



wwPDB EM Validation Summary Report ⓘ

Nov 12, 2024 – 05:30 AM JST

PDB ID : 8JJR
EMDB ID : EMD-36366
Title : Cryo-EM structure of Symbiodinium photosystem I
Authors : Zhao, L.S.; Wang, N.; Li, K.; Zhang, Y.Z.; Liu, L.N.
Deposited on : 2023-05-31
Resolution : 2.80 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.dev113
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

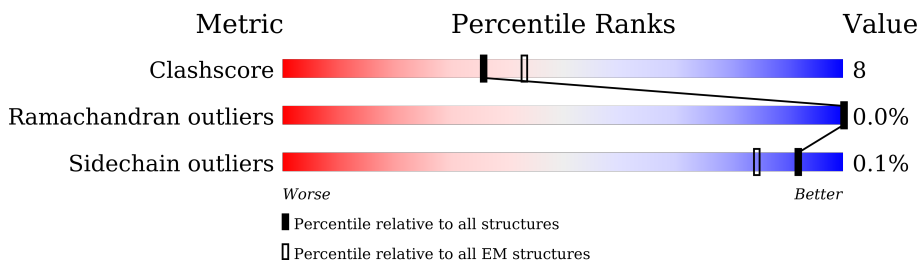
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY



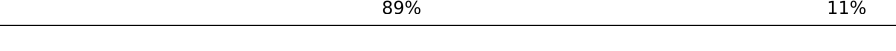
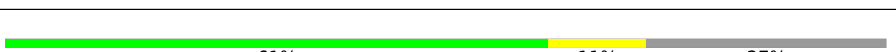


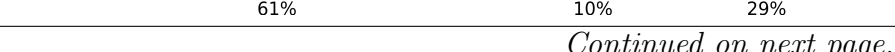

The reported resolution of this entry is 2.80 Å.

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.






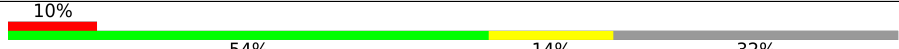

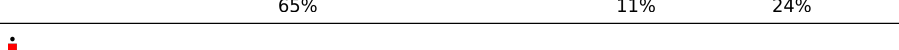
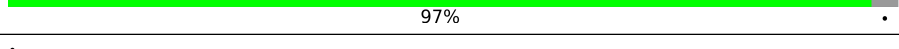
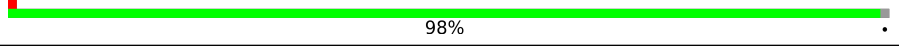

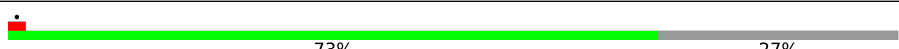





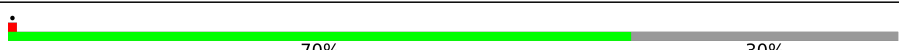

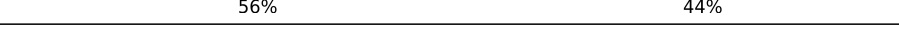
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	256	
2	B	269	
3	C	193	
4	D	177	
5	E	253	
6	F	286	
7	G	228	
8	H	271	

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Mol	Chain	Length	Quality of chain
9	I	246	
10	J	203	
11	K	226	
12	T	206	
13	U	137	
14	a	687	
15	b	669	
16	c	161	
17	d	295	
18	e	121	
19	f	279	
20	i	179	
21	j	141	
22	l	361	
23	m	142	
24	r	152	
25	x	121	
26	y	223	

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
27	CLA	A	601	X	-	-	-
27	CLA	A	602	X	-	-	-
27	CLA	A	603	X	-	-	-
27	CLA	A	604	X	-	-	-
27	CLA	A	605	X	-	-	-
27	CLA	A	606	X	-	-	-
27	CLA	A	607	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
27	CLA	A	609	X	-	-	-
27	CLA	A	610	X	-	-	-
27	CLA	A	611	X	-	-	-
27	CLA	A	612	X	-	-	-
27	CLA	B	601	X	-	-	-
27	CLA	B	603	X	-	-	-
27	CLA	B	604	X	-	-	-
27	CLA	B	605	X	-	-	-
27	CLA	B	606	X	-	-	-
27	CLA	B	607	X	-	-	-
27	CLA	B	609	X	-	-	-
27	CLA	B	610	X	-	-	-
27	CLA	C	201	X	-	-	-
27	CLA	C	202	X	-	-	-
27	CLA	C	203	X	-	-	-
27	CLA	C	204	X	-	-	-
27	CLA	C	205	X	-	-	-
27	CLA	C	206	X	-	-	-
27	CLA	C	207	X	-	-	-
27	CLA	C	208	X	-	-	-
27	CLA	C	209	X	-	-	-
27	CLA	C	211	X	-	-	-
27	CLA	C	212	X	-	-	-
27	CLA	D	601	X	-	-	-
27	CLA	D	602	X	-	-	-
27	CLA	D	603	X	-	-	-
27	CLA	D	604	X	-	-	-
27	CLA	D	605	X	-	-	-
27	CLA	D	606	X	-	-	-
27	CLA	D	607	X	-	-	-
27	CLA	D	608	X	-	-	-
27	CLA	D	609	X	-	-	-
27	CLA	D	610	X	-	-	-
27	CLA	D	611	X	-	-	-
27	CLA	D	612	X	-	-	-
27	CLA	E	602	X	-	-	-
27	CLA	E	603	X	-	-	-
27	CLA	E	604	X	-	-	-
27	CLA	E	605	X	-	-	-
27	CLA	E	606	X	-	-	-
27	CLA	E	607	X	-	-	-
27	CLA	E	608	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
27	CLA	E	609	X	-	-	-
27	CLA	E	611	X	-	-	-
27	CLA	E	612	X	-	-	-
27	CLA	F	601	X	-	-	-
27	CLA	F	602	X	-	-	-
27	CLA	F	603	X	-	-	-
27	CLA	F	604	X	-	-	-
27	CLA	F	605	X	-	-	-
27	CLA	F	606	X	-	-	-
27	CLA	F	607	X	-	-	-
27	CLA	F	608	X	-	-	-
27	CLA	F	610	X	-	-	-
27	CLA	F	617	X	-	-	-
27	CLA	F	619	X	-	-	-
27	CLA	G	602	X	-	-	-
27	CLA	G	603	X	-	-	-
27	CLA	G	604	X	-	-	-
27	CLA	G	605	X	-	-	-
27	CLA	G	606	X	-	-	-
27	CLA	G	607	X	-	-	-
27	CLA	G	608	X	-	-	-
27	CLA	G	609	X	-	-	-
27	CLA	G	610	X	-	-	-
27	CLA	G	611	X	-	-	-
27	CLA	H	303	X	-	-	-
27	CLA	H	304	X	-	-	-
27	CLA	H	305	X	-	-	-
27	CLA	H	306	X	-	-	-
27	CLA	H	307	X	-	-	-
27	CLA	H	308	X	-	-	-
27	CLA	H	309	X	-	-	-
27	CLA	H	310	X	-	-	-
27	CLA	H	312	X	-	-	-
27	CLA	H	313	X	-	-	-
27	CLA	H	319	X	-	-	-
27	CLA	I	601	X	-	-	-
27	CLA	I	602	X	-	-	-
27	CLA	I	603	X	-	-	-
27	CLA	I	605	X	-	-	-
27	CLA	I	606	X	-	-	-
27	CLA	I	607	X	-	-	-
27	CLA	I	608	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
27	CLA	I	609	X	-	-	-
27	CLA	I	610	X	-	-	-
27	CLA	I	611	X	-	-	-
27	CLA	I	616	X	-	-	-
27	CLA	J	601	X	-	-	-
27	CLA	J	603	X	-	-	-
27	CLA	J	605	X	-	-	-
27	CLA	J	607	X	-	-	-
27	CLA	J	609	X	-	-	-
27	CLA	K	601	X	-	-	-
27	CLA	K	602	X	-	-	-
27	CLA	K	603	X	-	-	-
27	CLA	K	604	X	-	-	-
27	CLA	K	605	X	-	-	-
27	CLA	K	606	X	-	-	-
27	CLA	K	608	X	-	-	-
27	CLA	T	601	X	-	-	-
27	CLA	T	602	X	-	-	-
27	CLA	T	603	X	-	-	-
27	CLA	T	604	X	-	-	-
27	CLA	T	605	X	-	-	-
27	CLA	T	606	X	-	-	-
27	CLA	T	607	X	-	-	-
27	CLA	T	609	X	-	-	-
27	CLA	U	601	X	-	-	-
27	CLA	U	603	X	-	-	-
27	CLA	U	605	X	-	-	-
27	CLA	U	606	X	-	-	-
27	CLA	a	801	X	-	-	-
27	CLA	a	802	X	-	-	-
27	CLA	a	803	X	-	-	-
27	CLA	a	804	X	-	-	-
27	CLA	a	805	X	-	-	-
27	CLA	a	806	X	-	-	-
27	CLA	a	807	X	-	-	-
27	CLA	a	808	X	-	-	-
27	CLA	a	809	X	-	-	-
27	CLA	a	810	X	-	-	-
27	CLA	a	811	X	-	-	-
27	CLA	a	812	X	-	-	-
27	CLA	a	813	X	-	-	-
27	CLA	a	814	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
27	CLA	a	815	X	-	-	-
27	CLA	a	816	X	-	-	-
27	CLA	a	817	X	-	-	-
27	CLA	a	818	X	-	-	-
27	CLA	a	819	X	-	-	-
27	CLA	a	820	X	-	-	-
27	CLA	a	821	X	-	-	-
27	CLA	a	822	X	-	-	-
27	CLA	a	823	X	-	-	-
27	CLA	a	824	X	-	-	-
27	CLA	a	825	X	-	-	-
27	CLA	a	826	X	-	-	-
27	CLA	a	827	X	-	-	-
27	CLA	a	828	X	-	-	-
27	CLA	a	829	X	-	-	-
27	CLA	a	830	X	-	-	-
27	CLA	a	831	X	-	-	-
27	CLA	a	837	X	-	-	-
27	CLA	a	839	X	-	-	-
27	CLA	b	701	X	-	-	-
27	CLA	b	702	X	-	-	-
27	CLA	b	703	X	-	-	-
27	CLA	b	704	X	-	-	-
27	CLA	b	705	X	-	-	-
27	CLA	b	706	X	-	-	-
27	CLA	b	707	X	-	-	-
27	CLA	b	708	X	-	-	-
27	CLA	b	709	X	-	-	-
27	CLA	b	710	X	-	-	-
27	CLA	b	711	X	-	-	-
27	CLA	b	712	X	-	-	-
27	CLA	b	713	X	-	-	-
27	CLA	b	714	X	-	-	-
27	CLA	b	715	X	-	-	-
27	CLA	b	716	X	-	-	-
27	CLA	b	717	X	-	-	-
27	CLA	b	718	X	-	-	-
27	CLA	b	719	X	-	-	-
27	CLA	b	720	X	-	-	-
27	CLA	b	721	X	-	-	-
27	CLA	b	722	X	-	-	-
27	CLA	b	723	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
27	CLA	b	724	X	-	-	-
27	CLA	b	725	X	-	-	-
27	CLA	b	726	X	-	-	-
27	CLA	b	727	X	-	-	-
27	CLA	b	728	X	-	-	-
27	CLA	f	302	X	-	-	-
27	CLA	f	303	X	-	-	-
27	CLA	j	202	X	-	-	-
27	CLA	l	402	X	-	-	-
27	CLA	l	403	X	-	-	-
27	CLA	l	404	X	-	-	-
27	CLA	l	405	X	-	-	-
27	CLA	l	406	X	-	-	-
27	CLA	l	407	X	-	-	-
27	CLA	l	408	X	-	-	-
27	CLA	l	409	X	-	-	-
27	CLA	l	410	X	-	-	-
27	CLA	l	411	X	-	-	-
27	CLA	l	412	X	-	-	-
27	CLA	r	203	X	-	-	-
27	CLA	r	204	X	-	-	-
30	DD6	D	613	X	-	-	-

2 Entry composition

There are 39 unique types of molecules in this entry. The entry contains 55980 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 PCPI-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	194	Total	C	N	O	S	0	0
			1461	941	239	274	7		

- Molecule 2 is a protein called PCPI-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	185	Total	C	N	O	S	0	0
			1412	900	237	264	11		

- Molecule 3 is a protein called PCP-11.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	192	Total	C	N	O	S	0	0
			1518	990	244	273	11		

- Molecule 4 is a protein called PCPI-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	177	Total	C	N	O	S	0	0
			1375	893	226	245	11		

- Molecule 5 is a protein called PCPI-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	184	Total	C	N	O	S	0	0
			1444	940	241	256	7		

- Molecule 6 is a protein called PCPI-8.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	225	Total	C	N	O	S	0	0
			1731	1118	282	314	17		

- Molecule 7 is a protein called PCPI-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	173	Total	C	N	O	S	0	0
			1329	861	220	238	10		

- Molecule 8 is a protein called PCPI-10.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	192	Total	C	N	O	S	0	0
			1458	948	241	261	8		

- Molecule 9 is a protein called PCPI-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	221	Total	C	N	O	S	0	0
			1736	1138	272	315	11		

- Molecule 10 is a protein called PCPI-9.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	173	Total	C	N	O	S	0	0
			1322	849	220	244	9		

- Molecule 11 is a protein called PCPI-13.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	154	Total	C	N	O	S	0	0
			1134	718	194	211	11		

- Molecule 12 is a protein called PCPI-12.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	T	140	Total	C	N	O	S	0	0
			1065	681	180	196	8		

- Molecule 13 is a protein called PCPI-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	U	104	Total	C	N	O	S	0	0
			828	535	144	142	7		

- Molecule 14 is a protein called PsaA.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	a	665	Total	C	N	O	S	0	0
			5250	3443	877	904	26		

- Molecule 15 is a protein called PsaB.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	b	659	Total	C	N	O	S	0	0
			5220	3437	845	918	20		

- Molecule 16 is a protein called PsaC.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	c	86	Total	C	N	O	S	0	0
			651	402	109	131	9		

- Molecule 17 is a protein called PsaD.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	d	216	Total	C	N	O	S	0	0
			1765	1123	308	321	13		

- Molecule 18 is a protein called PsaE.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	e	73	Total	C	N	O	0	0
			590	386	101	103		

- Molecule 19 is a protein called PsaF.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	f	169	Total	C	N	O	S	0	0
			1349	859	238	246	6		

- Molecule 20 is a protein called PsaI.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	i	120	Total	C	N	O	S	0	0
			971	627	165	177	2		

- Molecule 21 is a protein called PsaJ.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	j	99	Total	C	N	O	S	0	0
			791	507	130	153	1		

- Molecule 22 is a protein called PsaL.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	l	253	Total	C	N	O	S	0	0
			1974	1290	319	356	9		

- Molecule 23 is a protein called PsaM.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	m	79	Total	C	N	O	S	0	0
			598	391	102	104	1		

- Molecule 24 is a protein called PsaR.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	r	131	Total	C	N	O	S	0	0
			1082	714	168	194	6		

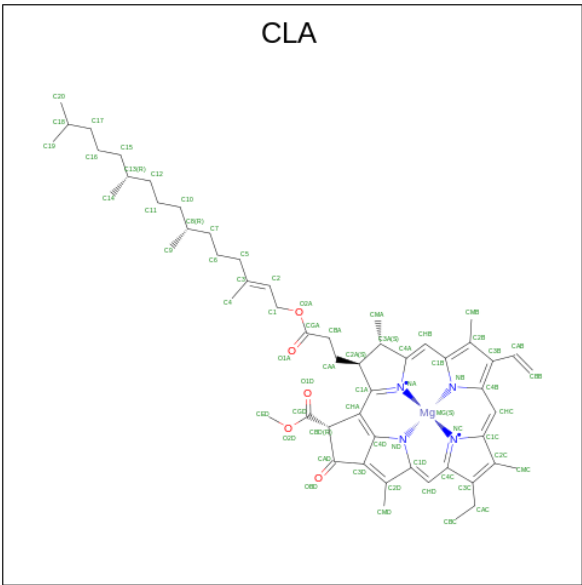
- Molecule 25 is a protein called PsaT.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	x	79	Total	C	N	O	S	0	0
			642	411	107	123	1		

- Molecule 26 is a protein called PsaU.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	y	130	Total	C	N	O	S	0	0
			1085	690	184	208	3		

- Molecule 27 is CHLOROPHYLL A (three-letter code: CLA) (formula: C₅₅H₇₂MgN₄O₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
27	A	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
27	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			47	37	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
27	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
27	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
27	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	B	1	Total 47	C 37	Mg 1	N 4	O 5	0
27	C	1	Total 42	C 34	Mg 1	N 4	O 3	0
27	C	1	Total 45	C 35	Mg 1	N 4	O 5	0
27	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	C	1	Total 55	C 45	Mg 1	N 4	O 5	0
27	C	1	Total 47	C 37	Mg 1	N 4	O 5	0
27	C	1	Total 60	C 50	Mg 1	N 4	O 5	0
27	C	1	Total 47	C 37	Mg 1	N 4	O 5	0
27	C	1	Total 45	C 35	Mg 1	N 4	O 5	0
27	C	1	Total 47	C 37	Mg 1	N 4	O 5	0
27	C	1	Total 47	C 37	Mg 1	N 4	O 5	0
27	D	1	Total 45	C 35	Mg 1	N 4	O 5	0
27	D	1	Total 55	C 45	Mg 1	N 4	O 5	0
27	D	1	Total 55	C 45	Mg 1	N 4	O 5	0
27	D	1	Total 55	C 45	Mg 1	N 4	O 5	0
27	D	1	Total 47	C 37	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
27	D	1	Total 45	C 35	Mg 1	N 4	O 5	0
27	D	1	Total 60	C 50	Mg 1	N 4	O 5	0
27	D	1	Total 55	C 45	Mg 1	N 4	O 5	0
27	D	1	Total 45	C 35	Mg 1	N 4	O 5	0
27	D	1	Total 47	C 37	Mg 1	N 4	O 5	0
27	D	1	Total 60	C 50	Mg 1	N 4	O 5	0
27	D	1	Total 55	C 45	Mg 1	N 4	O 5	0
27	E	1	Total 55	C 45	Mg 1	N 4	O 5	0
27	E	1	Total 47	C 37	Mg 1	N 4	O 5	0
27	E	1	Total 55	C 45	Mg 1	N 4	O 5	0
27	E	1	Total 45	C 35	Mg 1	N 4	O 5	0
27	E	1	Total 60	C 50	Mg 1	N 4	O 5	0
27	E	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	E	1	Total 60	C 50	Mg 1	N 4	O 5	0
27	E	1	Total 45	C 35	Mg 1	N 4	O 5	0
27	E	1	Total 60	C 50	Mg 1	N 4	O 5	0
27	E	1	Total 45	C 35	Mg 1	N 4	O 5	0
27	F	1	Total 60	C 50	Mg 1	N 4	O 5	0
27	F	1	Total 56	C 46	Mg 1	N 4	O 5	0
27	F	1	Total 52	C 42	Mg 1	N 4	O 5	0
27	F	1	Total 45	C 35	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
27	F	1	Total 45	C 35	Mg 1	N 4	O 5	0
27	F	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	F	1	Total 45	C 35	Mg 1	N 4	O 5	0
27	F	1	Total 45	C 35	Mg 1	N 4	O 5	0
27	F	1	Total 47	C 37	Mg 1	N 4	O 5	0
27	F	1	Total 60	C 50	Mg 1	N 4	O 5	0
27	F	1	Total 55	C 45	Mg 1	N 4	O 5	0
27	G	1	Total 55	C 45	Mg 1	N 4	O 5	0
27	G	1	Total 50	C 40	Mg 1	N 4	O 5	0
27	G	1	Total 47	C 37	Mg 1	N 4	O 5	0
27	G	1	Total 60	C 50	Mg 1	N 4	O 5	0
27	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	G	1	Total 45	C 35	Mg 1	N 4	O 5	0
27	G	1	Total 60	C 50	Mg 1	N 4	O 5	0
27	G	1	Total 55	C 45	Mg 1	N 4	O 5	0
27	G	1	Total 47	C 37	Mg 1	N 4	O 5	0
27	G	1	Total 45	C 35	Mg 1	N 4	O 5	0
27	H	1	Total 60	C 50	Mg 1	N 4	O 5	0
27	H	1	Total 60	C 50	Mg 1	N 4	O 5	0
27	H	1	Total 60	C 50	Mg 1	N 4	O 5	0
27	H	1	Total 45	C 35	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
27	H	1	Total 45	C 35	Mg 1	N 4	O 5	0
27	H	1	Total 55	C 45	Mg 1	N 4	O 5	0
27	H	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	H	1	Total 45	C 35	Mg 1	N 4	O 5	0
27	H	1	Total 42	C 34	Mg 1	N 4	O 3	0
27	H	1	Total 60	C 50	Mg 1	N 4	O 5	0
27	H	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	I	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	I	1	Total 55	C 45	Mg 1	N 4	O 5	0
27	I	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	I	1	Total 55	C 45	Mg 1	N 4	O 5	0
27	I	1	Total 55	C 45	Mg 1	N 4	O 5	0
27	I	1	Total 61	C 51	Mg 1	N 4	O 5	0
27	I	1	Total 60	C 50	Mg 1	N 4	O 5	0
27	I	1	Total 45	C 35	Mg 1	N 4	O 5	0
27	I	1	Total 55	C 45	Mg 1	N 4	O 5	0
27	I	1	Total 42	C 34	Mg 1	N 4	O 3	0
27	I	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	J	1	Total 45	C 35	Mg 1	N 4	O 5	0
27	J	1	Total 60	C 50	Mg 1	N 4	O 5	0
27	J	1	Total 60	C 50	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
27	J	1	Total 42	C 34	Mg 1	N 4	O 3	0
27	J	1	Total 41	C 33	Mg 1	N 4	O 3	0
27	K	1	Total 57	C 47	Mg 1	N 4	O 5	0
27	K	1	Total 55	C 45	Mg 1	N 4	O 5	0
27	K	1	Total 45	C 35	Mg 1	N 4	O 5	0
27	K	1	Total 57	C 47	Mg 1	N 4	O 5	0
27	K	1	Total 60	C 50	Mg 1	N 4	O 5	0
27	K	1	Total 41	C 33	Mg 1	N 4	O 3	0
27	K	1	Total 45	C 35	Mg 1	N 4	O 5	0
27	T	1	Total 47	C 37	Mg 1	N 4	O 5	0
27	T	1	Total 45	C 35	Mg 1	N 4	O 5	0
27	T	1	Total 45	C 35	Mg 1	N 4	O 5	0
27	T	1	Total 41	C 33	Mg 1	N 4	O 3	0
27	T	1	Total 45	C 35	Mg 1	N 4	O 5	0
27	T	1	Total 45	C 35	Mg 1	N 4	O 5	0
27	T	1	Total 45	C 35	Mg 1	N 4	O 5	0
27	T	1	Total 41	C 33	Mg 1	N 4	O 3	0
27	U	1	Total 43	C 35	Mg 1	N 4	O 3	0
27	U	1	Total 50	C 40	Mg 1	N 4	O 5	0
27	U	1	Total 60	C 50	Mg 1	N 4	O 5	0
27	U	1	Total 45	C 35	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
27	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	a	1	Total 55	C 45	Mg 1	N 4	O 5	0
27	a	1	Total 50	C 40	Mg 1	N 4	O 5	0
27	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	a	1	Total 55	C 45	Mg 1	N 4	O 5	0
27	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	a	1	Total 55	C 45	Mg 1	N 4	O 5	0
27	a	1	Total 47	C 37	Mg 1	N 4	O 5	0
27	a	1	Total 50	C 40	Mg 1	N 4	O 5	0
27	a	1	Total 48	C 38	Mg 1	N 4	O 5	0
27	a	1	Total 50	C 40	Mg 1	N 4	O 5	0
27	a	1	Total 48	C 38	Mg 1	N 4	O 5	0
27	a	1	Total 55	C 45	Mg 1	N 4	O 5	0
27	a	1	Total 60	C 50	Mg 1	N 4	O 5	0
27	a	1	Total 60	C 50	Mg 1	N 4	O 5	0
27	a	1	Total 55	C 45	Mg 1	N 4	O 5	0
27	a	1	Total 55	C 45	Mg 1	N 4	O 5	0
27	a	1	Total 60	C 50	Mg 1	N 4	O 5	0
27	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	a	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
27	a	1	Total 60	C 50	Mg 1	N 4	O 5	0
27	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	a	1	Total 55	C 45	Mg 1	N 4	O 5	0
27	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	a	1	Total 48	C 38	Mg 1	N 4	O 5	0
27	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	a	1	Total 55	C 45	Mg 1	N 4	O 5	0
27	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	a	1	Total 61	C 51	Mg 1	N 4	O 5	0
27	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	b	1	Total 65	C 55	Mg 1	N 4	O 5	0

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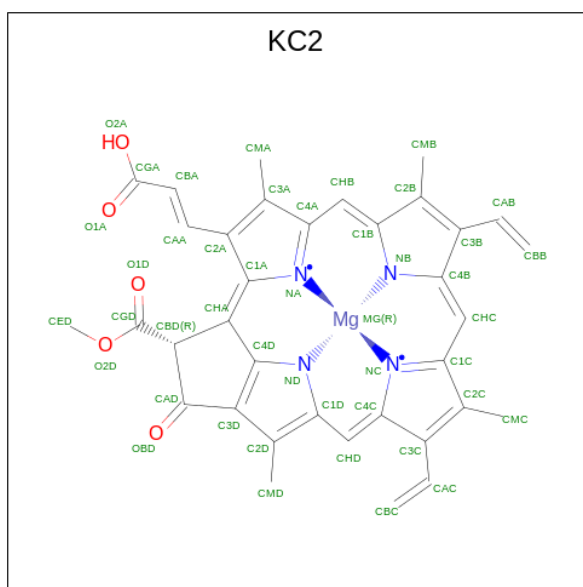
Mol	Chain	Residues	Atoms					AltConf
27	b	1	Total 55	C 45	Mg 1	N 4	O 5	0
27	b	1	Total 60	C 50	Mg 1	N 4	O 5	0
27	b	1	Total 48	C 38	Mg 1	N 4	O 5	0
27	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	b	1	Total 48	C 38	Mg 1	N 4	O 5	0
27	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	b	1	Total 48	C 38	Mg 1	N 4	O 5	0
27	b	1	Total 50	C 40	Mg 1	N 4	O 5	0
27	b	1	Total 48	C 38	Mg 1	N 4	O 5	0
27	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	b	1	Total 60	C 50	Mg 1	N 4	O 5	0
27	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	f	1	Total 48	C 38	Mg 1	N 4	O 5	0
27	f	1	Total 48	C 38	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
27	j	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
27	l	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
27	l	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	l	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
27	l	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
27	l	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	l	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
27	l	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
27	l	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	l	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
27	l	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
27	l	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	r	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
27	r	1	Total	C	Mg	N	O	0
			60	50	1	4	5	

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



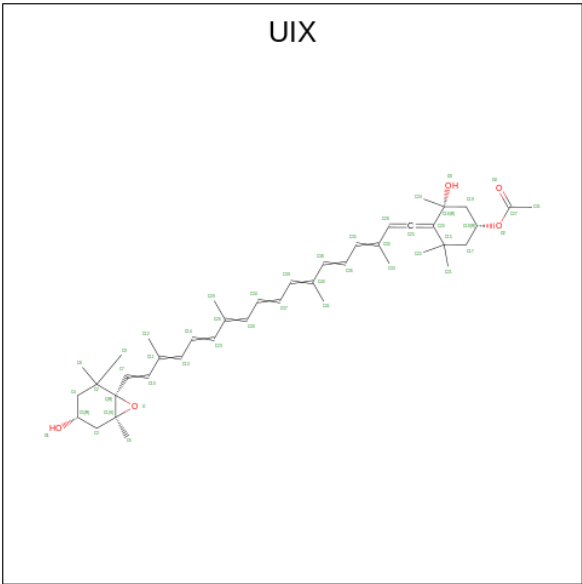
Mol	Chain	Residues	Atoms					AltConf
28	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
28	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
28	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
28	C	1	Total 45	C 35	Mg 1	N 4	O 5	0
28	E	1	Total 45	C 35	Mg 1	N 4	O 5	0
28	E	1	Total 45	C 35	Mg 1	N 4	O 5	0
28	F	1	Total 45	C 35	Mg 1	N 4	O 5	0
28	G	1	Total 45	C 35	Mg 1	N 4	O 5	0
28	H	1	Total 45	C 35	Mg 1	N 4	O 5	0
28	H	1	Total 45	C 35	Mg 1	N 4	O 5	0
28	I	1	Total 45	C 35	Mg 1	N 4	O 5	0
28	J	1	Total 45	C 35	Mg 1	N 4	O 5	0
28	J	1	Total 45	C 35	Mg 1	N 4	O 5	0
28	J	1	Total 45	C 35	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
28	J	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
28	J	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
28	K	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
28	T	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
28	U	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
28	U	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

- Molecule 29 is [(1 {S},5 {R})-3,3,5-trimethyl-5-oxidanyl-4-[(3 {E},5 {E},7 {E},9 {E},11 {E},13 {E},15 {E},17 {E})-3,7,12,16-tetramethyl-18-[(1 {S},4 {S},6 {R})-2,2,6-trimethyl-4-oxidanyl-7-oxabicyclo[4.1.0]heptan-1-yl]octadeca-1,3,5,7,9,11,13,15,17-nonaenylidene]cyclohexyl] ethanoate (three-letter code: UIX) (formula: C₄₂H₅₈O₅) (labeled as "Ligand of Interest" by depositor).



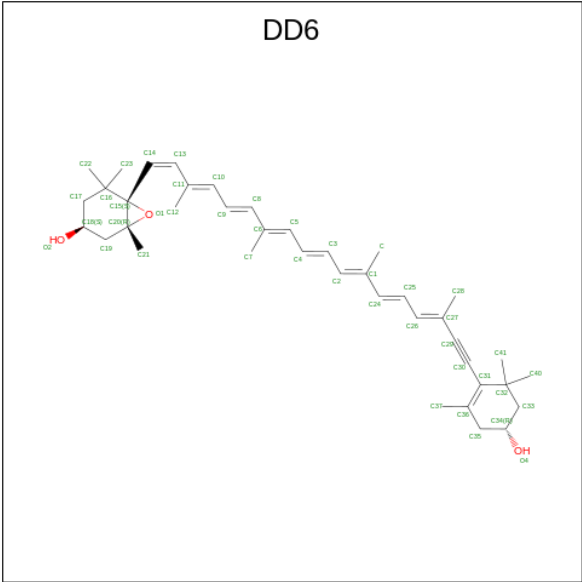
Mol	Chain	Residues	Atoms			AltConf
29	A	1	Total	C	O	0
			47	42	5	
29	A	1	Total	C	O	0
			47	42	5	
29	B	1	Total	C	O	0
			47	42	5	

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Mol	Chain	Residues	Atoms			AltConf
29	B	1	Total	C	O	0
			47	42	5	
29	C	1	Total	C	O	0
			47	42	5	
29	C	1	Total	C	O	0
			47	42	5	
29	D	1	Total	C	O	0
			47	42	5	
29	E	1	Total	C	O	0
			47	42	5	
29	F	1	Total	C	O	0
			47	42	5	
29	G	1	Total	C	O	0
			47	42	5	
29	H	1	Total	C	O	0
			47	42	5	
29	H	1	Total	C	O	0
			47	42	5	
29	I	1	Total	C	O	0
			47	42	5	
29	J	1	Total	C	O	0
			47	42	5	
29	T	1	Total	C	O	0
			47	42	5	
29	j	1	Total	C	O	0
			47	42	5	

- Molecule 30 is (3S,3'R,5R,6S,7cis)-7',8'-didehydro-5,6-dihydro-5,6-epoxy-beta,beta-carotene-3,3'-diol (three-letter code: DD6) (formula: C₄₀H₅₄O₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
30	A	1	Total	C	O	0
			43	40	3	
30	A	1	Total	C	O	0
			43	40	3	
30	A	1	Total	C	O	0
			43	40	3	
30	B	1	Total	C	O	0
			43	40	3	
30	B	1	Total	C	O	0
			43	40	3	
30	B	1	Total	C	O	0
			43	40	3	
30	C	1	Total	C	O	0
			43	40	3	
30	C	1	Total	C	O	0
			43	40	3	
30	D	1	Total	C	O	0
			43	40	3	
30	D	1	Total	C	O	0
			43	40	3	
30	D	1	Total	C	O	0
			43	40	3	
30	D	1	Total	C	O	0
			43	40	3	
30	D	1	Total	C	O	0
			43	40	3	
30	E	1	Total	C	O	0
			43	40	3	

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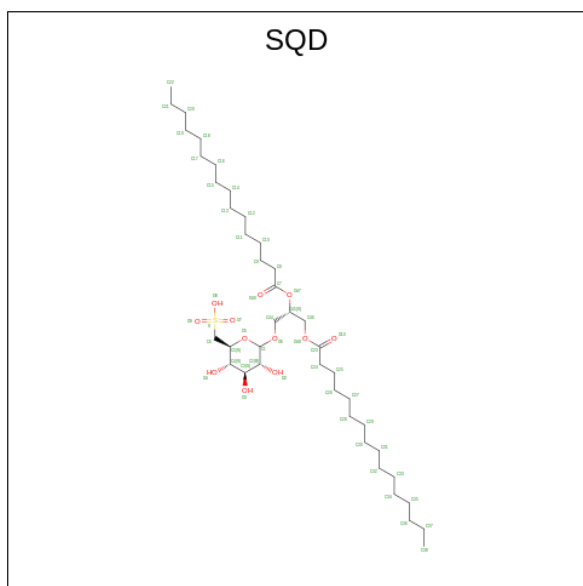
Mol	Chain	Residues	Atoms			AltConf
30	E	1	Total 43	C 40	O 3	0
30	E	1	Total 43	C 40	O 3	0
30	E	1	Total 43	C 40	O 3	0
30	F	1	Total 43	C 40	O 3	0
30	F	1	Total 43	C 40	O 3	0
30	G	1	Total 43	C 40	O 3	0
30	G	1	Total 43	C 40	O 3	0
30	G	1	Total 43	C 40	O 3	0
30	G	1	Total 43	C 40	O 3	0
30	H	1	Total 43	C 40	O 3	0
30	H	1	Total 43	C 40	O 3	0
30	H	1	Total 43	C 40	O 3	0
30	H	1	Total 43	C 40	O 3	0
30	I	1	Total 43	C 40	O 3	0
30	I	1	Total 43	C 40	O 3	0
30	J	1	Total 43	C 40	O 3	0
30	K	1	Total 43	C 40	O 3	0
30	K	1	Total 43	C 40	O 3	0
30	K	1	Total 43	C 40	O 3	0
30	T	1	Total 43	C 40	O 3	0
30	T	1	Total 43	C 40	O 3	0

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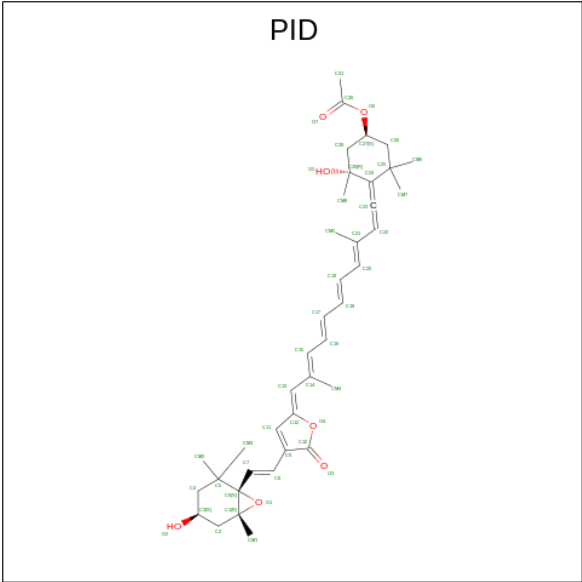
Mol	Chain	Residues	Atoms			AltConf
30	U	1	Total	C	O	0
			43	40	3	
30	b	1	Total	C	O	0
			43	40	3	
30	i	1	Total	C	O	0
			43	40	3	
30	r	1	Total	C	O	0
			43	40	3	
30	r	1	Total	C	O	0
			43	40	3	
30	r	1	Total	C	O	0
			43	40	3	

- Molecule 31 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula: $C_{41}H_{78}O_{12}S$).



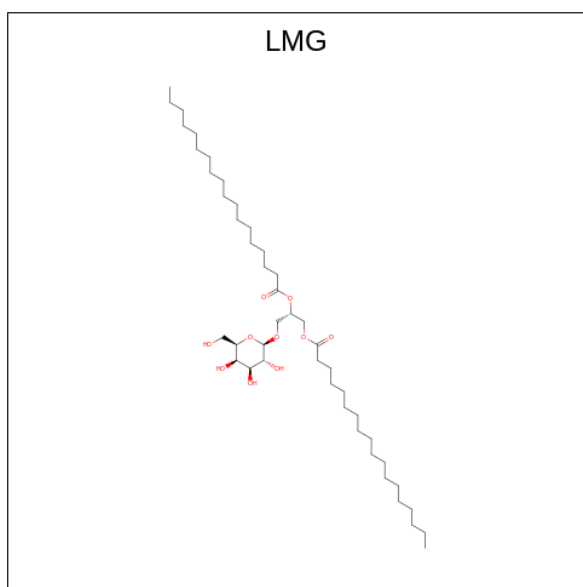
Mol	Chain	Residues	Atoms				AltConf
31	A	1	Total	C	O	S	0
			28	15	12	1	
31	H	1	Total	C	O	S	0
			46	33	12	1	
31	y	1	Total	C	O	S	0
			46	33	12	1	

- Molecule 32 is PERIDININ (three-letter code: PID) (formula: $C_{39}H_{50}O_7$) (labeled as "Ligand of Interest" by depositor).



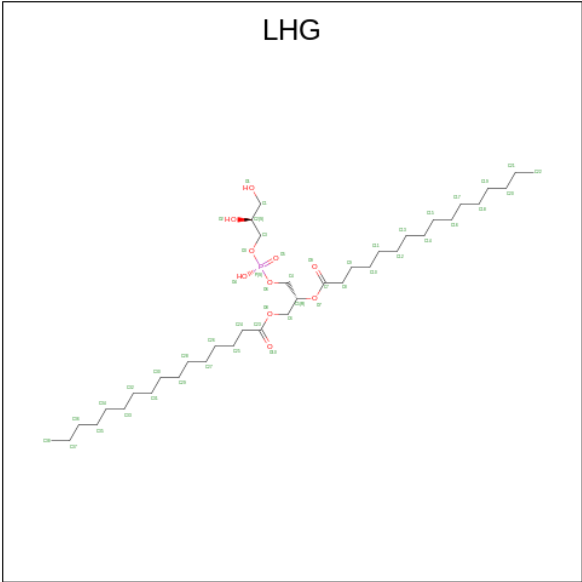
Mol	Chain	Residues	Atoms			AltConf
32	B	1	Total	C	O	0
			46	39	7	
32	F	1	Total	C	O	0
			46	39	7	
32	F	1	Total	C	O	0
			46	39	7	
32	I	1	Total	C	O	0
			46	39	7	
32	J	1	Total	C	O	0
			46	39	7	
32	J	1	Total	C	O	0
			46	39	7	
32	J	1	Total	C	O	0
			46	39	7	
32	J	1	Total	C	O	0
			46	39	7	
32	K	1	Total	C	O	0
			46	39	7	
32	U	1	Total	C	O	0
			46	39	7	

- Molecule 33 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: C₄₅H₈₆O₁₀).



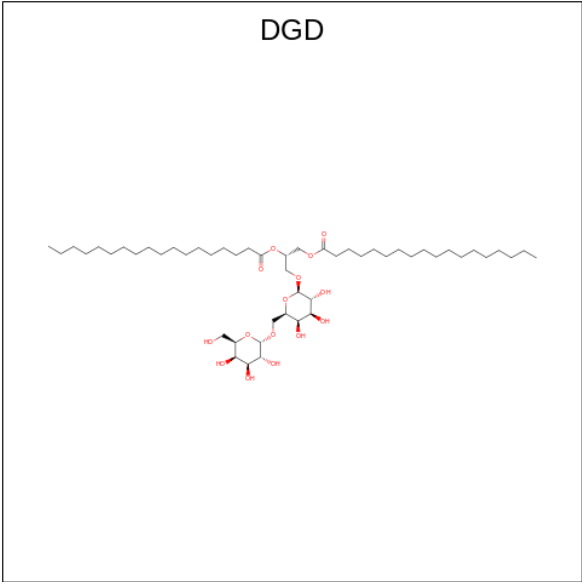
Mol	Chain	Residues	Atoms			AltConf
33	C	1	Total	C	O	0
			34	24	10	
33	D	1	Total	C	O	0
			35	25	10	
33	D	1	Total	C	O	0
			46	36	10	
33	F	1	Total	C	O	0
			46	36	10	
33	K	1	Total	C	O	0
			42	32	10	
33	b	1	Total	C	O	0
			55	45	10	
33	l	1	Total	C	O	0
			50	40	10	

- Molecule 34 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: $C_{38}H_{75}O_{10}P$).



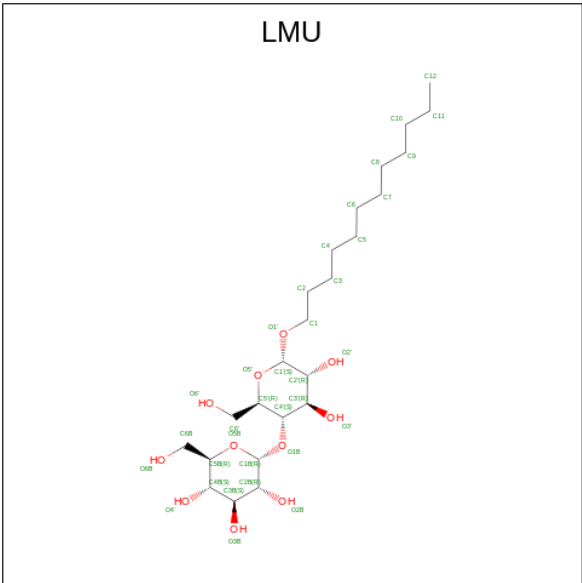
Mol	Chain	Residues	Atoms				AltConf
34	D	1	Total	C	O	P	0
			46	35	10	1	
34	F	1	Total	C	O	P	0
			37	26	10	1	
34	G	1	Total	C	O	P	0
			34	23	10	1	
34	a	1	Total	C	O	P	0
			48	37	10	1	
34	j	1	Total	C	O	P	0
			37	26	10	1	
34	l	1	Total	C	O	P	0
			46	35	10	1	
34	r	1	Total	C	O	P	0
			46	35	10	1	

- Molecule 35 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: C₅₁H₉₆O₁₅).



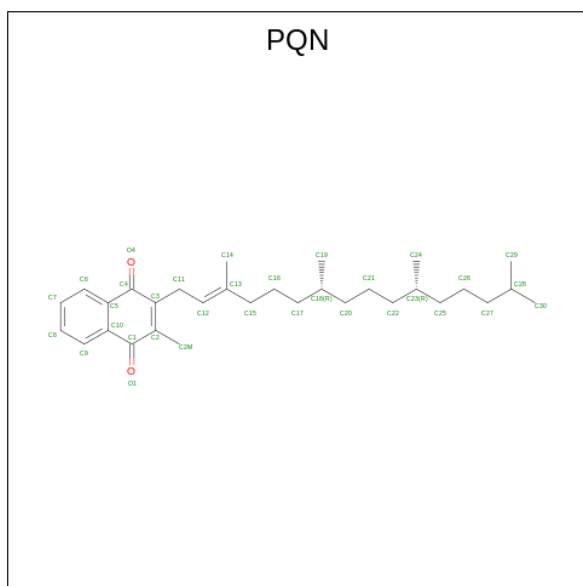
Mol	Chain	Residues	Atoms			AltConf
35	K	1	Total	C	O	0
			47	32	15	
35	f	1	Total	C	O	0
			52	37	15	
35	j	1	Total	C	O	0
			60	45	15	
35	l	1	Total	C	O	0
			55	40	15	

- Molecule 36 is DODECYL-ALPHA-D-MALTOSIDE (three-letter code: LMU) (formula: C₂₄H₄₆O₁₁).



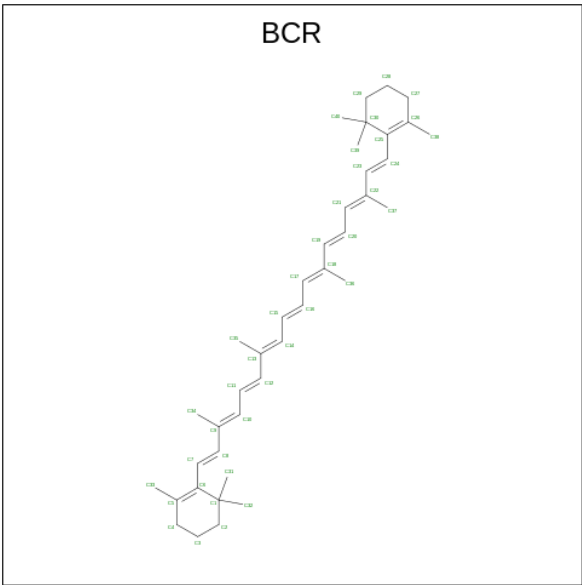
Mol	Chain	Residues	Atoms			AltConf
36	T	1	Total	C	O	0
			35	24	11	

- Molecule 37 is PHYLLOQUINONE (three-letter code: PQN) (formula: $C_{31}H_{46}O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
37	a	1	Total	C	O	0
			33	31	2	
37	b	1	Total	C	O	0
			33	31	2	

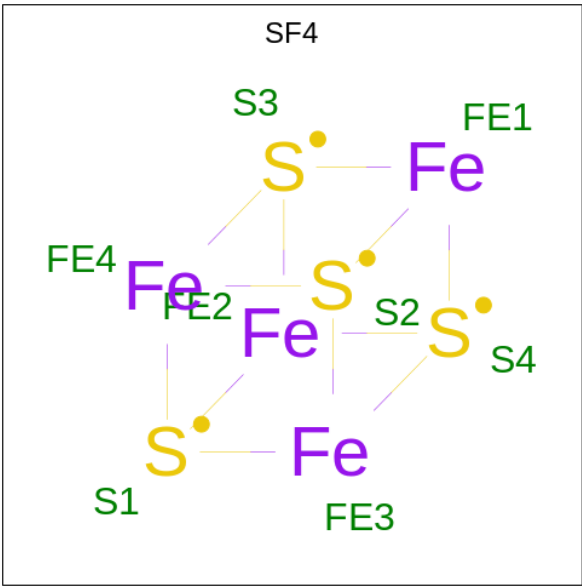
- Molecule 38 is BETA-CAROTENE (three-letter code: BCR) (formula: $C_{40}H_{56}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
38	a	1	Total C 40 40	0
38	a	1	Total C 40 40	0
38	a	1	Total C 40 40	0
38	b	1	Total C 40 40	0
38	b	1	Total C 40 40	0
38	f	1	Total C 40 40	0
38	f	1	Total C 40 40	0
38	i	1	Total C 40 40	0
38	j	1	Total C 40 40	0
38	l	1	Total C 40 40	0
38	l	1	Total C 40 40	0
38	l	1	Total C 40 40	0
38	m	1	Total C 40 40	0

- Molecule 39 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄) (labeled

as "Ligand of Interest" by depositor).

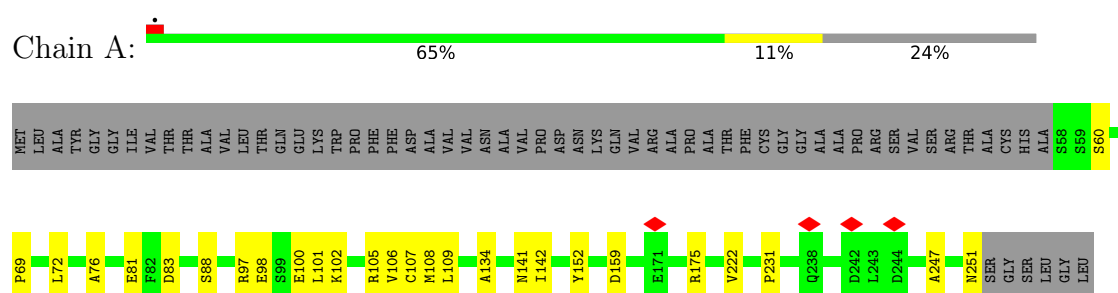


Mol	Chain	Residues	Atoms			AltConf
39	a	1	Total	Fe	S	0
			8	4	4	
39	c	1	Total	Fe	S	0
			8	4	4	
39	c	1	Total	Fe	S	0
			8	4	4	

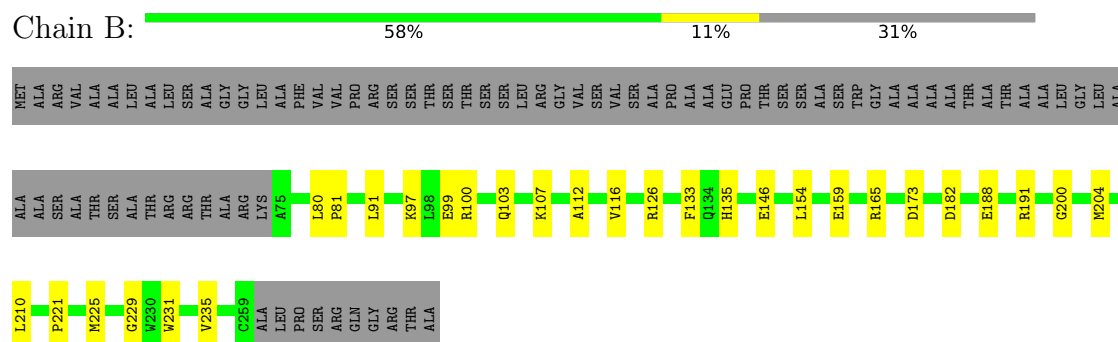
3 Residue-property plots

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.

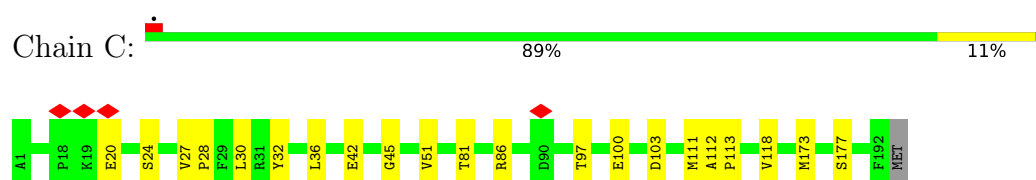
• Molecule 1: PCPI-7



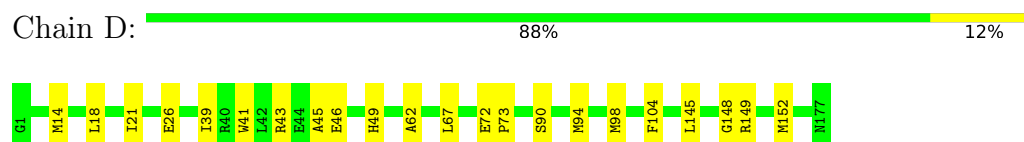
• Molecule 2: PCPI-1



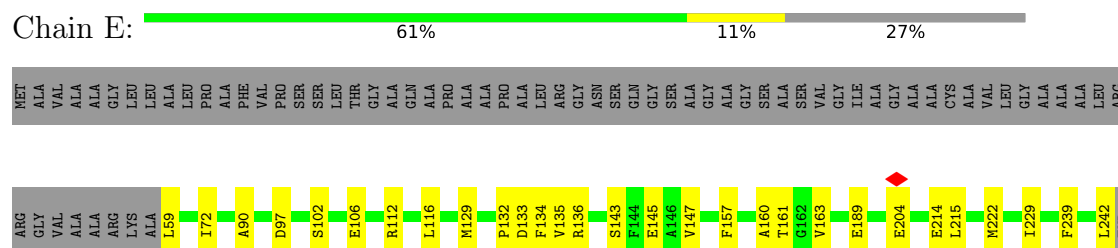
• Molecule 3: PCP-11



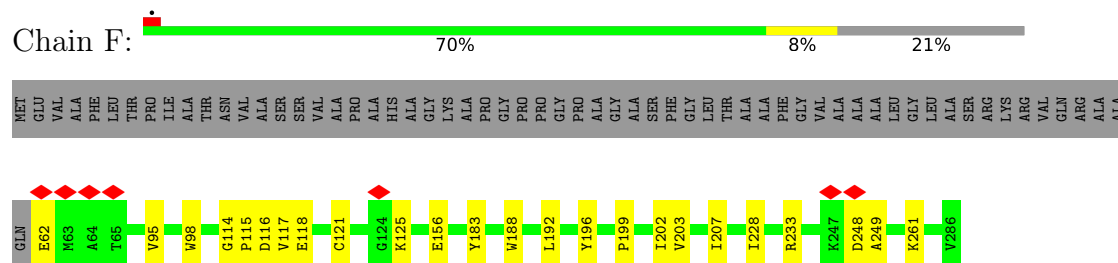
• Molecule 4: PCPI-6



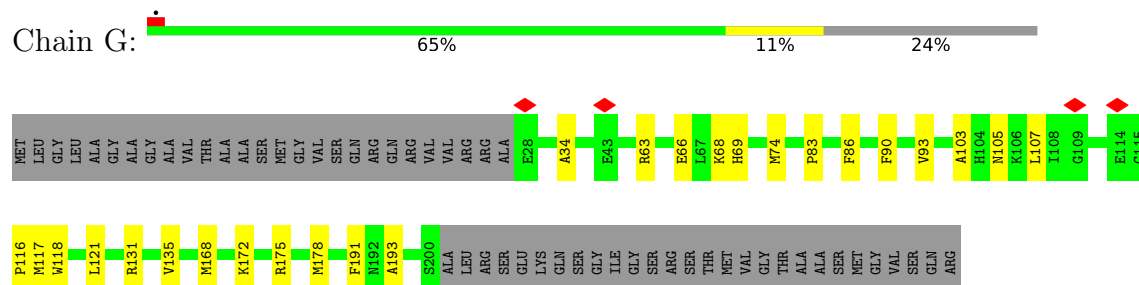
- Molecule 5: PCPI-5



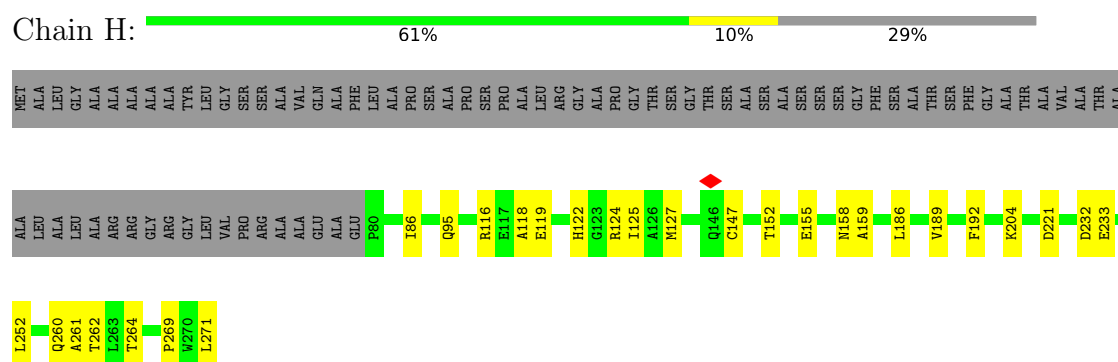
- Molecule 6: PCPI-8



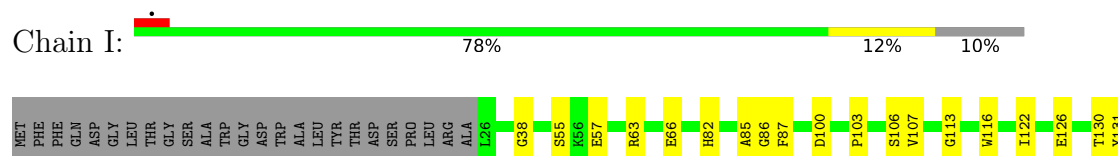
- Molecule 7: PCPI-4

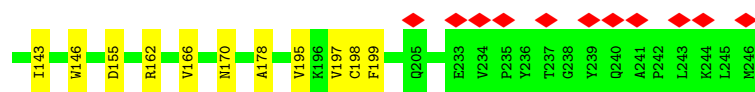


- Molecule 8: PCPI-10

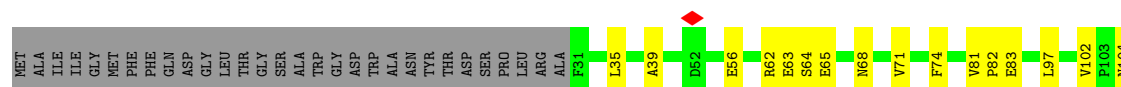


- Molecule 9: PCPI-3

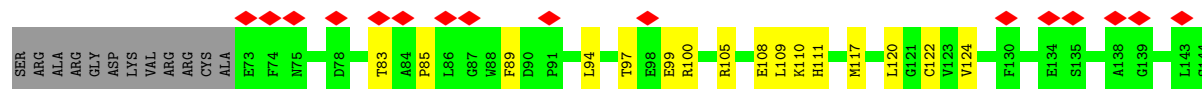
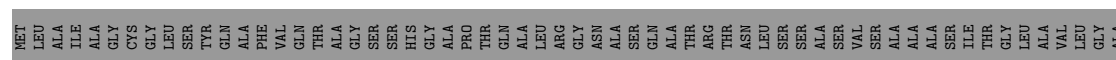




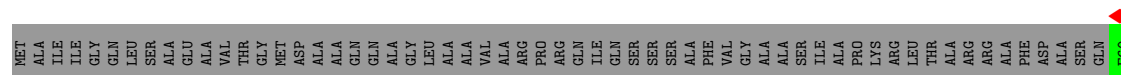
• Molecule 10: PCPI-9



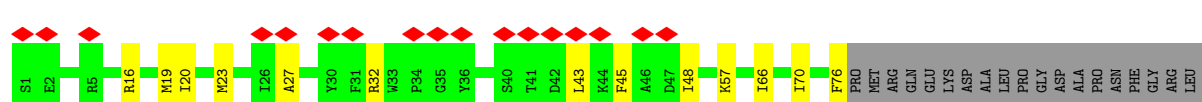
• Molecule 11: PCPI-13

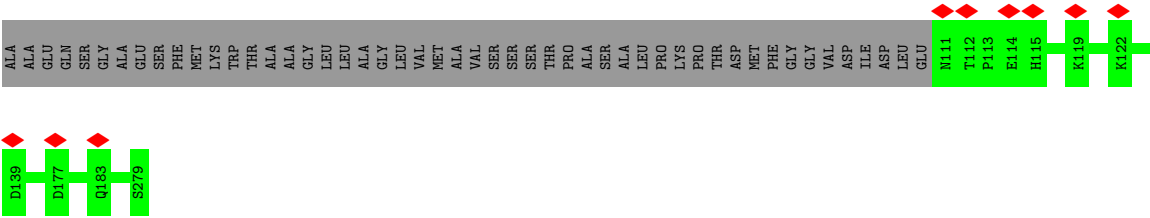


• Molecule 12: PCPI-12

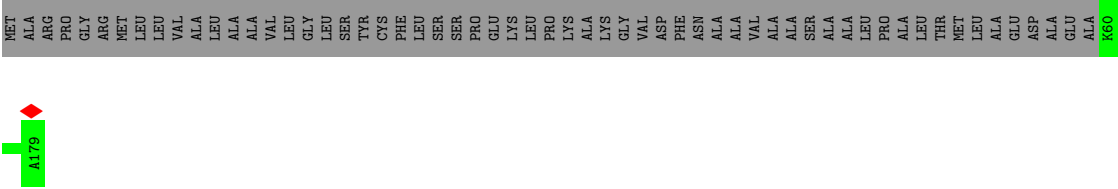


• Molecule 13: PCPI-2

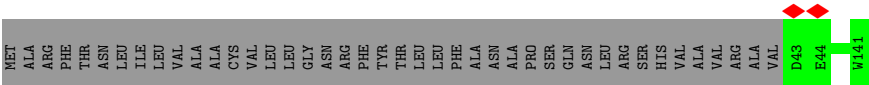




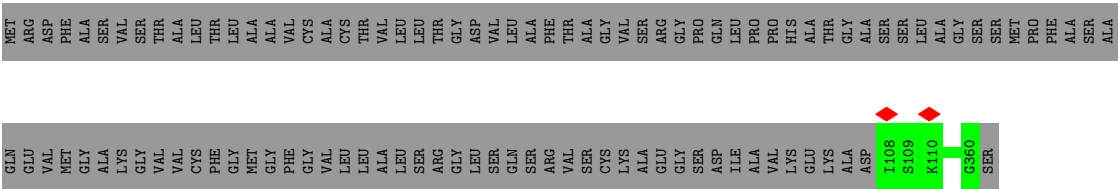
• Molecule 20: PsaI



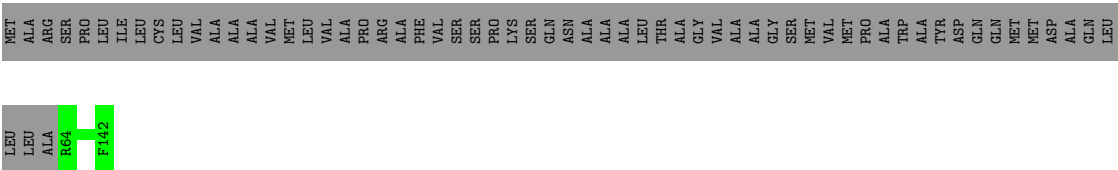
• Molecule 21: PsaJ



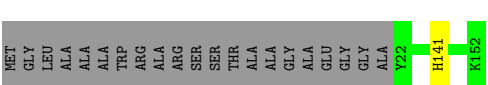
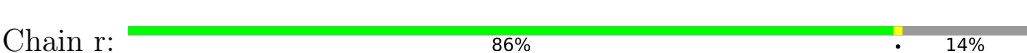
• Molecule 22: PsaL



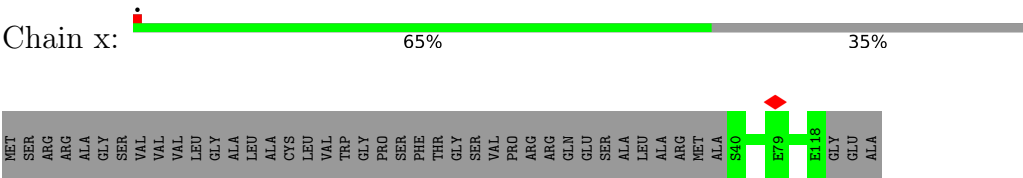
• Molecule 23: PsaM



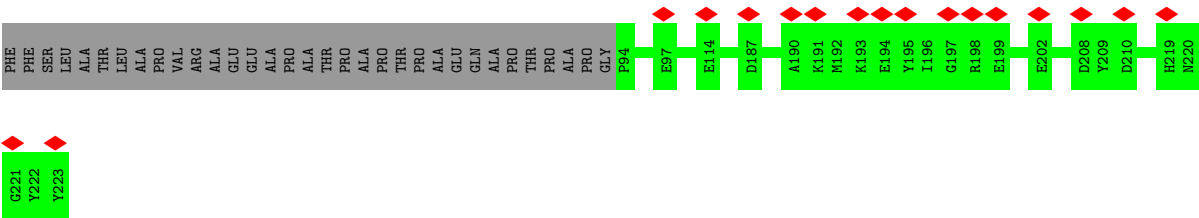
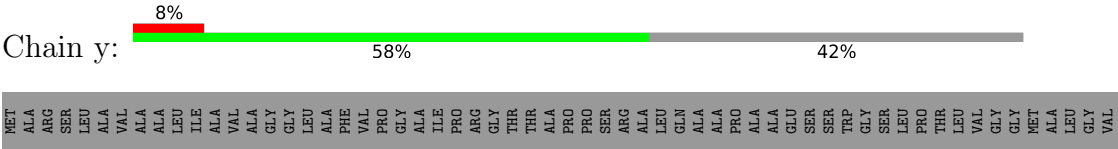
• Molecule 24: PsaR



● Molecule 25: PsaT



● Molecule 26: PsaU



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	161863	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	2.960	Depositor
Minimum map value	-0.099	Depositor
Average map value	0.041	Depositor
Map value standard deviation	0.089	Depositor
Recommended contour level	0.35	Depositor
Map size (Å)	339.19998, 339.19998, 339.19998	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BCR, LHG, DD6, PQN, DGD, LMU, SF4, SQD, UX, KC2, PID, CLA, LMG

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	0.27	0/1501	0.45	0/2037
2	B	0.32	0/1443	0.50	0/1954
3	C	0.26	0/1562	0.43	0/2114
4	D	0.28	0/1413	0.46	0/1912
5	E	0.28	0/1484	0.51	0/2006
6	F	0.27	0/1785	0.44	0/2426
7	G	0.31	0/1365	0.48	0/1841
8	H	0.26	0/1499	0.44	0/2030
9	I	0.34	0/1794	0.48	0/2454
10	J	0.30	0/1355	0.50	0/1835
11	K	0.37	0/1162	0.50	0/1565
12	T	0.32	0/1090	0.52	0/1477
13	U	0.28	0/847	0.50	0/1140
14	a	0.28	0/5412	0.44	0/7363
15	b	0.40	0/5390	0.49	0/7368
16	c	0.36	0/661	0.55	0/901
17	d	0.27	0/1803	0.50	0/2419
18	e	0.27	0/611	0.44	0/836
19	f	0.41	0/1384	0.48	0/1873
20	i	0.27	0/1001	0.47	0/1357
21	j	0.27	0/808	0.47	0/1104
22	l	0.28	0/2031	0.46	0/2755
23	m	0.35	0/608	0.52	0/820
24	r	0.31	0/1118	0.45	0/1513
25	x	0.28	0/667	0.43	0/908
26	y	0.28	0/1119	0.50	0/1515
All	All	0.31	0/40913	0.47	0/55523

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1461	0	1420	19	0
2	B	1412	0	1384	18	0
3	C	1518	0	1491	18	0
4	D	1375	0	1359	15	0
5	E	1444	0	1418	18	0
6	F	1731	0	1691	19	0
7	G	1329	0	1301	27	0
8	H	1458	0	1426	18	0
9	I	1736	0	1687	23	0
10	J	1322	0	1296	19	0
11	K	1134	0	1085	51	0
12	T	1065	0	1042	20	0
13	U	828	0	828	16	0
14	a	5250	0	5201	0	0
15	b	5220	0	5122	0	0
16	c	651	0	634	0	0
17	d	1765	0	1785	0	0
18	e	590	0	582	0	0
19	f	1349	0	1334	0	0
20	i	971	0	951	0	0
21	j	791	0	783	0	0
22	l	1974	0	1950	0	0
23	m	598	0	641	0	0
24	r	1082	0	1041	0	0
25	x	642	0	594	0	0
26	y	1085	0	1025	0	0
27	A	543	0	441	9	0
27	B	454	0	437	5	0
27	C	565	0	489	11	0
27	D	624	0	532	8	0
27	E	537	0	481	4	0
27	F	575	0	500	14	0
27	G	529	0	463	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	H	602	0	559	10	0
27	I	623	0	596	17	0
27	J	248	0	211	7	0
27	K	360	0	309	19	0
27	T	354	0	258	12	0
27	U	198	0	164	12	0
27	a	1927	0	1885	0	0
27	b	1717	0	1790	0	0
27	f	96	0	72	0	0
27	j	56	0	51	0	0
27	l	627	0	600	0	0
27	r	108	0	95	0	0
28	A	45	0	0	0	0
28	B	90	0	0	0	0
28	C	45	0	0	0	0
28	E	90	0	0	0	0
28	F	45	0	0	0	0
28	G	45	0	0	0	0
28	H	90	0	0	0	0
28	I	45	0	0	0	0
28	J	225	0	0	5	0
28	K	45	0	0	6	0
28	T	45	0	0	0	0
28	U	90	0	0	0	0
29	A	94	0	0	0	0
29	B	94	0	0	0	0
29	C	94	0	0	0	0
29	D	47	0	0	0	0
29	E	47	0	0	0	0
29	F	47	0	0	0	0
29	G	47	0	0	0	0
29	H	94	0	0	1	0
29	I	47	0	0	1	0
29	J	47	0	0	0	0
29	T	47	0	0	0	0
29	j	47	0	0	0	0
30	A	129	0	0	2	0
30	B	129	0	0	2	0
30	C	86	0	0	2	0
30	D	215	0	0	3	0
30	E	172	0	0	2	0
30	F	86	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	G	172	0	0	4	0
30	H	172	0	0	3	0
30	I	86	0	0	2	0
30	J	43	0	0	1	0
30	K	129	0	0	3	0
30	T	86	0	0	1	0
30	U	43	0	0	1	0
30	b	43	0	0	0	0
30	i	43	0	0	0	0
30	r	129	0	0	0	0
31	A	28	0	20	0	0
31	H	46	0	56	0	0
31	y	46	0	56	0	0
32	B	46	0	50	1	0
32	F	92	0	100	8	0
32	I	46	0	50	5	0
32	J	184	0	200	21	0
32	K	46	0	50	12	0
32	U	46	0	50	0	0
33	C	34	0	38	1	0
33	D	81	0	105	2	0
33	F	46	0	65	0	0
33	K	42	0	57	1	0
33	b	55	0	86	0	0
33	l	50	0	73	0	0
34	D	46	0	65	0	0
34	F	37	0	44	0	0
34	G	34	0	38	0	0
34	a	48	0	69	0	0
34	j	37	0	44	0	0
34	l	46	0	65	0	0
34	r	46	0	65	0	0
35	K	47	0	52	4	0
35	f	52	0	62	0	0
35	j	60	0	81	0	0
35	l	55	0	71	0	0
36	T	35	0	46	1	0
37	a	33	0	46	0	0
37	b	33	0	46	0	0
38	a	120	0	168	0	0
38	b	80	0	112	0	0
38	f	80	0	112	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	i	40	0	56	0	0
38	j	40	0	56	0	0
38	l	120	0	168	0	0
38	m	40	0	56	0	0
39	a	8	0	0	0	0
39	c	16	0	0	0	0
All	All	55980	0	51582	380	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 8.

