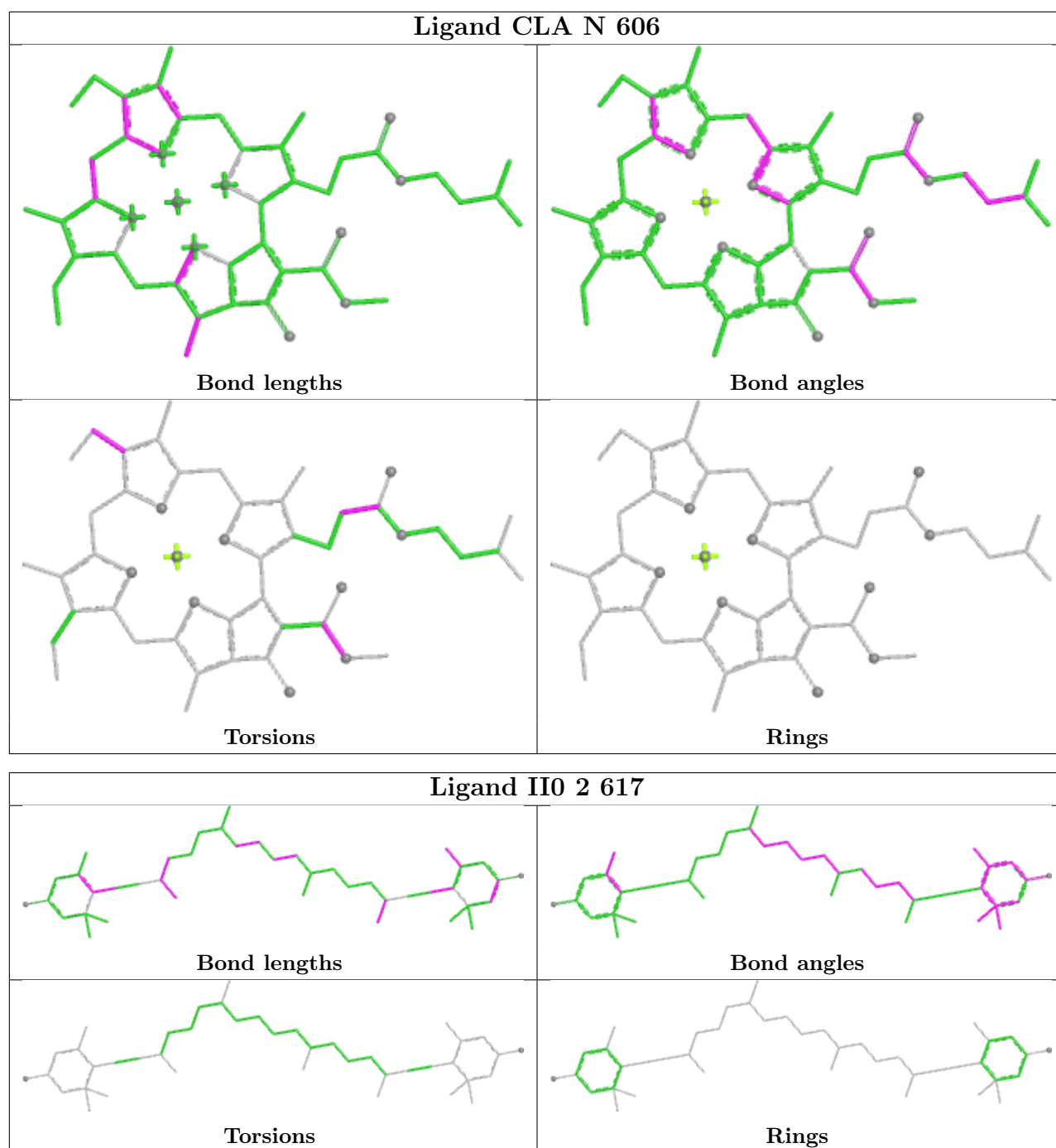
Ligand KC2 4 605



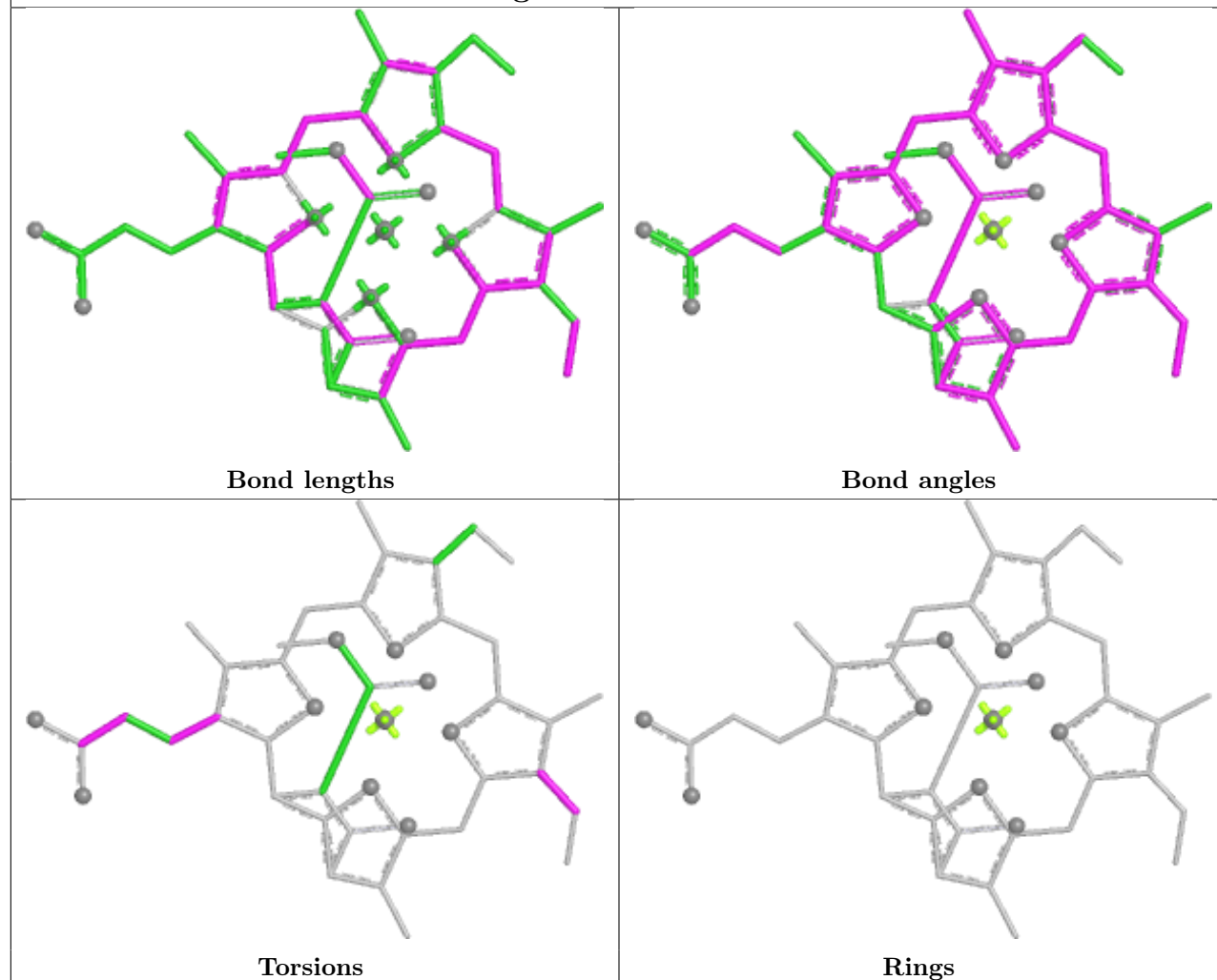
Ligand CLA C 524



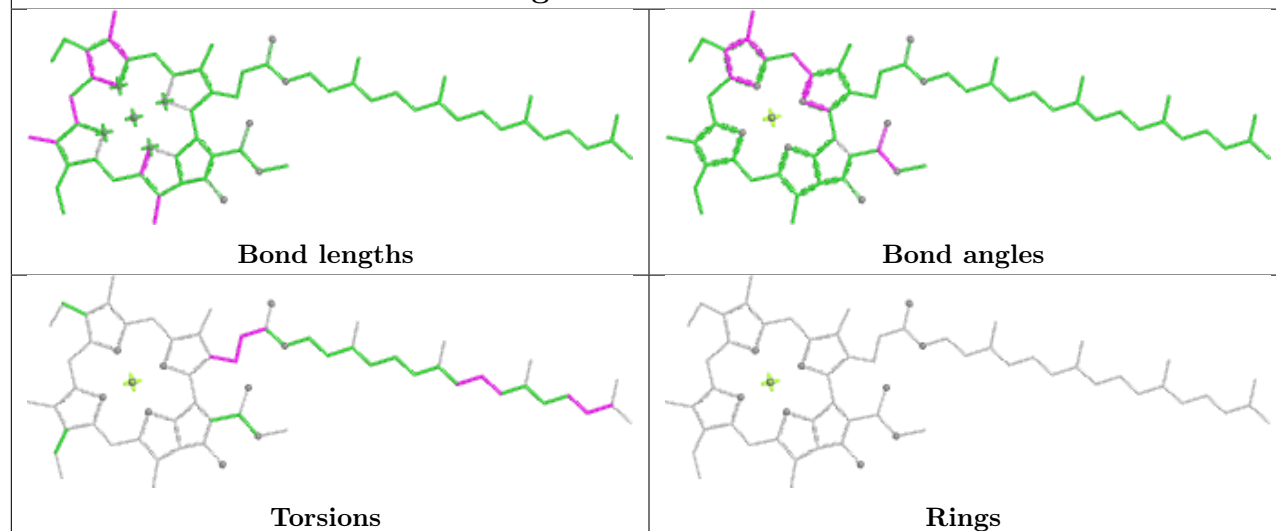


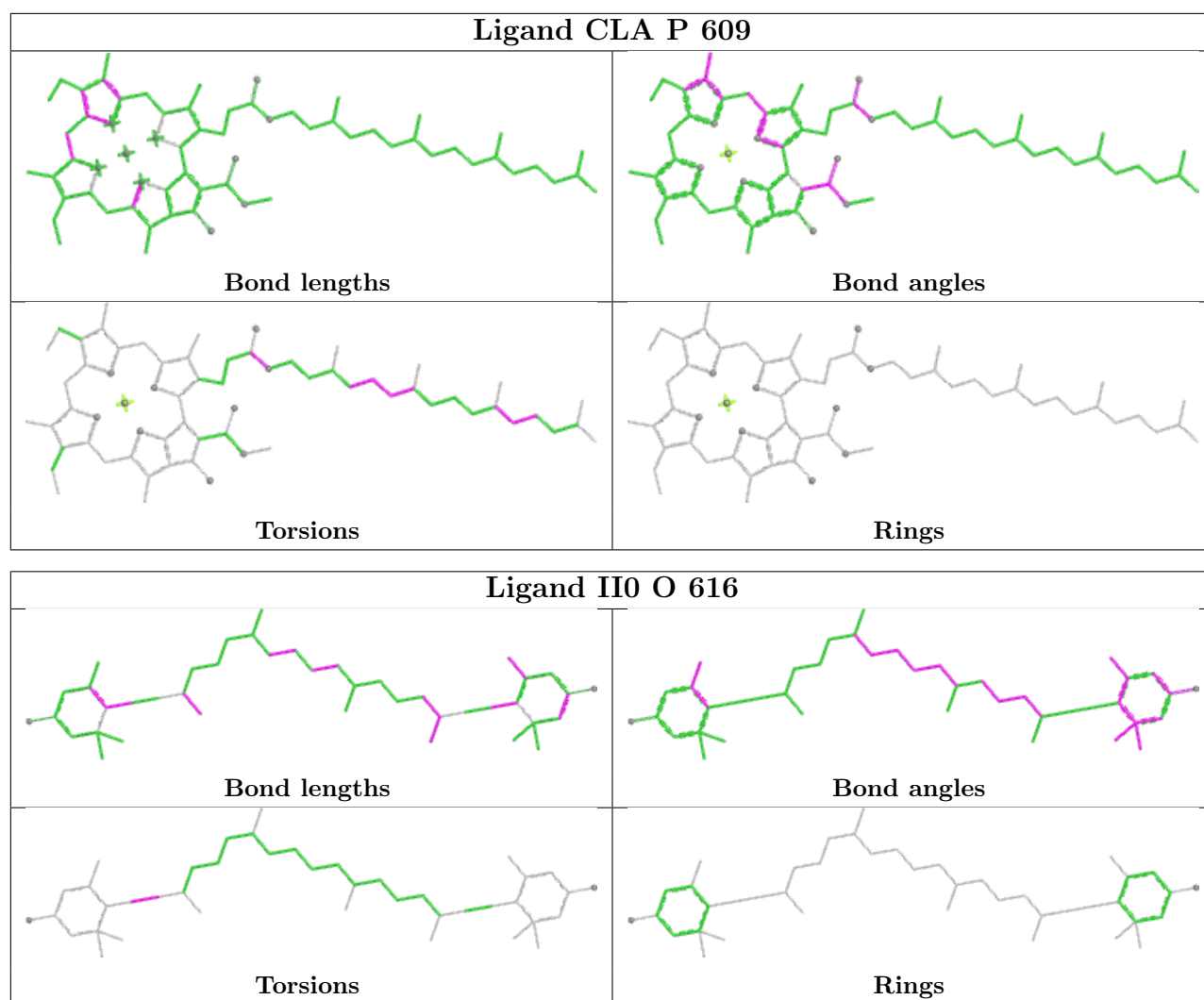


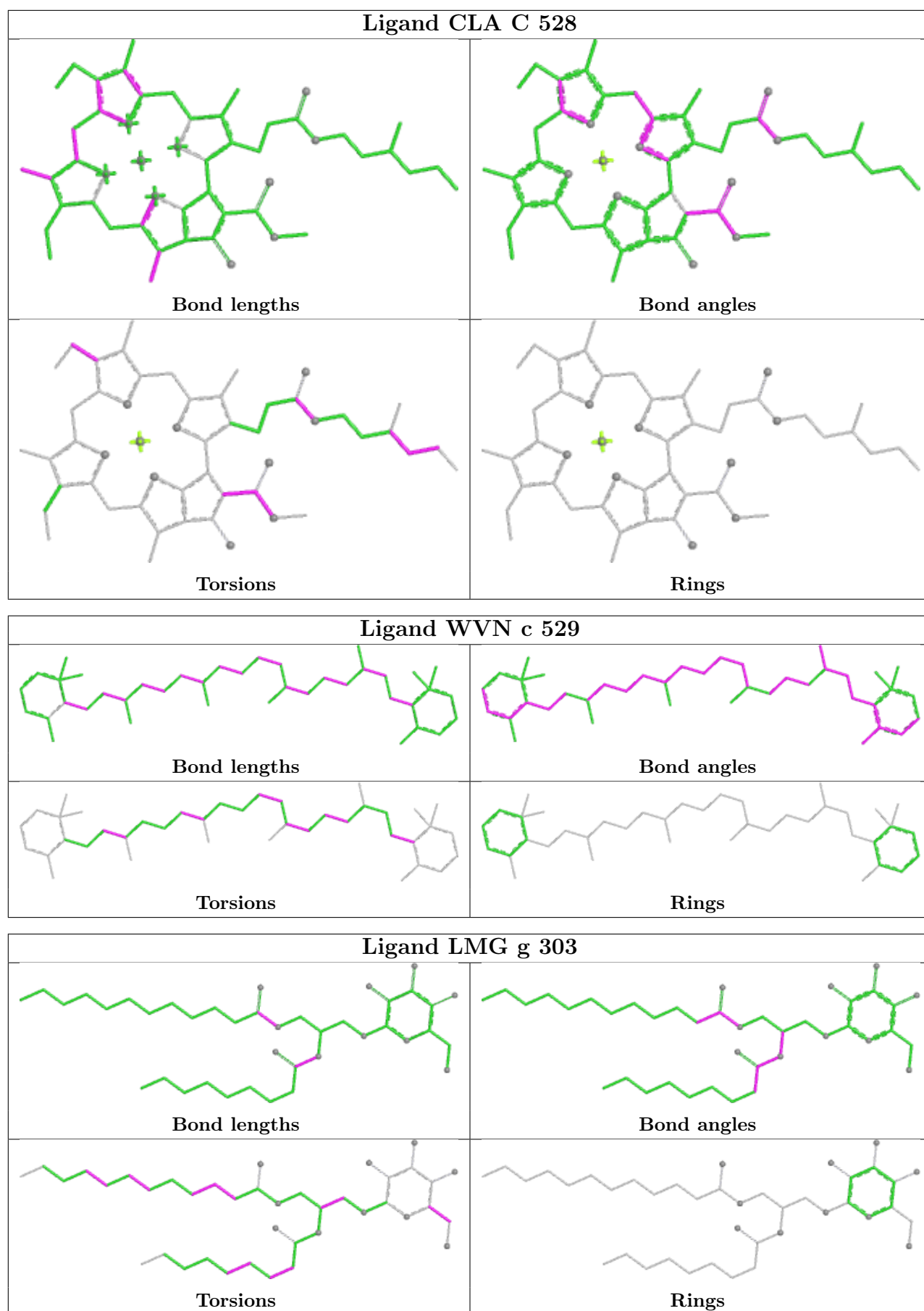
Ligand KC2 6 612



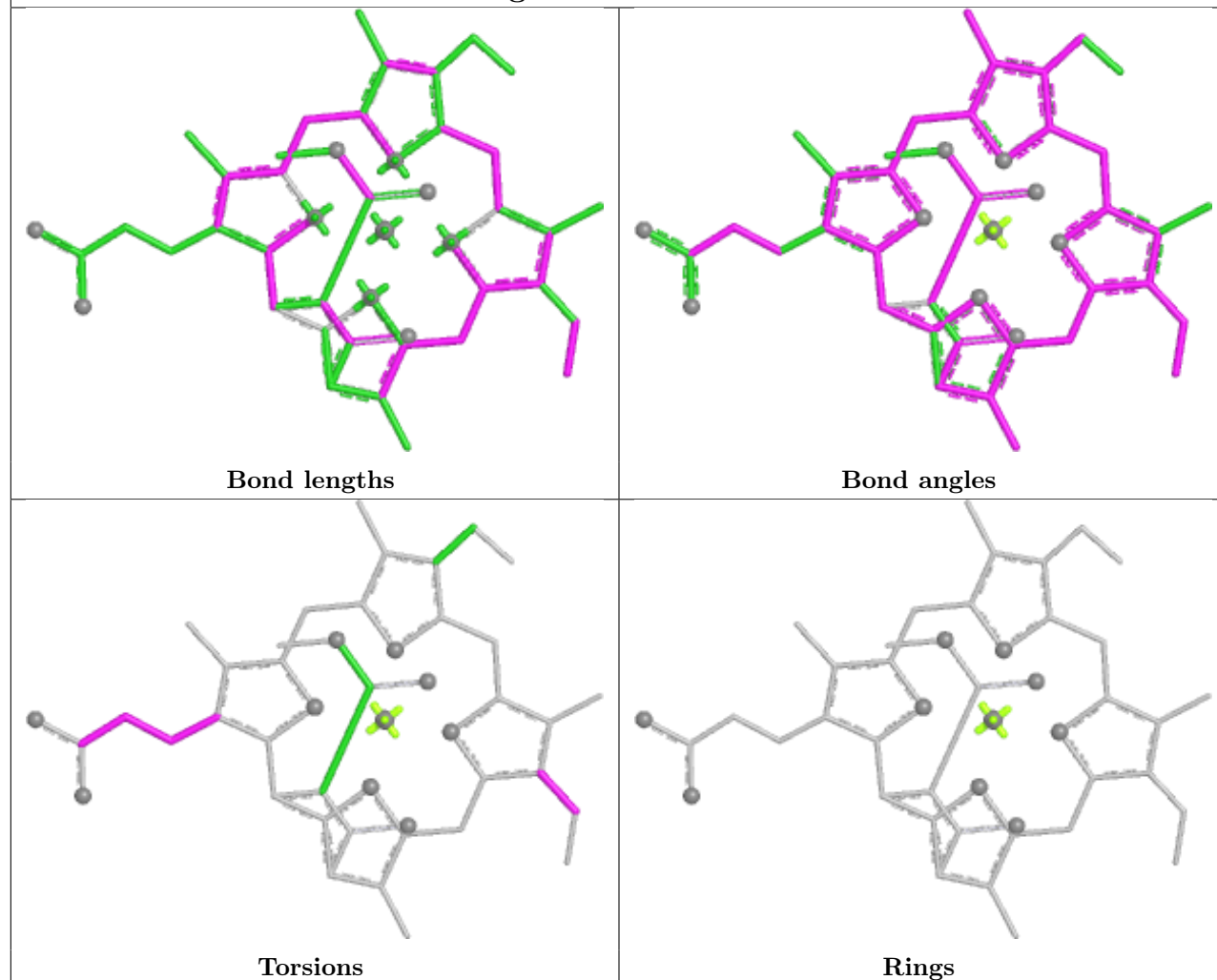
Ligand CLA O 603



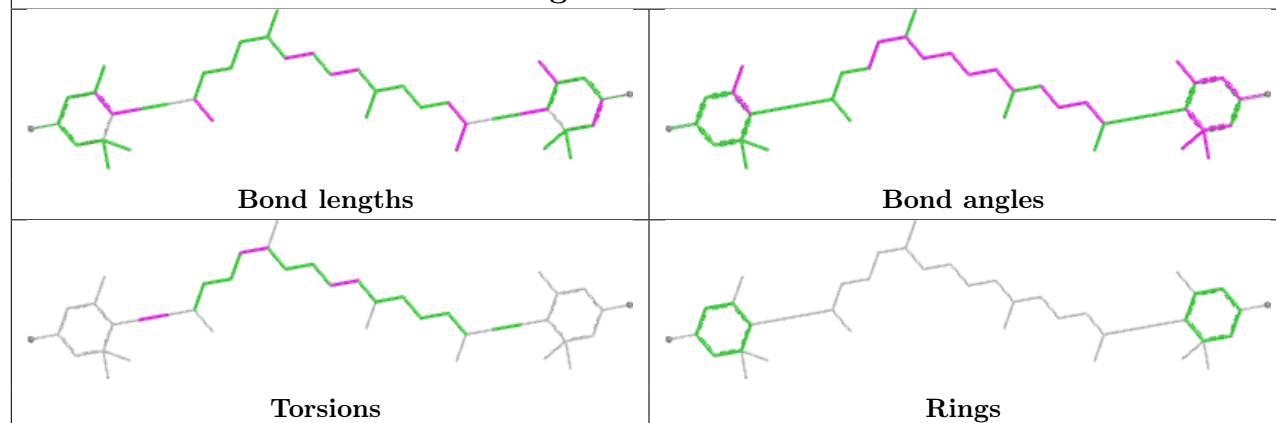


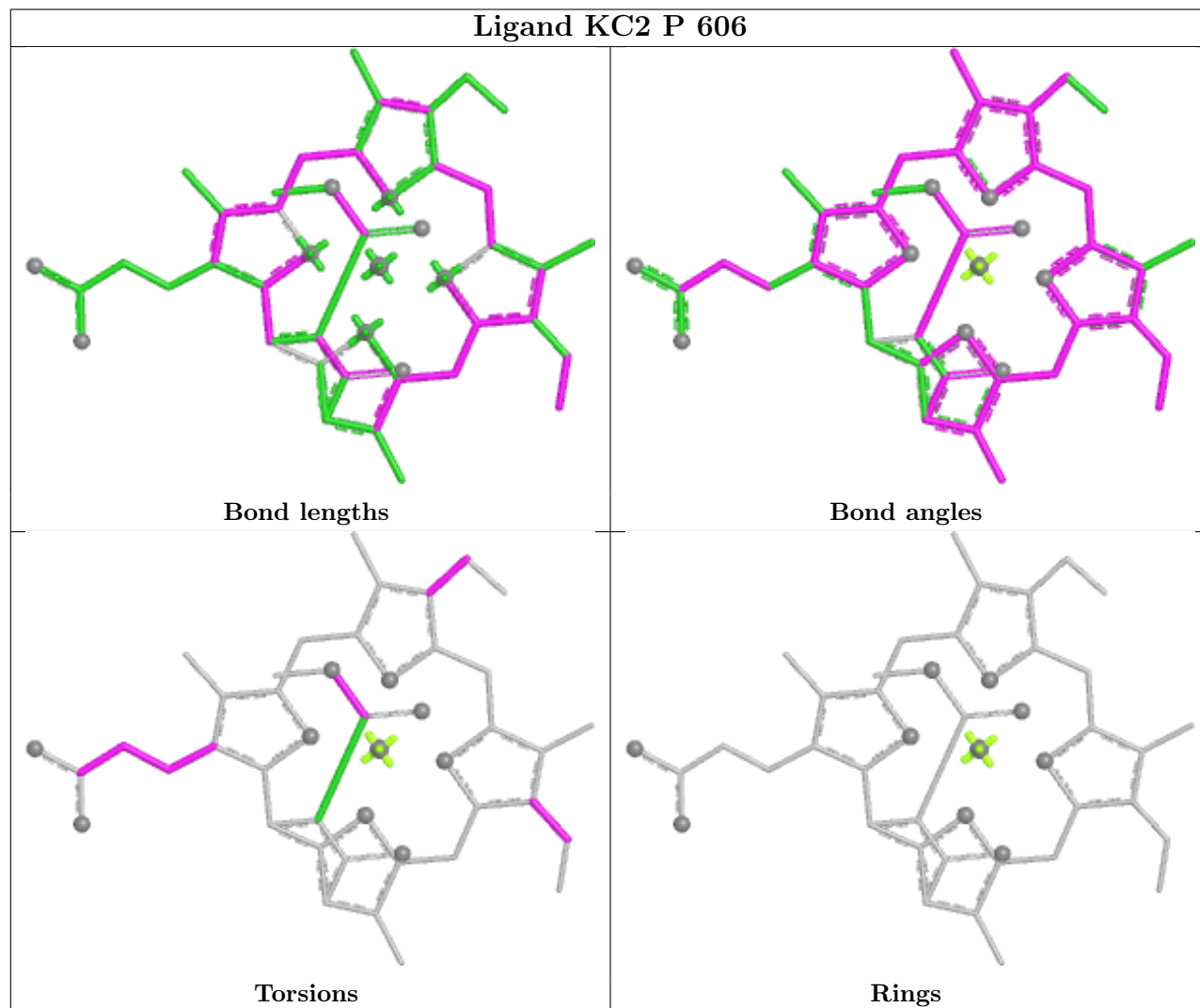
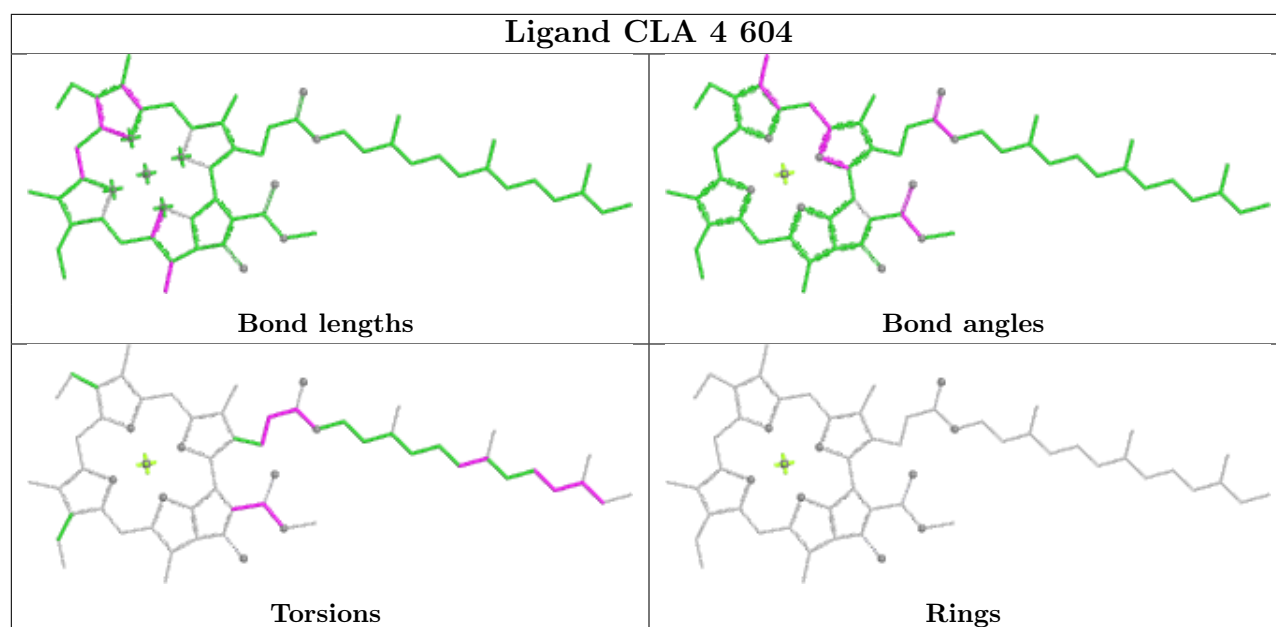


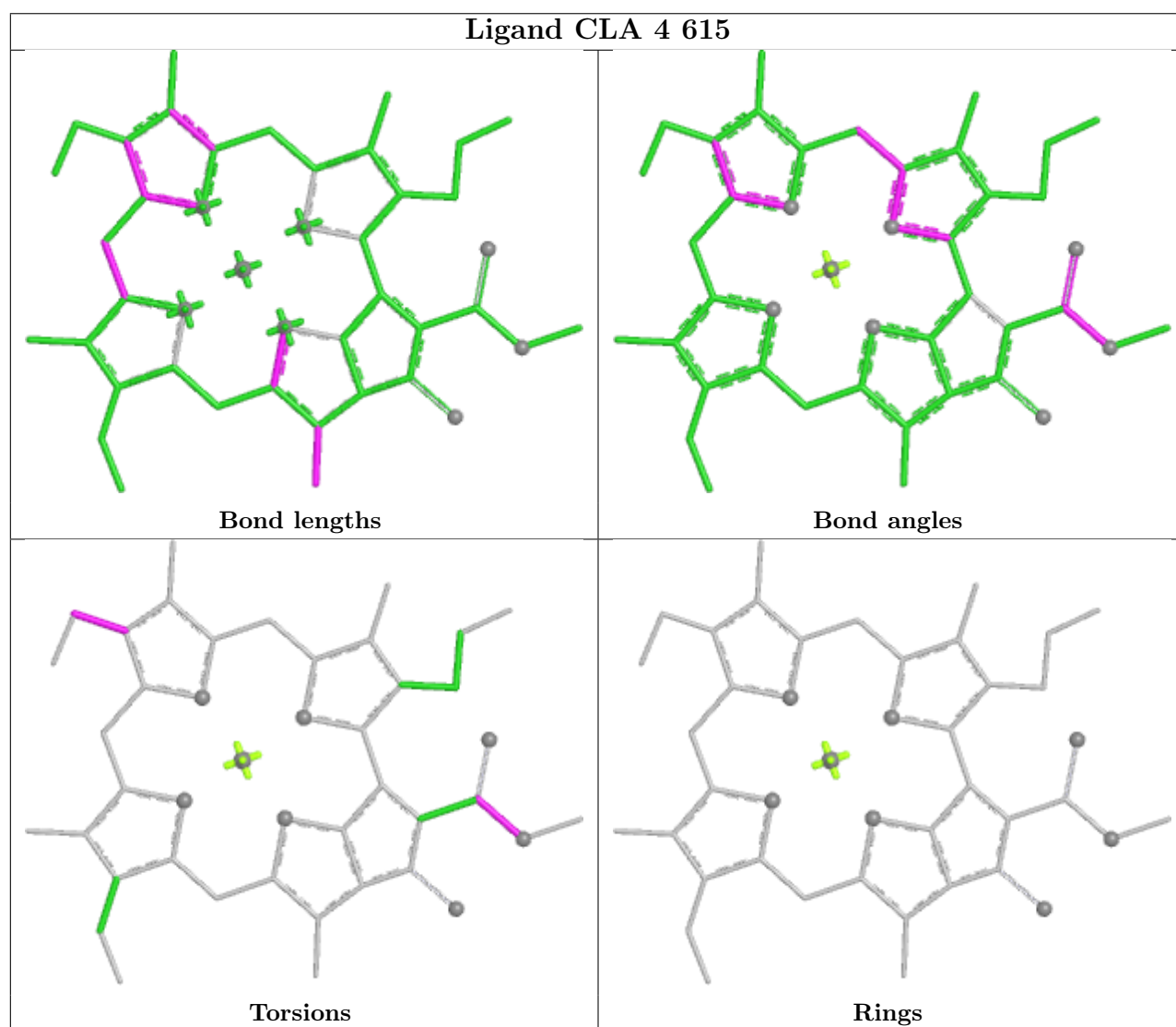
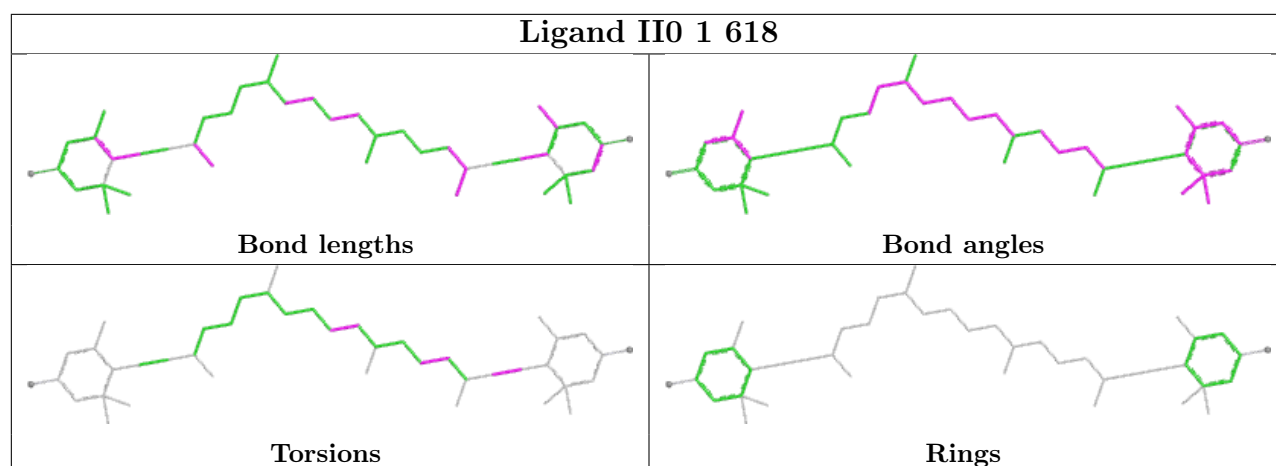
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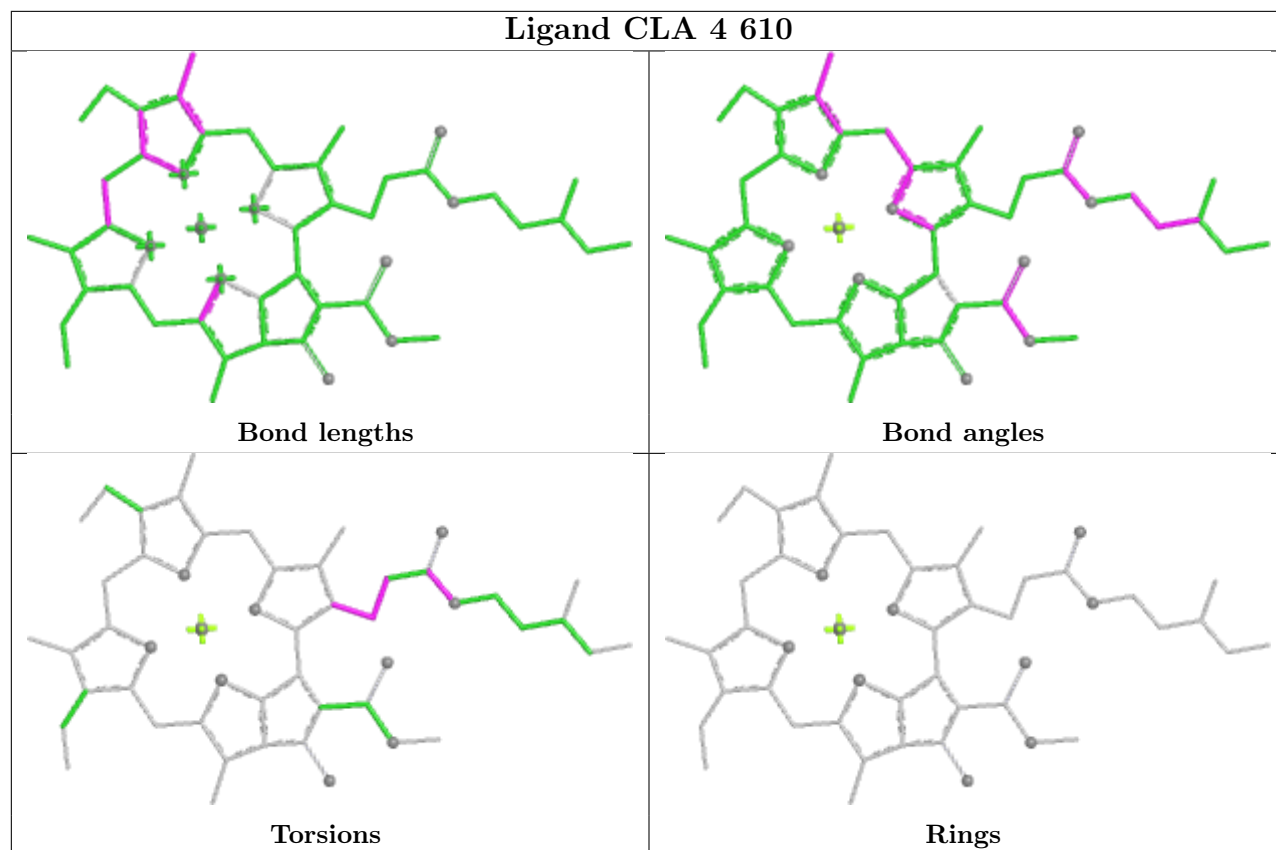
Ligand II0 S 619