The worst 5 of 380 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)
7:G:90:PHE:CE1	7:G:93:VAL:HG13	1.79	1.17
11:K:120:LEU:HD12	27:K:603:CLA:HAC1	1.37	1.02
11:K:120:LEU:CD1	27:K:603:CLA:HAC1	1.95	0.96
7:G:90:PHE:HE1	7:G:93:VAL:HG13	1.32	0.90
11:K:120:LEU:HD13	11:K:120:LEU:O	1.71	0.90

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	192/256 (75%)	186 (97%)	6 (3%)	0	100	100
2	B	183/269 (68%)	177 (97%)	6 (3%)	0	100	100
3	C	190/193 (98%)	186 (98%)	4 (2%)	0	100	100
4	D	175/177 (99%)	170 (97%)	5 (3%)	0	100	100
5	E	182/253 (72%)	175 (96%)	7 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	F	223/286 (78%)	212 (95%)	10 (4%)	1 (0%)	30	61
7	G	171/228 (75%)	162 (95%)	9 (5%)	0	100	100
8	H	190/271 (70%)	186 (98%)	4 (2%)	0	100	100
9	I	219/246 (89%)	207 (94%)	12 (6%)	0	100	100
10	J	171/203 (84%)	168 (98%)	3 (2%)	0	100	100
11	K	152/226 (67%)	147 (97%)	5 (3%)	0	100	100
12	T	138/206 (67%)	128 (93%)	10 (7%)	0	100	100
13	U	100/137 (73%)	96 (96%)	4 (4%)	0	100	100
14	a	659/687 (96%)	642 (97%)	17 (3%)	0	100	100
15	b	655/669 (98%)	634 (97%)	20 (3%)	1 (0%)	44	73
16	c	84/161 (52%)	78 (93%)	6 (7%)	0	100	100
17	d	212/295 (72%)	206 (97%)	6 (3%)	0	100	100
18	e	71/121 (59%)	68 (96%)	3 (4%)	0	100	100
19	f	167/279 (60%)	162 (97%)	5 (3%)	0	100	100
20	i	118/179 (66%)	116 (98%)	2 (2%)	0	100	100
21	j	97/141 (69%)	96 (99%)	1 (1%)	0	100	100
22	l	251/361 (70%)	246 (98%)	5 (2%)	0	100	100
23	m	77/142 (54%)	75 (97%)	2 (3%)	0	100	100
24	r	129/152 (85%)	126 (98%)	3 (2%)	0	100	100
25	x	77/121 (64%)	73 (95%)	4 (5%)	0	100	100
26	y	128/223 (57%)	127 (99%)	1 (1%)	0	100	100
All	All	5011/6482 (77%)	4849 (97%)	160 (3%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	F	117	VAL
15	b	454	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	149/195 (76%)	149 (100%)	0	100	100
2	B	149/202 (74%)	149 (100%)	0	100	100
3	C	155/156 (99%)	155 (100%)	0	100	100
4	D	140/140 (100%)	140 (100%)	0	100	100
5	E	145/181 (80%)	145 (100%)	0	100	100
6	F	183/220 (83%)	183 (100%)	0	100	100
7	G	134/172 (78%)	134 (100%)	0	100	100
8	H	143/188 (76%)	143 (100%)	0	100	100
9	I	186/205 (91%)	185 (100%)	1 (0%)	86	95
10	J	134/156 (86%)	134 (100%)	0	100	100
11	K	107/155 (69%)	107 (100%)	0	100	100
12	T	108/152 (71%)	108 (100%)	0	100	100
13	U	83/110 (76%)	83 (100%)	0	100	100
14	a	565/584 (97%)	565 (100%)	0	100	100
15	b	559/568 (98%)	557 (100%)	2 (0%)	89	96
16	c	75/119 (63%)	75 (100%)	0	100	100
17	d	193/242 (80%)	193 (100%)	0	100	100
18	e	64/93 (69%)	64 (100%)	0	100	100
19	f	140/212 (66%)	140 (100%)	0	100	100
20	i	102/143 (71%)	102 (100%)	0	100	100
21	j	90/124 (73%)	90 (100%)	0	100	100
22	l	201/280 (72%)	201 (100%)	0	100	100
23	m	63/108 (58%)	63 (100%)	0	100	100
24	r	115/124 (93%)	114 (99%)	1 (1%)	75	92
25	x	67/97 (69%)	67 (100%)	0	100	100
26	y	115/175 (66%)	115 (100%)	0	100	100
All	All	4165/5101 (82%)	4161 (100%)	4 (0%)	92	98

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
9	I	198	CYS
15	b	98	HIS
15	b	227	PHE
24	r	141	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
15	b	495	HIS
17	d	220	HIS
24	r	51	HIS
20	i	93	GLN
11	K	213	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

323 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
38	BCR	b	732	-	41,41,41	0.30	0	56,56,56	0.75	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	DD6	B	614	-	39,45,45	0.42	0	52,67,67	0.85	1 (1%)
27	CLA	b	718	-	65,73,73	2.15	8 (12%)	76,113,113	1.52	8 (10%)
35	DGD	l	416	-	56,56,67	0.92	2 (3%)	70,70,81	1.40	7 (10%)
27	CLA	f	302	-	48,56,73	2.60	8 (16%)	55,92,113	1.60	8 (14%)
28	KC2	J	602	10	48,53,53	1.50	8 (16%)	54,89,89	1.06	4 (7%)
27	CLA	F	607	6	45,53,73	2.66	8 (17%)	52,89,113	1.72	7 (13%)
38	BCR	m	201	-	41,41,41	0.30	0	56,56,56	0.69	0
27	CLA	J	609	-	41,49,73	2.89	9 (21%)	47,84,113	1.87	7 (14%)
30	DD6	i	202	-	39,45,45	0.18	0	52,67,67	0.87	2 (3%)
27	CLA	G	605	-	60,68,73	2.32	8 (13%)	70,107,113	1.56	8 (11%)
28	KC2	I	604	9	48,53,53	1.51	8 (16%)	54,89,89	1.09	5 (9%)
27	CLA	F	603	-	52,60,73	2.44	8 (15%)	60,97,113	1.55	7 (11%)
27	CLA	b	722	-	48,56,73	2.57	8 (16%)	55,92,113	1.66	7 (12%)
27	CLA	a	820	-	65,73,73	2.20	8 (12%)	76,113,113	1.36	7 (9%)
30	DD6	J	612	-	39,45,45	0.19	0	52,67,67	0.67	2 (3%)
30	DD6	D	615	-	39,45,45	0.16	0	52,67,67	0.63	1 (1%)
27	CLA	G	603	-	50,58,73	2.50	8 (16%)	58,95,113	1.58	8 (13%)
27	CLA	H	313	-	60,68,73	2.33	8 (13%)	70,107,113	1.45	7 (10%)
27	CLA	E	602	5	55,63,73	2.41	8 (14%)	64,101,113	1.53	7 (10%)
27	CLA	H	308	8	55,63,73	2.36	8 (14%)	64,101,113	1.47	7 (10%)
27	CLA	I	610	-	55,63,73	2.41	8 (14%)	64,101,113	1.63	6 (9%)
30	DD6	D	613	-	39,45,45	0.43	0	52,67,67	0.81	3 (5%)
30	DD6	b	730	-	39,45,45	0.18	0	52,67,67	0.61	1 (1%)
38	BCR	b	731	-	41,41,41	0.31	0	56,56,56	0.73	1 (1%)
27	CLA	l	403	-	65,73,73	2.18	8 (12%)	76,113,113	1.35	7 (9%)
27	CLA	F	617	-	60,68,73	2.30	8 (13%)	70,107,113	1.45	7 (10%)
27	CLA	a	827	-	65,73,73	2.23	8 (12%)	76,113,113	1.51	8 (10%)
38	BCR	i	201	-	41,41,41	0.31	0	56,56,56	0.94	1 (1%)
28	KC2	J	604	10	48,53,53	1.51	8 (16%)	54,89,89	1.08	5 (9%)
27	CLA	l	412	22	65,73,73	2.19	8 (12%)	76,113,113	1.42	8 (10%)
27	CLA	b	707	-	65,73,73	2.15	8 (12%)	76,113,113	1.43	7 (9%)
27	CLA	a	808	14	55,63,73	2.45	8 (14%)	64,101,113	1.54	9 (14%)
30	DD6	H	316	-	39,45,45	0.20	0	52,67,67	0.77	3 (5%)
27	CLA	E	604	-	55,63,73	2.40	8 (14%)	64,101,113	1.53	8 (12%)
35	DGD	j	201	-	61,61,67	0.92	4 (6%)	75,75,81	1.44	13 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	CLA	G	611	-	45,53,73	2.69	8 (17%)	52,89,113	1.65	7 (13%)
27	CLA	J	607	-	42,50,73	2.81	8 (19%)	48,85,113	1.73	7 (14%)
27	CLA	a	813	-	48,56,73	2.63	8 (16%)	55,92,113	1.62	7 (12%)
27	CLA	D	605	4	47,55,73	2.59	8 (17%)	54,91,113	1.57	8 (14%)
27	CLA	C	211	-	47,55,73	2.62	8 (17%)	54,91,113	1.59	7 (12%)
27	CLA	a	837	-	65,73,73	2.06	8 (12%)	76,113,113	1.40	7 (9%)
34	LHG	l	401	-	45,45,48	0.52	0	48,51,54	0.47	0
27	CLA	G	604	-	47,55,73	2.66	8 (17%)	54,91,113	1.70	5 (9%)
27	CLA	D	604	-	55,63,73	2.39	8 (14%)	64,101,113	1.53	7 (10%)
27	CLA	a	805	-	65,73,73	2.22	8 (12%)	76,113,113	1.39	7 (9%)
27	CLA	E	608	5	60,68,73	2.31	8 (13%)	70,107,113	1.47	5 (7%)
27	CLA	G	602	7	55,63,73	2.41	8 (14%)	64,101,113	1.51	7 (10%)
27	CLA	C	201	-	42,50,73	2.79	8 (19%)	48,85,113	1.77	9 (18%)
27	CLA	b	712	-	48,56,73	2.58	8 (16%)	55,92,113	1.66	8 (14%)
27	CLA	j	202	27	56,64,73	2.42	7 (12%)	65,102,113	1.44	7 (10%)
27	CLA	b	721	-	50,58,73	2.55	8 (16%)	58,95,113	1.60	7 (12%)
27	CLA	D	609	-	45,53,73	2.70	8 (17%)	52,89,113	1.67	7 (13%)
32	PID	K	611	-	41,49,49	1.62	5 (12%)	49,76,76	3.72	19 (38%)
27	CLA	H	319	-	65,73,73	2.20	8 (12%)	76,113,113	1.39	7 (9%)
27	CLA	l	410	-	48,56,73	2.62	8 (16%)	55,92,113	1.68	7 (12%)
27	CLA	a	839	-	61,69,73	2.25	8 (13%)	71,108,113	1.40	7 (9%)
27	CLA	G	609	7	55,63,73	2.42	8 (14%)	64,101,113	1.51	9 (14%)
30	DD6	r	201	-	39,45,45	0.16	0	52,67,67	0.87	2 (3%)
27	CLA	E	603	-	47,55,73	2.61	8 (17%)	54,91,113	1.64	7 (12%)
31	SQD	A	618	-	27,28,54	1.50	4 (14%)	36,39,65	1.32	4 (11%)
27	CLA	b	703	-	65,73,73	2.16	8 (12%)	76,113,113	1.44	11 (14%)
28	KC2	B	602	-	48,53,53	1.46	7 (14%)	54,89,89	1.04	5 (9%)
27	CLA	B	609	2	65,73,73	2.20	8 (12%)	76,113,113	1.38	8 (10%)
27	CLA	b	705	-	65,73,73	2.21	8 (12%)	76,113,113	1.49	5 (6%)
32	PID	J	613	-	41,49,49	1.61	6 (14%)	49,76,76	4.24	20 (40%)
27	CLA	C	209	-	45,53,73	2.71	8 (17%)	52,89,113	1.69	8 (15%)
30	DD6	U	607	-	39,45,45	0.14	0	52,67,67	0.59	1 (1%)
37	PQN	b	729	-	34,34,34	0.36	0	42,45,45	0.61	1 (2%)
27	CLA	H	306	-	45,53,73	2.65	8 (17%)	52,89,113	1.64	8 (15%)
30	DD6	T	610	-	39,45,45	0.15	0	52,67,67	0.64	1 (1%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	CLA	I	607	-	61,69,73	2.28	8 (13%)	71,108,113	1.43	7 (9%)
27	CLA	a	804	-	65,73,73	2.19	8 (12%)	76,113,113	1.49	10 (13%)
27	CLA	l	408	-	47,55,73	2.61	8 (17%)	54,91,113	1.70	7 (12%)
30	DD6	T	611	-	39,45,45	0.17	0	52,67,67	0.77	4 (7%)
28	KC2	A	608	-	48,53,53	1.48	7 (14%)	54,89,89	1.15	6 (11%)
33	LMG	D	618	-	35,35,55	0.55	0	43,43,63	0.78	1 (2%)
30	DD6	E	615	-	39,45,45	0.17	0	52,67,67	0.71	3 (5%)
34	LHG	r	202	-	45,45,48	0.53	0	48,51,54	0.51	0
28	KC2	J	610	-	48,53,53	1.49	8 (16%)	54,89,89	1.10	5 (9%)
28	KC2	H	311	-	48,53,53	1.51	8 (16%)	54,89,89	1.09	5 (9%)
30	DD6	I	615	-	39,45,45	0.18	0	52,67,67	0.59	2 (3%)
27	CLA	B	606	-	65,73,73	2.22	8 (12%)	76,113,113	1.45	8 (10%)
30	DD6	r	205	-	39,45,45	0.18	0	52,67,67	0.86	2 (3%)
27	CLA	K	605	11	60,68,73	2.29	8 (13%)	70,107,113	1.42	6 (8%)
29	UIX	G	615	-	41,49,49	1.24	3 (7%)	52,74,74	1.97	17 (32%)
27	CLA	l	405	22	61,69,73	2.28	8 (13%)	71,108,113	1.44	7 (9%)
27	CLA	a	810	-	50,58,73	2.54	8 (16%)	58,95,113	1.60	9 (15%)
29	UIX	C	215	-	41,49,49	1.22	3 (7%)	52,74,74	2.12	21 (40%)
27	CLA	b	714	-	48,56,73	2.60	8 (16%)	55,92,113	1.74	7 (12%)
27	CLA	D	603	-	55,63,73	2.40	8 (14%)	64,101,113	1.55	7 (10%)
33	LMG	F	616	-	46,46,55	0.52	0	54,54,63	0.69	0
27	CLA	B	607	-	60,68,73	2.30	8 (13%)	70,107,113	1.42	8 (11%)
27	CLA	U	605	13	60,68,73	2.34	8 (13%)	70,107,113	1.39	7 (10%)
27	CLA	T	605	12	45,53,73	2.62	8 (17%)	52,89,113	1.59	6 (11%)
27	CLA	l	407	-	48,56,73	2.62	8 (16%)	55,92,113	1.61	7 (12%)
27	CLA	B	610	-	47,55,73	2.61	8 (17%)	54,91,113	1.66	7 (12%)
27	CLA	D	610	4	47,55,73	2.64	8 (17%)	54,91,113	1.60	8 (14%)
27	CLA	H	303	8	60,68,73	2.26	8 (13%)	70,107,113	1.46	8 (11%)
27	CLA	b	713	-	65,73,73	2.20	8 (12%)	76,113,113	1.48	8 (10%)
29	UIX	J	616	-	41,49,49	1.22	3 (7%)	52,74,74	1.87	14 (26%)
27	CLA	K	602	-	55,63,73	2.43	8 (14%)	64,101,113	1.51	8 (12%)
33	LMG	l	417	-	50,50,55	0.49	0	58,58,63	0.61	0
27	CLA	B	603	-	65,73,73	2.25	8 (12%)	76,113,113	1.50	7 (9%)
27	CLA	b	701	-	65,73,73	2.20	8 (12%)	76,113,113	1.37	7 (9%)
27	CLA	J	601	-	45,53,73	2.68	8 (17%)	52,89,113	1.75	6 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	CLA	a	812	-	50,58,73	2.59	8 (16%)	58,95,113	1.71	10 (17%)
33	LMG	b	733	-	55,55,55	0.48	0	63,63,63	0.57	0
27	CLA	r	203	-	48,56,73	2.61	8 (16%)	55,92,113	1.65	5 (9%)
28	KC2	E	610	5	48,53,53	1.51	8 (16%)	54,89,89	1.08	5 (9%)
29	UIX	B	611	-	41,49,49	1.31	4 (9%)	52,74,74	2.00	21 (40%)
27	CLA	a	809	-	47,55,73	2.64	8 (17%)	54,91,113	1.74	5 (9%)
27	CLA	b	728	-	65,73,73	2.19	8 (12%)	76,113,113	1.36	8 (10%)
27	CLA	U	601	-	43,51,73	2.80	8 (18%)	49,86,113	1.87	6 (12%)
27	CLA	F	619	-	55,63,73	2.38	8 (14%)	64,101,113	1.50	7 (10%)
29	UIX	H	317	-	41,49,49	1.21	3 (7%)	52,74,74	1.91	16 (30%)
30	DD6	F	612	-	39,45,45	0.16	0	52,67,67	0.50	0
27	CLA	a	806	-	55,63,73	2.41	8 (14%)	64,101,113	1.51	6 (9%)
27	CLA	T	603	-	45,53,73	2.66	8 (17%)	52,89,113	1.62	7 (13%)
34	LHG	j	205	-	36,36,48	0.57	0	39,42,54	0.53	0
27	CLA	a	818	-	55,63,73	2.36	8 (14%)	64,101,113	1.49	6 (9%)
27	CLA	U	606	-	45,53,73	2.75	8 (17%)	52,89,113	1.67	7 (13%)
27	CLA	a	826	-	55,63,73	2.32	8 (14%)	64,101,113	1.47	7 (10%)
28	KC2	J	606	-	48,53,53	1.49	7 (14%)	54,89,89	1.07	4 (7%)
27	CLA	D	611	-	60,68,73	2.30	8 (13%)	70,107,113	1.42	8 (11%)
30	DD6	E	613	-	39,45,45	0.18	0	52,67,67	0.87	4 (7%)
30	DD6	I	613	-	39,45,45	0.19	0	52,67,67	0.89	4 (7%)
33	LMG	K	613	-	42,42,55	0.53	0	50,50,63	0.66	0
38	BCR	l	415	-	41,41,41	0.33	0	56,56,56	0.57	0
38	BCR	a	834	-	41,41,41	0.28	0	56,56,56	0.53	0
27	CLA	f	303	19	48,56,73	2.62	8 (16%)	55,92,113	1.59	8 (14%)
30	DD6	K	612	-	39,45,45	0.15	0	52,67,67	0.68	3 (5%)
27	CLA	D	606	-	45,53,73	2.63	8 (17%)	52,89,113	1.66	7 (13%)
28	KC2	T	608	-	48,53,53	1.57	7 (14%)	54,89,89	1.09	4 (7%)
27	CLA	C	208	-	47,55,73	2.61	8 (17%)	54,91,113	1.63	7 (12%)
27	CLA	E	605	5	45,53,73	2.69	8 (17%)	52,89,113	1.73	8 (15%)
27	CLA	H	304	-	60,68,73	2.30	8 (13%)	70,107,113	1.51	11 (15%)
27	CLA	H	310	-	45,53,73	2.73	8 (17%)	52,89,113	1.75	8 (15%)
32	PID	I	614	-	41,49,49	1.58	5 (12%)	49,76,76	3.86	22 (44%)
30	DD6	F	611	-	39,45,45	0.16	0	52,67,67	0.93	4 (7%)
27	CLA	a	803	27	50,58,73	2.52	8 (16%)	58,95,113	1.67	6 (10%)
28	KC2	F	609	6	48,53,53	1.54	8 (16%)	54,89,89	1.07	5 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	CLA	l	402	-	60,68,73	2.33	8 (13%)	70,107,113	1.49	7 (10%)
29	UIX	A	613	-	41,49,49	1.23	3 (7%)	52,74,74	1.86	13 (25%)
27	CLA	H	309	-	65,73,73	2.23	8 (12%)	76,113,113	1.41	7 (9%)
27	CLA	b	704	-	65,73,73	2.19	8 (12%)	76,113,113	1.37	7 (9%)
27	CLA	a	822	-	60,68,73	2.31	8 (13%)	70,107,113	1.45	8 (11%)
27	CLA	T	601	12	47,55,73	2.67	8 (17%)	54,91,113	1.70	8 (14%)
32	PID	F	614	-	41,49,49	1.55	5 (12%)	49,76,76	3.83	17 (34%)
27	CLA	a	821	-	65,73,73	2.16	8 (12%)	76,113,113	1.38	7 (9%)
27	CLA	G	606	7	65,73,73	2.22	8 (12%)	76,113,113	1.45	9 (11%)
27	CLA	b	723	-	65,73,73	2.21	8 (12%)	76,113,113	1.42	7 (9%)
28	KC2	C	210	-	48,53,53	1.53	8 (16%)	54,89,89	1.07	5 (9%)
27	CLA	E	612	-	45,53,73	2.70	8 (17%)	52,89,113	1.64	7 (13%)
27	CLA	H	312	-	42,50,73	2.72	8 (19%)	48,85,113	1.74	8 (16%)
30	DD6	C	216	-	39,45,45	0.16	0	52,67,67	0.77	2 (3%)
27	CLA	a	801	-	65,73,73	2.10	7 (10%)	76,113,113	1.30	9 (11%)
27	CLA	E	611	5	60,68,73	2.32	8 (13%)	70,107,113	1.49	8 (11%)
28	KC2	E	601	27	48,53,53	1.52	8 (16%)	54,89,89	1.10	5 (9%)
27	CLA	F	602	-	56,64,73	2.39	8 (14%)	65,102,113	1.50	8 (12%)
30	DD6	A	617	-	39,45,45	0.18	0	52,67,67	0.66	2 (3%)
27	CLA	a	815	-	60,68,73	2.27	8 (13%)	70,107,113	1.44	7 (10%)
27	CLA	b	726	-	60,68,73	2.30	8 (13%)	70,107,113	1.43	7 (10%)
27	CLA	a	830	-	65,73,73	2.19	8 (12%)	76,113,113	1.38	7 (9%)
27	CLA	C	212	-	47,55,73	2.65	8 (17%)	54,91,113	1.64	7 (12%)
27	CLA	I	601	9	65,73,73	2.20	8 (12%)	76,113,113	1.39	7 (9%)
27	CLA	G	610	7	47,55,73	2.64	8 (17%)	54,91,113	1.61	7 (12%)
38	BCR	a	833	-	41,41,41	0.30	0	56,56,56	0.61	0
27	CLA	D	608	4	55,63,73	2.39	8 (14%)	64,101,113	1.55	8 (12%)
34	LHG	G	617	-	33,33,48	0.60	0	36,39,54	0.55	0
27	CLA	I	609	9	45,53,73	2.66	8 (17%)	52,89,113	1.72	8 (15%)
39	SF4	c	202	-	0,12,12	-	-	-	-	-
27	CLA	C	204	-	65,73,73	2.21	8 (12%)	76,113,113	1.42	8 (10%)
30	DD6	G	613	-	39,45,45	0.15	0	52,67,67	0.78	2 (3%)
29	UIX	F	613	-	41,49,49	1.21	3 (7%)	52,74,74	2.03	14 (26%)
27	CLA	I	608	9	60,68,73	2.30	8 (13%)	70,107,113	1.39	8 (11%)
30	DD6	A	615	-	39,45,45	0.16	0	52,67,67	0.86	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	CLA	C	205	-	55,63,73	2.43	8 (14%)	64,101,113	1.70	7 (10%)
27	CLA	a	802	-	55,63,73	2.37	8 (14%)	64,101,113	1.47	8 (12%)
27	CLA	D	607	4	60,68,73	2.30	8 (13%)	70,107,113	1.44	7 (10%)
27	CLA	a	816	-	60,68,73	2.33	8 (13%)	70,107,113	1.46	7 (10%)
27	CLA	E	609	28	45,53,73	2.69	8 (17%)	52,89,113	1.63	7 (13%)
27	CLA	B	604	2	47,55,73	2.67	8 (17%)	54,91,113	1.69	7 (12%)
27	CLA	A	612	1	47,55,73	2.64	8 (17%)	54,91,113	1.86	10 (18%)
35	DGD	K	614	-	48,48,67	1.00	3 (6%)	62,62,81	1.43	10 (16%)
27	CLA	F	605	6	45,53,73	2.67	8 (17%)	52,89,113	1.71	8 (15%)
27	CLA	E	607	5	65,73,73	2.17	8 (12%)	76,113,113	1.33	8 (10%)
27	CLA	a	825	-	65,73,73	2.22	8 (12%)	76,113,113	1.37	7 (9%)
38	BCR	l	413	-	41,41,41	0.32	0	56,56,56	0.54	0
30	DD6	B	612	-	39,45,45	0.17	0	52,67,67	0.64	2 (3%)
27	CLA	I	605	9	55,63,73	2.37	8 (14%)	64,101,113	1.46	7 (10%)
27	CLA	A	601	1	42,50,73	2.74	8 (19%)	48,85,113	1.73	8 (16%)
27	CLA	F	604	-	45,53,73	2.59	8 (17%)	52,89,113	1.64	8 (15%)
27	CLA	A	602	1	60,68,73	2.33	8 (13%)	70,107,113	1.48	7 (10%)
27	CLA	A	609	-	47,55,73	2.60	8 (17%)	54,91,113	1.62	7 (12%)
32	PID	B	613	-	41,49,49	1.56	7 (17%)	49,76,76	3.46	21 (42%)
28	KC2	G	601	-	48,53,53	1.50	8 (16%)	54,89,89	1.13	6 (11%)
27	CLA	I	603	-	65,73,73	2.18	8 (12%)	76,113,113	1.44	9 (11%)
30	DD6	H	315	-	39,45,45	0.17	0	52,67,67	0.65	1 (1%)
27	CLA	A	611	27	45,53,73	2.71	8 (17%)	52,89,113	1.68	7 (13%)
27	CLA	A	606	1	47,55,73	2.59	8 (17%)	54,91,113	1.65	7 (12%)
27	CLA	A	604	-	45,53,73	2.67	8 (17%)	52,89,113	1.66	7 (13%)
27	CLA	F	601	6	60,68,73	2.32	8 (13%)	70,107,113	1.46	7 (10%)
30	DD6	D	621	-	39,45,45	0.18	0	52,67,67	0.75	2 (3%)
27	CLA	b	711	-	60,68,73	2.31	8 (13%)	70,107,113	1.47	7 (10%)
27	CLA	b	708	-	65,73,73	2.12	8 (12%)	76,113,113	1.30	6 (7%)
27	CLA	T	604	12	41,49,73	2.86	9 (21%)	47,84,113	1.77	7 (14%)
27	CLA	a	824	-	65,73,73	2.19	8 (12%)	76,113,113	1.41	8 (10%)
27	CLA	b	717	-	65,73,73	2.15	8 (12%)	76,113,113	1.38	7 (9%)
27	CLA	a	817	-	55,63,73	2.43	8 (14%)	64,101,113	1.52	8 (12%)
29	UIX	H	314	-	41,49,49	1.23	3 (7%)	52,74,74	1.94	18 (34%)
38	BCR	l	414	-	41,41,41	0.33	0	56,56,56	0.81	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	CLA	a	829	27	65,73,73	2.23	8 (12%)	76,113,113	1.39	7 (9%)
30	DD6	E	614	-	39,45,45	0.17	0	52,67,67	0.52	0
27	CLA	l	404	-	55,63,73	2.32	8 (14%)	64,101,113	1.55	8 (12%)
28	KC2	U	602	-	48,53,53	1.52	8 (16%)	54,89,89	1.07	5 (9%)
30	DD6	D	617	-	39,45,45	0.19	0	52,67,67	0.64	3 (5%)
27	CLA	T	609	-	41,49,73	2.91	9 (21%)	47,84,113	1.83	7 (14%)
27	CLA	l	409	-	65,73,73	2.17	8 (12%)	76,113,113	1.38	7 (9%)
27	CLA	C	203	3	65,73,73	2.19	8 (12%)	76,113,113	1.44	8 (10%)
30	DD6	D	614	-	39,45,45	0.15	0	52,67,67	0.66	2 (3%)
27	CLA	b	720	-	48,56,73	2.59	8 (16%)	55,92,113	1.62	7 (12%)
29	UIX	I	612	-	41,49,49	1.29	3 (7%)	52,74,74	2.14	18 (34%)
27	CLA	T	606	12	45,53,73	2.72	8 (17%)	52,89,113	1.66	5 (9%)
36	LMU	T	613	-	36,36,36	0.41	0	47,47,47	0.95	2 (4%)
27	CLA	a	828	-	48,56,73	2.65	8 (16%)	55,92,113	1.73	6 (10%)
27	CLA	I	602	-	55,63,73	2.37	8 (14%)	64,101,113	1.45	7 (10%)
34	LHG	a	835	-	47,47,48	0.52	0	50,53,54	0.53	0
27	CLA	F	610	6	47,55,73	2.67	8 (17%)	54,91,113	1.66	7 (12%)
29	UIX	T	612	-	41,49,49	1.24	4 (9%)	52,74,74	2.02	18 (34%)
27	CLA	J	603	-	60,68,73	2.32	8 (13%)	70,107,113	1.46	7 (10%)
27	CLA	A	610	-	55,63,73	2.39	8 (14%)	64,101,113	1.51	7 (10%)
34	LHG	F	618	-	36,36,48	0.58	0	39,42,54	0.56	0
30	DD6	H	318	28	39,45,45	0.15	0	52,67,67	0.74	3 (5%)
27	CLA	G	608	-	60,68,73	2.35	8 (13%)	70,107,113	1.51	7 (10%)
27	CLA	b	702	-	65,73,73	2.09	8 (12%)	76,113,113	1.28	9 (11%)
27	CLA	T	607	-	45,53,73	2.71	8 (17%)	52,89,113	1.67	7 (13%)
27	CLA	U	603	-	50,58,73	2.56	8 (16%)	58,95,113	1.69	7 (12%)
27	CLA	a	823	-	65,73,73	2.22	8 (12%)	76,113,113	1.47	8 (10%)
27	CLA	D	602	-	55,63,73	2.39	8 (14%)	64,101,113	1.57	6 (9%)
30	DD6	H	301	-	39,45,45	0.19	0	52,67,67	0.75	2 (3%)
27	CLA	D	612	-	55,63,73	2.42	8 (14%)	64,101,113	1.52	7 (10%)
27	CLA	K	601	11	57,65,73	2.38	8 (14%)	66,103,113	1.52	7 (10%)
38	BCR	j	203	-	41,41,41	0.32	0	56,56,56	0.57	0
32	PID	U	608	-	41,49,49	1.55	6 (14%)	49,76,76	3.57	17 (34%)
38	BCR	f	301	-	41,41,41	0.30	0	56,56,56	0.73	0
27	CLA	B	601	-	60,68,73	2.26	8 (13%)	70,107,113	1.49	8 (11%)
27	CLA	b	727	-	65,73,73	2.20	8 (12%)	76,113,113	1.44	8 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	KC2	J	608	-	48,53,53	1.53	7 (14%)	54,89,89	1.09	5 (9%)
29	UIX	E	616	-	41,49,49	1.24	4 (9%)	52,74,74	1.97	15 (28%)
29	UIX	C	213	-	41,49,49	1.26	3 (7%)	52,74,74	1.89	16 (30%)
27	CLA	A	605	1	55,63,73	2.42	8 (14%)	64,101,113	1.51	7 (10%)
27	CLA	K	604	-	57,65,73	2.36	8 (14%)	66,103,113	1.46	6 (9%)
27	CLA	I	606	9	55,63,73	2.41	8 (14%)	64,101,113	1.53	7 (10%)
29	UIX	B	615	-	41,49,49	1.25	4 (9%)	52,74,74	1.89	15 (28%)
27	CLA	b	715	-	65,73,73	2.21	8 (12%)	76,113,113	1.51	9 (11%)
39	SF4	a	838	14	0,12,12	-	-	-		
28	KC2	K	607	-	48,53,53	1.53	7 (14%)	54,89,89	1.09	5 (9%)
27	CLA	b	724	-	65,73,73	2.21	8 (12%)	76,113,113	1.38	7 (9%)
29	UIX	j	204	-	41,49,49	1.25	3 (7%)	52,74,74	2.02	18 (34%)
31	SQD	y	301	-	45,46,54	1.29	4 (8%)	54,57,65	1.08	5 (9%)
32	PID	J	614	-	41,49,49	1.54	5 (12%)	49,76,76	3.27	15 (30%)
33	LMG	D	619	-	46,46,55	0.52	0	54,54,63	0.71	1 (1%)
32	PID	F	615	-	41,49,49	1.53	5 (12%)	49,76,76	3.48	16 (32%)
30	DD6	A	614	-	39,45,45	0.16	0	52,67,67	0.71	2 (3%)
27	CLA	b	706	-	65,73,73	2.19	8 (12%)	76,113,113	1.37	8 (10%)
34	LHG	D	620	-	45,45,48	0.53	0	48,51,54	0.51	0
28	KC2	H	302	30	48,53,53	1.50	8 (16%)	54,89,89	1.11	5 (9%)
27	CLA	D	601	4	45,53,73	2.66	8 (17%)	52,89,113	1.64	7 (13%)
32	PID	J	615	-	41,49,49	1.51	5 (12%)	49,76,76	3.56	18 (36%)
27	CLA	E	606	-	60,68,73	2.33	8 (13%)	70,107,113	1.46	7 (10%)
27	CLA	B	605	2	45,53,73	2.64	8 (17%)	52,89,113	1.67	8 (15%)
27	CLA	l	411	22	48,56,73	2.55	8 (16%)	55,92,113	1.66	7 (12%)
27	CLA	b	709	15	65,73,73	2.12	8 (12%)	76,113,113	1.34	7 (9%)
27	CLA	A	607	-	45,53,73	2.70	8 (17%)	52,89,113	1.66	7 (13%)
30	DD6	G	616	-	39,45,45	0.15	0	52,67,67	0.47	0
37	PQN	a	832	-	34,34,34	0.35	0	42,45,45	0.68	0
38	BCR	f	304	-	41,41,41	0.30	0	56,56,56	0.52	0
27	CLA	C	202	3	45,53,73	2.69	8 (17%)	52,89,113	1.68	7 (13%)
27	CLA	C	206	-	47,55,73	2.58	8 (17%)	54,91,113	1.61	7 (12%)
29	UIX	A	616	-	41,49,49	1.27	4 (9%)	52,74,74	1.91	16 (30%)
27	CLA	a	819	-	60,68,73	2.29	8 (13%)	70,107,113	1.43	7 (10%)
27	CLA	H	305	-	60,68,73	2.31	8 (13%)	70,107,113	1.54	10 (14%)
39	SF4	c	201	16	0,12,12	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
33	LMG	C	217	-	34,34,55	0.58	0	42,42,63	0.71	1 (2%)
32	PID	J	611	-	41,49,49	1.53	6 (14%)	49,76,76	4.07	21 (42%)
27	CLA	C	207	3	60,68,73	2.31	8 (13%)	70,107,113	1.46	8 (11%)
27	CLA	a	831	-	55,63,73	2.39	8 (14%)	64,101,113	1.52	8 (12%)
27	CLA	r	204	-	60,68,73	2.30	8 (13%)	70,107,113	1.41	7 (10%)
30	DD6	K	609	-	39,45,45	0.16	0	52,67,67	0.59	1 (1%)
28	KC2	U	604	13	48,53,53	1.54	8 (16%)	54,89,89	1.08	5 (9%)
27	CLA	b	716	-	65,73,73	2.21	8 (12%)	76,113,113	1.37	7 (9%)
27	CLA	I	611	-	42,50,73	2.85	8 (19%)	48,85,113	1.84	9 (18%)
27	CLA	K	603	-	45,53,73	2.73	8 (17%)	52,89,113	1.71	7 (13%)
28	KC2	B	608	2	48,53,53	1.47	8 (16%)	54,89,89	1.09	5 (9%)
30	DD6	G	614	-	39,45,45	0.16	0	52,67,67	0.75	3 (5%)
27	CLA	I	616	-	65,73,73	2.25	8 (12%)	76,113,113	1.33	7 (9%)
30	DD6	B	616	-	39,45,45	0.14	0	52,67,67	0.58	0
27	CLA	l	406	-	65,73,73	2.20	8 (12%)	76,113,113	1.36	8 (10%)
30	DD6	r	206	-	39,45,45	0.18	0	52,67,67	0.83	3 (5%)
27	CLA	H	307	-	45,53,73	2.66	8 (17%)	52,89,113	1.64	7 (13%)
30	DD6	C	214	-	39,45,45	0.19	0	52,67,67	0.69	2 (3%)
29	UIX	D	616	-	41,49,49	1.22	3 (7%)	52,74,74	2.11	16 (30%)
27	CLA	F	608	6	45,53,73	2.72	8 (17%)	52,89,113	1.67	7 (13%)
27	CLA	a	807	-	65,73,73	2.21	8 (12%)	76,113,113	1.43	9 (11%)
38	BCR	a	836	-	41,41,41	0.85	2 (4%)	56,56,56	2.18	19 (33%)
27	CLA	b	725	-	65,73,73	2.16	8 (12%)	76,113,113	1.38	8 (10%)
27	CLA	b	719	-	65,73,73	2.20	8 (12%)	76,113,113	1.36	7 (9%)
27	CLA	b	710	-	55,63,73	2.42	8 (14%)	64,101,113	1.55	8 (12%)
27	CLA	a	814	-	55,63,73	2.42	8 (14%)	64,101,113	1.49	7 (10%)
27	CLA	K	608	-	45,53,73	2.73	8 (17%)	52,89,113	1.67	8 (15%)
30	DD6	K	610	-	39,45,45	0.17	0	52,67,67	0.81	2 (3%)
31	SQD	H	320	-	45,46,54	1.27	4 (8%)	54,57,65	1.09	6 (11%)
30	DD6	E	617	-	39,45,45	0.15	0	52,67,67	0.82	2 (3%)
27	CLA	T	602	-	45,53,73	2.70	8 (17%)	52,89,113	1.65	7 (13%)
27	CLA	K	606	-	41,49,73	2.91	9 (21%)	47,84,113	1.90	8 (17%)
27	CLA	J	605	10	60,68,73	2.29	8 (13%)	70,107,113	1.39	7 (10%)
27	CLA	F	606	6	65,73,73	2.19	8 (12%)	76,113,113	1.38	7 (9%)
27	CLA	G	607	7	45,53,73	2.67	8 (17%)	52,89,113	1.76	7 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	CLA	A	603	-	55,63,73	2.38	8 (14%)	64,101,113	1.51	8 (12%)
30	DD6	G	612	-	39,45,45	0.17	0	52,67,67	0.94	3 (5%)
27	CLA	a	811	-	48,56,73	2.63	8 (16%)	55,92,113	1.63	8 (14%)
35	DGD	f	305	-	53,53,67	0.97	3 (5%)	67,67,81	1.51	11 (16%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
38	BCR	b	732	-	-	1/29/63/63	0/2/2/2
30	DD6	B	614	-	-	5/26/80/80	0/3/3/3
27	CLA	b	718	-	1/1/15/20	7/37/115/115	-
35	DGD	l	416	-	-	17/44/84/95	0/2/2/2
27	CLA	f	302	-	1/1/11/20	1/17/95/115	-
28	KC2	J	602	10	-	6/15/71/71	-
27	CLA	F	607	6	1/1/11/20	5/13/91/115	-
38	BCR	m	201	-	-	10/29/63/63	0/2/2/2
27	CLA	J	609	-	1/1/10/20	5/8/86/115	-
30	DD6	i	202	-	-	3/26/80/80	0/3/3/3
27	CLA	G	605	-	1/1/14/20	2/31/109/115	-
28	KC2	I	604	9	-	2/15/71/71	-
27	CLA	F	603	-	1/1/12/20	6/22/100/115	-
27	CLA	b	722	-	1/1/11/20	5/17/95/115	-
27	CLA	a	820	-	1/1/15/20	8/37/115/115	-
30	DD6	J	612	-	-	1/26/80/80	0/3/3/3
30	DD6	D	615	-	-	2/26/80/80	0/3/3/3
27	CLA	G	603	-	1/1/12/20	4/19/97/115	-
27	CLA	H	313	-	1/1/14/20	2/31/109/115	-
27	CLA	E	602	5	1/1/13/20	0/25/103/115	-
27	CLA	H	308	8	1/1/13/20	2/25/103/115	-
27	CLA	I	610	-	1/1/13/20	4/25/103/115	-
30	DD6	D	613	-	1/1/12/24	2/26/80/80	0/3/3/3
30	DD6	b	730	-	-	1/26/80/80	0/3/3/3
38	BCR	b	731	-	-	8/29/63/63	0/2/2/2
27	CLA	l	403	-	1/1/15/20	7/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	CLA	F	617	-	1/1/14/20	8/31/109/115	-
27	CLA	a	827	-	1/1/15/20	12/37/115/115	-
38	BCR	i	201	-	-	6/29/63/63	0/2/2/2
28	KC2	J	604	10	-	5/15/71/71	-
27	CLA	l	412	22	1/1/15/20	10/37/115/115	-
27	CLA	b	707	-	1/1/15/20	3/37/115/115	-
27	CLA	a	808	14	1/1/13/20	5/25/103/115	-
30	DD6	H	316	-	-	1/26/80/80	0/3/3/3
27	CLA	E	604	-	1/1/13/20	4/25/103/115	-
35	DGD	j	201	-	-	17/49/89/95	0/2/2/2
27	CLA	G	611	-	1/1/11/20	1/13/91/115	-
27	CLA	J	607	-	1/1/10/20	2/10/88/115	-
27	CLA	a	813	-	1/1/11/20	4/17/95/115	-
27	CLA	D	605	4	1/1/11/20	0/16/94/115	-
27	CLA	C	211	-	1/1/11/20	2/16/94/115	-
27	CLA	a	837	-	1/1/15/20	3/37/115/115	-
34	LHG	l	401	-	-	23/50/50/53	-
27	CLA	G	604	-	1/1/11/20	1/16/94/115	-
27	CLA	D	604	-	1/1/13/20	8/25/103/115	-
27	CLA	a	805	-	1/1/15/20	9/37/115/115	-
27	CLA	E	608	5	1/1/14/20	5/31/109/115	-
27	CLA	G	602	7	1/1/13/20	2/25/103/115	-
27	CLA	C	201	-	1/1/10/20	2/10/88/115	-
27	CLA	b	712	-	1/1/11/20	3/17/95/115	-
27	CLA	j	202	27	1/1/13/20	5/27/105/115	-
27	CLA	b	721	-	1/1/12/20	2/19/97/115	-
27	CLA	D	609	-	1/1/11/20	2/13/91/115	-
32	PID	K	611	-	-	6/24/93/93	1/4/4/4
27	CLA	H	319	-	1/1/15/20	8/37/115/115	-
27	CLA	l	410	-	1/1/11/20	3/17/95/115	-
27	CLA	a	839	-	1/1/14/20	7/33/111/115	-
27	CLA	G	609	7	1/1/13/20	6/25/103/115	-
30	DD6	r	201	-	-	2/26/80/80	0/3/3/3
27	CLA	E	603	-	1/1/11/20	1/16/94/115	-
31	SQD	A	618	-	-	8/22/42/69	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	CLA	b	703	-	1/1/15/20	7/37/115/115	-
28	KC2	B	602	-	-	2/15/71/71	-
27	CLA	B	609	2	1/1/15/20	6/37/115/115	-
27	CLA	b	705	-	1/1/15/20	9/37/115/115	-
32	PID	J	613	-	-	3/24/93/93	0/4/4/4
27	CLA	C	209	-	1/1/11/20	1/13/91/115	-
30	DD6	U	607	-	-	0/26/80/80	0/3/3/3
37	PQN	b	729	-	-	10/23/43/43	0/2/2/2
27	CLA	H	306	-	1/1/11/20	3/13/91/115	-
30	DD6	T	610	-	-	4/26/80/80	0/3/3/3
27	CLA	I	607	-	1/1/14/20	3/33/111/115	-
27	CLA	a	804	-	1/1/15/20	12/37/115/115	-
27	CLA	l	408	-	1/1/11/20	3/16/94/115	-
30	DD6	T	611	-	-	2/26/80/80	0/3/3/3
28	KC2	A	608	-	-	6/15/71/71	-
33	LMG	D	618	-	-	17/30/50/70	0/1/1/1
30	DD6	E	615	-	-	1/26/80/80	0/3/3/3
34	LHG	r	202	-	-	20/50/50/53	-
28	KC2	J	610	-	-	6/15/71/71	-
28	KC2	H	311	-	-	10/15/71/71	-
30	DD6	I	615	-	-	0/26/80/80	0/3/3/3
27	CLA	B	606	-	1/1/15/20	8/37/115/115	-
30	DD6	r	205	-	-	3/26/80/80	0/3/3/3
27	CLA	K	605	11	1/1/14/20	8/31/109/115	-
29	UIX	G	615	-	-	4/31/87/87	0/3/3/3
27	CLA	l	405	22	1/1/14/20	5/33/111/115	-
27	CLA	a	810	-	1/1/12/20	1/19/97/115	-
29	UIX	C	215	-	-	3/31/87/87	0/3/3/3
27	CLA	b	714	-	1/1/11/20	5/17/95/115	-
27	CLA	D	603	-	1/1/13/20	3/25/103/115	-
33	LMG	F	616	-	-	14/41/61/70	0/1/1/1
27	CLA	B	607	-	1/1/14/20	7/31/109/115	-
27	CLA	U	605	13	1/1/14/20	6/31/109/115	-
27	CLA	T	605	12	1/1/11/20	0/13/91/115	-
27	CLA	l	407	-	1/1/11/20	4/17/95/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	CLA	B	610	-	1/1/11/20	5/16/94/115	-
27	CLA	D	610	4	1/1/11/20	4/16/94/115	-
27	CLA	H	303	8	1/1/14/20	4/31/109/115	-
27	CLA	b	713	-	1/1/15/20	7/37/115/115	-
29	UIX	J	616	-	-	3/31/87/87	0/3/3/3
27	CLA	K	602	-	1/1/13/20	8/25/103/115	-
33	LMG	l	417	-	-	21/45/65/70	0/1/1/1
27	CLA	B	603	-	1/1/15/20	9/37/115/115	-
27	CLA	b	701	-	1/1/15/20	9/37/115/115	-
27	CLA	J	601	-	1/1/11/20	4/13/91/115	-
27	CLA	a	812	-	1/1/12/20	2/19/97/115	-
33	LMG	b	733	-	-	26/50/70/70	0/1/1/1
27	CLA	r	203	-	1/1/11/20	4/17/95/115	-
28	KC2	E	610	5	-	7/15/71/71	-
29	UIX	B	611	-	-	2/31/87/87	0/3/3/3
27	CLA	a	809	-	1/1/11/20	3/16/94/115	-
27	CLA	b	728	-	1/1/15/20	8/37/115/115	-
27	CLA	U	601	-	1/1/10/20	3/11/89/115	-
27	CLA	F	619	-	1/1/13/20	5/25/103/115	-
29	UIX	H	317	-	-	4/31/87/87	0/3/3/3
30	DD6	F	612	-	-	0/26/80/80	0/3/3/3
27	CLA	a	806	-	1/1/13/20	4/25/103/115	-
27	CLA	T	603	-	1/1/11/20	4/13/91/115	-
34	LHG	j	205	-	-	16/41/41/53	-
27	CLA	a	818	-	1/1/13/20	5/25/103/115	-
27	CLA	U	606	-	1/1/11/20	7/13/91/115	-
27	CLA	a	826	-	1/1/13/20	4/25/103/115	-
28	KC2	J	606	-	-	5/15/71/71	-
27	CLA	D	611	-	1/1/14/20	6/31/109/115	-
30	DD6	E	613	-	-	1/26/80/80	0/3/3/3
30	DD6	I	613	-	-	1/26/80/80	0/3/3/3
33	LMG	K	613	-	-	11/37/57/70	0/1/1/1
38	BCR	l	415	-	-	12/29/63/63	0/2/2/2
38	BCR	a	834	-	-	5/29/63/63	0/2/2/2
27	CLA	f	303	19	1/1/11/20	0/17/95/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	DD6	K	612	-	-	5/26/80/80	0/3/3/3
27	CLA	D	606	-	1/1/11/20	2/13/91/115	-
28	KC2	T	608	-	-	5/15/71/71	-
27	CLA	C	208	-	1/1/11/20	2/16/94/115	-
27	CLA	E	605	5	1/1/11/20	4/13/91/115	-
27	CLA	H	304	-	1/1/14/20	9/31/109/115	-
27	CLA	H	310	-	1/1/11/20	5/13/91/115	-
32	PID	I	614	-	-	5/24/93/93	0/4/4/4
30	DD6	F	611	-	-	2/26/80/80	0/3/3/3
27	CLA	a	803	27	1/1/12/20	2/19/97/115	-
28	KC2	F	609	6	-	7/15/71/71	-
27	CLA	l	402	-	1/1/14/20	3/31/109/115	-
29	UIX	A	613	-	-	2/31/87/87	0/3/3/3
27	CLA	H	309	-	1/1/15/20	6/37/115/115	-
27	CLA	b	704	-	1/1/15/20	9/37/115/115	-
27	CLA	a	822	-	1/1/14/20	7/31/109/115	-
27	CLA	T	601	12	1/1/11/20	3/16/94/115	-
32	PID	F	614	-	-	5/24/93/93	0/4/4/4
27	CLA	a	821	-	1/1/15/20	8/37/115/115	-
27	CLA	G	606	7	1/1/15/20	8/37/115/115	-
27	CLA	b	723	-	1/1/15/20	5/37/115/115	-
28	KC2	C	210	-	-	6/15/71/71	-
27	CLA	E	612	-	1/1/11/20	0/13/91/115	-
27	CLA	H	312	-	1/1/10/20	5/10/88/115	-
30	DD6	C	216	-	-	1/26/80/80	0/3/3/3
27	CLA	a	801	-	1/1/15/20	6/37/115/115	-
27	CLA	E	611	5	1/1/14/20	6/31/109/115	-
28	KC2	E	601	27	-	10/15/71/71	-
27	CLA	F	602	-	1/1/13/20	5/27/105/115	-
30	DD6	A	617	-	-	4/26/80/80	0/3/3/3
27	CLA	a	815	-	1/1/14/20	5/31/109/115	-
27	CLA	b	726	-	1/1/14/20	4/31/109/115	-
27	CLA	a	830	-	1/1/15/20	11/37/115/115	-
27	CLA	C	212	-	1/1/11/20	0/16/94/115	-
27	CLA	I	601	9	1/1/15/20	7/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	CLA	G	610	7	1/1/11/20	4/16/94/115	-
38	BCR	a	833	-	-	8/29/63/63	0/2/2/2
27	CLA	D	608	4	1/1/13/20	2/25/103/115	-
34	LHG	G	617	-	-	23/38/38/53	-
27	CLA	I	609	9	1/1/11/20	3/13/91/115	-
39	SF4	c	202	-	-	-	0/6/5/5
27	CLA	C	204	-	1/1/15/20	7/37/115/115	-
30	DD6	G	613	-	-	2/26/80/80	0/3/3/3
29	UIX	F	613	-	-	4/31/87/87	0/3/3/3
27	CLA	I	608	9	1/1/14/20	4/31/109/115	-
30	DD6	A	615	-	-	3/26/80/80	0/3/3/3
27	CLA	C	205	-	1/1/13/20	7/25/103/115	-
27	CLA	a	802	-	1/1/13/20	4/25/103/115	-
27	CLA	D	607	4	1/1/14/20	3/31/109/115	-
27	CLA	a	816	-	1/1/14/20	7/31/109/115	-
27	CLA	E	609	28	1/1/11/20	2/13/91/115	-
27	CLA	B	604	2	1/1/11/20	0/16/94/115	-
27	CLA	A	612	1	1/1/11/20	3/16/94/115	-
35	DGD	K	614	-	-	19/36/76/95	0/2/2/2
27	CLA	F	605	6	1/1/11/20	7/13/91/115	-
27	CLA	E	607	5	1/1/15/20	9/37/115/115	-
27	CLA	a	825	-	1/1/15/20	9/37/115/115	-
38	BCR	l	413	-	-	3/29/63/63	0/2/2/2
30	DD6	B	612	-	-	1/26/80/80	0/3/3/3
27	CLA	I	605	9	1/1/13/20	3/25/103/115	-
27	CLA	A	601	1	1/1/10/20	2/10/88/115	-
27	CLA	F	604	-	1/1/11/20	4/13/91/115	-
27	CLA	A	602	1	1/1/14/20	2/31/109/115	-
27	CLA	A	609	-	1/1/11/20	2/16/94/115	-
32	PID	B	613	-	-	3/24/93/93	0/4/4/4
28	KC2	G	601	-	-	8/15/71/71	-
27	CLA	I	603	-	1/1/15/20	8/37/115/115	-
30	DD6	H	315	-	-	0/26/80/80	0/3/3/3
27	CLA	A	611	27	1/1/11/20	3/13/91/115	-
27	CLA	A	606	1	1/1/11/20	3/16/94/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	CLA	A	604	-	1/1/11/20	4/13/91/115	-
27	CLA	F	601	6	1/1/14/20	5/31/109/115	-
30	DD6	D	621	-	-	5/26/80/80	0/3/3/3
27	CLA	b	711	-	1/1/14/20	6/31/109/115	-
27	CLA	b	708	-	1/1/15/20	8/37/115/115	-
27	CLA	T	604	12	1/1/10/20	0/8/86/115	-
27	CLA	a	824	-	1/1/15/20	10/37/115/115	-
27	CLA	b	717	-	1/1/15/20	7/37/115/115	-
27	CLA	a	817	-	1/1/13/20	3/25/103/115	-
29	UIX	H	314	-	-	2/31/87/87	0/3/3/3
38	BCR	l	414	-	-	5/29/63/63	0/2/2/2
27	CLA	a	829	27	1/1/15/20	16/37/115/115	-
30	DD6	E	614	-	-	0/26/80/80	0/3/3/3
27	CLA	l	404	-	1/1/13/20	1/25/103/115	-
28	KC2	U	602	-	-	5/15/71/71	-
30	DD6	D	617	-	-	0/26/80/80	0/3/3/3
27	CLA	T	609	-	1/1/10/20	0/8/86/115	-
27	CLA	l	409	-	1/1/15/20	12/37/115/115	-
27	CLA	C	203	3	1/1/15/20	4/37/115/115	-
30	DD6	D	614	-	-	0/26/80/80	0/3/3/3
27	CLA	b	720	-	1/1/11/20	1/17/95/115	-
29	UIX	I	612	-	-	2/31/87/87	1/3/3/3
27	CLA	T	606	12	1/1/11/20	1/13/91/115	-
36	LMU	T	613	-	-	5/21/61/61	0/2/2/2
27	CLA	a	828	-	1/1/11/20	6/17/95/115	-
27	CLA	I	602	-	1/1/13/20	7/25/103/115	-
34	LHG	a	835	-	-	21/52/52/53	-
27	CLA	F	610	6	1/1/11/20	6/16/94/115	-
29	UIX	T	612	-	-	5/31/87/87	0/3/3/3
27	CLA	J	603	-	1/1/14/20	4/31/109/115	-
27	CLA	A	610	-	1/1/13/20	4/25/103/115	-
34	LHG	F	618	-	-	21/41/41/53	-
30	DD6	H	318	28	-	0/26/80/80	0/3/3/3
27	CLA	G	608	-	1/1/14/20	5/31/109/115	-
27	CLA	b	702	-	1/1/15/20	13/37/115/115	-
27	CLA	T	607	-	1/1/11/20	3/13/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	CLA	U	603	-	1/1/12/20	6/19/97/115	-
27	CLA	a	823	-	1/1/15/20	13/37/115/115	-
27	CLA	D	602	-	1/1/13/20	7/25/103/115	-
30	DD6	H	301	-	-	3/26/80/80	0/3/3/3
27	CLA	D	612	-	1/1/13/20	5/25/103/115	-
27	CLA	K	601	11	1/1/13/20	1/28/106/115	-
38	BCR	j	203	-	-	10/29/63/63	0/2/2/2
32	PID	U	608	-	-	4/24/93/93	1/4/4/4
38	BCR	f	301	-	-	9/29/63/63	0/2/2/2
27	CLA	B	601	-	1/1/14/20	4/31/109/115	-
27	CLA	b	727	-	1/1/15/20	11/37/115/115	-
28	KC2	J	608	-	-	4/15/71/71	-
29	UIX	E	616	-	-	3/31/87/87	0/3/3/3
29	UIX	C	213	-	-	2/31/87/87	0/3/3/3
27	CLA	A	605	1	1/1/13/20	4/25/103/115	-
27	CLA	K	604	-	1/1/13/20	6/28/106/115	-
27	CLA	I	606	9	1/1/13/20	3/25/103/115	-
29	UIX	B	615	-	-	3/31/87/87	1/3/3/3
27	CLA	b	715	-	1/1/15/20	6/37/115/115	-
39	SF4	a	838	14	-	-	0/6/5/5
28	KC2	K	607	-	-	3/15/71/71	-
27	CLA	b	724	-	1/1/15/20	6/37/115/115	-
29	UIX	j	204	-	-	6/31/87/87	0/3/3/3
31	SQD	y	301	-	-	6/41/61/69	0/1/1/1
32	PID	J	614	-	-	0/24/93/93	0/4/4/4
33	LMG	D	619	-	-	21/41/61/70	0/1/1/1
32	PID	F	615	-	-	4/24/93/93	0/4/4/4
30	DD6	A	614	-	-	1/26/80/80	0/3/3/3
27	CLA	b	706	-	1/1/15/20	11/37/115/115	-
34	LHG	D	620	-	-	22/50/50/53	-
28	KC2	H	302	30	-	8/15/71/71	-
27	CLA	D	601	4	1/1/11/20	3/13/91/115	-
32	PID	J	615	-	-	6/24/93/93	0/4/4/4
27	CLA	E	606	-	1/1/14/20	8/31/109/115	-
27	CLA	B	605	2	1/1/11/20	5/13/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	CLA	l	411	22	1/1/11/20	1/17/95/115	-
27	CLA	b	709	15	1/1/15/20	7/37/115/115	-
27	CLA	A	607	-	1/1/11/20	0/13/91/115	-
30	DD6	G	616	-	-	1/26/80/80	0/3/3/3
37	PQN	a	832	-	-	6/23/43/43	0/2/2/2
38	BCR	f	304	-	-	3/29/63/63	0/2/2/2
27	CLA	C	202	3	1/1/11/20	1/13/91/115	-
27	CLA	C	206	-	1/1/11/20	2/16/94/115	-
29	UIX	A	616	-	-	6/31/87/87	0/3/3/3
27	CLA	a	819	-	1/1/14/20	5/31/109/115	-
27	CLA	H	305	-	1/1/14/20	14/31/109/115	-
39	SF4	c	201	16	-	-	0/6/5/5
33	LMG	C	217	-	-	14/29/49/70	0/1/1/1
32	PID	J	611	-	-	4/24/93/93	0/4/4/4
27	CLA	C	207	3	1/1/14/20	4/31/109/115	-
27	CLA	a	831	-	1/1/13/20	2/25/103/115	-
27	CLA	r	204	-	1/1/14/20	12/31/109/115	-
30	DD6	K	609	-	-	4/26/80/80	0/3/3/3
28	KC2	U	604	13	-	8/15/71/71	-
27	CLA	b	716	-	1/1/15/20	5/37/115/115	-
27	CLA	I	611	-	1/1/10/20	4/10/88/115	-
27	CLA	K	603	-	1/1/11/20	3/13/91/115	-
28	KC2	B	608	2	-	4/15/71/71	-
30	DD6	G	614	-	-	2/26/80/80	0/3/3/3
27	CLA	I	616	-	1/1/15/20	1/37/115/115	-
30	DD6	B	616	-	-	2/26/80/80	0/3/3/3
27	CLA	l	406	-	1/1/15/20	3/37/115/115	-
30	DD6	r	206	-	-	3/26/80/80	0/3/3/3
27	CLA	H	307	-	1/1/11/20	4/13/91/115	-
30	DD6	C	214	-	-	1/26/80/80	0/3/3/3
29	UIX	D	616	-	-	5/31/87/87	0/3/3/3
27	CLA	F	608	6	1/1/11/20	1/13/91/115	-
27	CLA	a	807	-	1/1/15/20	10/37/115/115	-
38	BCR	a	836	-	-	13/29/63/63	0/2/2/2
27	CLA	b	725	-	1/1/15/20	4/37/115/115	-
27	CLA	b	719	-	1/1/15/20	7/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	CLA	b	710	-	1/1/13/20	3/25/103/115	-
27	CLA	a	814	-	1/1/13/20	2/25/103/115	-
27	CLA	K	608	-	1/1/11/20	2/13/91/115	-
30	DD6	K	610	-	-	3/26/80/80	0/3/3/3
31	SQD	H	320	-	-	15/41/61/69	0/1/1/1
30	DD6	E	617	-	-	2/26/80/80	0/3/3/3
27	CLA	T	602	-	1/1/11/20	5/13/91/115	-
27	CLA	K	606	-	1/1/10/20	0/8/86/115	-
27	CLA	J	605	10	1/1/14/20	4/31/109/115	-
27	CLA	F	606	6	1/1/15/20	12/37/115/115	-
27	CLA	G	607	7	1/1/11/20	7/13/91/115	-
27	CLA	A	603	-	1/1/13/20	1/25/103/115	-
30	DD6	G	612	-	-	0/26/80/80	0/3/3/3
27	CLA	a	811	-	1/1/11/20	2/17/95/115	-
35	DGD	f	305	-	-	17/41/81/95	0/2/2/2

The worst 5 of 1858 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	K	603	CLA	C1B-NB	10.82	1.44	1.35
27	I	611	CLA	C1B-NB	10.78	1.44	1.35
27	U	606	CLA	C1B-NB	10.77	1.44	1.35
27	B	604	CLA	C1B-NB	10.77	1.44	1.35
27	K	606	CLA	C1B-NB	10.75	1.44	1.35

The worst 5 of 2164 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	J	613	PID	O4-C12-C11	16.67	117.47	107.36
32	J	615	PID	O4-C12-C11	16.54	117.39	107.36
32	J	611	PID	O4-C12-C11	16.54	117.39	107.36
32	U	608	PID	O4-C12-C11	16.19	117.17	107.36
32	F	614	PID	O4-C12-C11	16.13	117.14	107.36

5 of 197 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
27	A	601	CLA	ND
27	A	602	CLA	ND

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Mol	Chain	Res	Type	Atom
27	A	603	CLA	ND
27	A	604	CLA	ND
27	A	605	CLA	ND

5 of 1715 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
27	A	601	CLA	C1A-C2A-CAA-CBA
27	A	602	CLA	CHA-CBD-CGD-O1D
27	A	602	CLA	CHA-CBD-CGD-O2D
27	A	604	CLA	C1A-C2A-CAA-CBA
27	A	606	CLA	C1A-C2A-CAA-CBA

All (4) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
32	K	611	PID	C24-C25-C26-C27-C28-C29
29	B	615	UIX	C15-C16-C17-C18-C19-C20
29	I	612	UIX	C15-C16-C17-C18-C19-C20
32	U	608	PID	C24-C25-C26-C27-C28-C29

115 monomers are involved in 212 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	J	609	CLA	3	0
27	G	605	CLA	3	0
30	J	612	DD6	1	0
30	D	615	DD6	2	0
27	H	313	CLA	1	0
27	H	308	CLA	1	0
27	I	610	CLA	3	0
28	J	604	KC2	3	0
30	H	316	DD6	1	0
27	G	611	CLA	1	0
27	J	607	CLA	1	0
27	D	605	CLA	2	0
27	C	211	CLA	1	0
27	E	608	CLA	1	0
27	G	602	CLA	1	0
27	D	609	CLA	1	0
32	K	611	PID	12	0
27	H	319	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	G	609	CLA	1	0
32	J	613	PID	10	0
30	U	607	DD6	1	0
27	H	306	CLA	2	0
27	I	607	CLA	1	0
30	T	611	DD6	1	0
33	D	618	LMG	1	0
27	B	606	CLA	2	0
27	K	605	CLA	2	0
27	D	603	CLA	1	0
27	U	605	CLA	3	0
27	T	605	CLA	2	0
27	B	610	CLA	1	0
27	D	610	CLA	1	0
27	H	303	CLA	1	0
27	K	602	CLA	1	0
27	J	601	CLA	1	0
27	U	601	CLA	1	0
27	F	619	CLA	2	0
30	F	612	DD6	2	0
27	T	603	CLA	4	0
30	E	613	DD6	1	0
30	I	613	DD6	2	0
33	K	613	LMG	1	0
27	E	605	CLA	1	0
27	H	304	CLA	3	0
32	I	614	PID	5	0
27	T	601	CLA	3	0
32	F	614	PID	6	0
27	G	606	CLA	3	0
30	C	216	DD6	2	0
27	E	611	CLA	1	0
27	F	602	CLA	2	0
27	I	601	CLA	4	0
27	D	608	CLA	1	0
27	I	609	CLA	1	0
27	C	204	CLA	1	0
30	G	613	DD6	1	0
30	A	615	DD6	1	0
27	C	205	CLA	4	0
27	E	609	CLA	1	0
27	A	612	CLA	1	0

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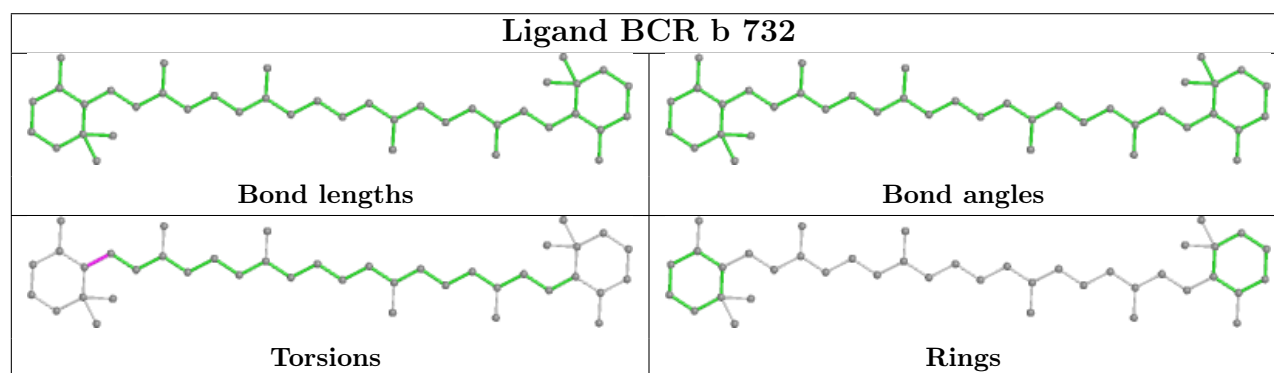
Mol	Chain	Res	Type	Clashes	Symm-Clashes
35	K	614	DGD	4	0
27	F	605	CLA	2	0
30	B	612	DD6	2	0
27	I	605	CLA	2	0
27	A	601	CLA	1	0
27	F	604	CLA	6	0
32	B	613	PID	1	0
27	I	603	CLA	5	0
30	H	315	DD6	1	0
27	A	606	CLA	2	0
27	A	604	CLA	4	0
27	F	601	CLA	1	0
30	D	621	DD6	1	0
29	H	314	UIX	1	0
30	E	614	DD6	1	0
27	C	203	CLA	2	0
29	I	612	UIX	1	0
27	T	606	CLA	2	0
36	T	613	LMU	1	0
27	I	602	CLA	1	0
30	H	318	DD6	1	0
27	G	608	CLA	2	0
27	T	607	CLA	1	0
27	U	603	CLA	8	0
27	D	602	CLA	1	0
27	D	612	CLA	1	0
27	K	601	CLA	4	0
27	B	601	CLA	1	0
28	J	608	KC2	2	0
27	A	605	CLA	1	0
27	K	604	CLA	1	0
27	I	606	CLA	3	0
28	K	607	KC2	6	0
32	J	614	PID	4	0
33	D	619	LMG	1	0
32	F	615	PID	2	0
30	A	614	DD6	1	0
32	J	615	PID	3	0
27	B	605	CLA	1	0
30	G	616	DD6	1	0
27	C	202	CLA	1	0
27	C	206	CLA	1	0

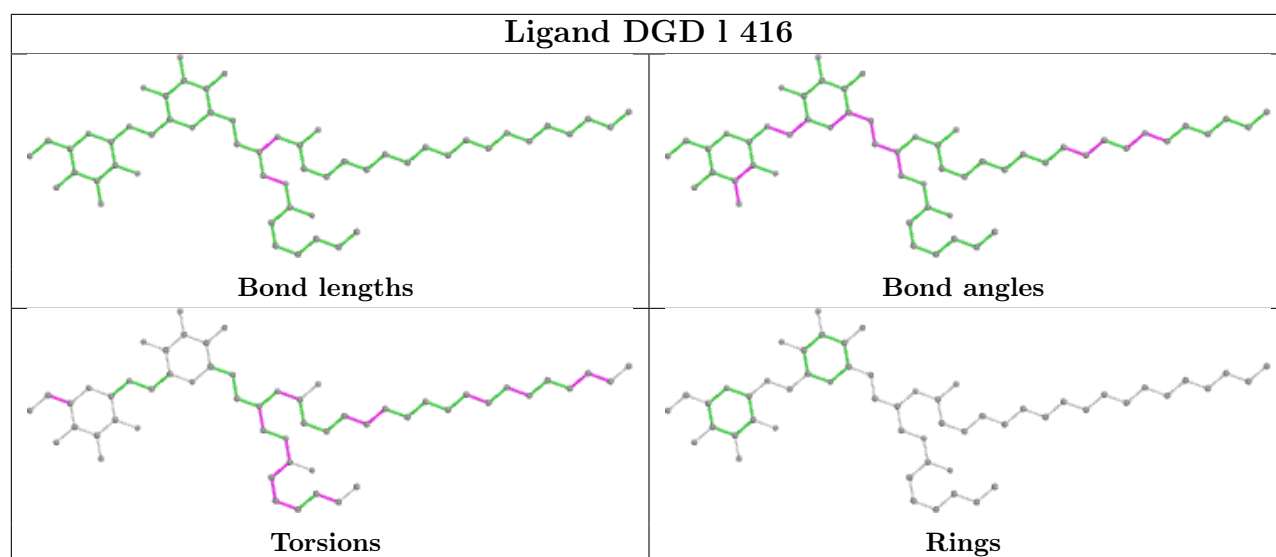
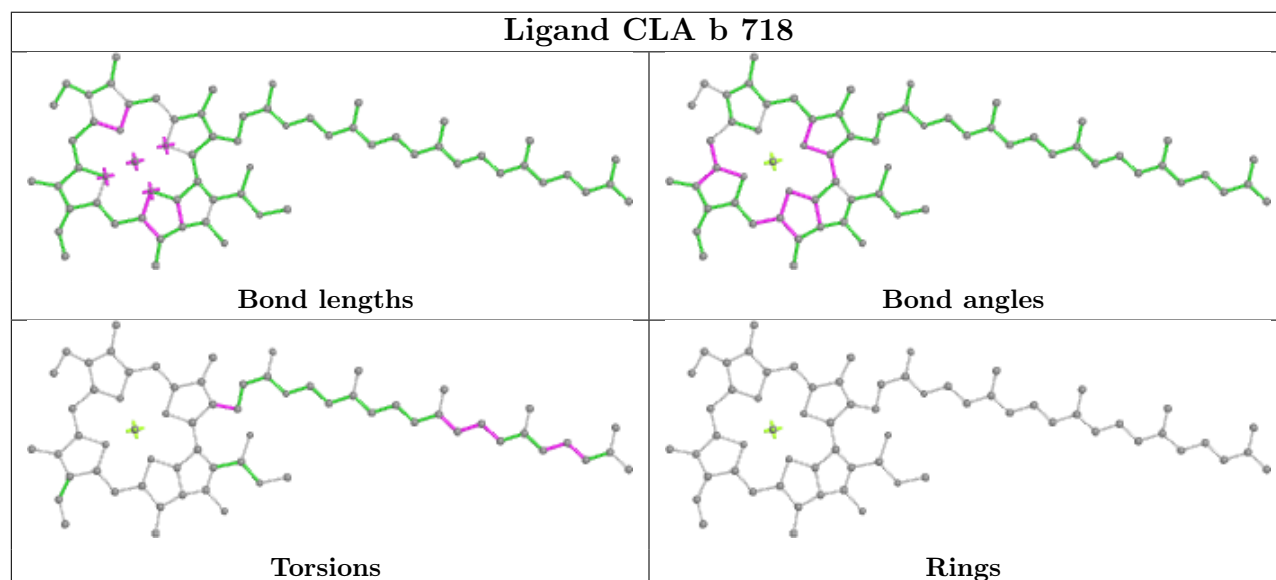
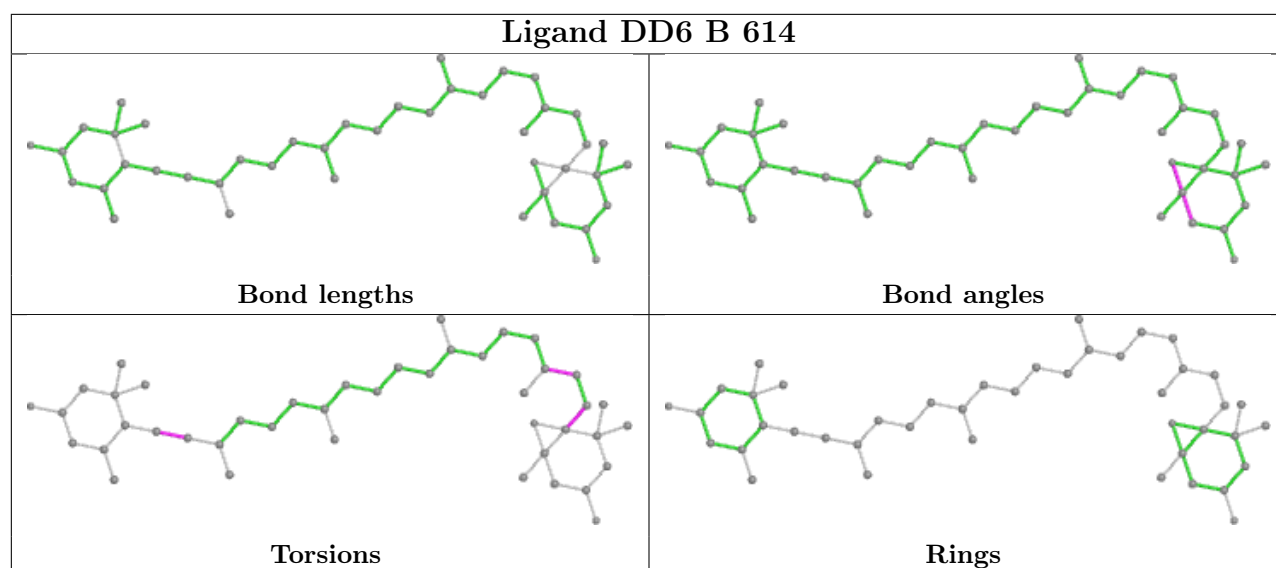
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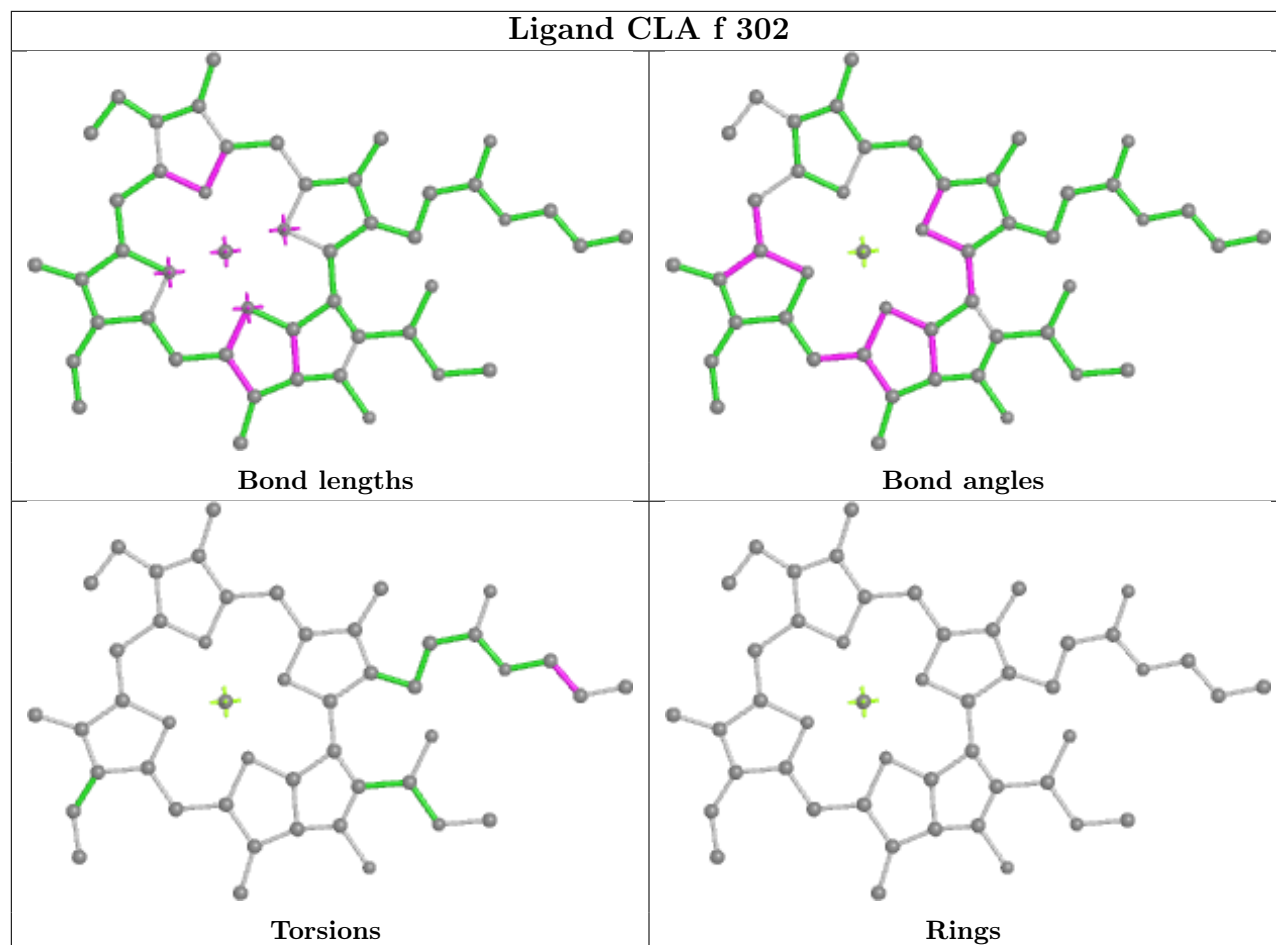
Mol	Chain	Res	Type	Clashes	Symm-Clashes
33	C	217	LMG	1	0
32	J	611	PID	6	0
27	C	207	CLA	1	0
30	K	609	DD6	1	0
27	K	603	CLA	11	0
30	G	614	DD6	1	0
27	F	608	CLA	1	0
30	K	610	DD6	2	0
27	T	602	CLA	1	0
27	J	605	CLA	2	0
27	F	606	CLA	1	0
27	G	607	CLA	3	0
30	G	612	DD6	1	0