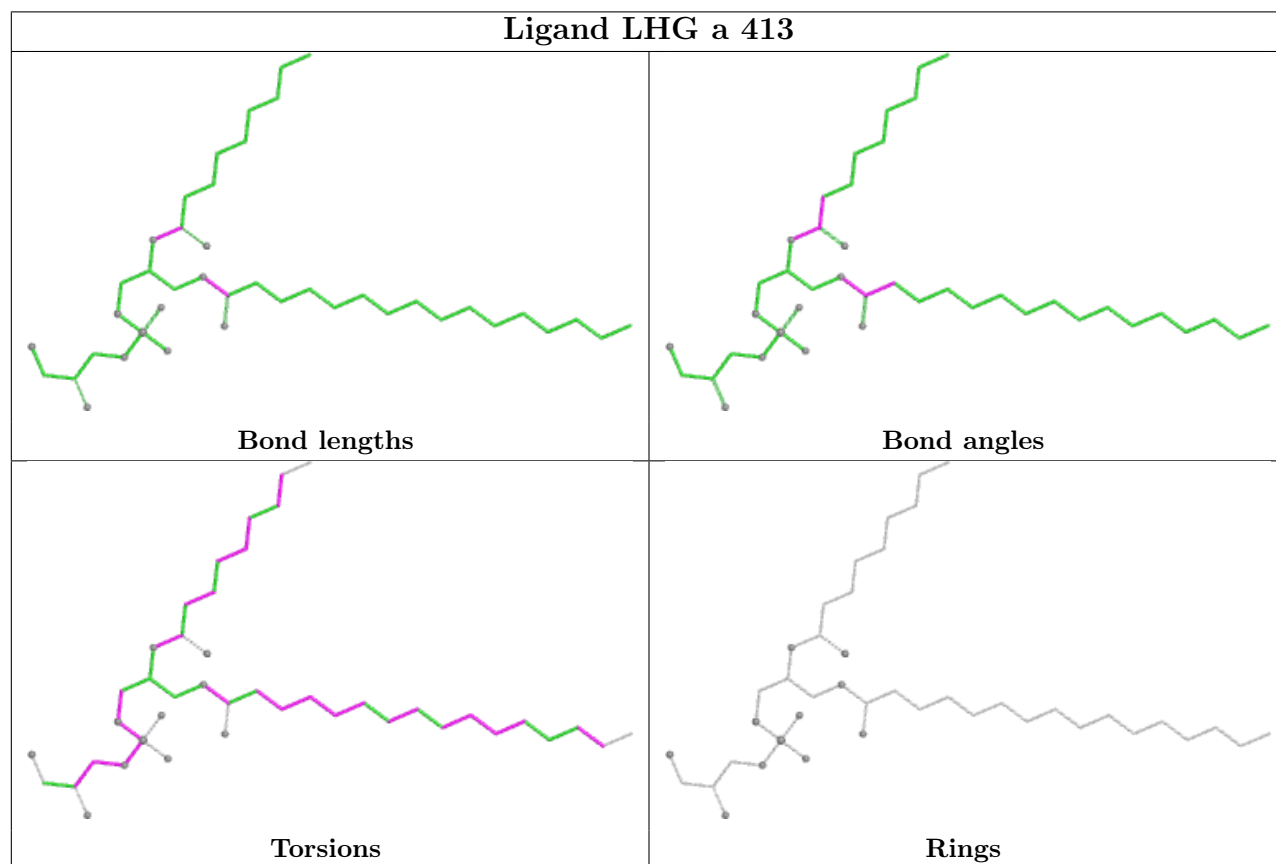


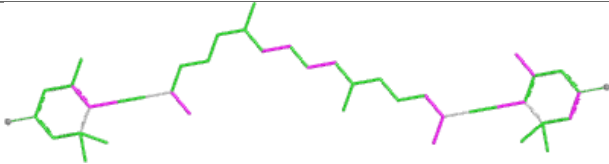
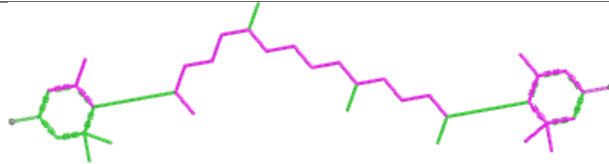
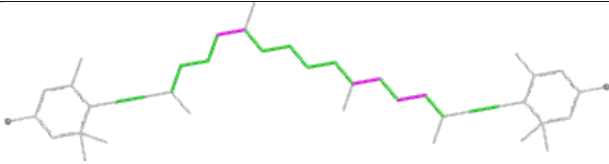
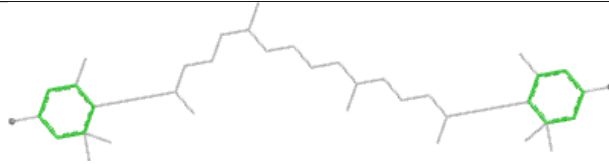


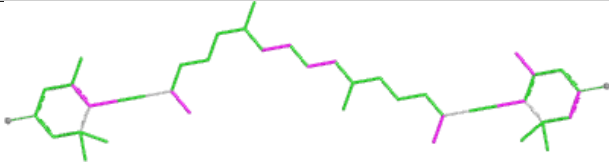
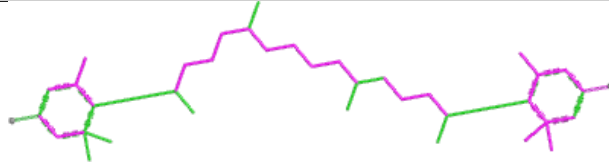
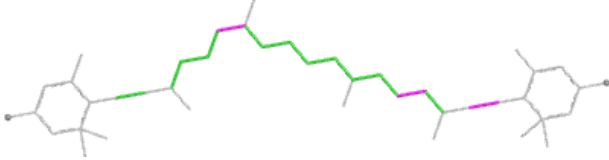
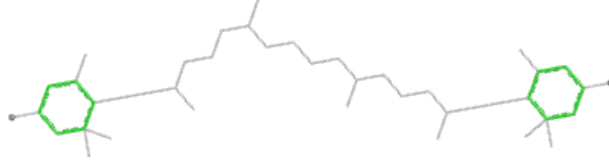
Ligand CLA 4 610

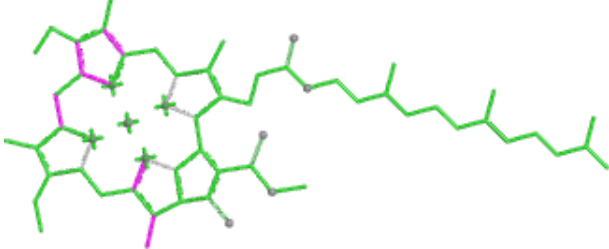
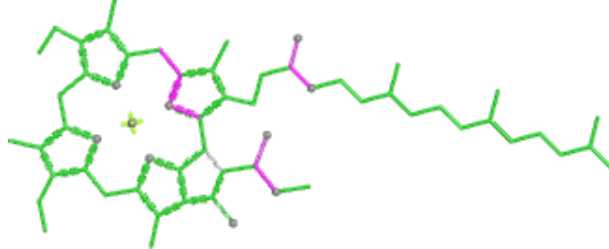
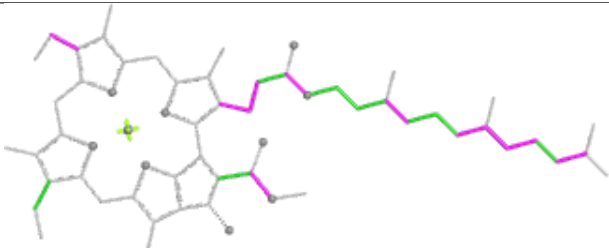
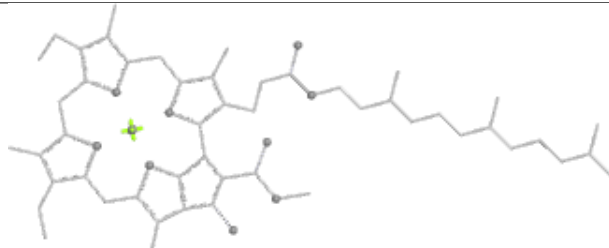


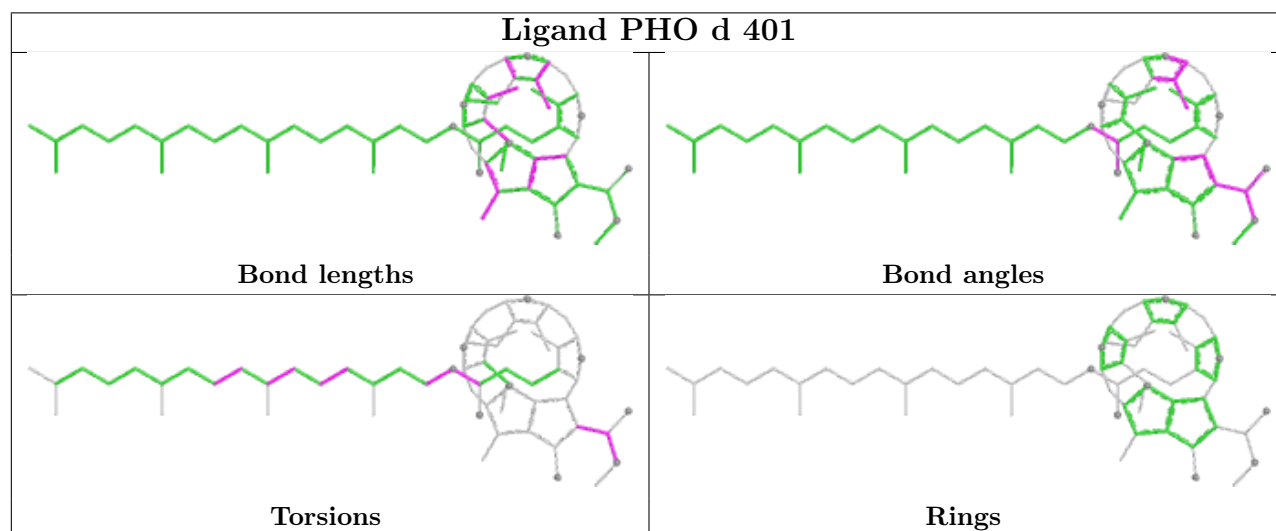
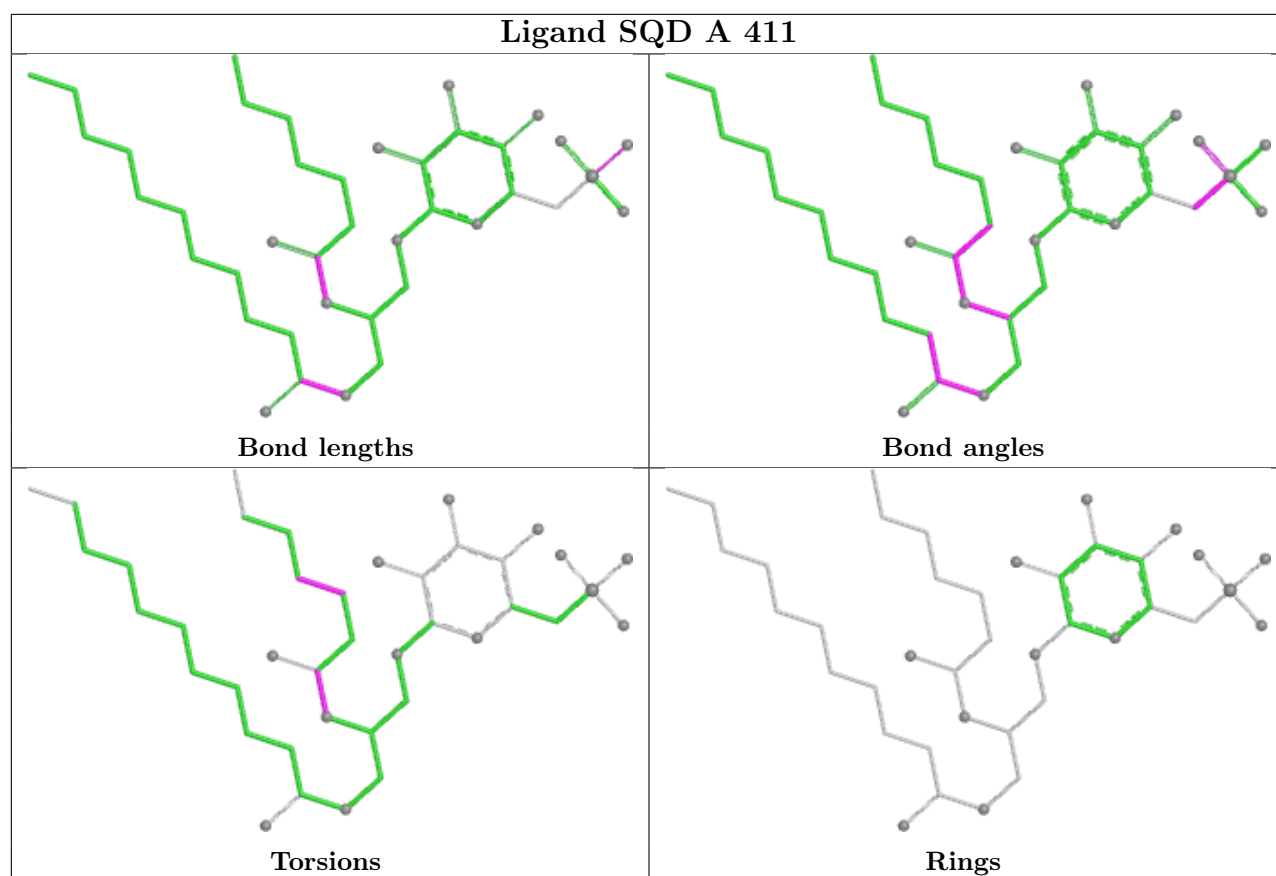
Ligand LHG a 413

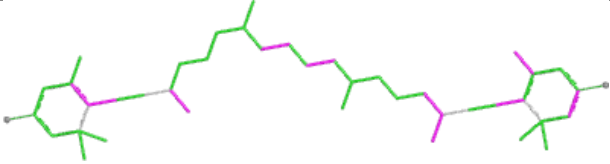
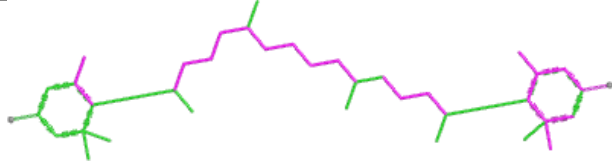
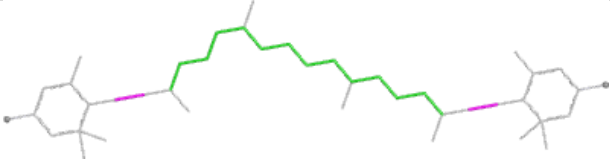
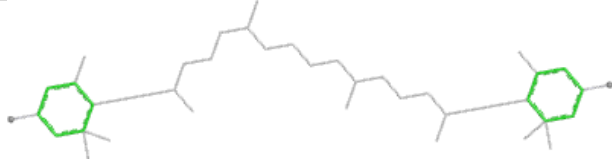
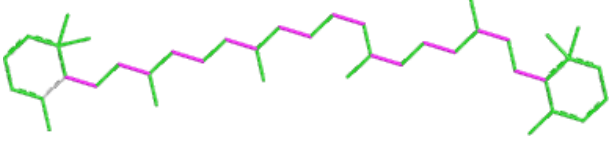
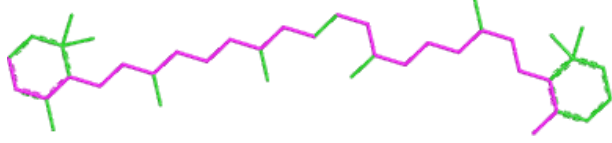
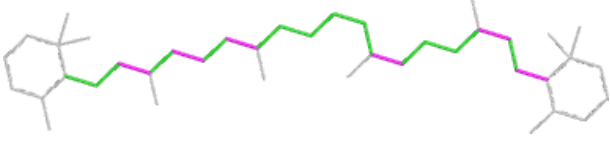
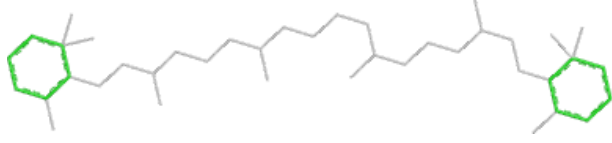
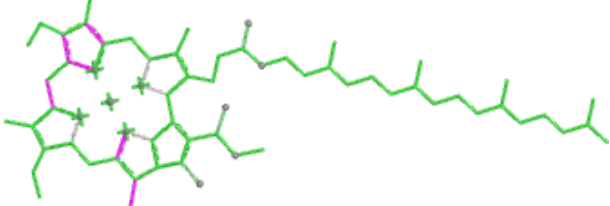
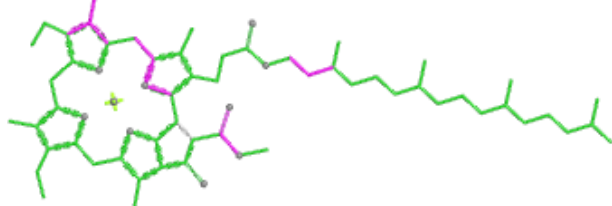
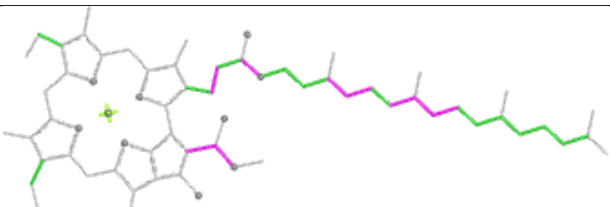
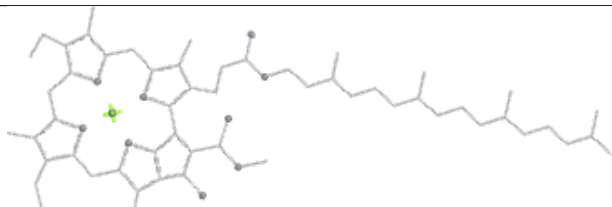


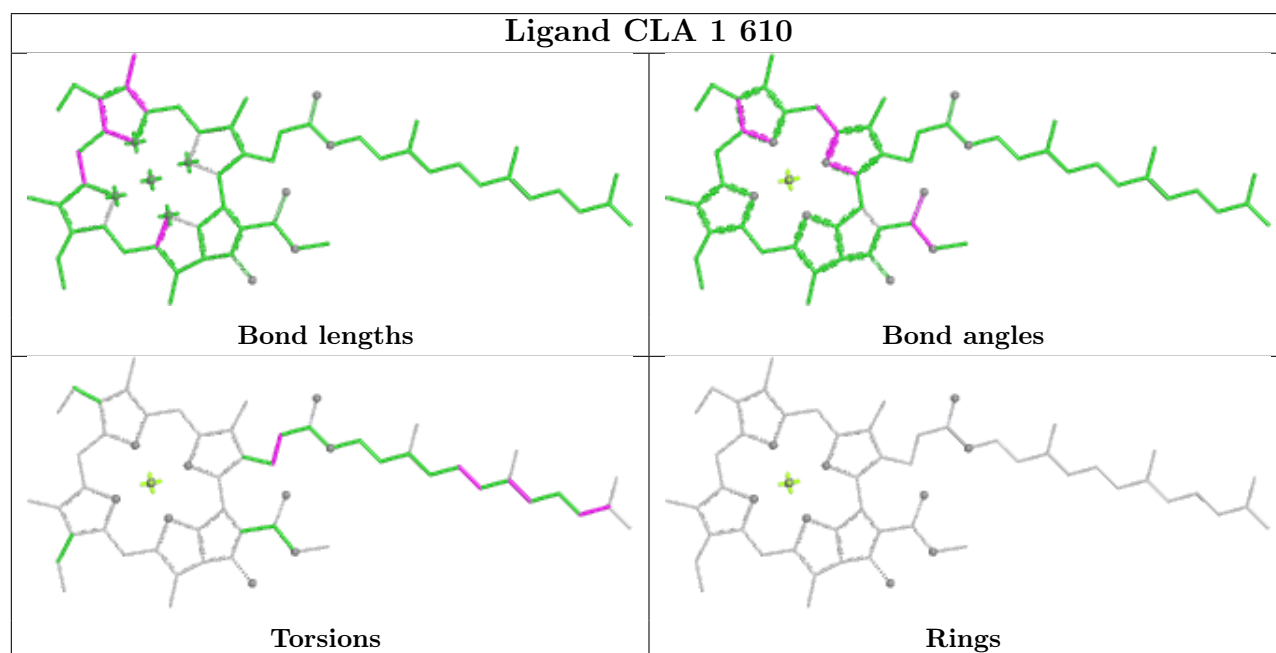
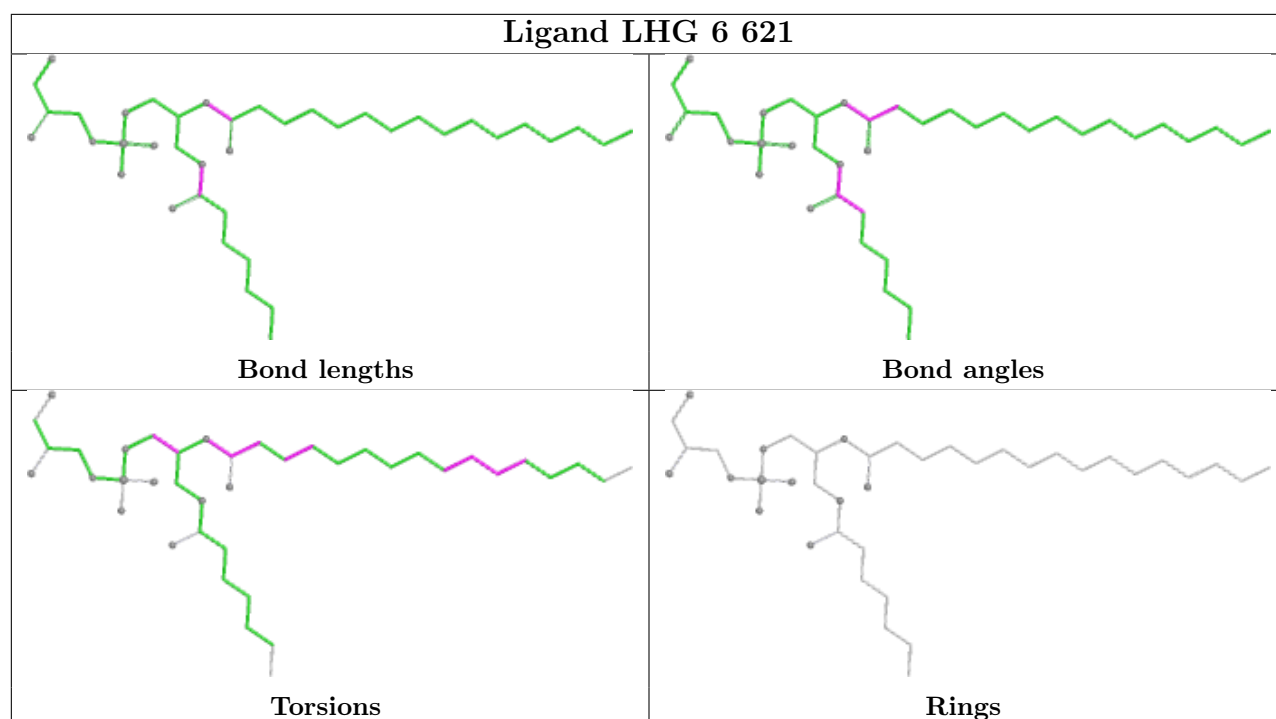
Ligand II0 2 619	
	
Bond lengths	Bond angles
	
Torsions	Rings

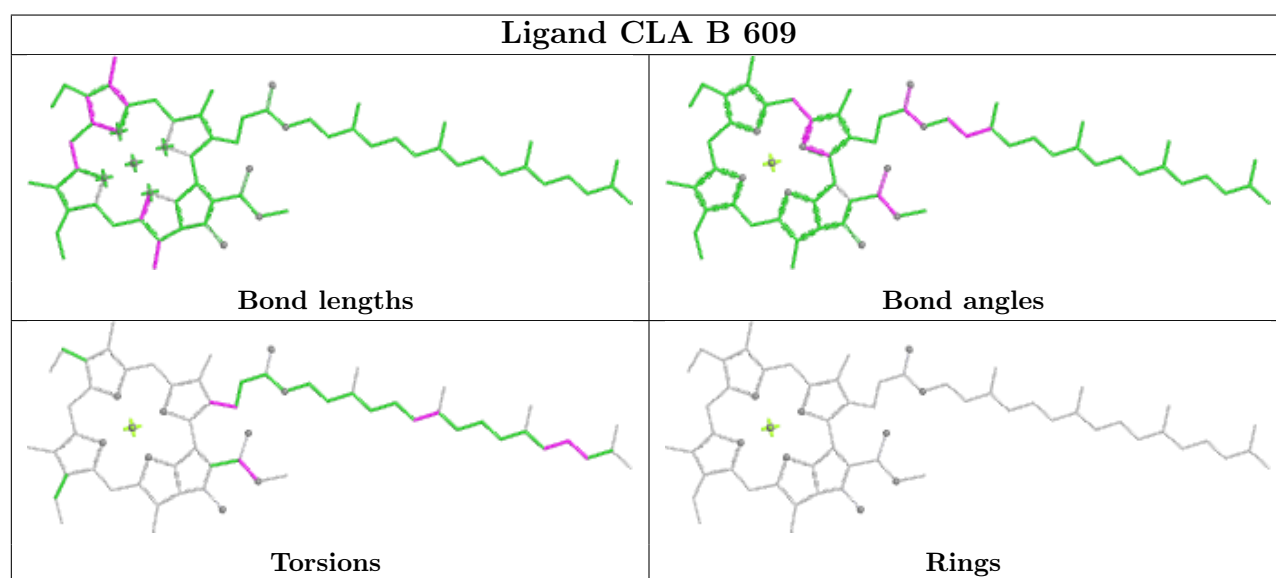
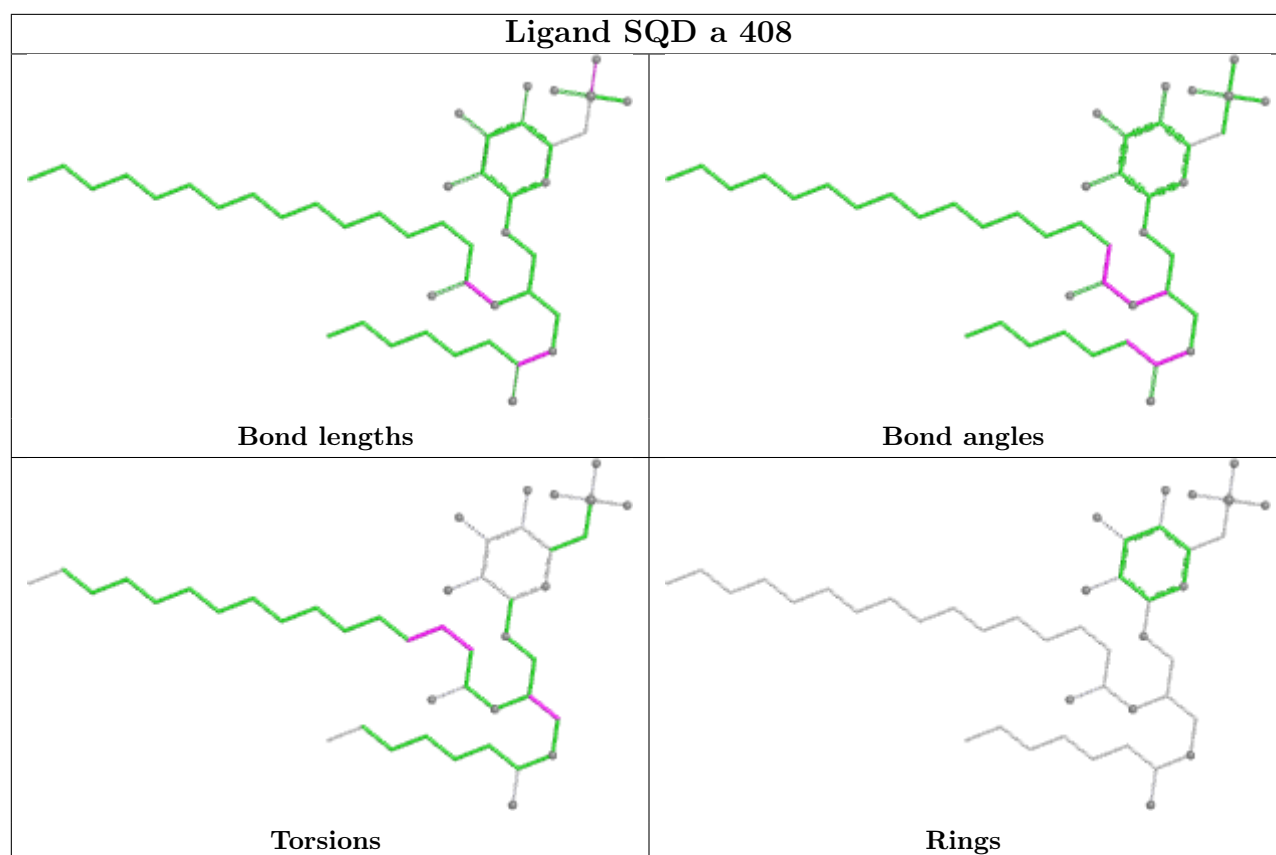
Ligand II0 6 618	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA 2 611	
	
Bond lengths	Bond angles
	
Torsions	Rings

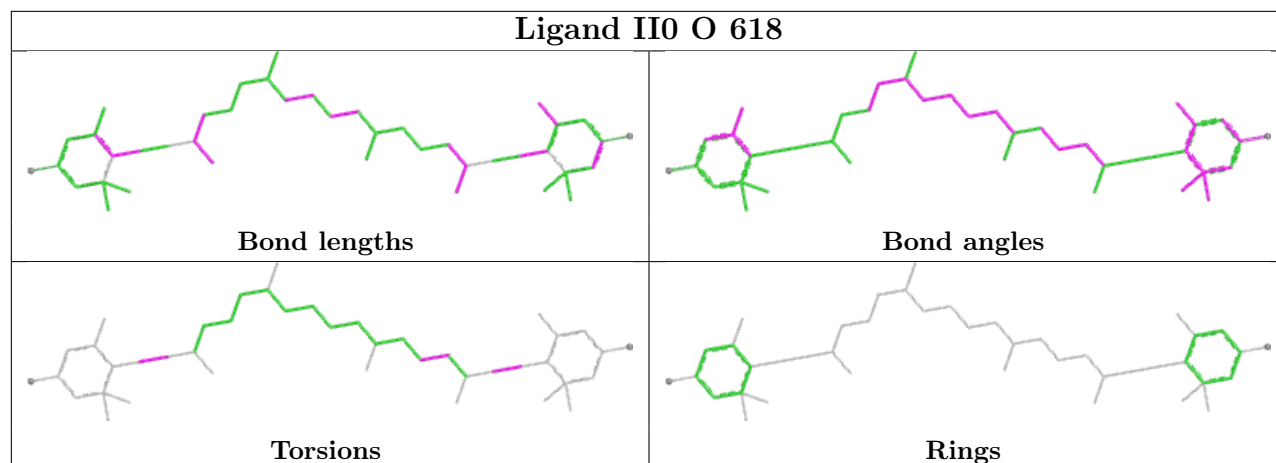


Ligand II0 Q 618	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand WVN B 618	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CLA C 525	
 Bond lengths	 Bond angles
 Torsions	 Rings

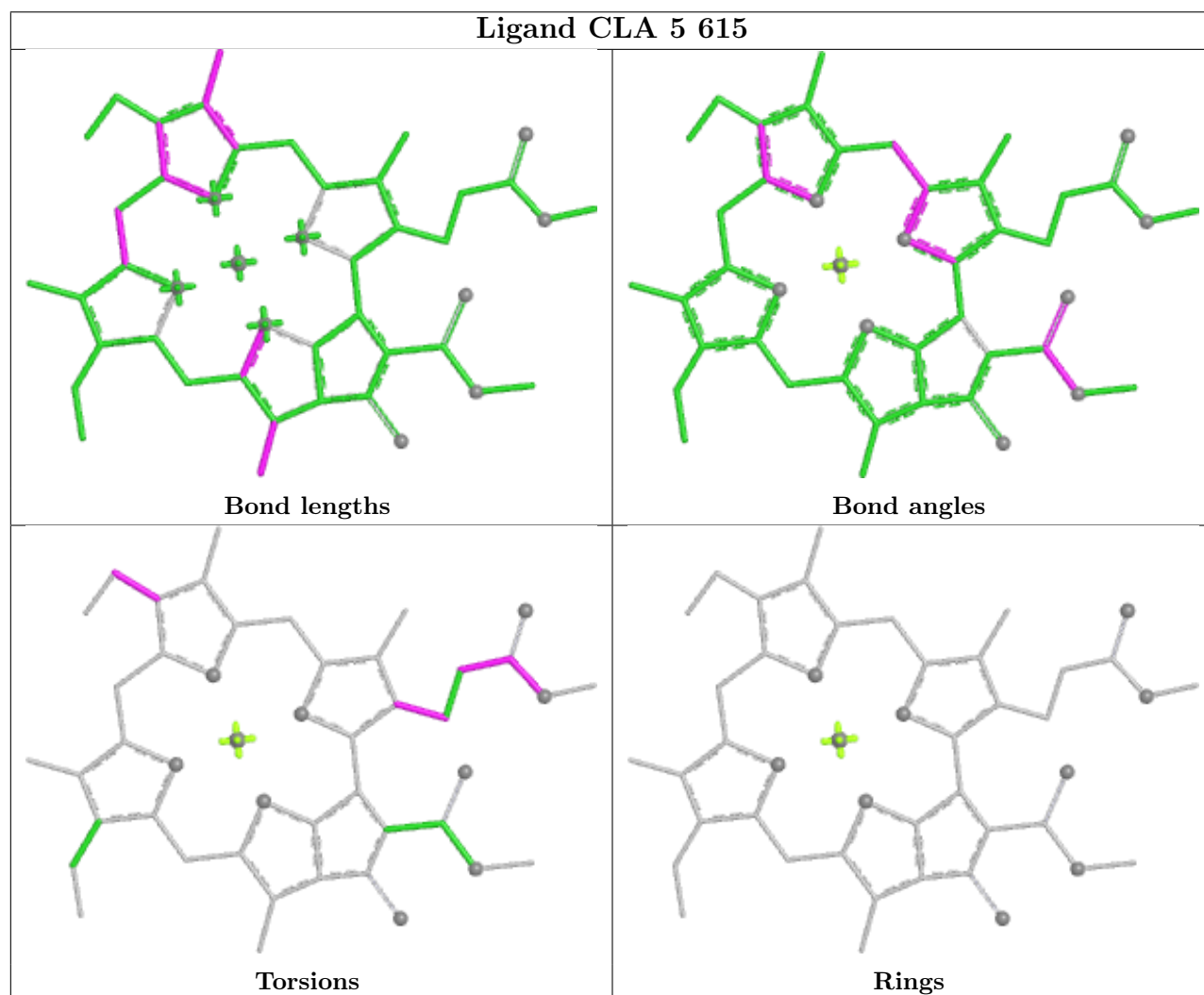




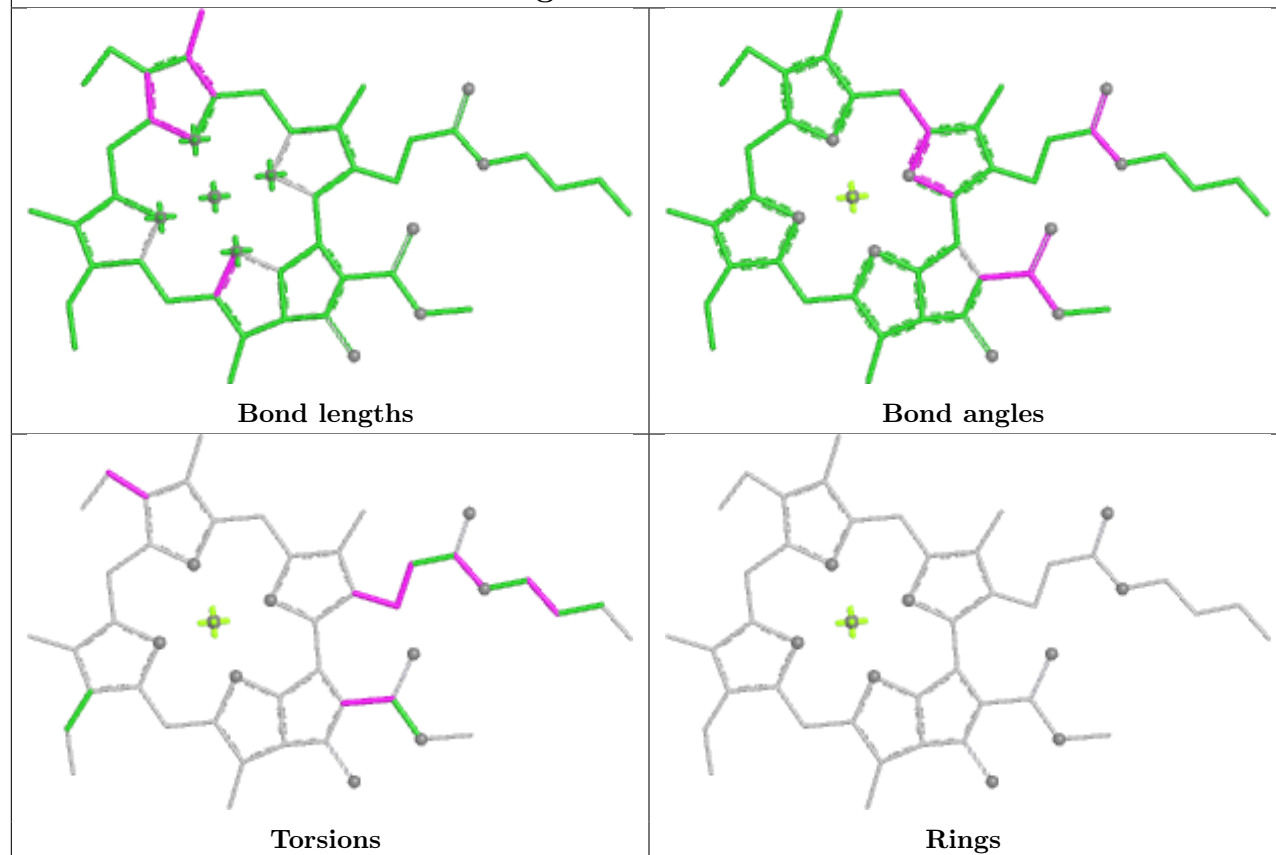
Ligand II0 O 618



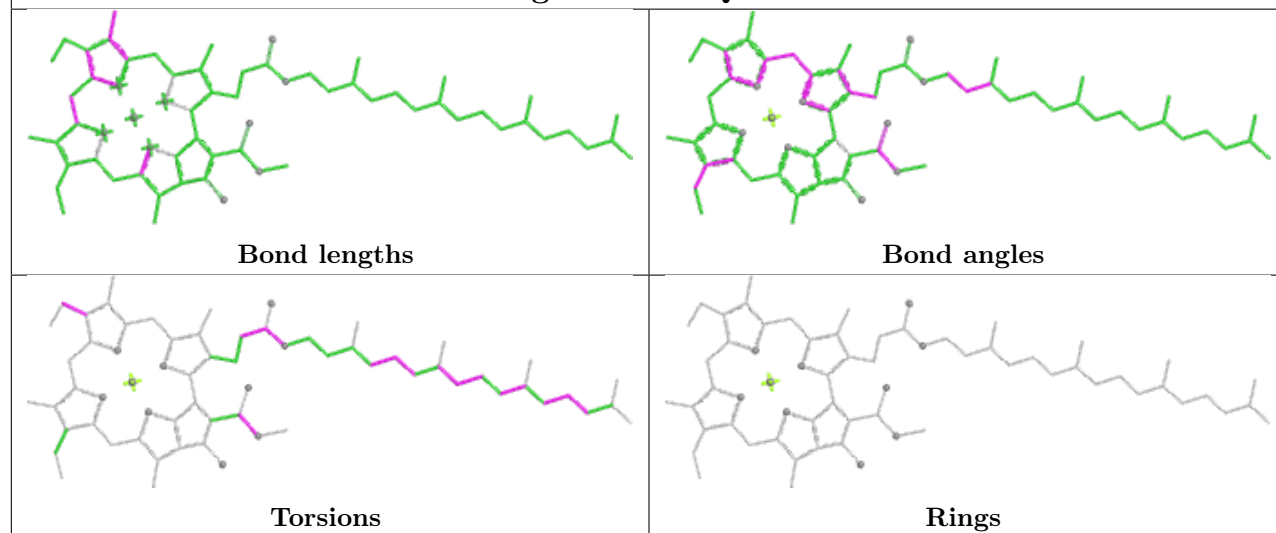
Ligand CLA 5 615

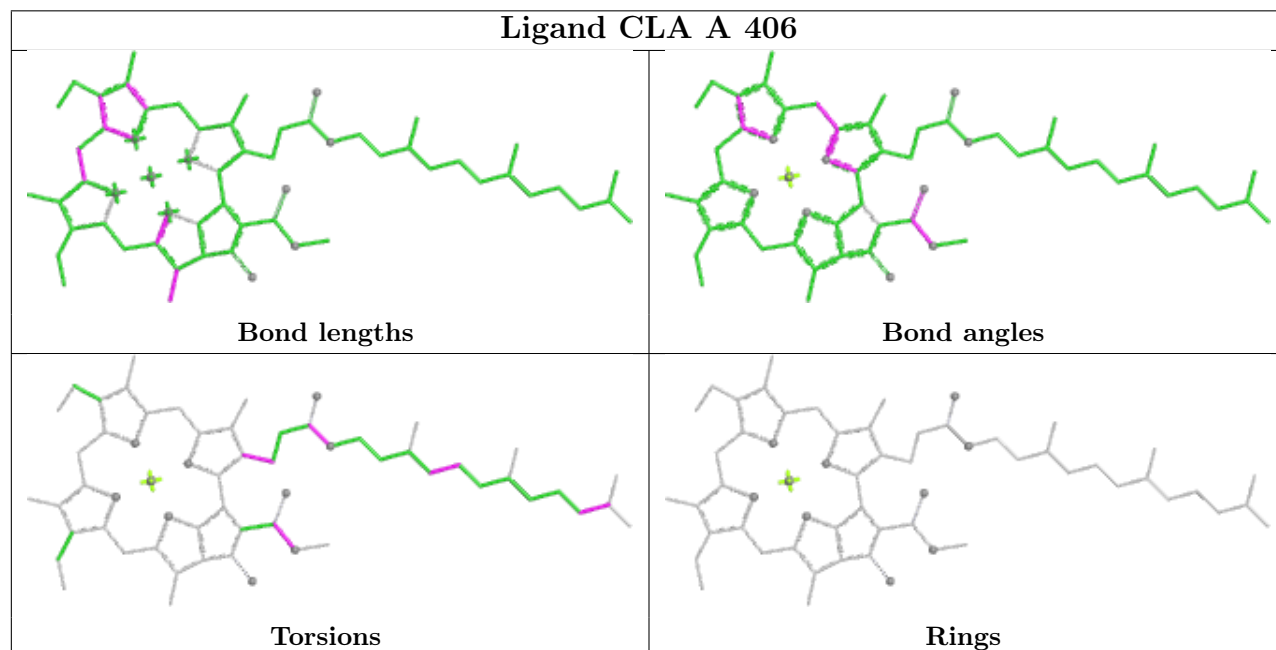
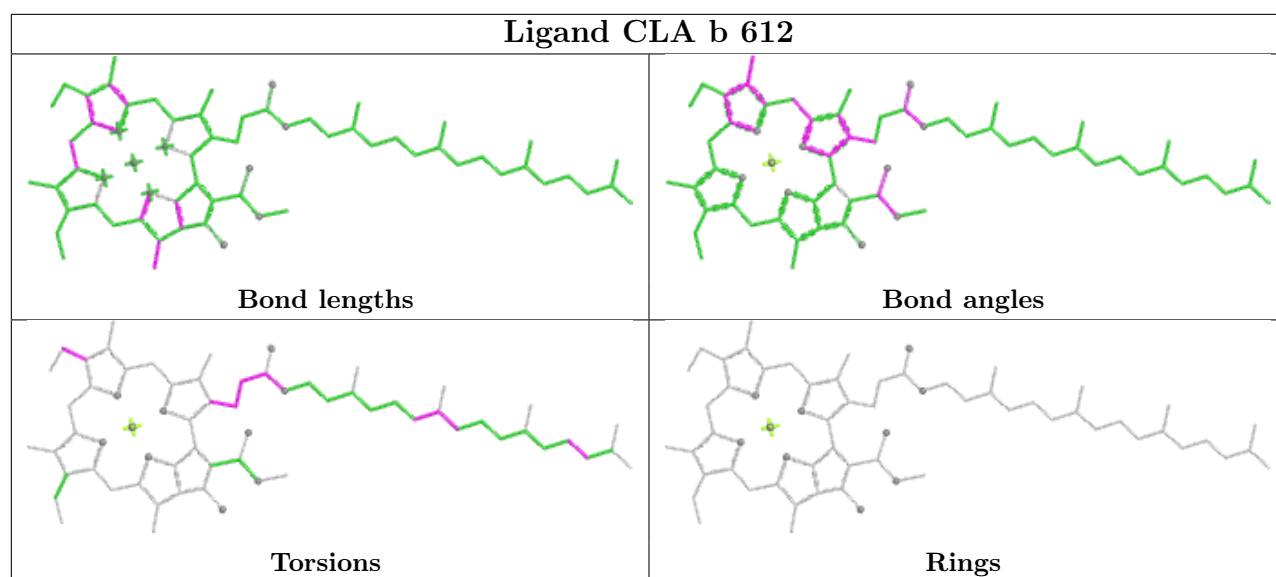


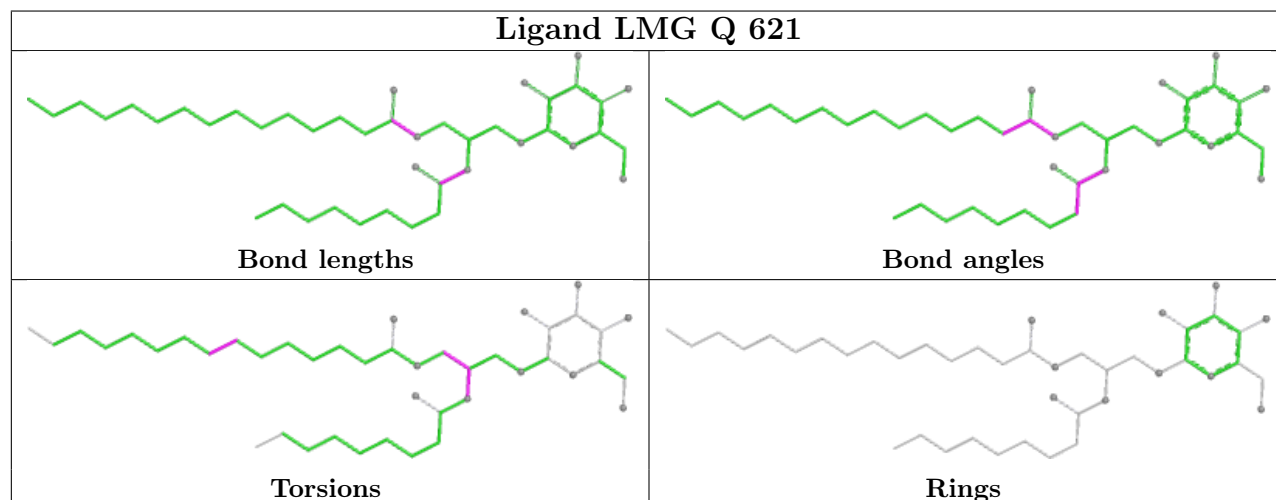
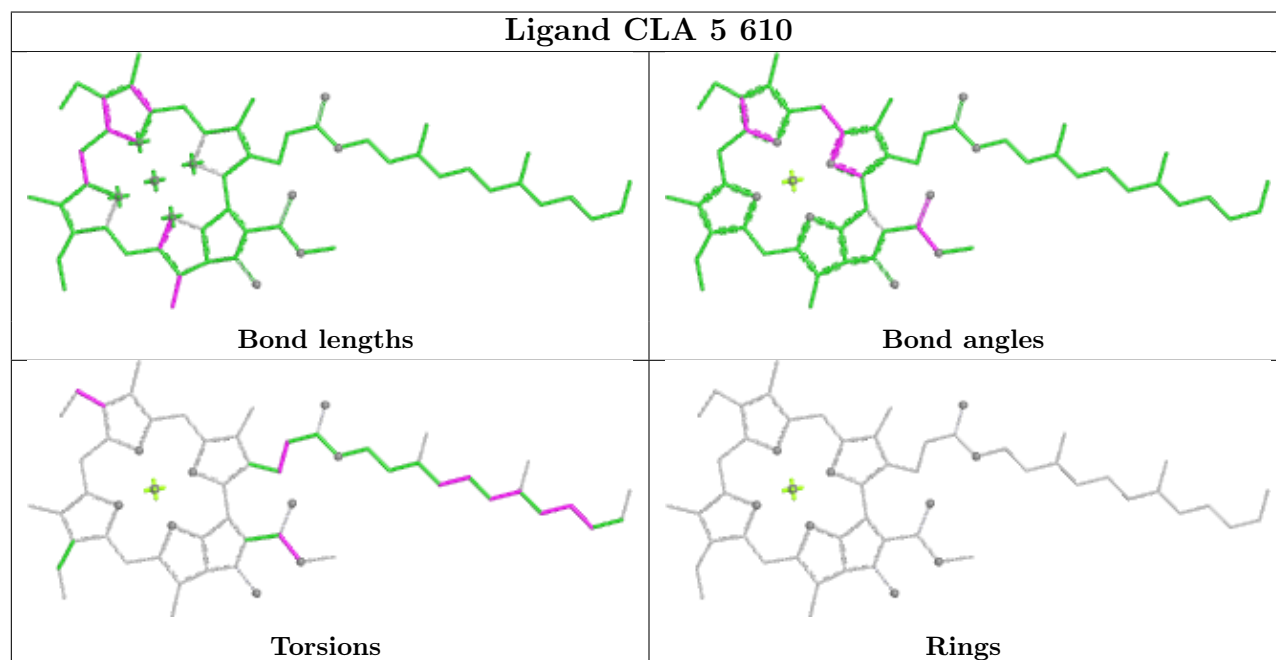
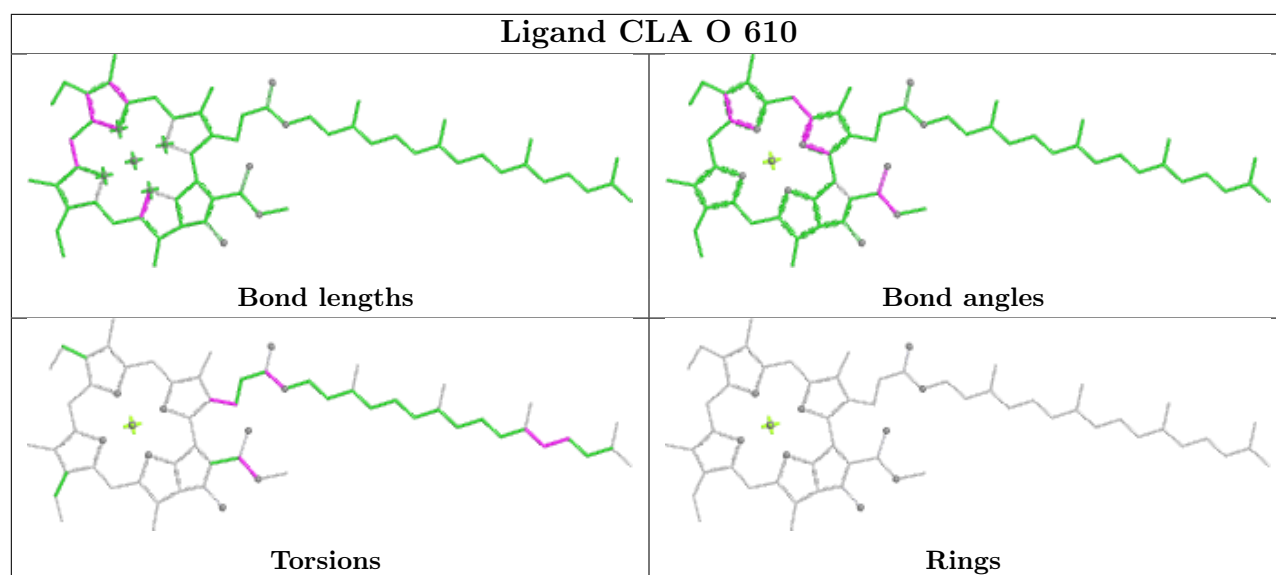
Ligand CLA 2 601

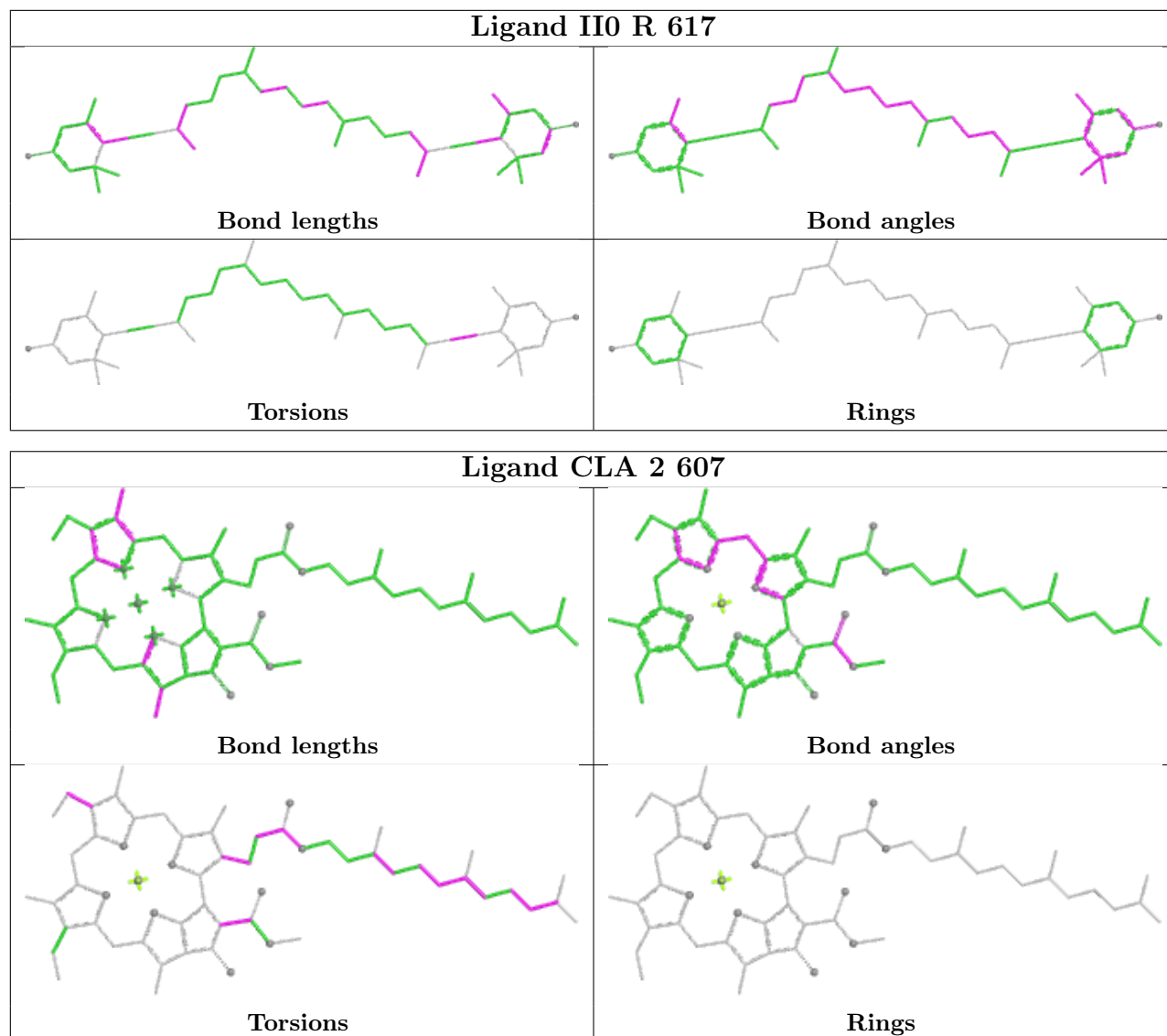


Ligand CLA Q 603

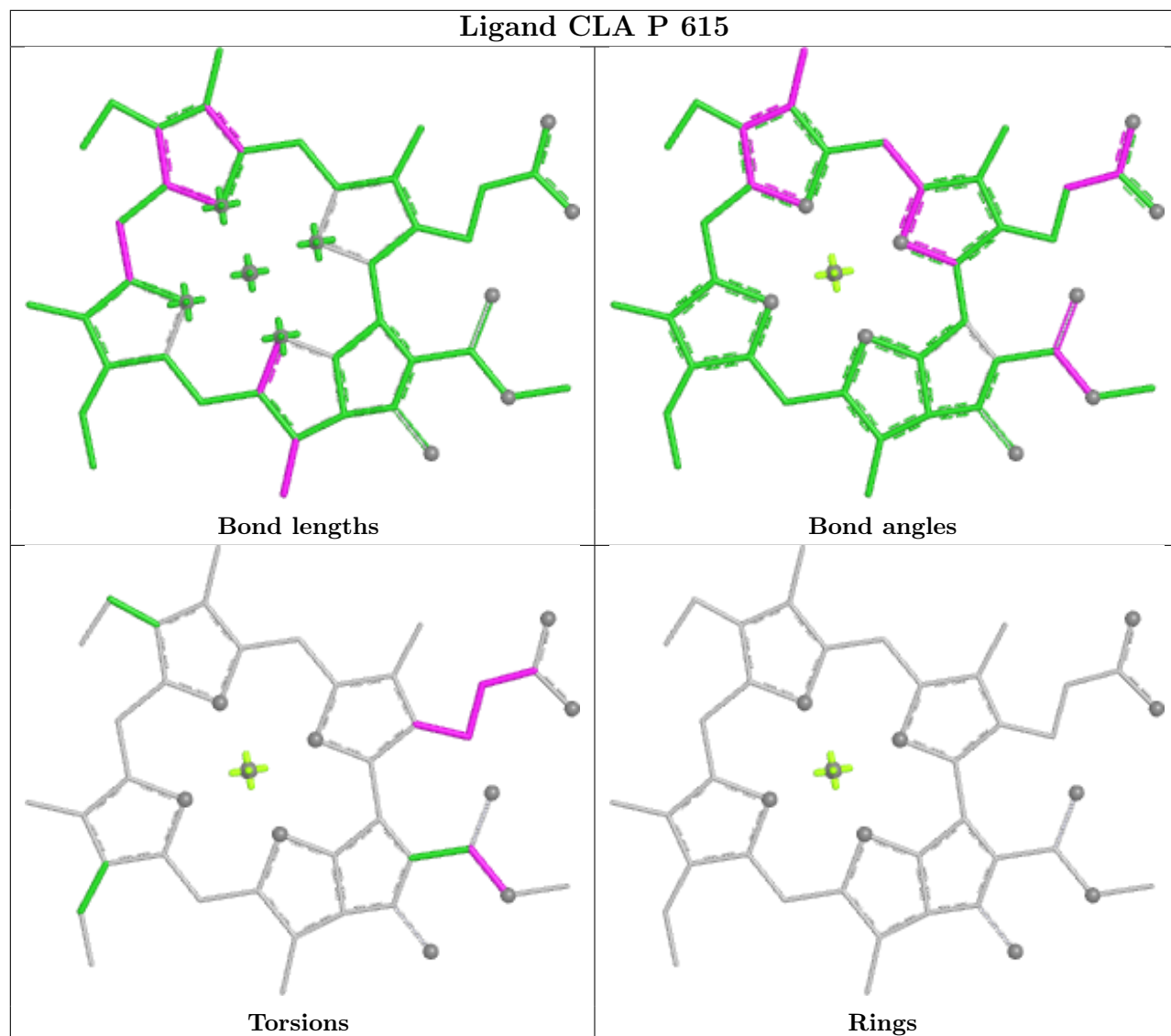


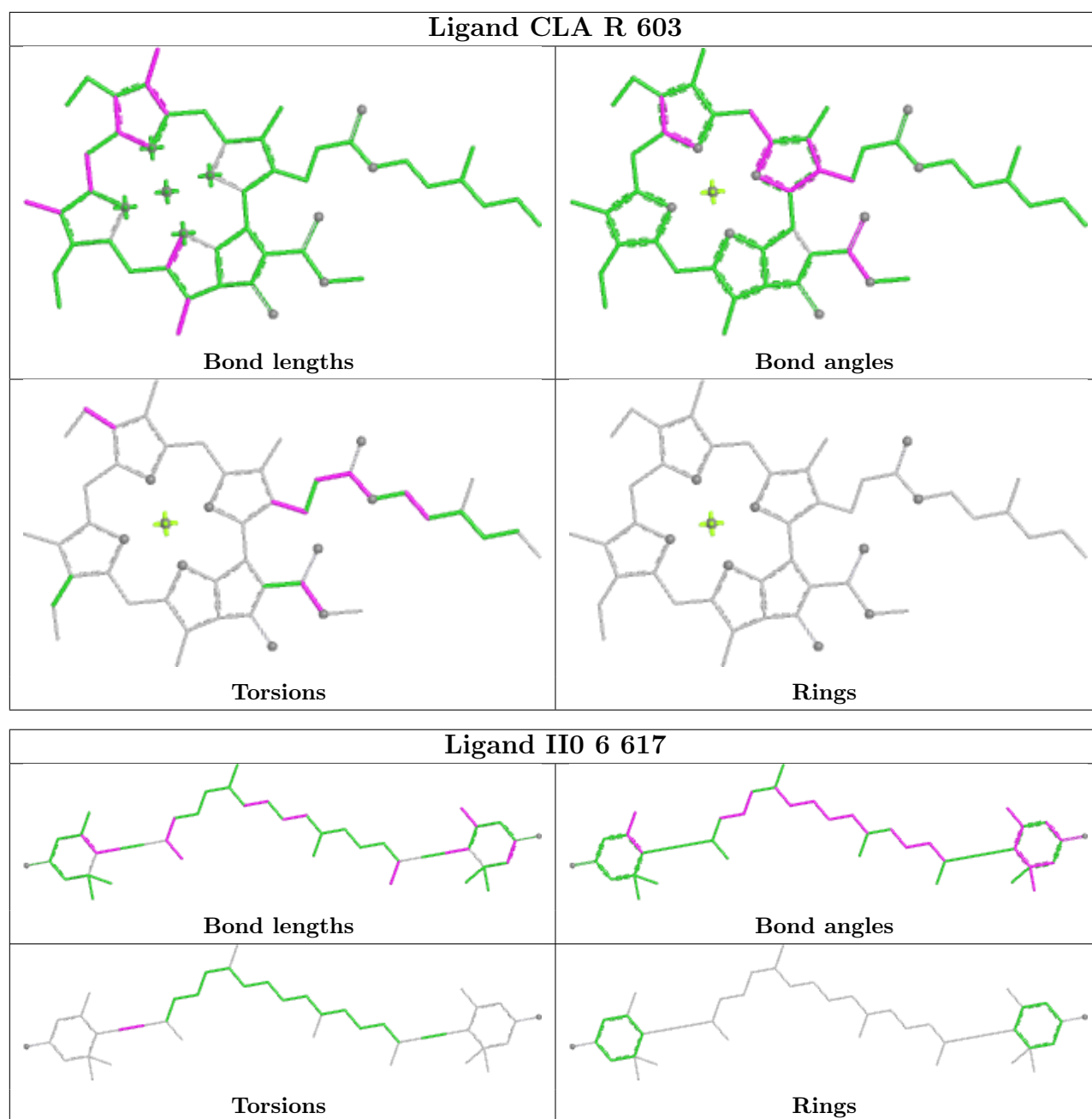


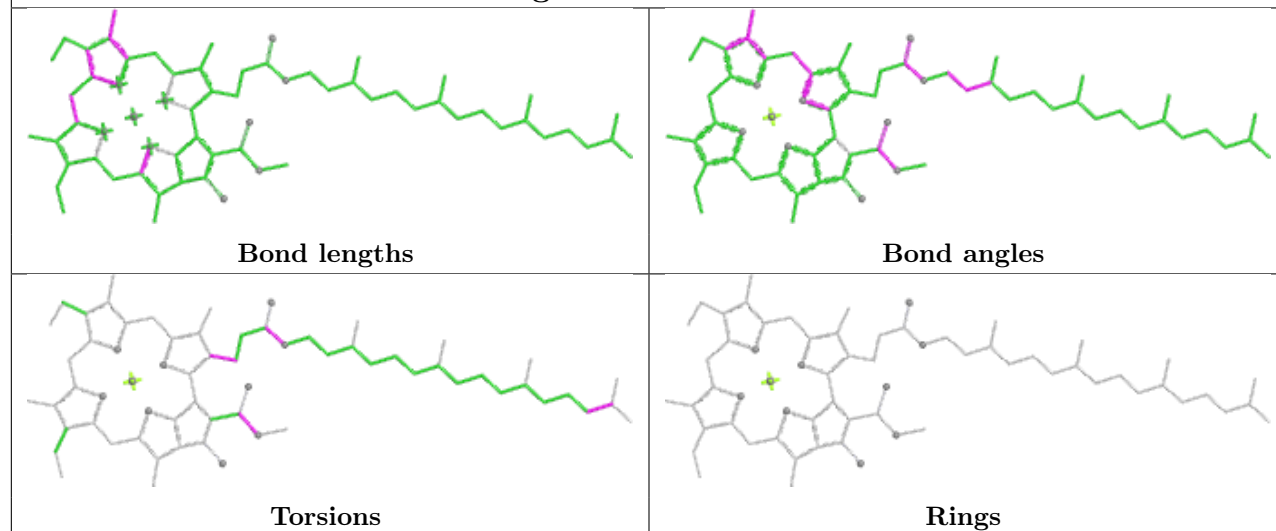
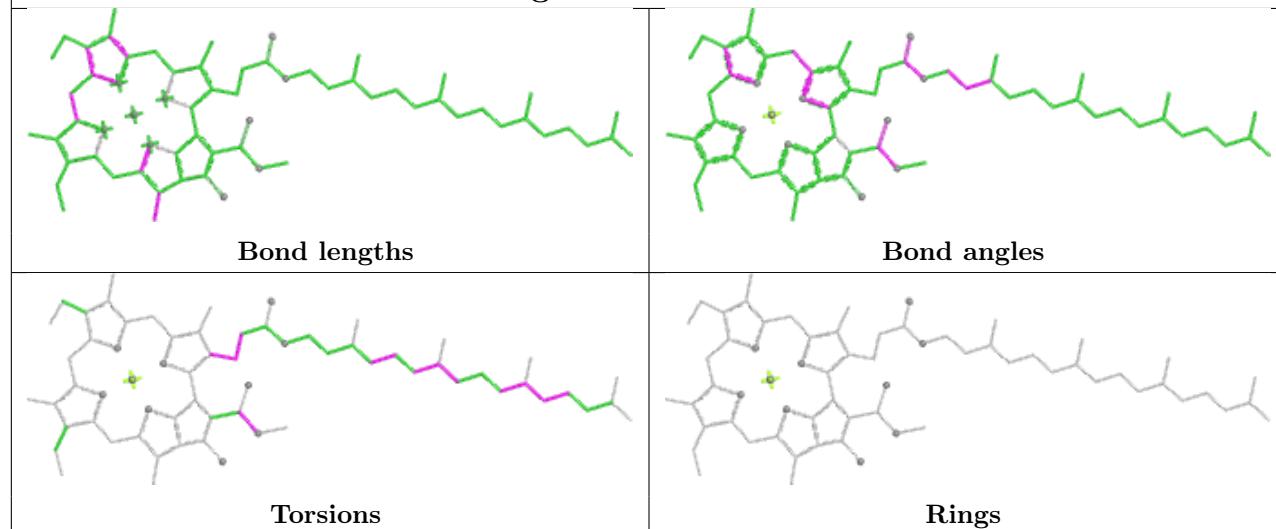
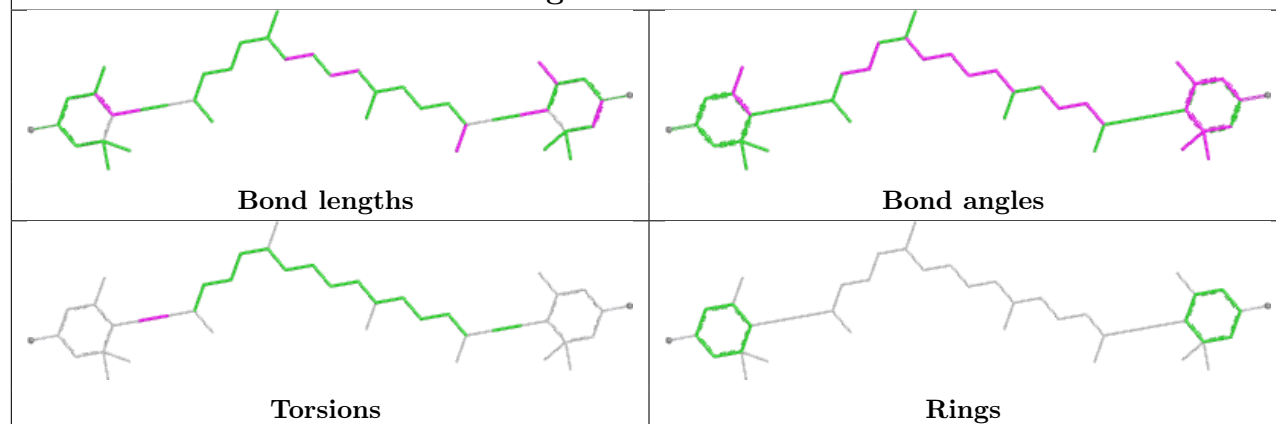