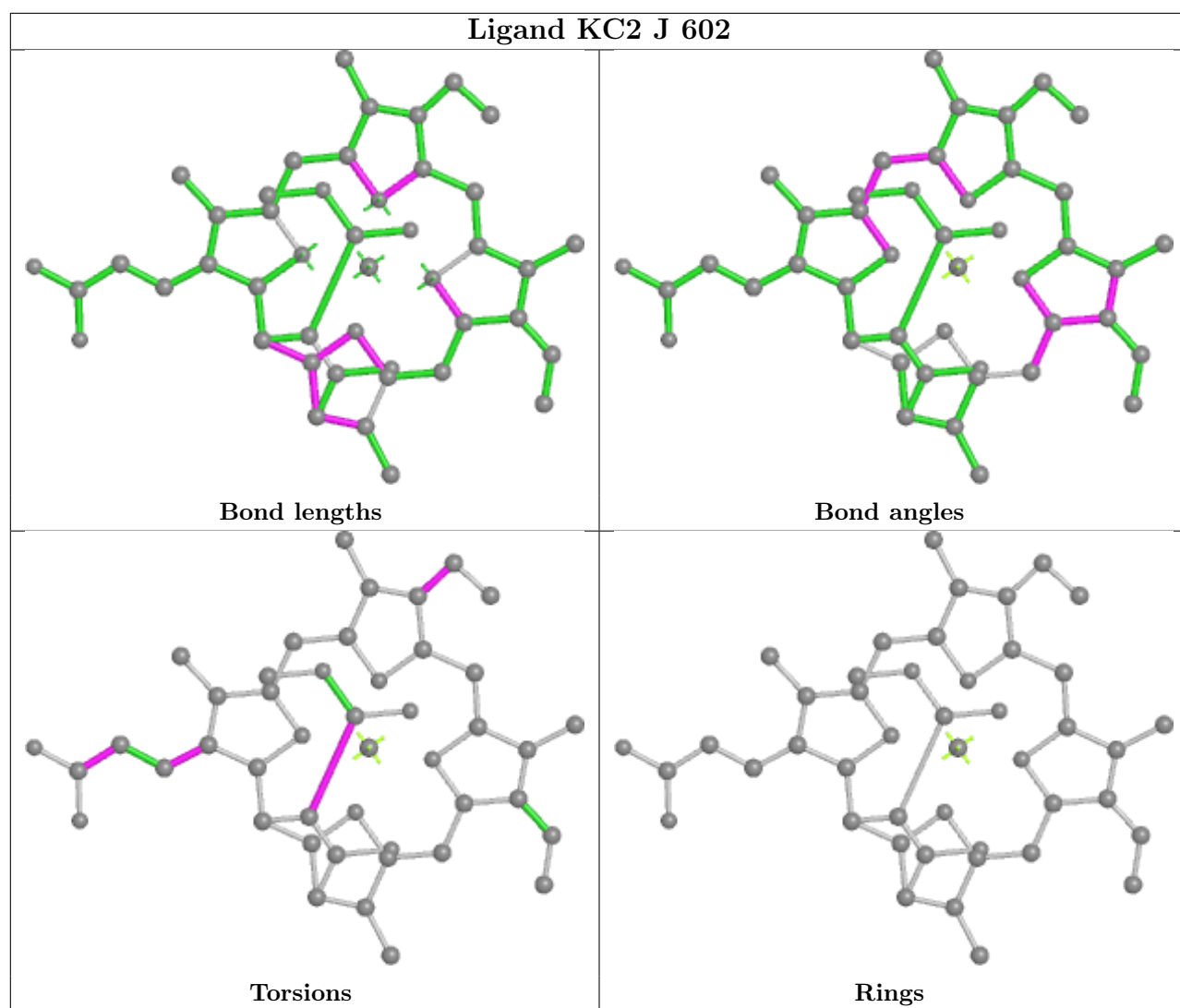
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



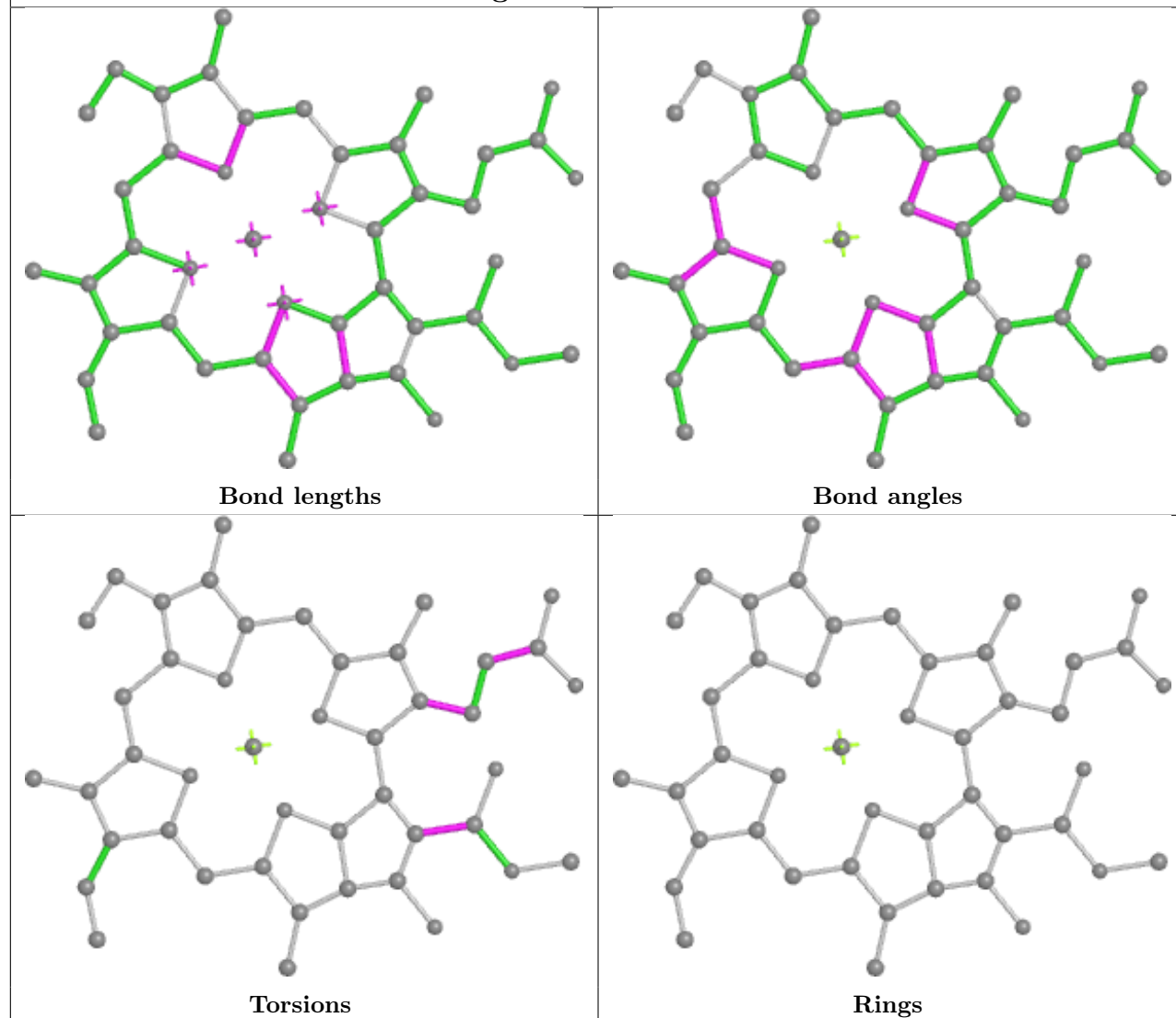


Ligand CLA f 302

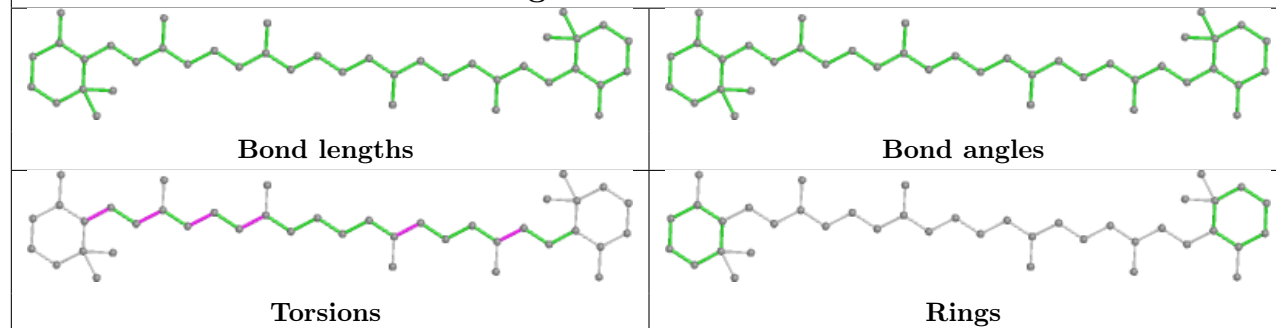




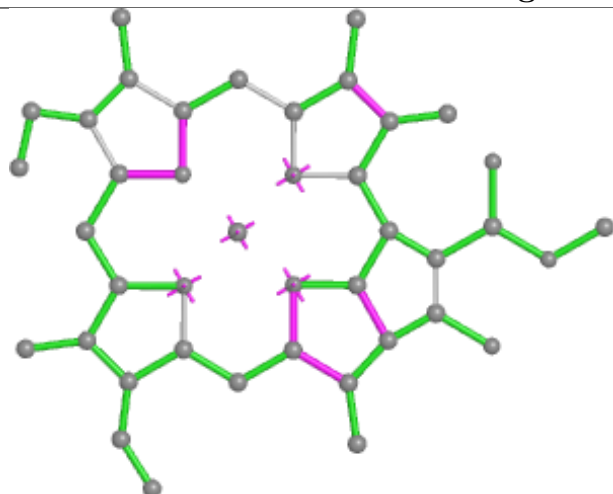
Ligand CLA F 607



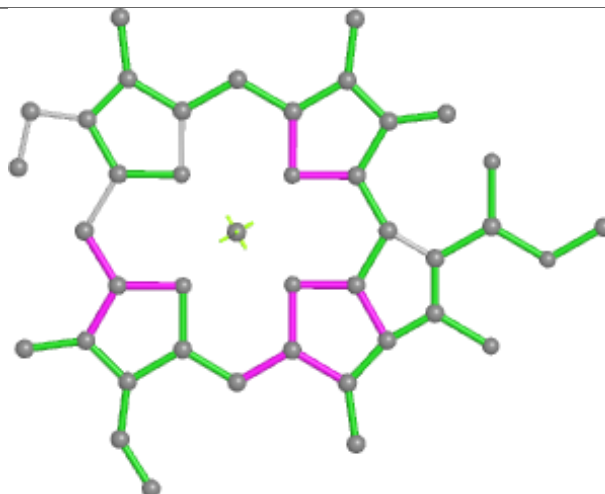
Ligand BCR m 201



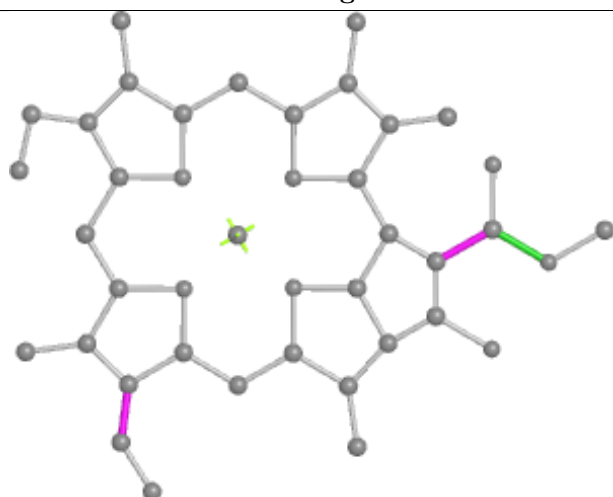
Ligand CLA J 609



Bond lengths



Bond angles

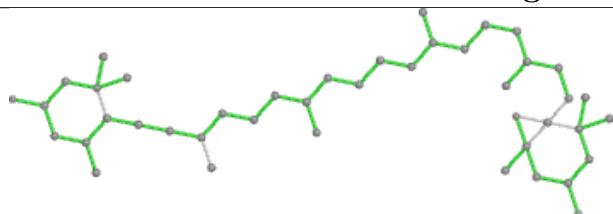


Torsions

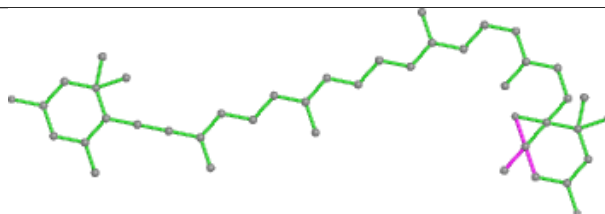


Rings

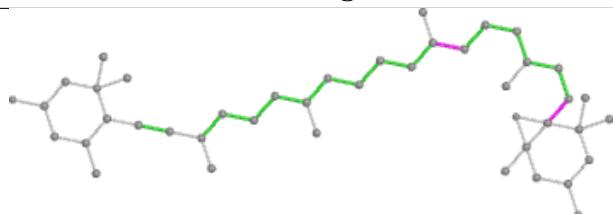
Ligand DD6 i 202



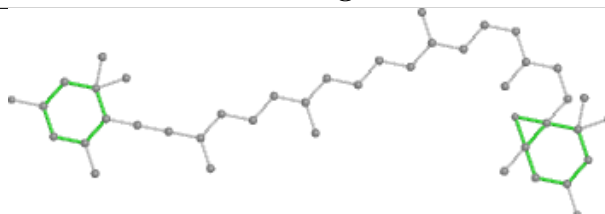
Bond lengths



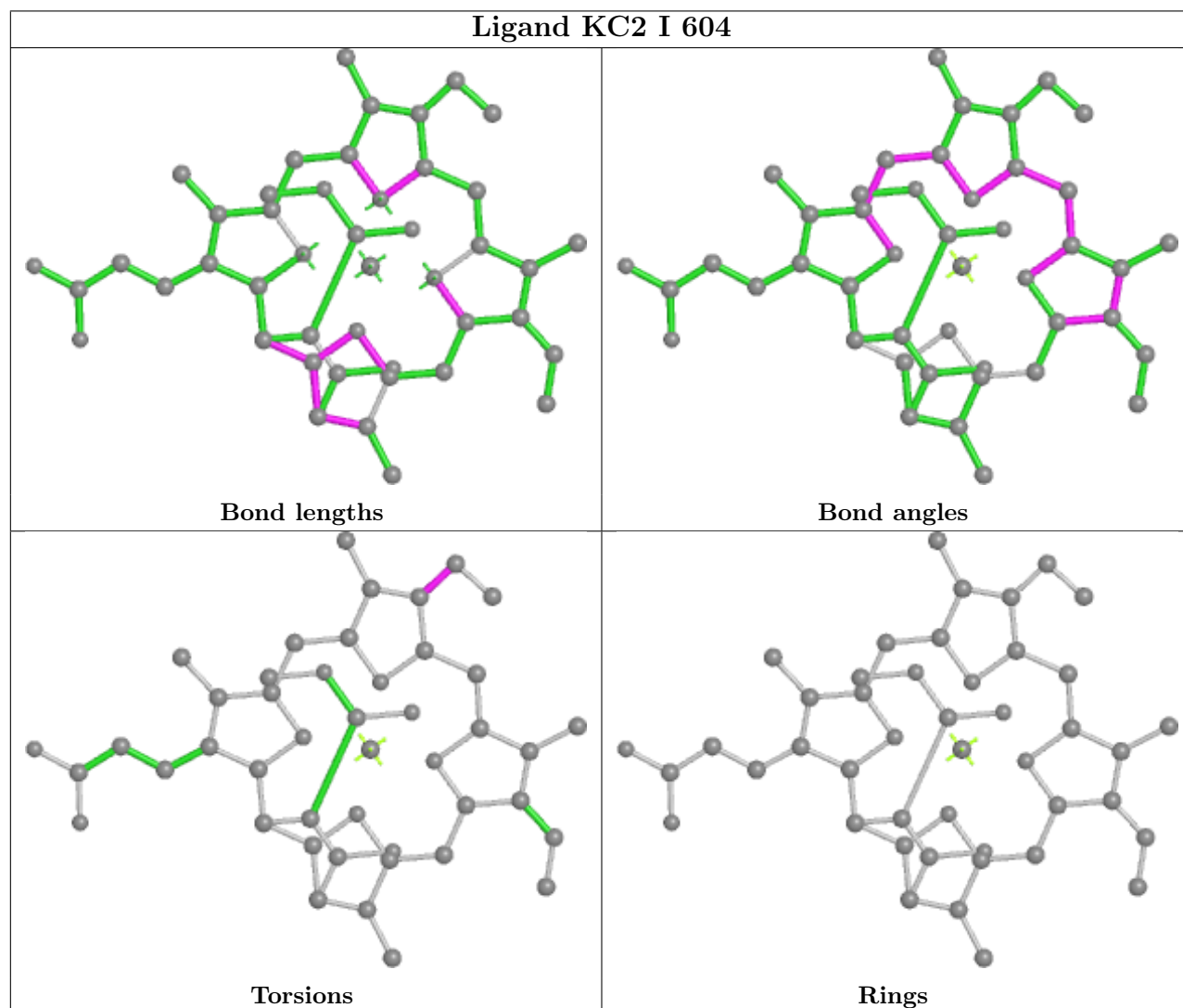
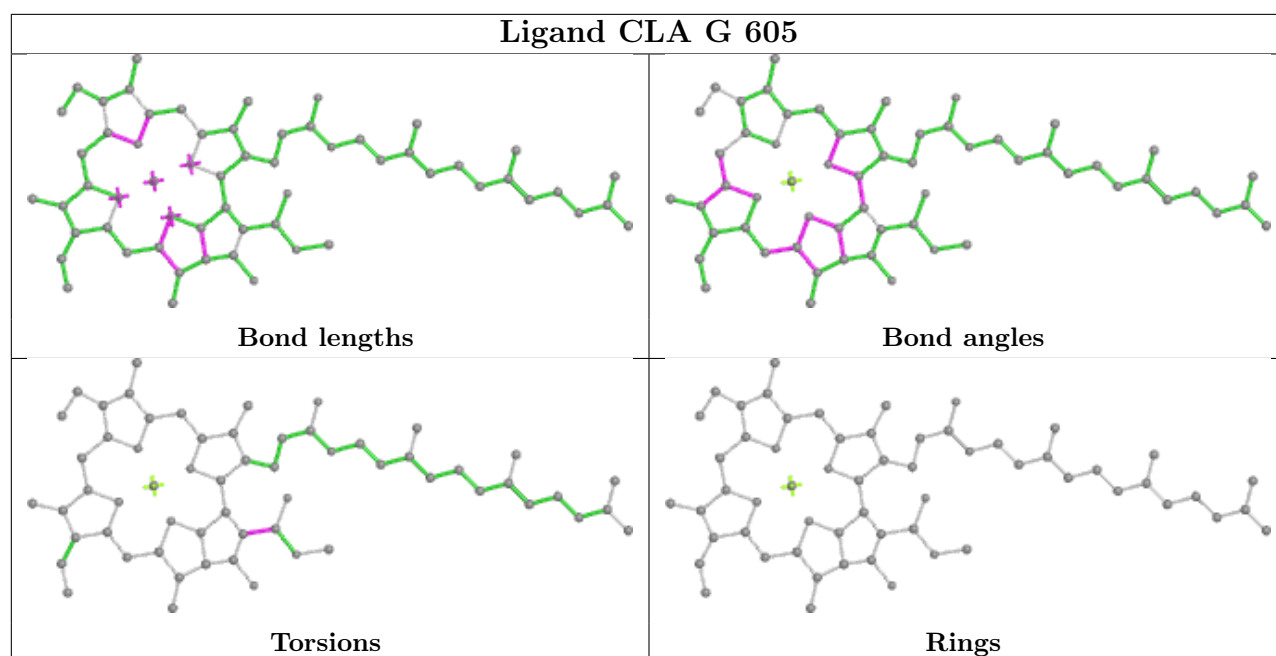
Bond angles



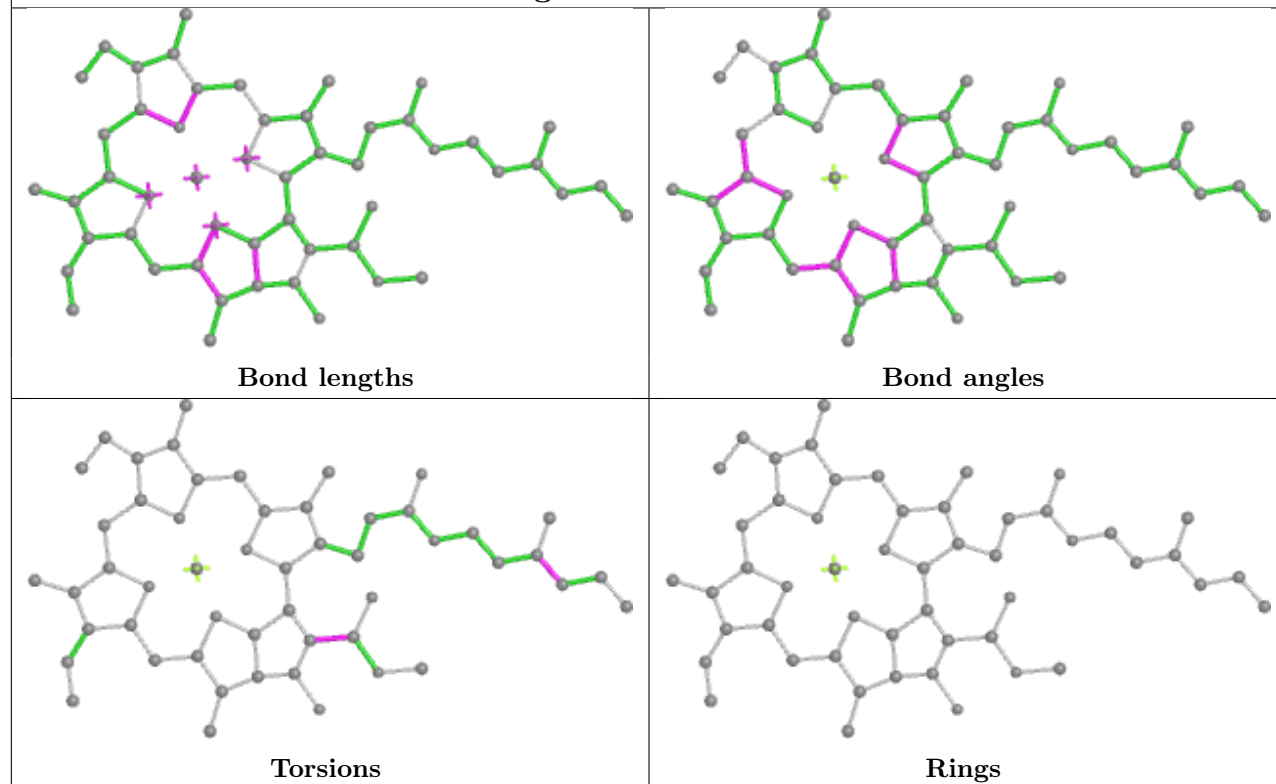
Torsions



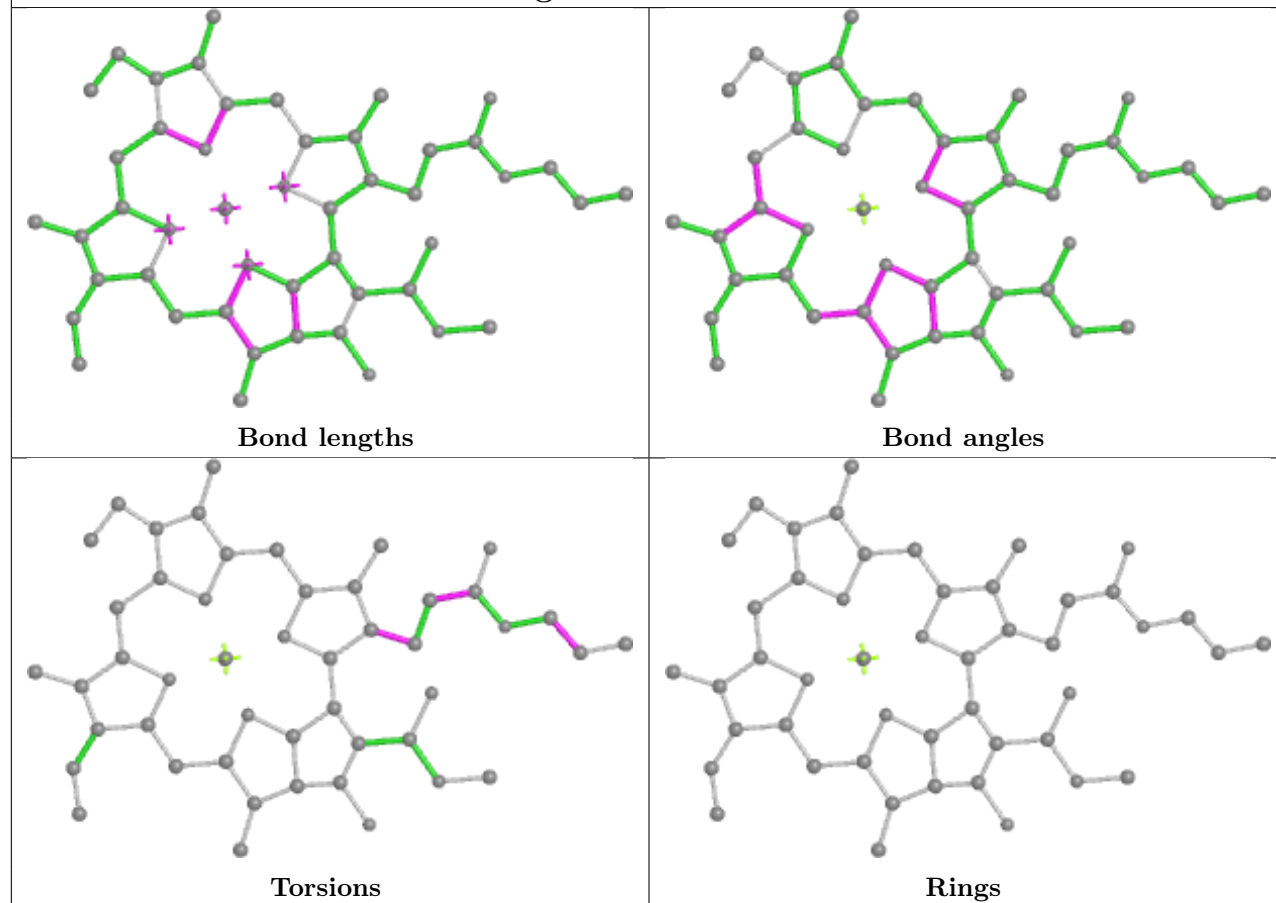
Rings

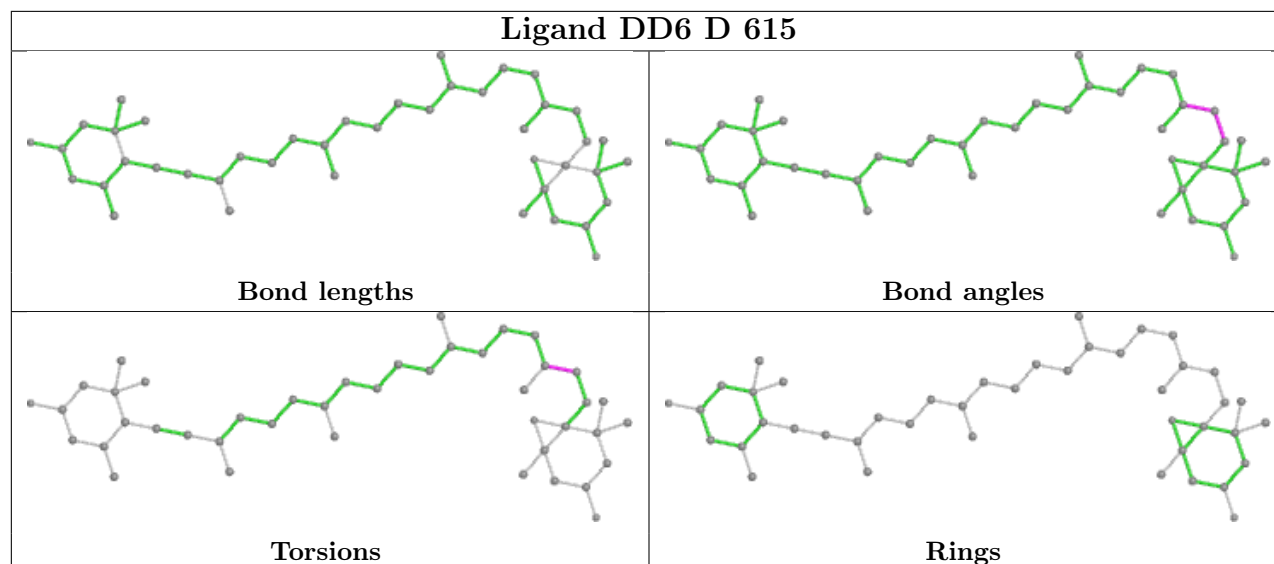
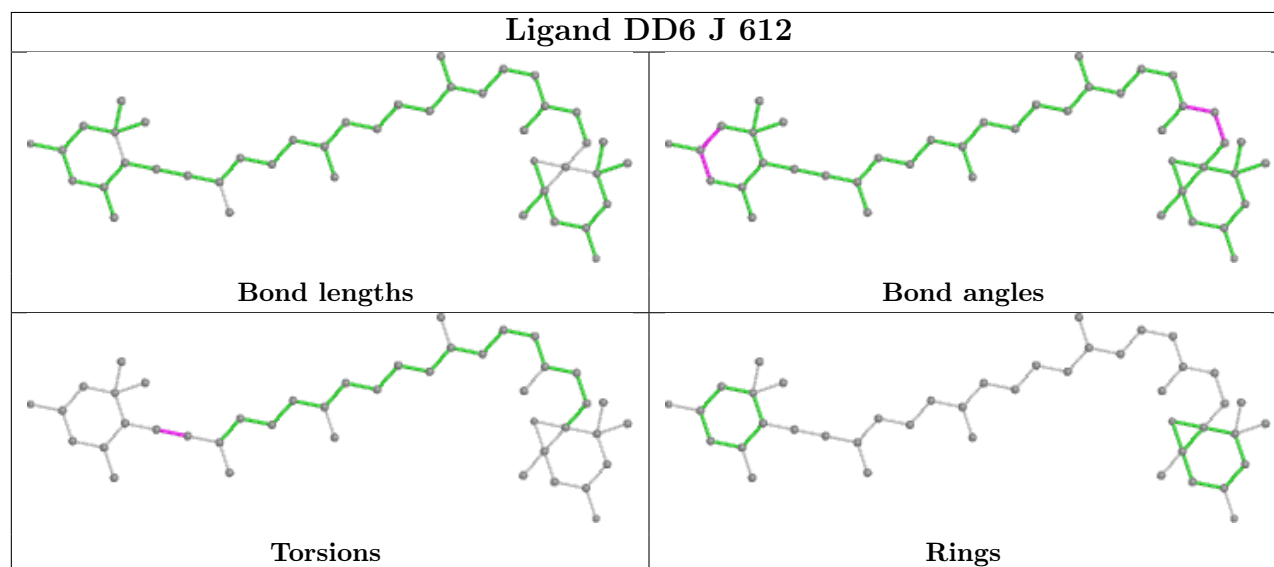
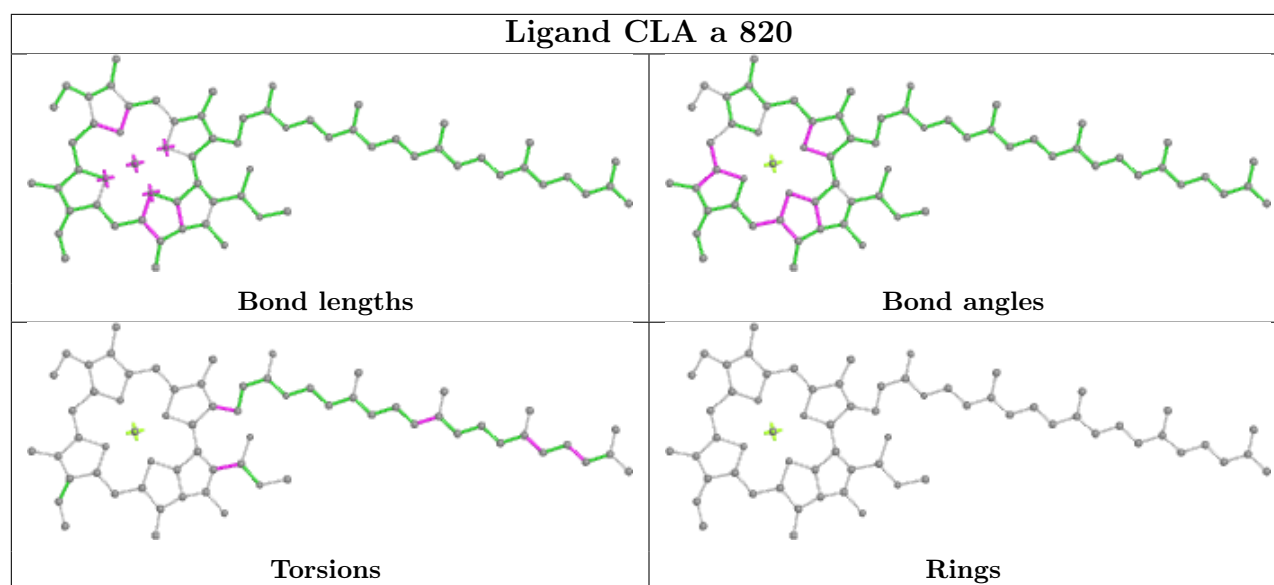


Ligand CLA F 603

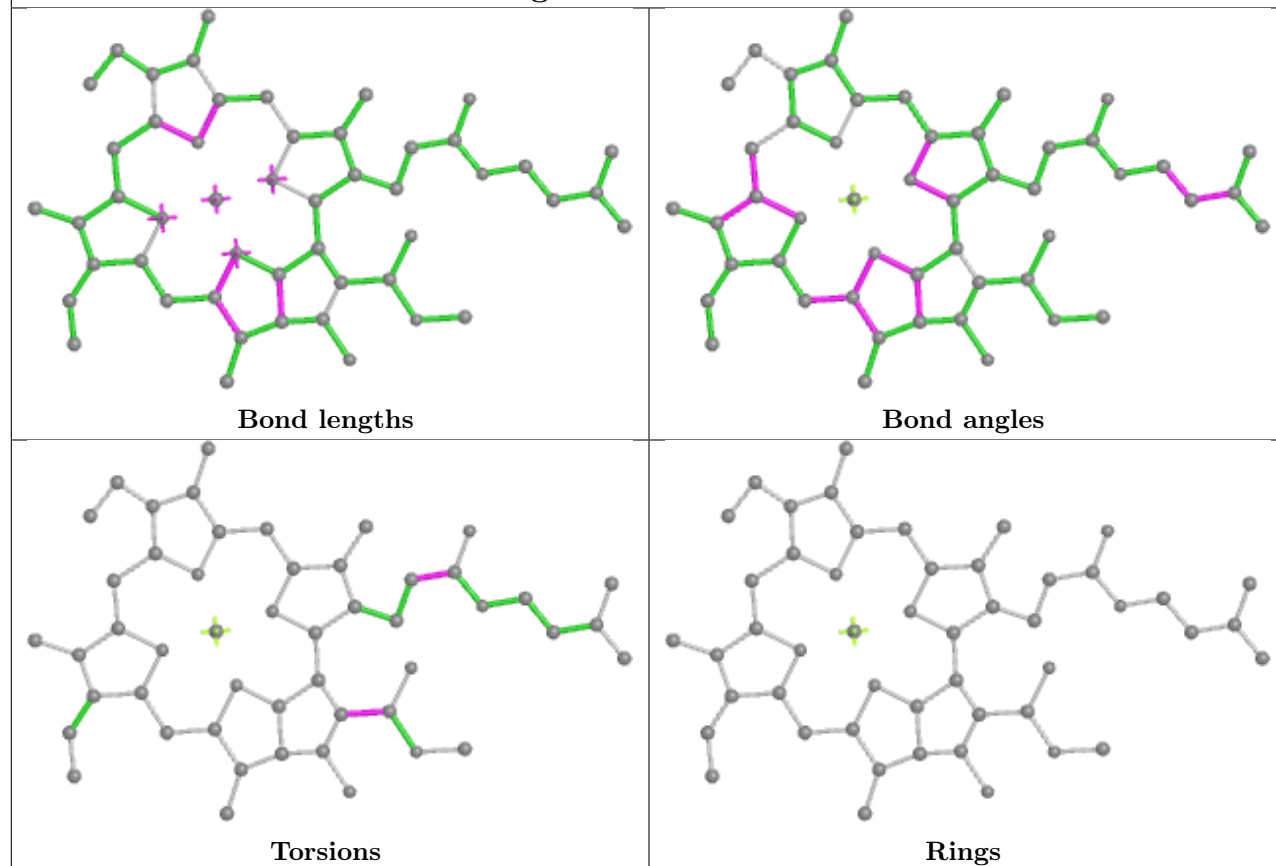


Ligand CLA b 722

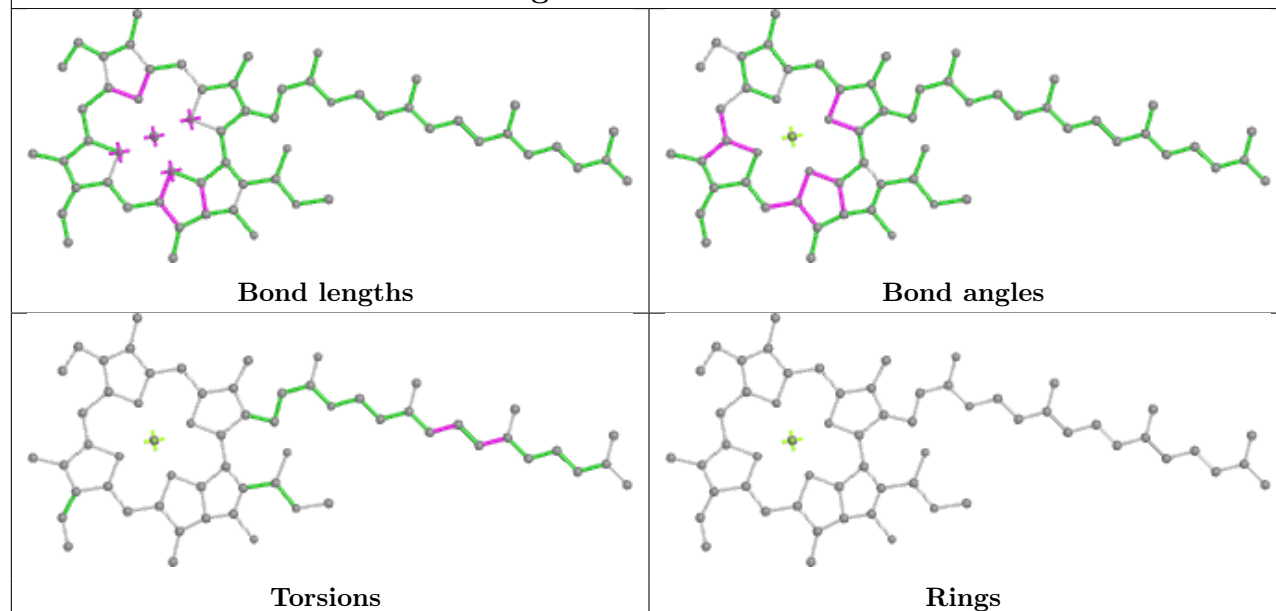




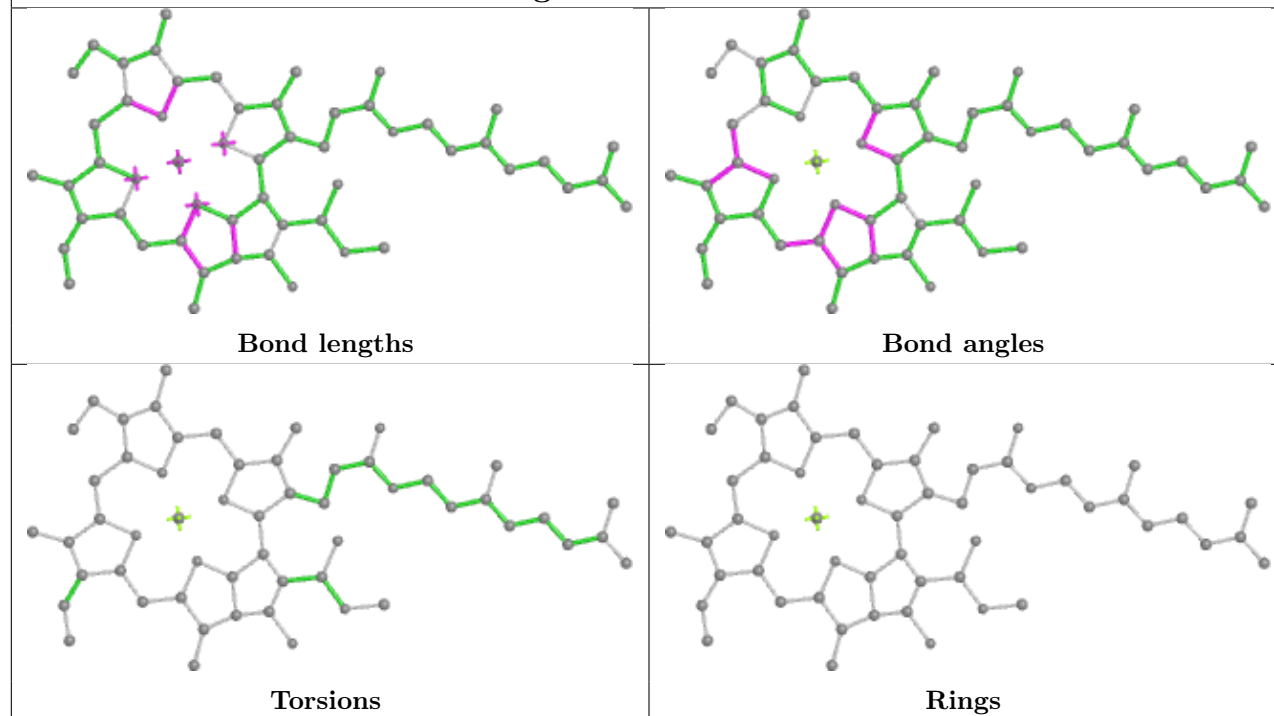
Ligand CLA G 603



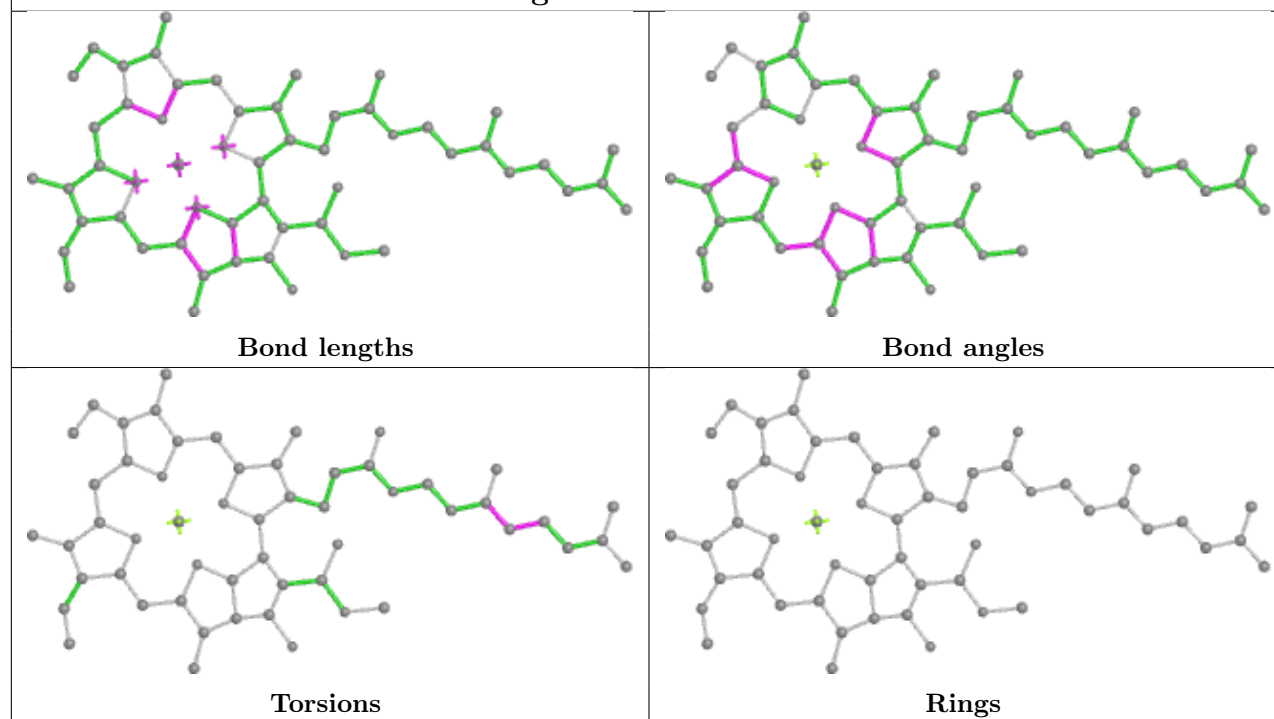
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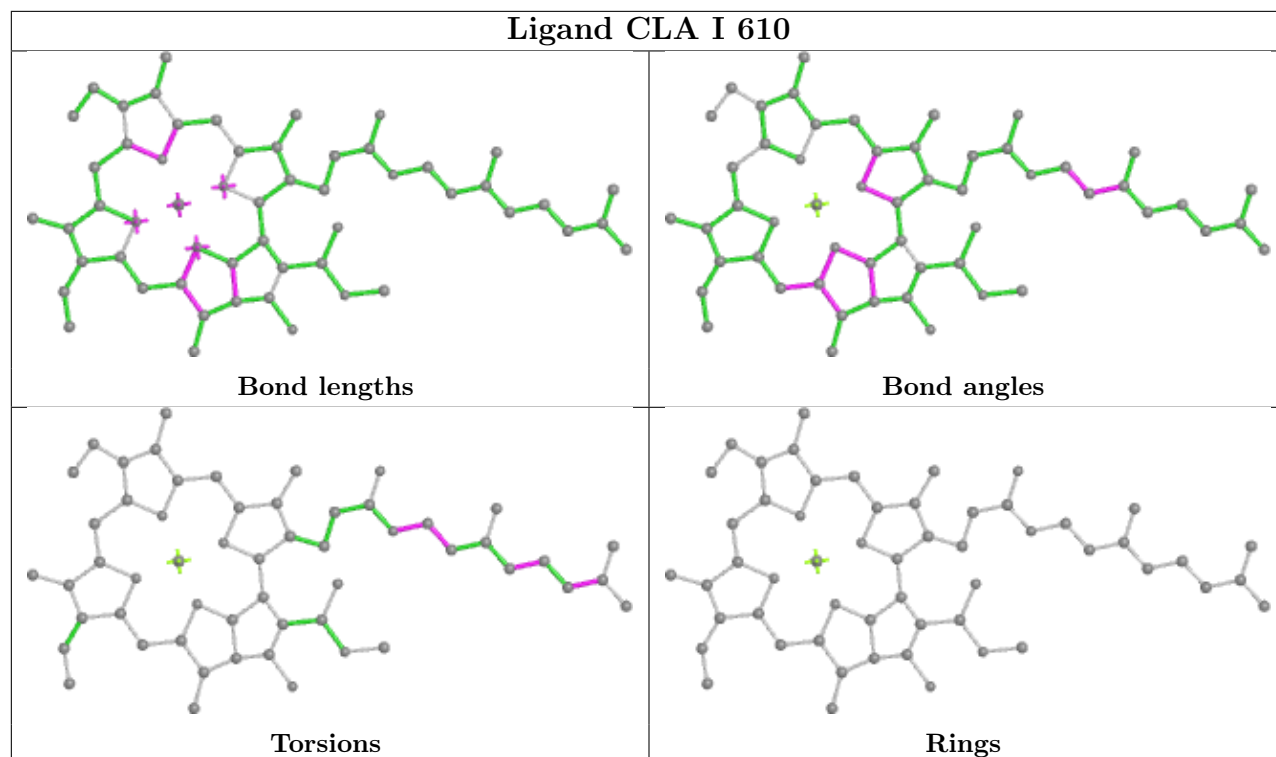
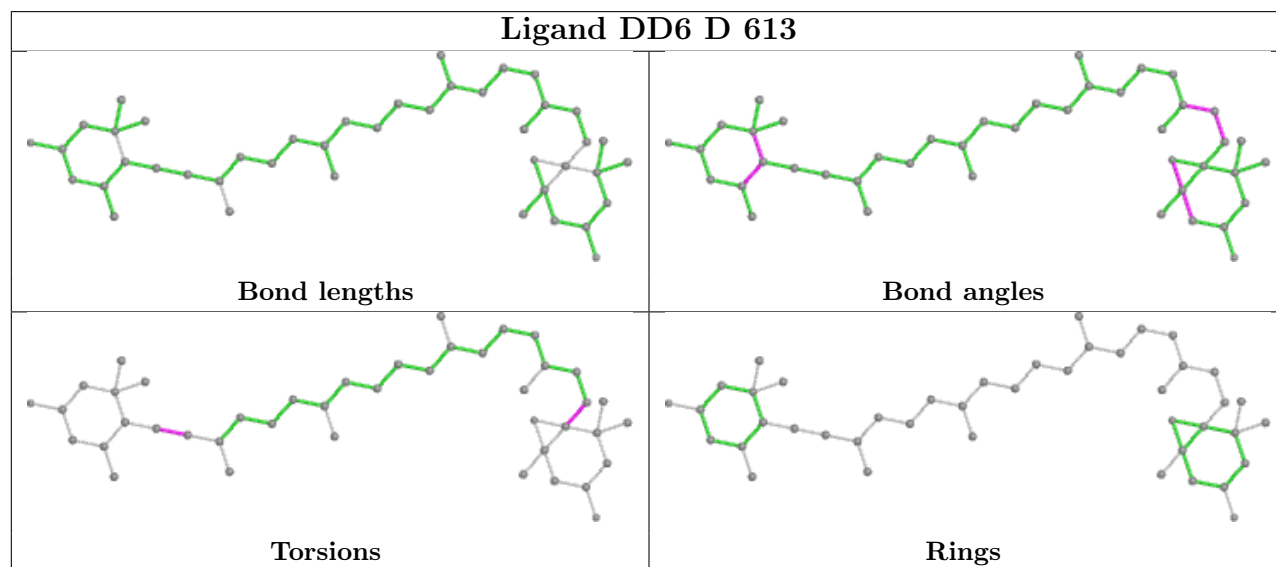


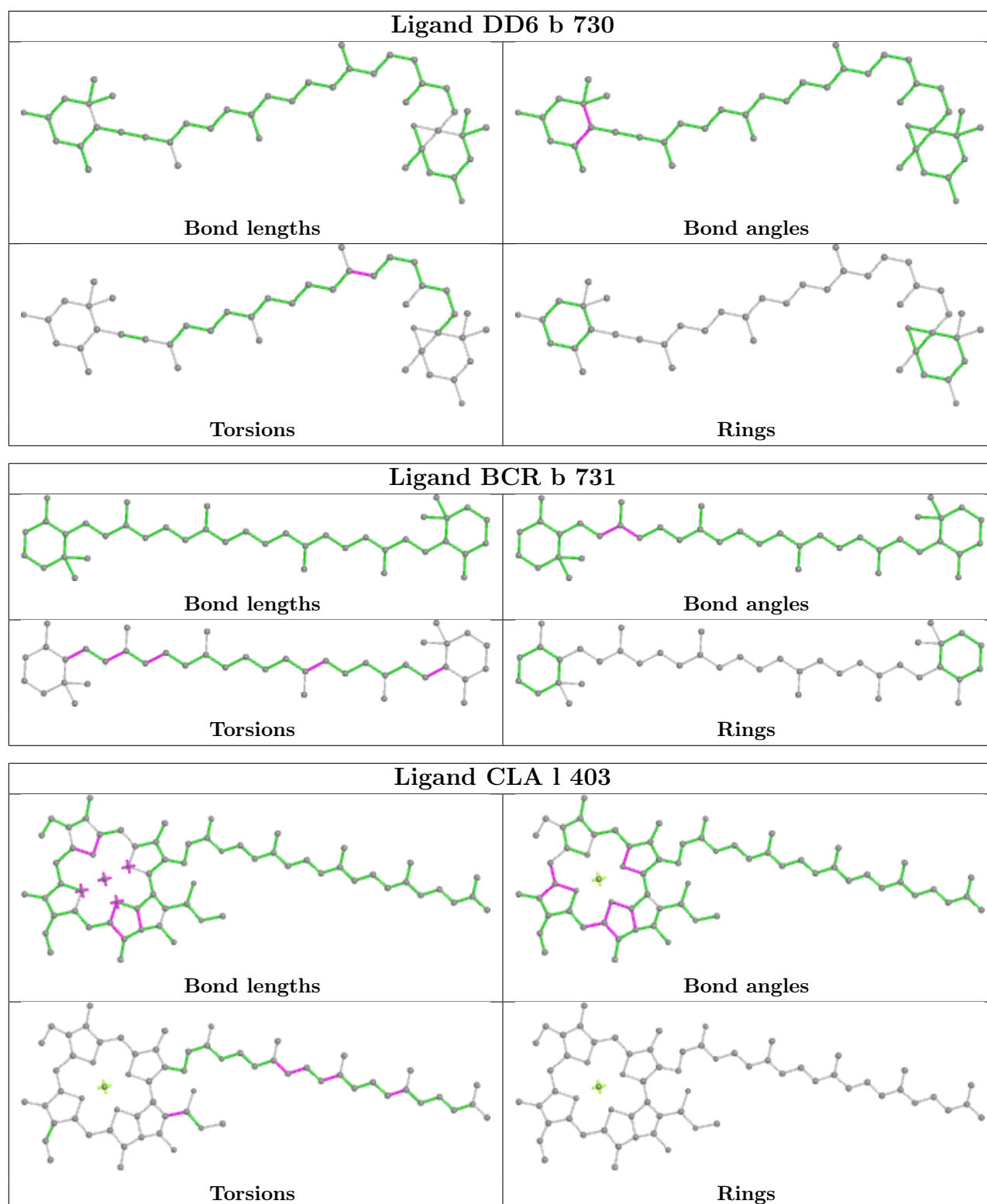
Ligand CLA E 602

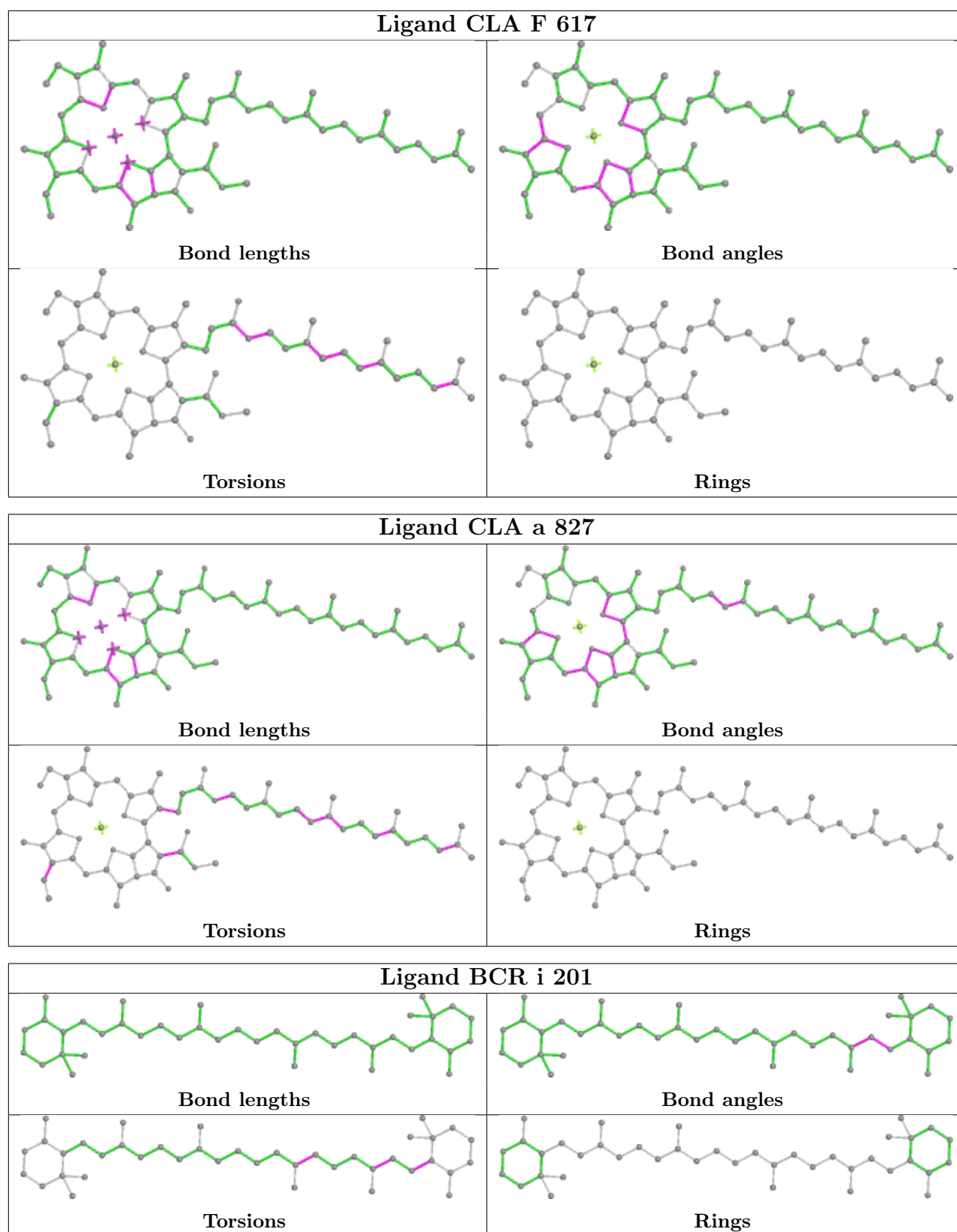


Ligand CLA H 308

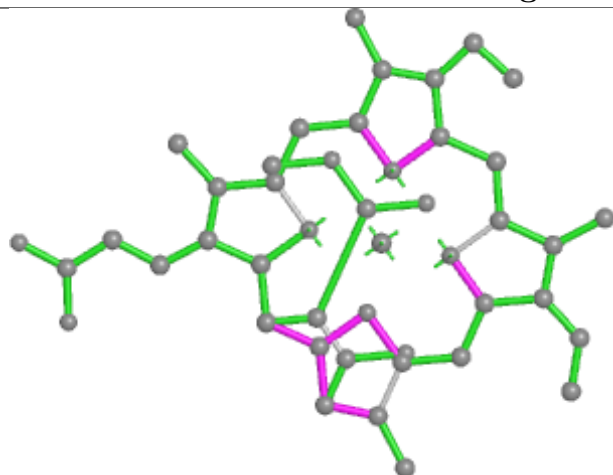


Ligand CLA I 610**Ligand DD6 D 613**

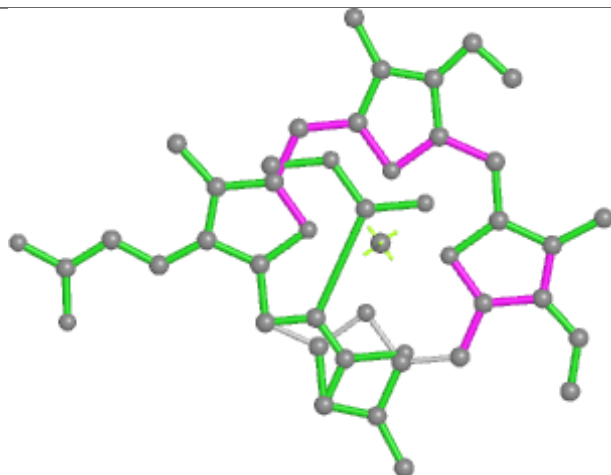




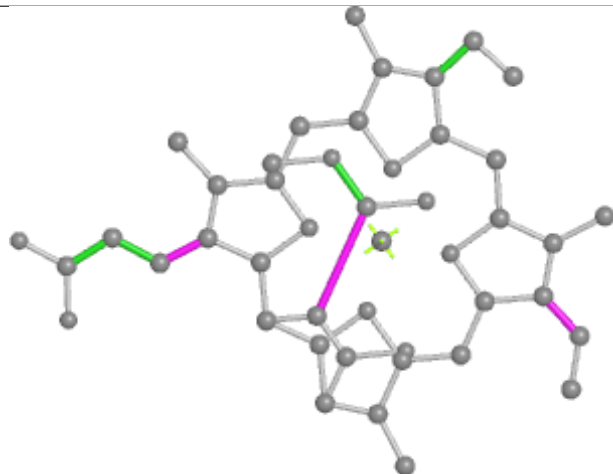
Ligand KC2 J 604



Bond lengths



Bond angles

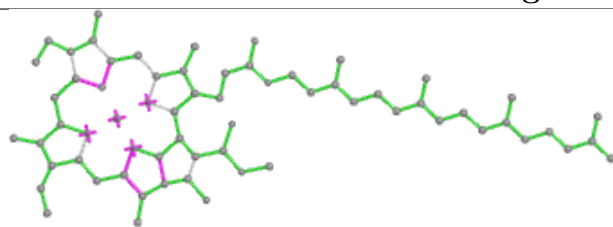


Torsions

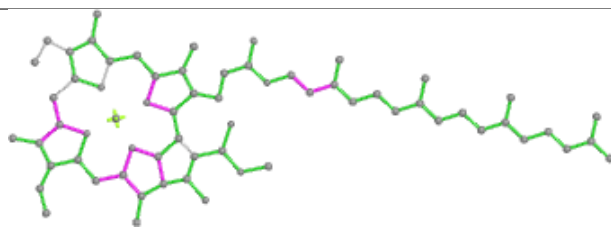


Rings

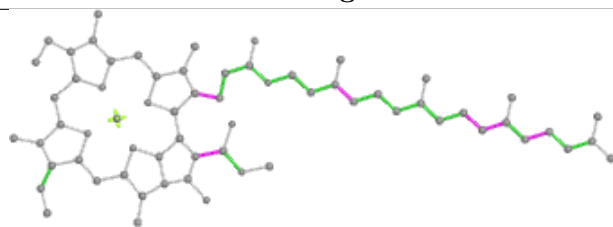
Ligand CLA I 412



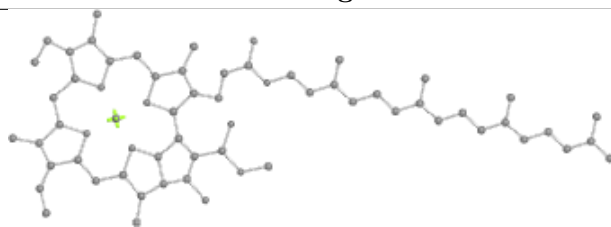
Bond lengths



Bond angles

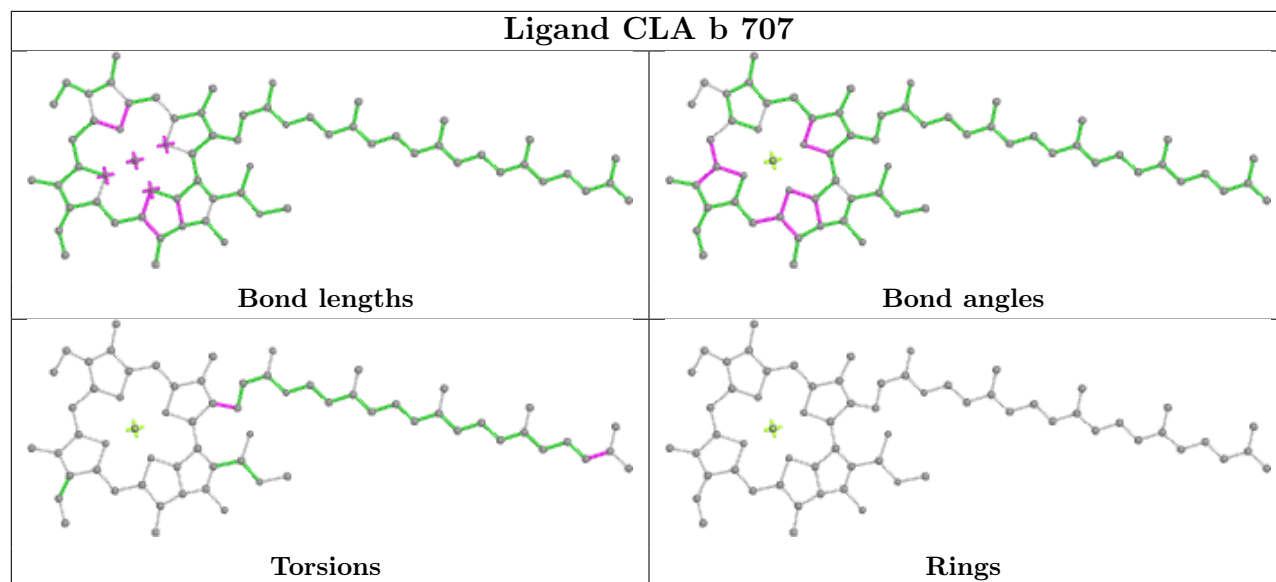


Torsions

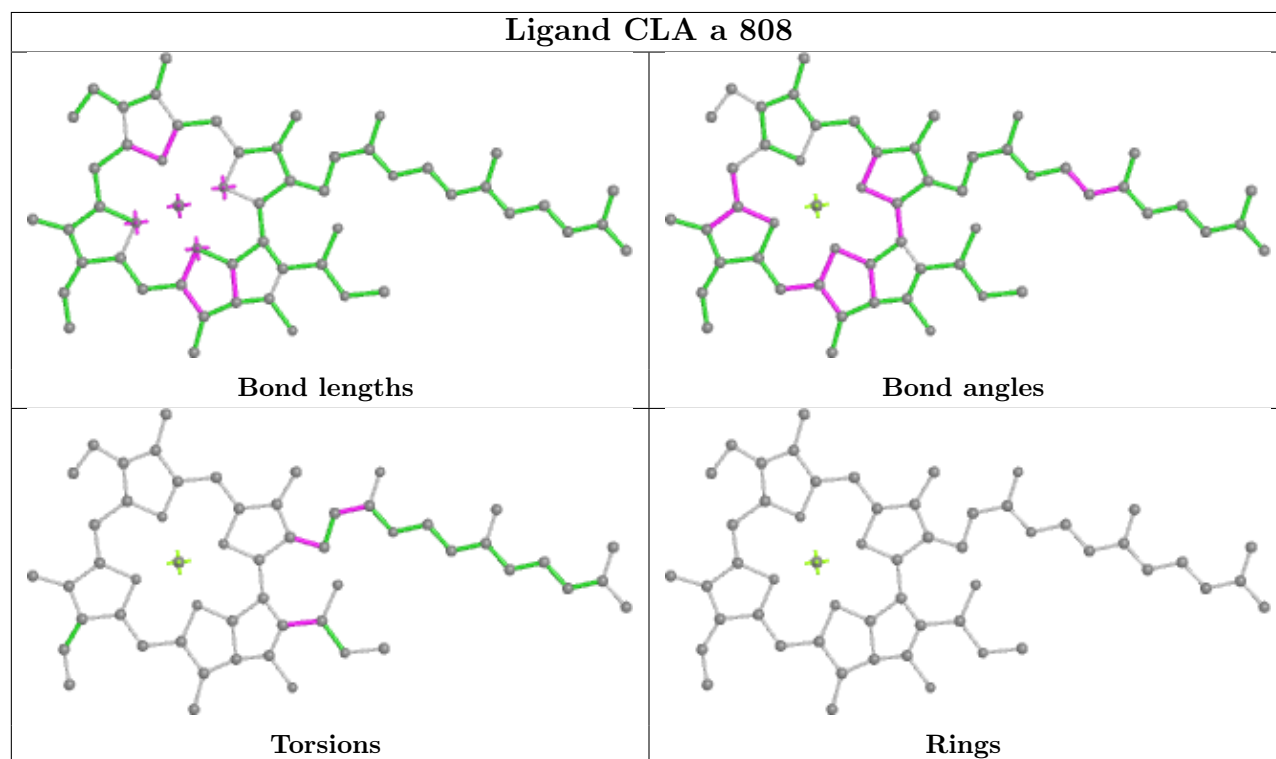


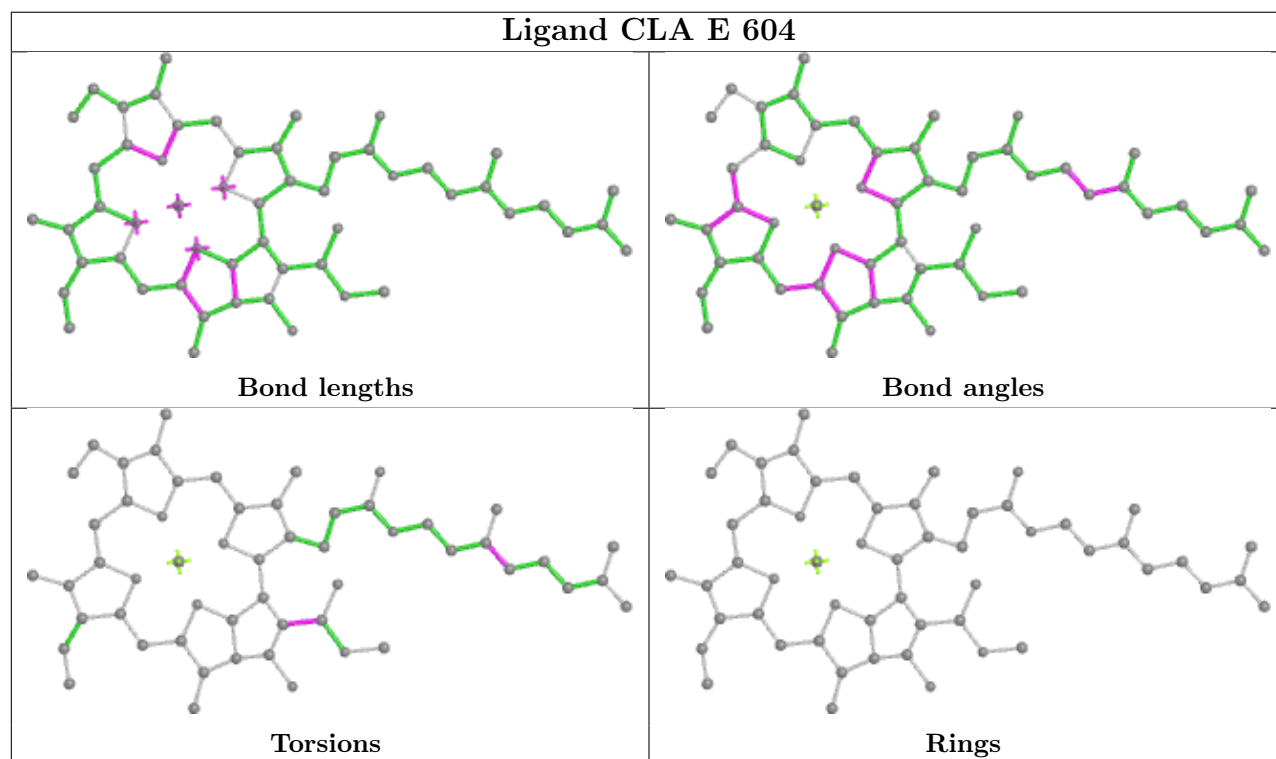
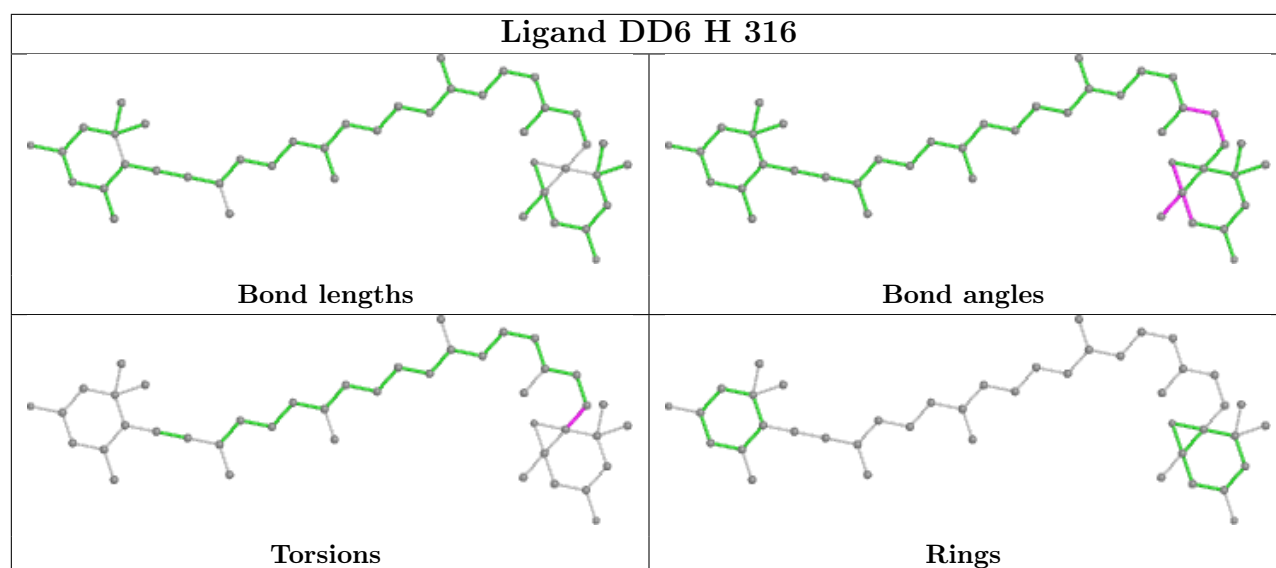
Rings