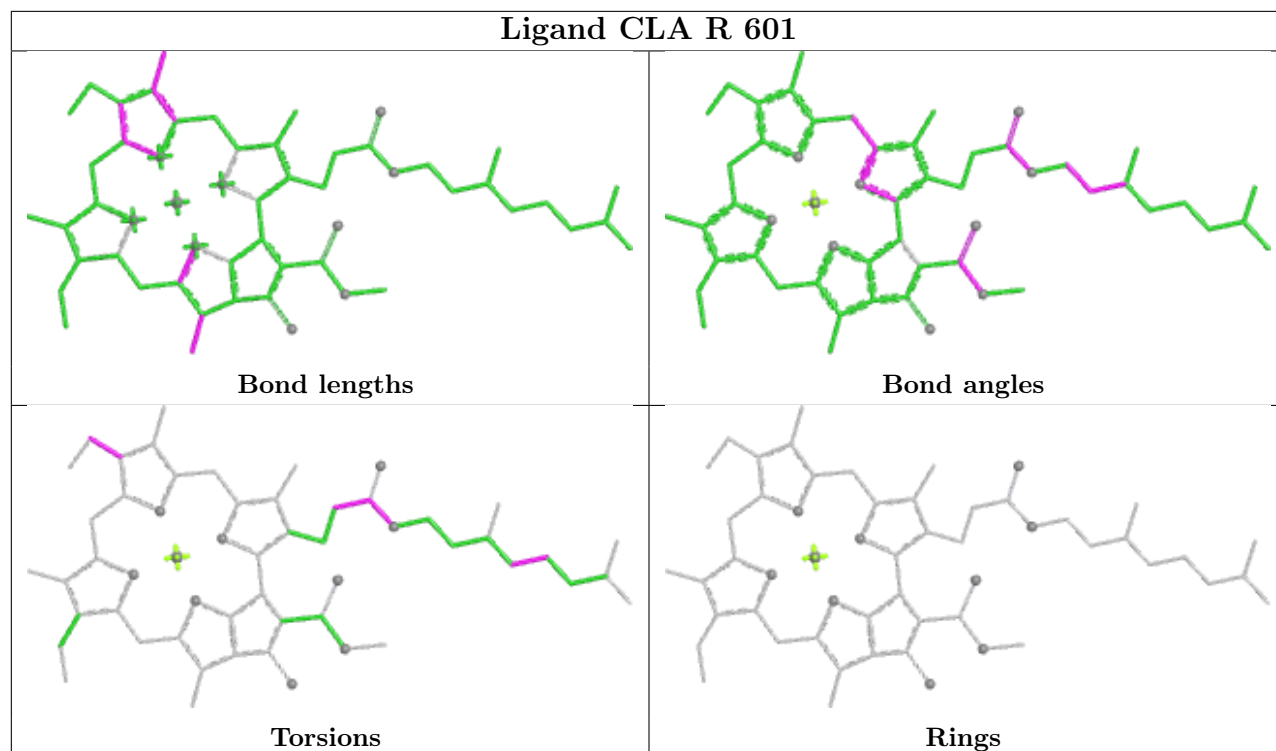
Ligand CLA P 615



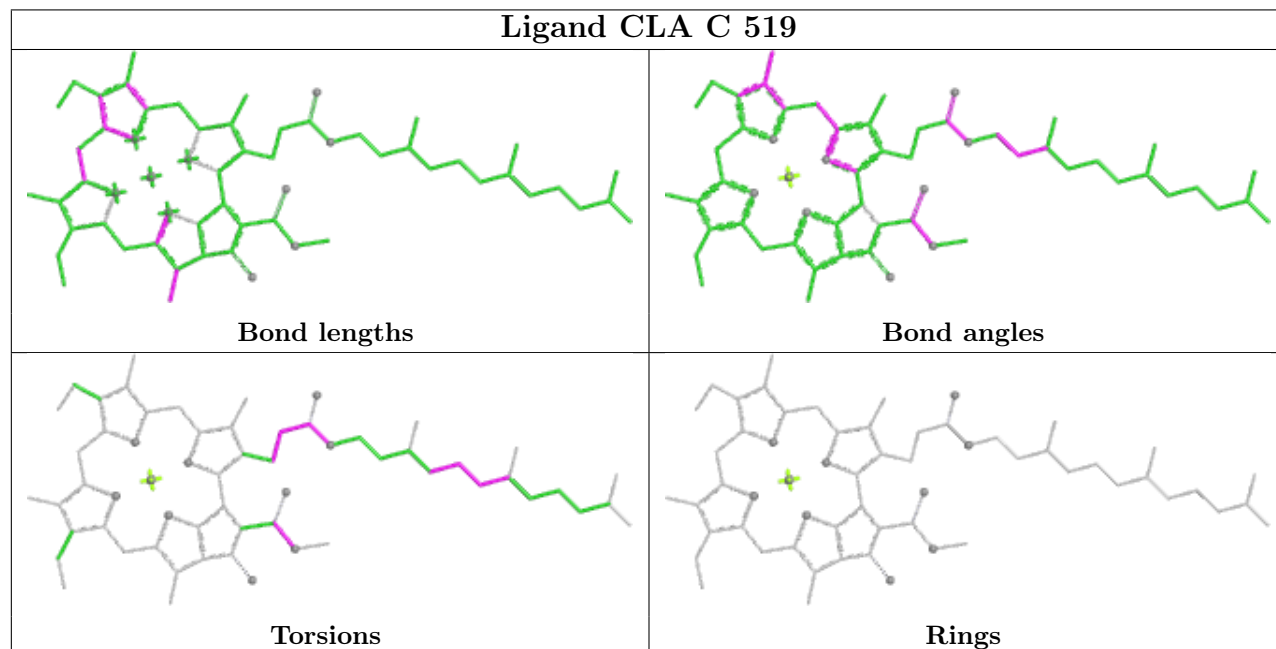


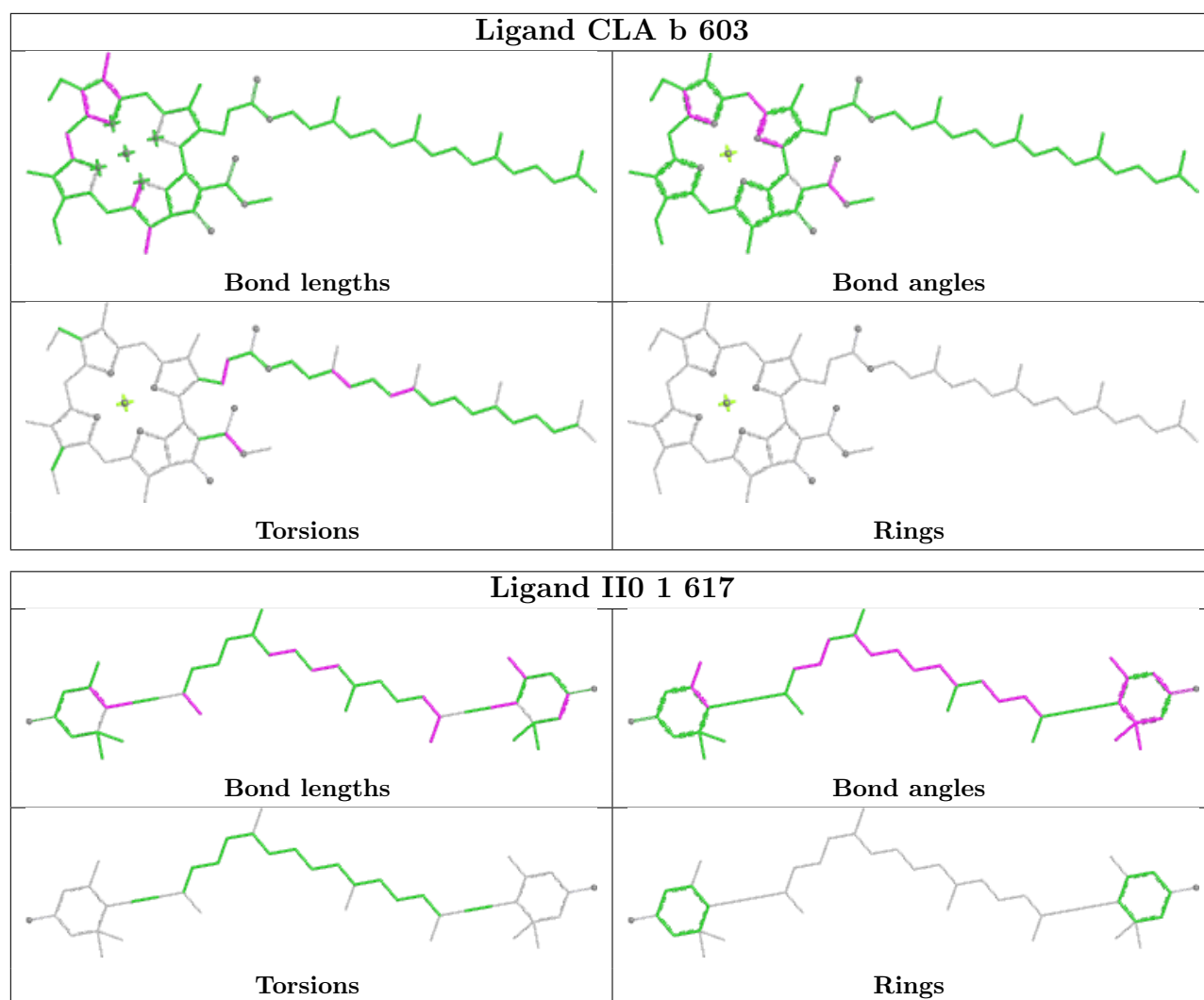
Ligand CLA C 521**Ligand CLA O 602****Ligand II0 O 617**

Ligand CLA R 601

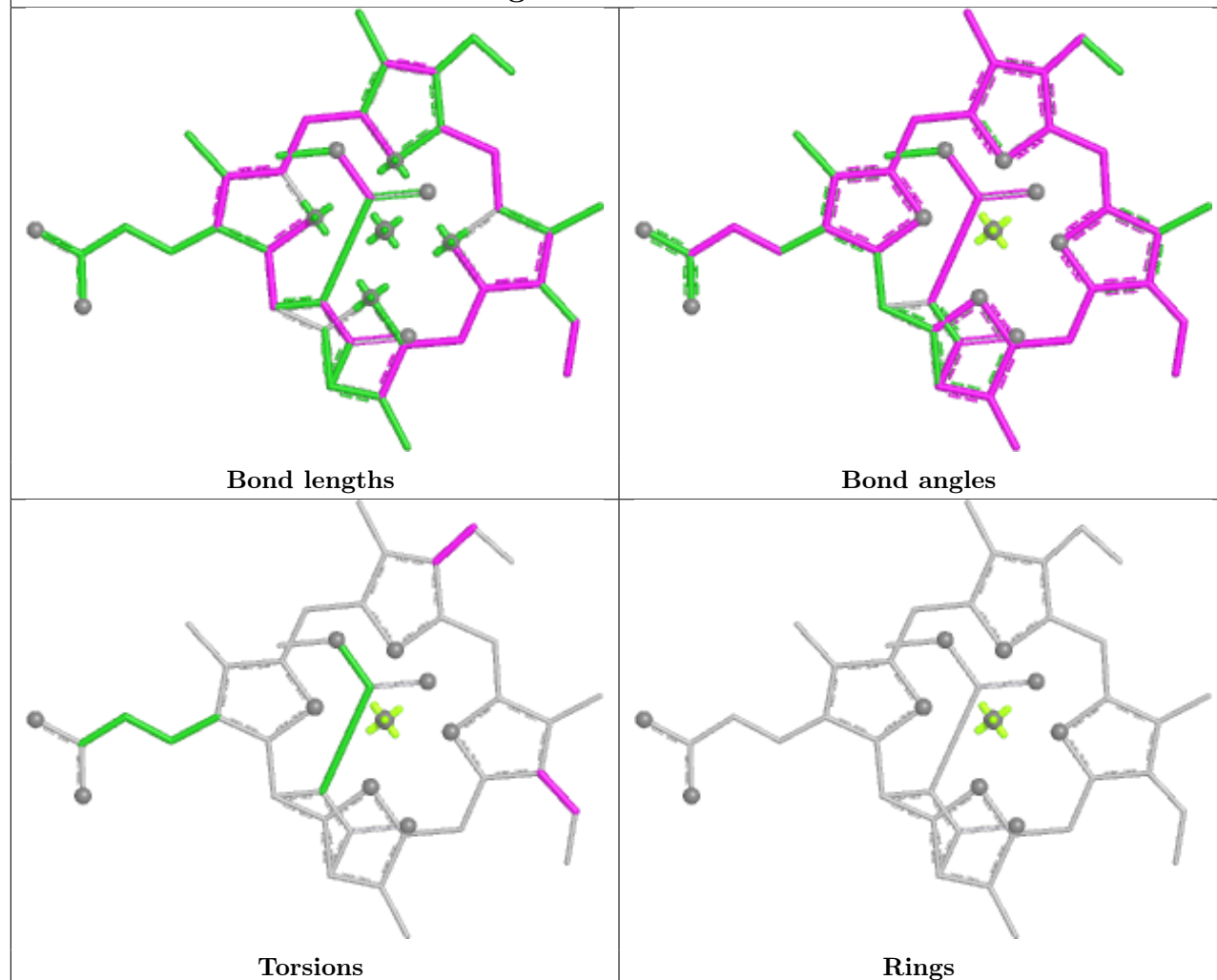


Ligand CLA C 519

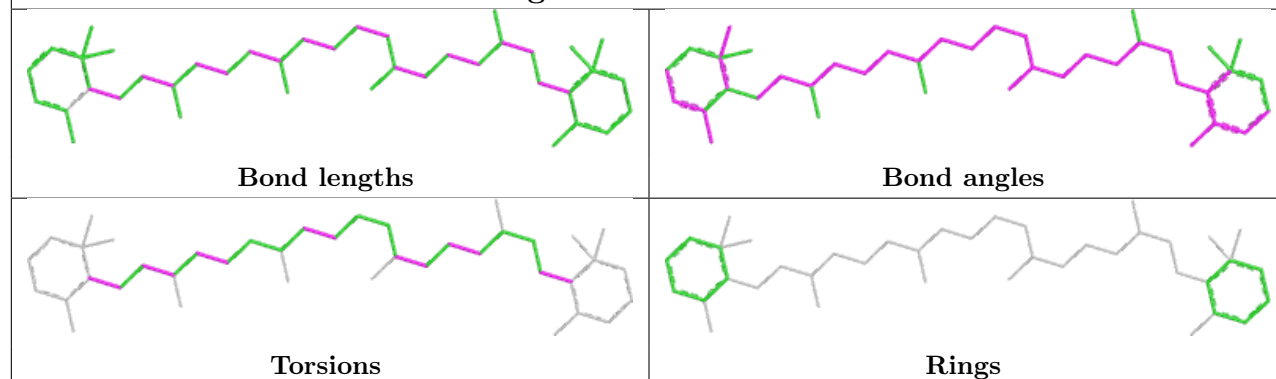




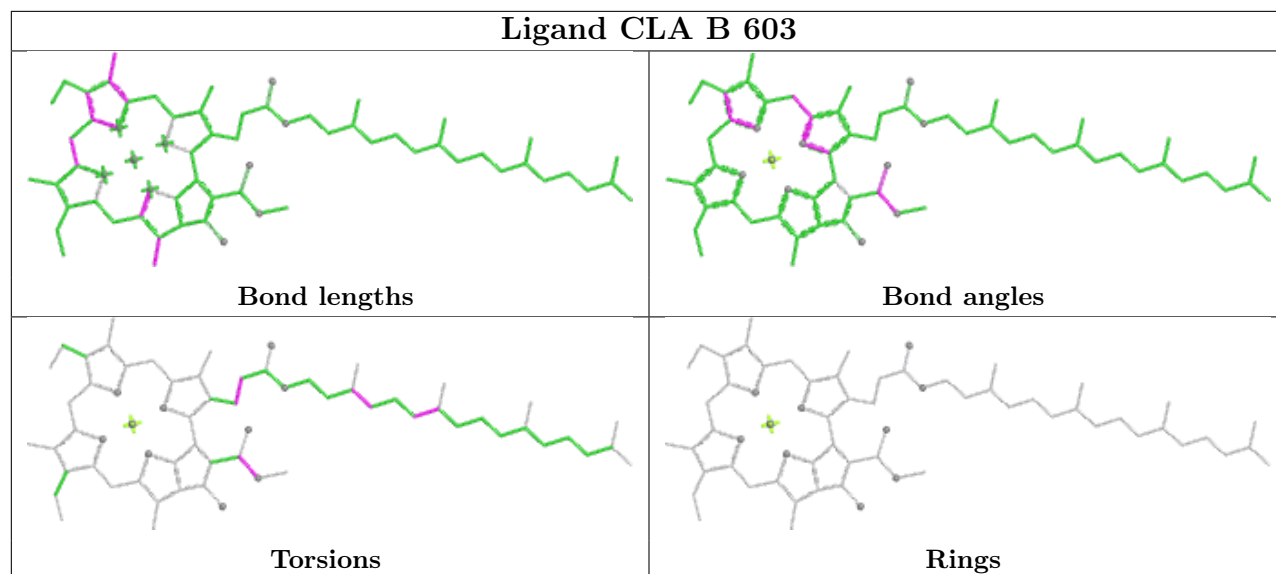
Ligand KC2 N 611



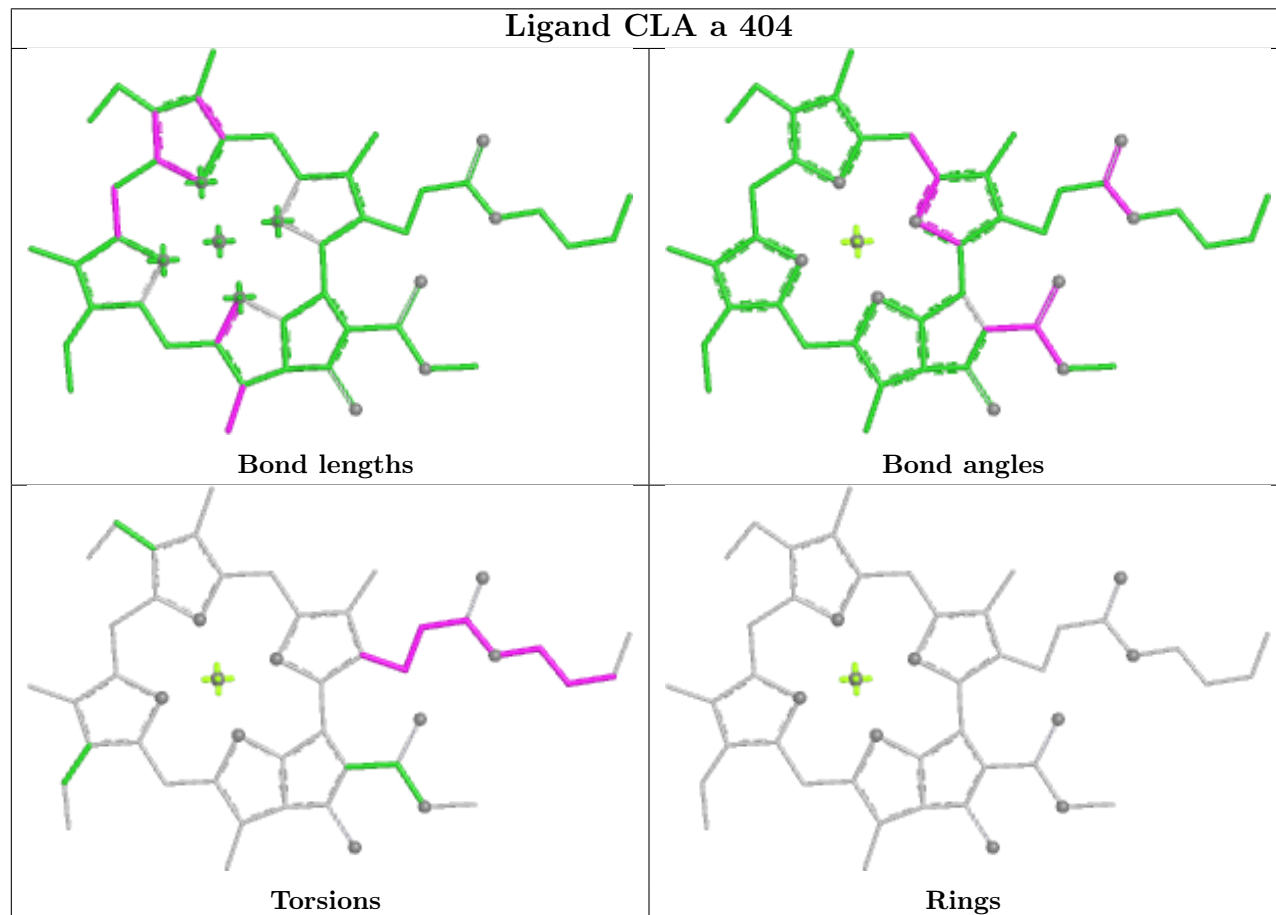
Ligand WVN a 407



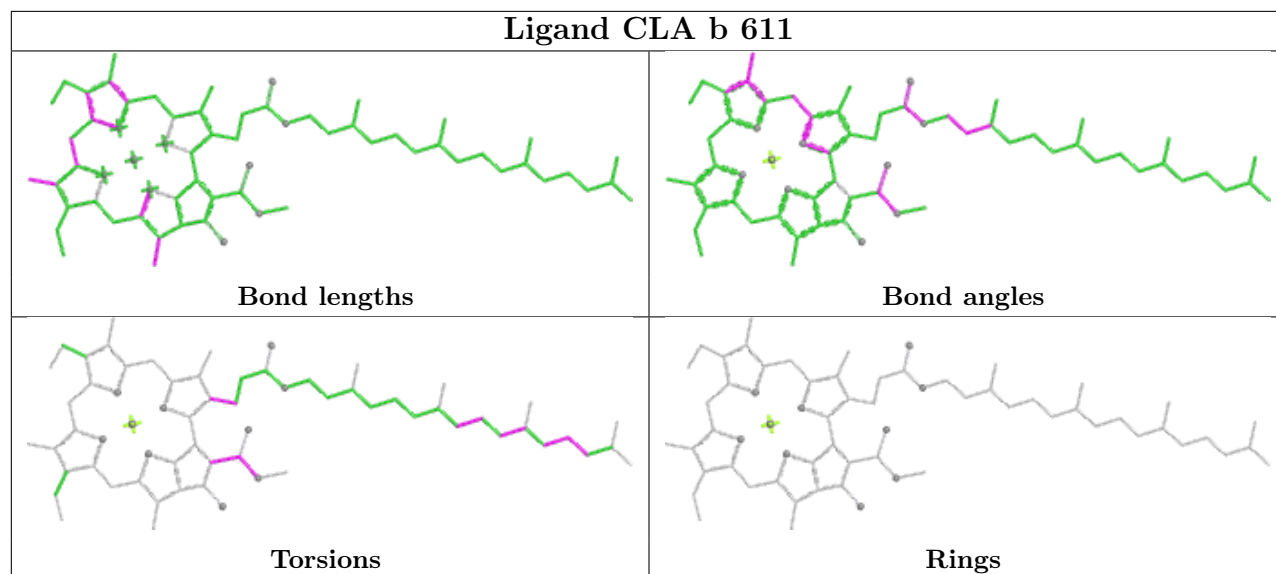
Ligand CLA B 603



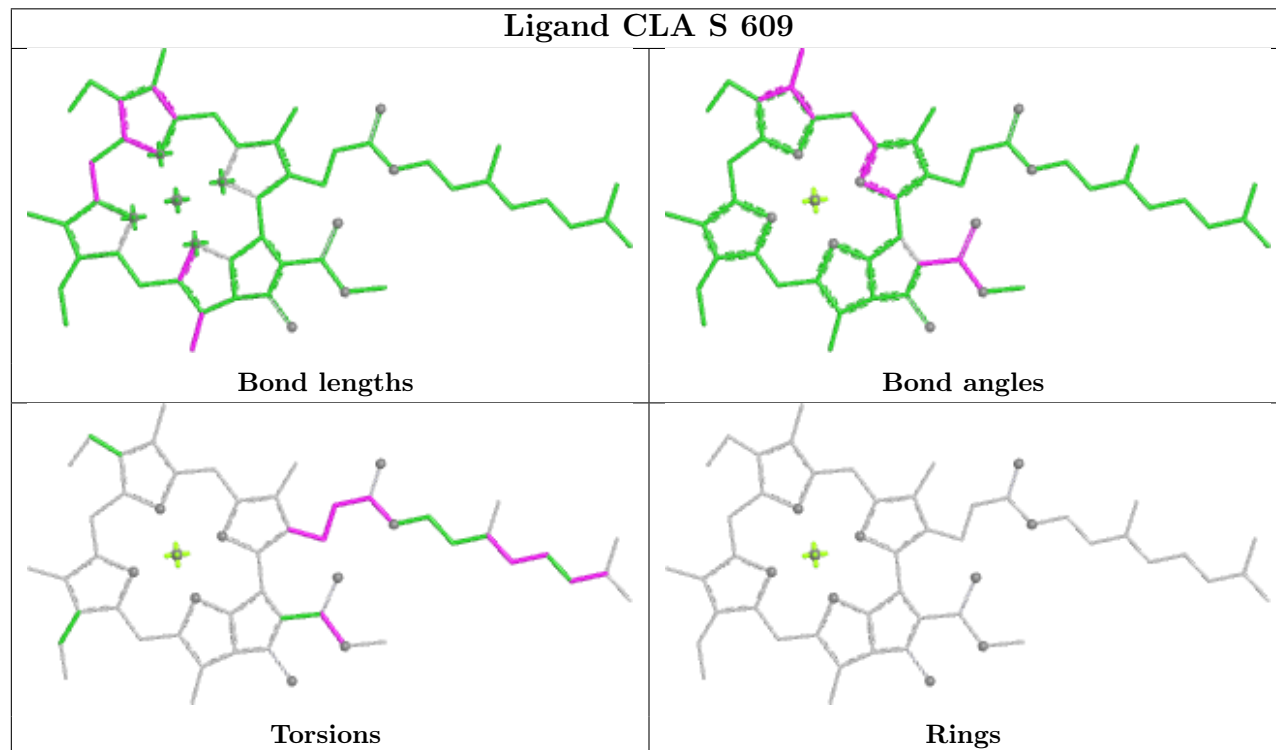
Ligand CLA a 404



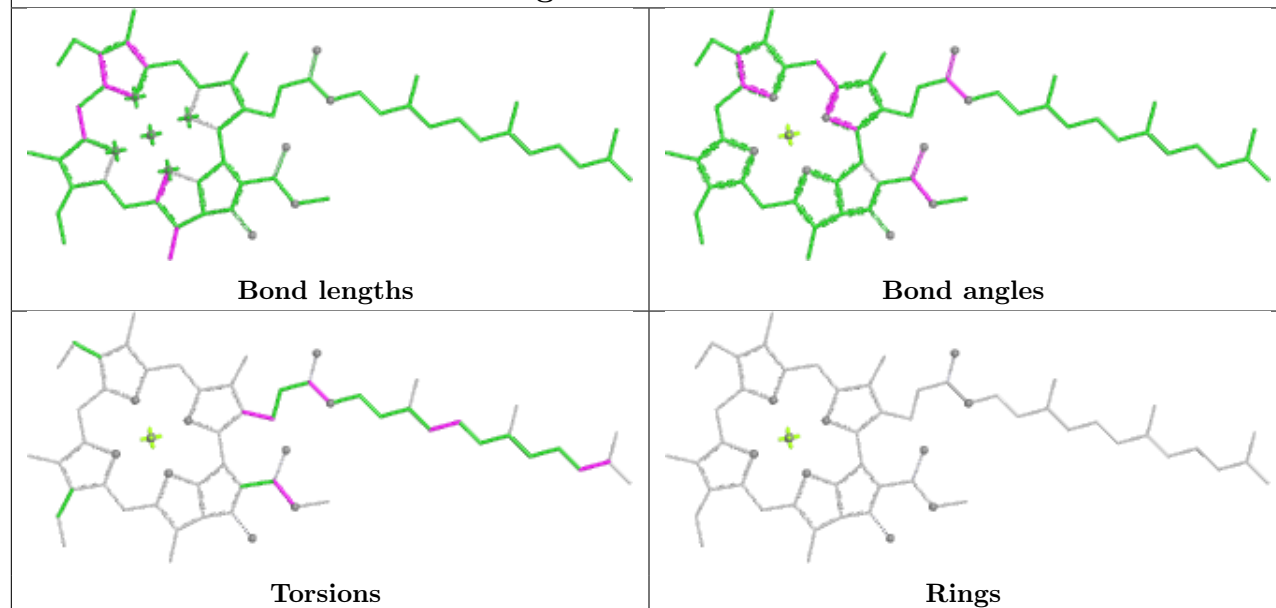
Ligand CLA b 611



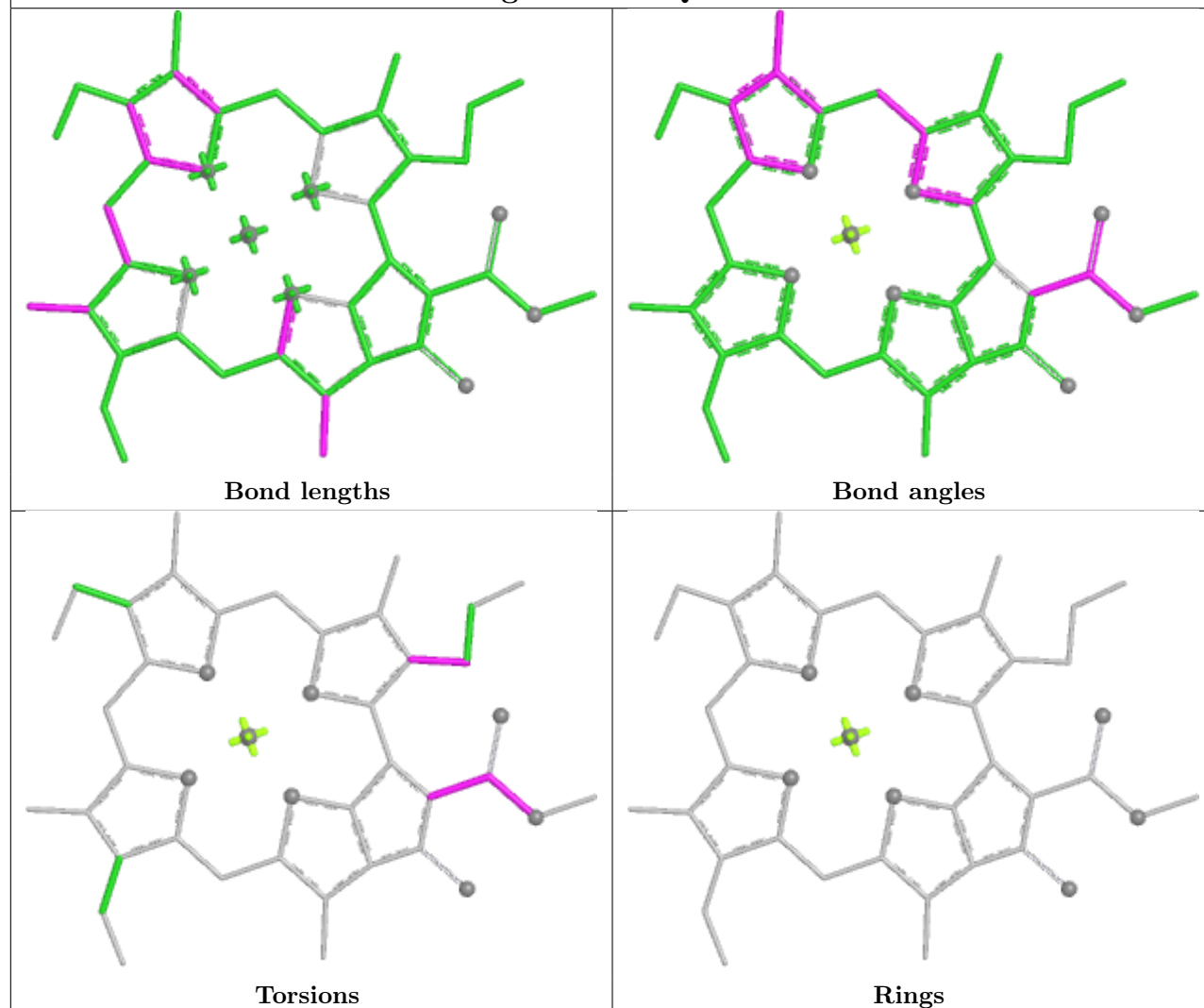
Ligand CLA S 609

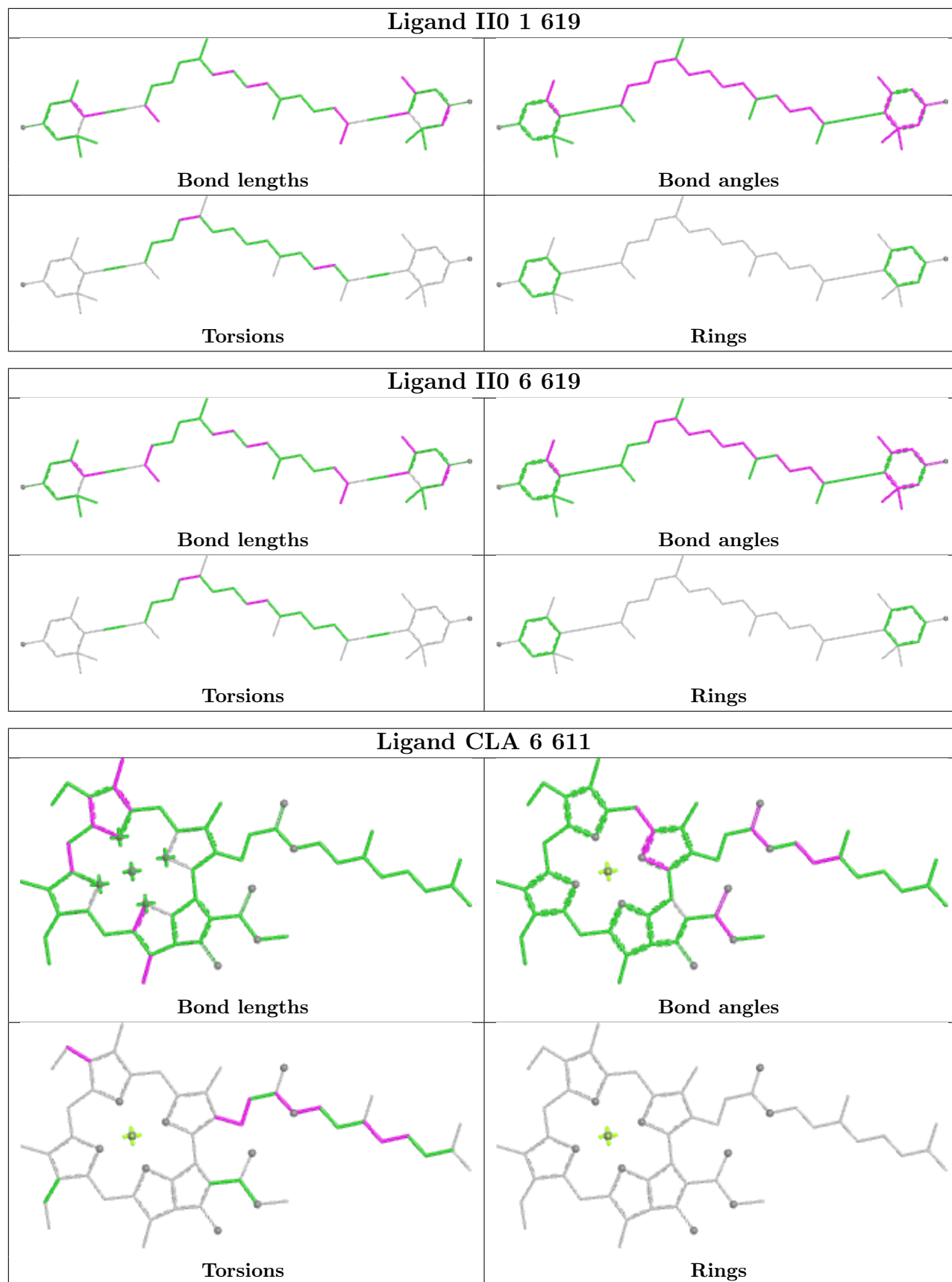


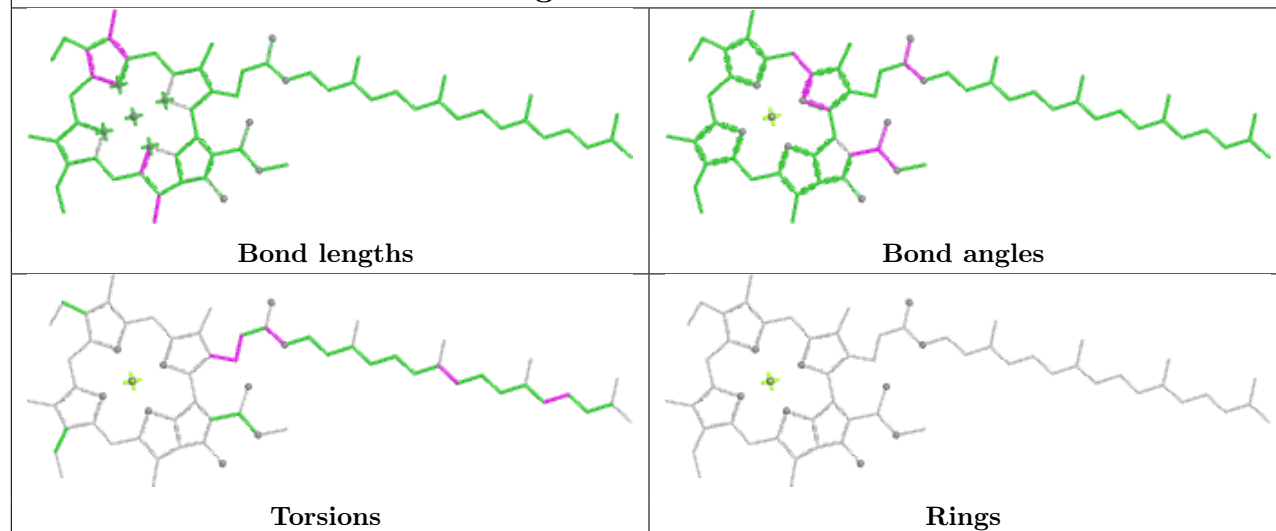
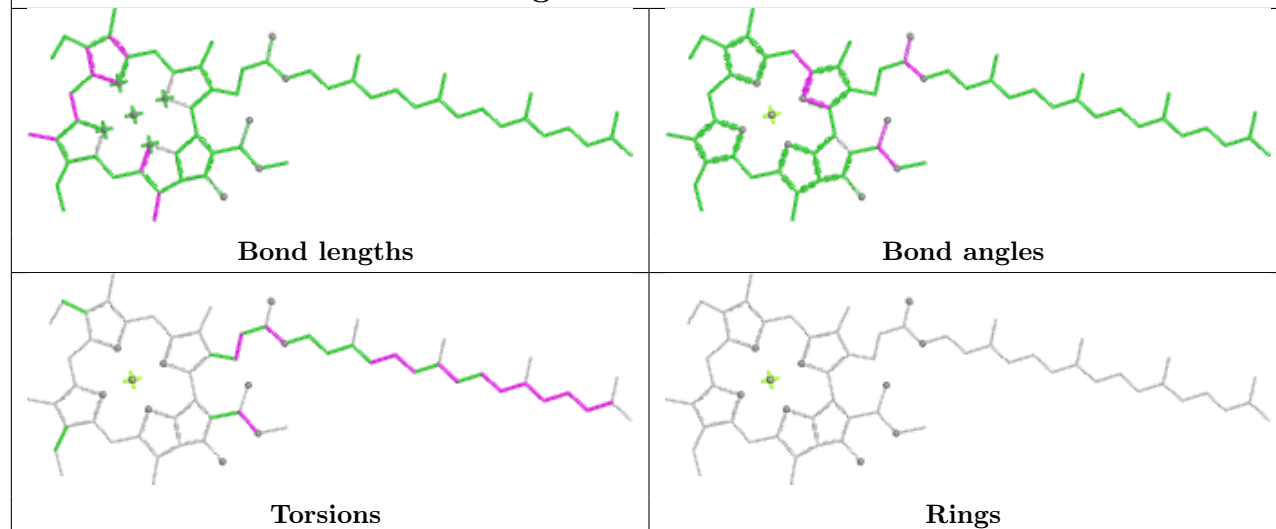
Ligand CLA a 406



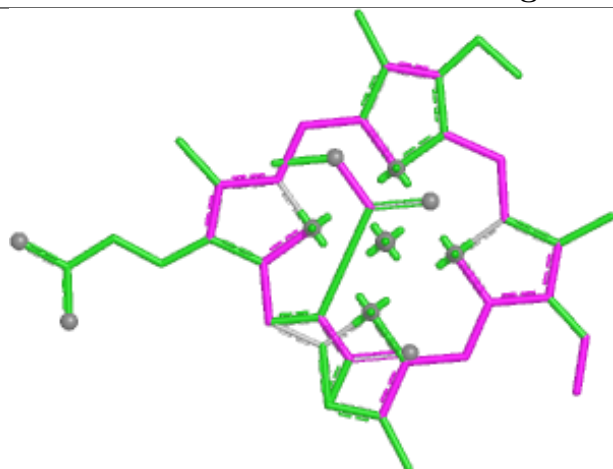
Ligand CLA Q 613



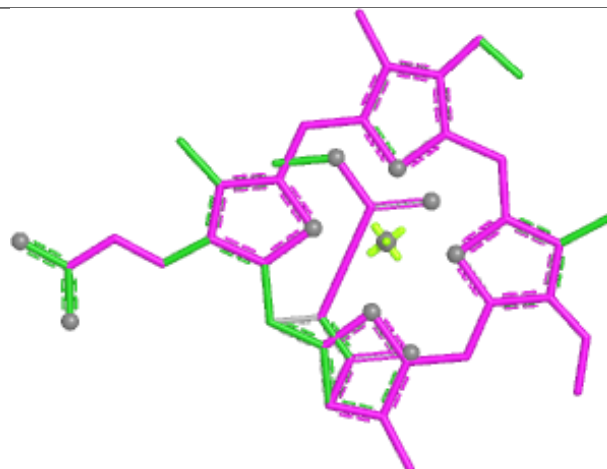


Ligand CLA d 400**Ligand CLA B 616**

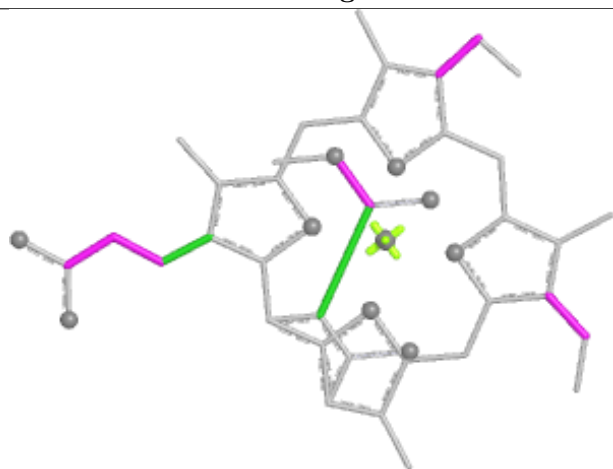
Ligand KC2 1 613



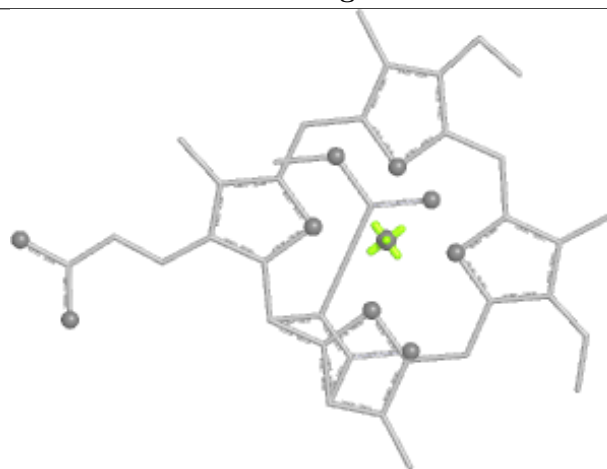
Bond lengths



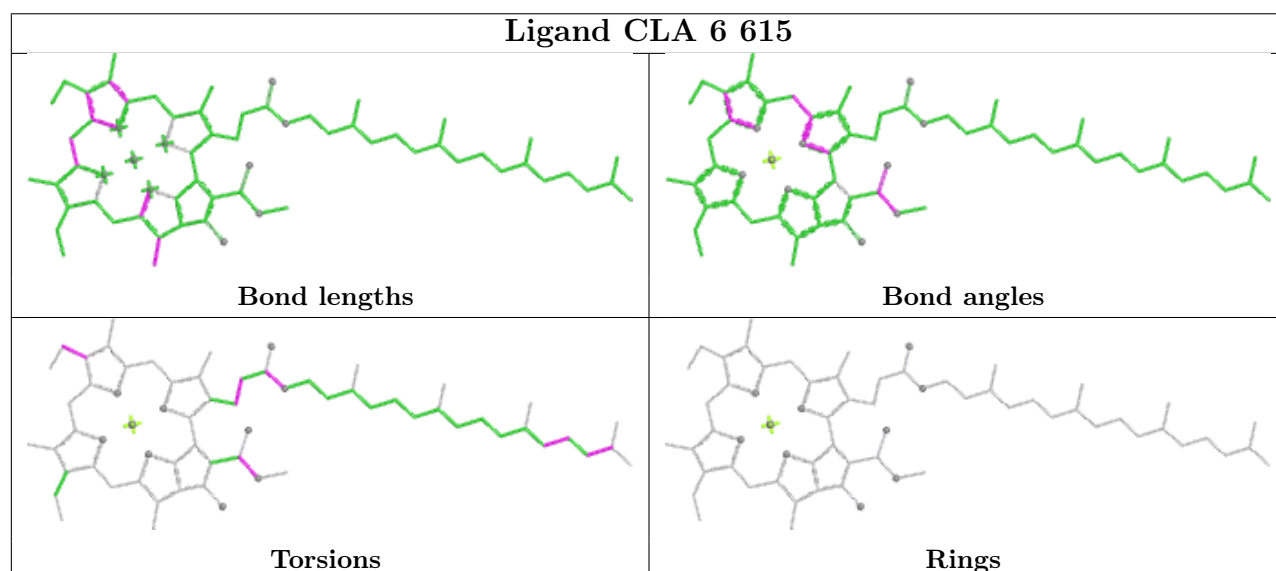
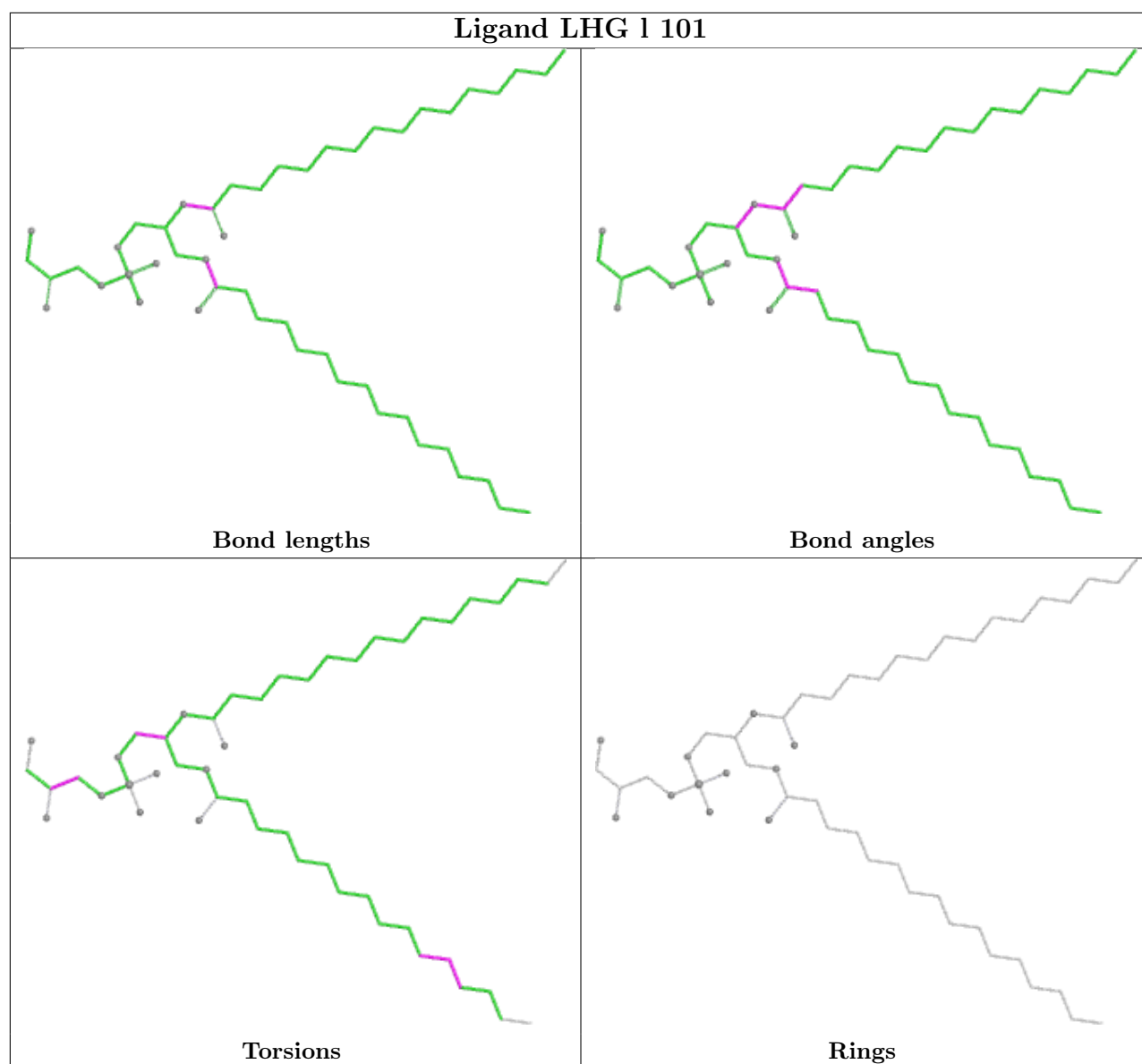
Bond angles

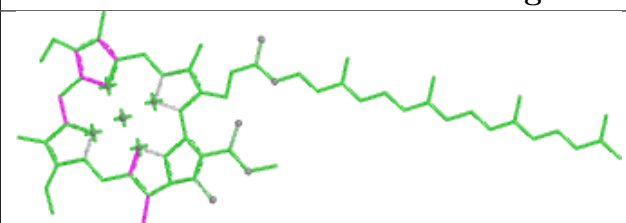
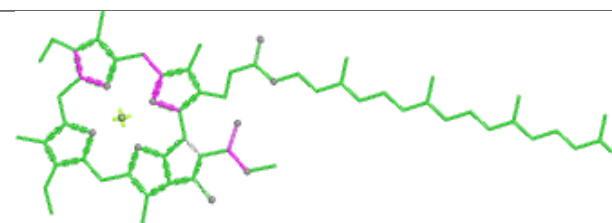
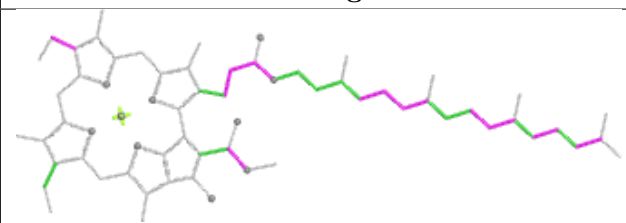
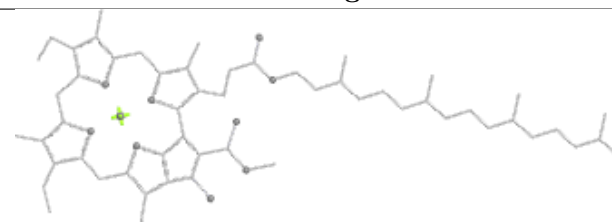


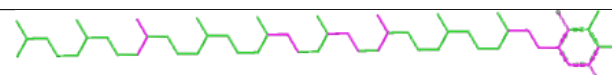
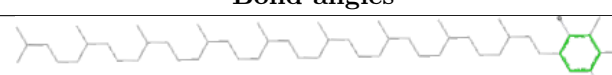
Torsions

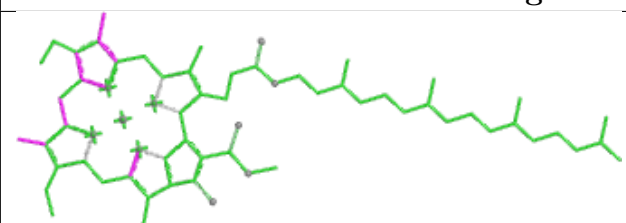
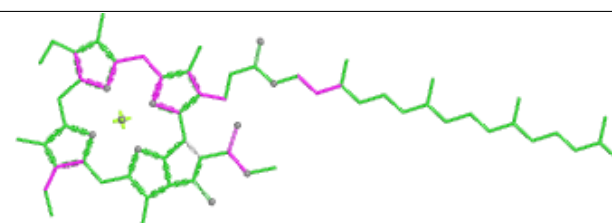
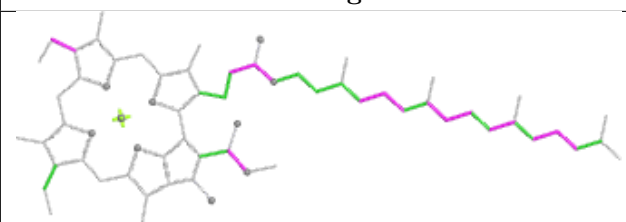
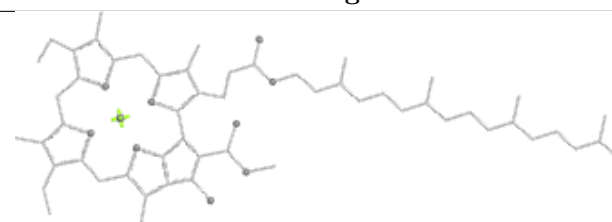


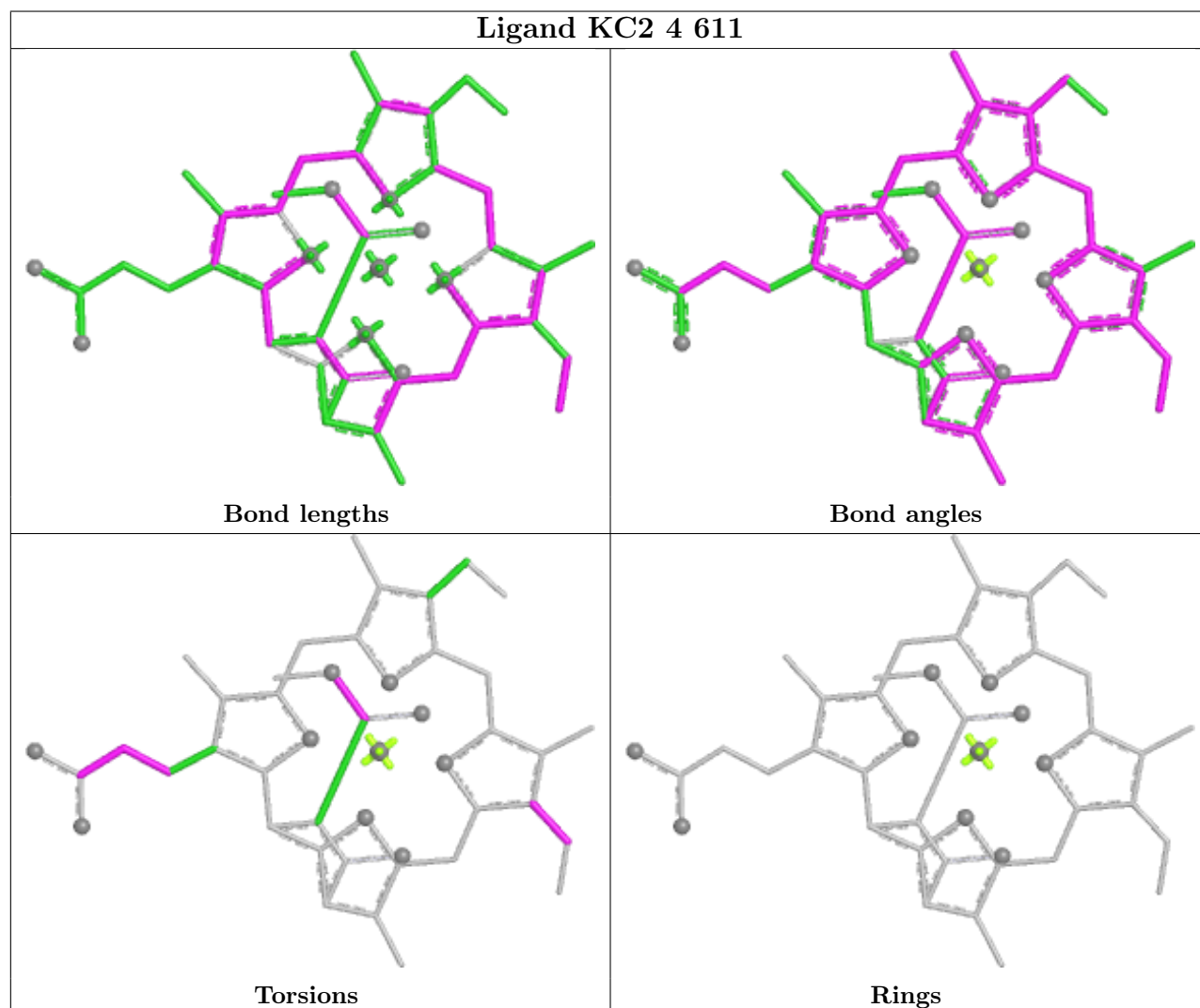
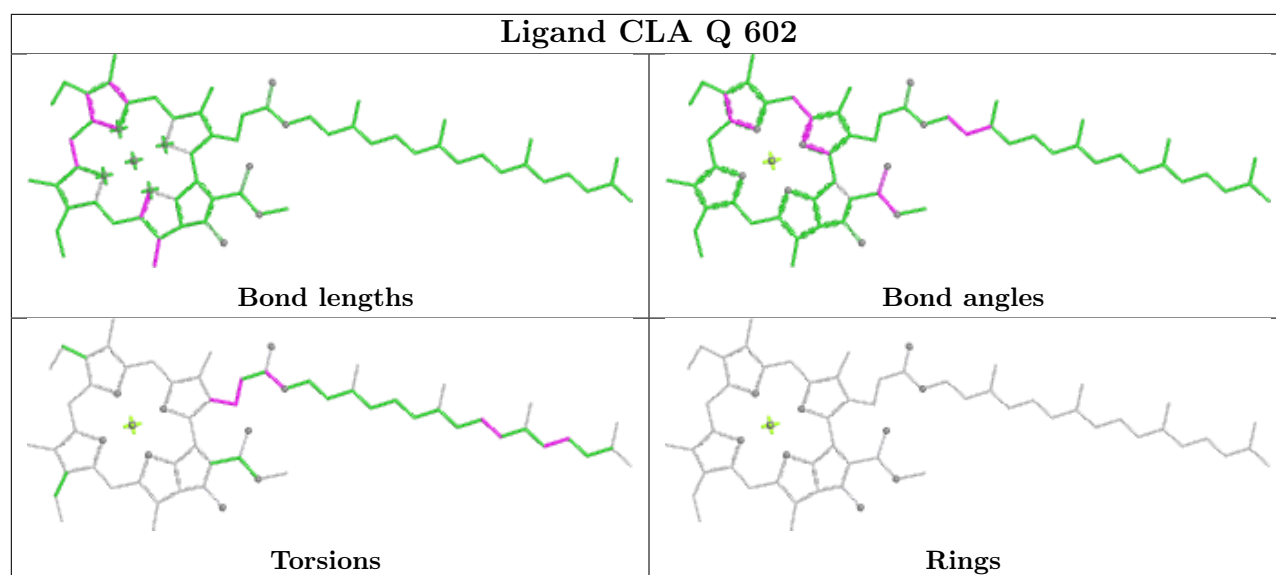
Rings

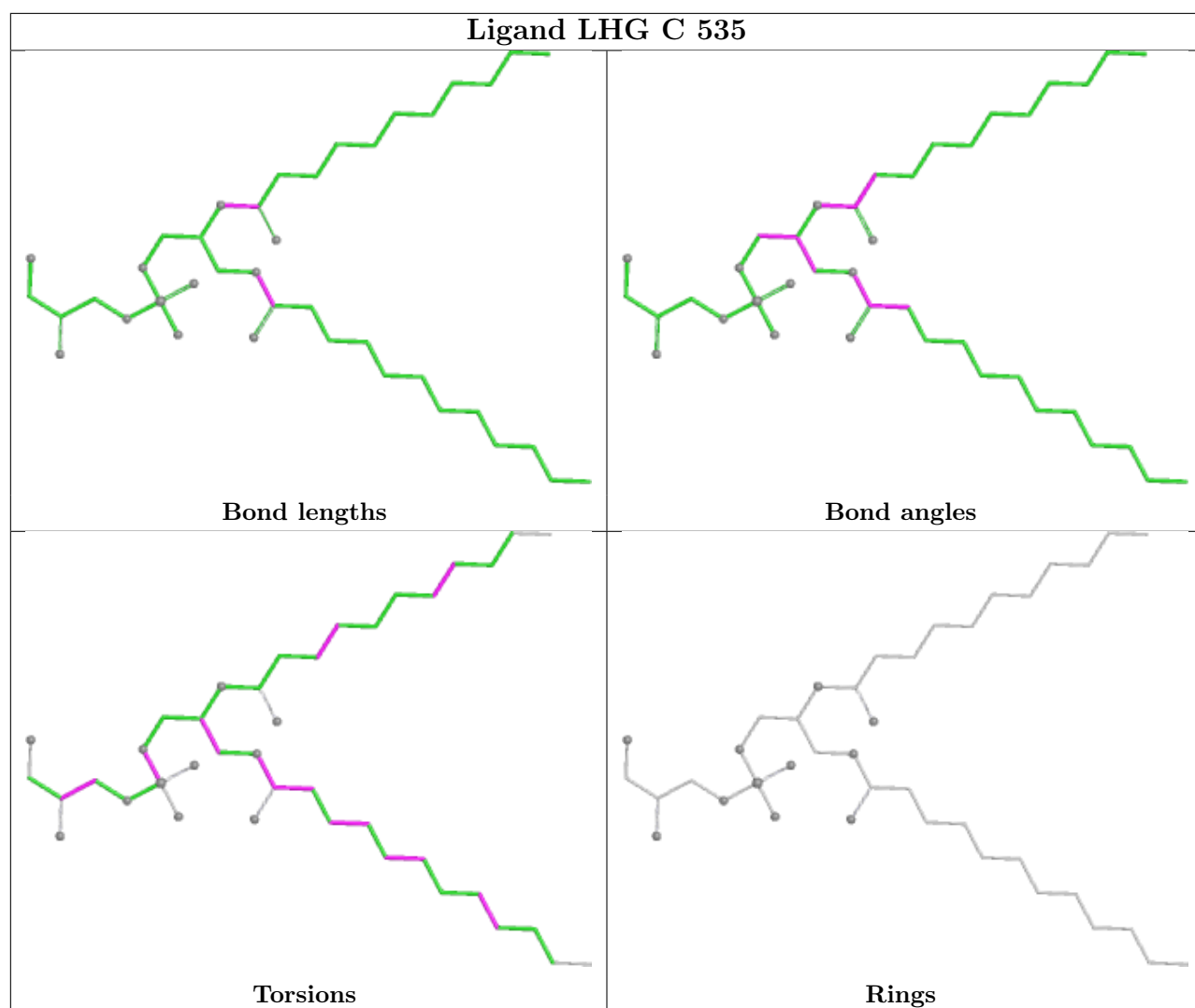


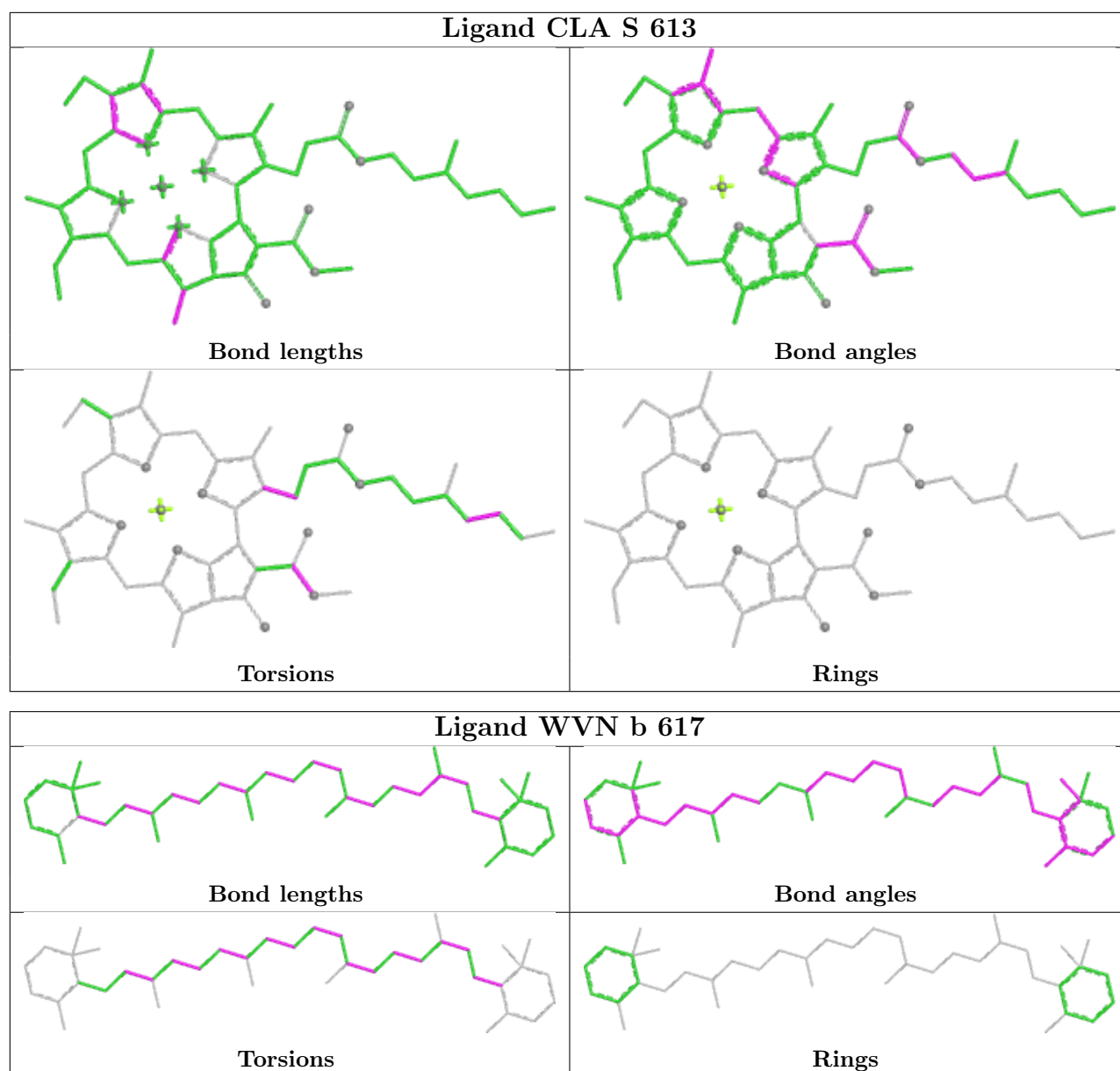
Ligand CLA b 613	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand PL9 D 405	
	