Ligand CLA b 707

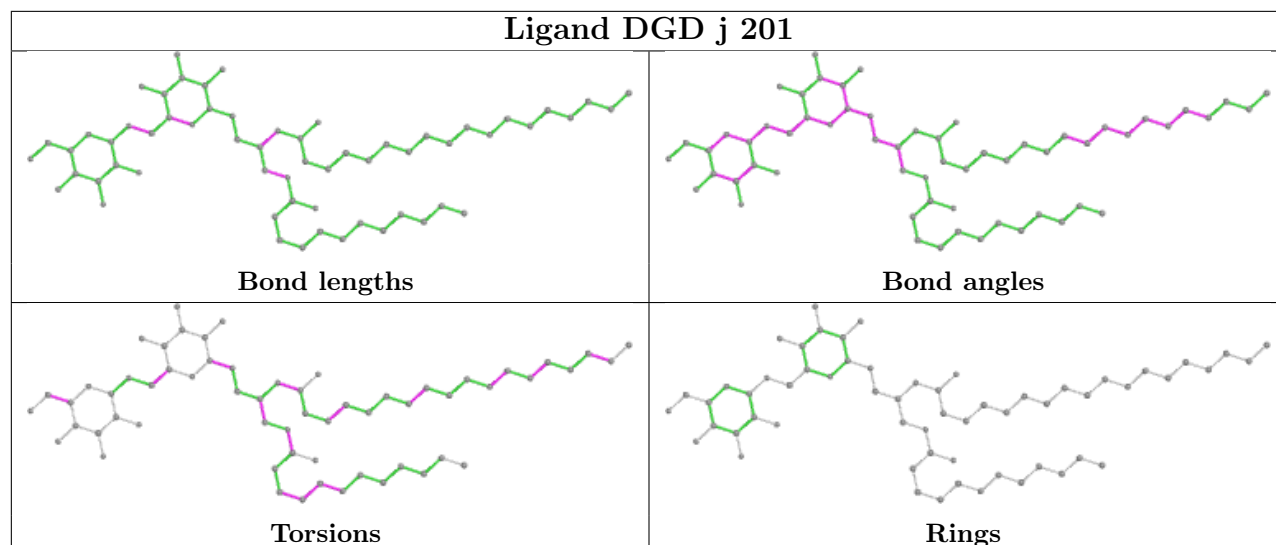


Ligand CLA a 808

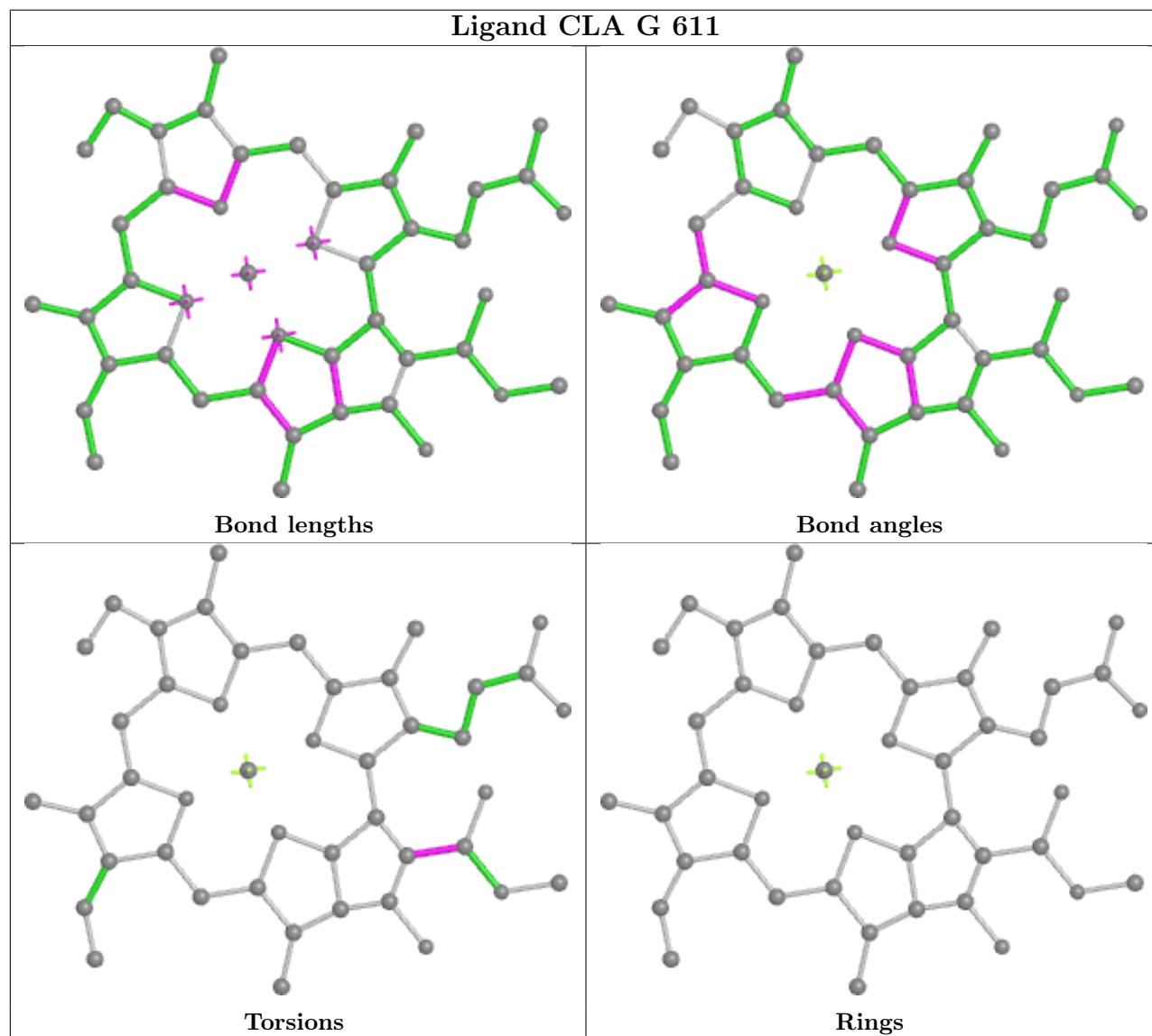




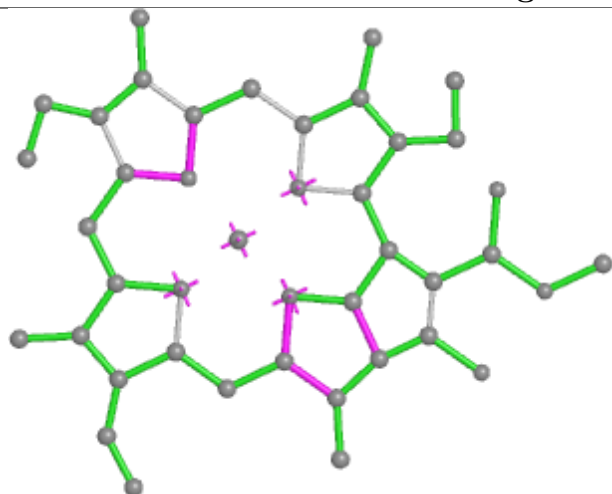
Ligand DGD j 201



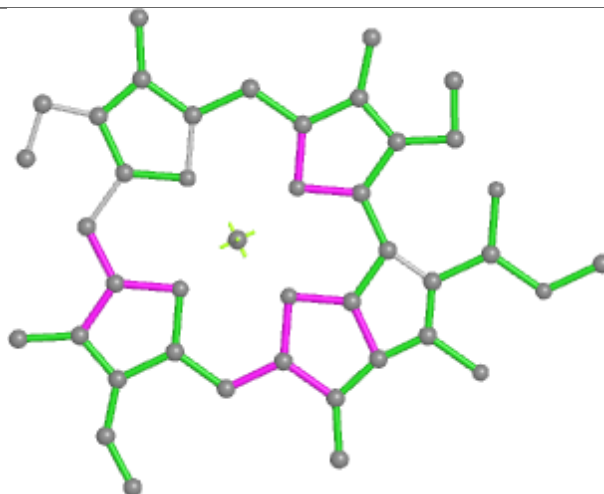
Ligand CLA G 611



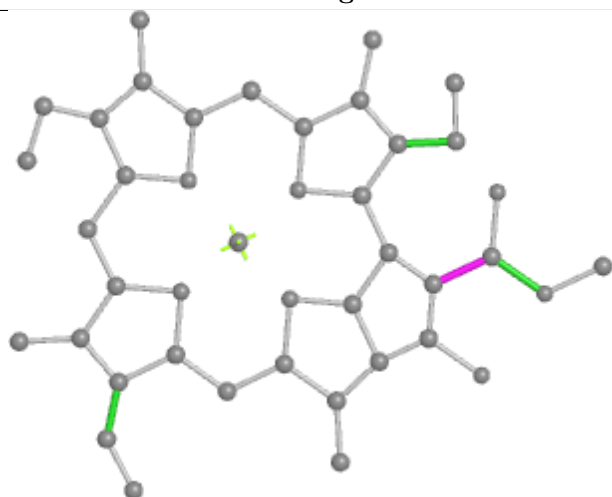
Ligand CLA J 607



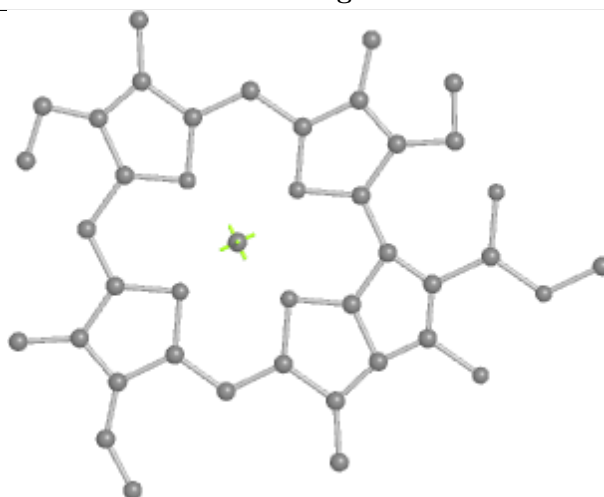
Bond lengths



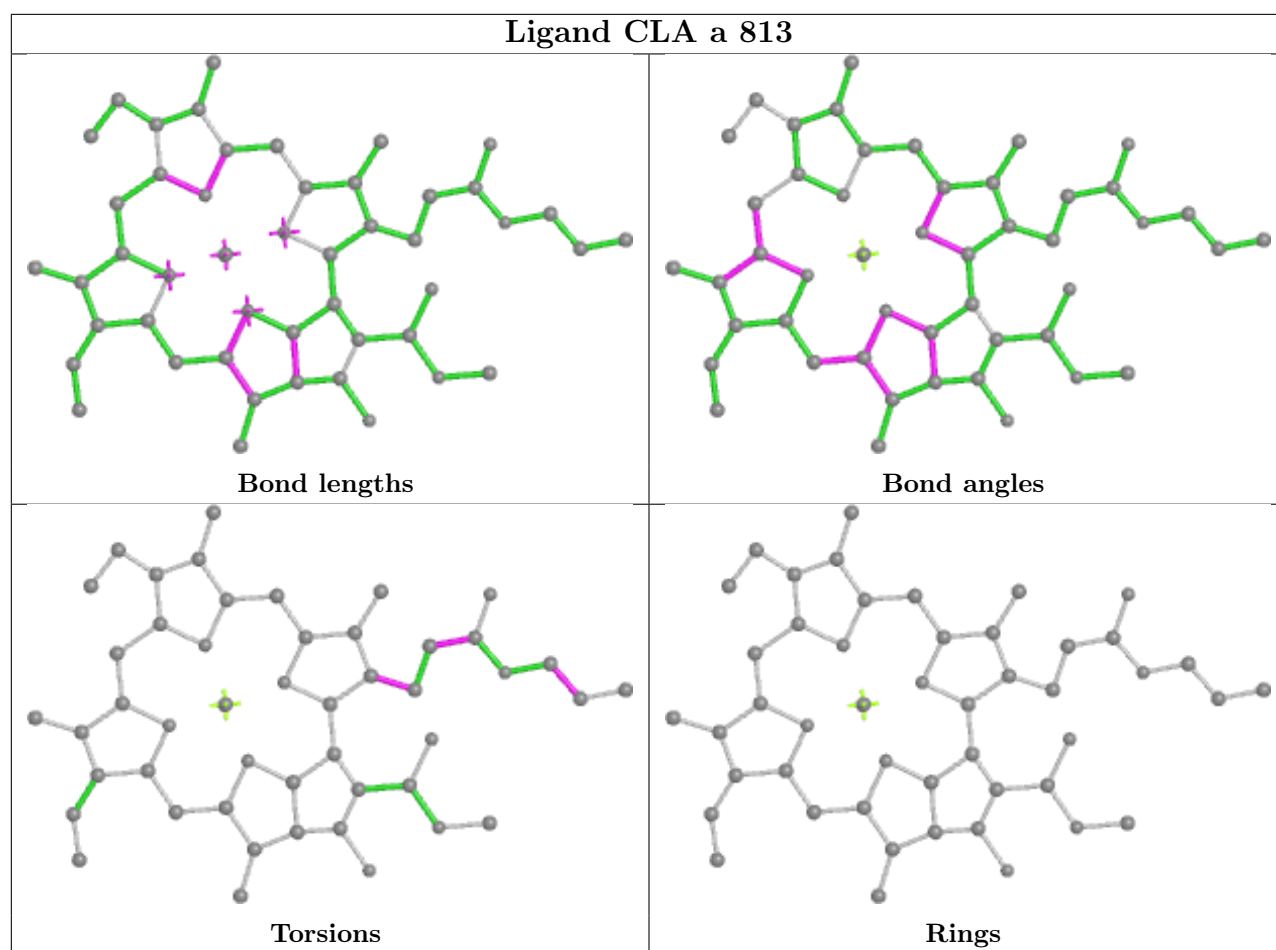
Bond angles

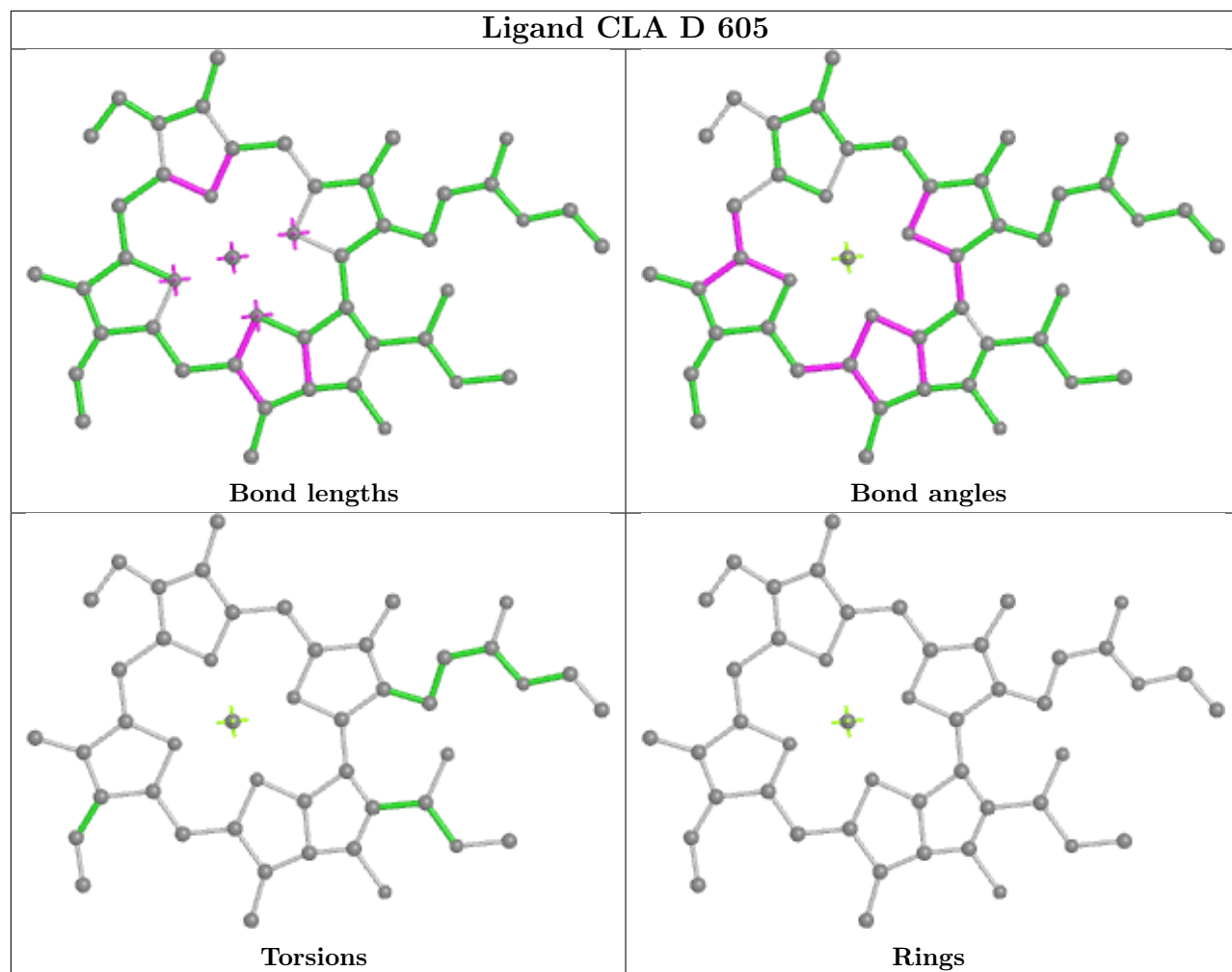


Torsions

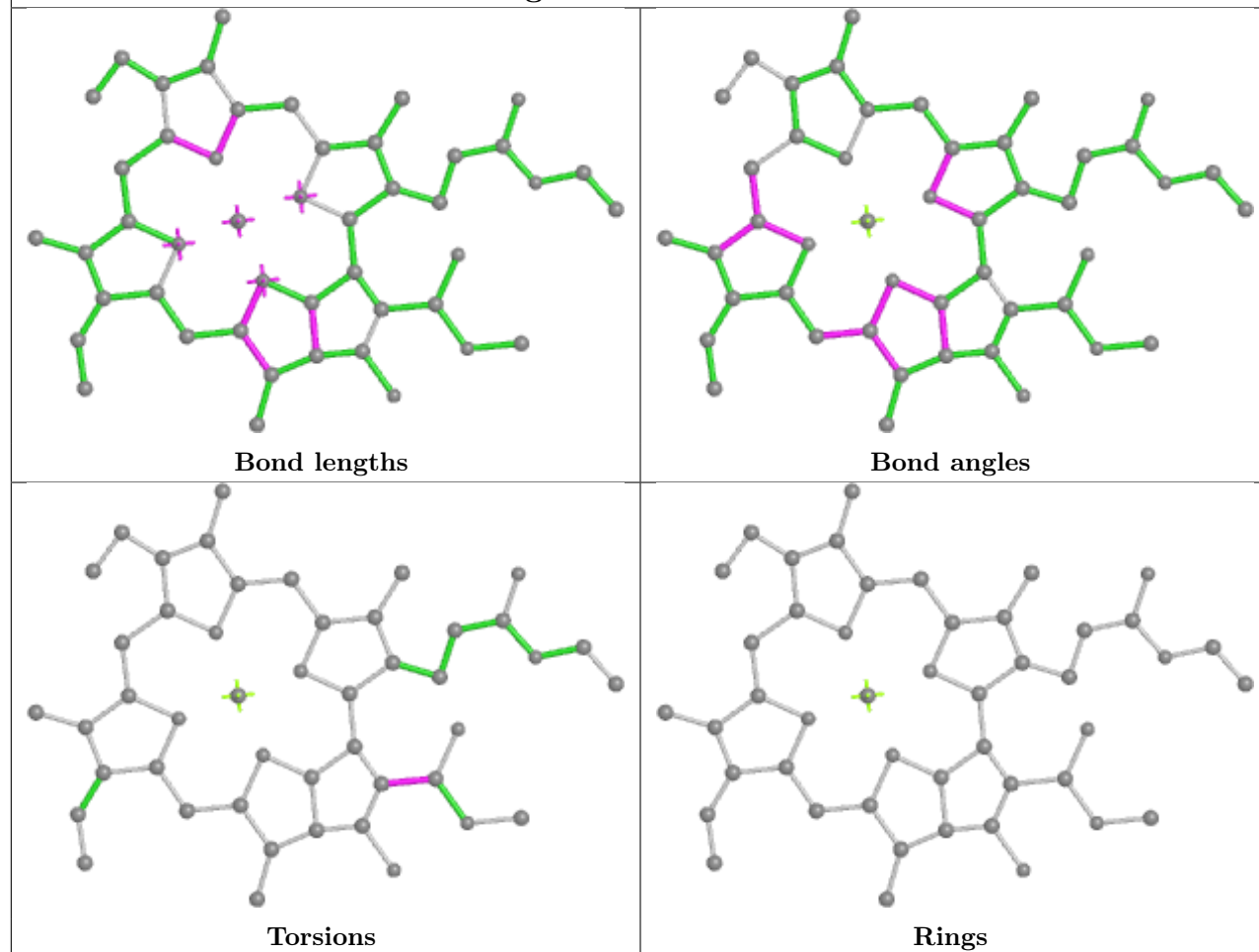


Rings

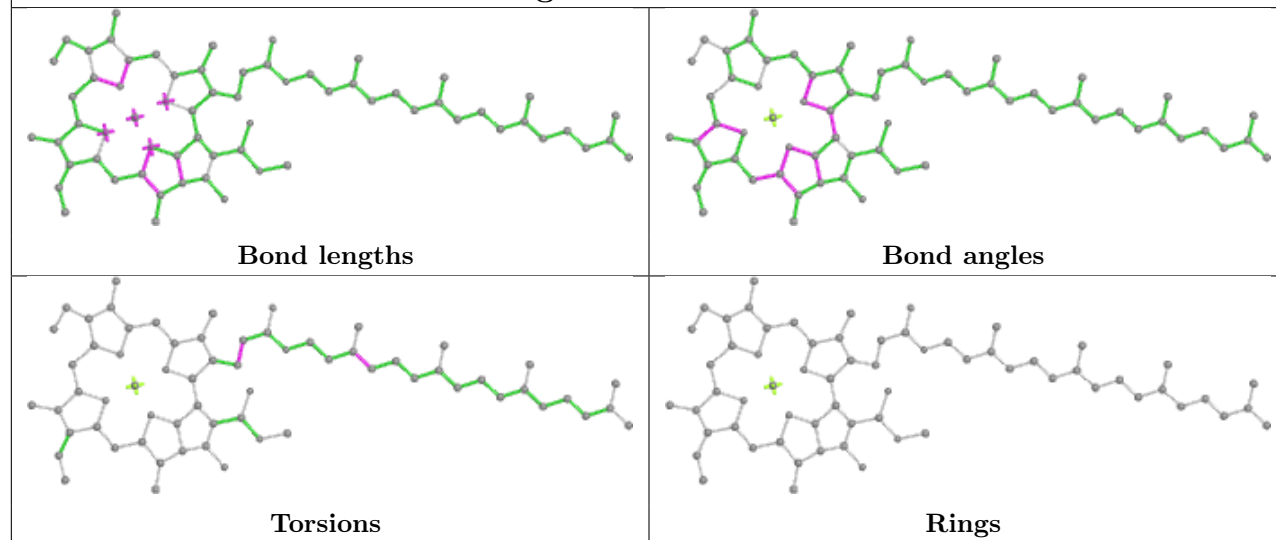


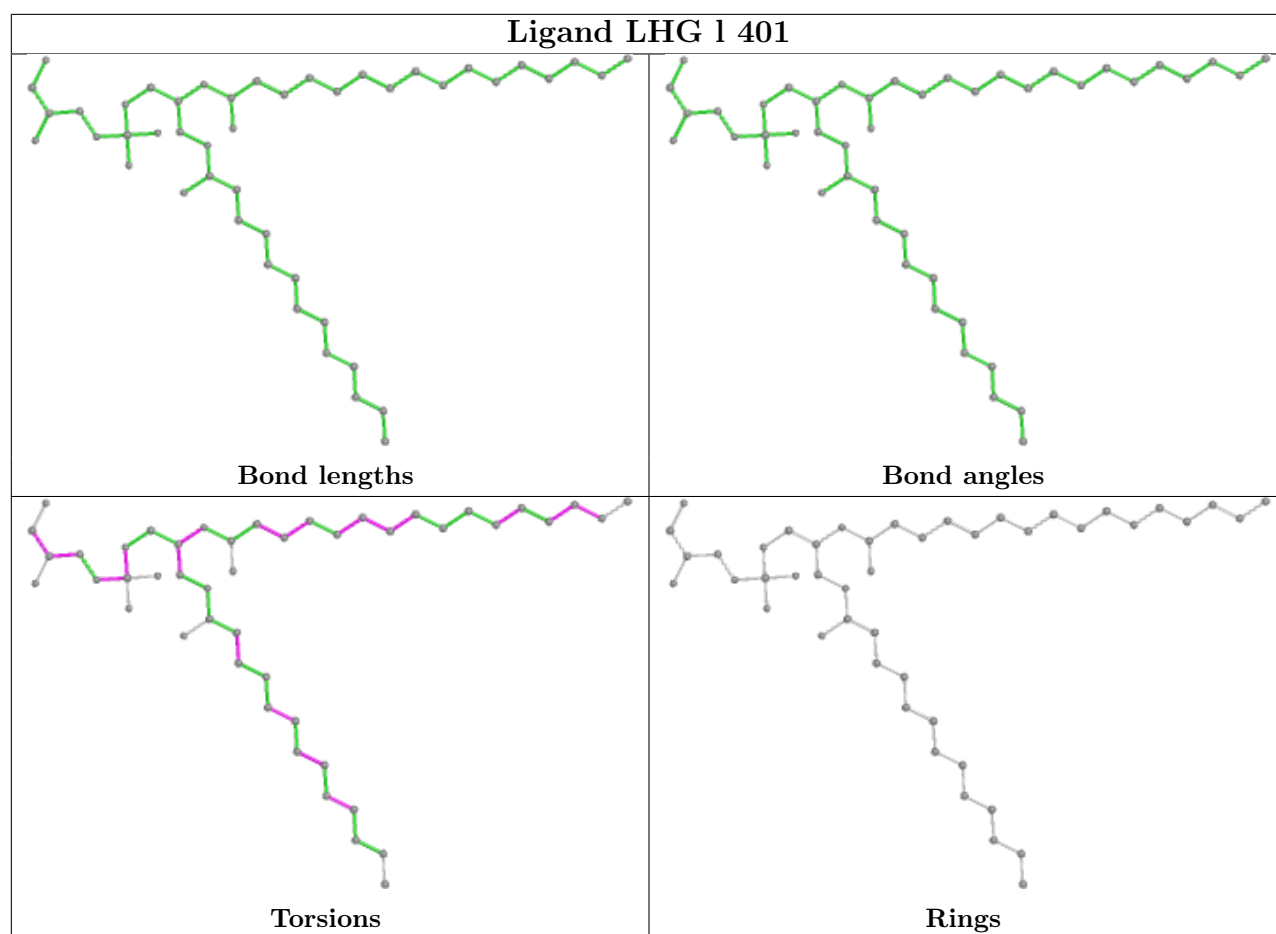


Ligand CLA C 211

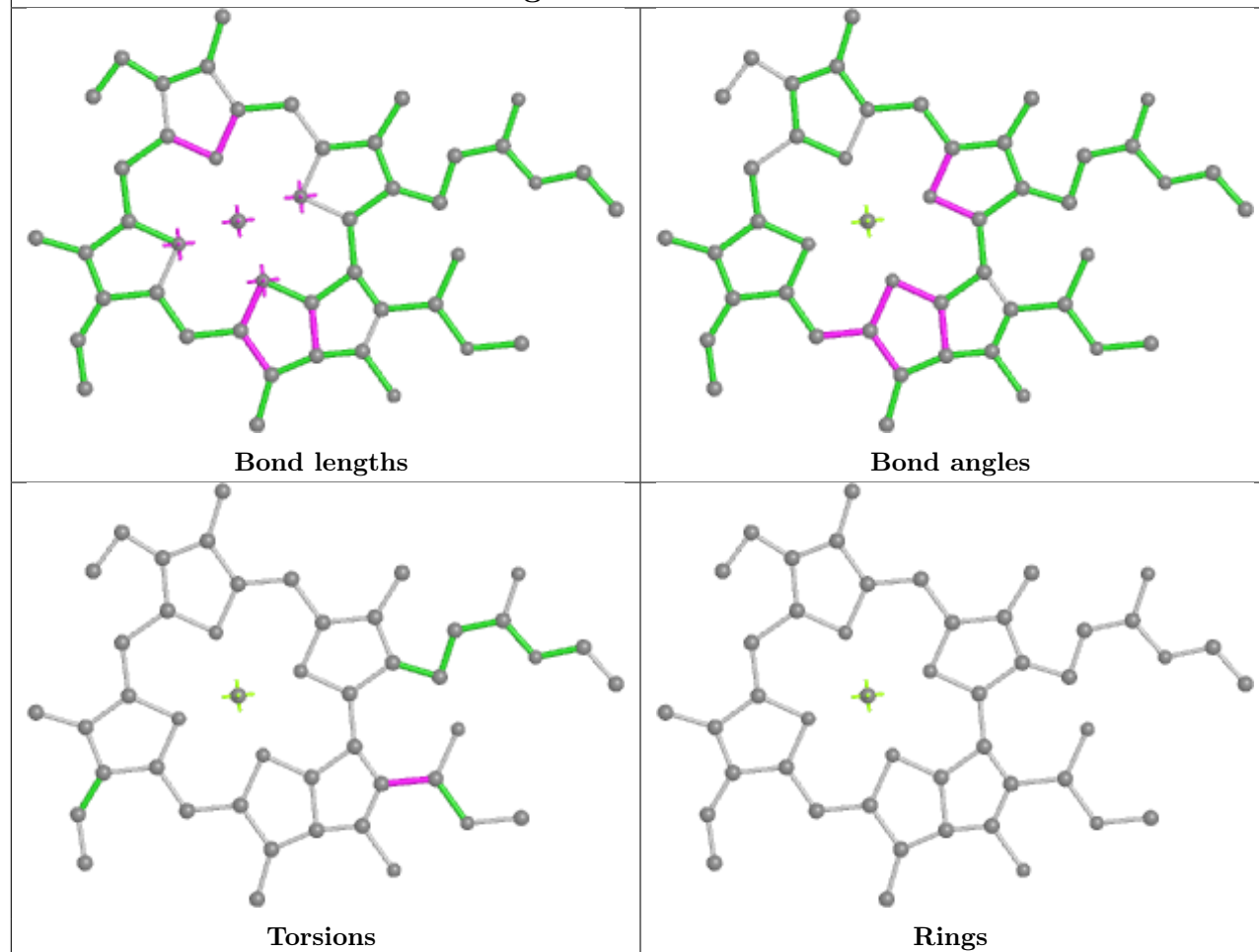


Ligand CLA a 837

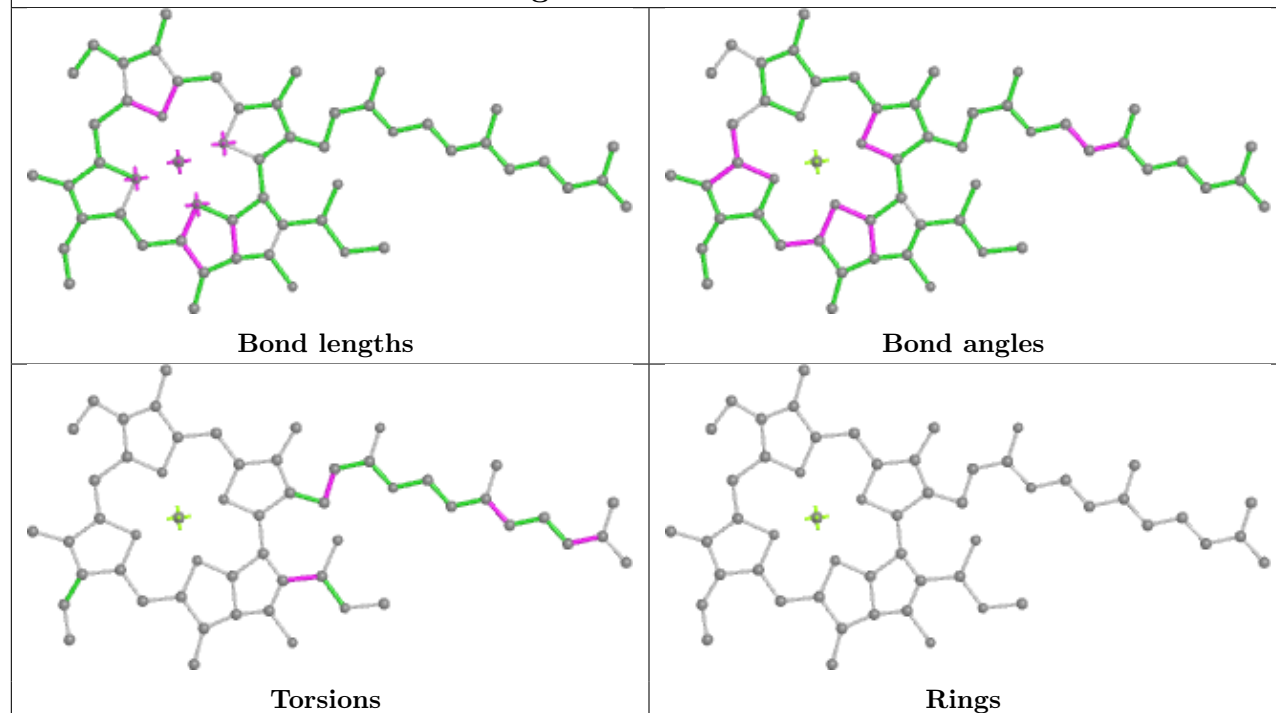


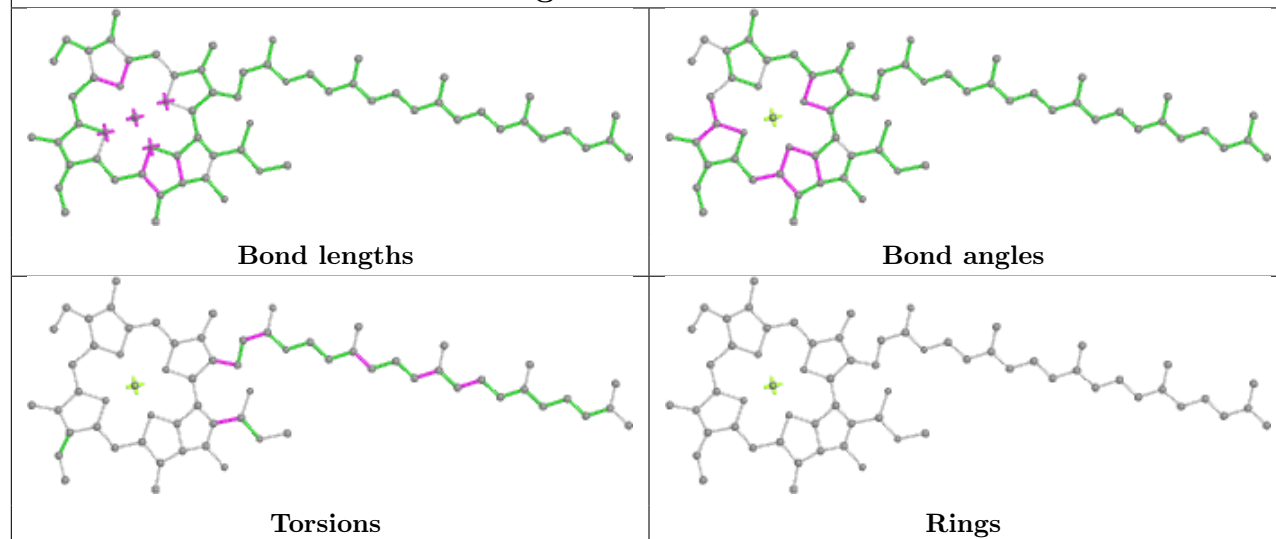
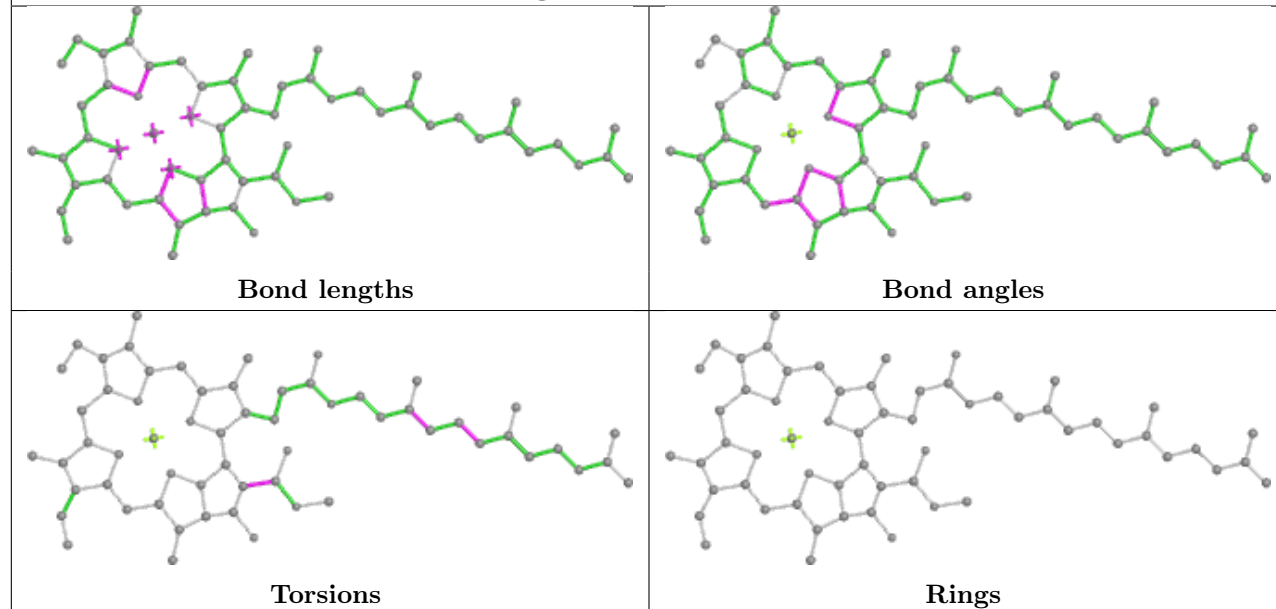


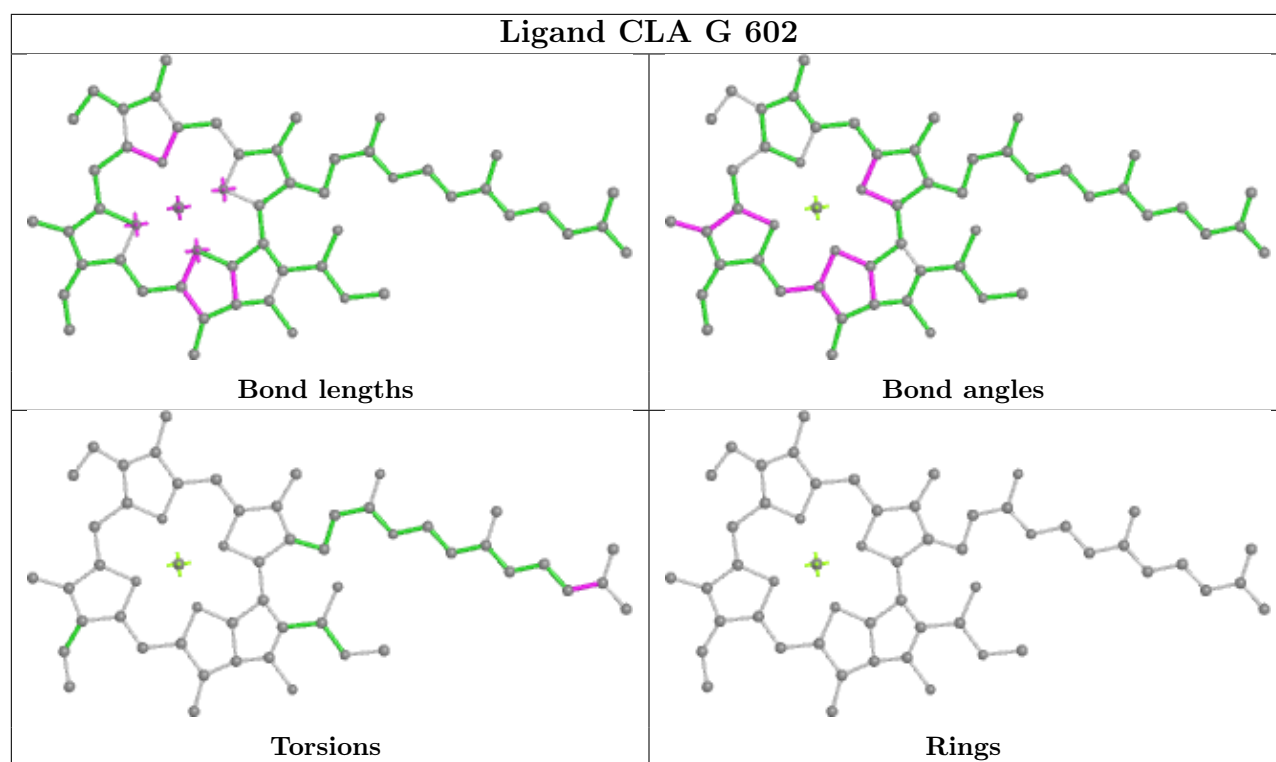
Ligand CLA G 604



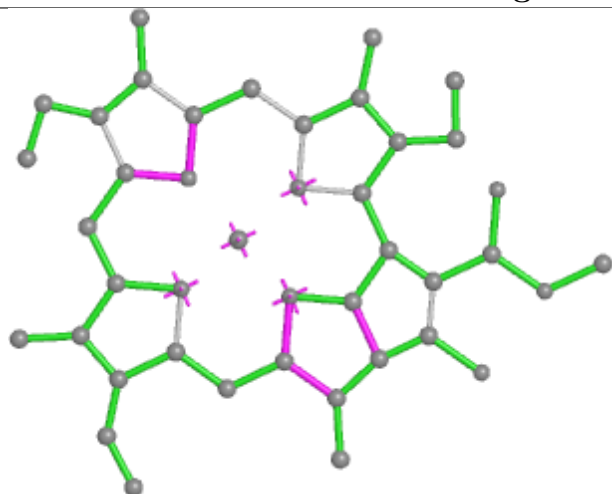
Ligand CLA D 604



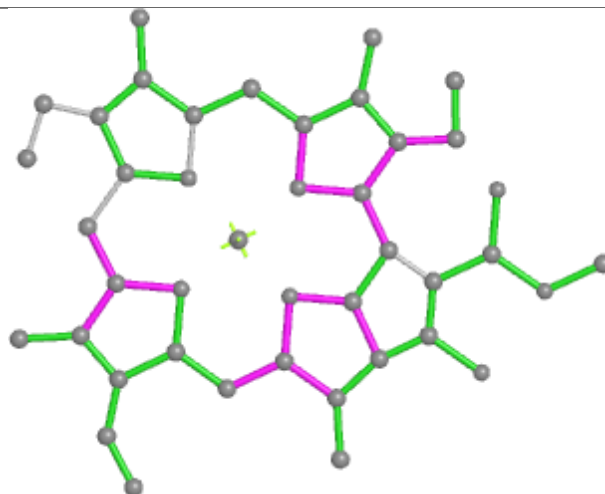
Ligand CLA a 805**Ligand CLA E 608**



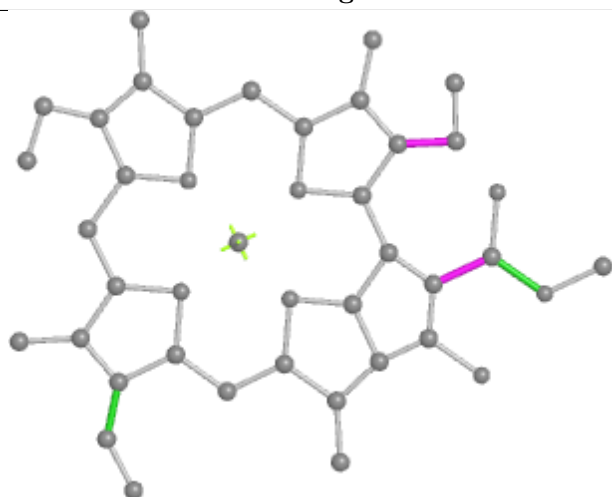
Ligand CLA C 201



Bond lengths



Bond angles

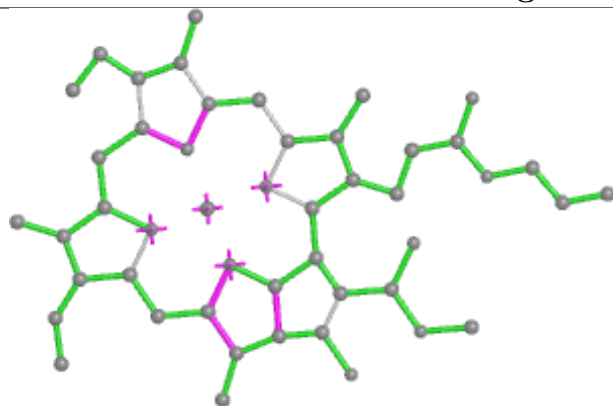


Torsions

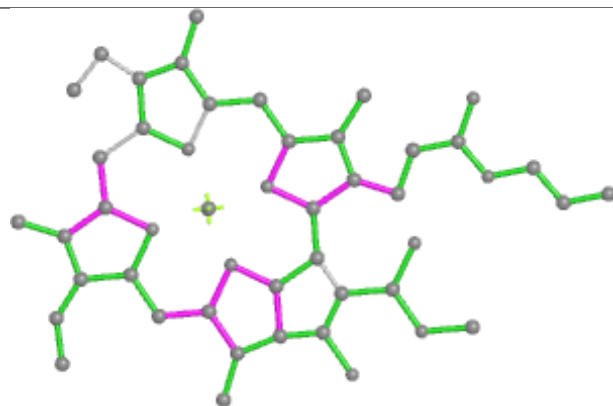


Rings

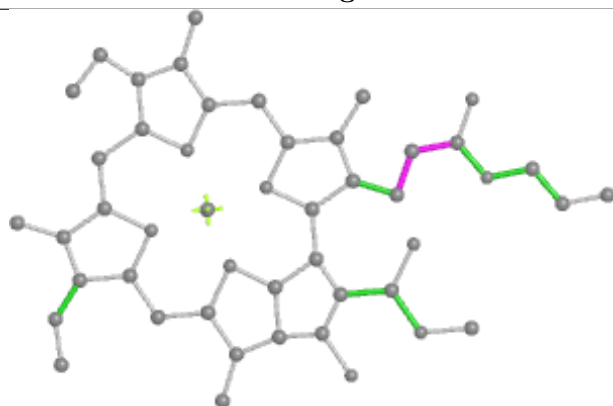
Ligand CLA b 712



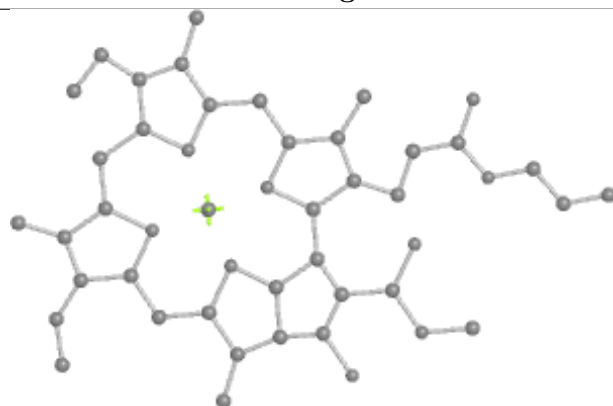
Bond lengths



Bond angles

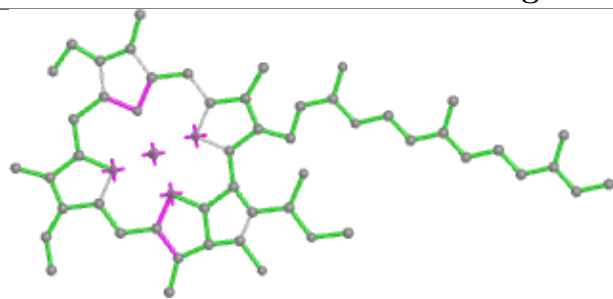


Torsions

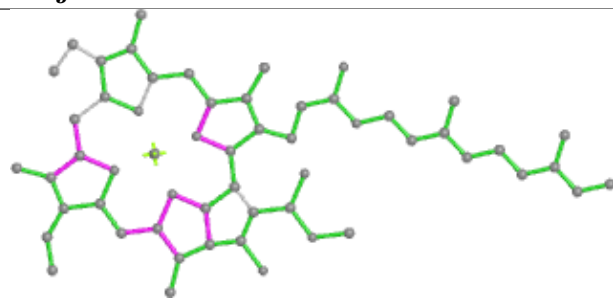


Rings

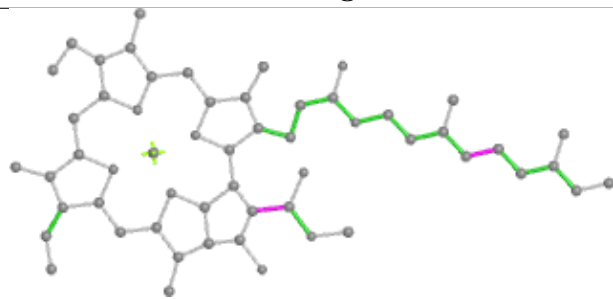
Ligand CLA j 202



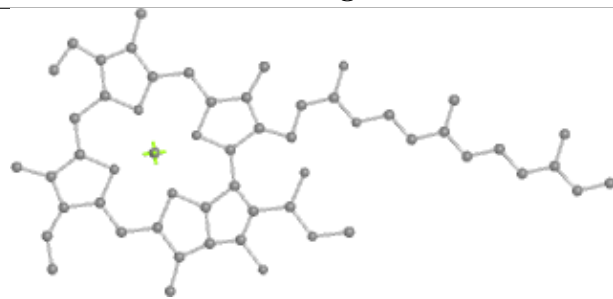
Bond lengths



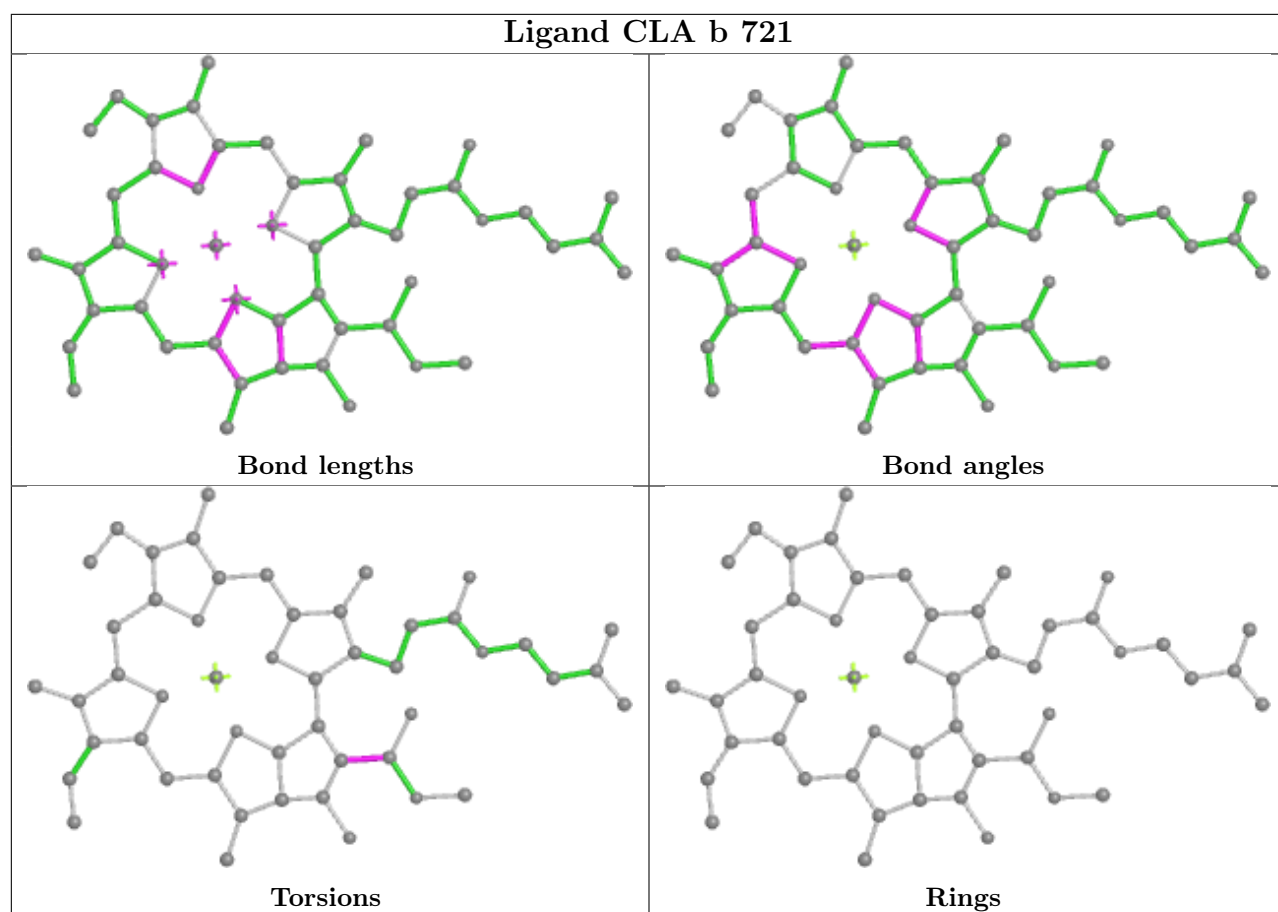
Bond angles



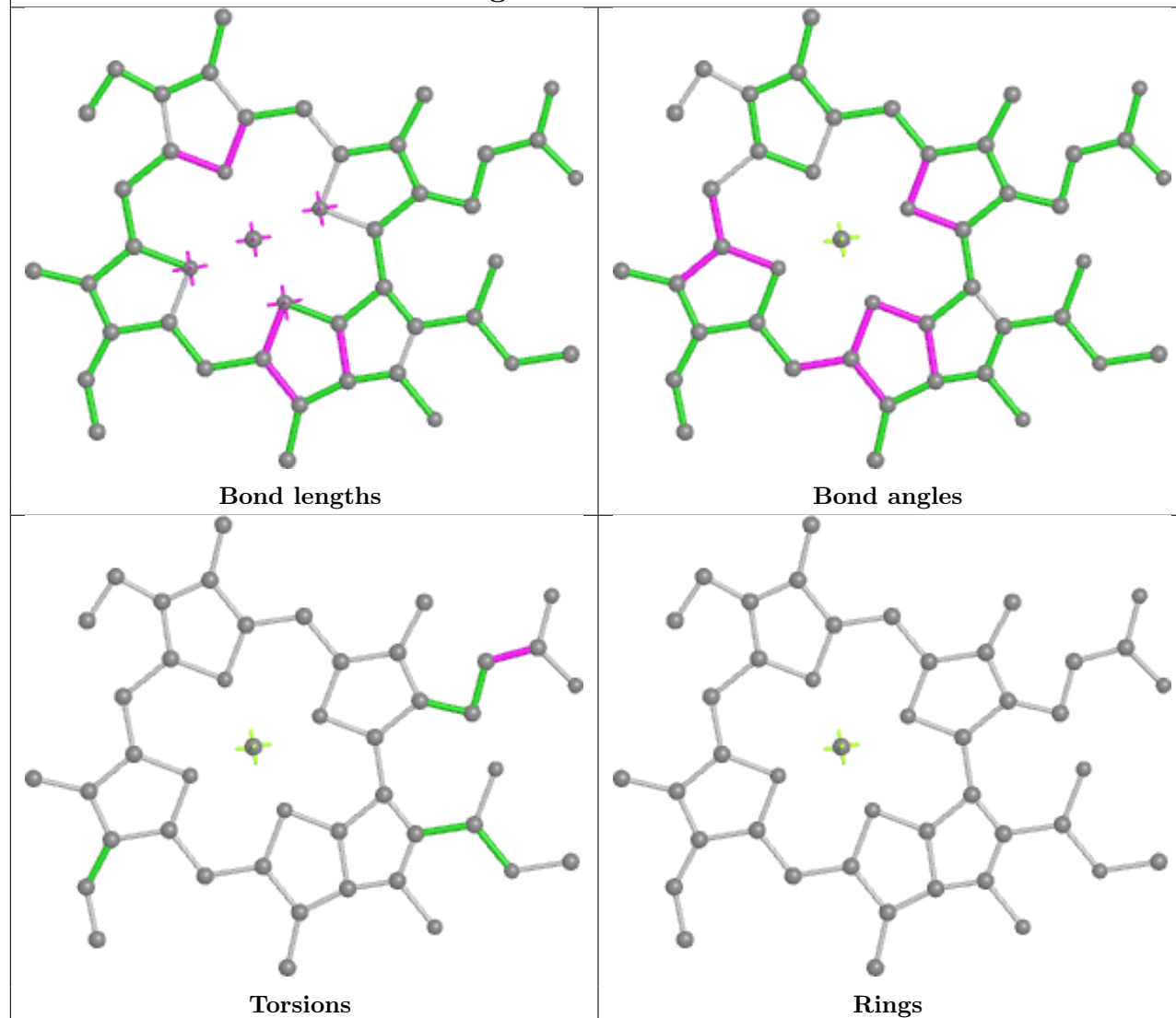
Torsions



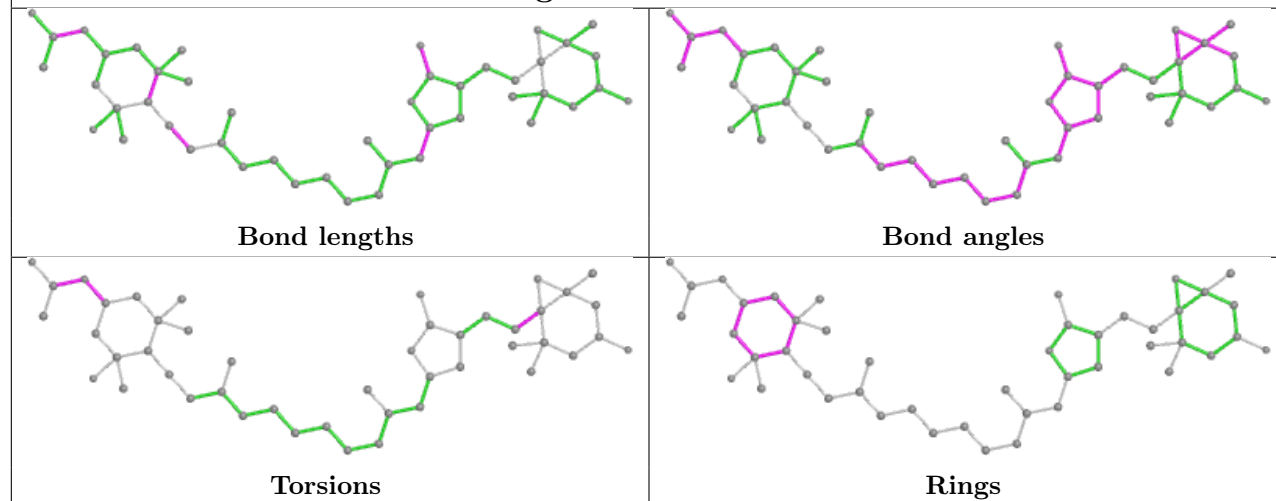
Rings



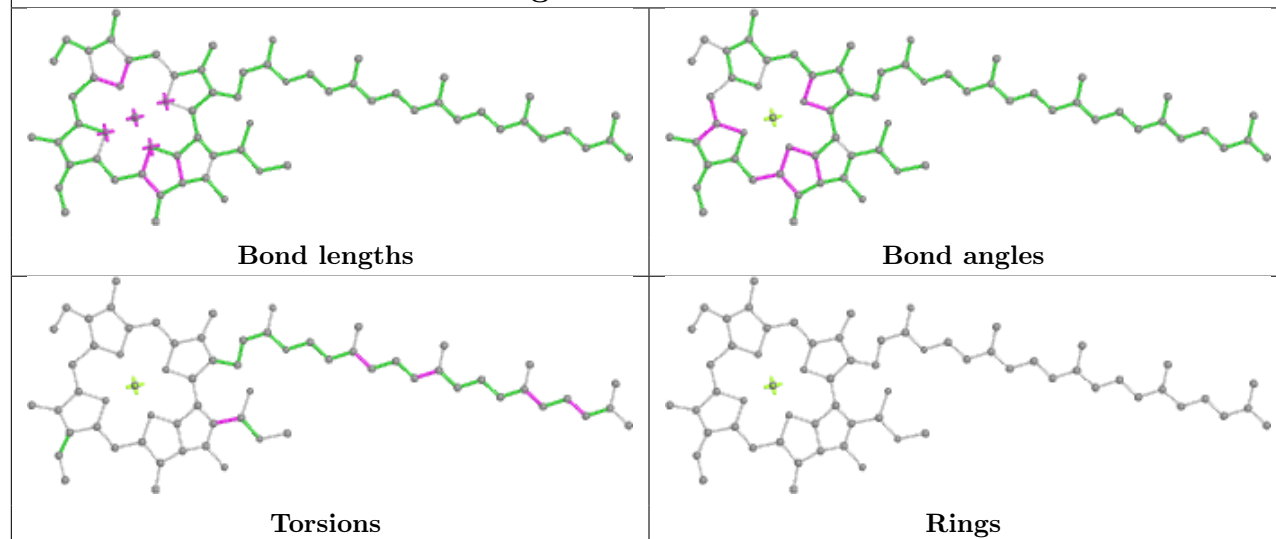
Ligand CLA D 609



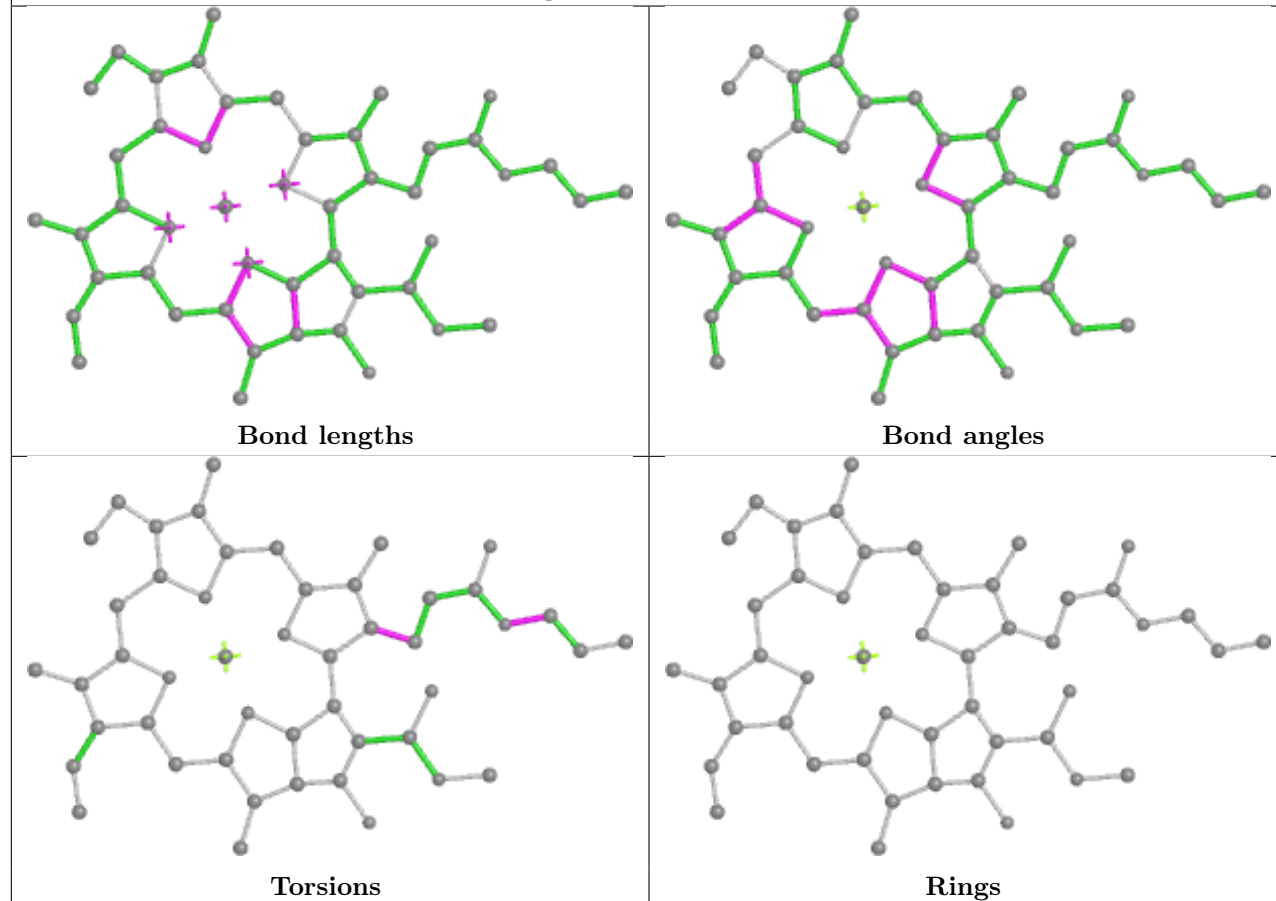
Ligand PID K 611

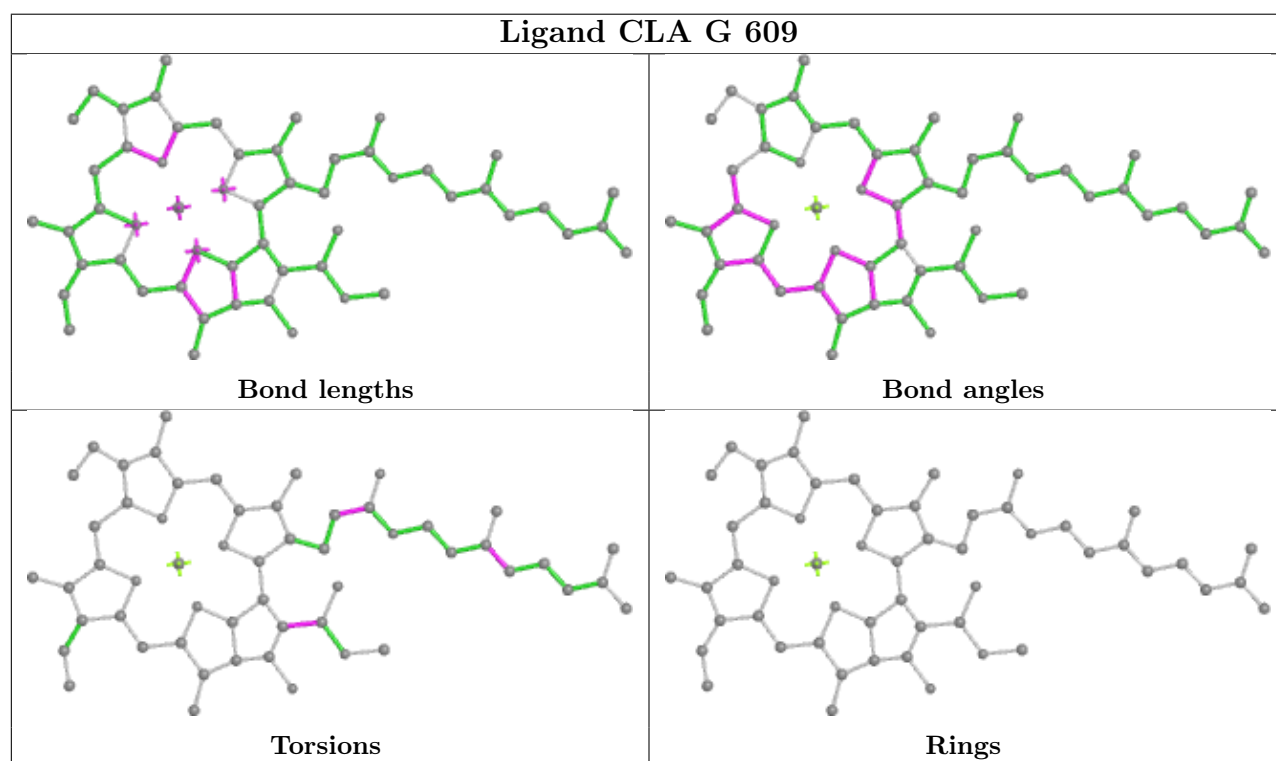
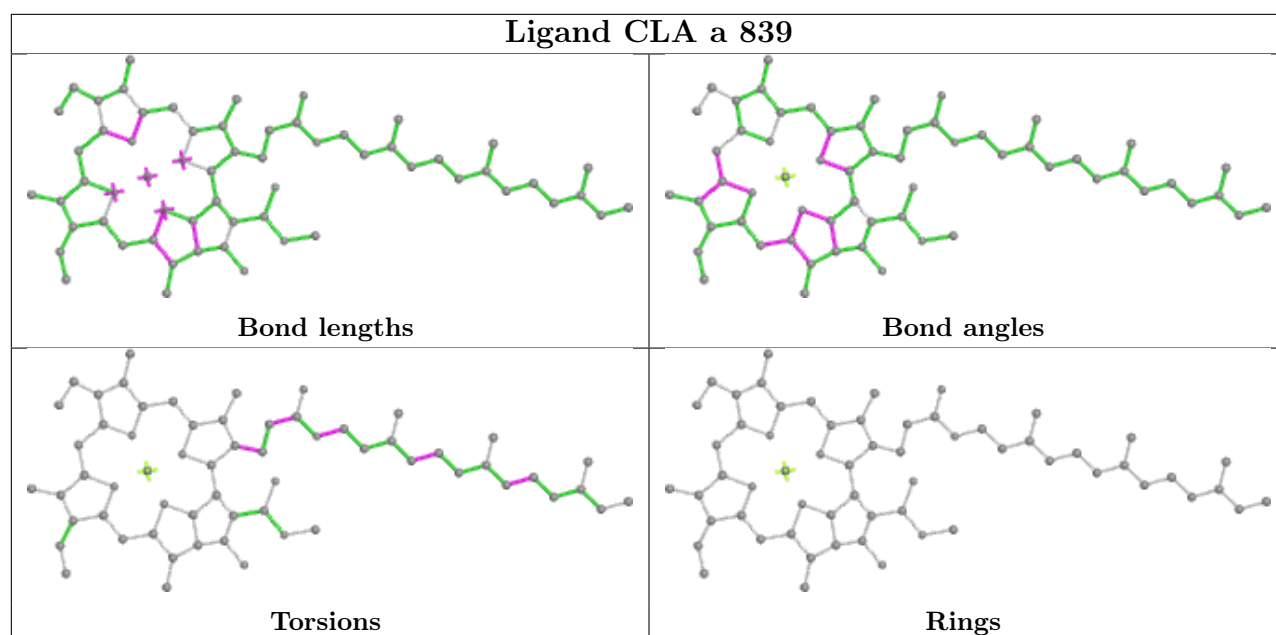