Bond lengths	Bond angles
	
Torsions	Rings

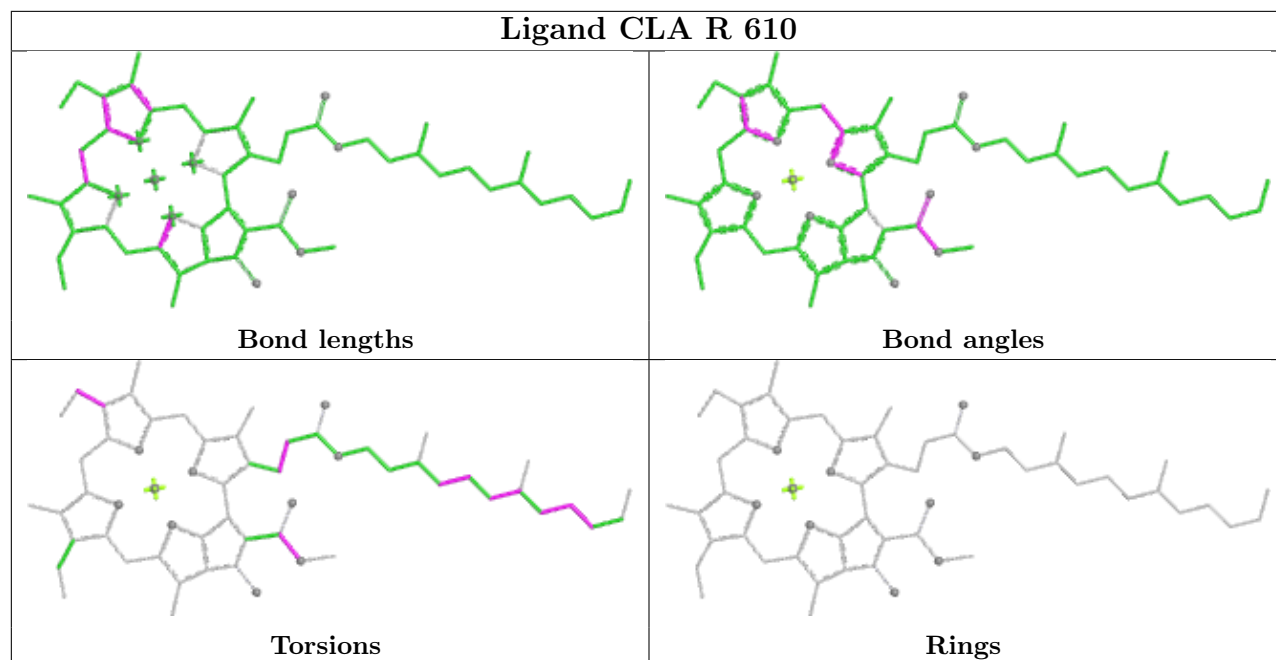
Ligand CLA 4 603	
	
Bond lengths	Bond angles
	
Torsions	Rings



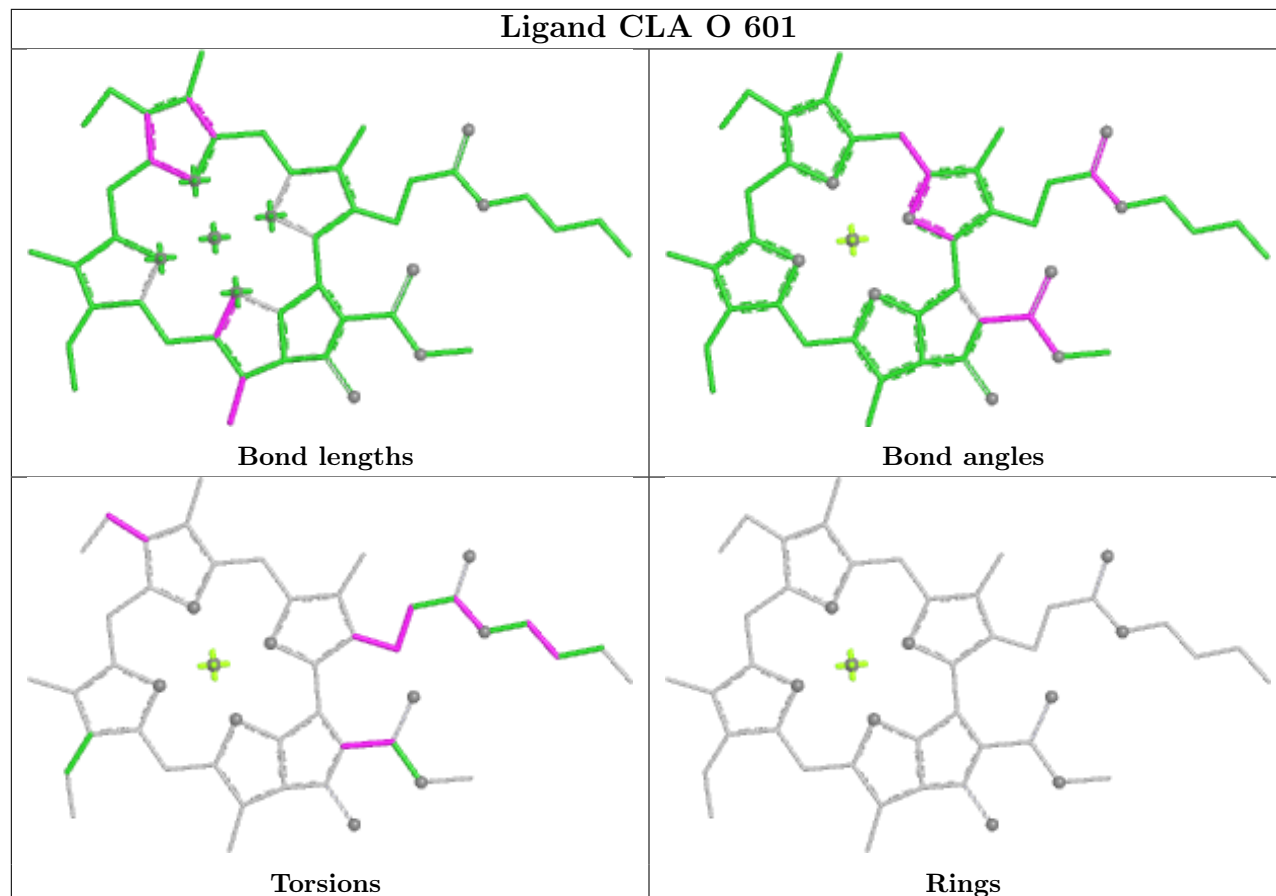


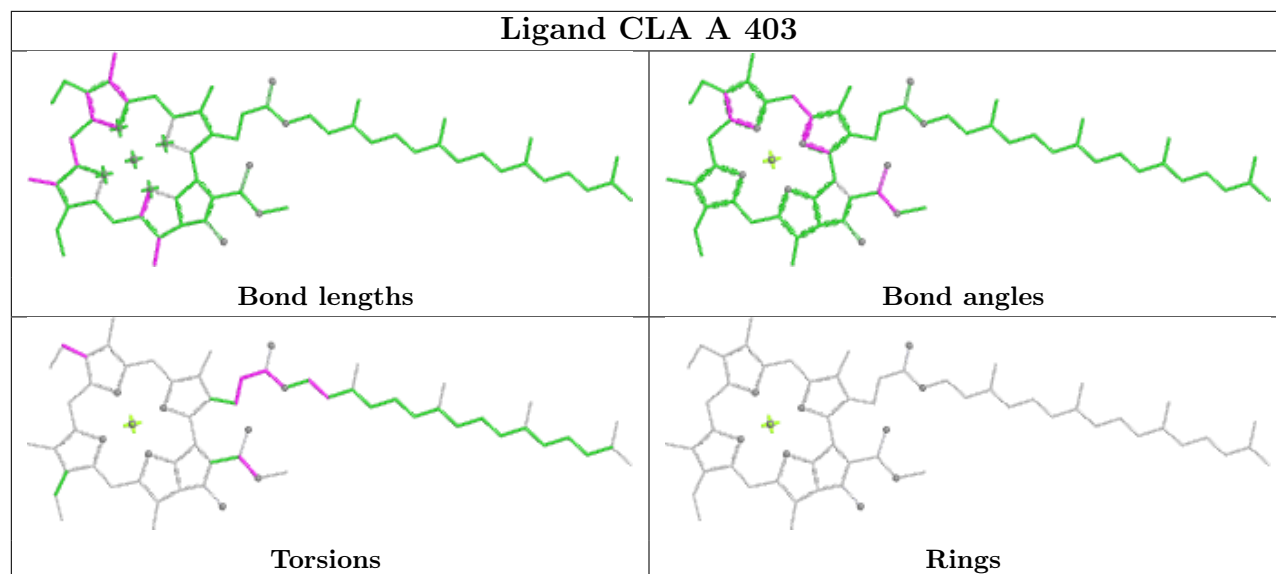
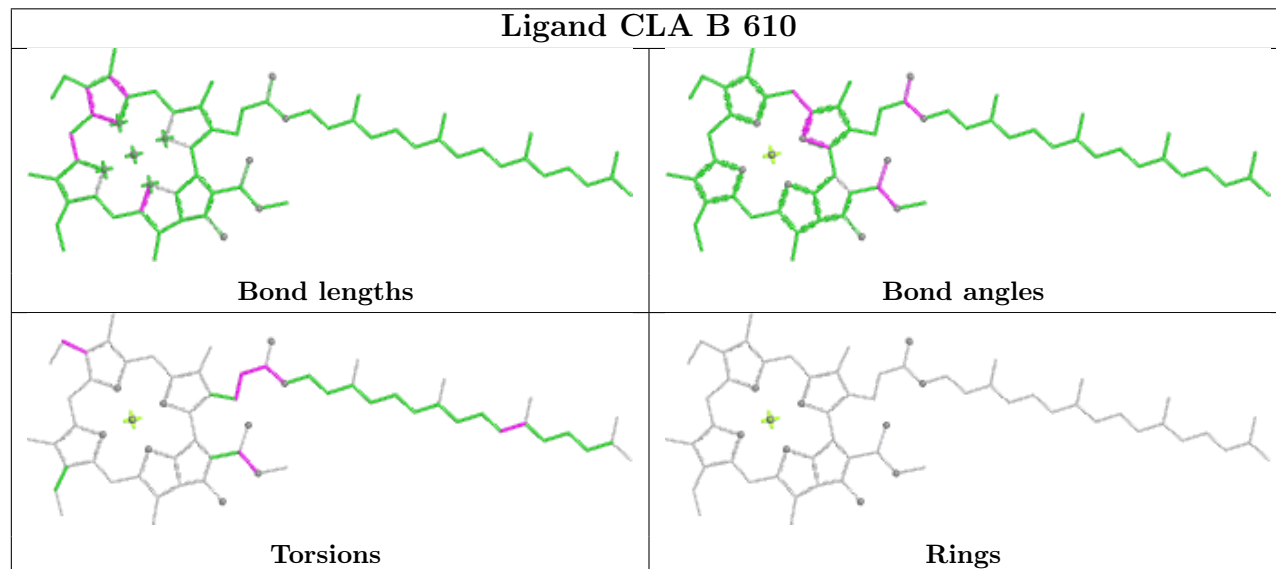


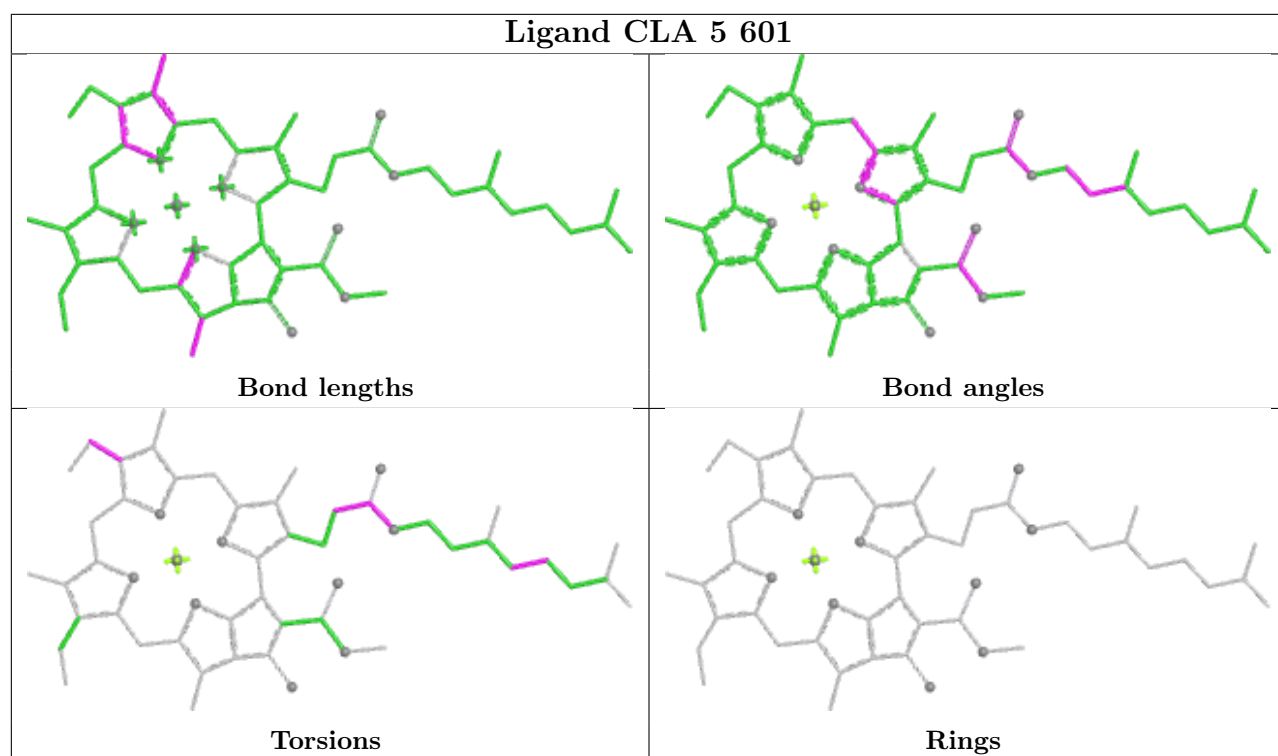
Ligand CLA R 610

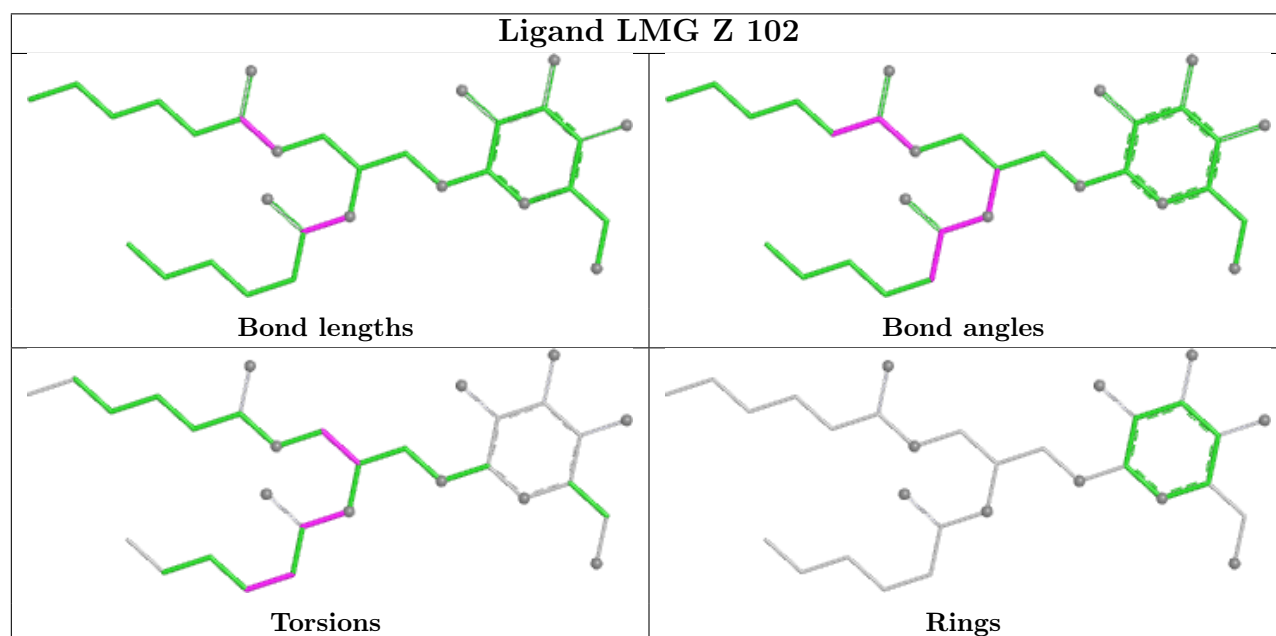
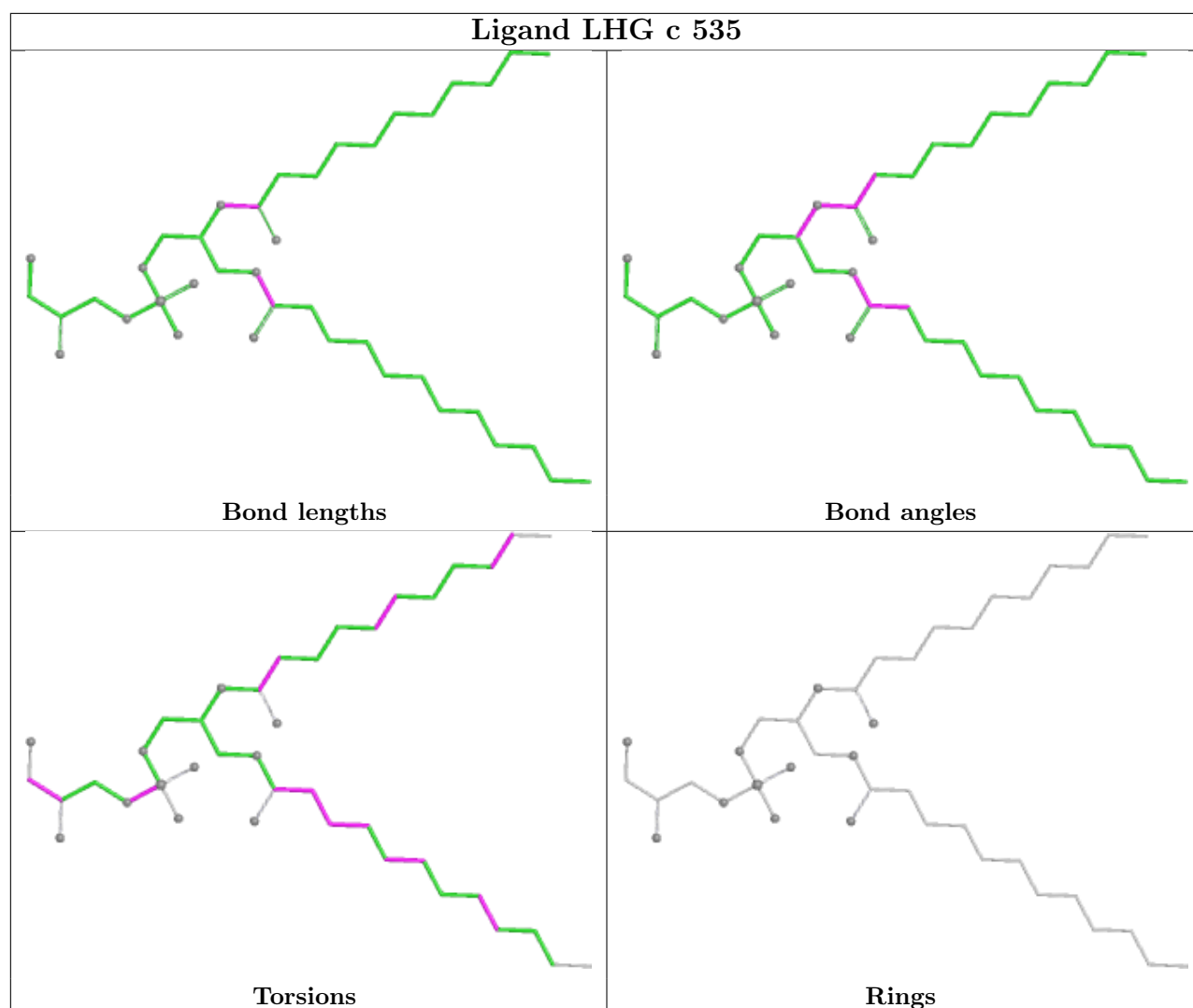


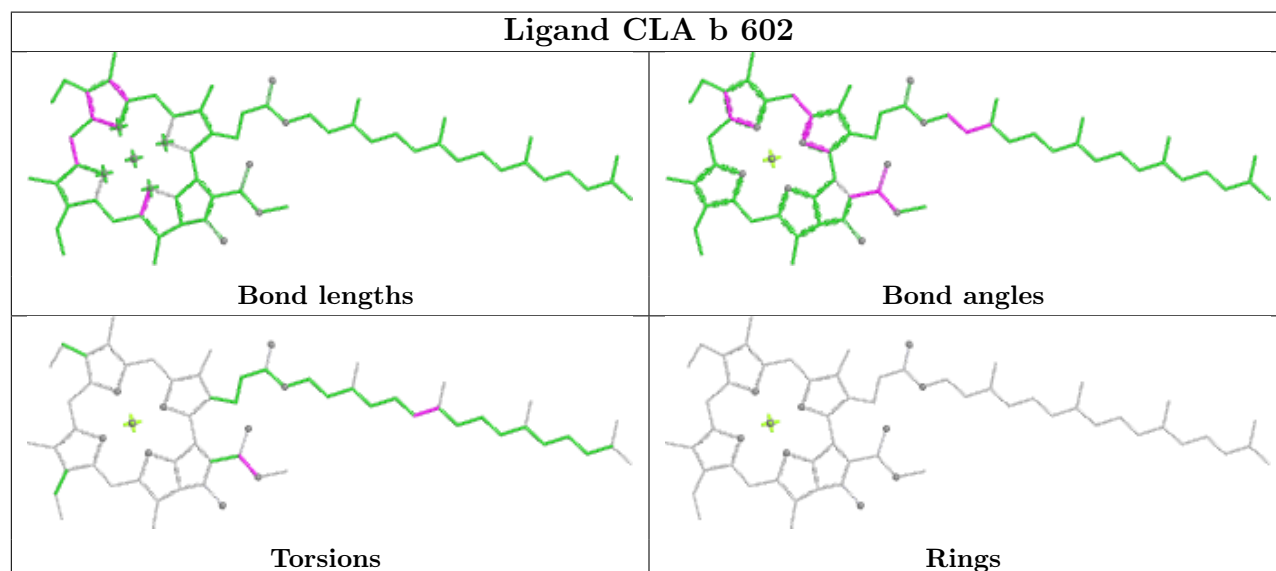
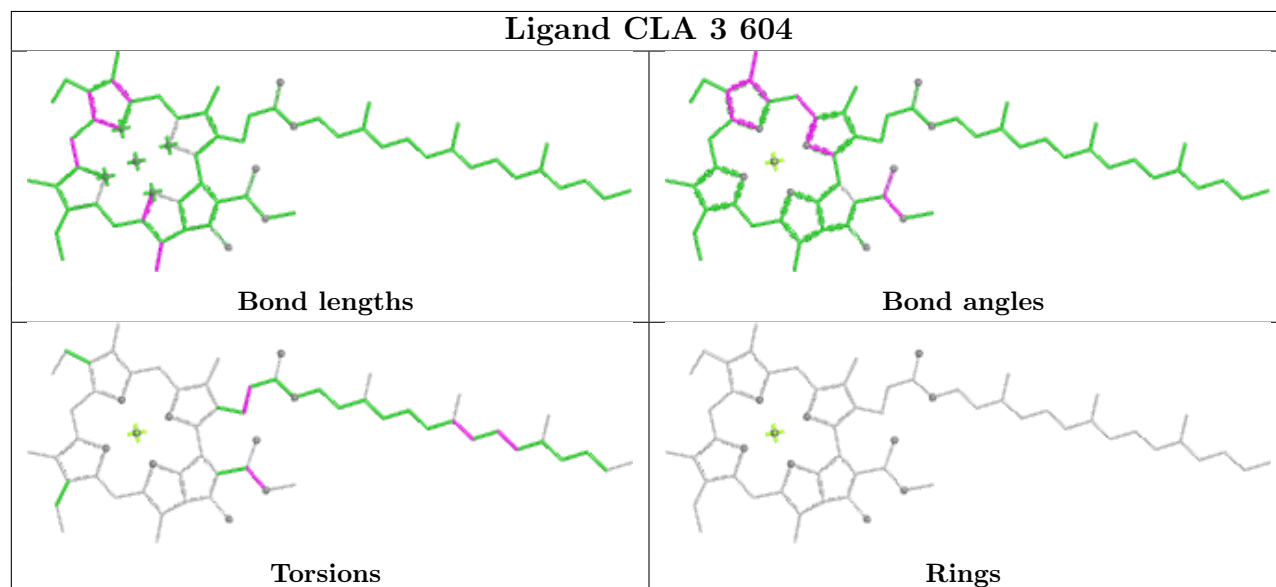
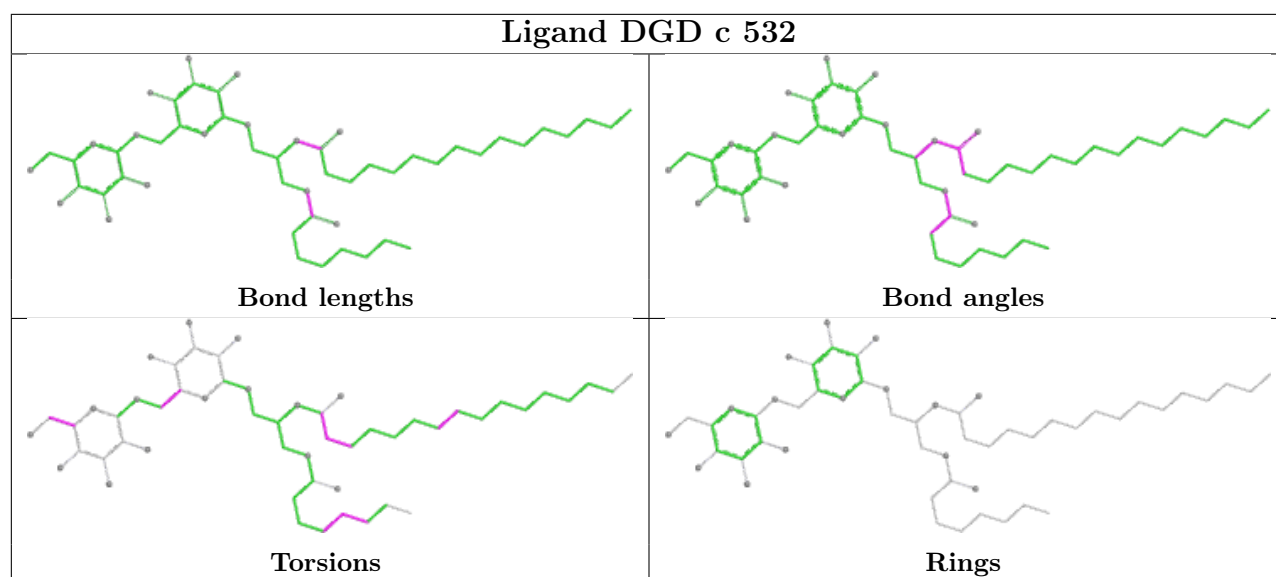
Ligand CLA O 601

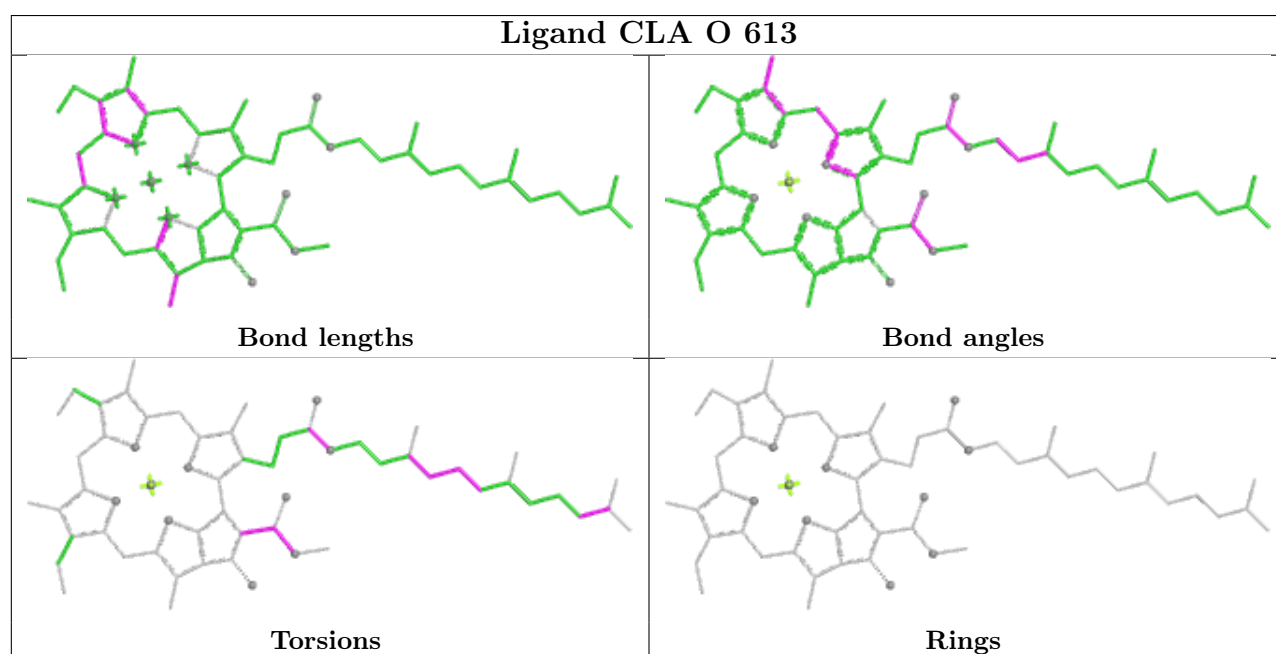
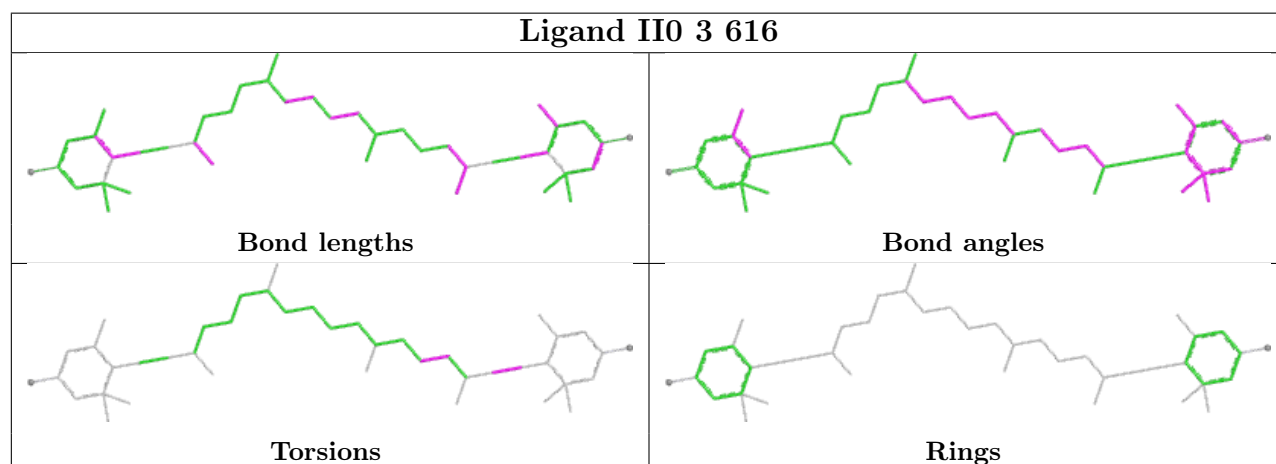
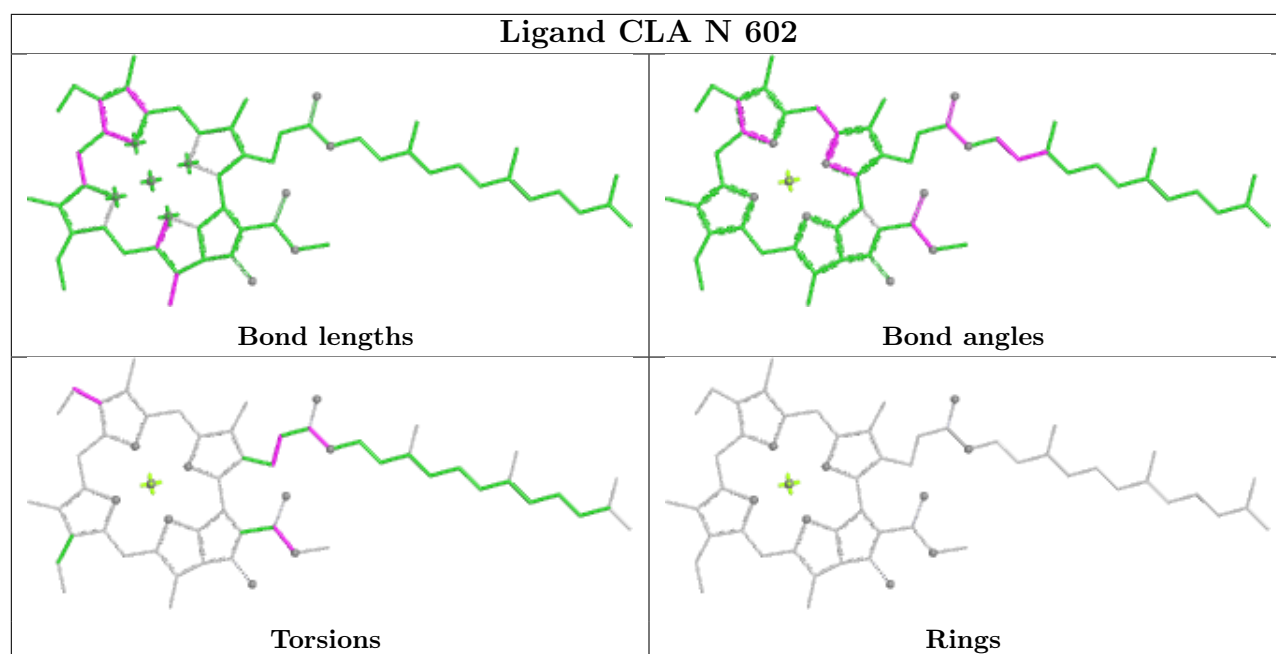