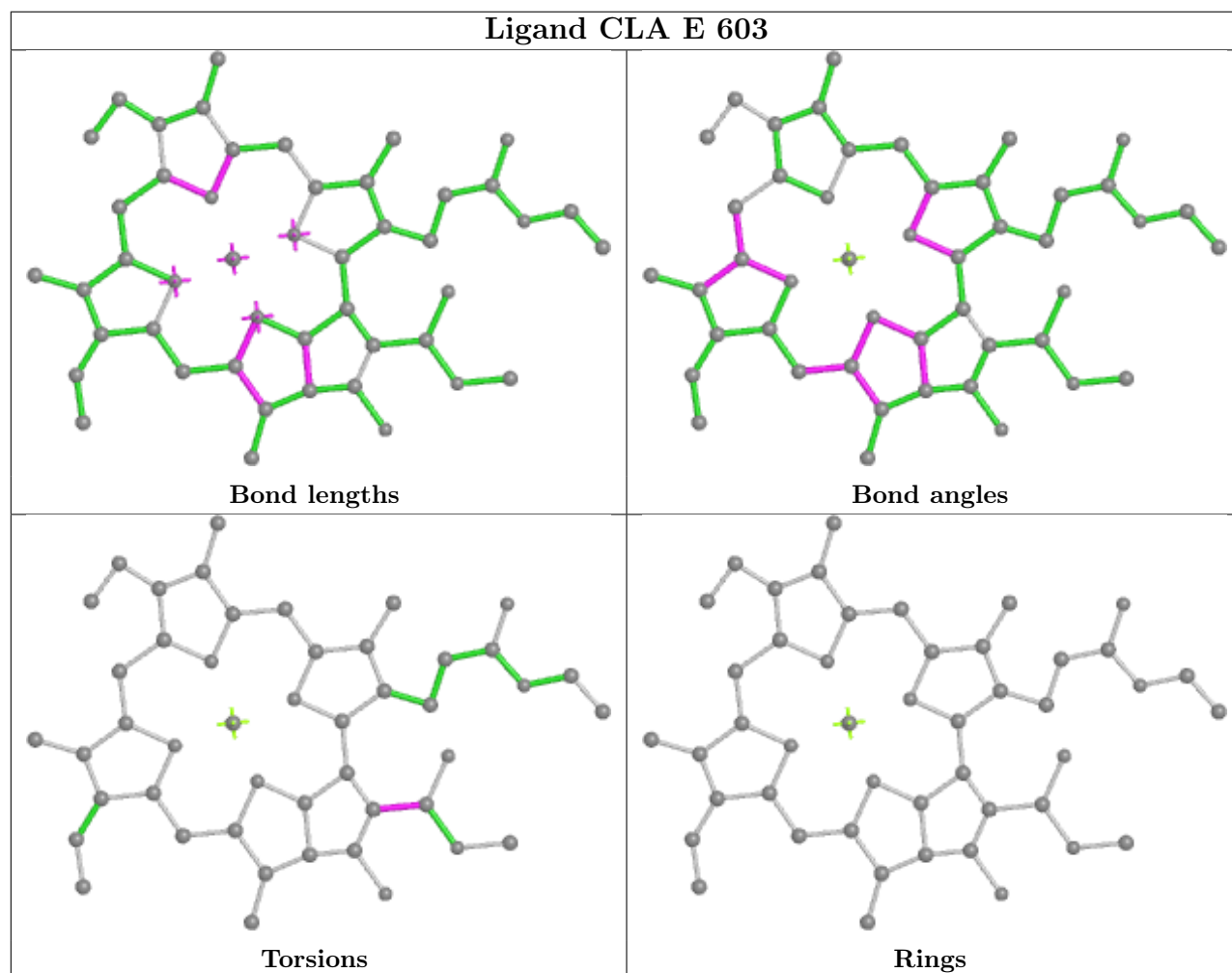
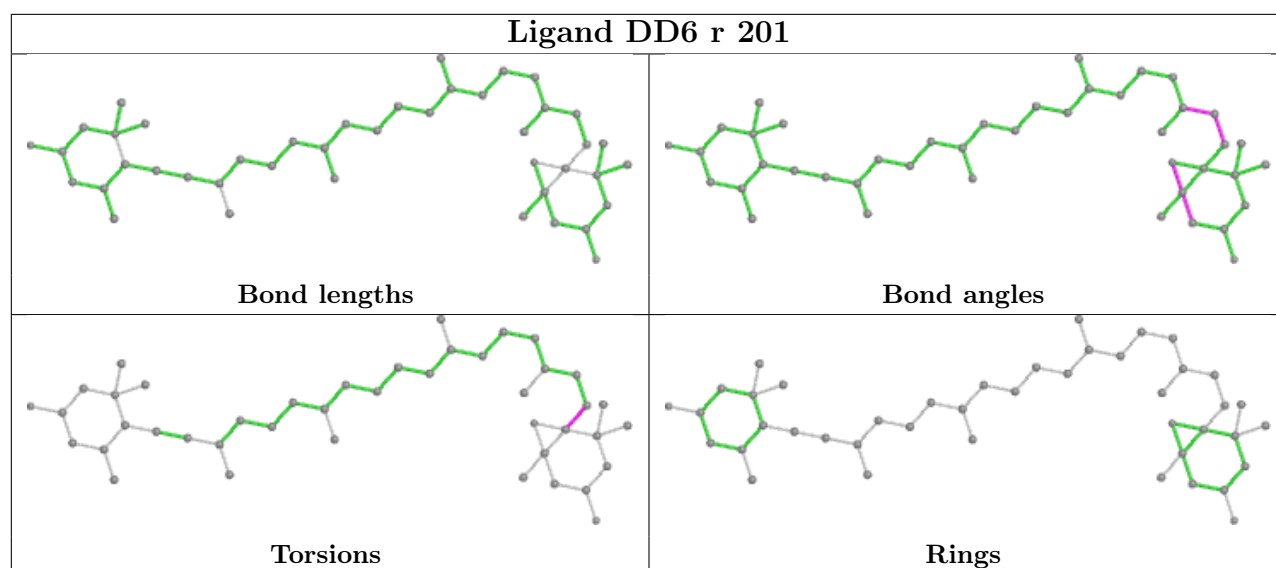
Ligand CLA H 319

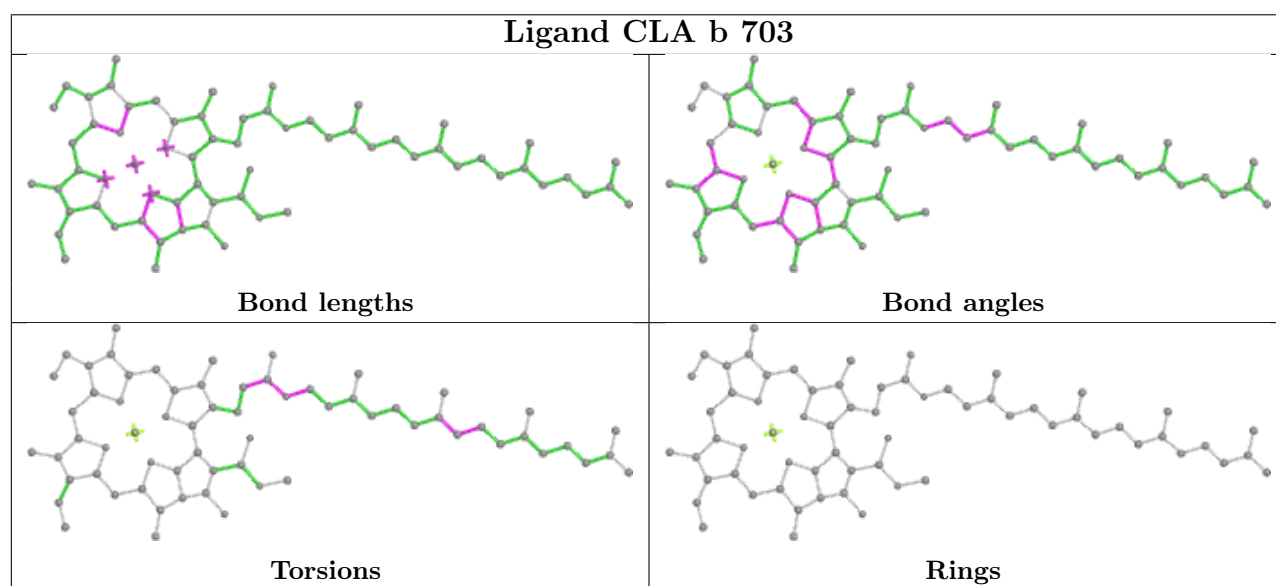
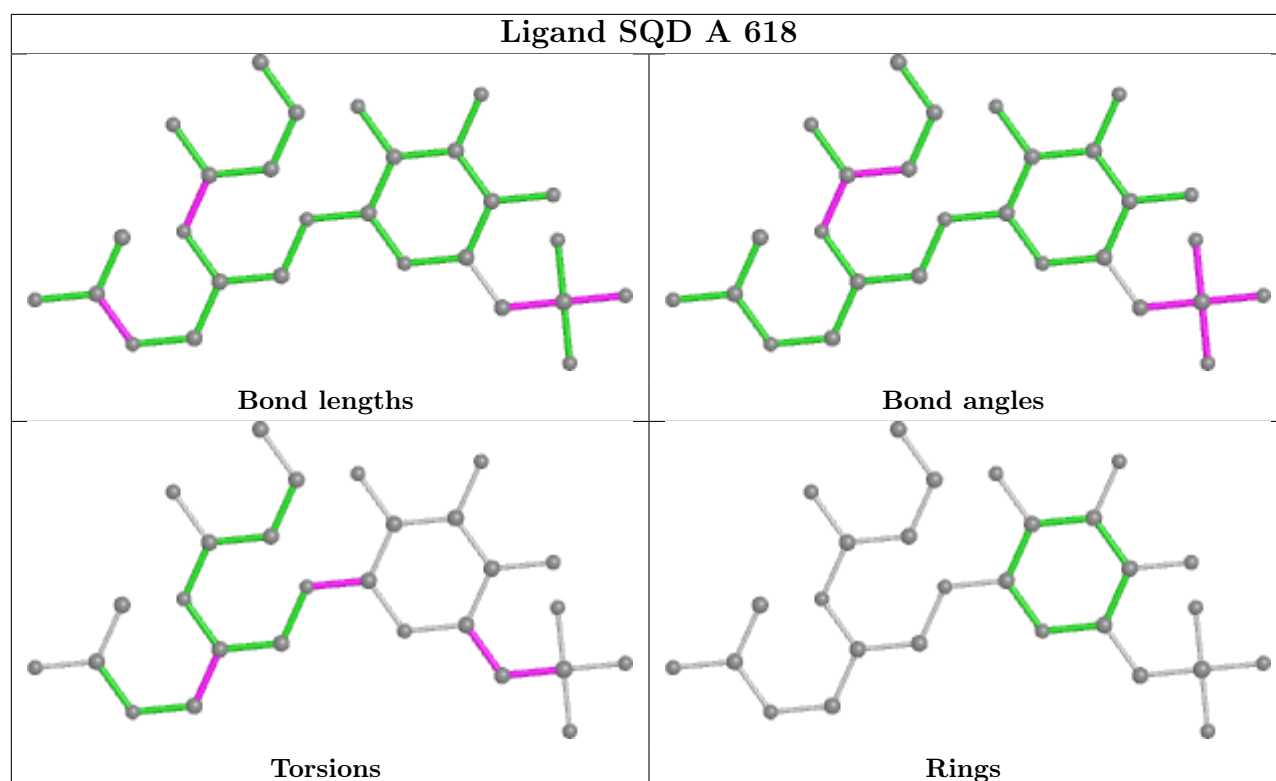


Ligand CLA I 410

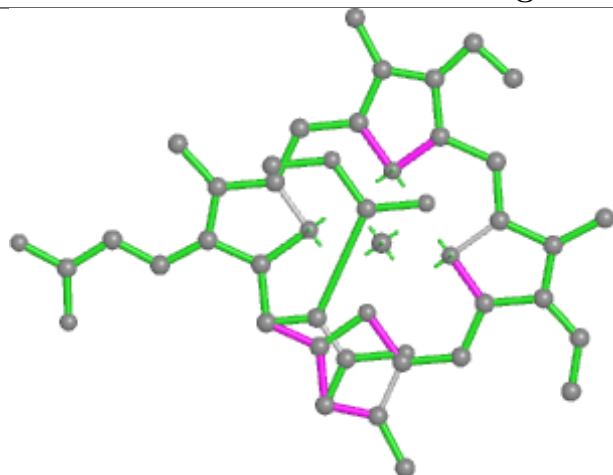




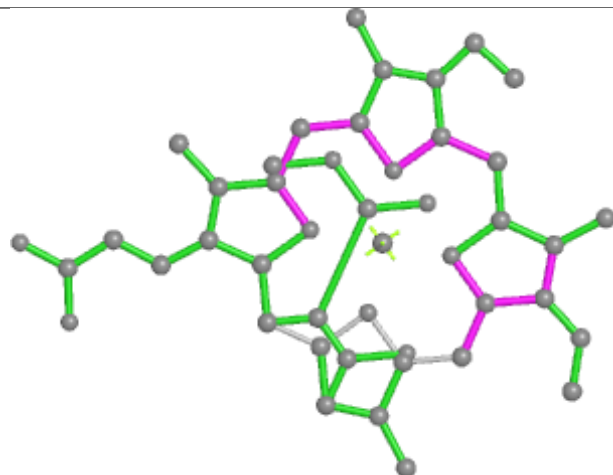




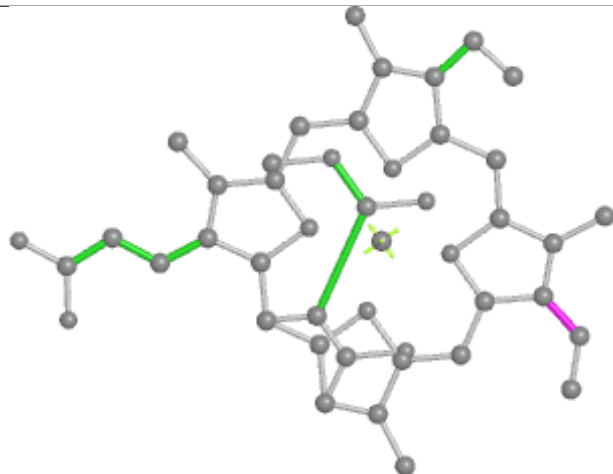
Ligand KC2 B 602



Bond lengths



Bond angles

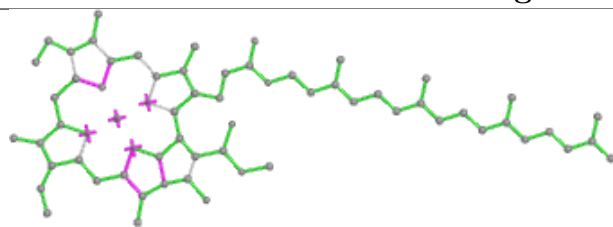


Torsions

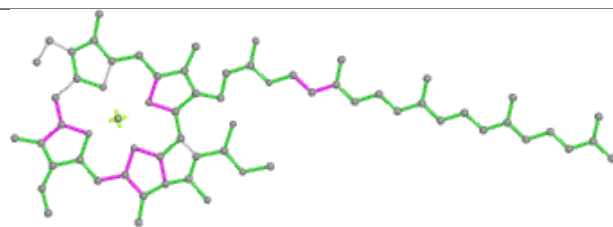


Rings

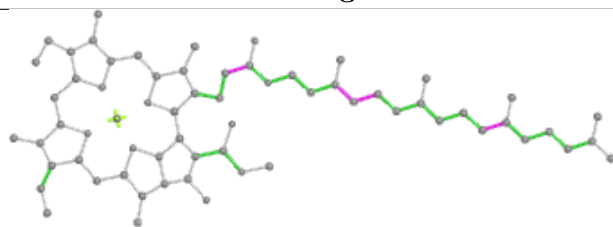
Ligand CLA B 609



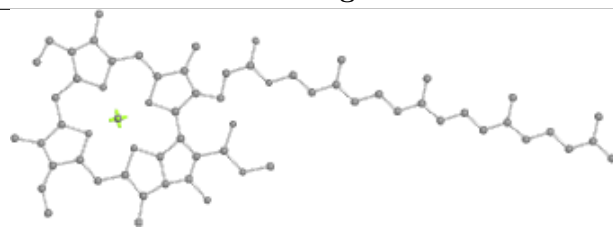
Bond lengths



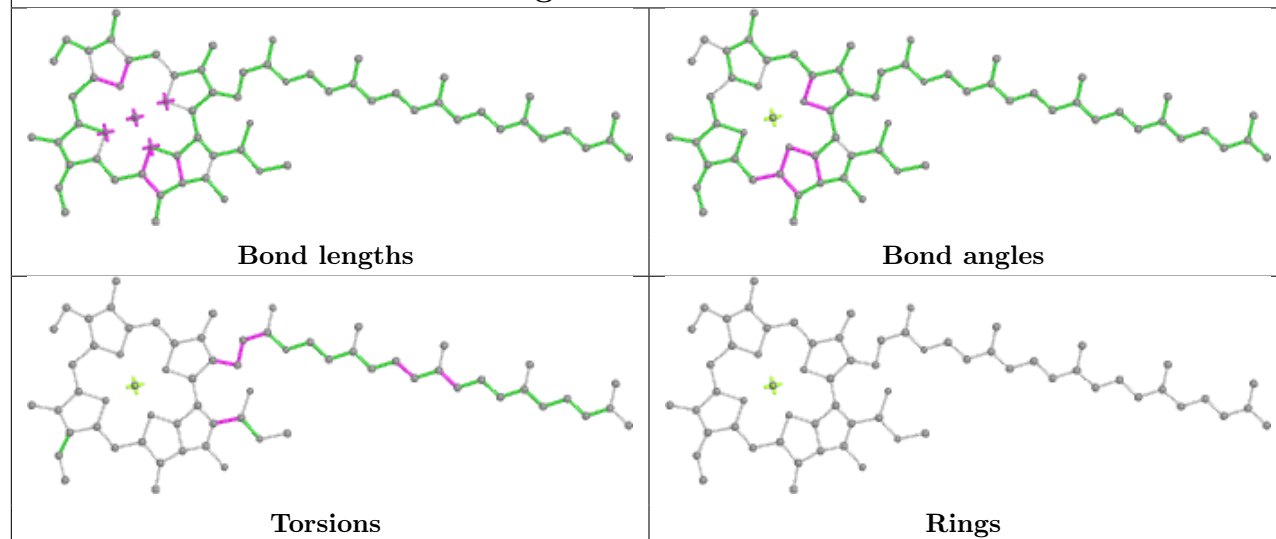
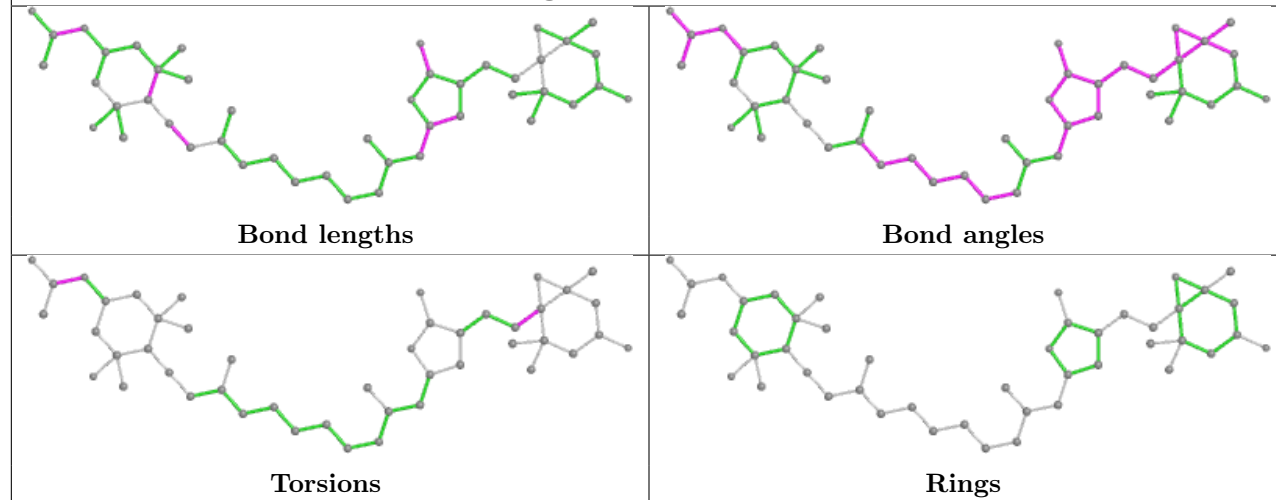
Bond angles



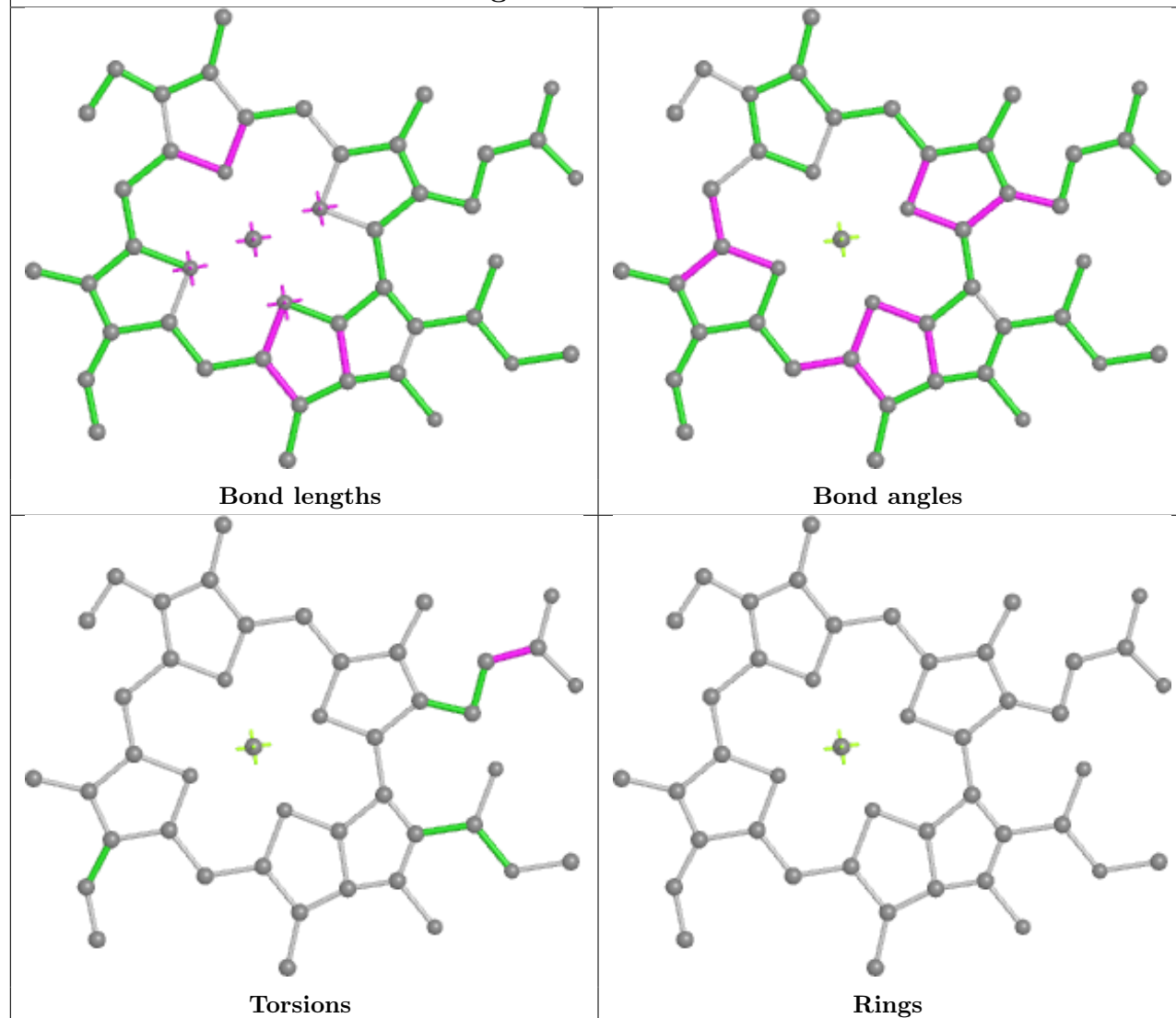
Torsions



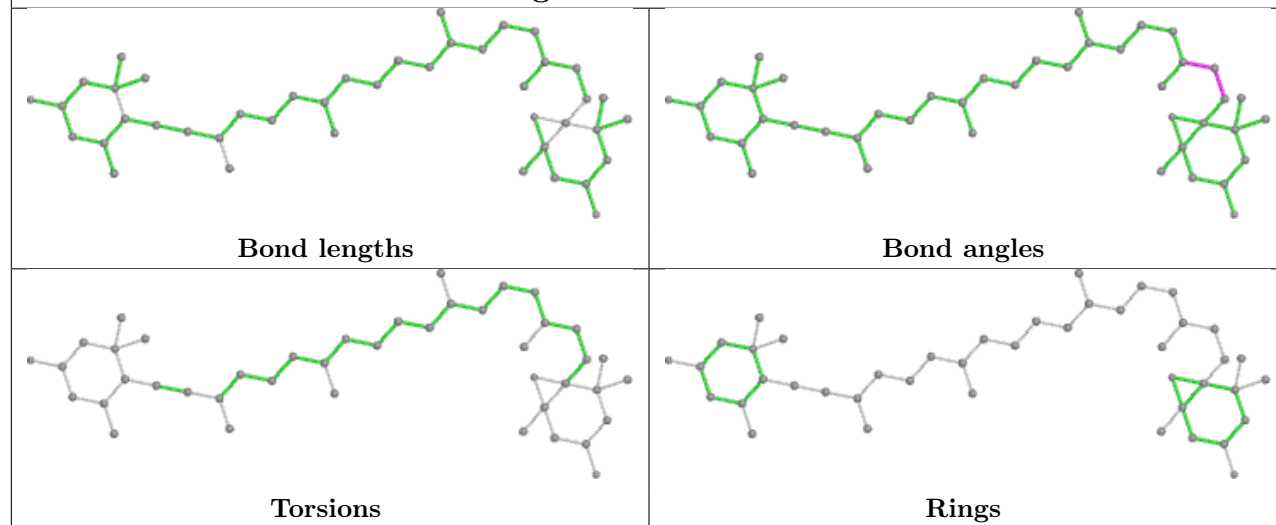
Rings

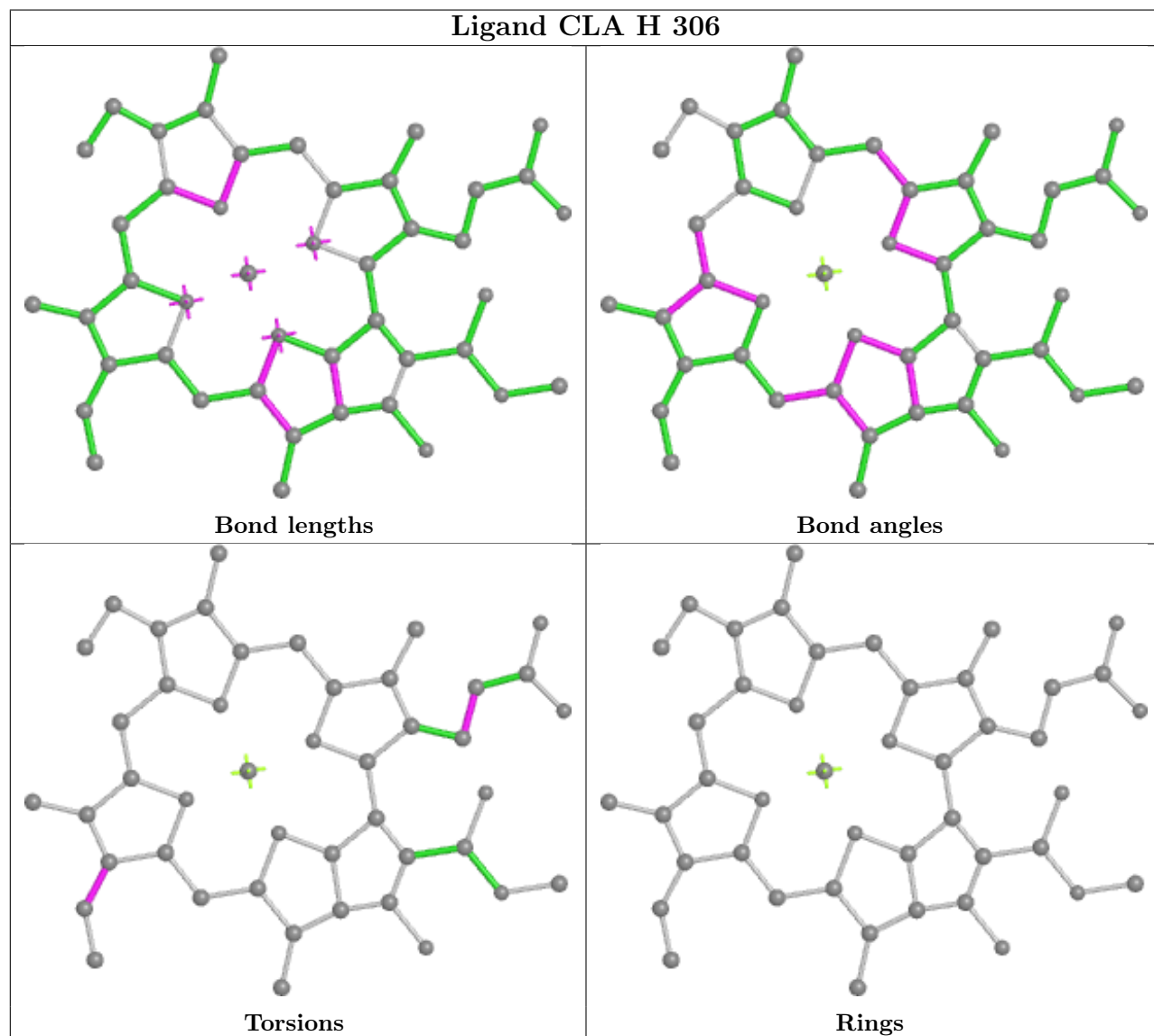
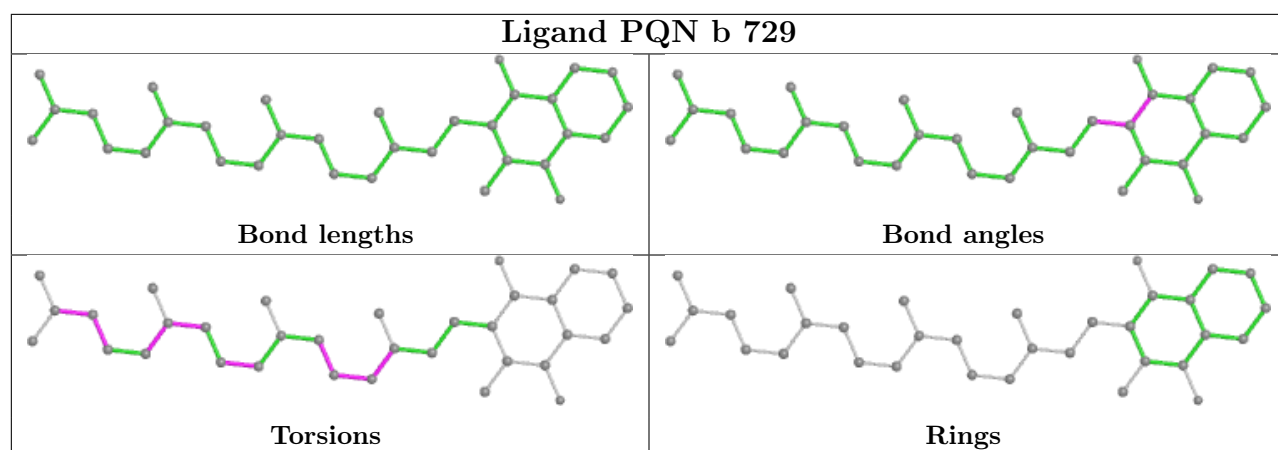
Ligand CLA b 705**Ligand PID J 613**

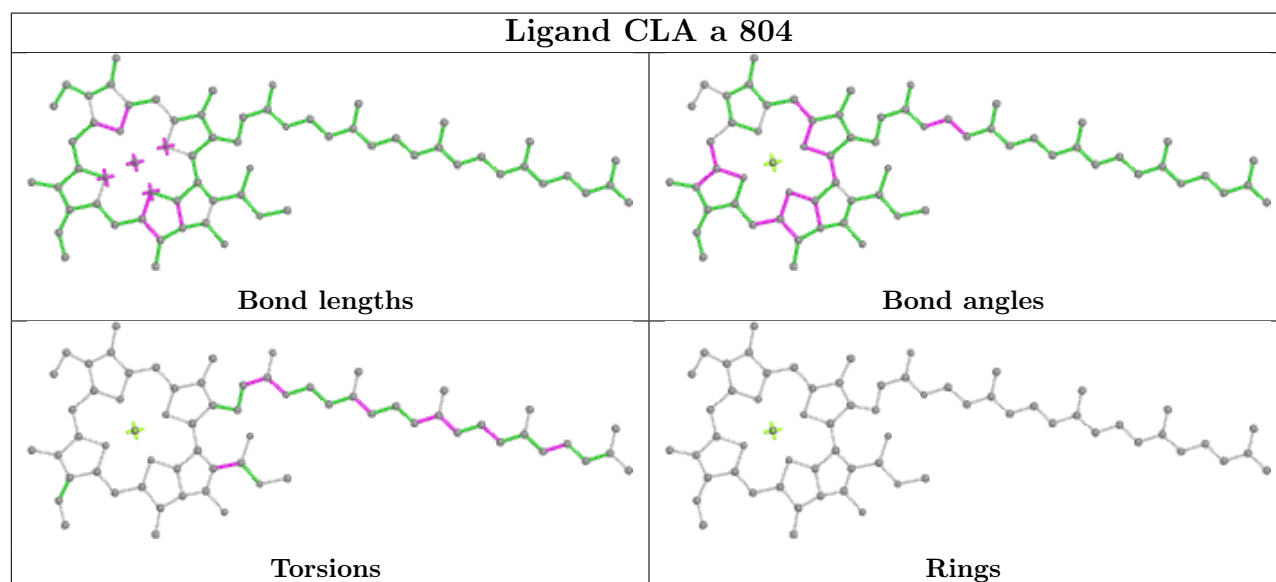
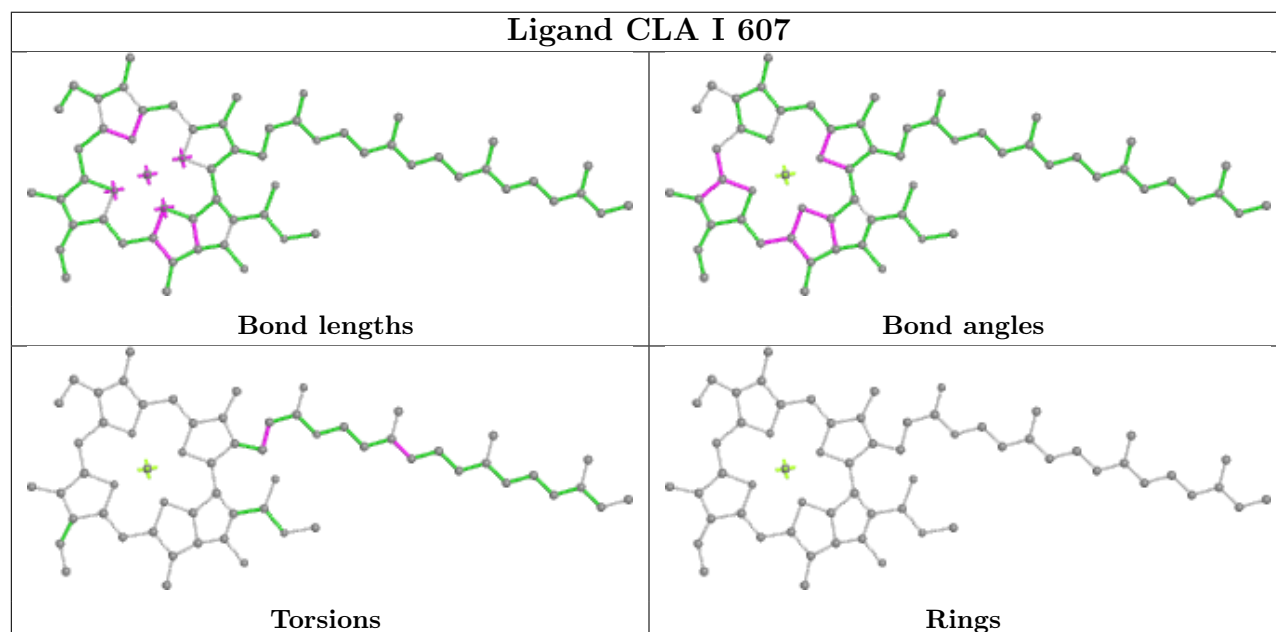
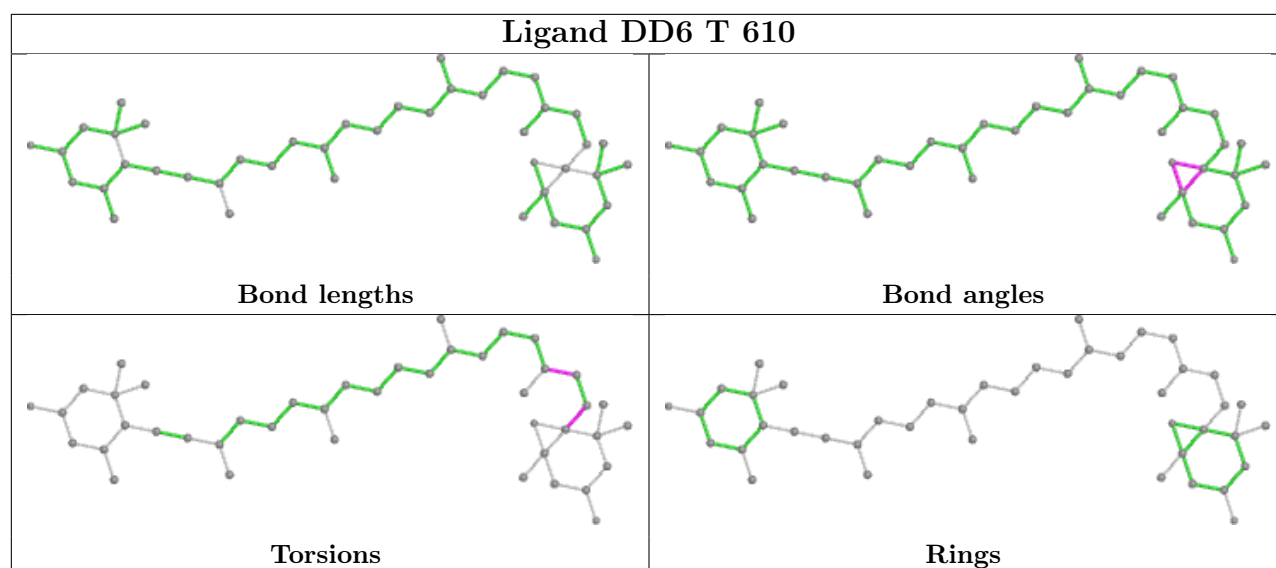
Ligand CLA C 209



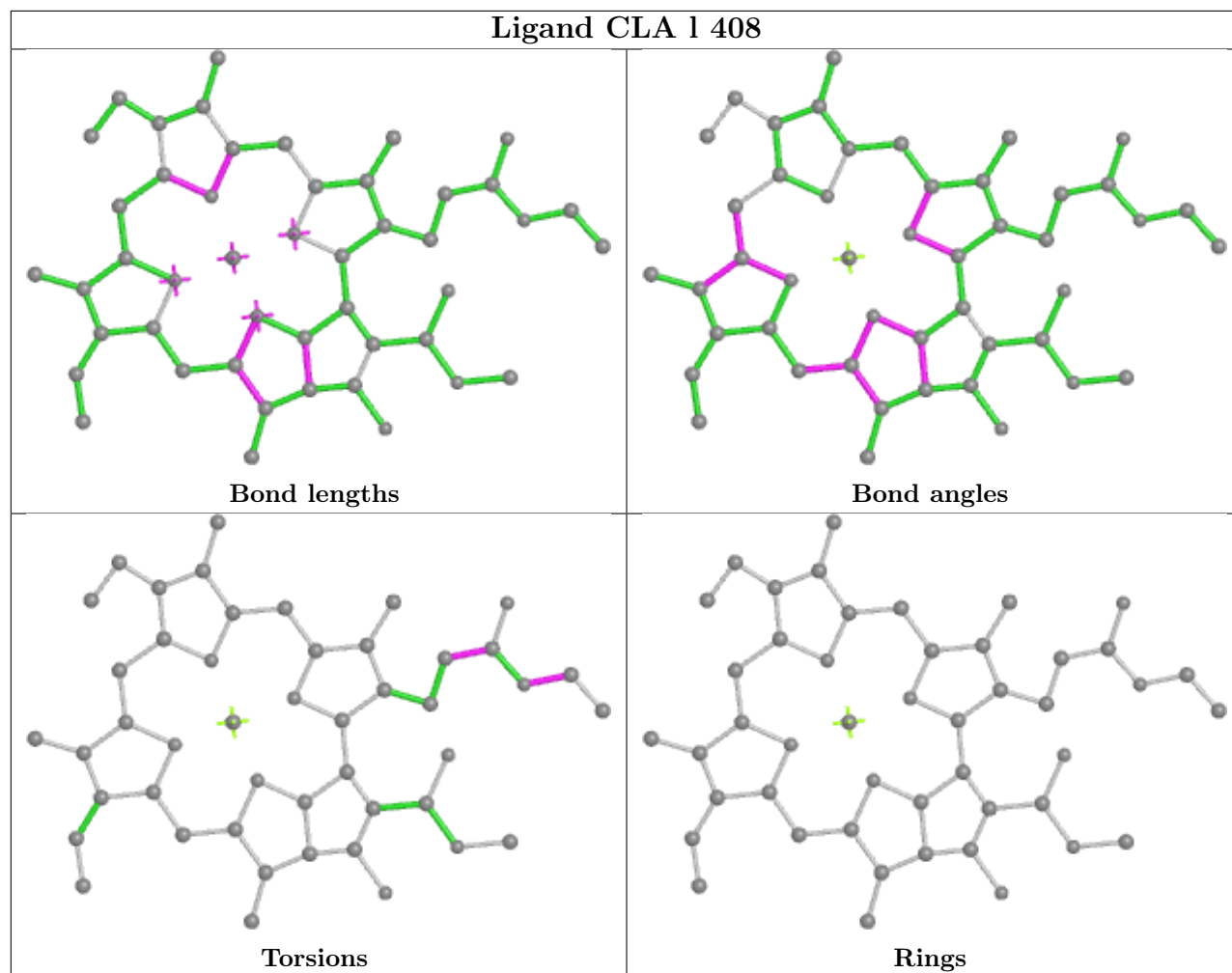
Ligand DD6 U 607



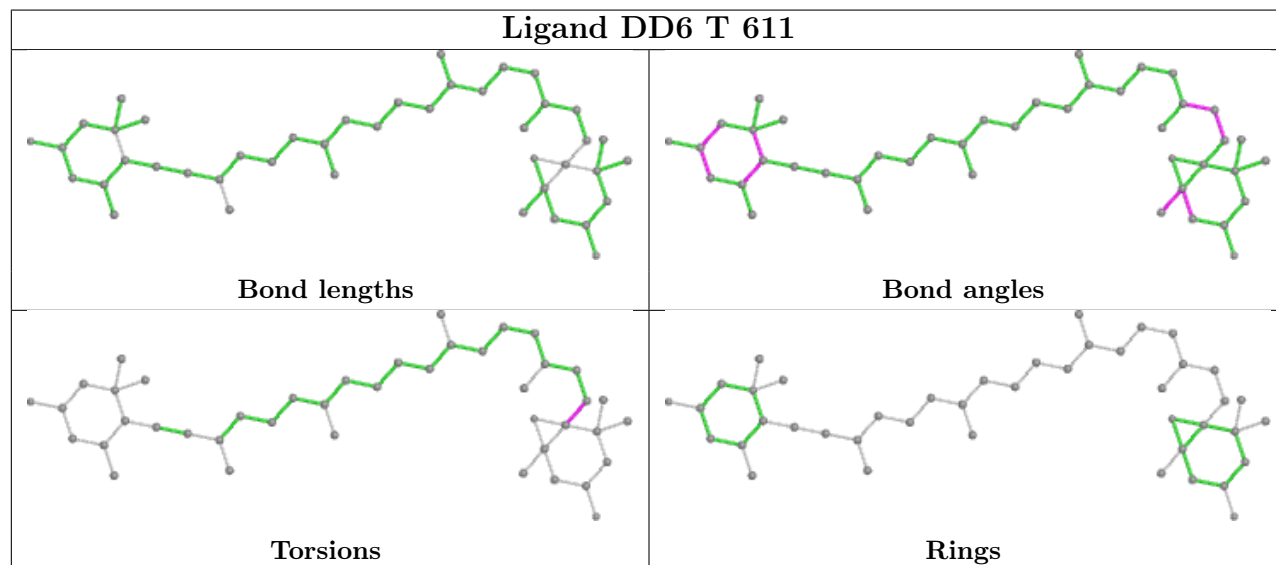




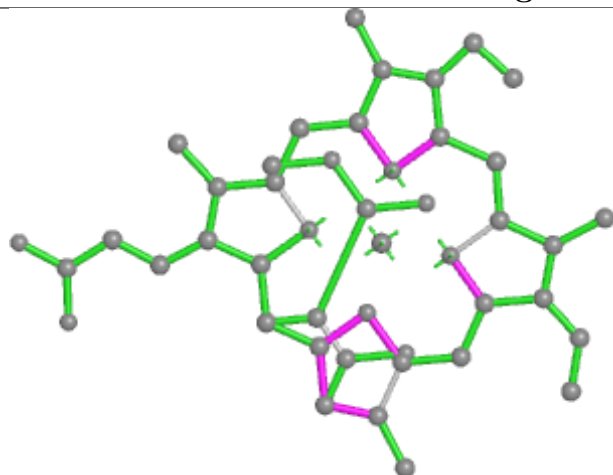
Ligand CLA 1 408



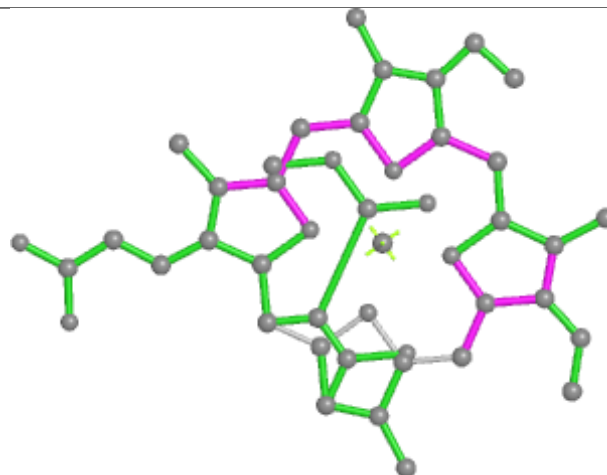
Ligand DD6 T 611



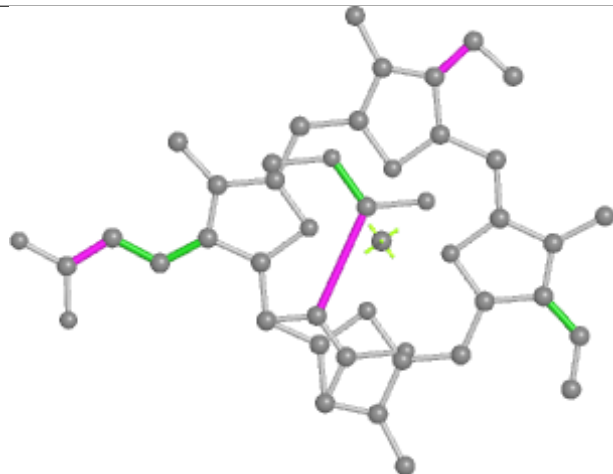
Ligand KC2 A 608



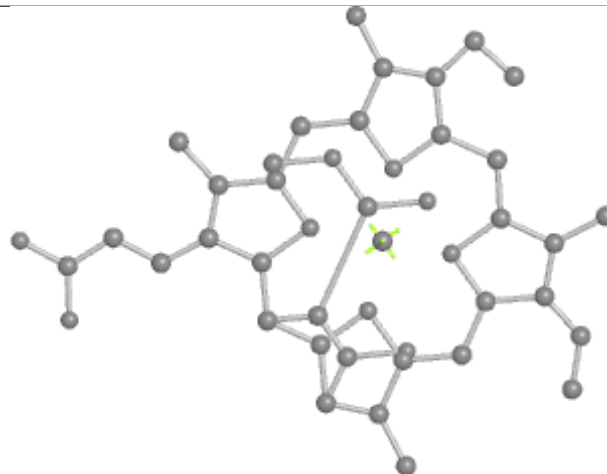
Bond lengths



Bond angles

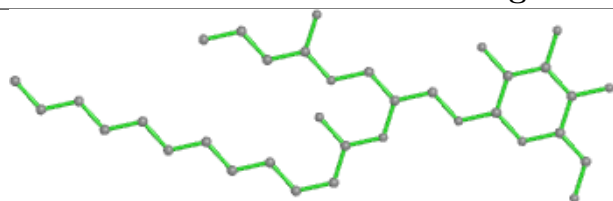


Torsions

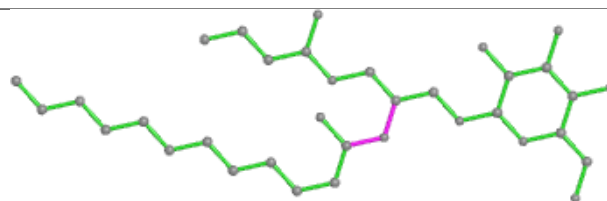


Rings

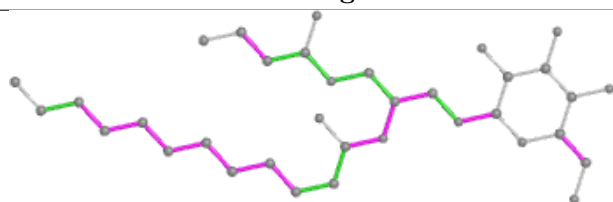
Ligand LMG D 618



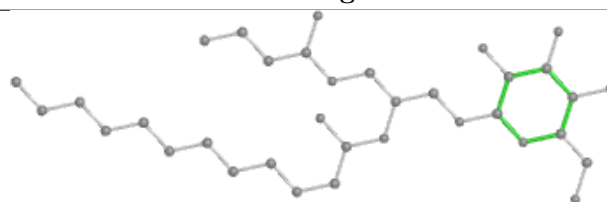
Bond lengths



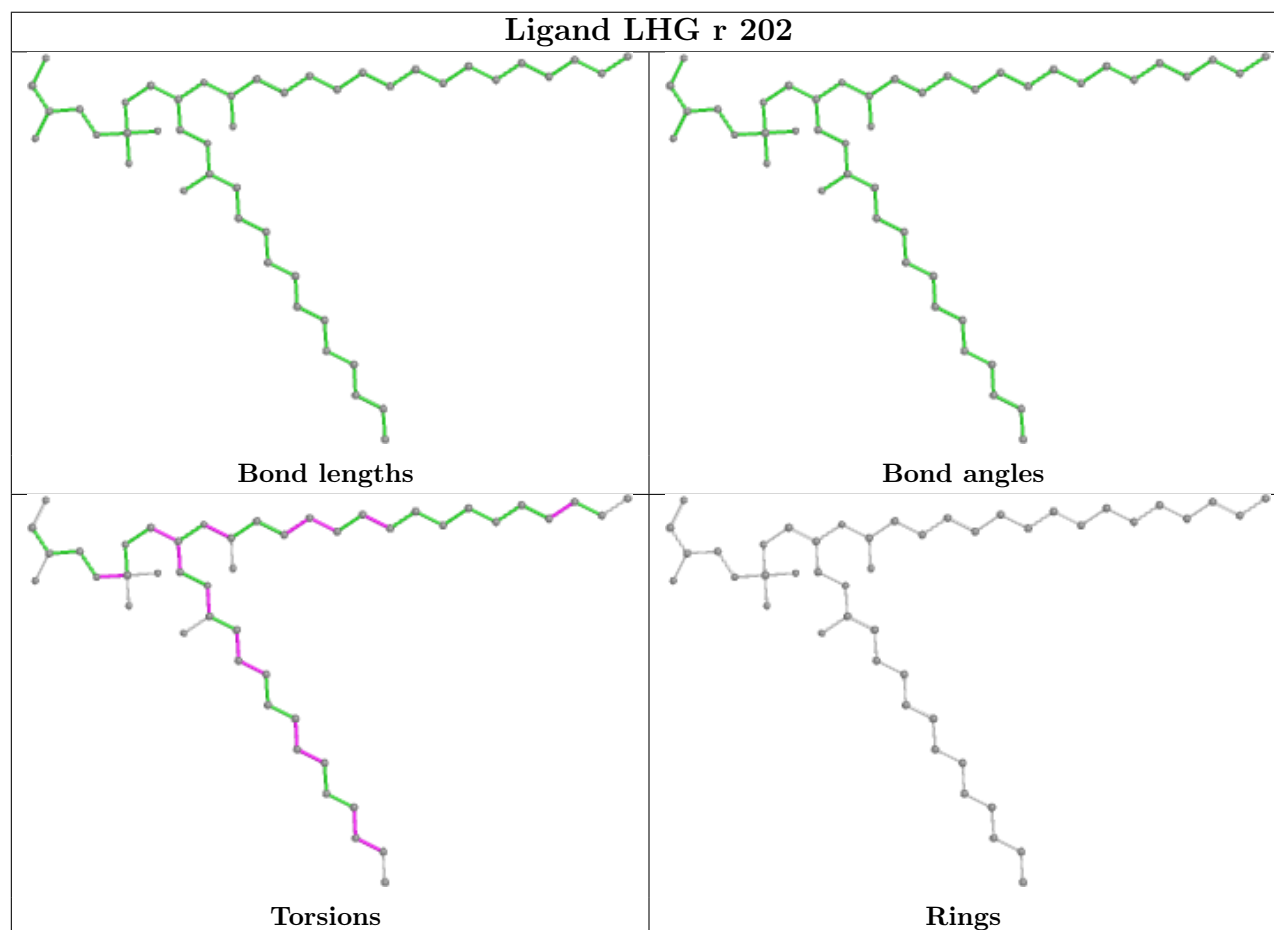
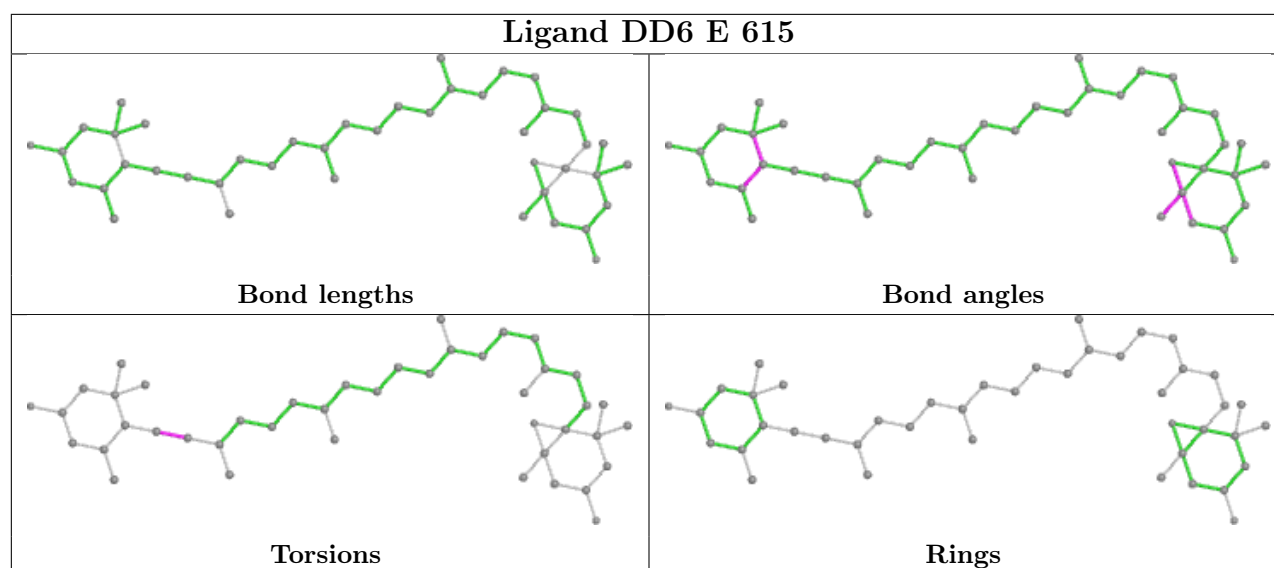
Bond angles