Ligand CLA A 403**Ligand CLA B 610**

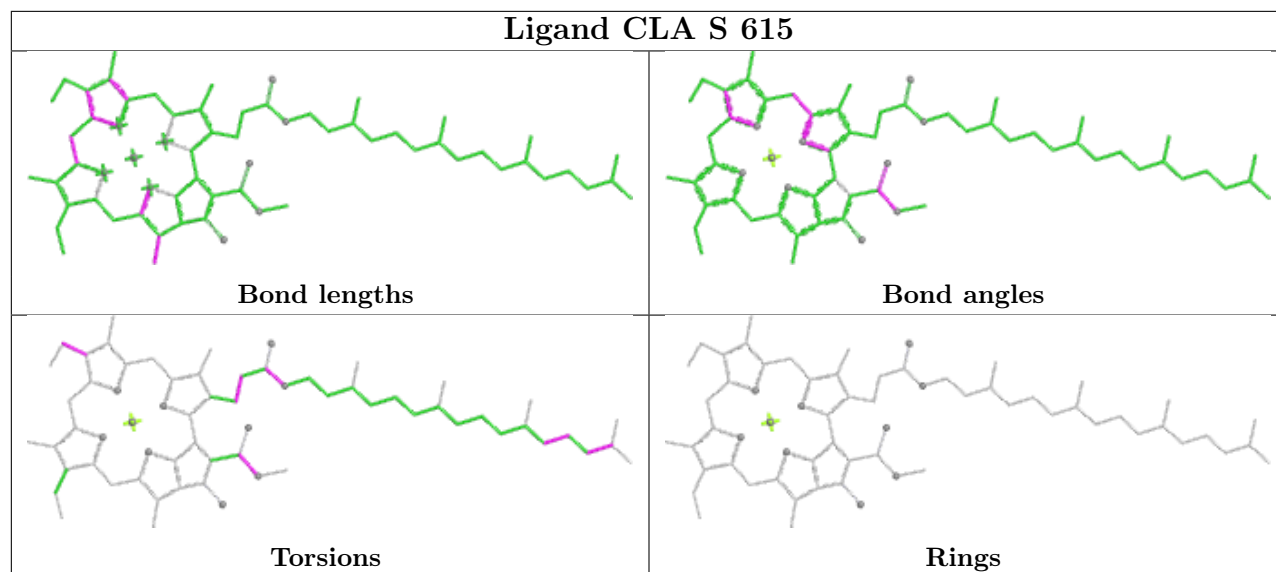




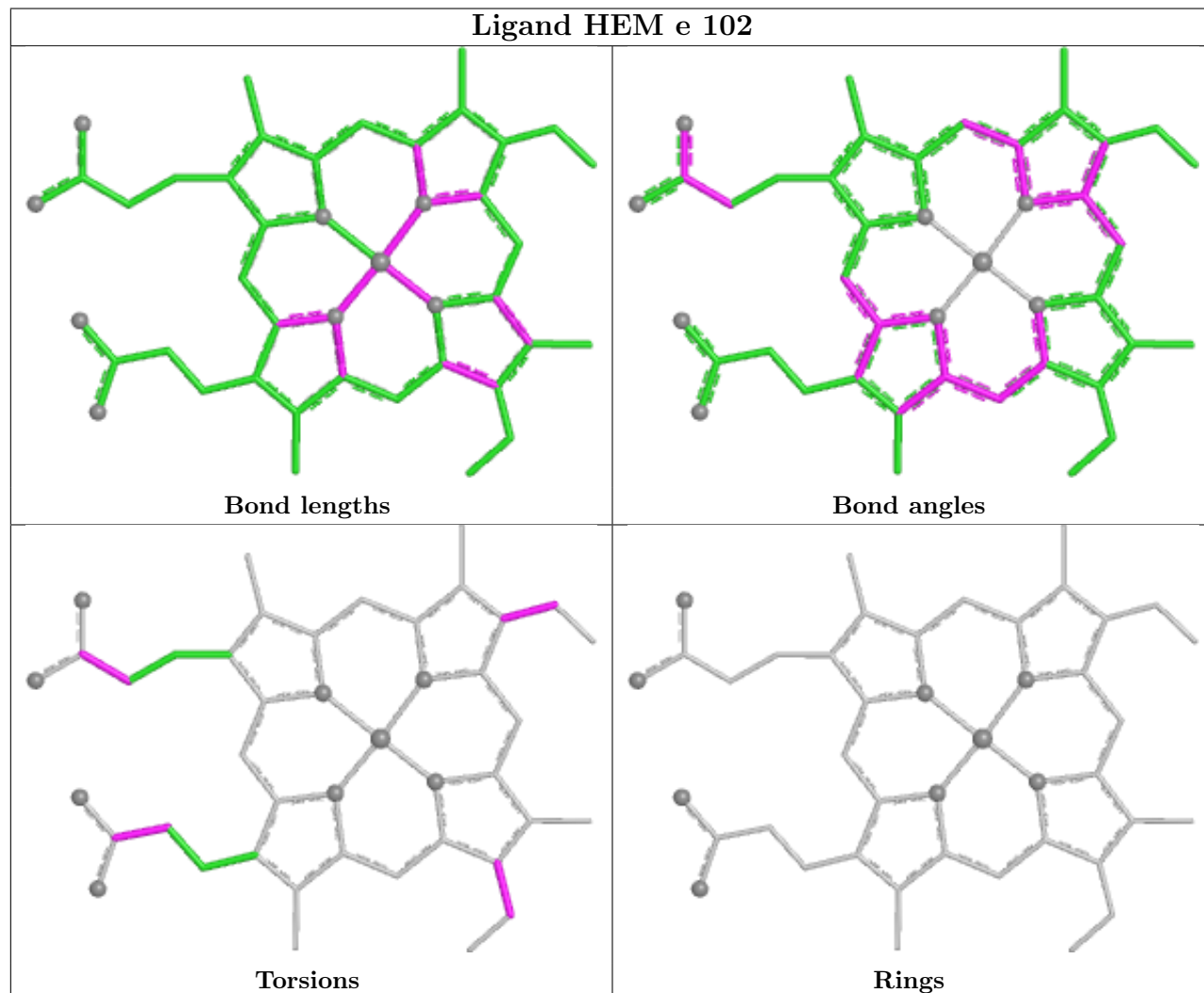




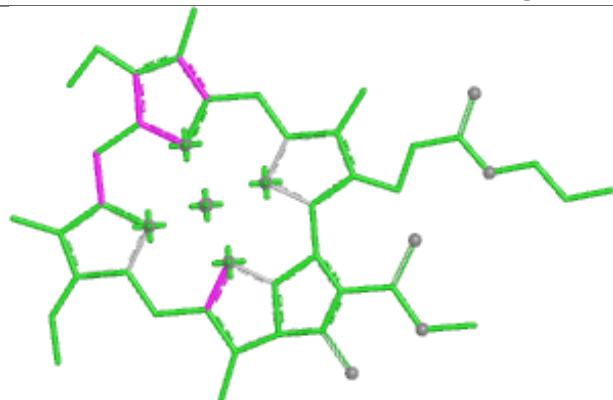
Ligand CLA S 615



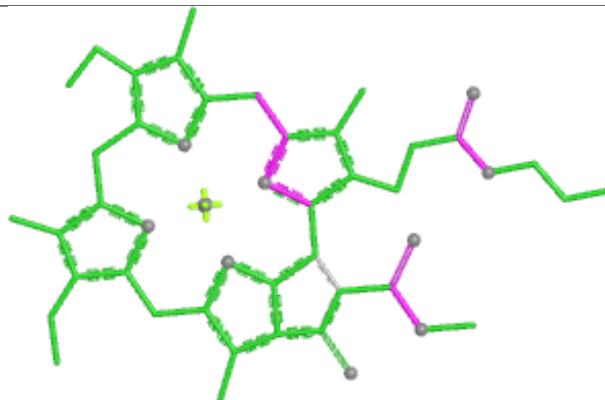
Ligand HEM e 102



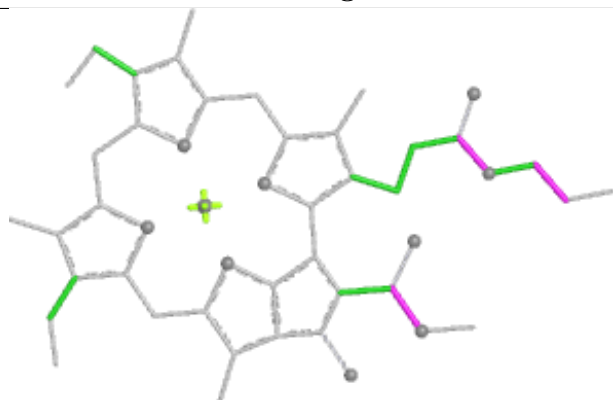
Ligand CLA 1 614



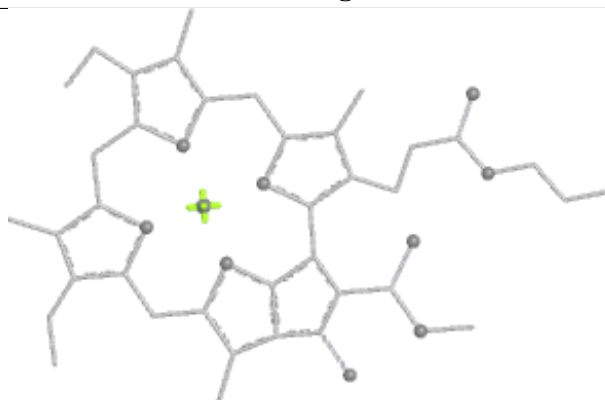
Bond lengths



Bond angles

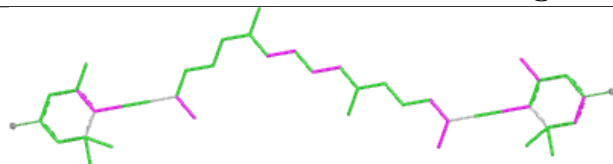


Torsions

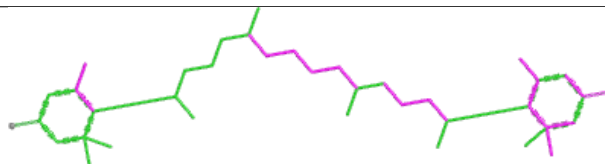


Rings

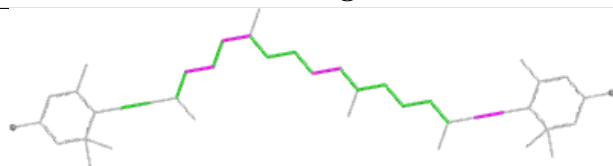
Ligand II0 6 616



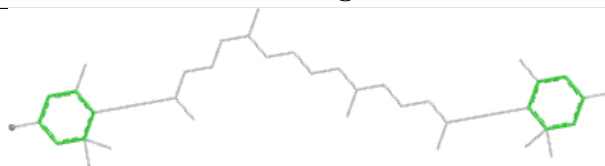
Bond lengths



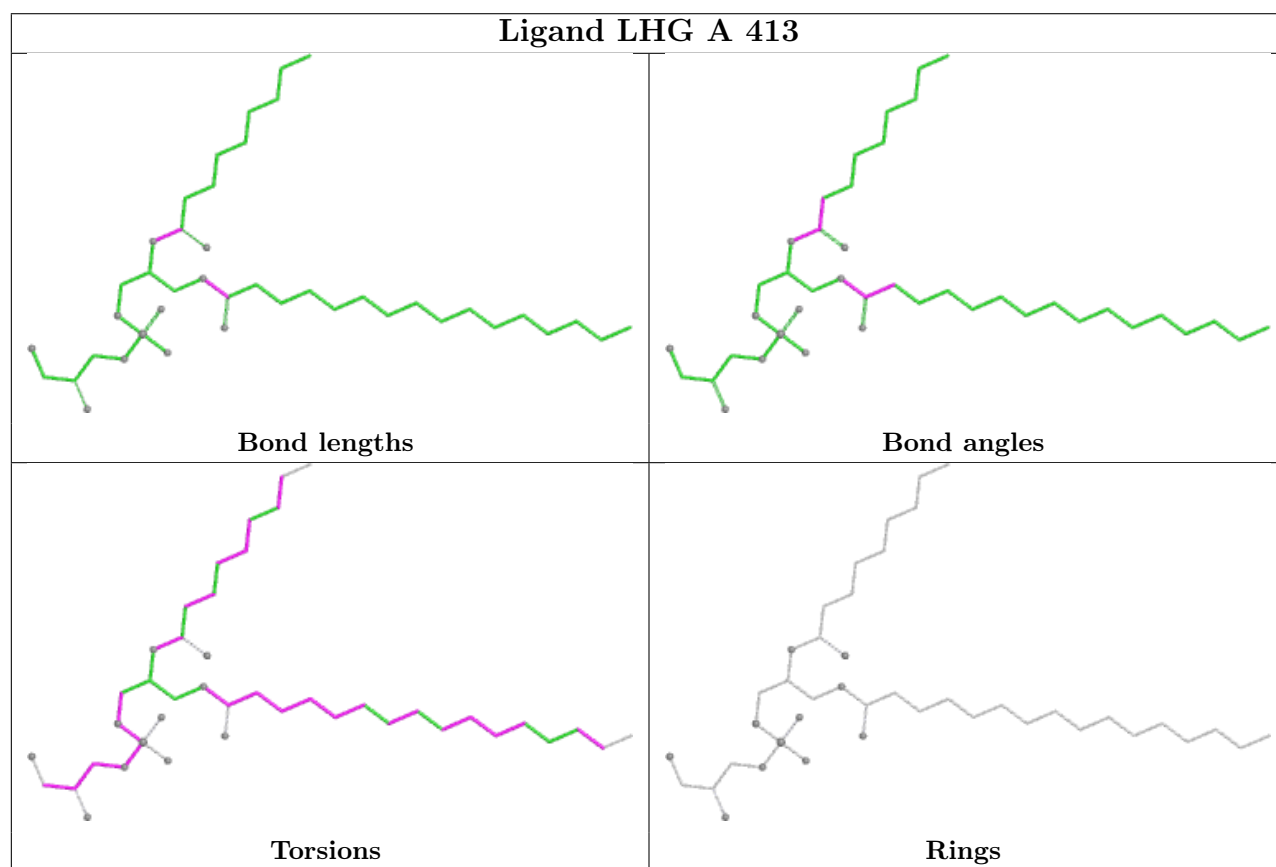
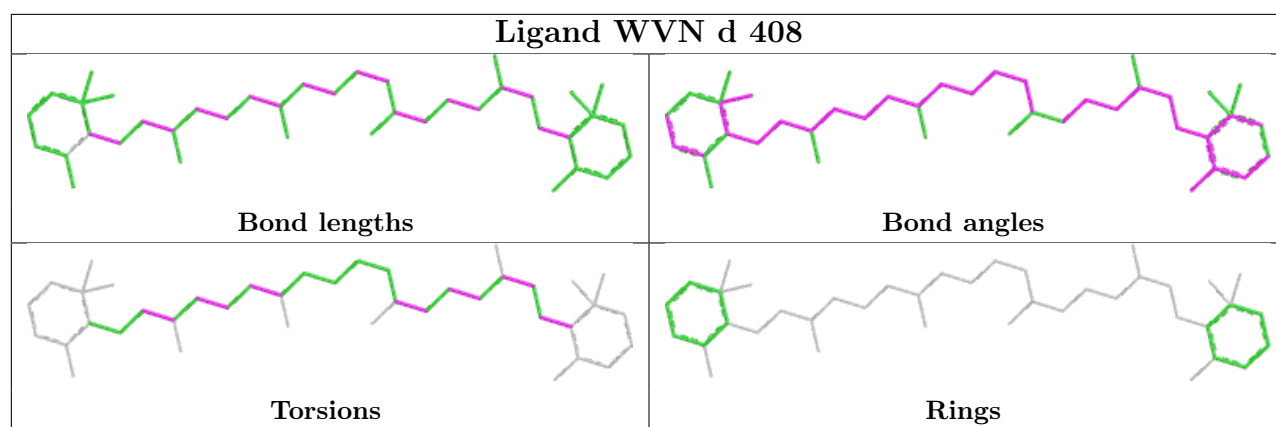
Bond angles



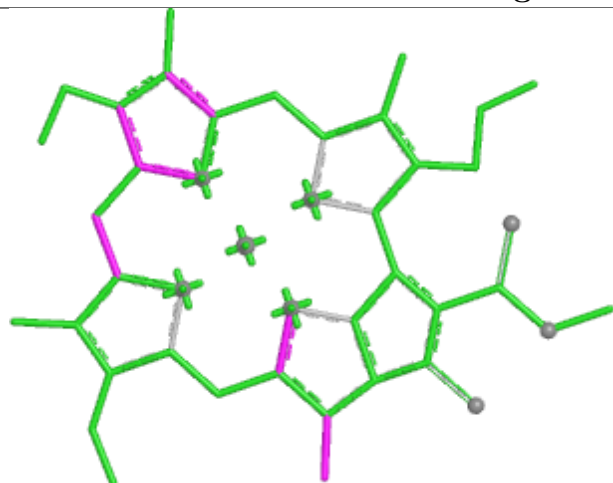
Torsions



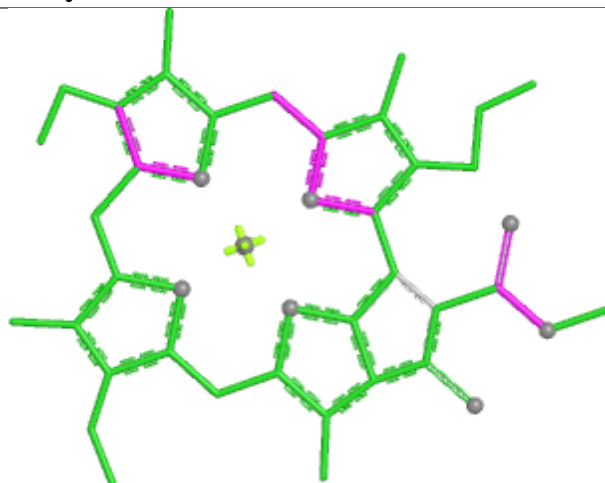
Rings



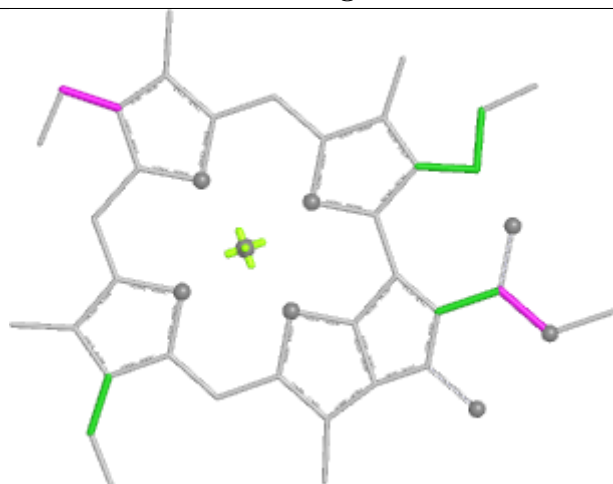
Ligand CLA Q 615



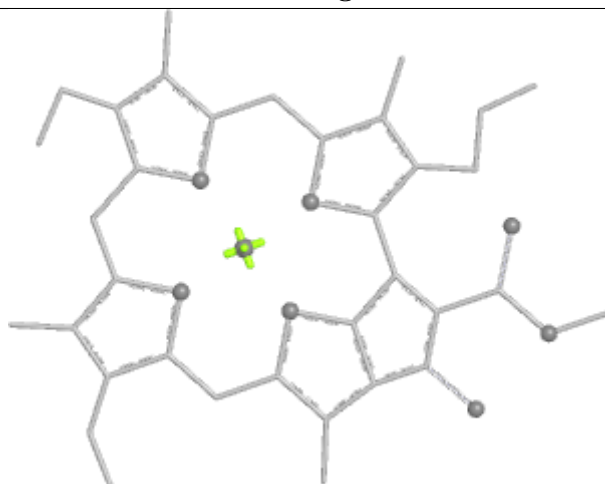
Bond lengths



Bond angles

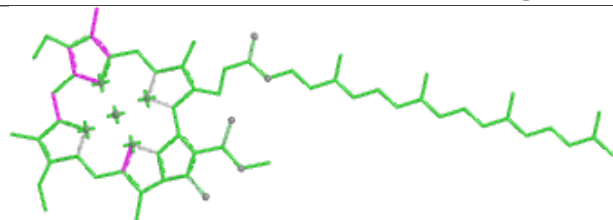


Torsions

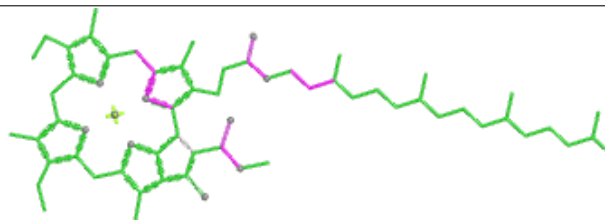


Rings

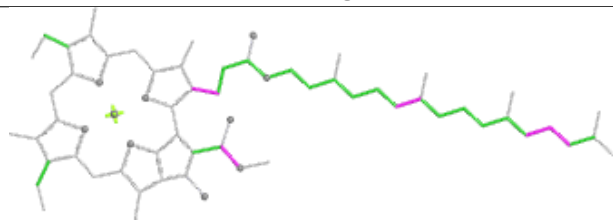
Ligand CLA b 609



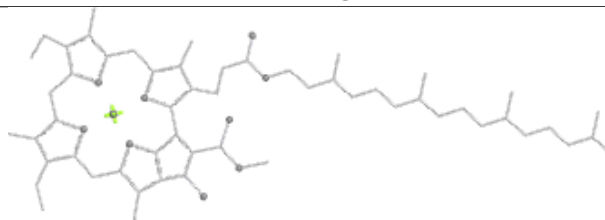
Bond lengths



Bond angles

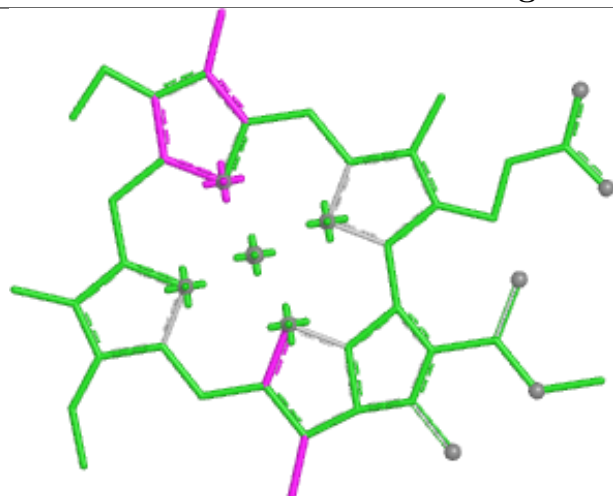


Torsions

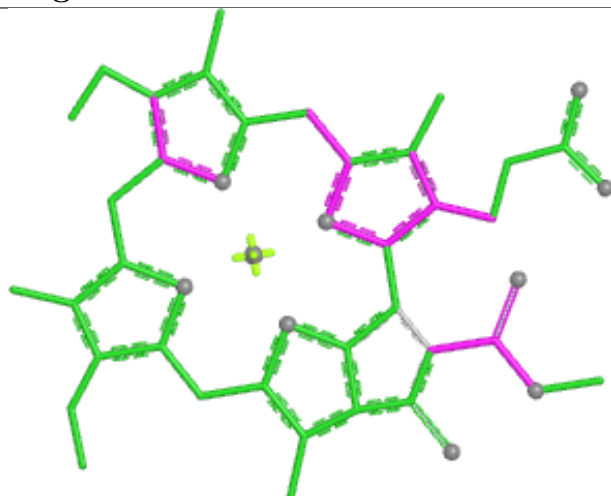


Rings

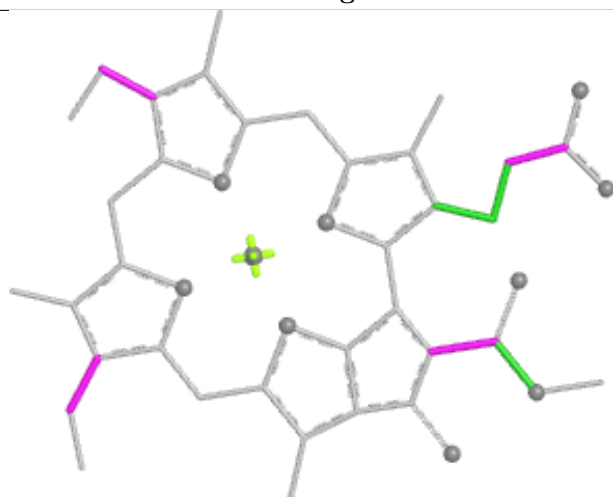
Ligand CLA g 302



Bond lengths



Bond angles

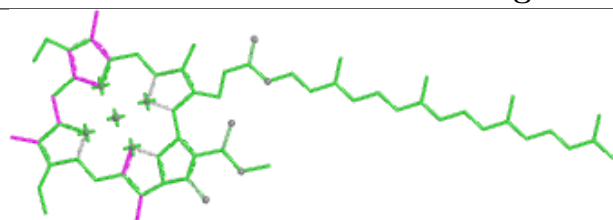


Torsions

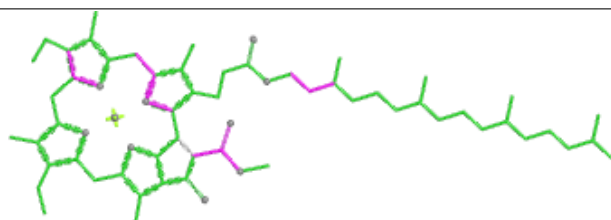


Rings

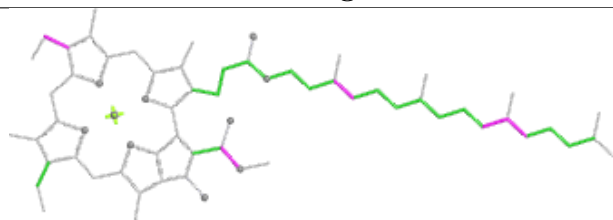
Ligand CLA R 609



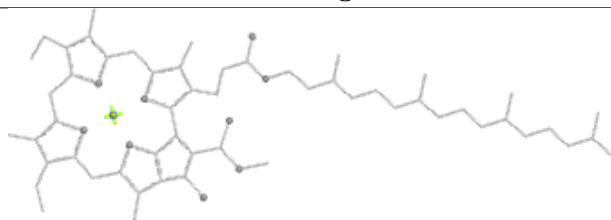
Bond lengths



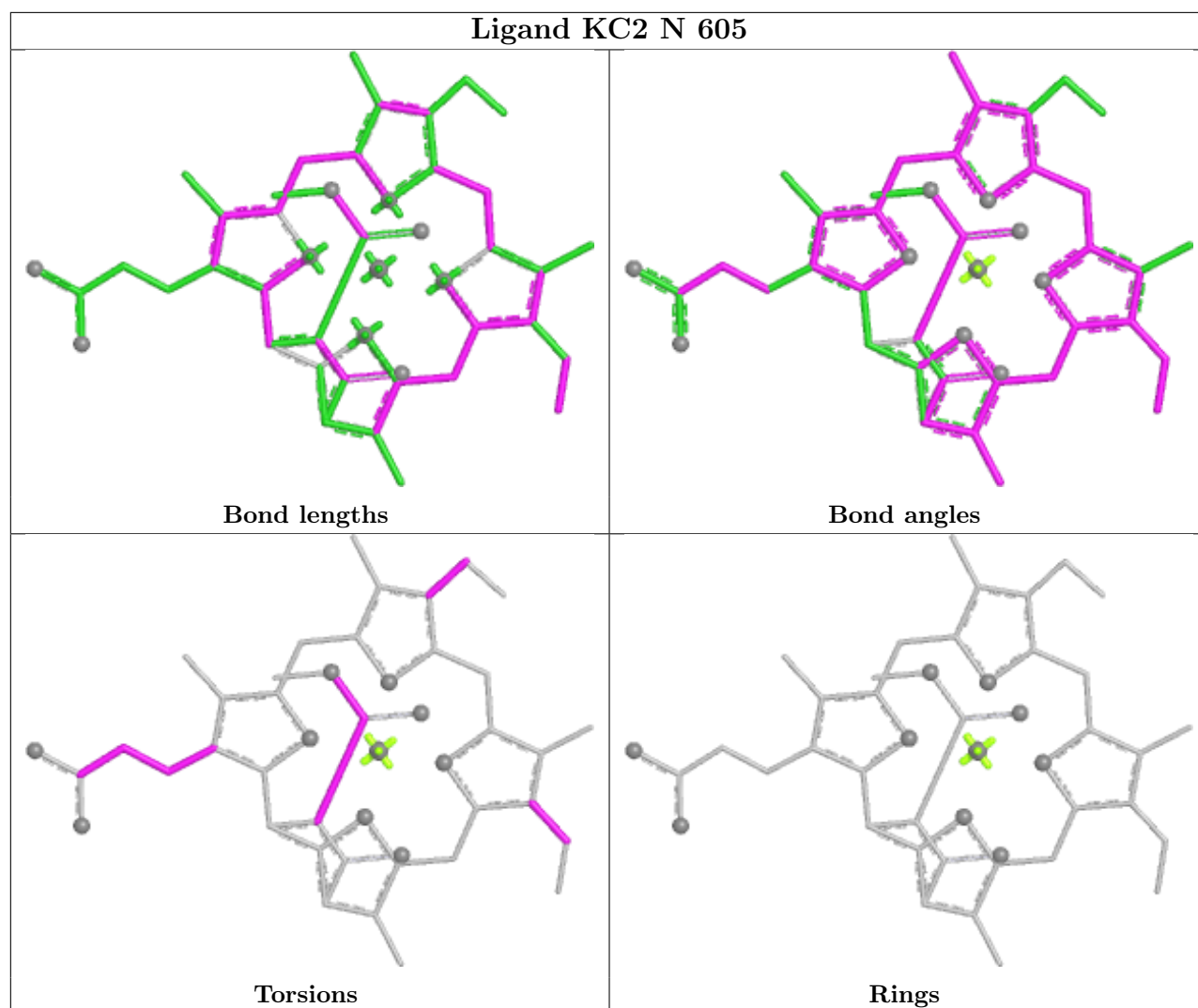
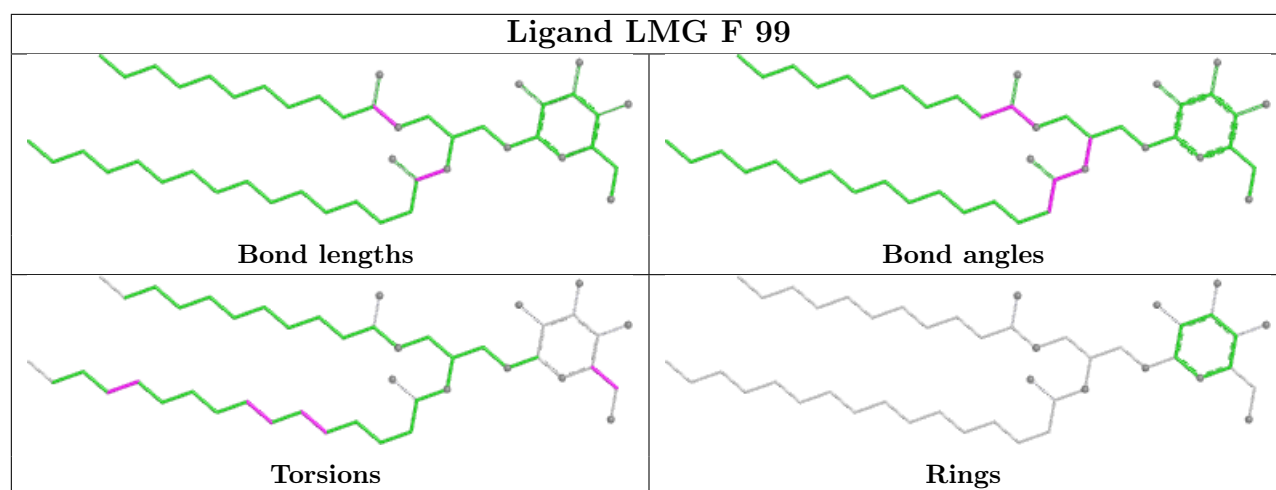
Bond angles