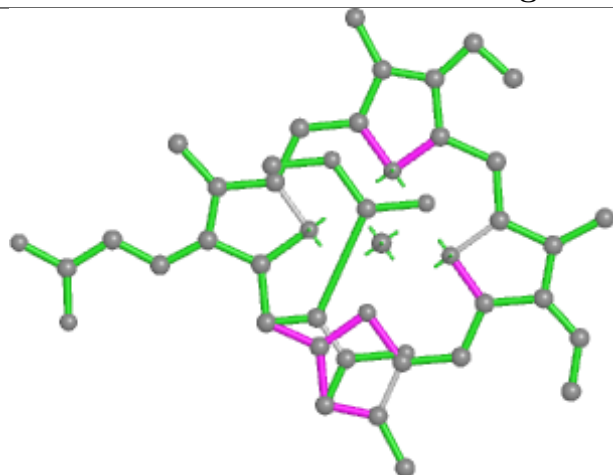
Torsions



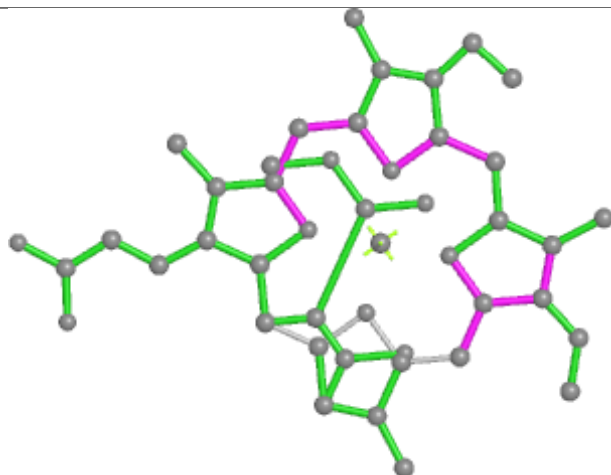
Rings



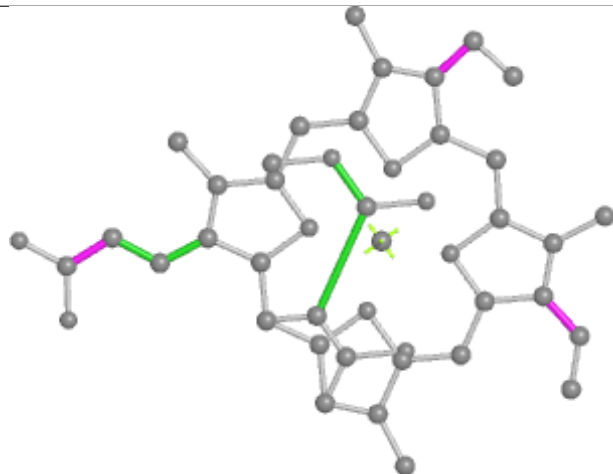
Ligand KC2 J 610



Bond lengths



Bond angles

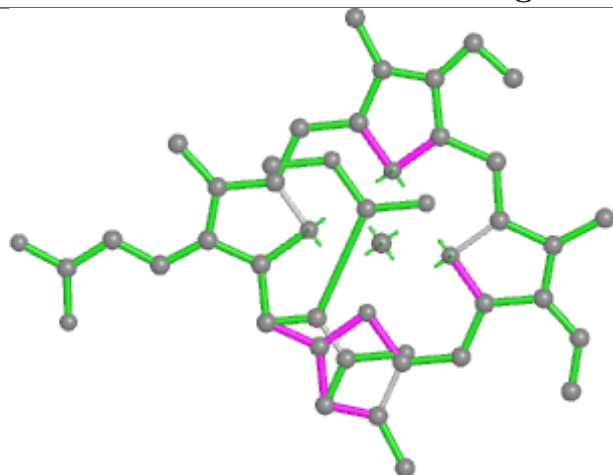


Torsions

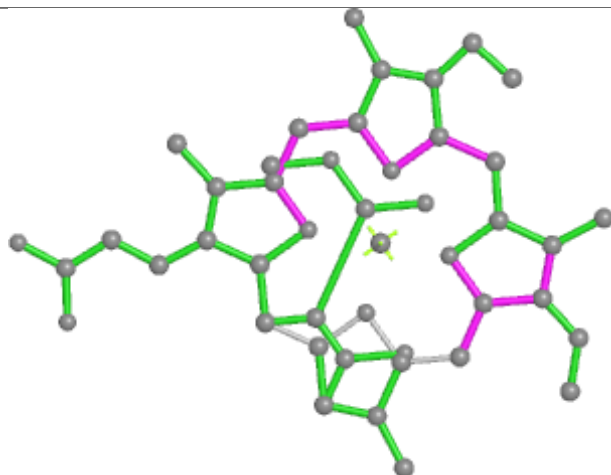


Rings

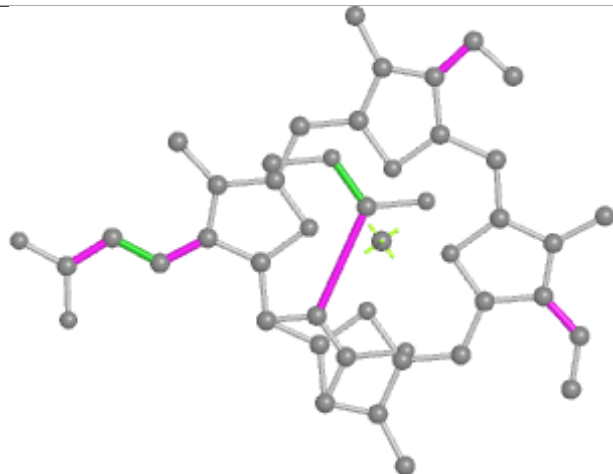
Ligand KC2 H 311



Bond lengths



Bond angles

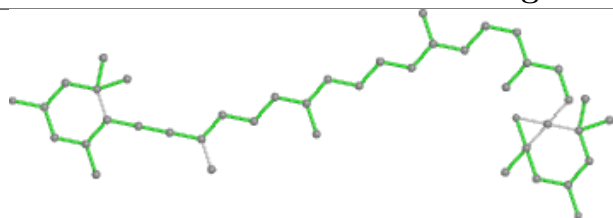


Torsions

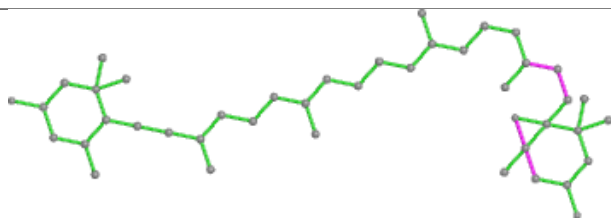


Rings

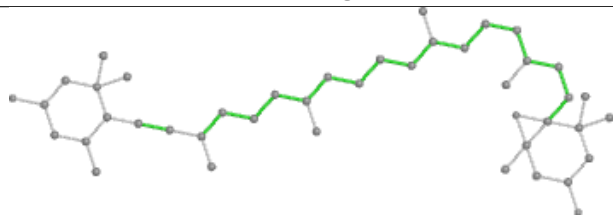
Ligand DD6 I 615



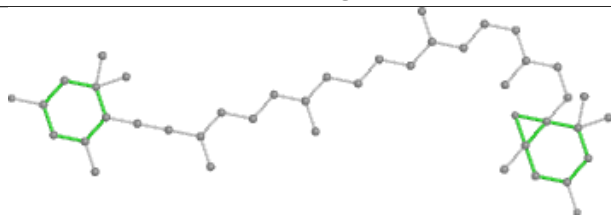
Bond lengths



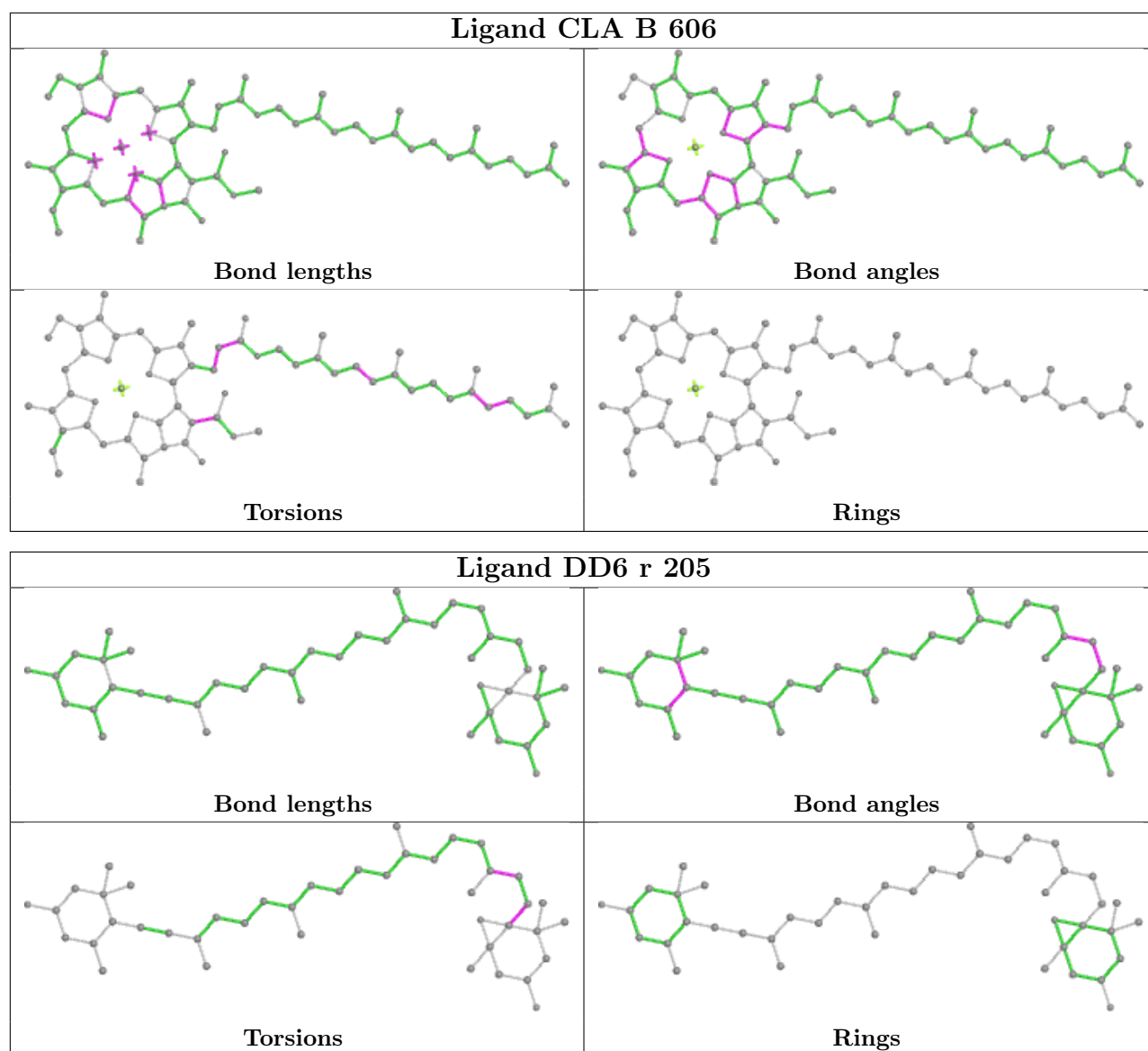
Bond angles

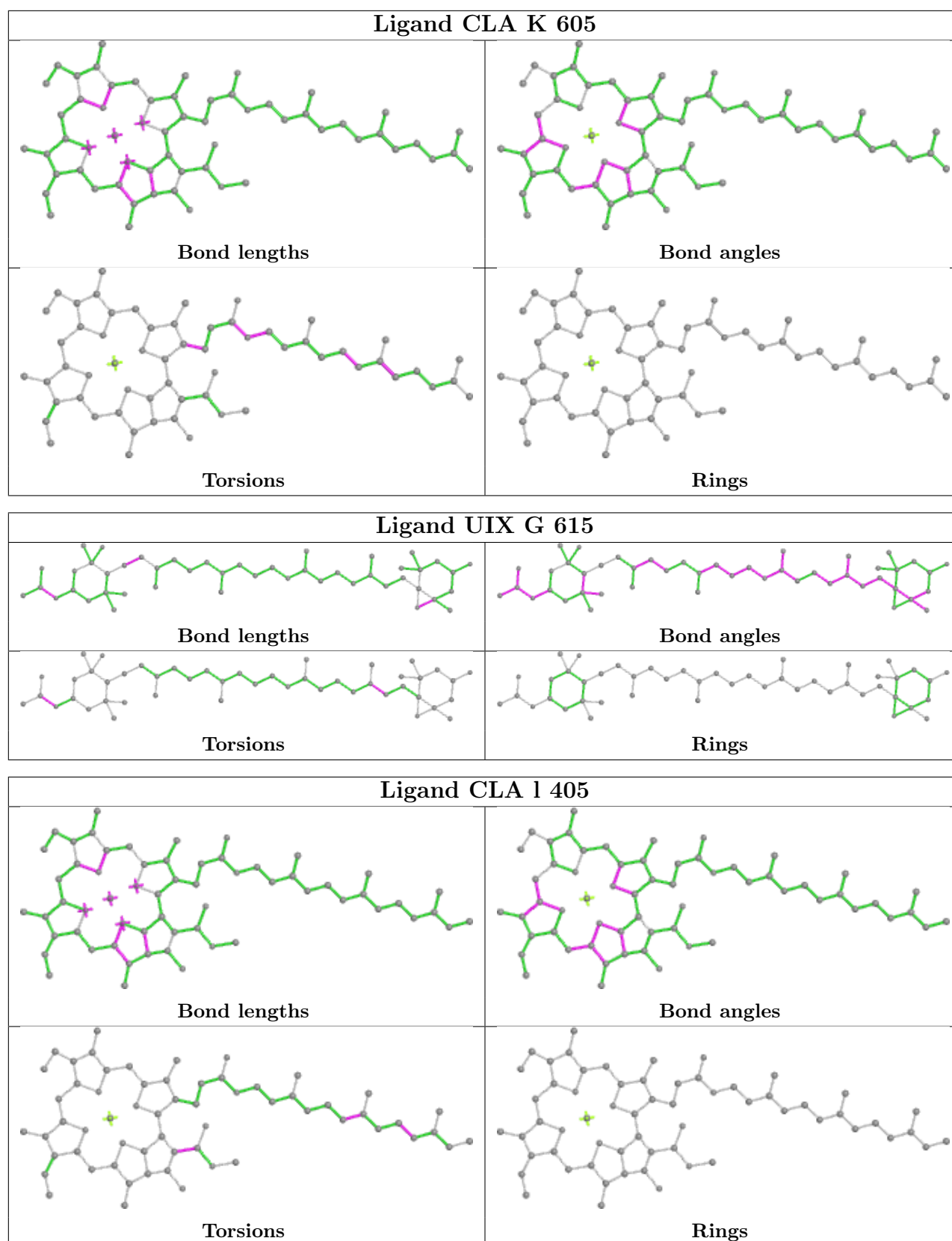


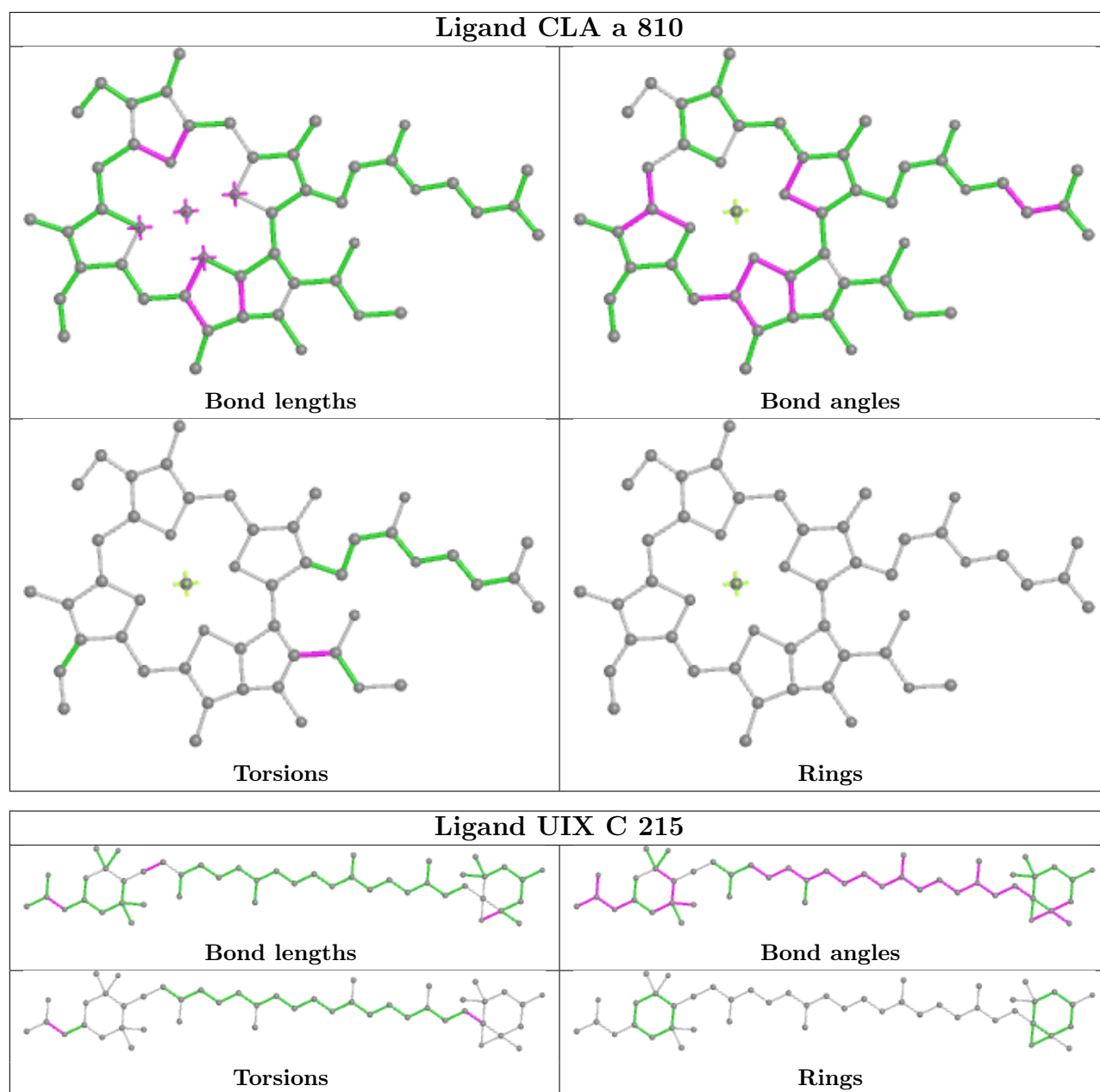
Torsions



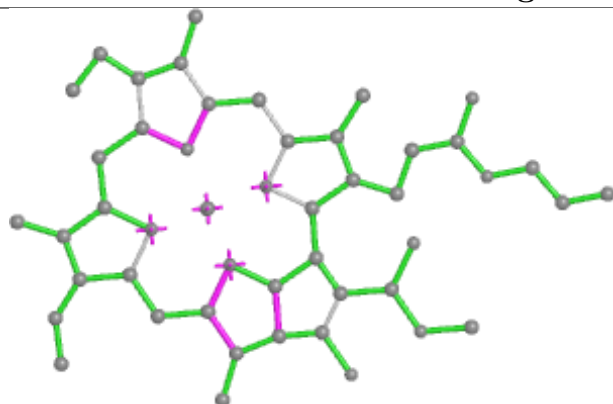
Rings



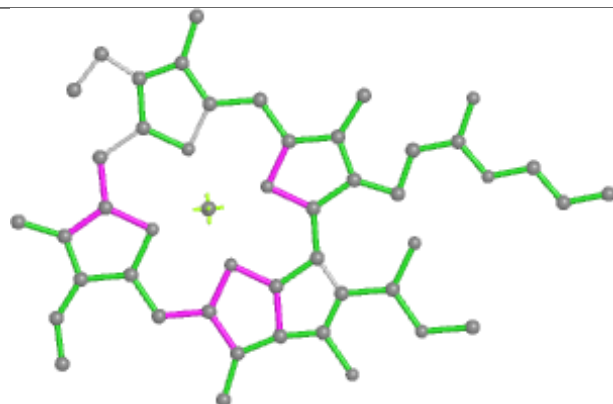




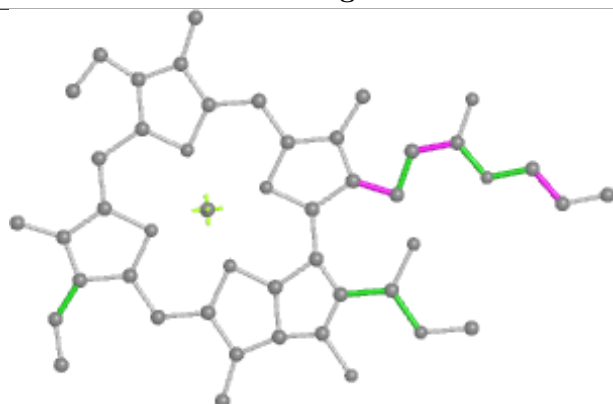
Ligand CLA b 714



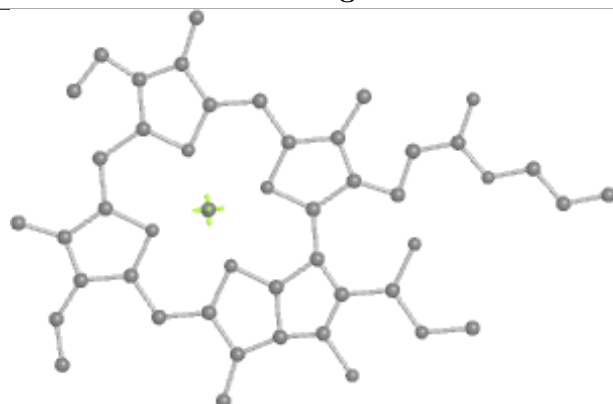
Bond lengths



Bond angles

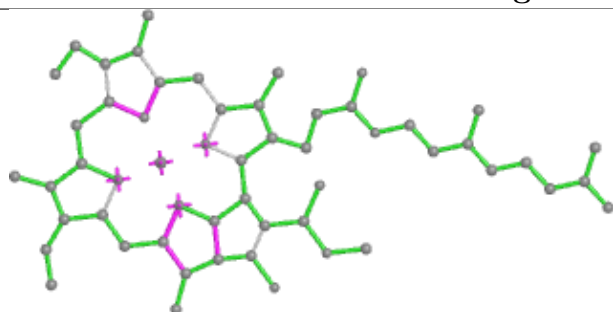


Torsions

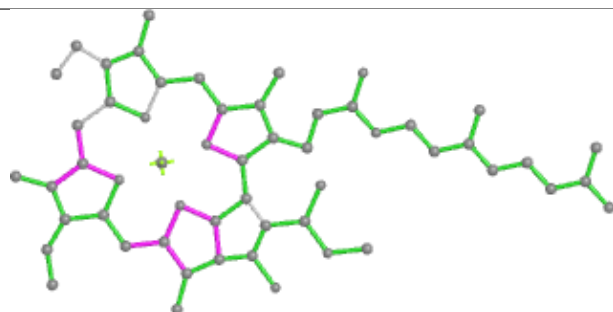


Rings

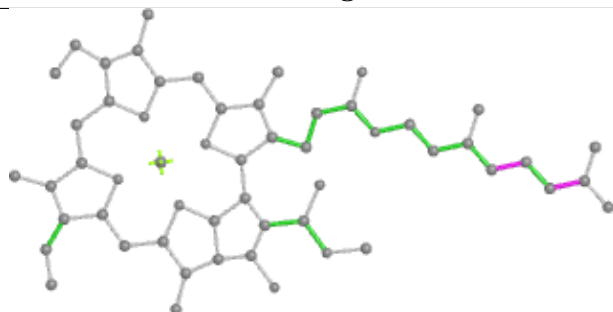
Ligand CLA D 603



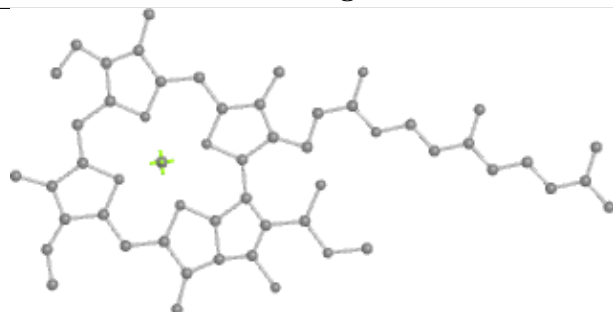
Bond lengths



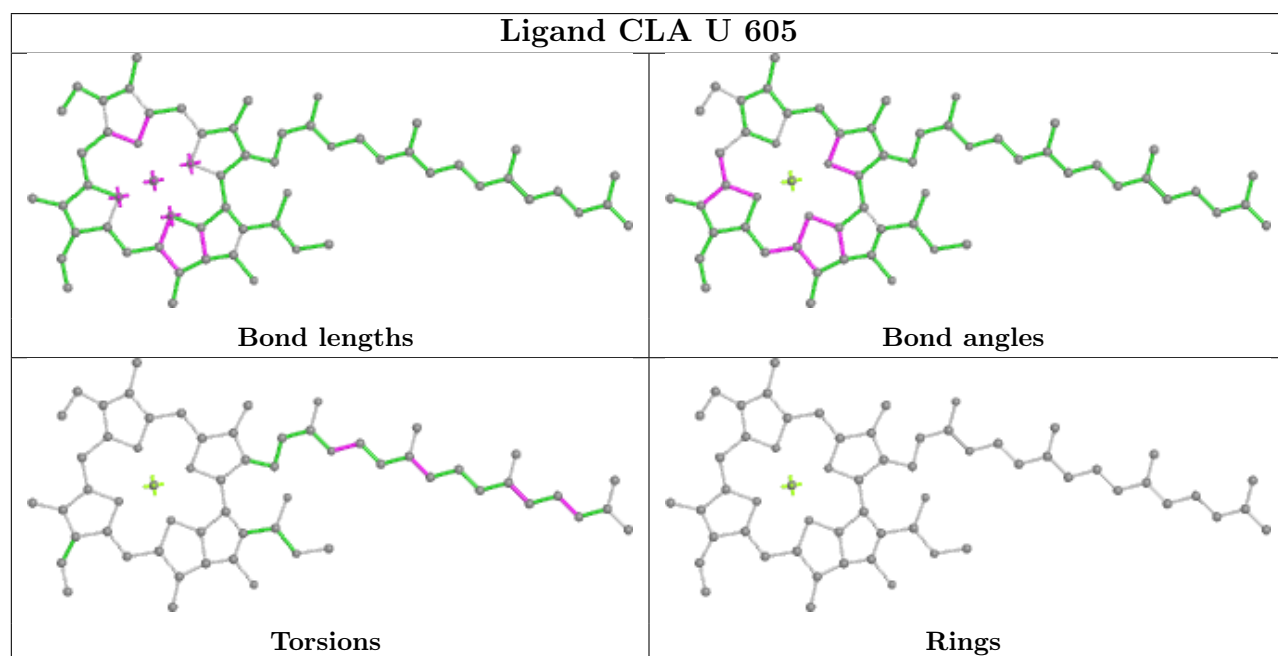
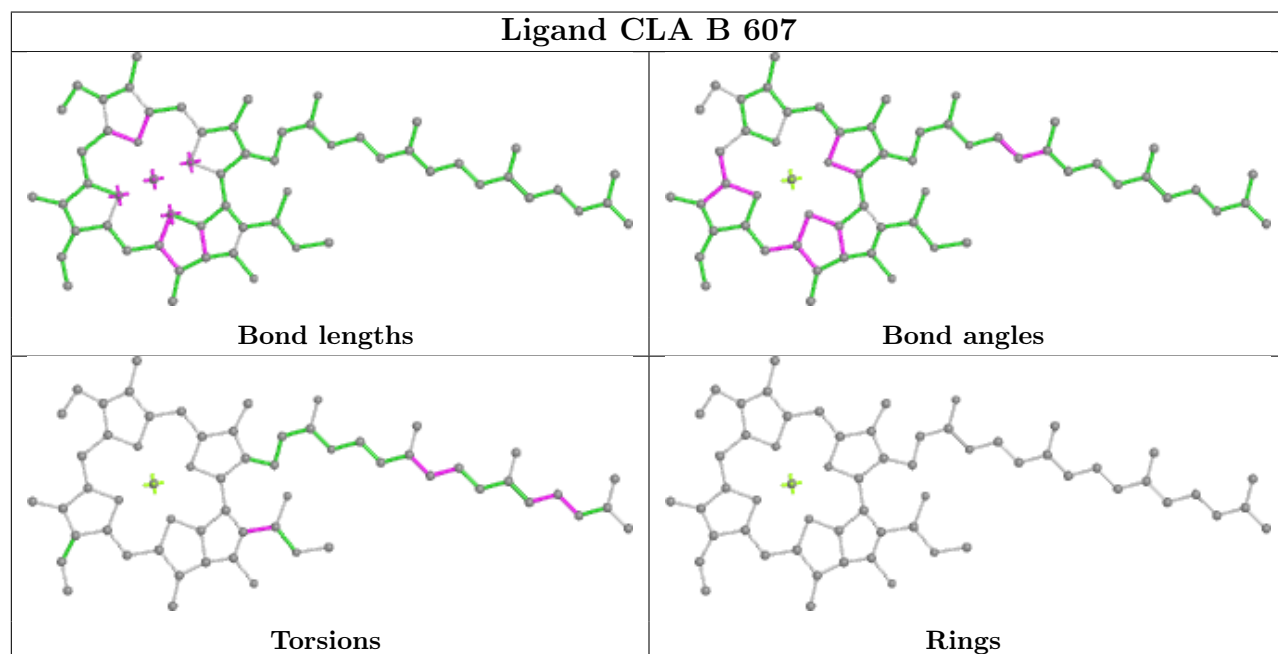
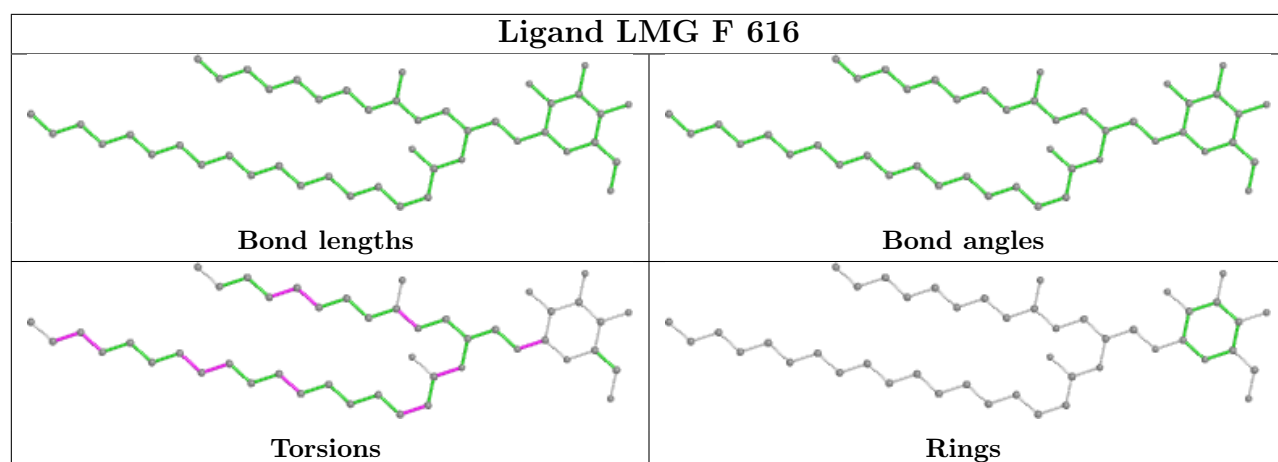
Bond angles



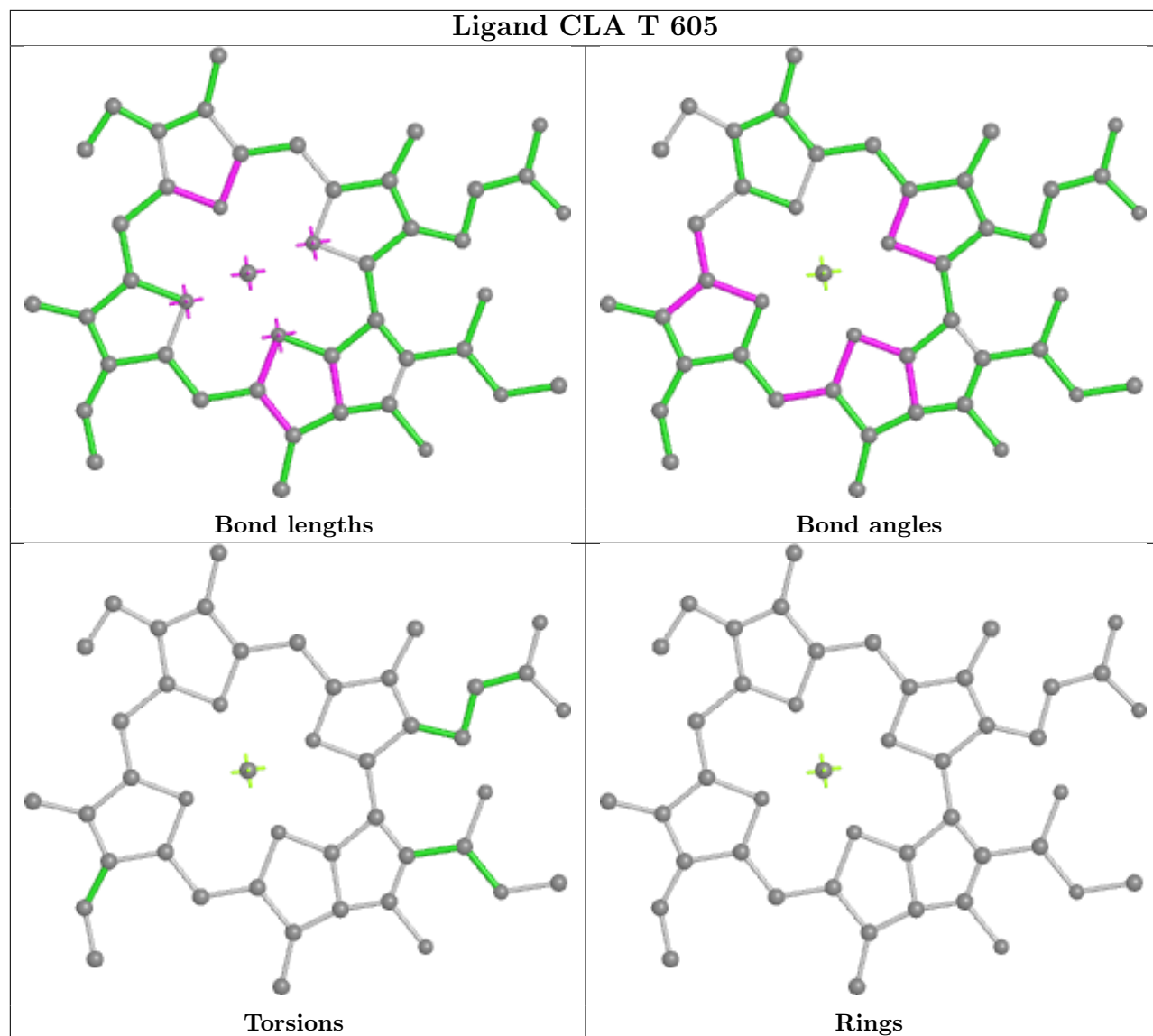
Torsions



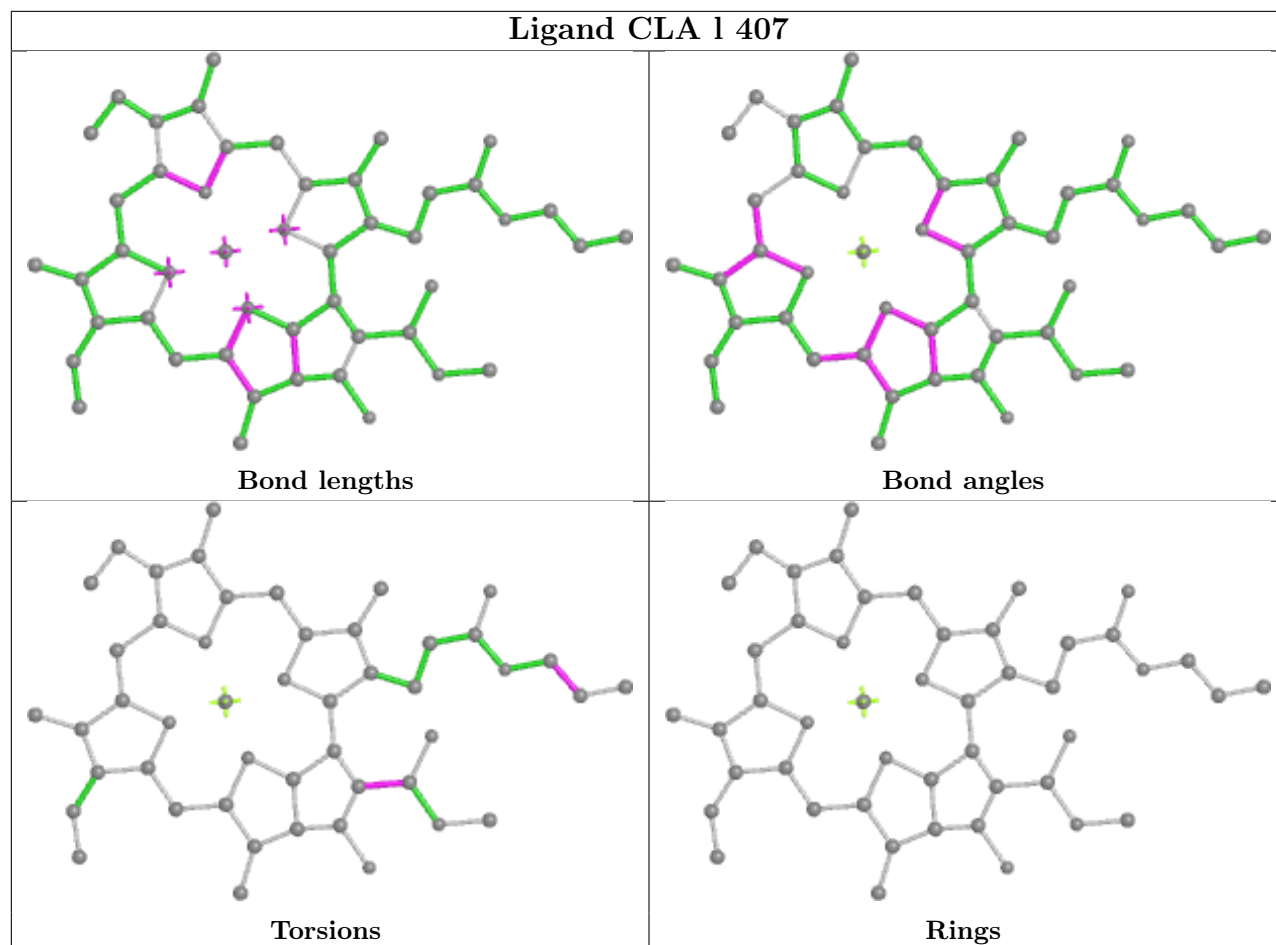
Rings



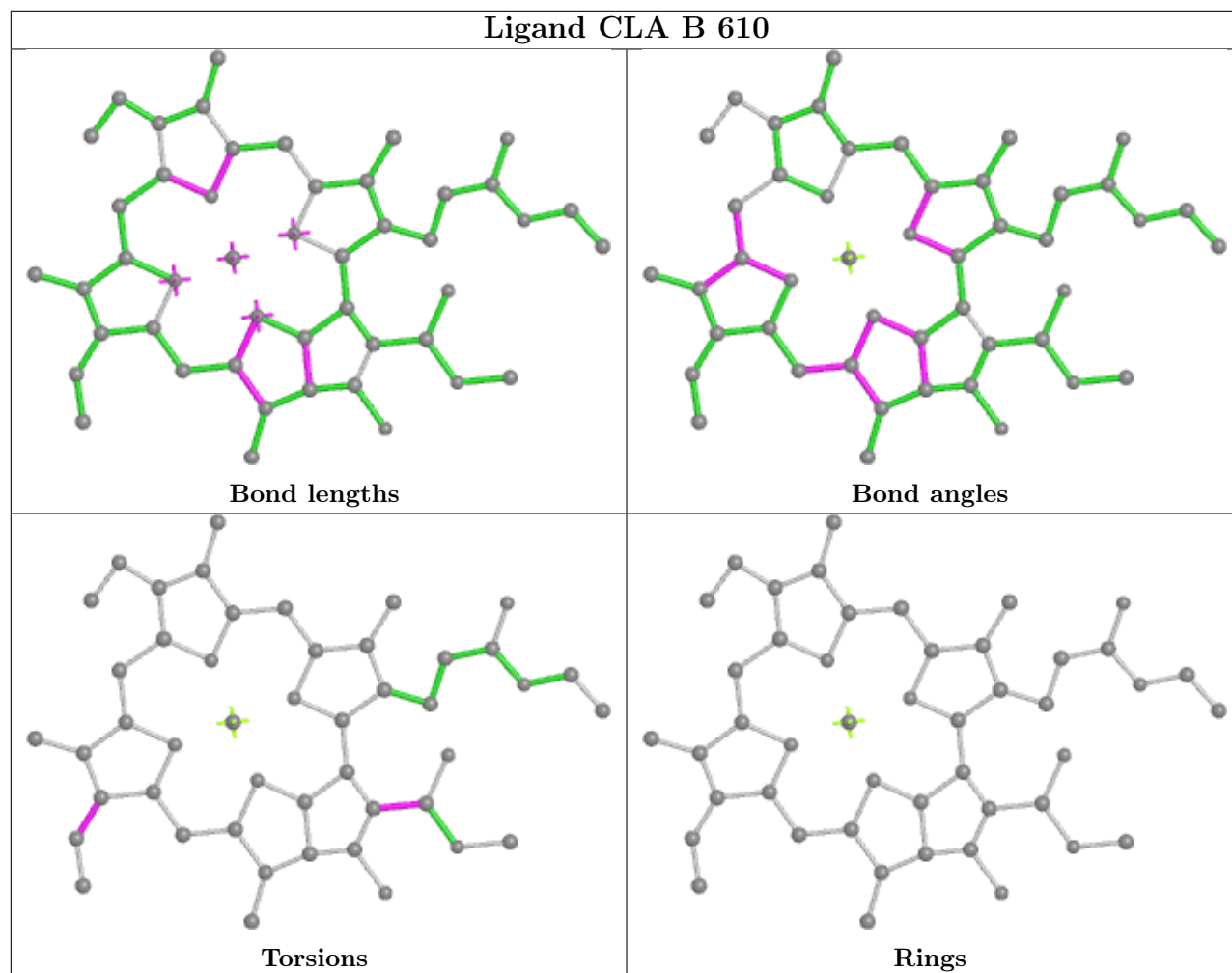
Ligand CLA T 605



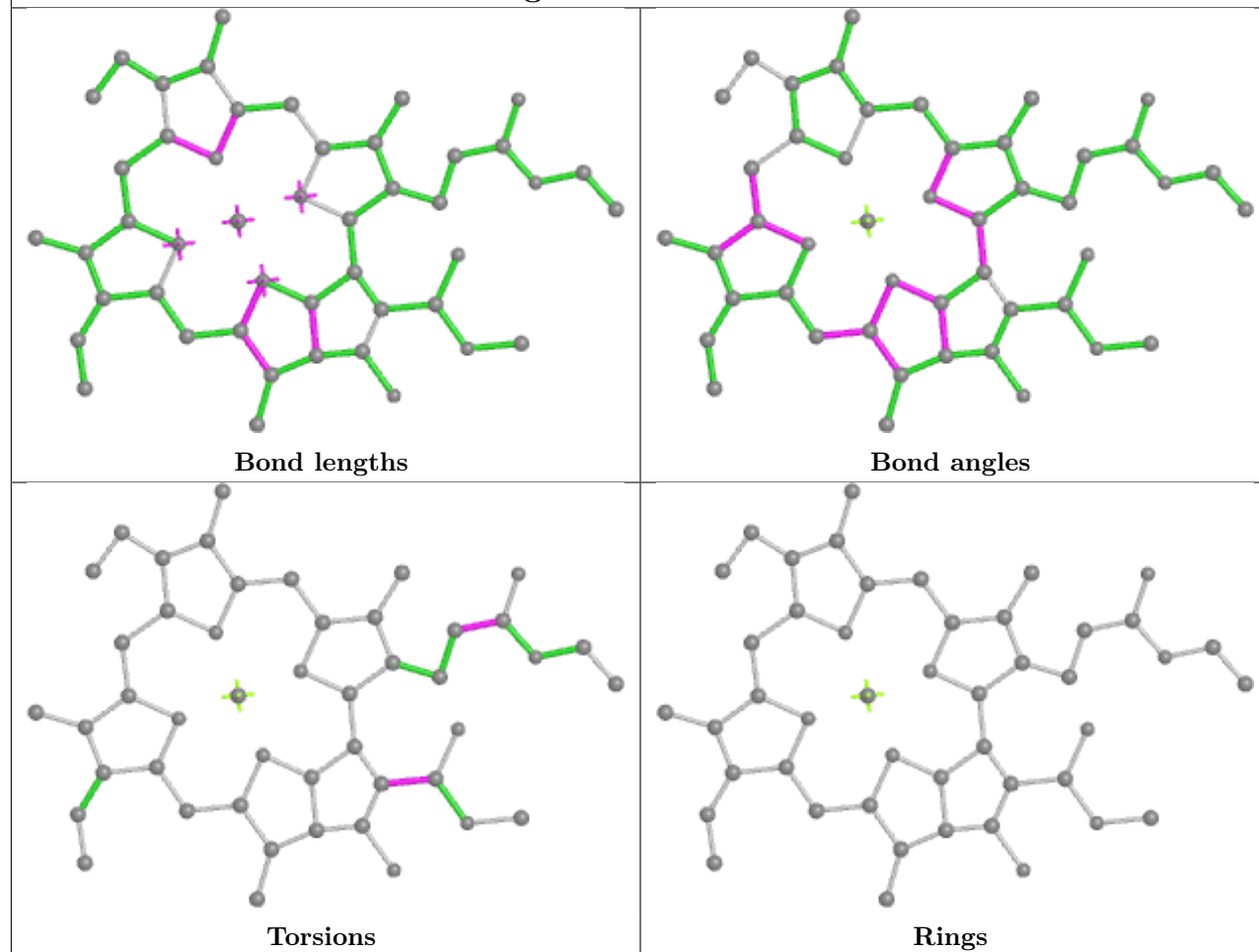
Ligand CLA 1 407



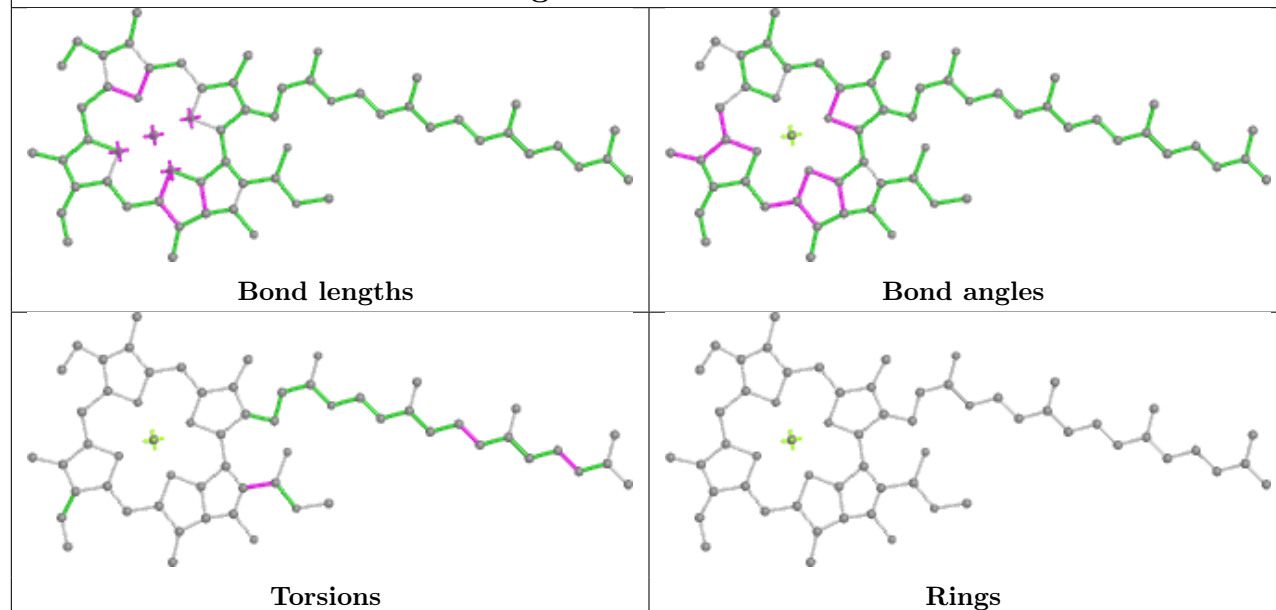
Ligand CLA B 610

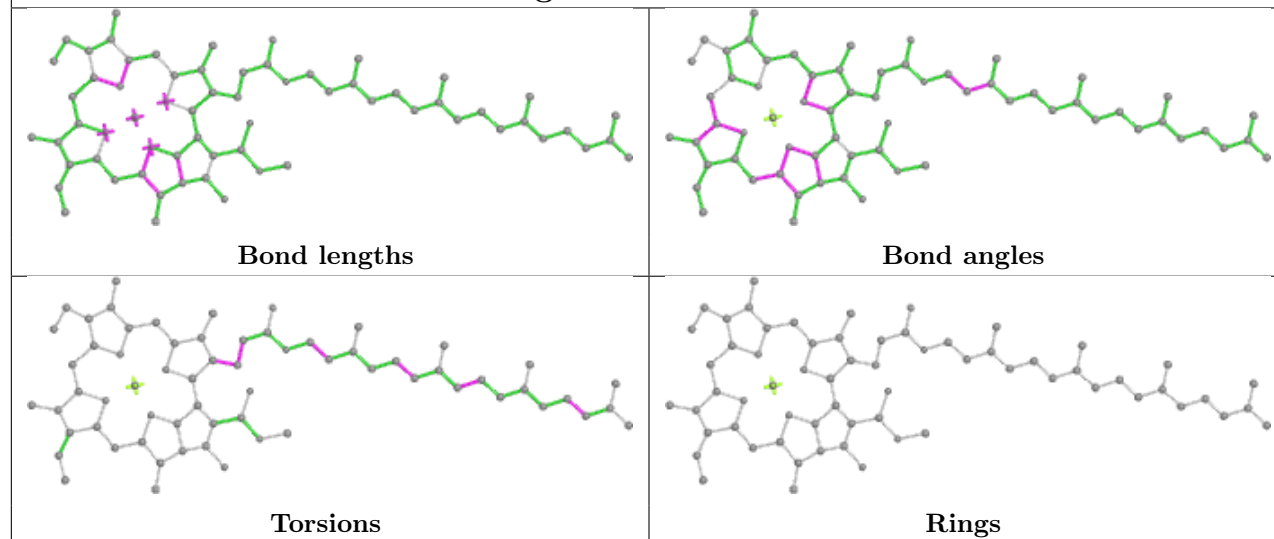
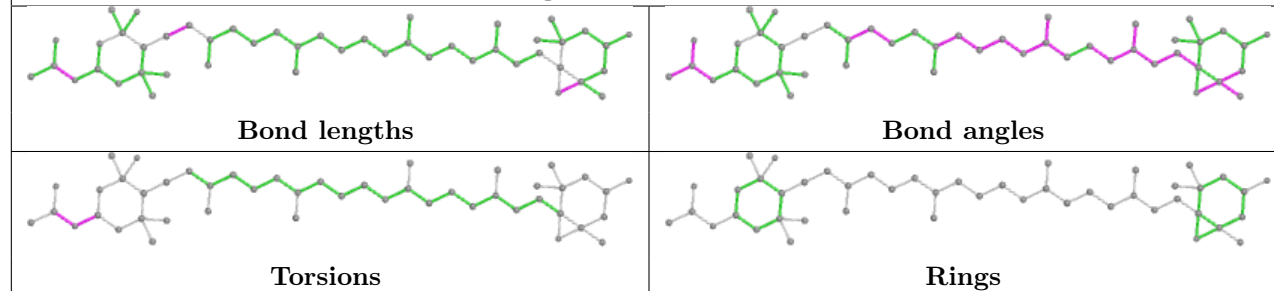
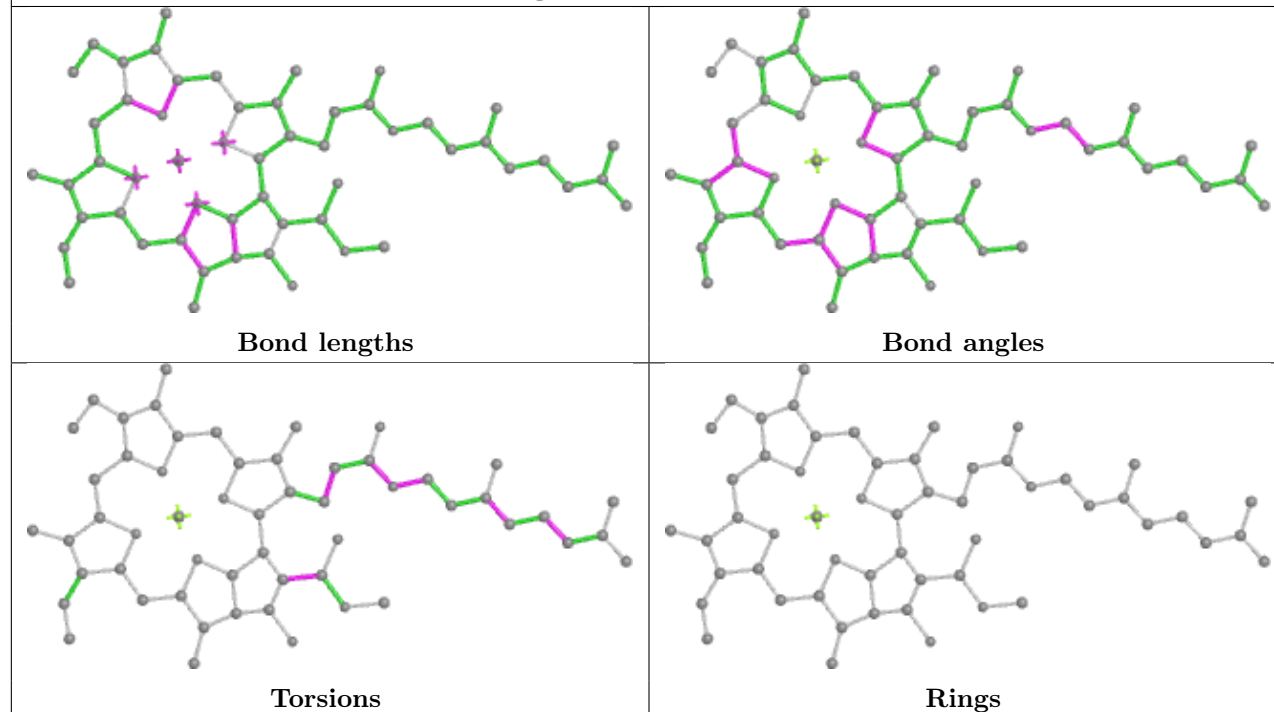


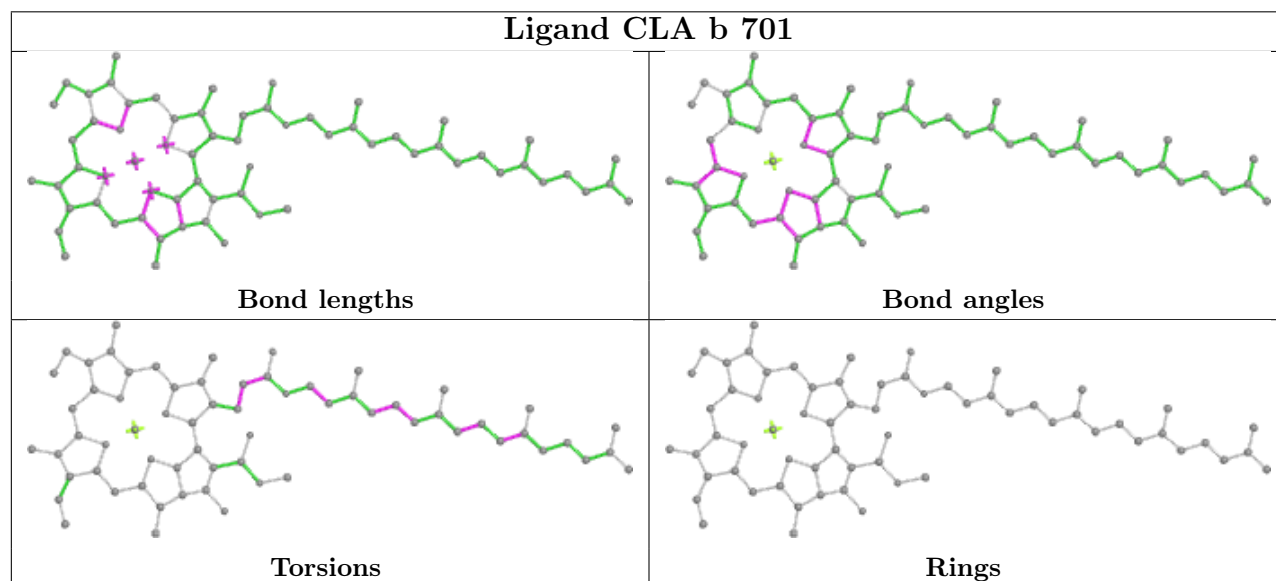
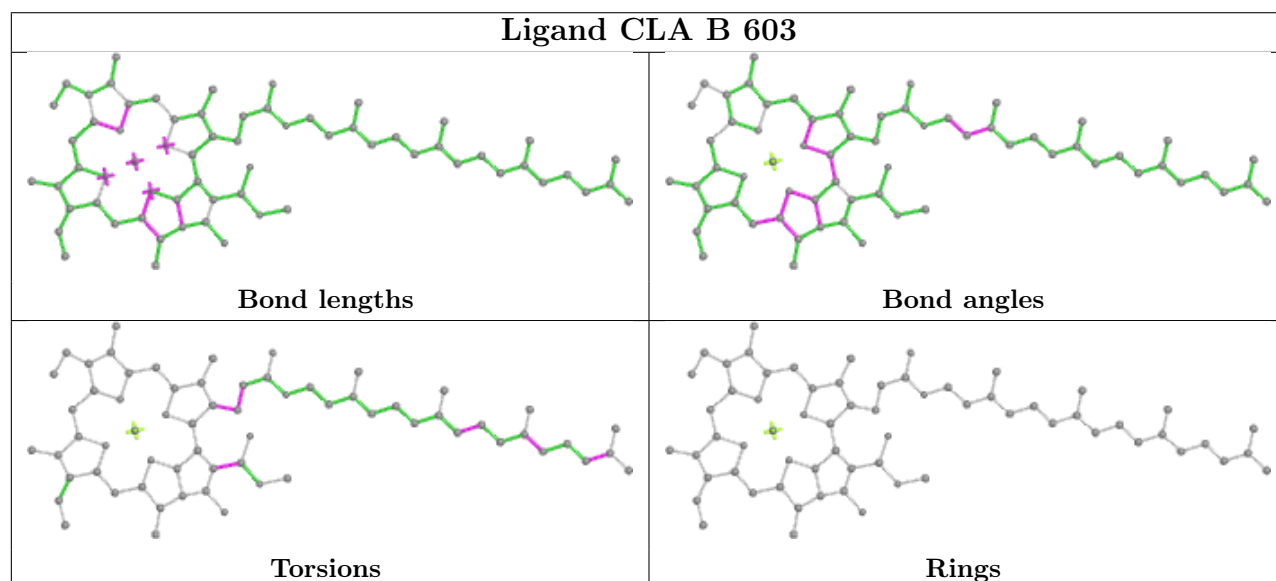
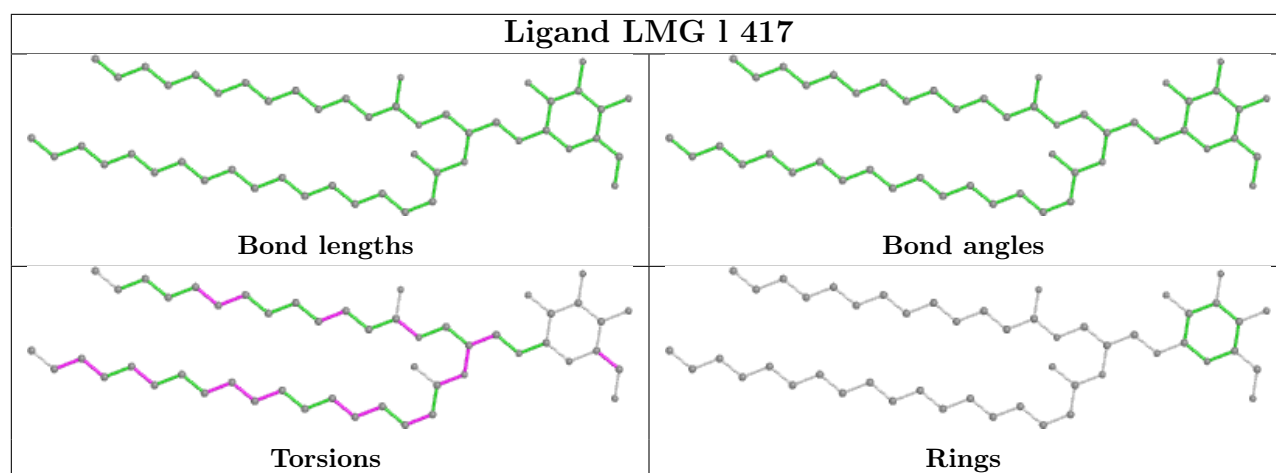
Ligand CLA D 610



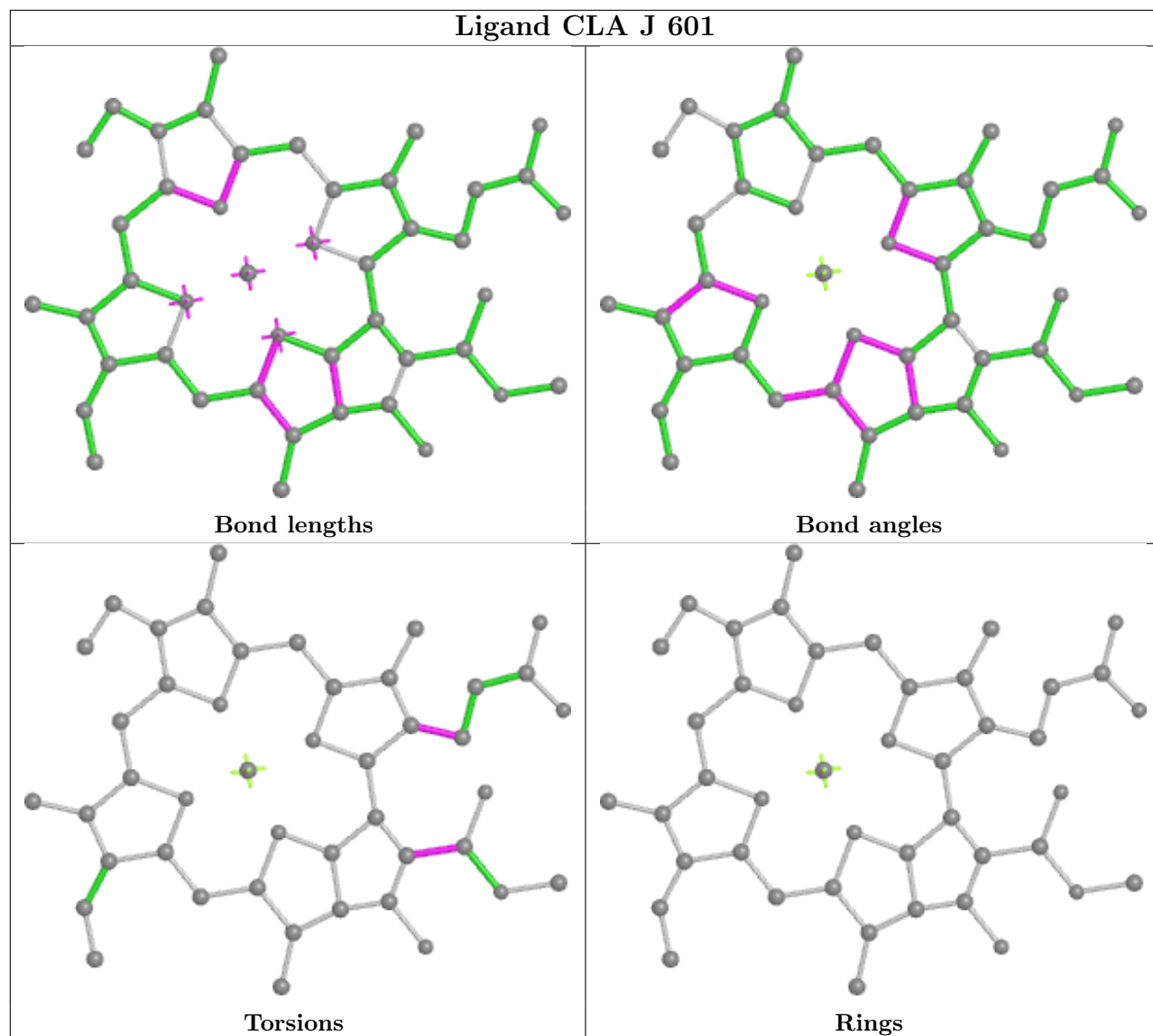
Ligand CLA H 303

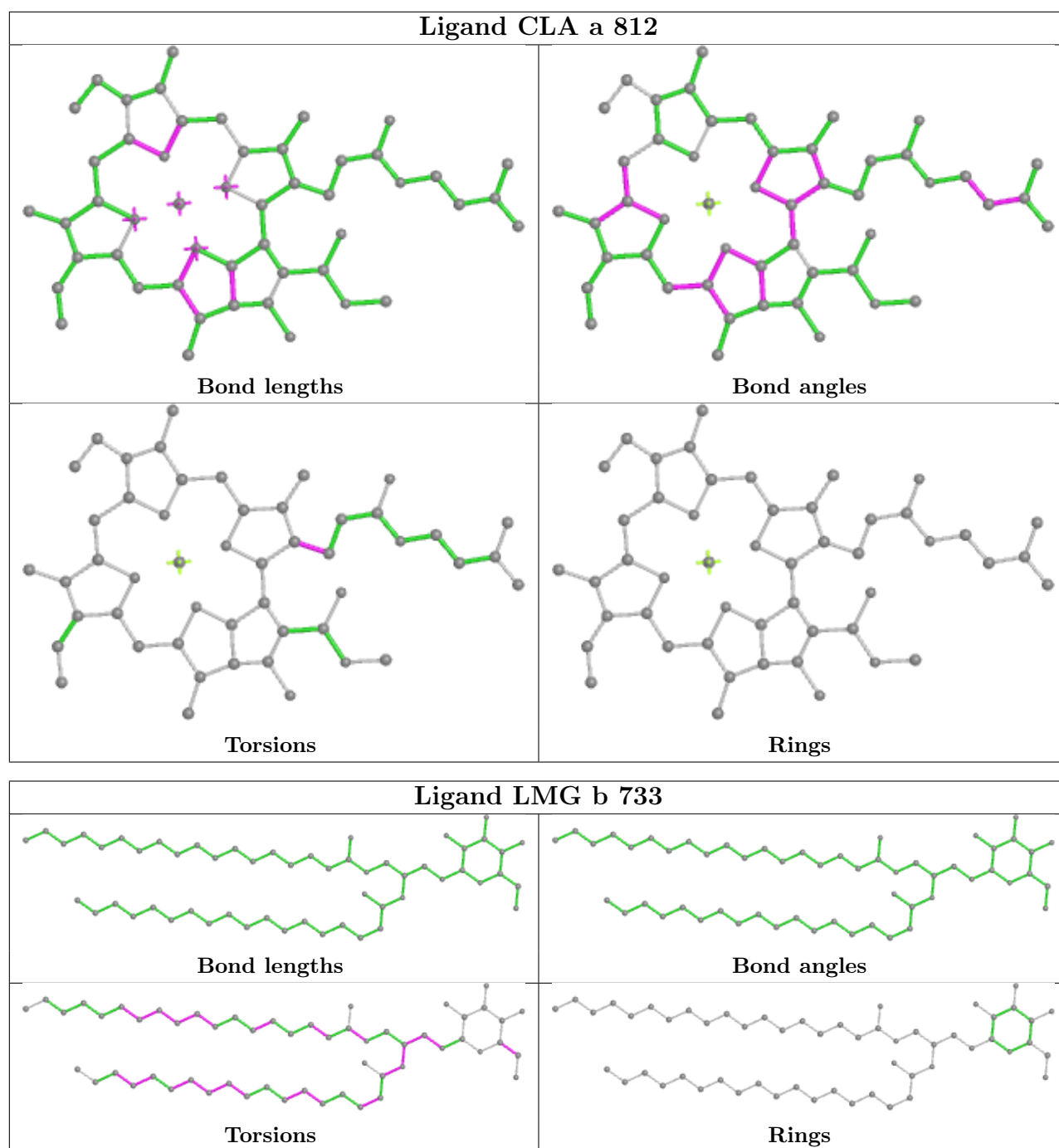


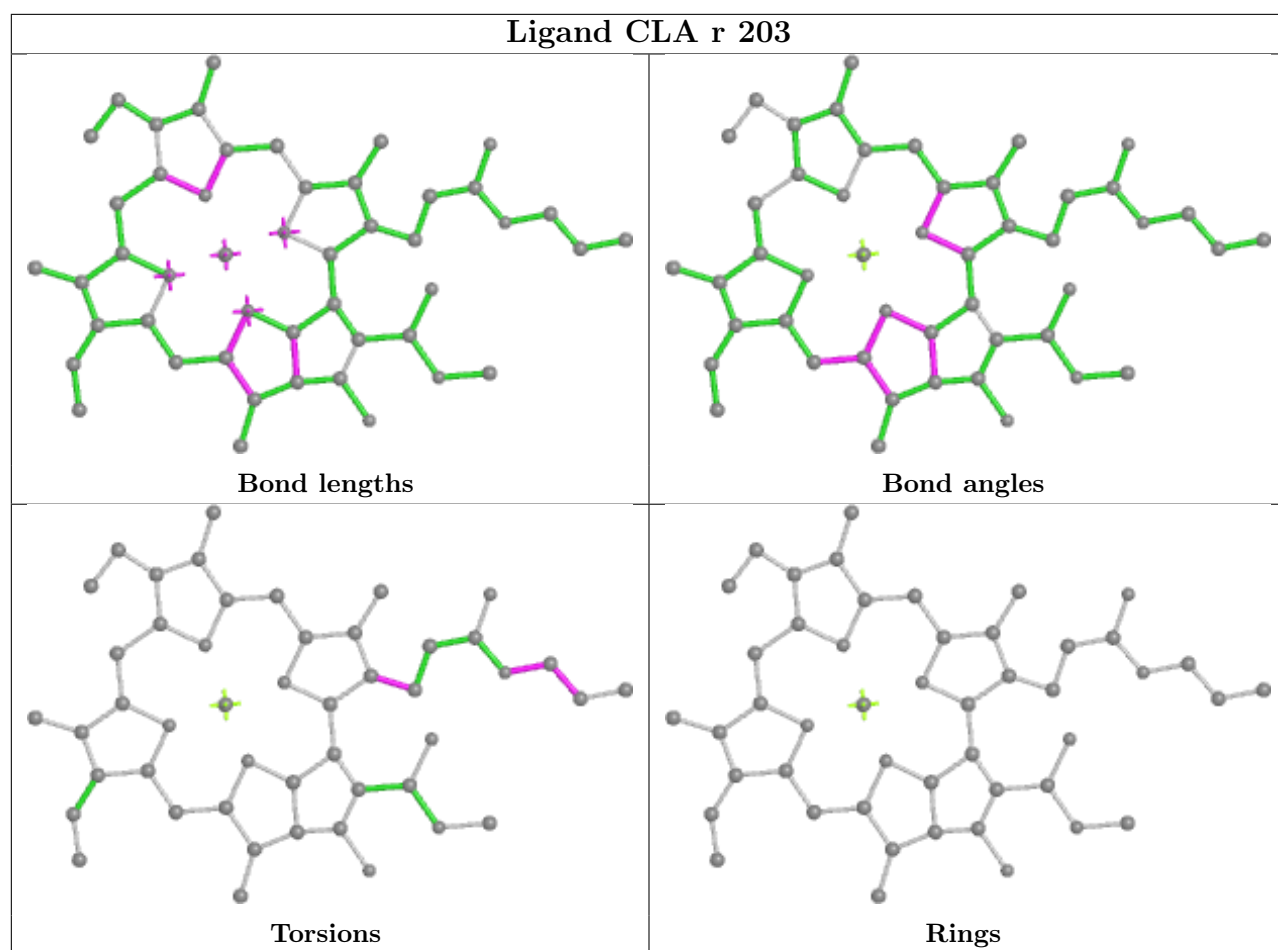
Ligand CLA b 713**Ligand UIX J 616****Ligand CLA K 602**



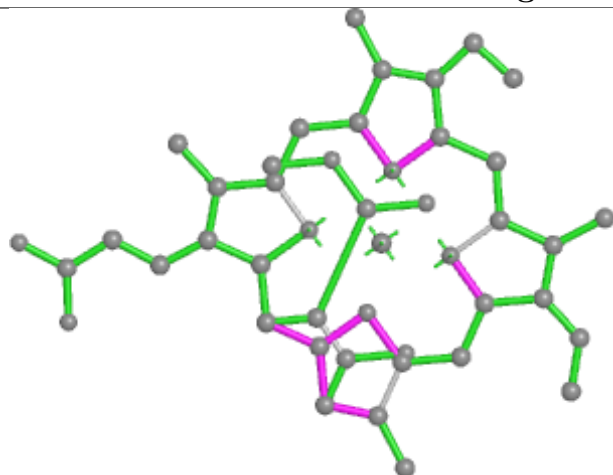
Ligand CLA J 601



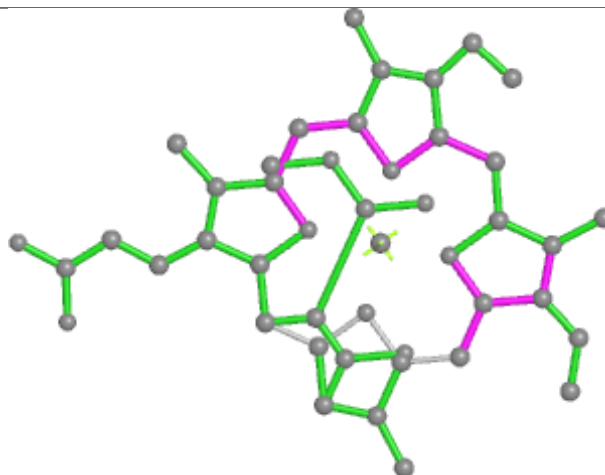




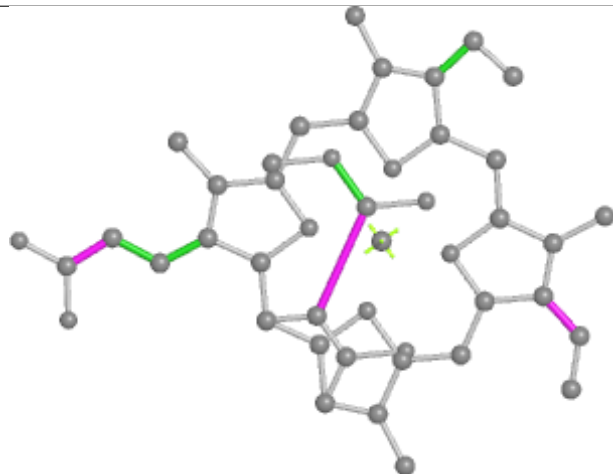
Ligand KC2 E 610



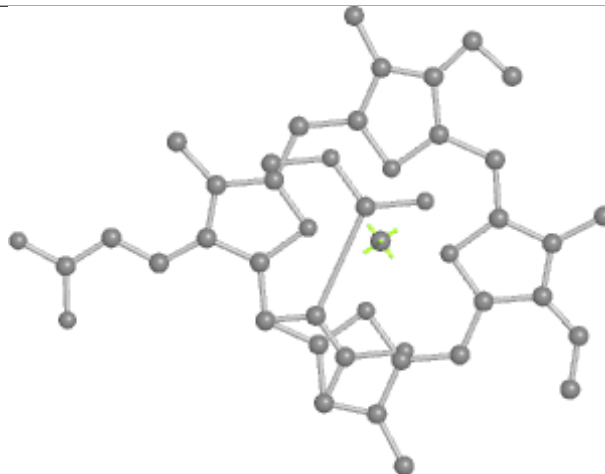
Bond lengths



Bond angles

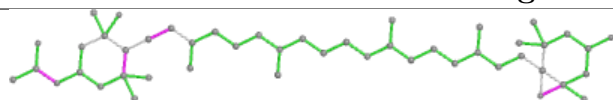


Torsions

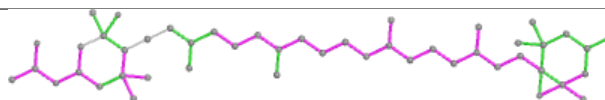


Rings

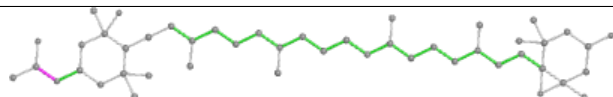
Ligand UIX B 611



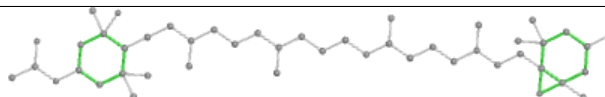
Bond lengths



Bond angles

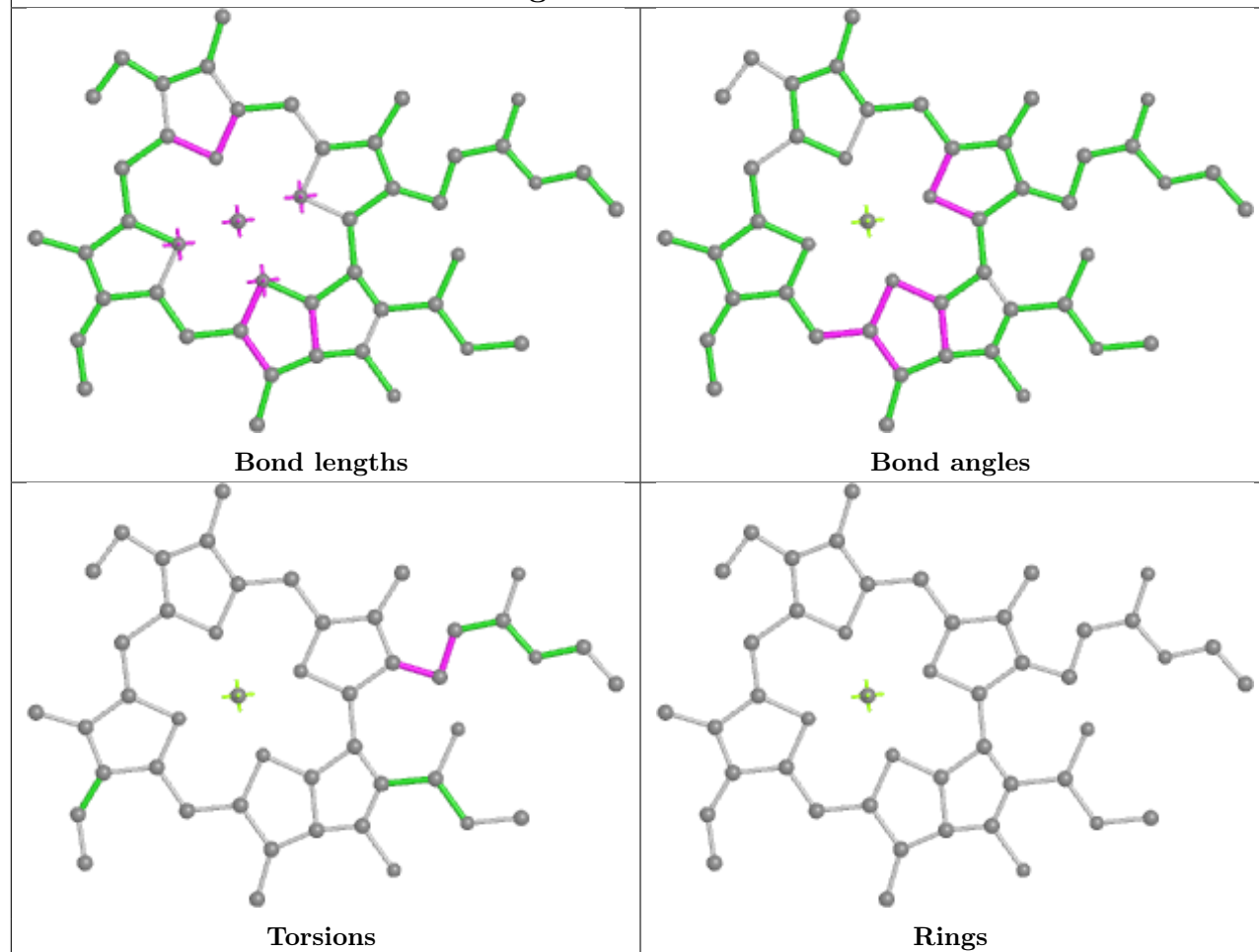


Torsions

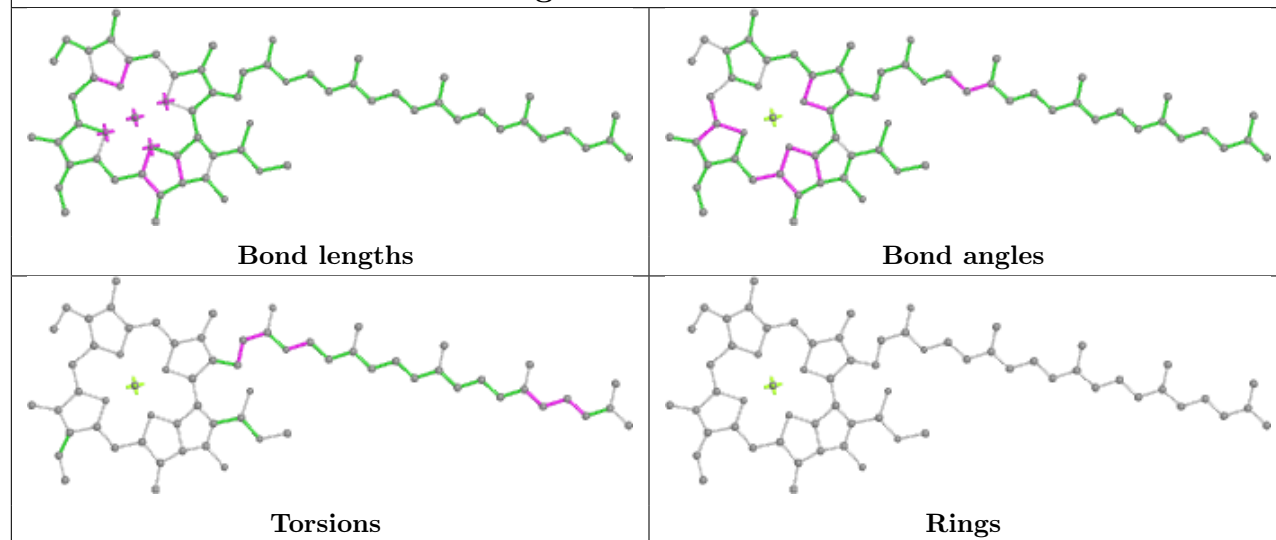


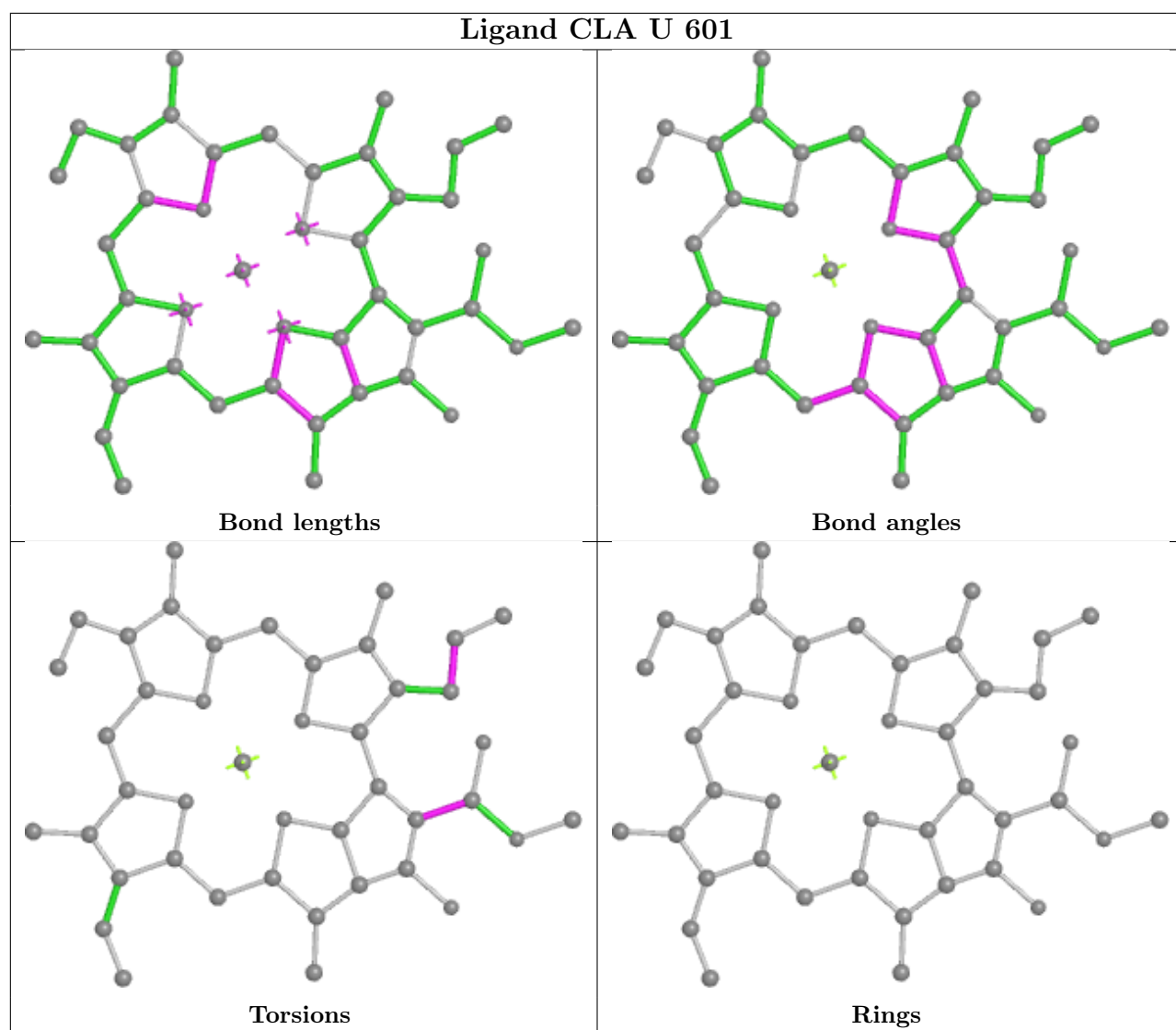
Rings

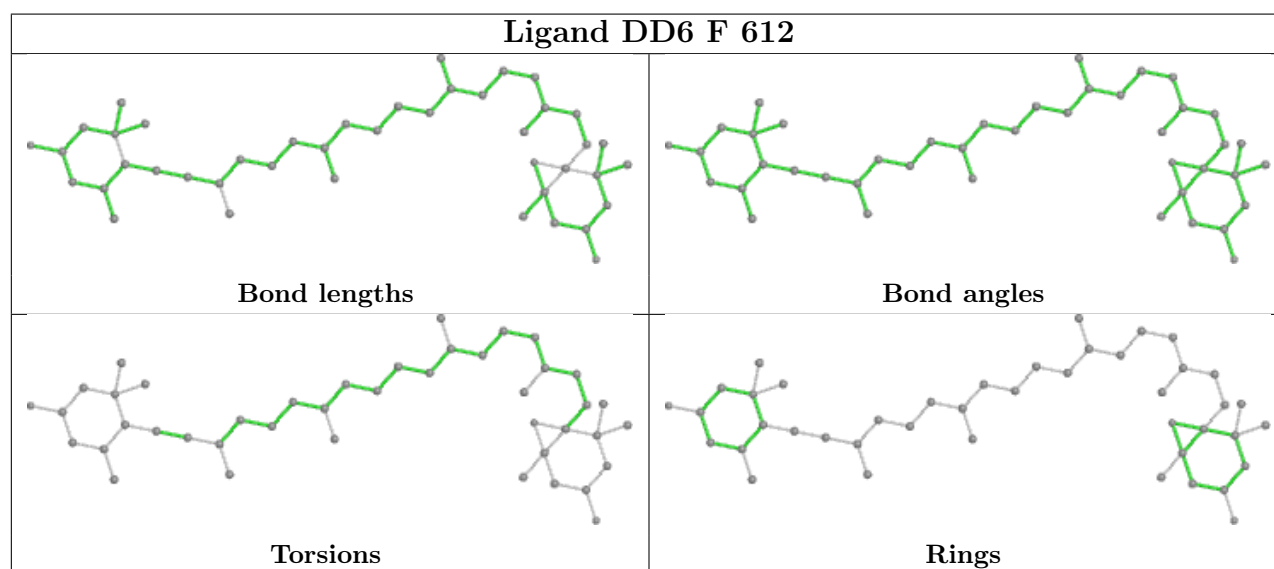
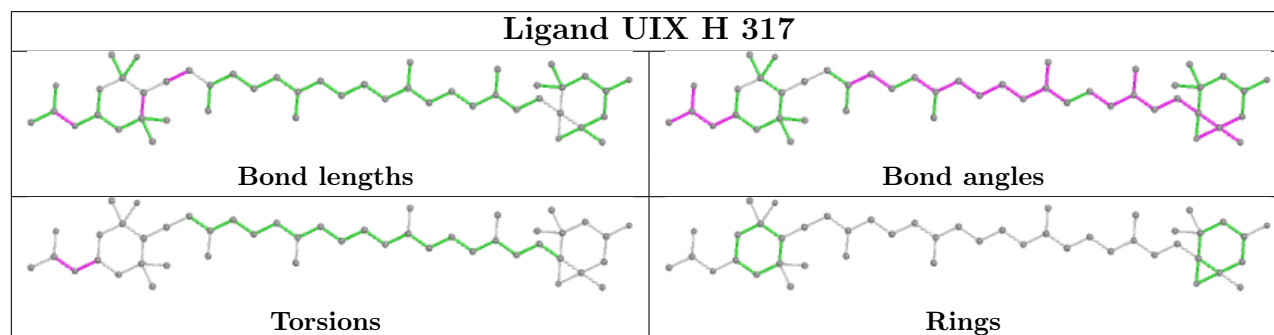
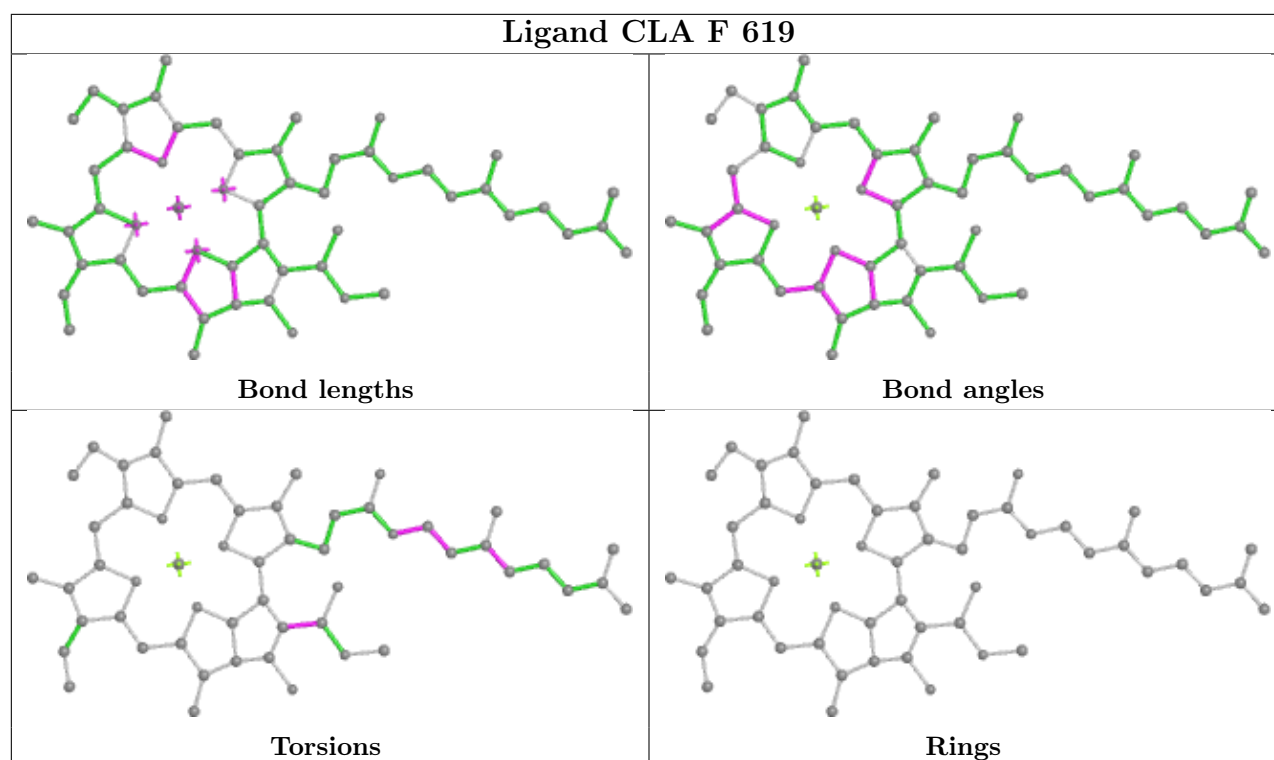
Ligand CLA a 809