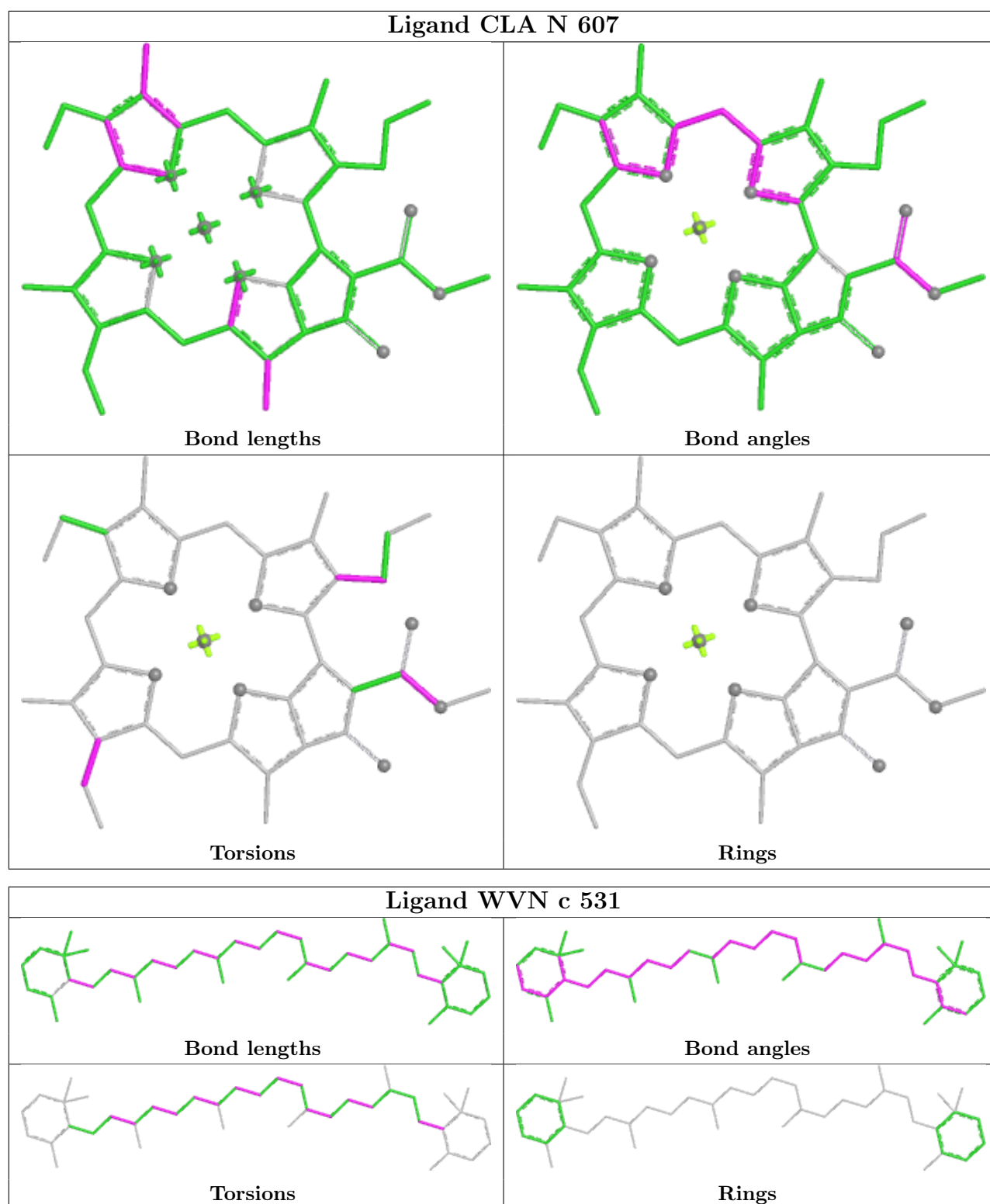


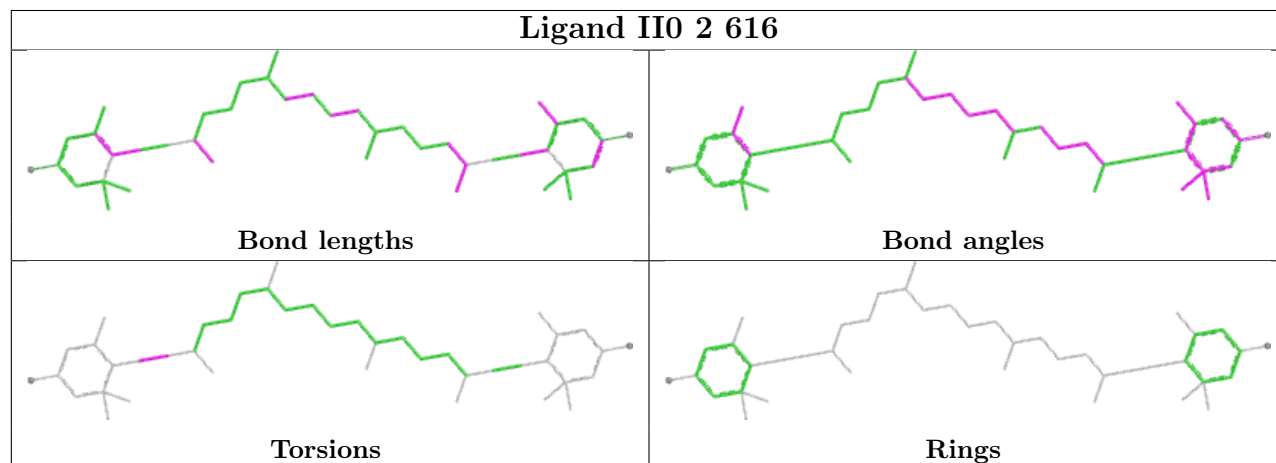
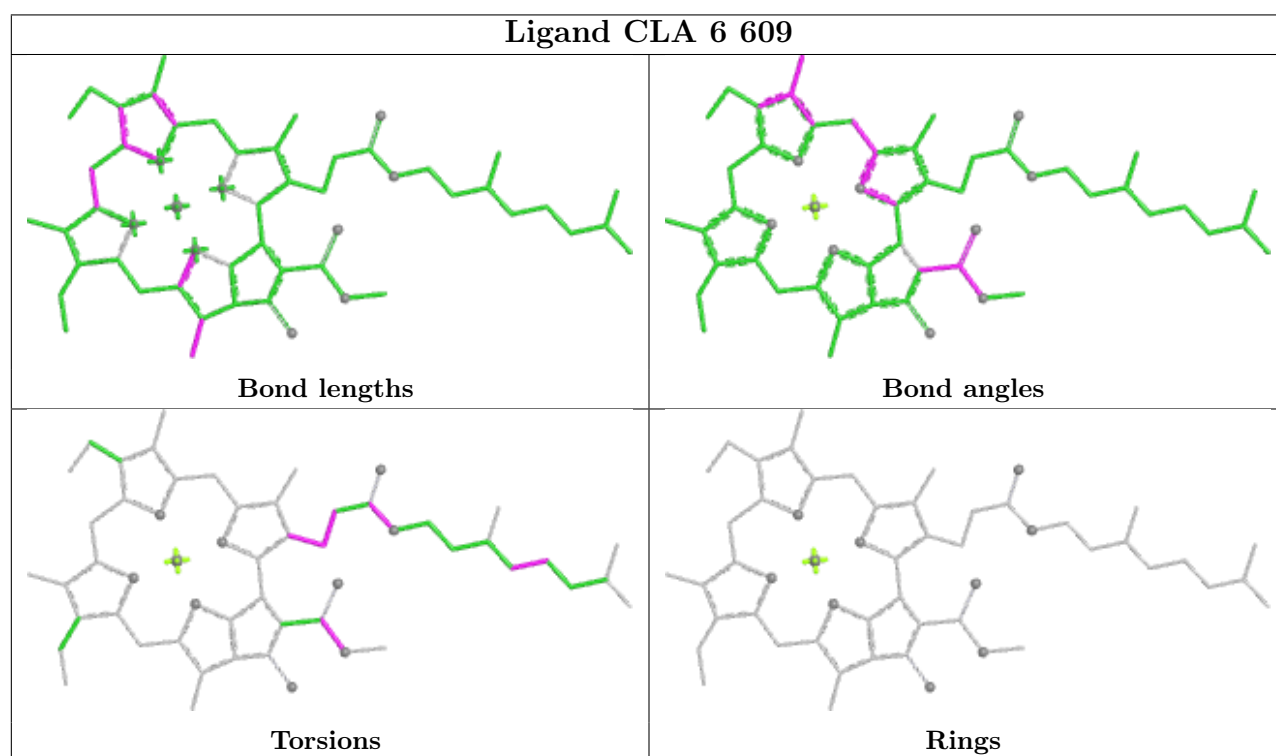
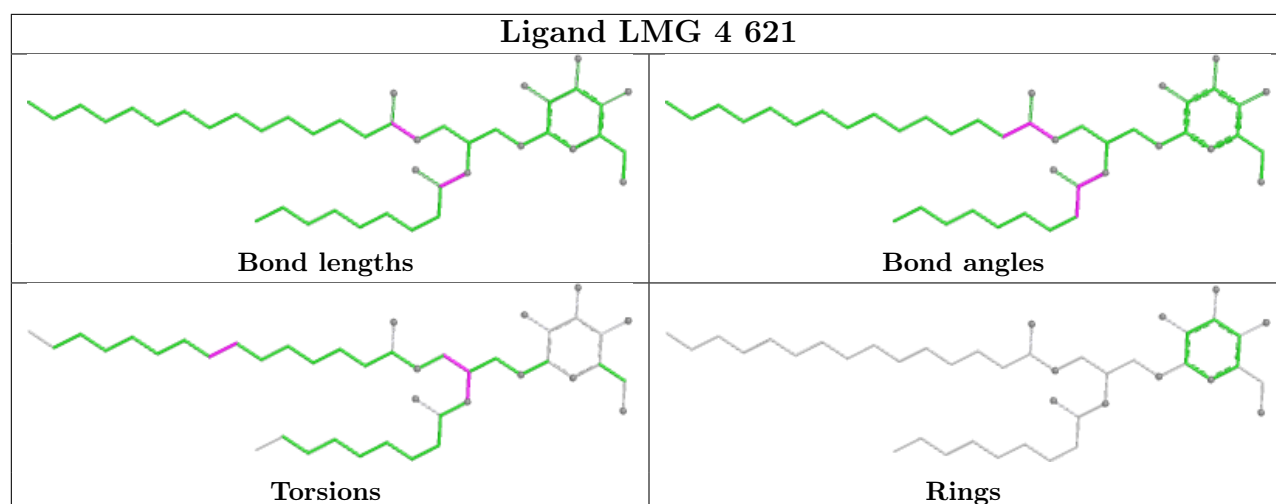
Torsions



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.

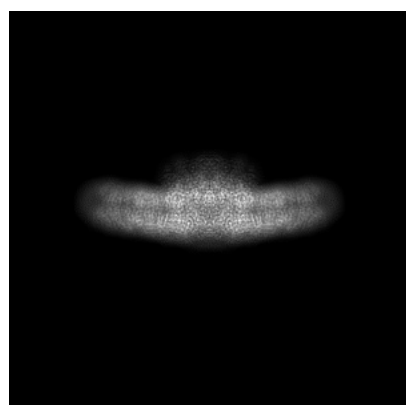
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-38455. These allow visual inspection of the internal detail of the map and identification of artifacts.

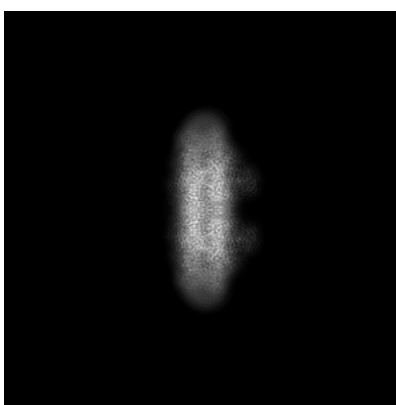
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

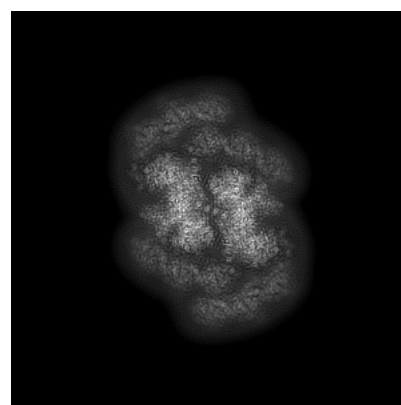
6.1.1 Primary map



X



Y

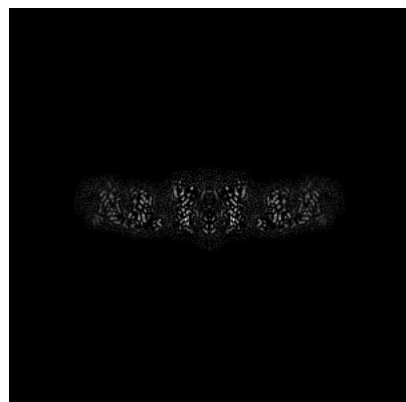


Z

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

6.2 Central slices [i](#)

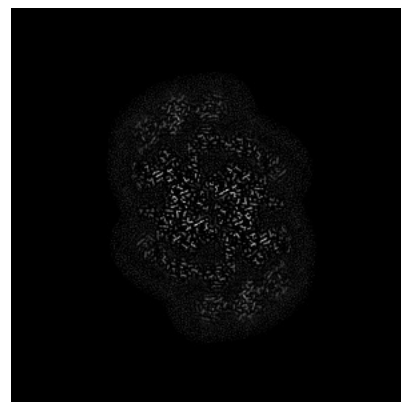
6.2.1 Primary map



X Index: 208



Y Index: 208

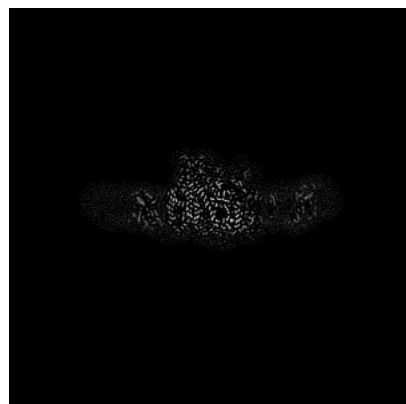


Z Index: 208

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

6.3 Largest variance slices [i](#)

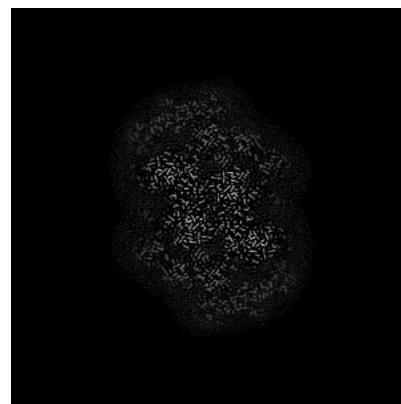
6.3.1 Primary map



X Index: 182



Y Index: 222

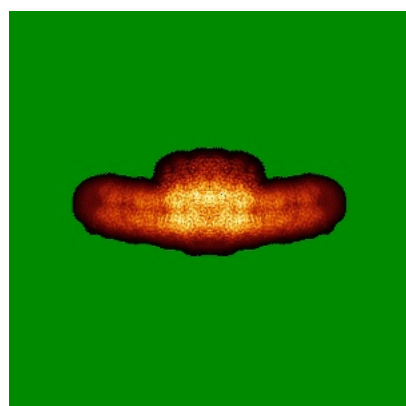


Z Index: 198

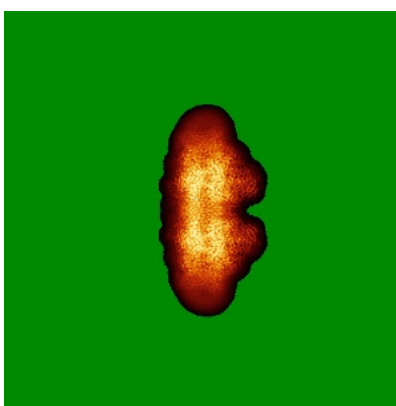
The images above show the largest variance slices of the map in three orthogonal directions.

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

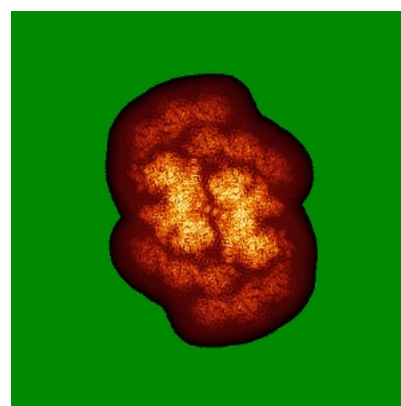
6.4.1 Primary map



X



Y

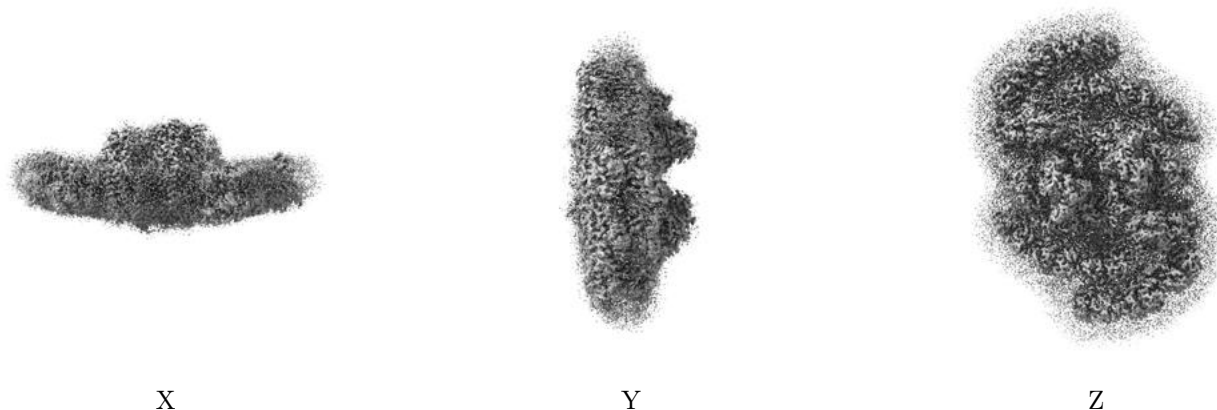


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.024. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

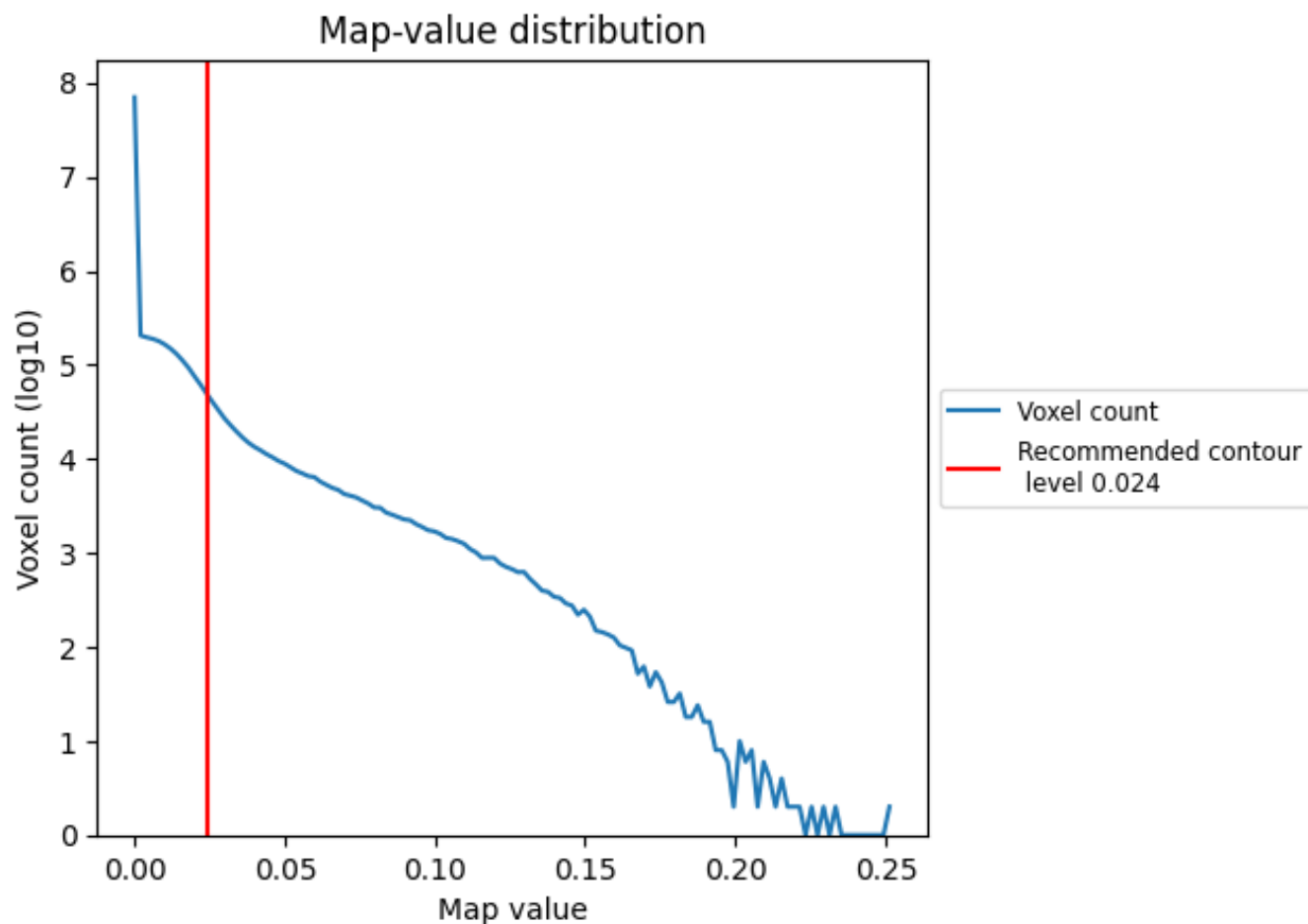
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

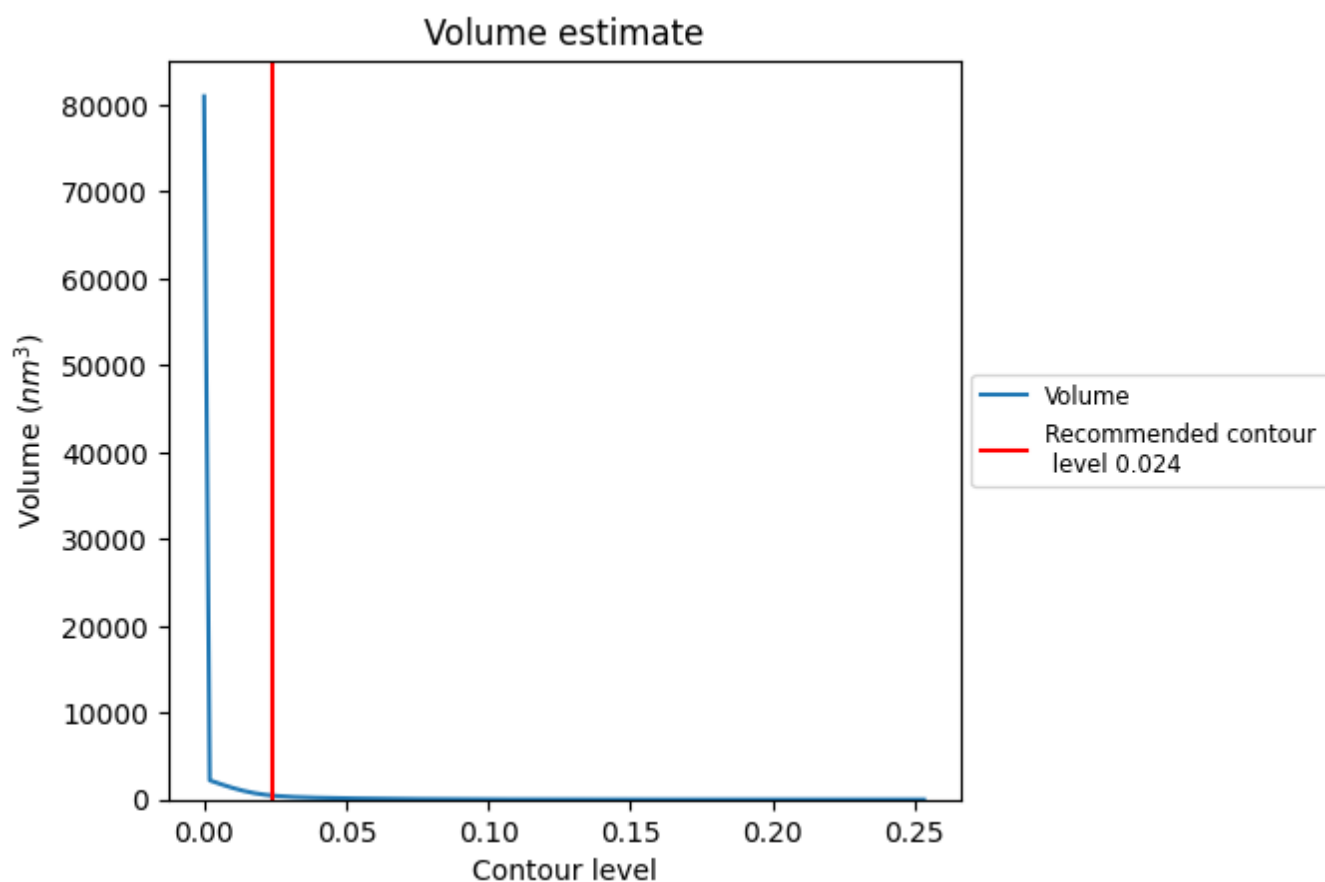
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

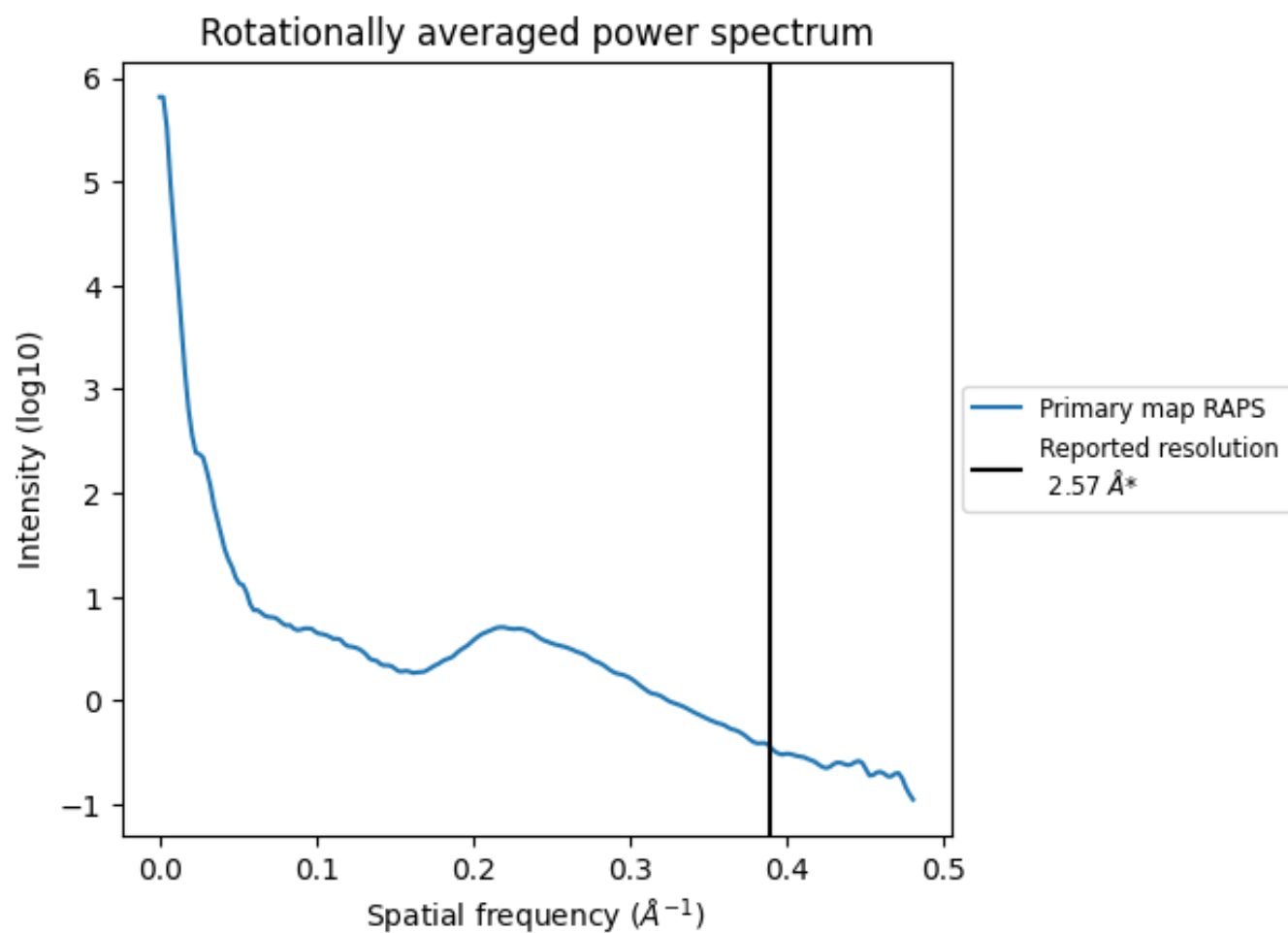
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 462 nm^3 ; this corresponds to an approximate mass of 417 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 0.389 Å⁻¹

8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

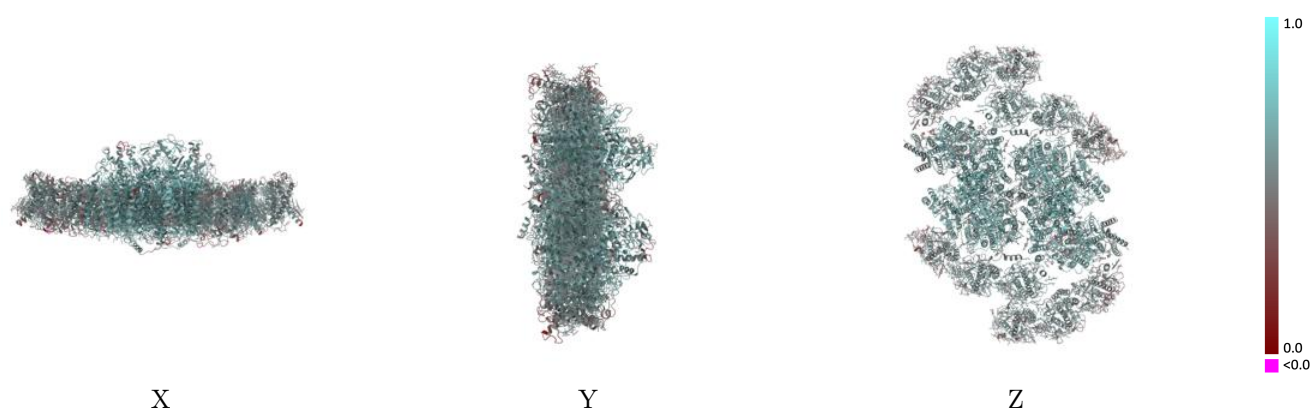
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-38455 and PDB model 8XLP. Per-residue inclusion information can be found in section 3 on page 40.

9.1 Map-model overlay [i](#)

This section was not generated.

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

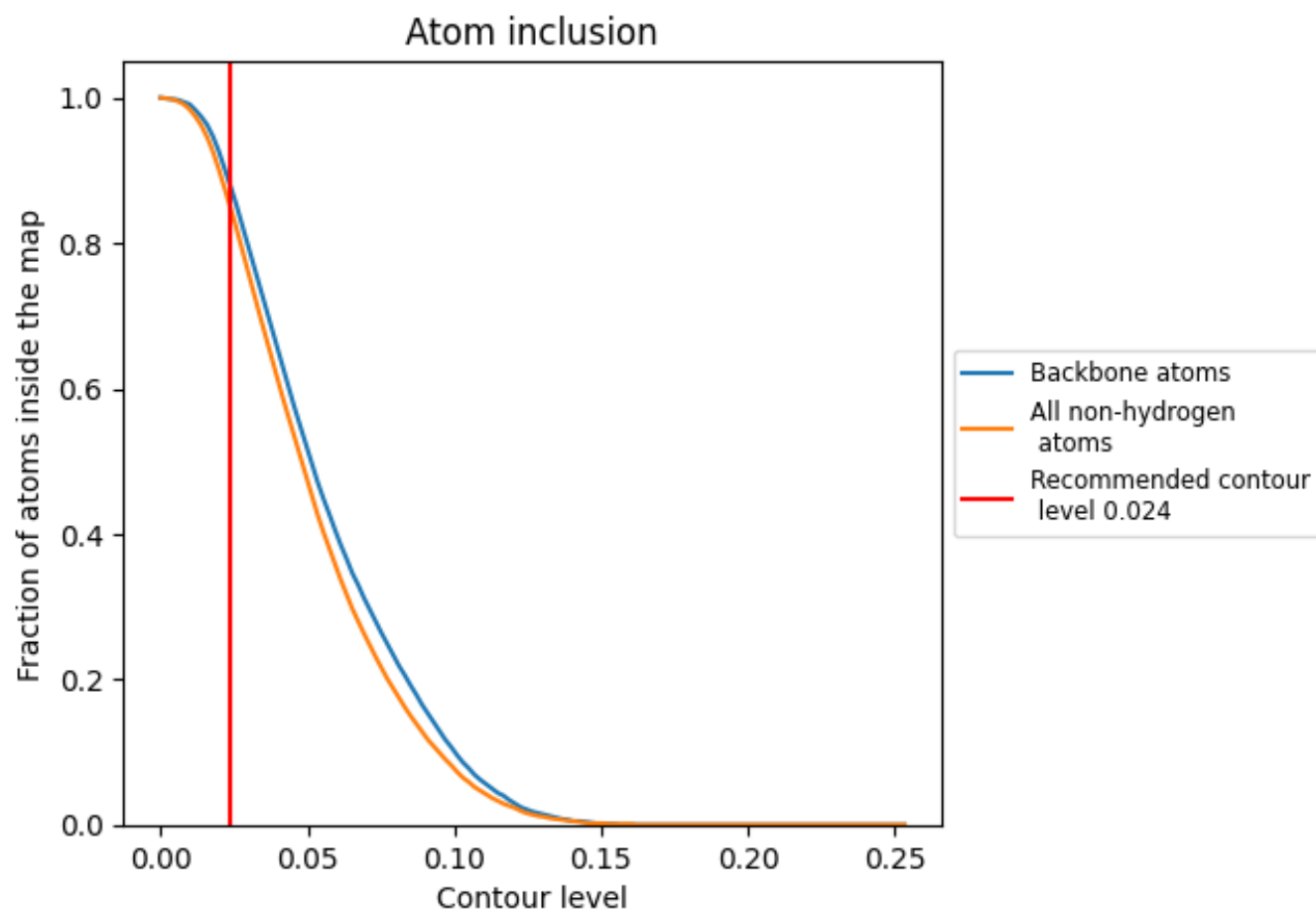


The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 85% 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 (0.024) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8460	 0.5980
1	 0.7140	 0.5020
2	 0.8310	 0.5580
3	 0.8790	 0.5930
4	 0.7750	 0.5350
5	 0.7940	 0.5290
6	 0.6910	 0.4620
A	 0.9410	 0.6790
B	 0.9180	 0.6570
C	 0.8900	 0.6360
D	 0.9550	 0.6820
E	 0.7920	 0.5820
F	 0.7420	 0.5460
G	 0.7280	 0.5440
H	 0.9280	 0.6440
I	 0.9790	 0.6960
K	 0.8700	 0.6110
L	 0.9620	 0.6660
M	 0.8390	 0.5970
N	 0.6900	 0.4630
O	 0.8340	 0.5610
P	 0.8800	 0.5980
Q	 0.7760	 0.5270
R	 0.8050	 0.5410
S	 0.6950	 0.4870
T	 0.9410	 0.6690
W	 0.8860	 0.6330
X	 0.8830	 0.6140
Y	 0.6100	 0.5300
Z	 0.6220	 0.4910
a	 0.9440	 0.6800
b	 0.9160	 0.6570
c	 0.8870	 0.6360
d	 0.9540	 0.6820
e	 0.7830	 0.5780



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Chain	Atom inclusion	Q-score
f	 0.7520	 0.5470
g	 0.7260	 0.5500
h	 0.9230	 0.6430
i	 0.9790	 0.6900
k	 0.8870	 0.6100
l	 0.9650	 0.6690
m	 0.8290	 0.5940
t	 0.9330	 0.6710
w	 0.8590	 0.6060
x	 0.8910	 0.6090
y	 0.5990	 0.5230
z	 0.6160	 0.5020