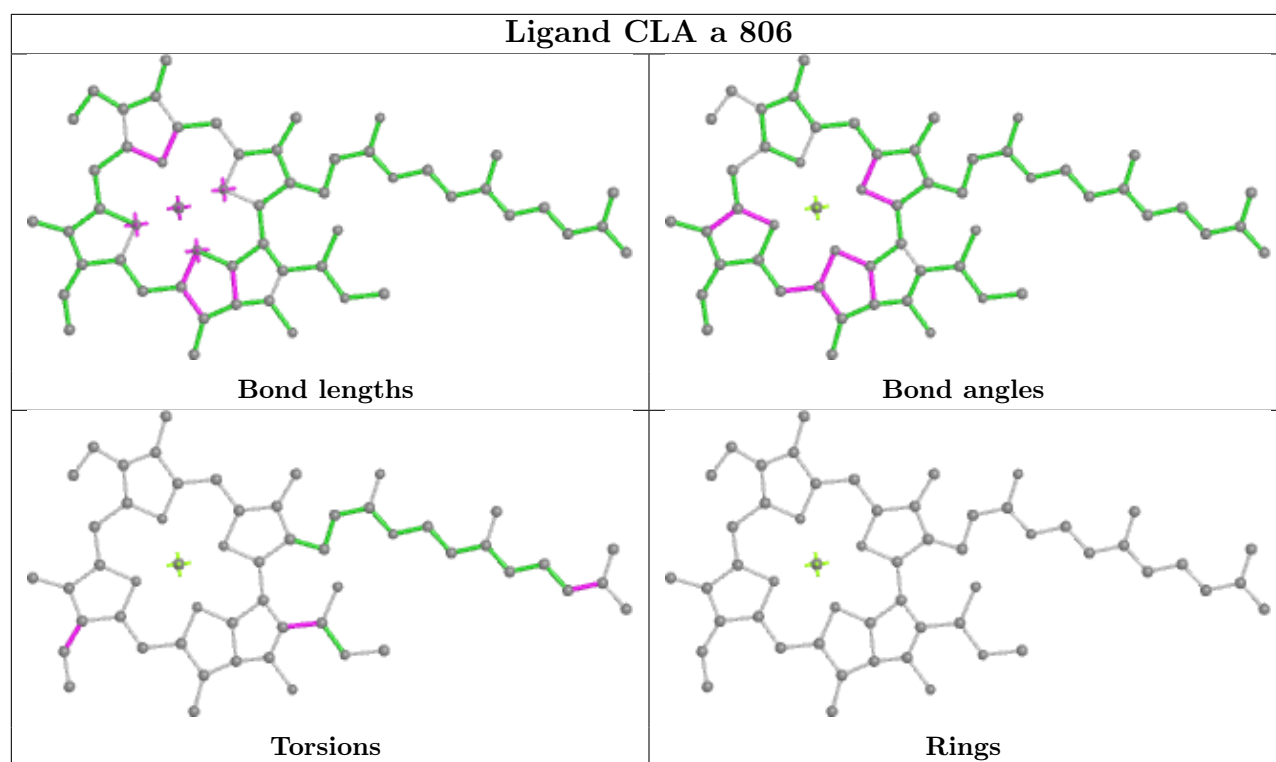


Ligand CLA b 728

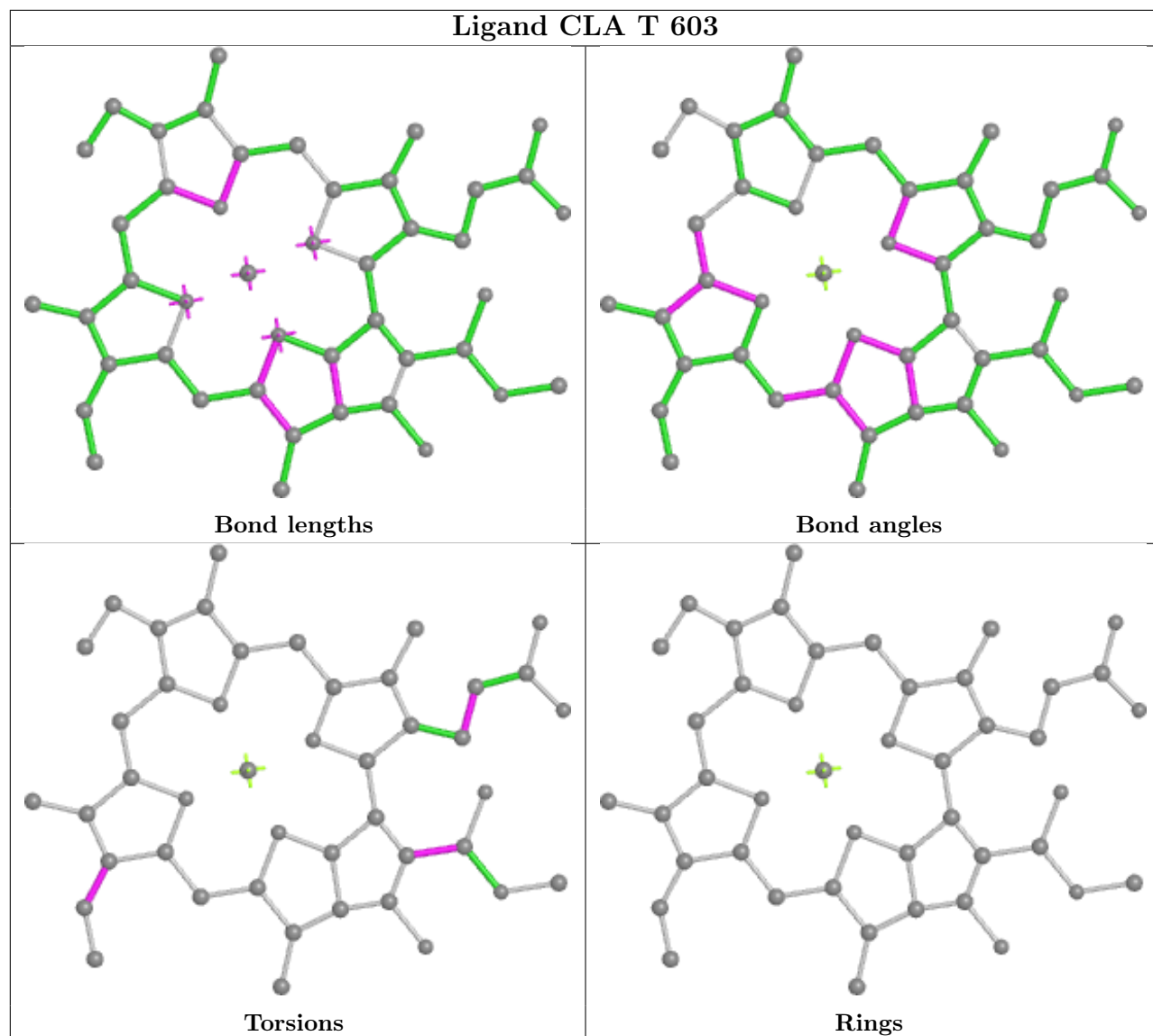


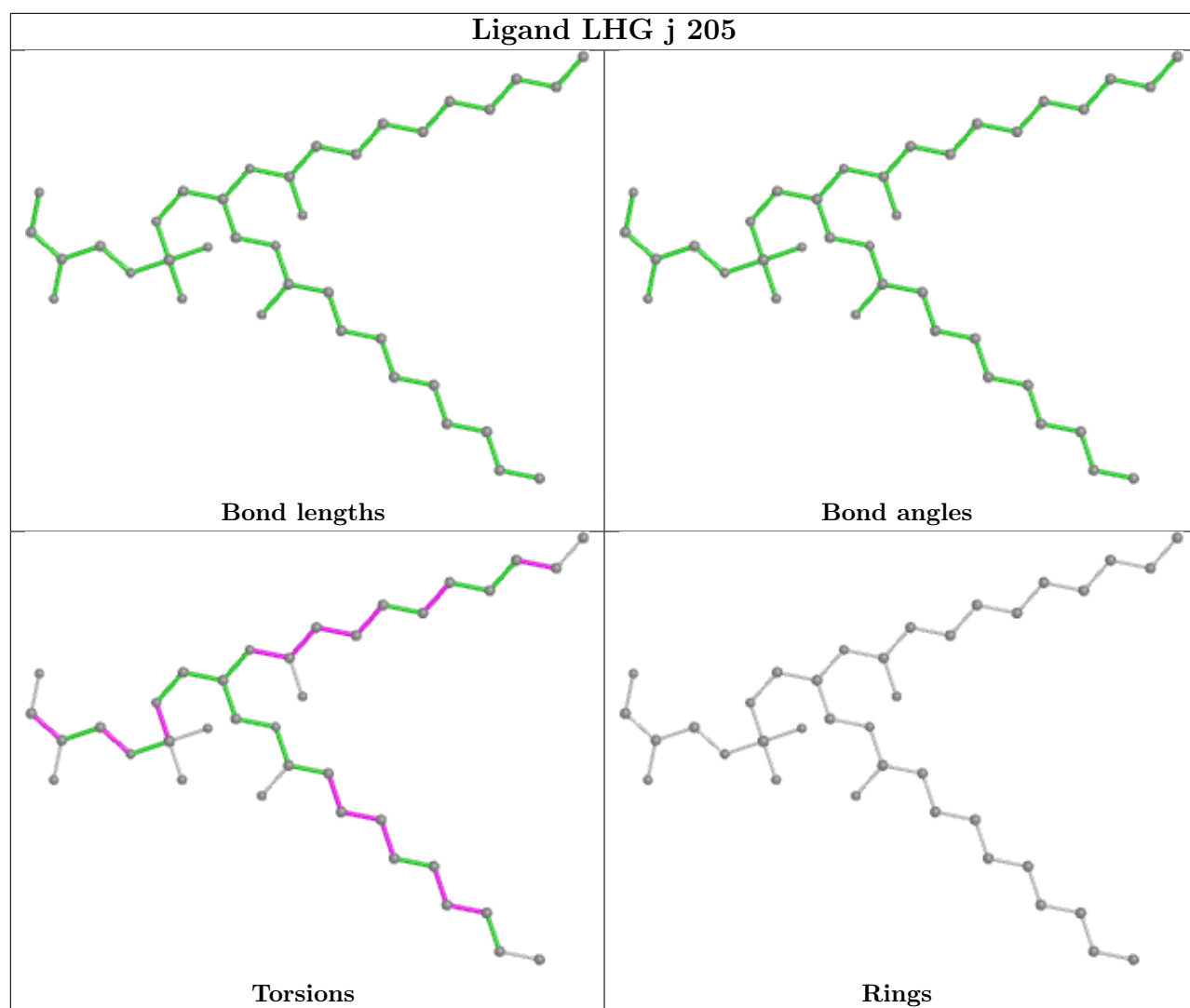


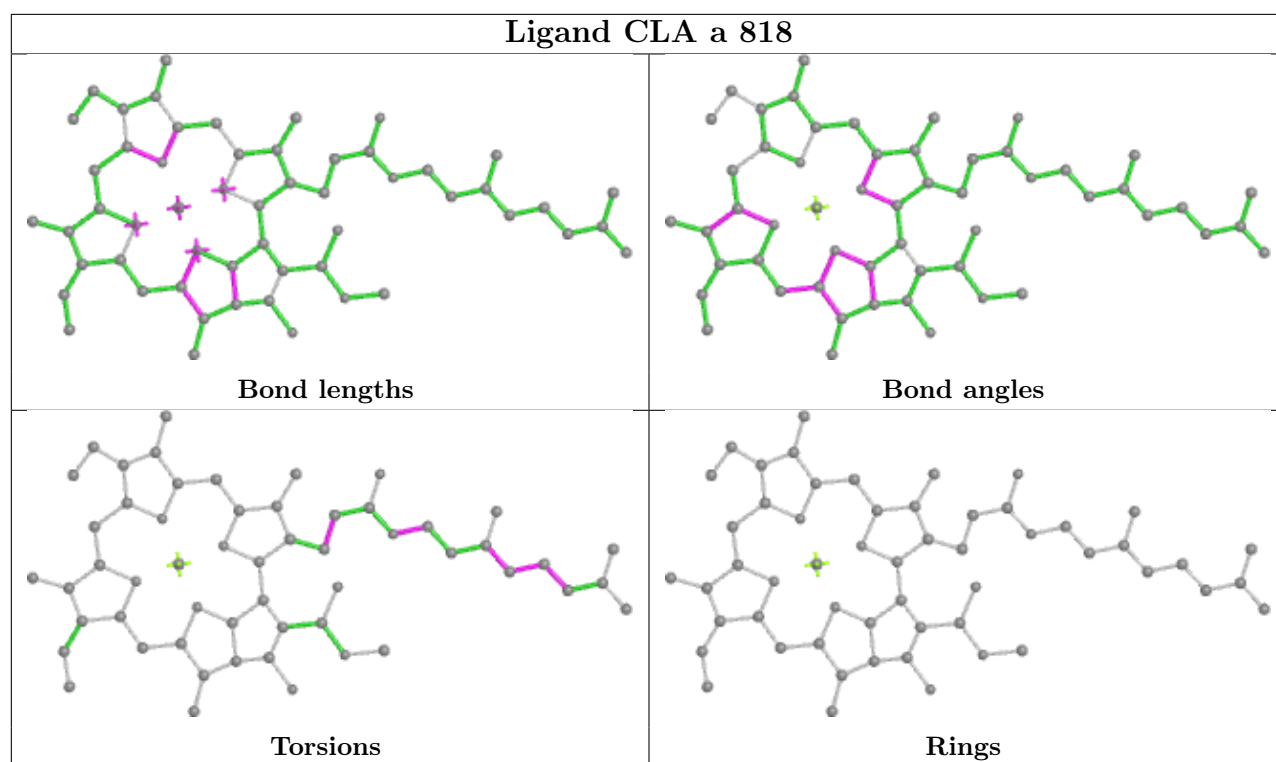




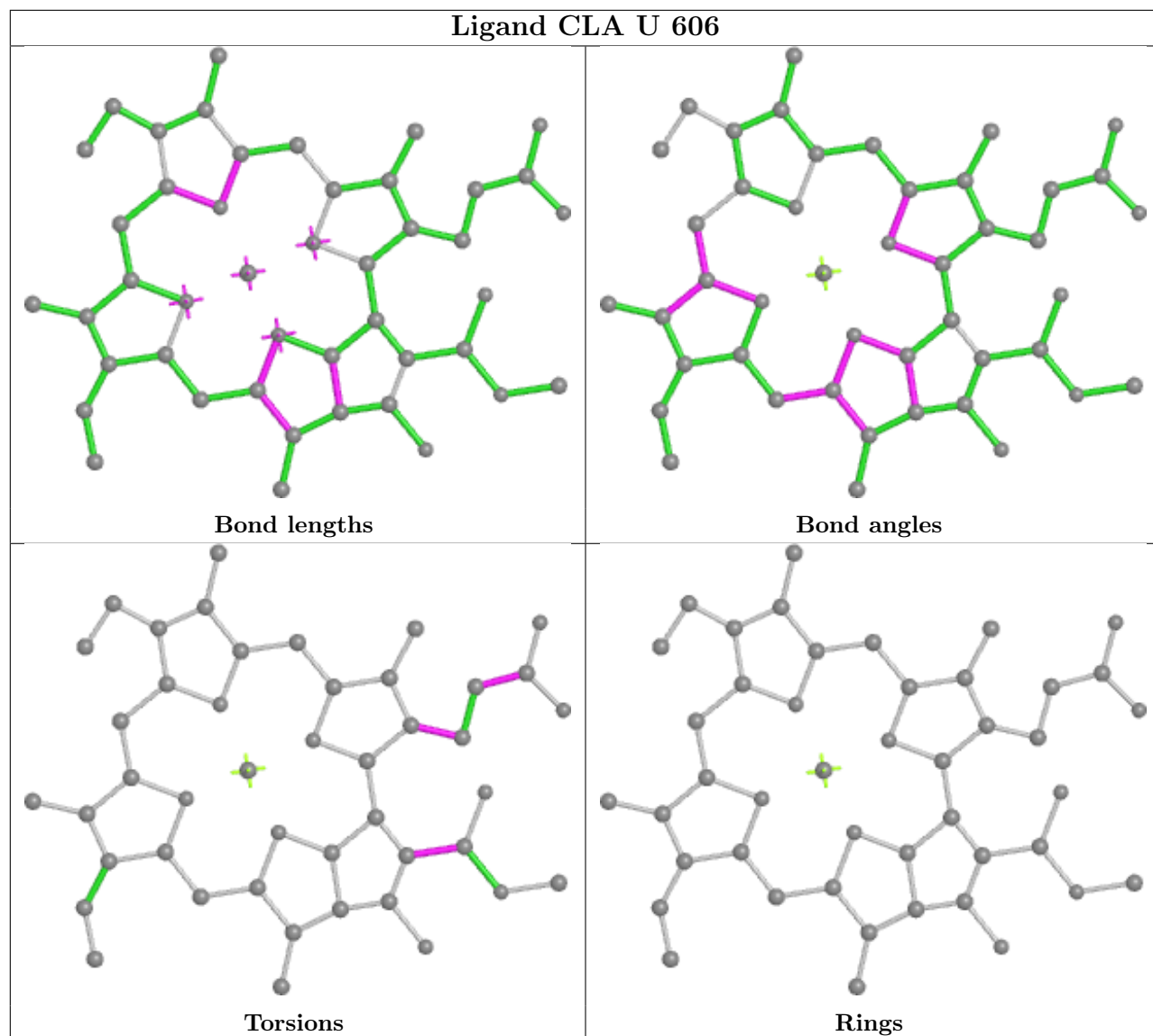
Ligand CLA T 603

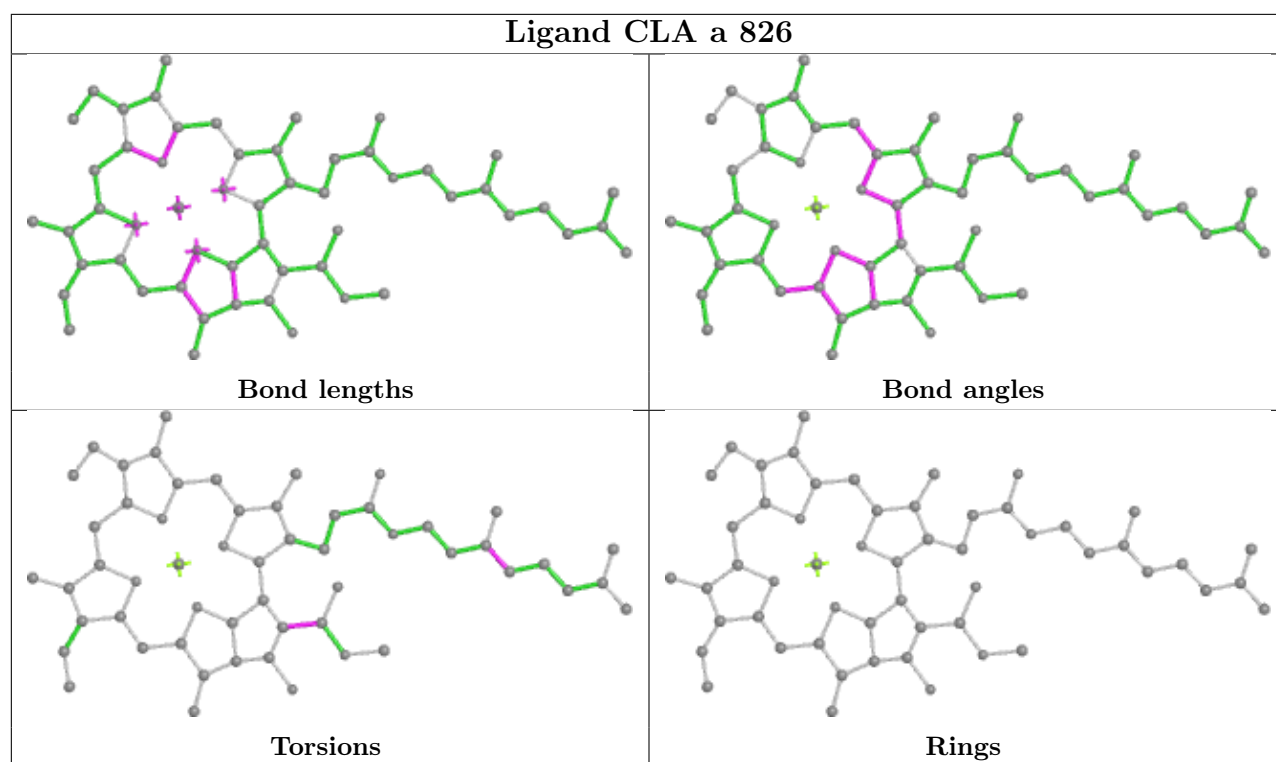




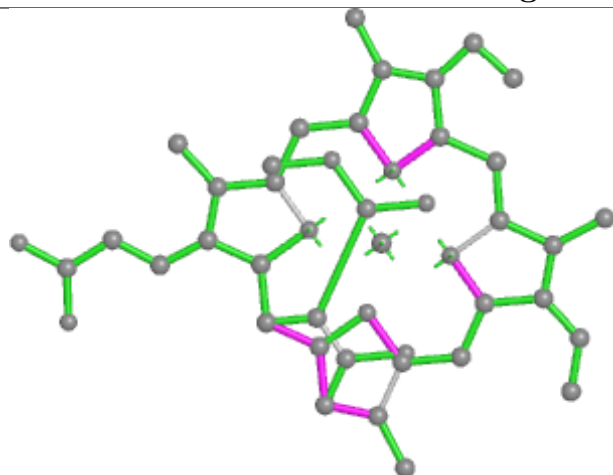


Ligand CLA U 606

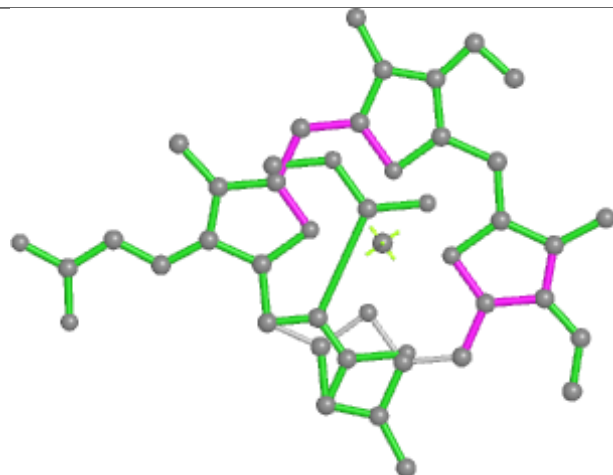




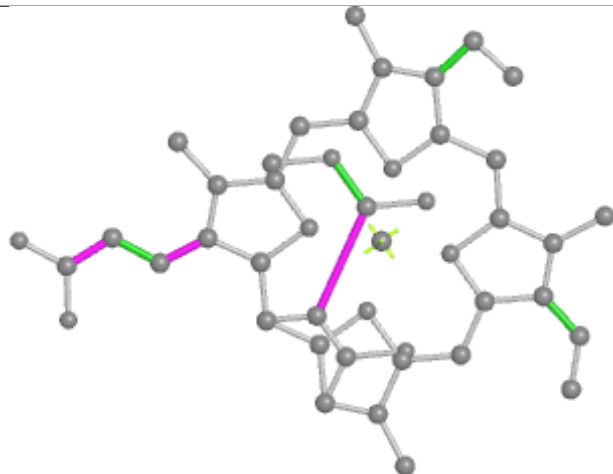
Ligand KC2 J 606



Bond lengths



Bond angles

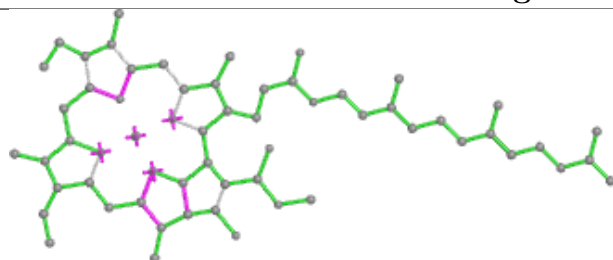


Torsions

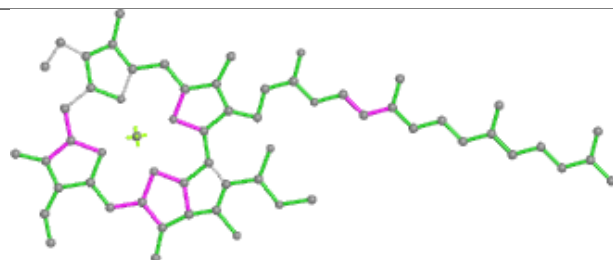


Rings

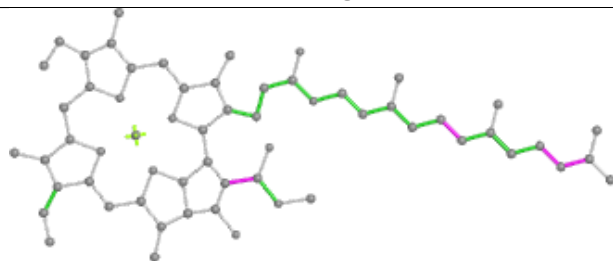
Ligand CLA D 611



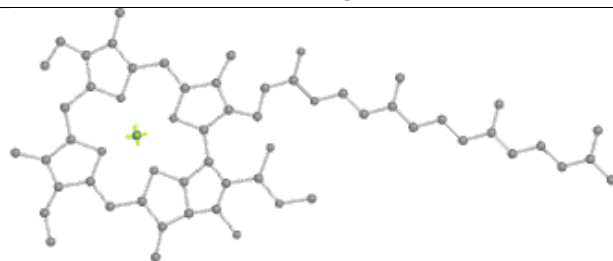
Bond lengths



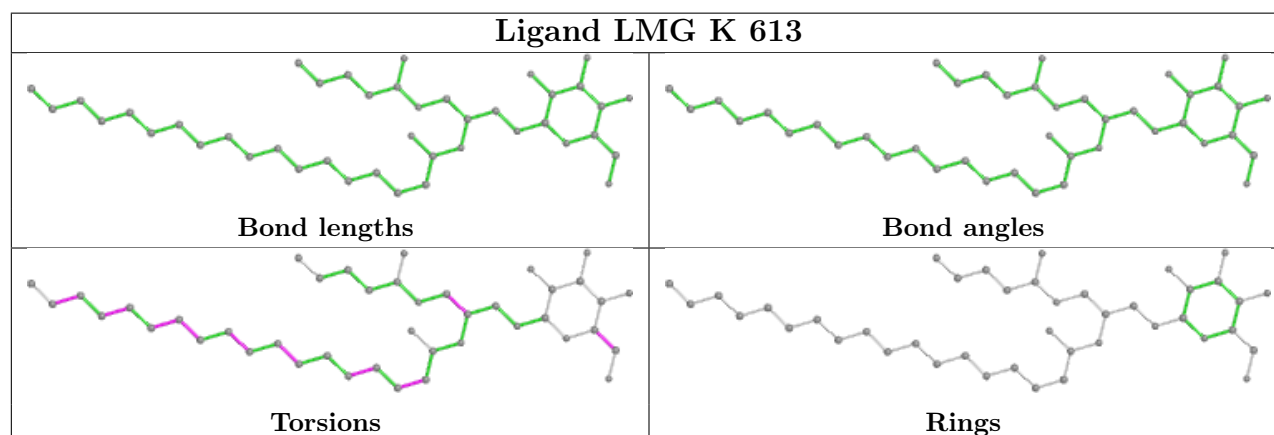
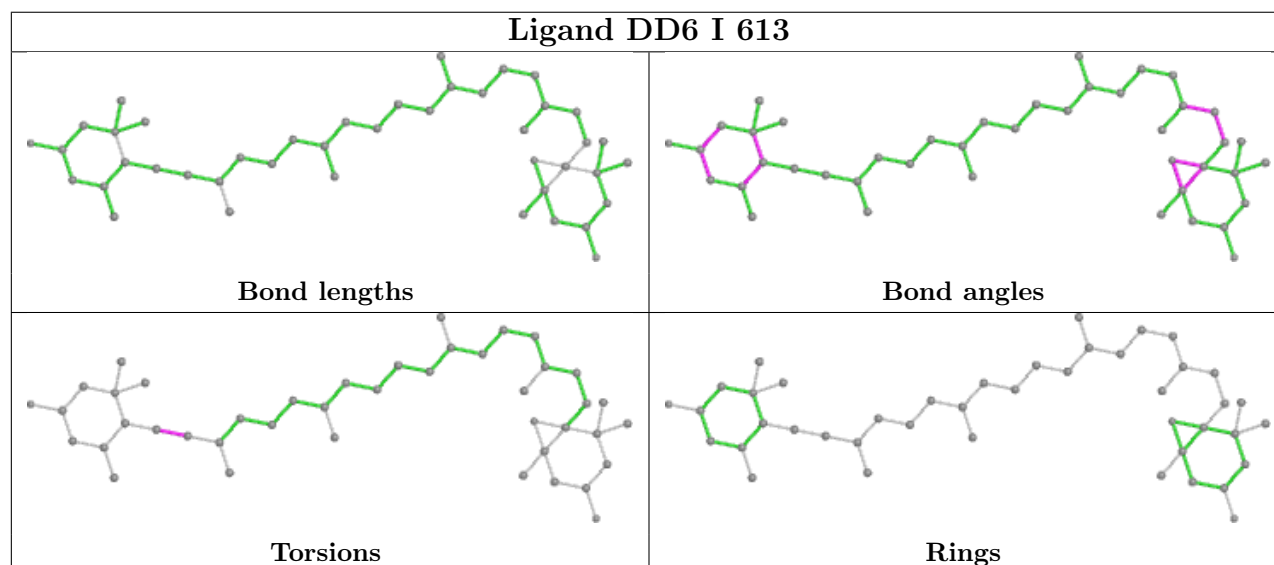
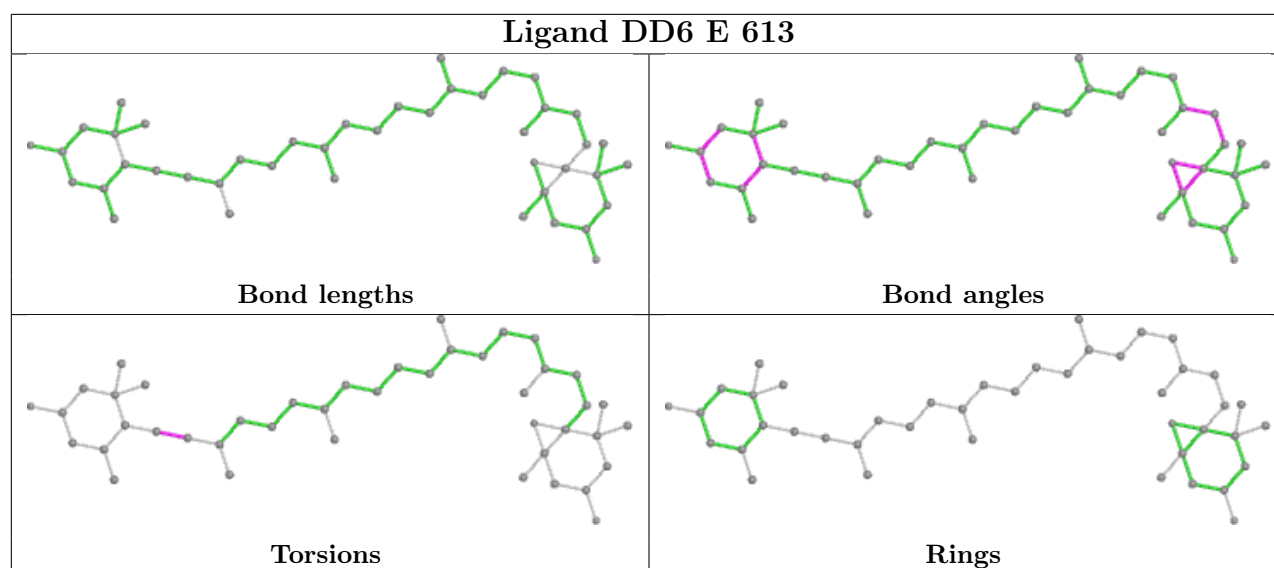
Bond angles

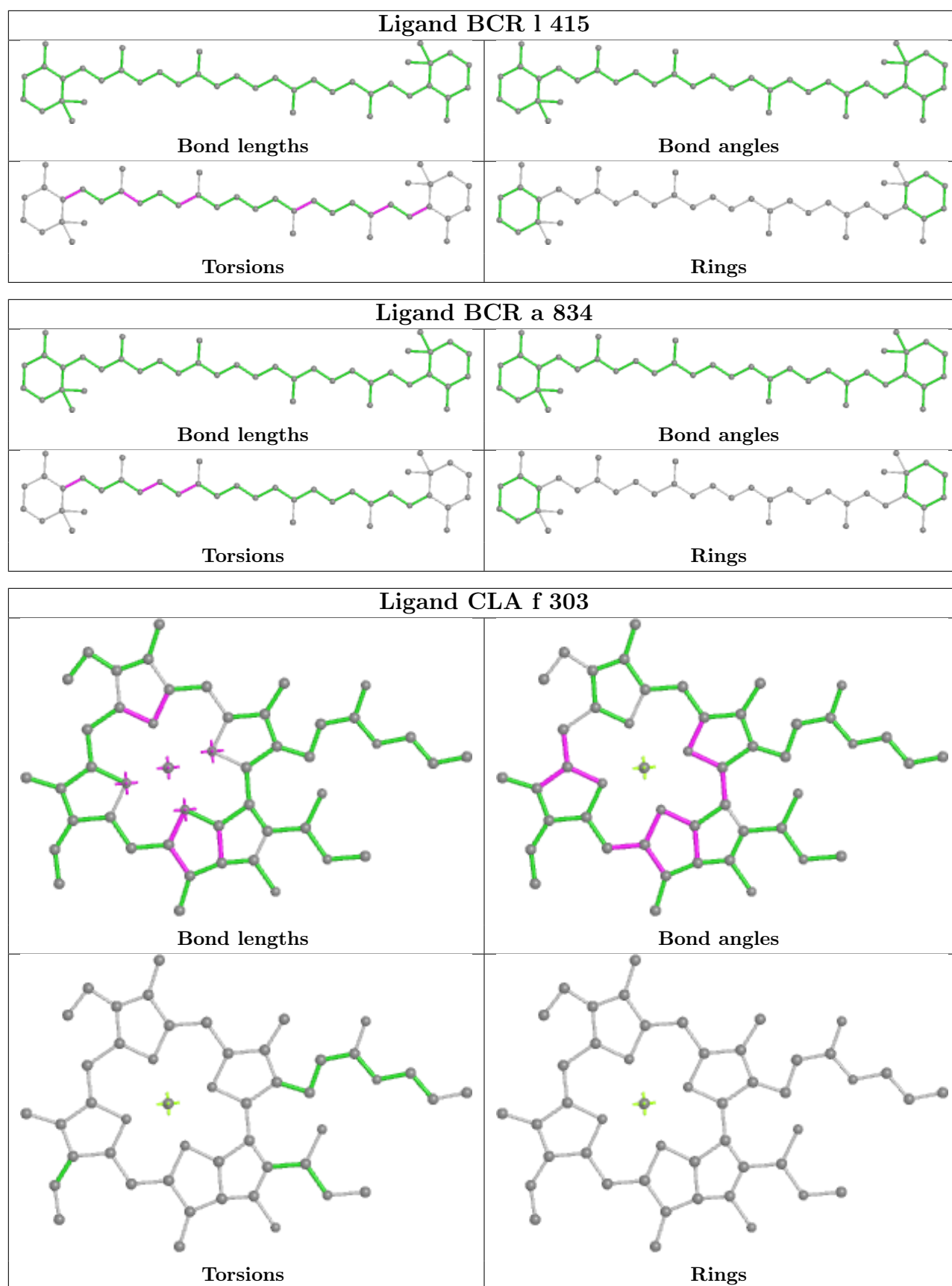


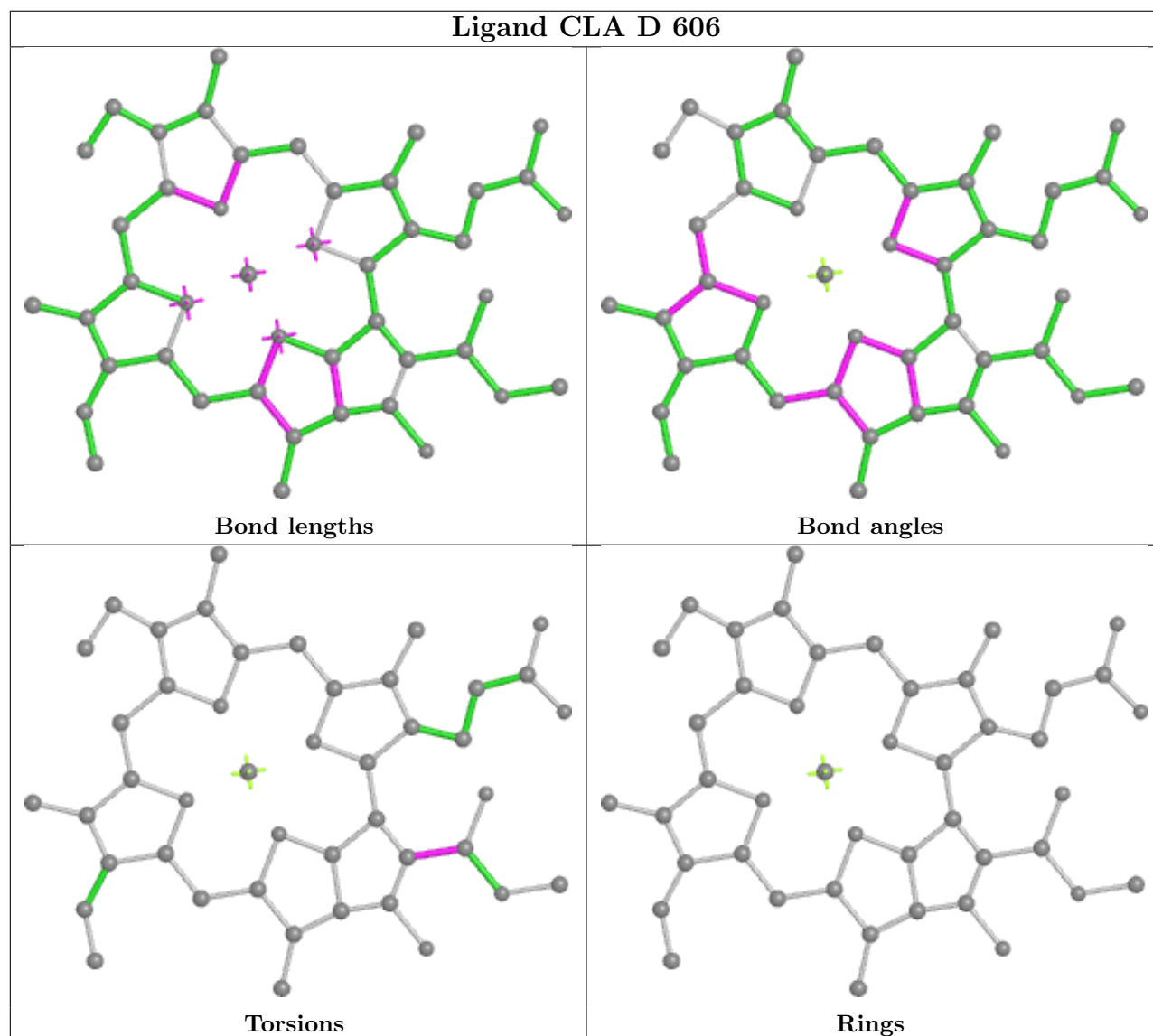
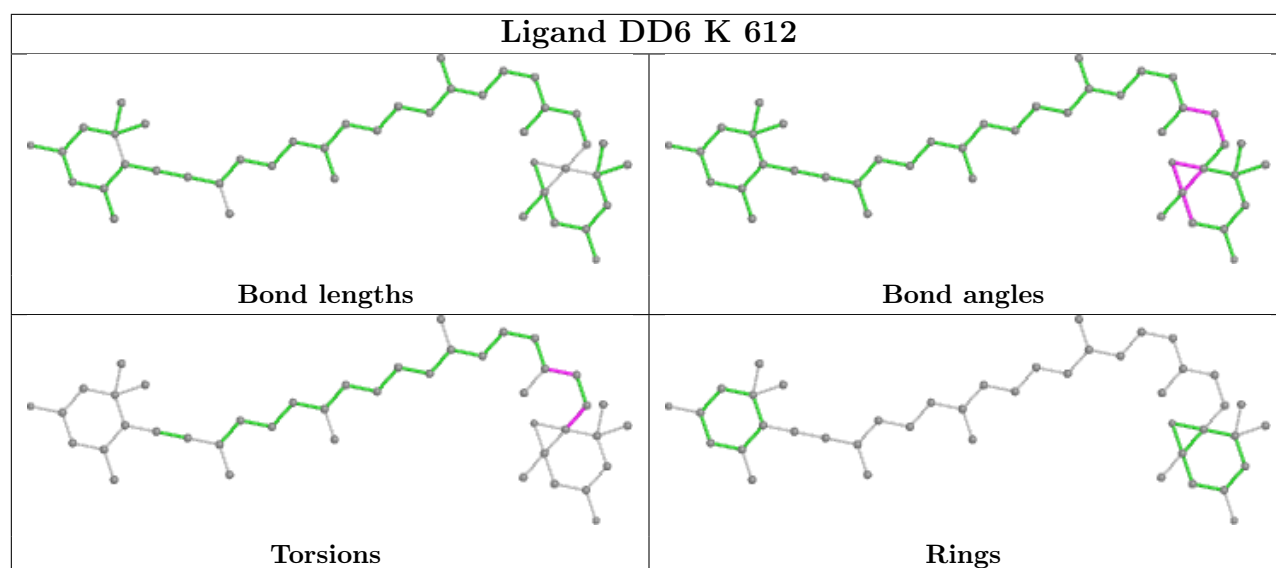
Torsions



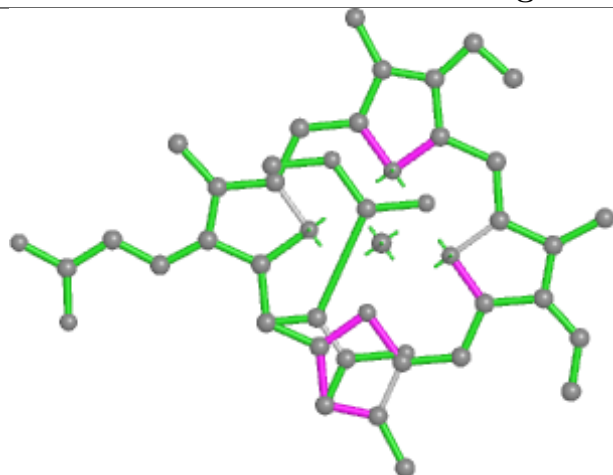
Rings



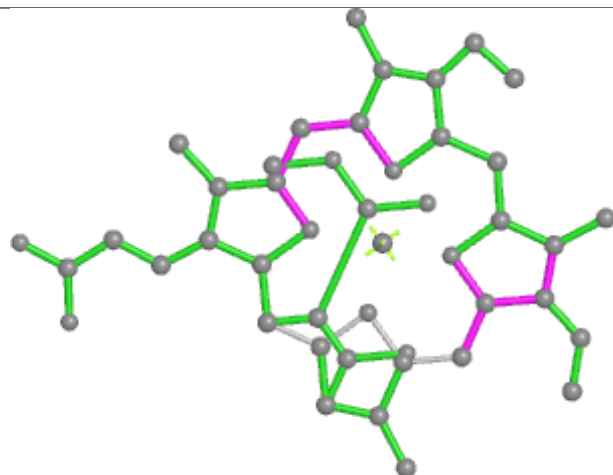




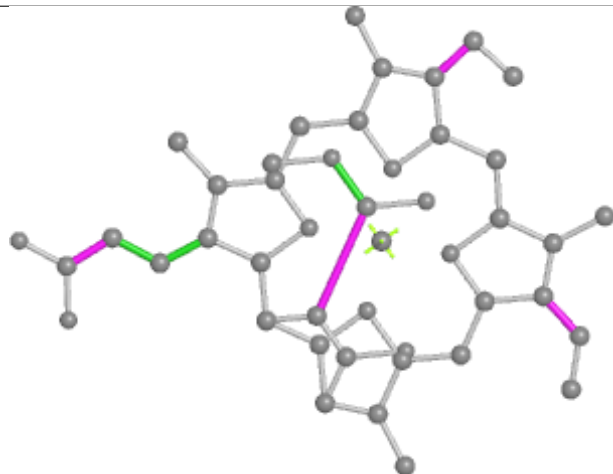
Ligand KC2 T 608



Bond lengths



Bond angles

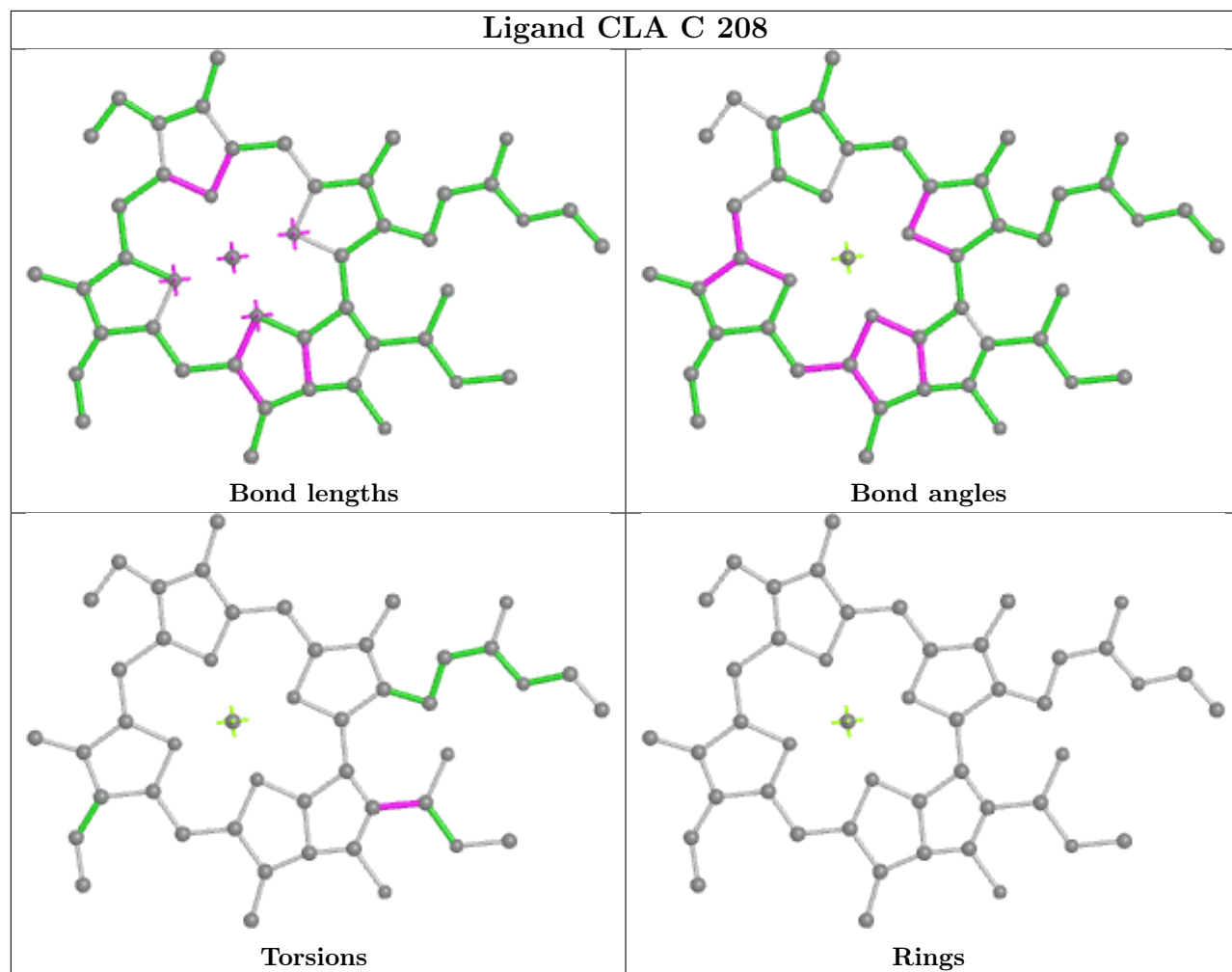


Torsions

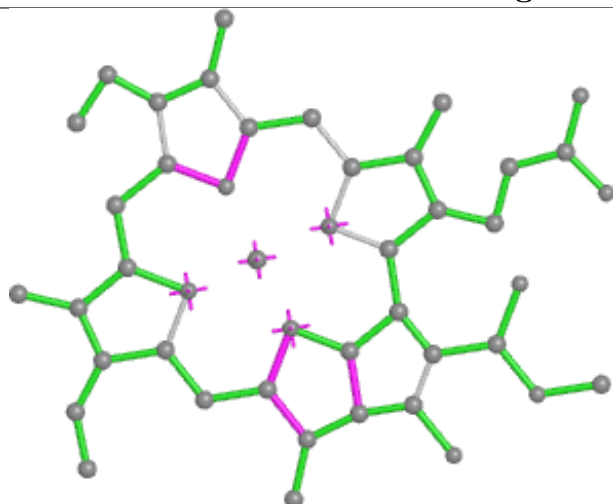


Rings

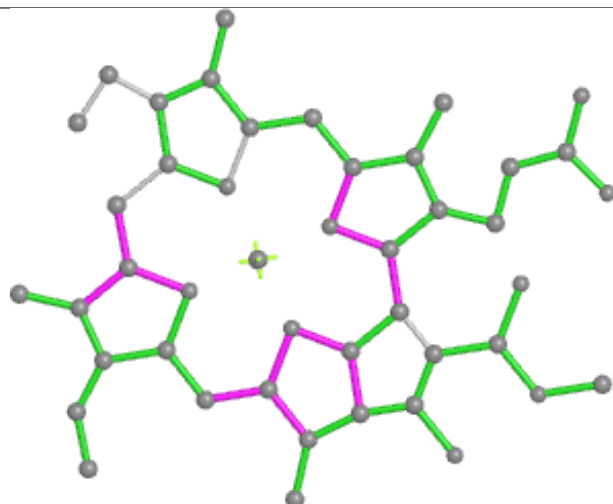
Ligand CLA C 208



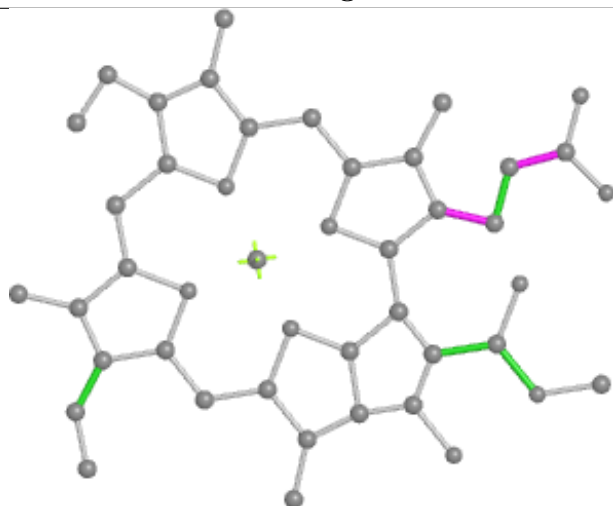
Ligand CLA E 605



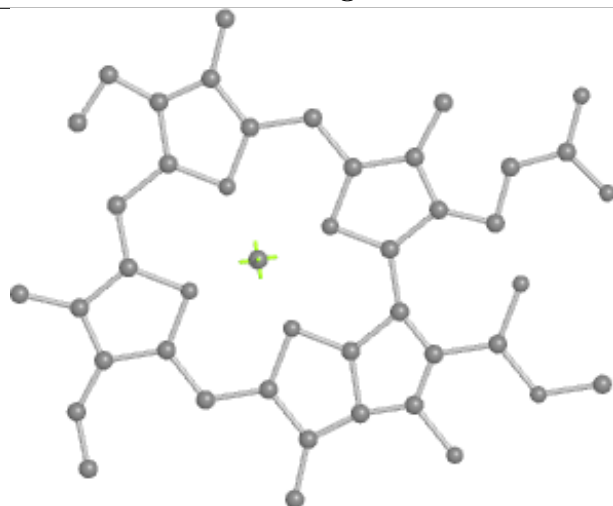
Bond lengths



Bond angles

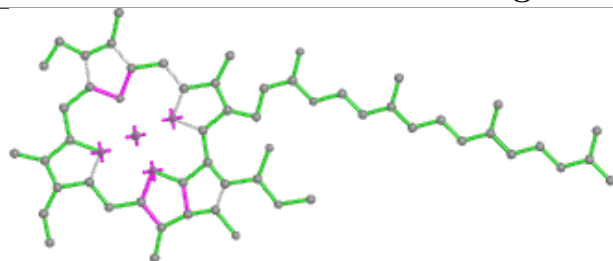


Torsions

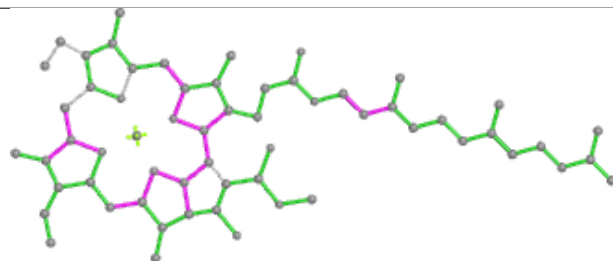


Rings

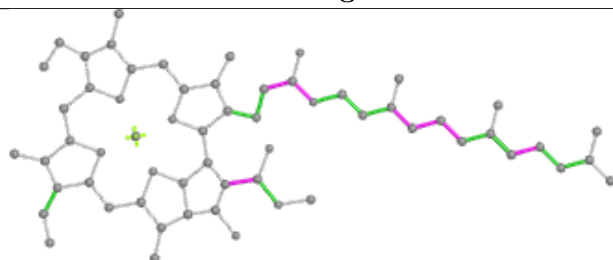
Ligand CLA H 304



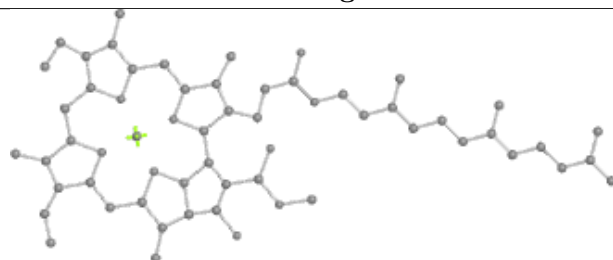
Bond lengths



Bond angles

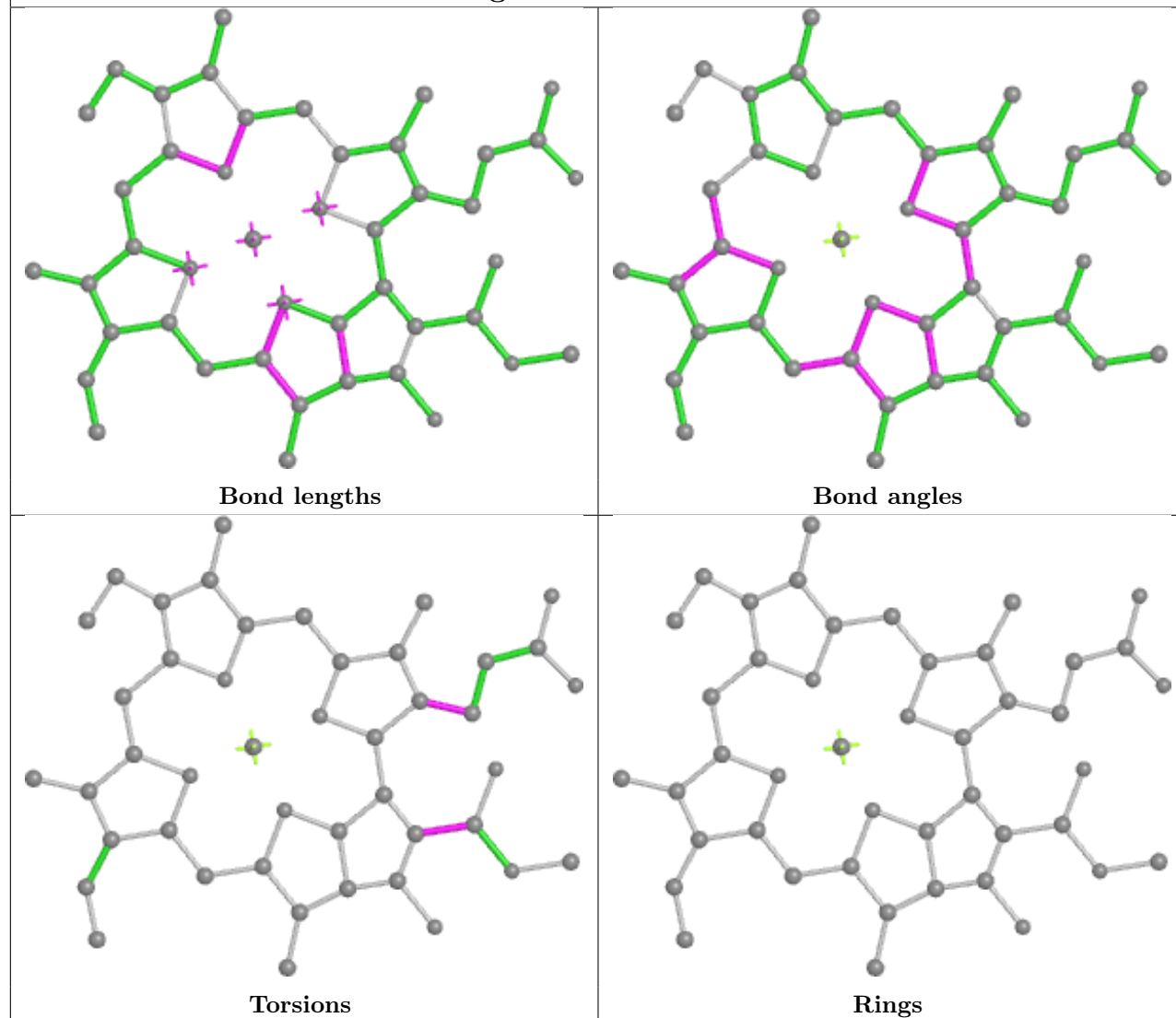


Torsions

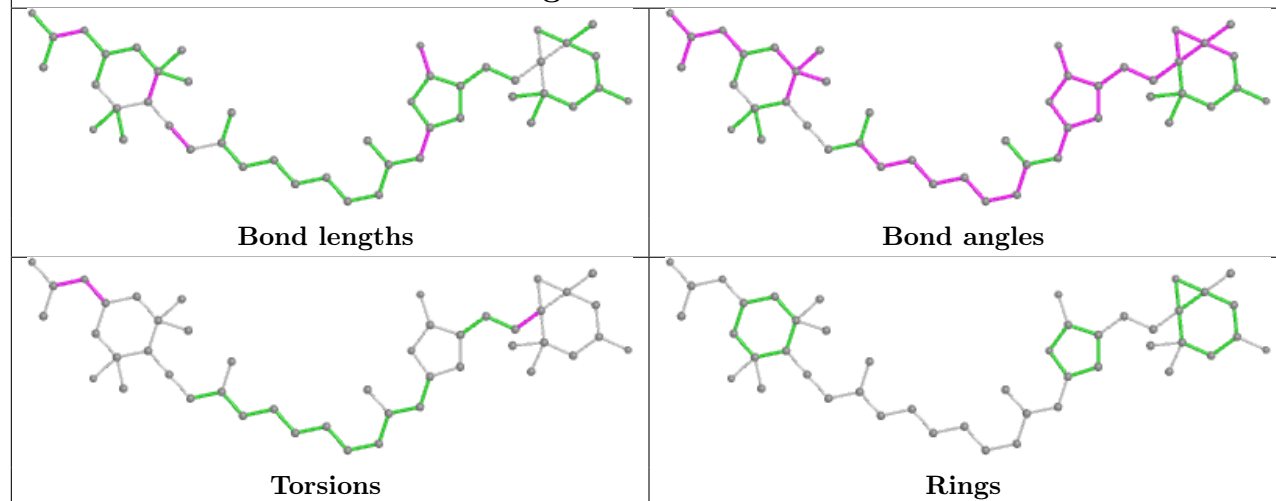


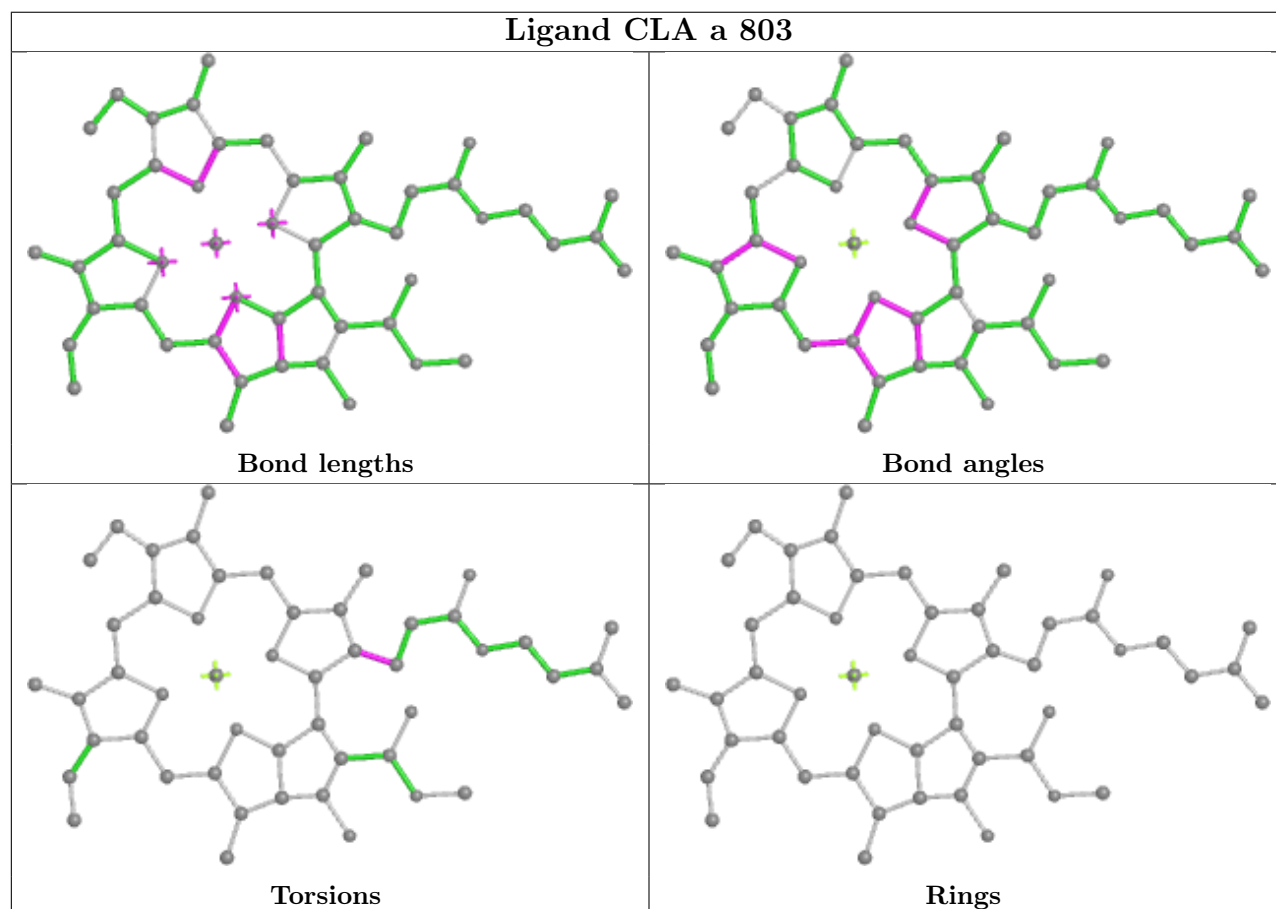
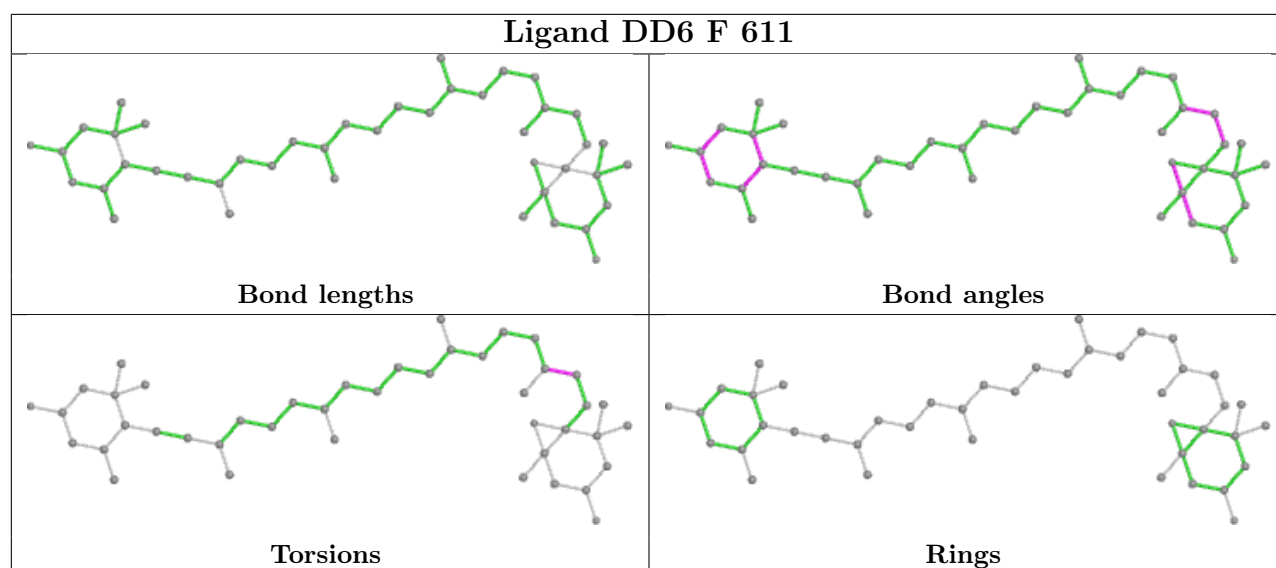
Rings

Ligand CLA H 310

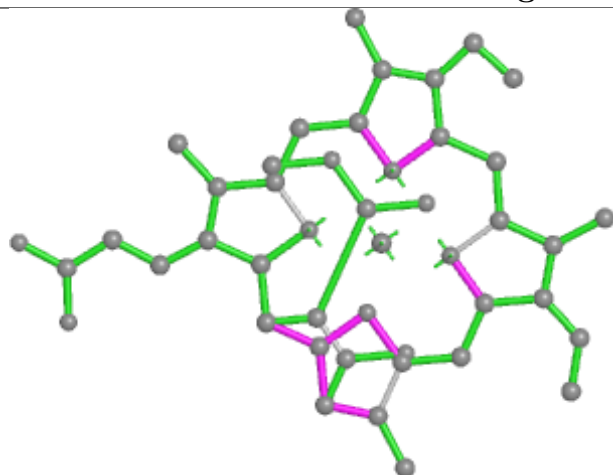


Ligand PID I 614

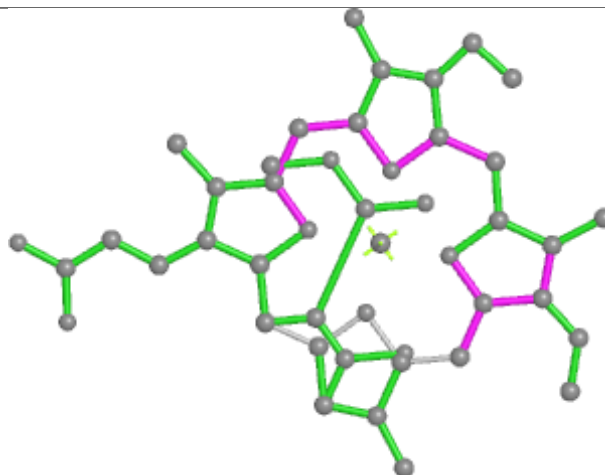




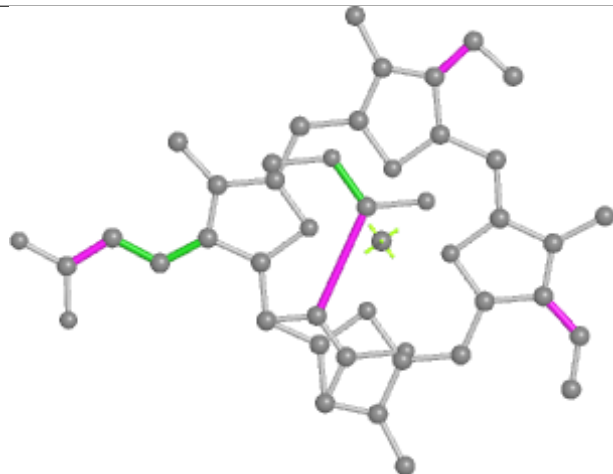
Ligand KC2 F 609



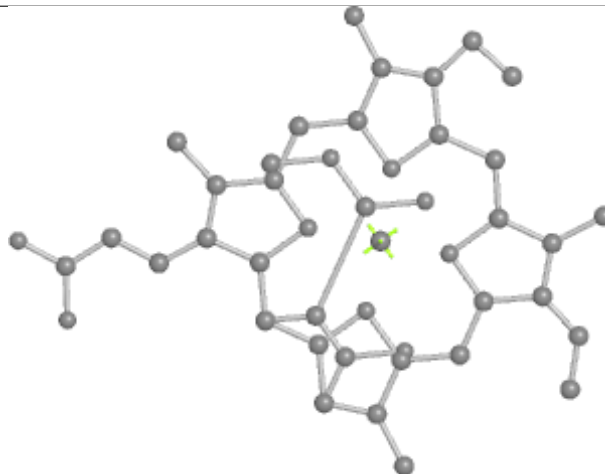
Bond lengths



Bond angles

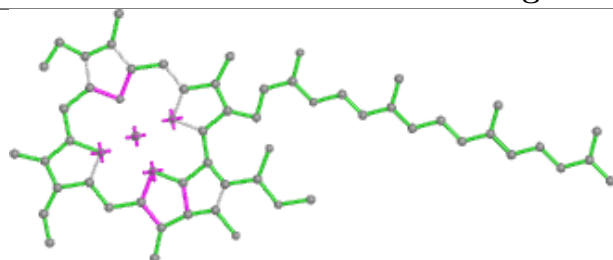


Torsions

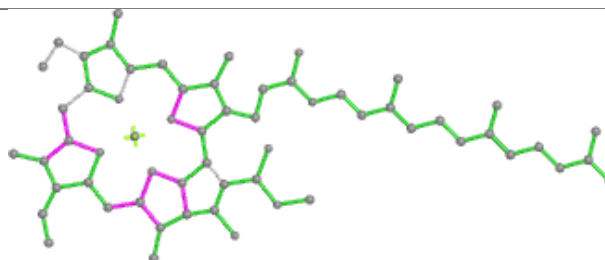


Rings

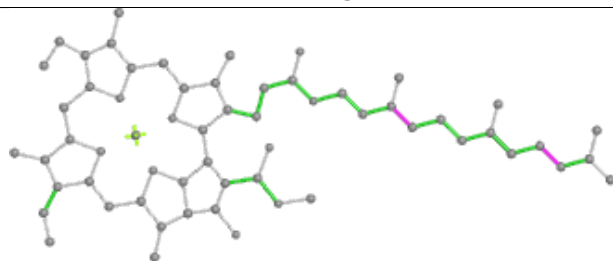
Ligand CLA 1 402



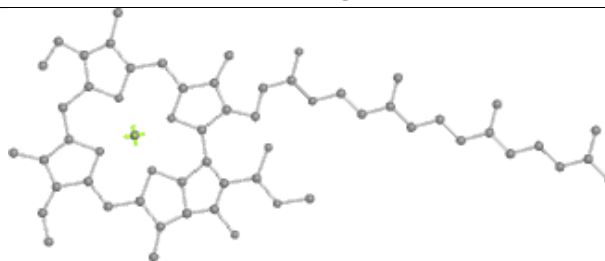
Bond lengths



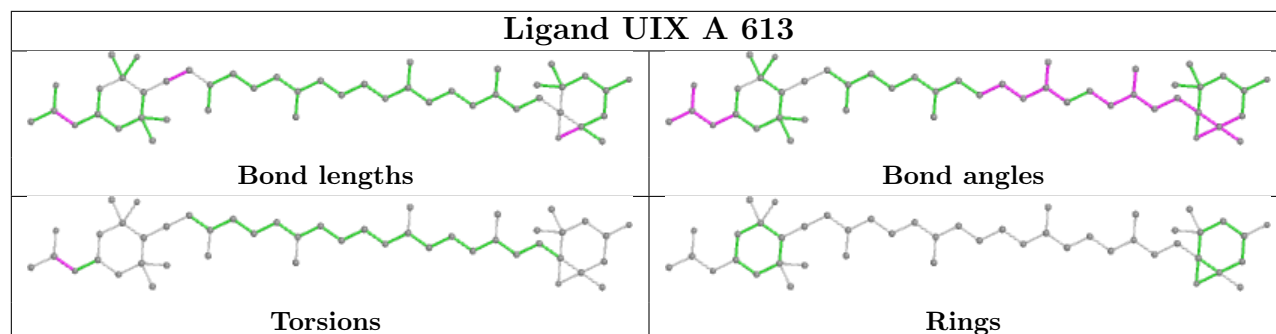
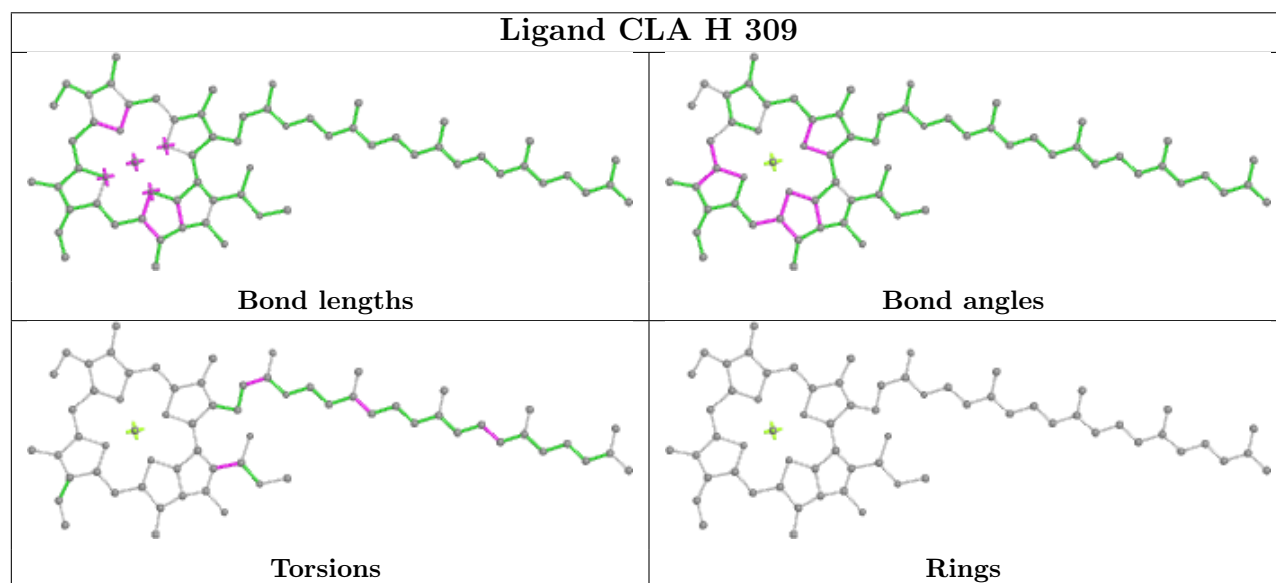
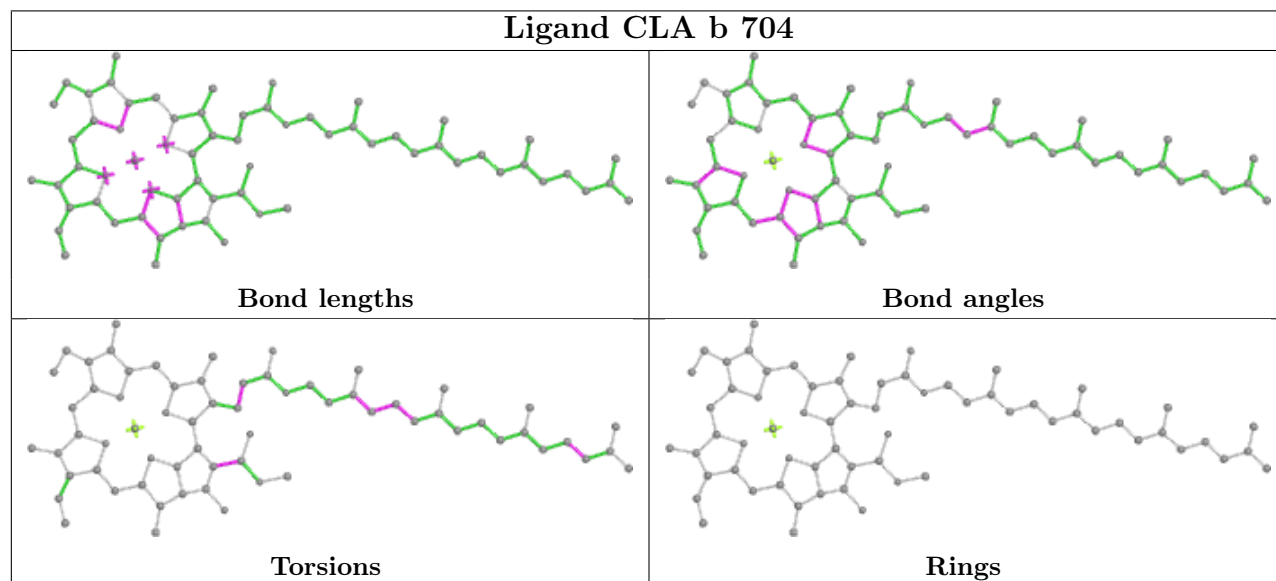
Bond angles



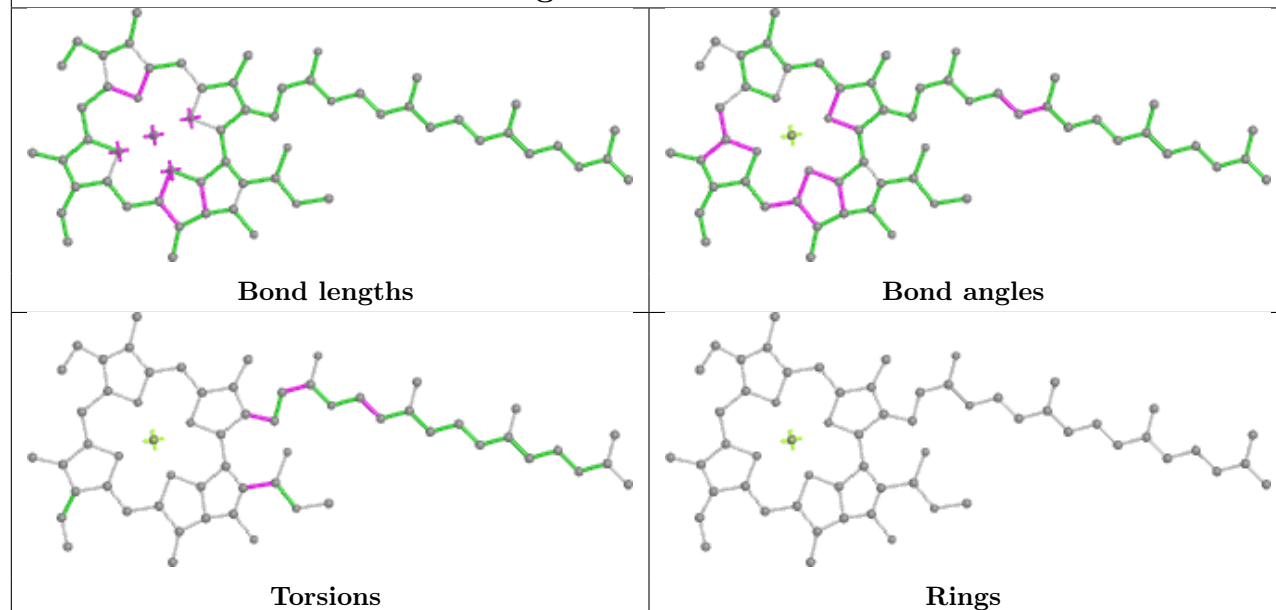
Torsions



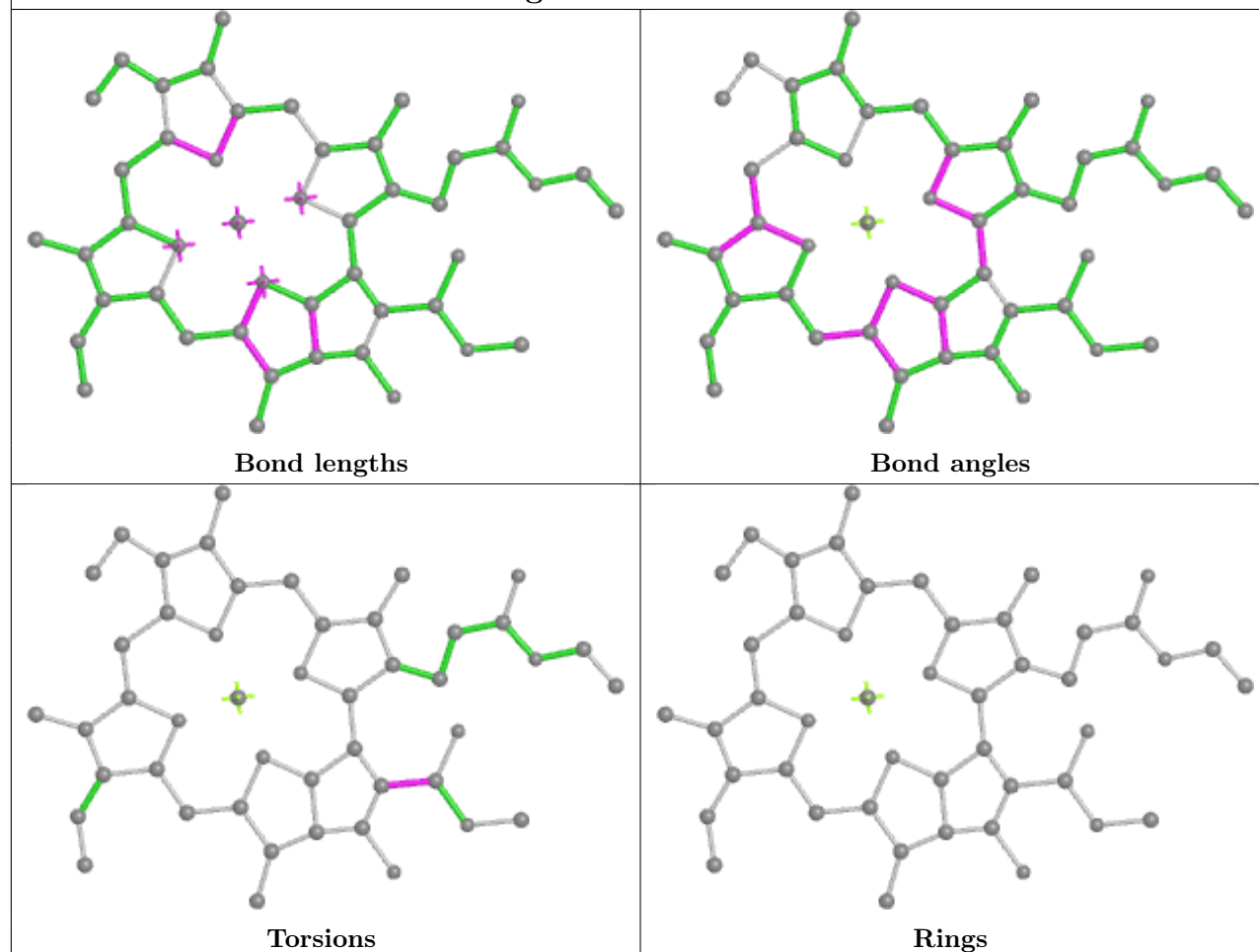
Rings

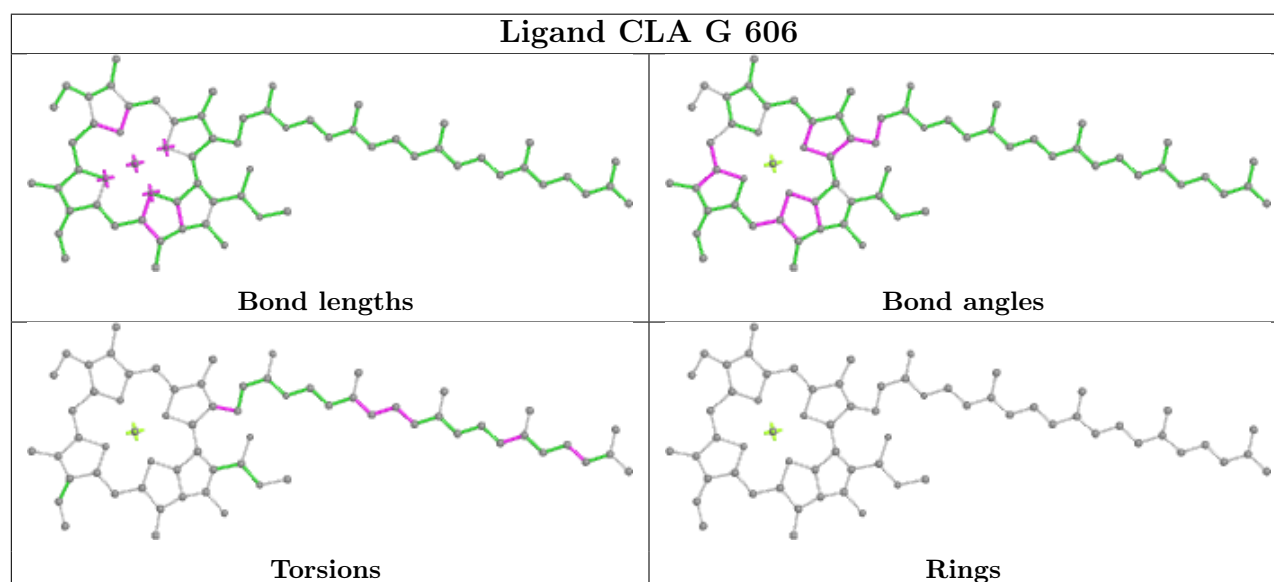
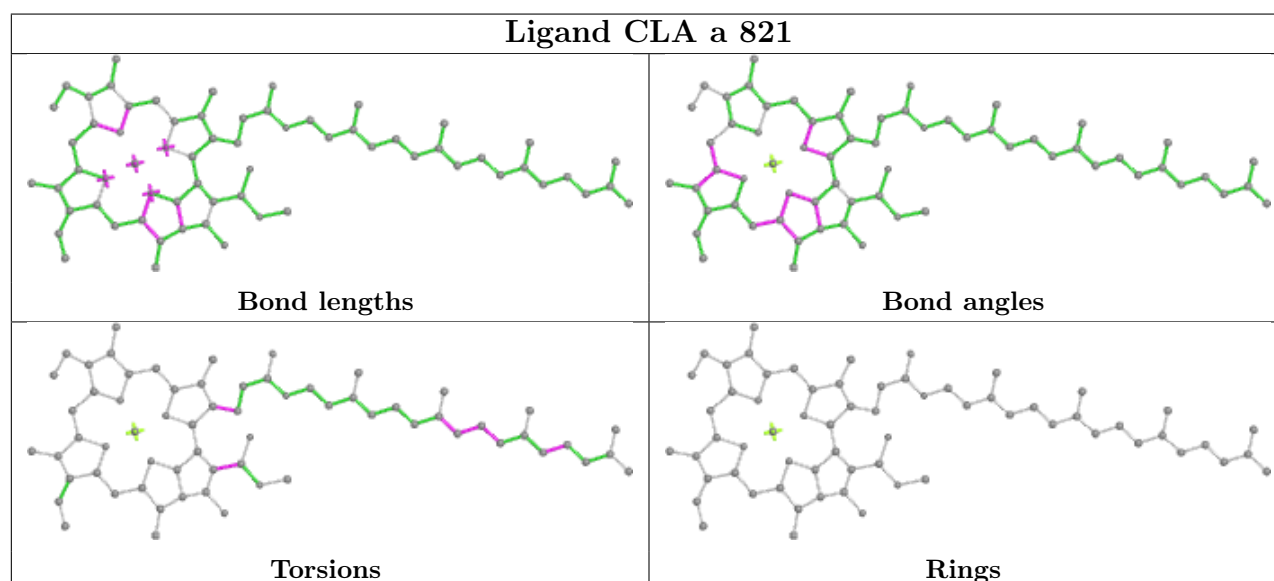
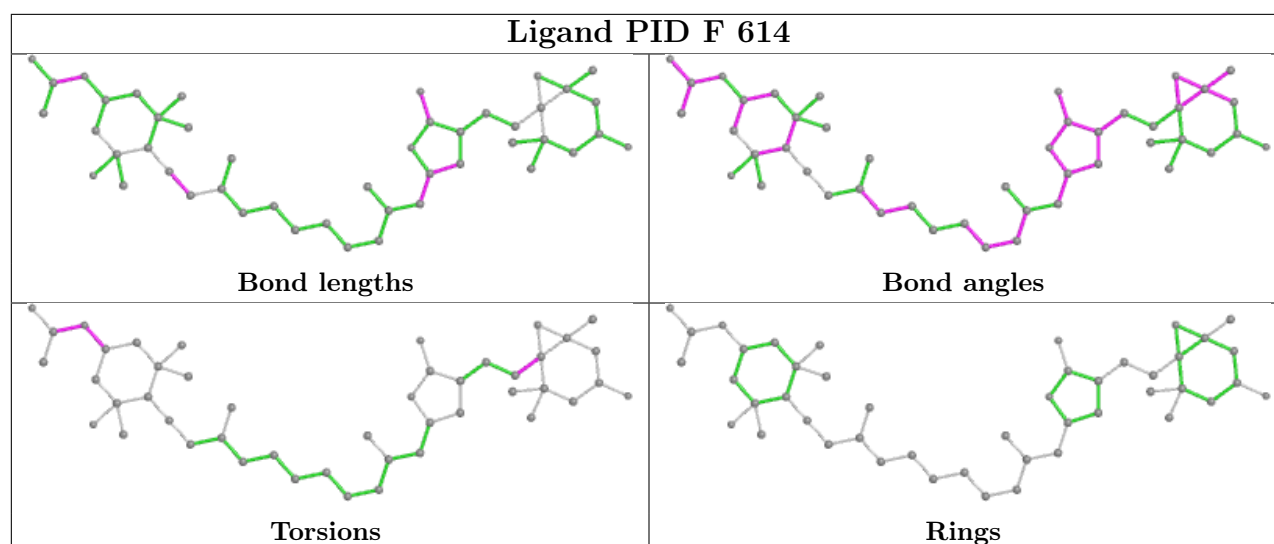
Ligand UIX A 613**Ligand CLA H 309****Ligand CLA b 704**

Ligand CLA a 822

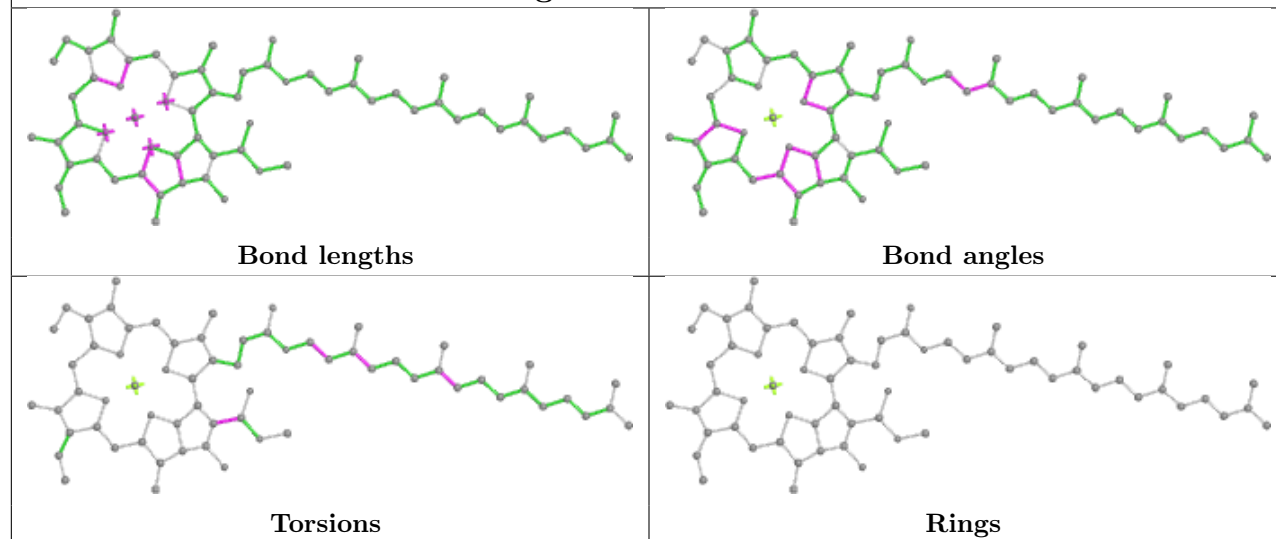


Ligand CLA T 601

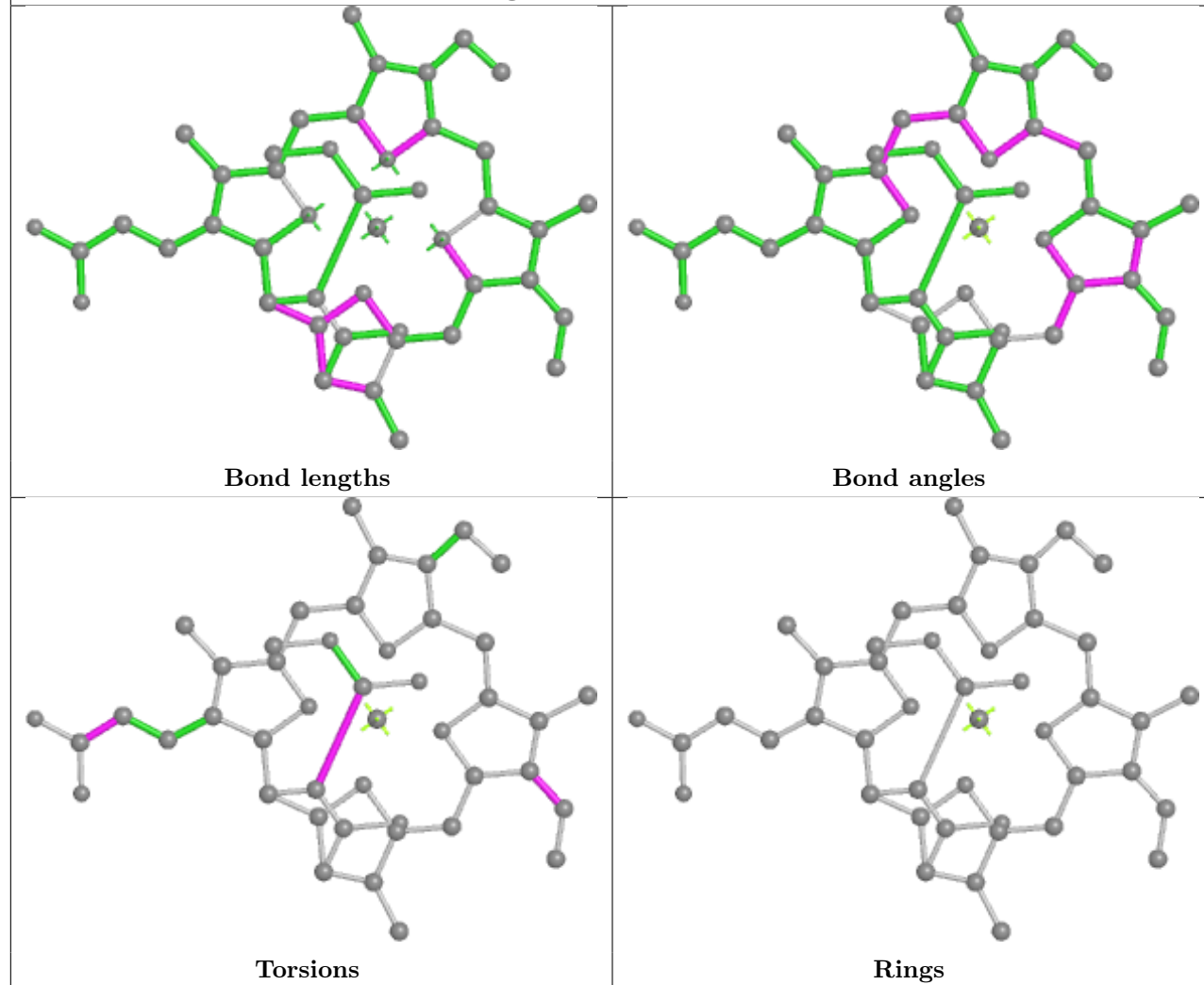




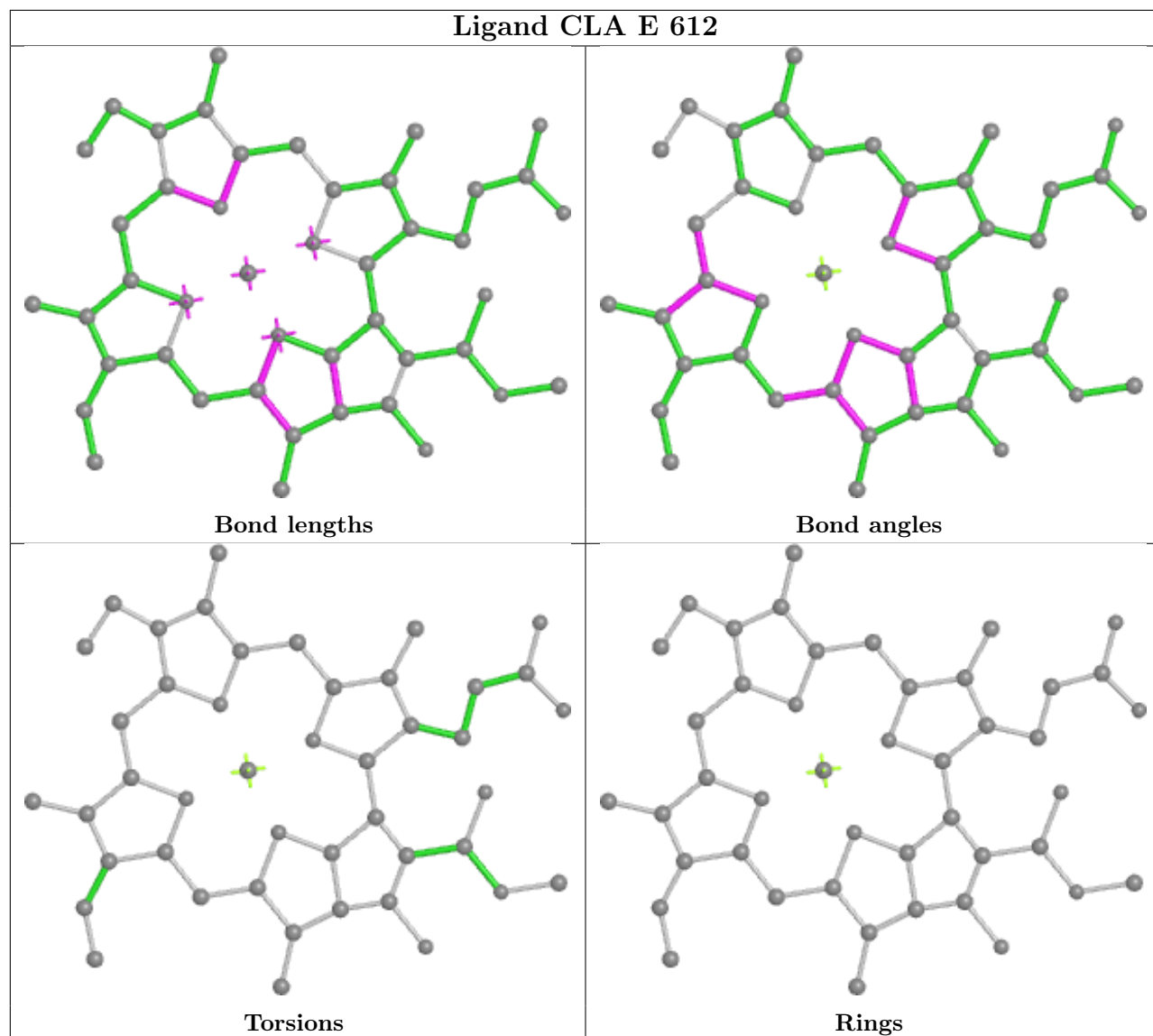
Ligand CLA b 723



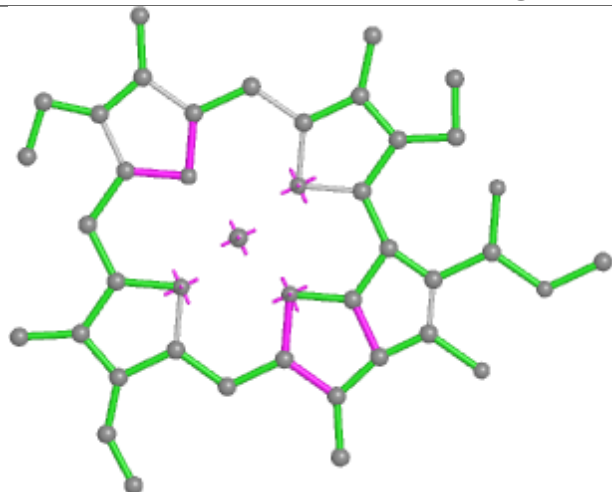
Ligand KC2 C 210



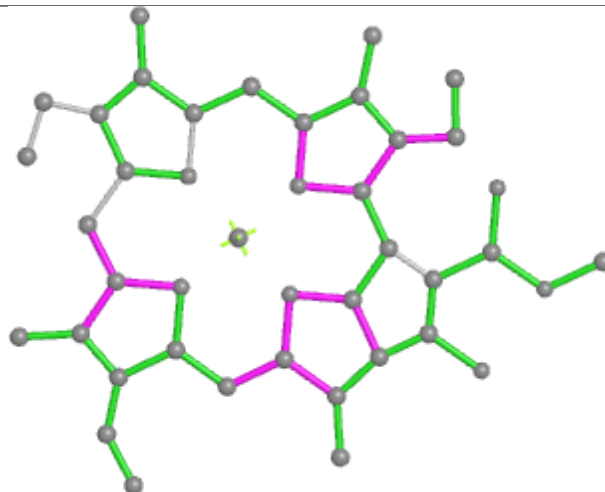
Ligand CLA E 612



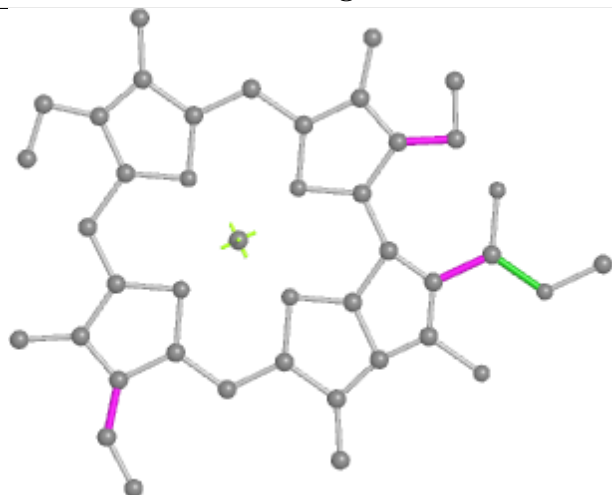
Ligand CLA H 312



Bond lengths



Bond angles

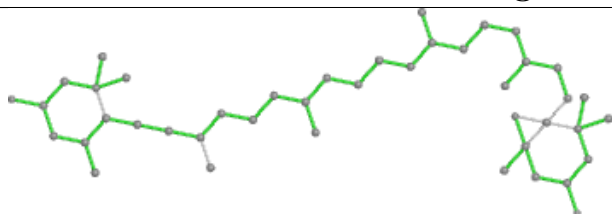


Torsions

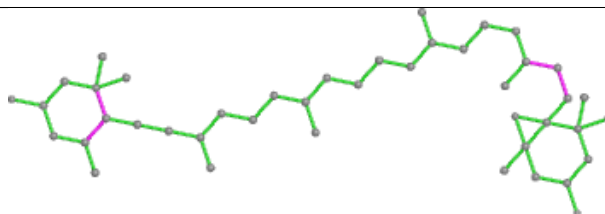


Rings

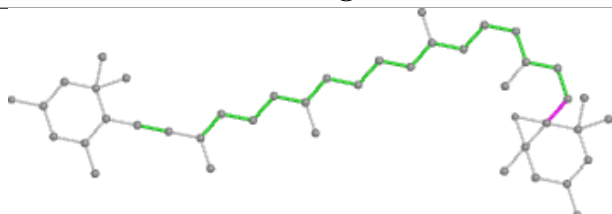
Ligand DD6 C 216



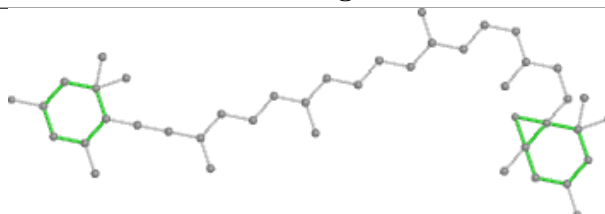
Bond lengths



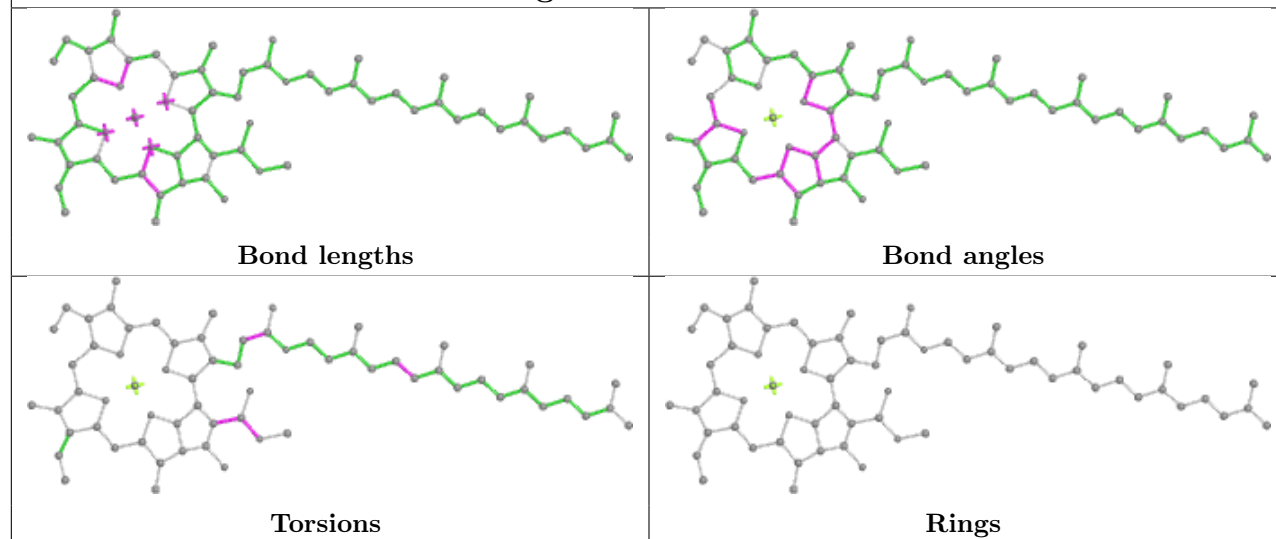
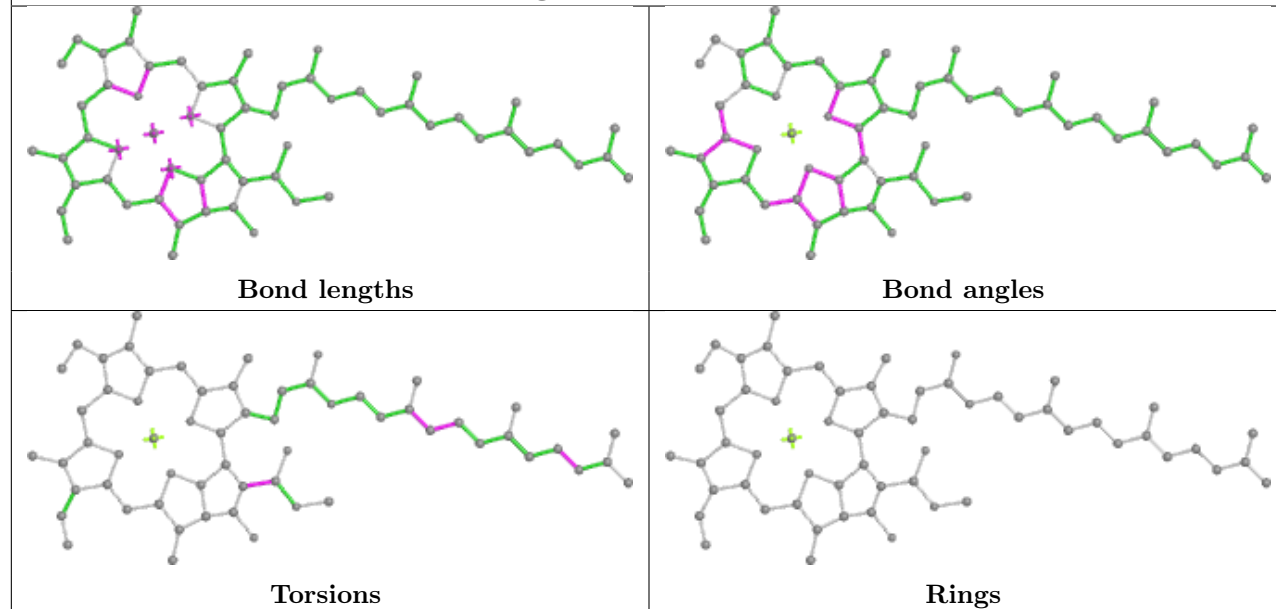
Bond angles



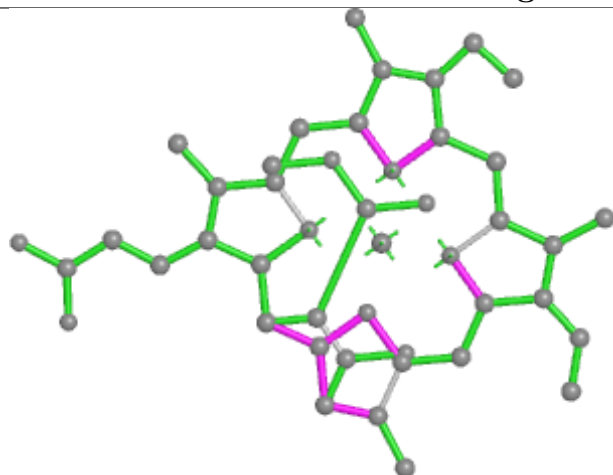
Torsions



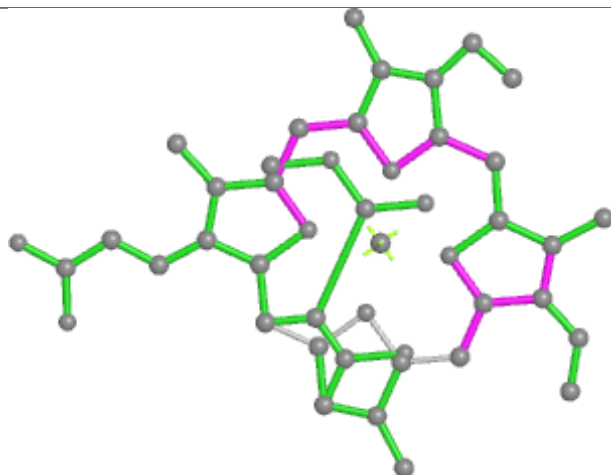
Rings

Ligand CLA a 801**Ligand CLA E 611**

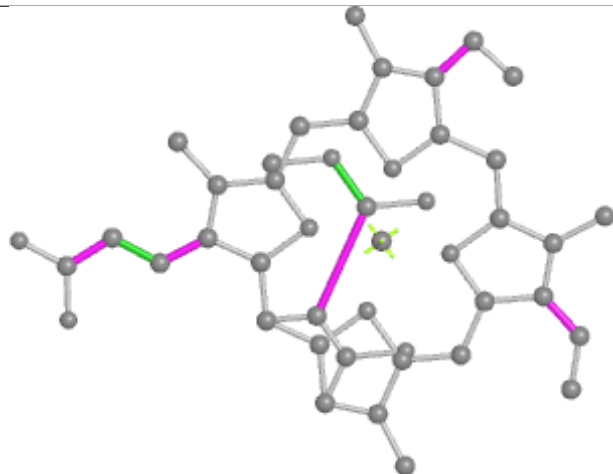
Ligand KC2 E 601



Bond lengths



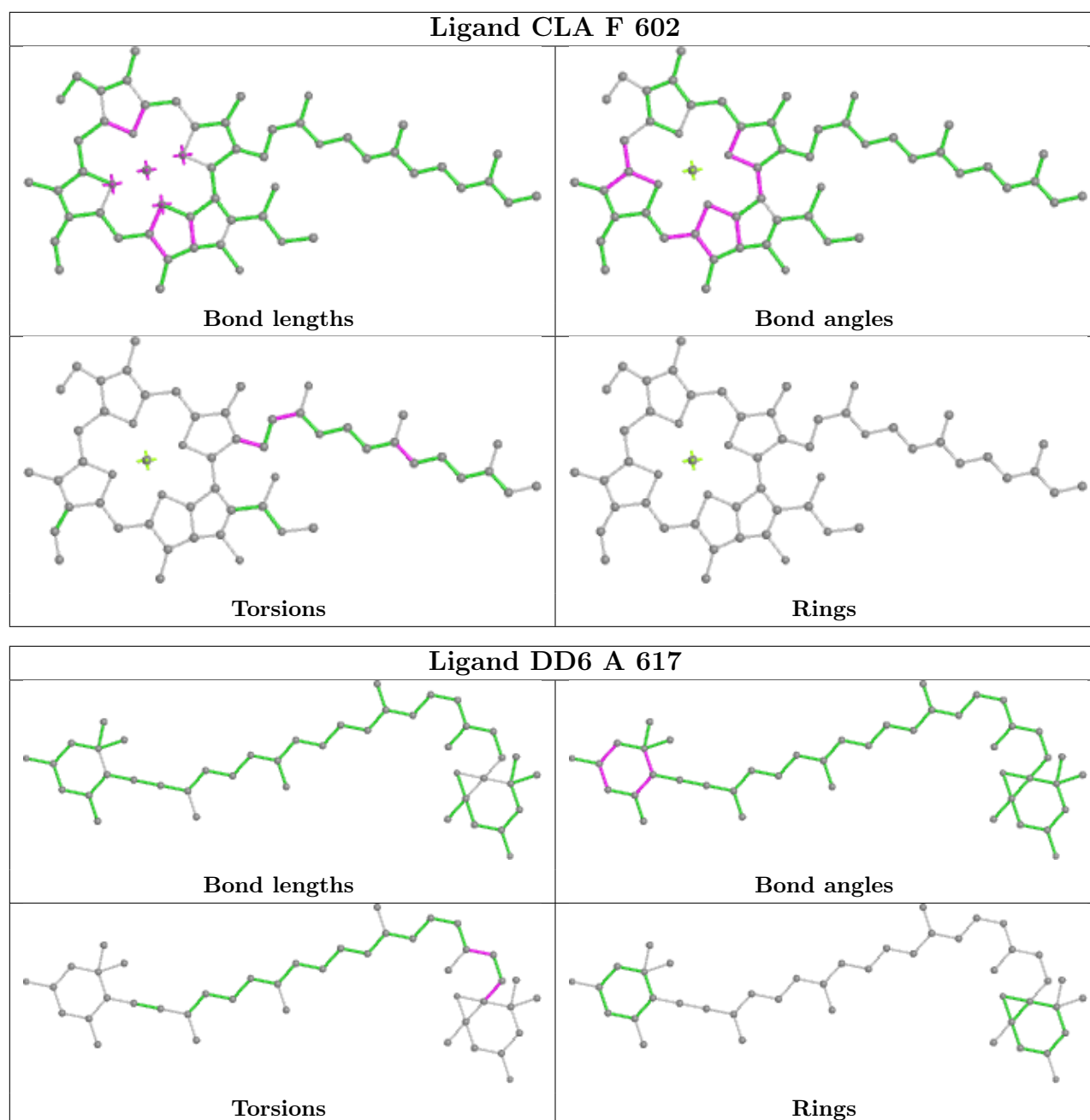
Bond angles

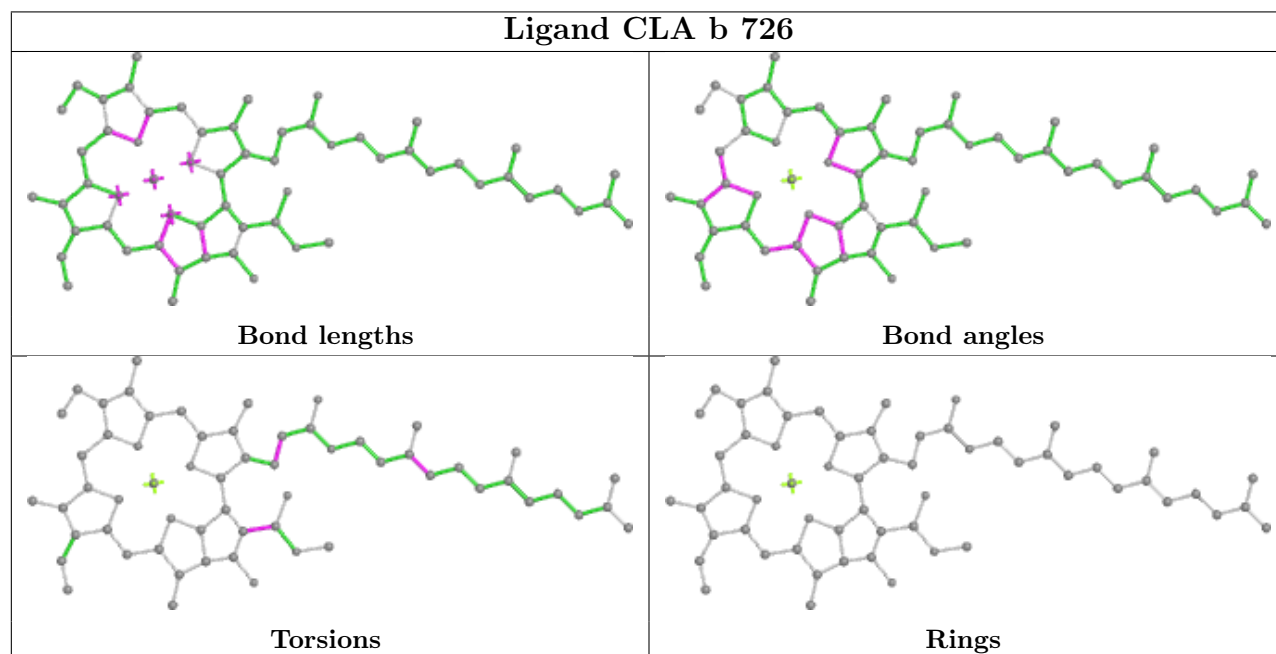
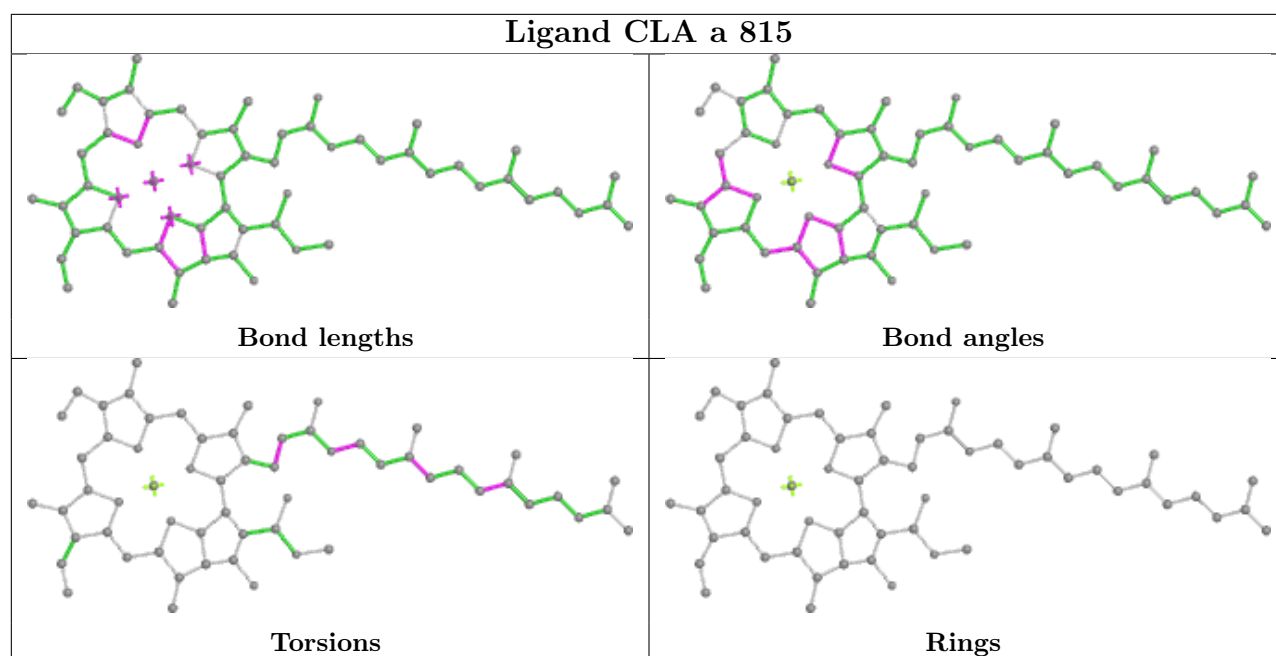


Torsions

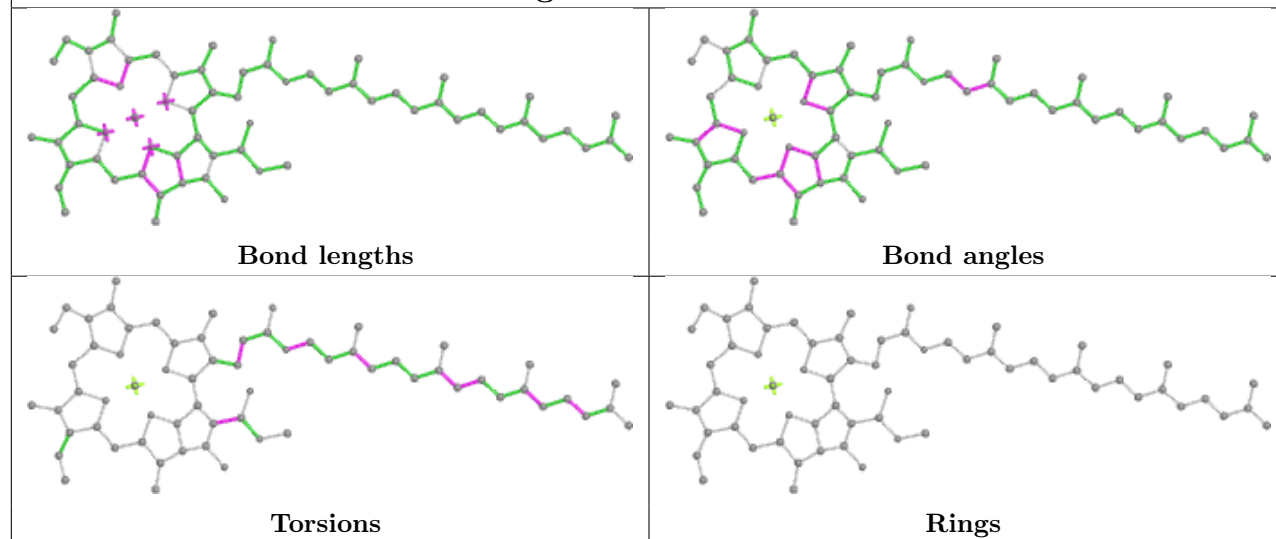


Rings

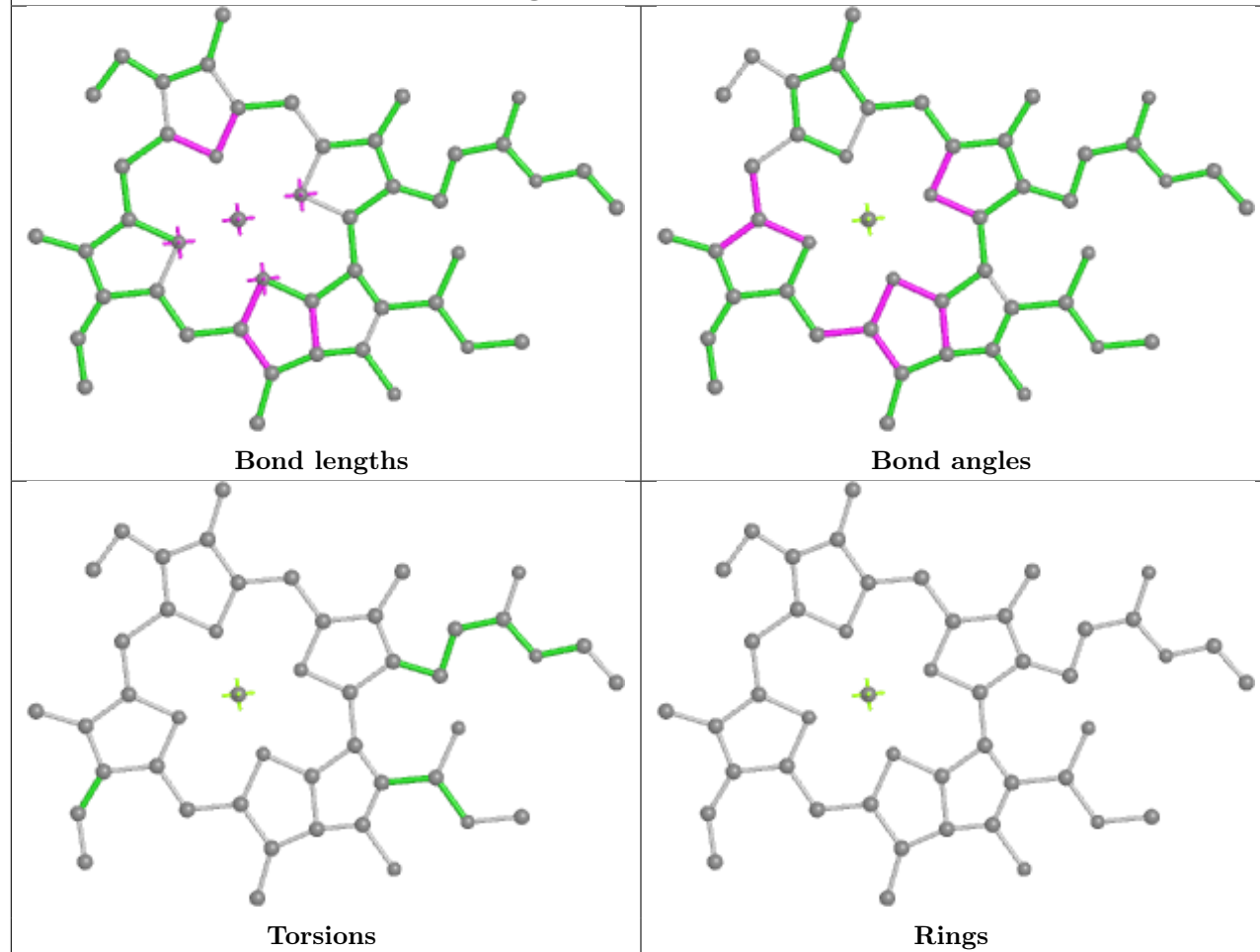




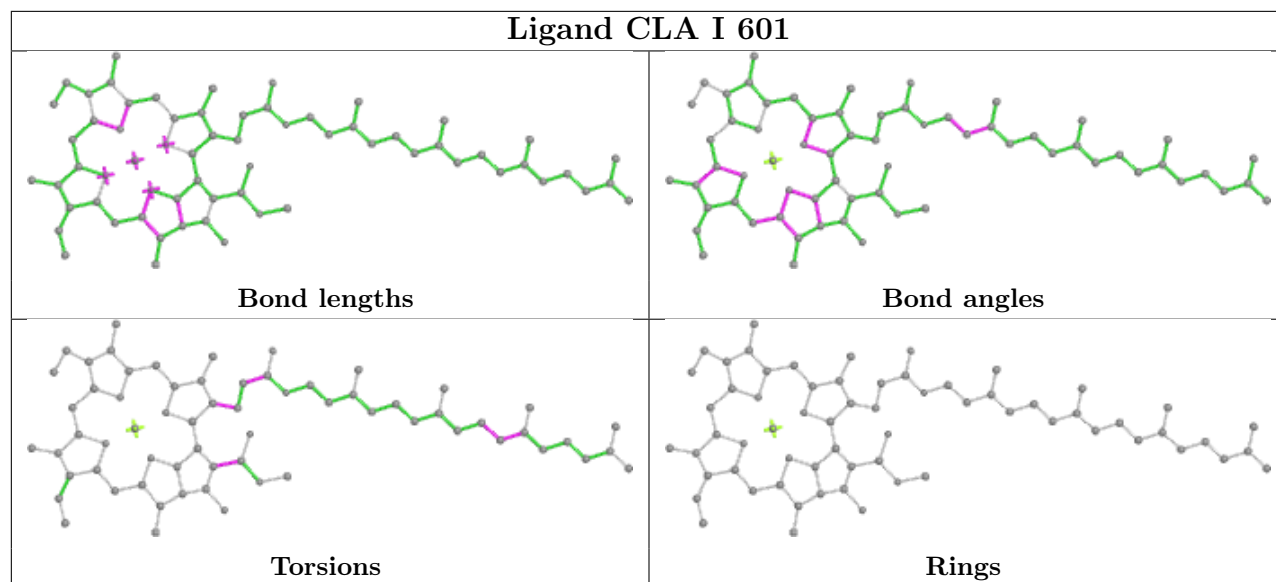
Ligand CLA a 830



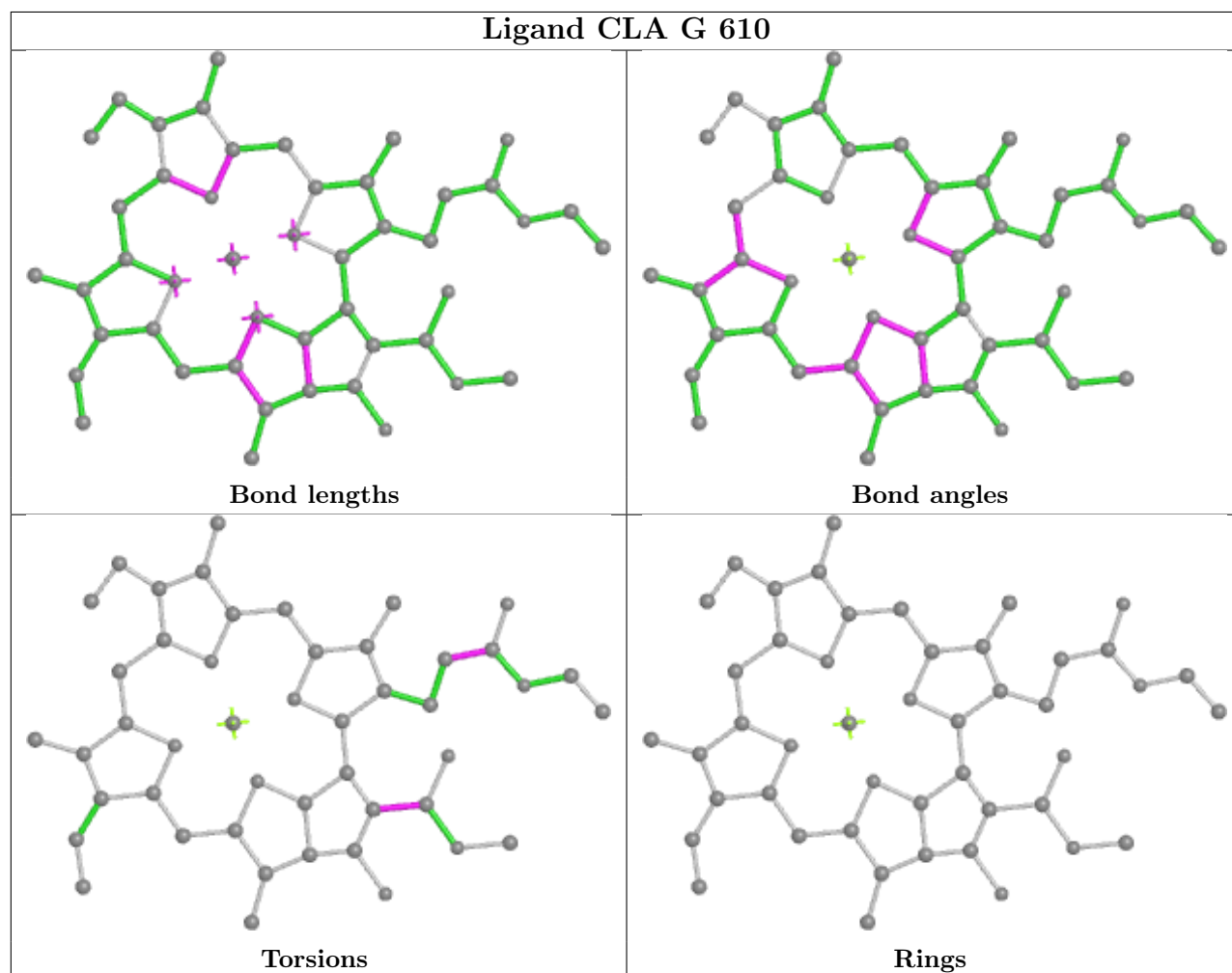
Ligand CLA C 212

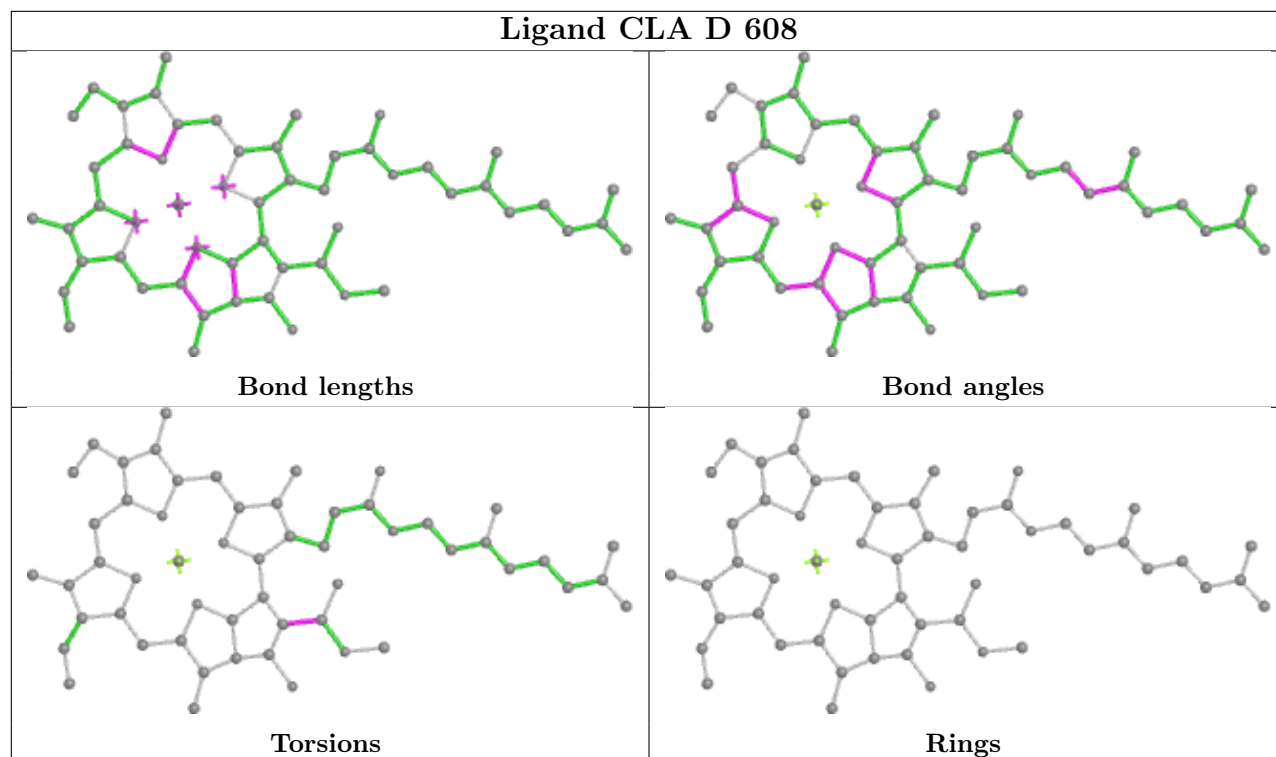
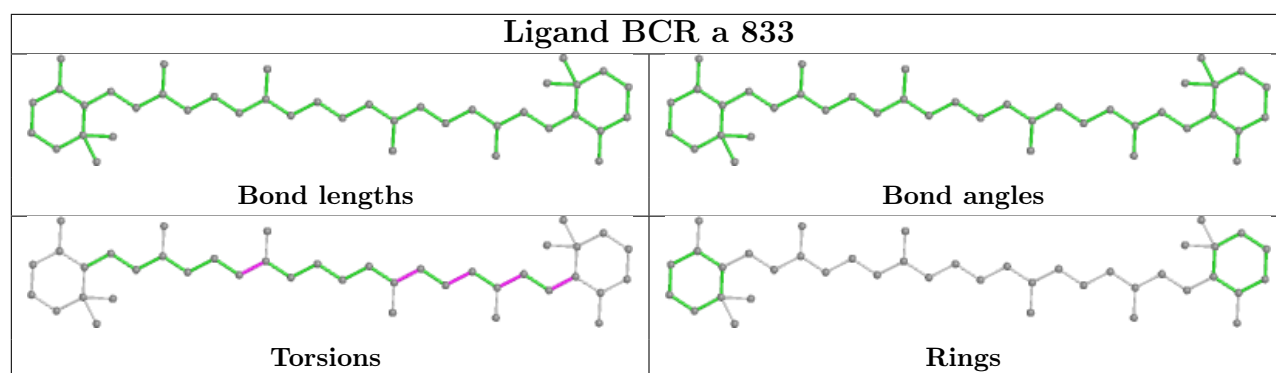


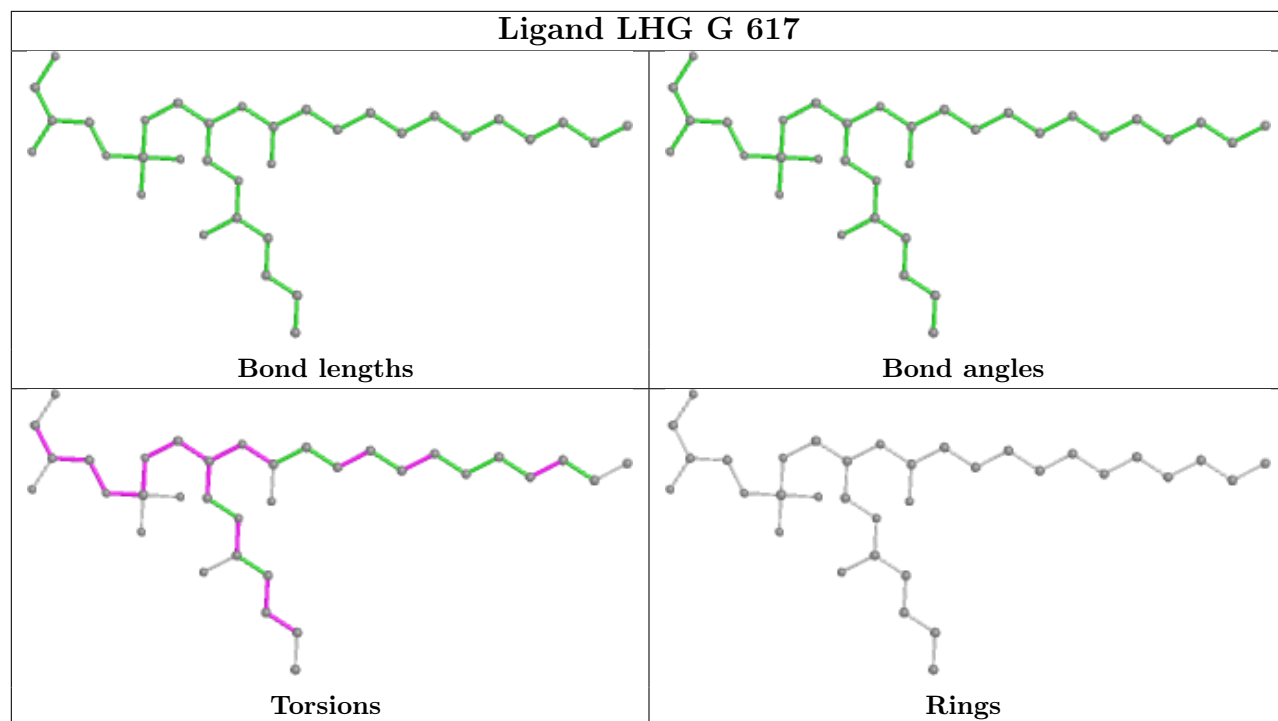
Ligand CLA I 601



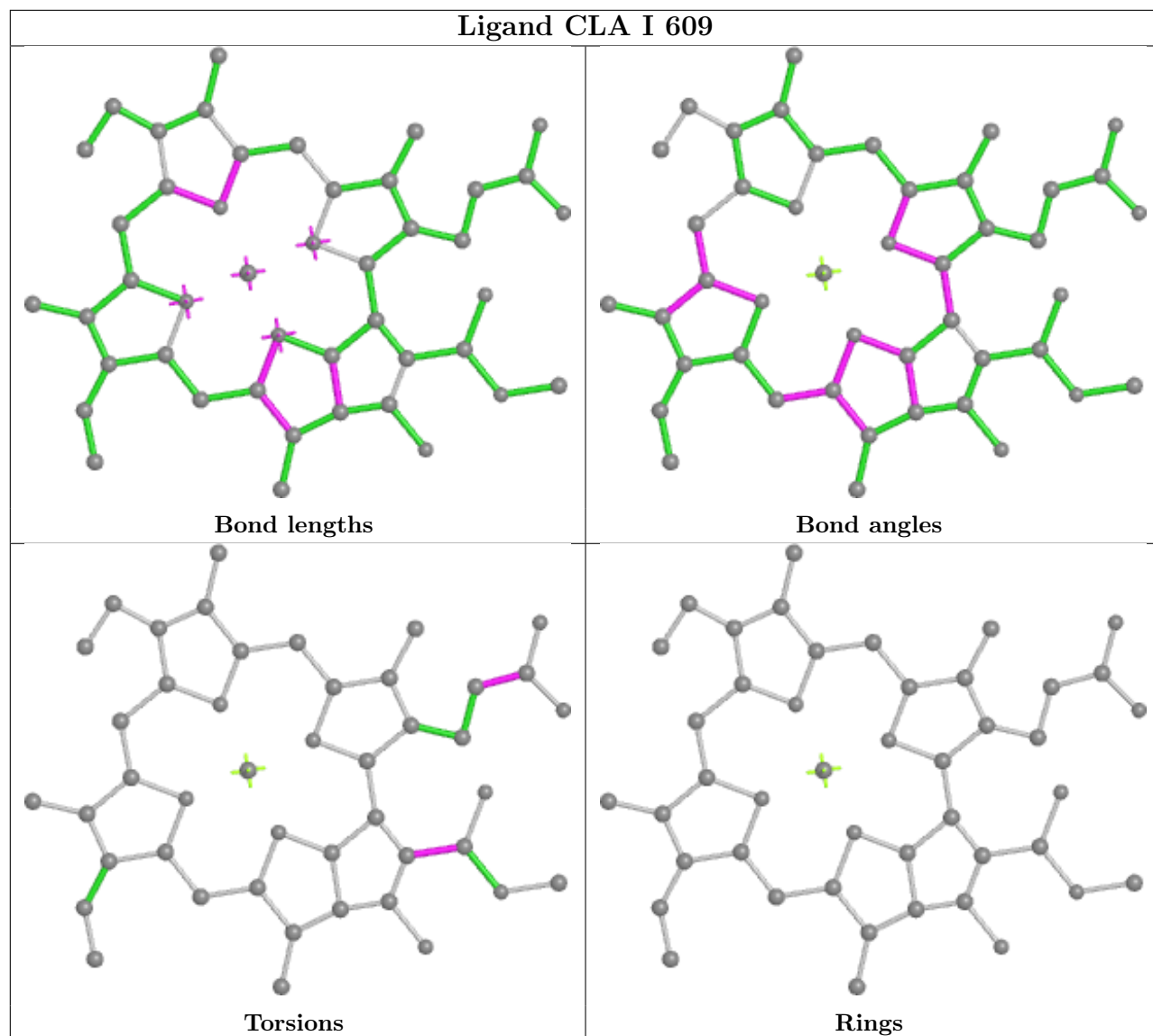
Ligand CLA G 610

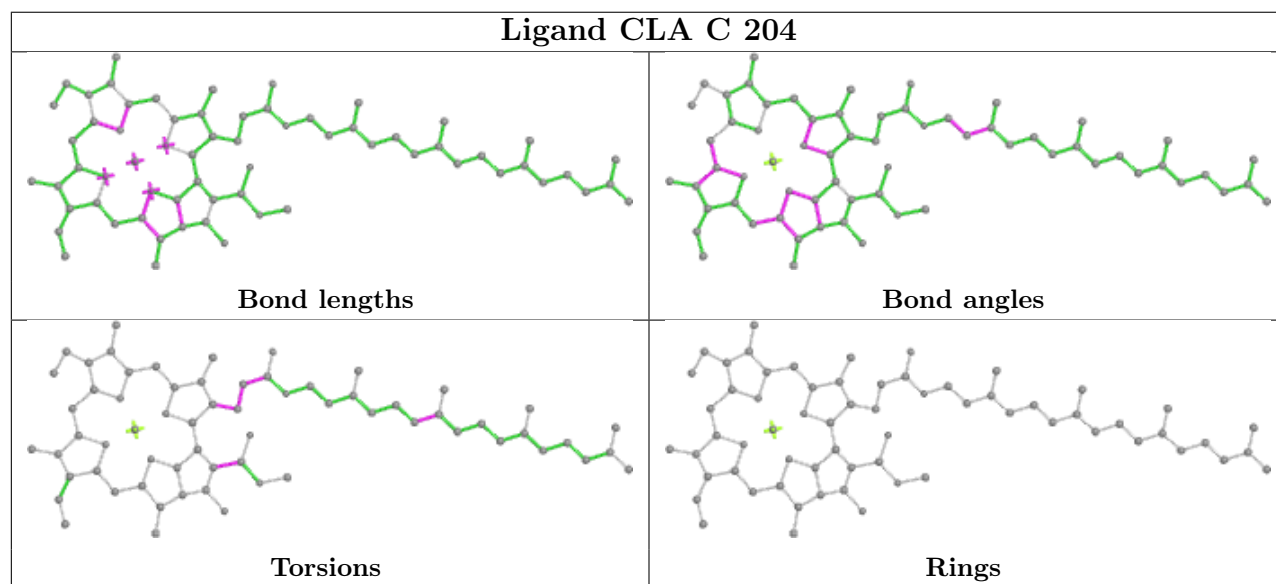
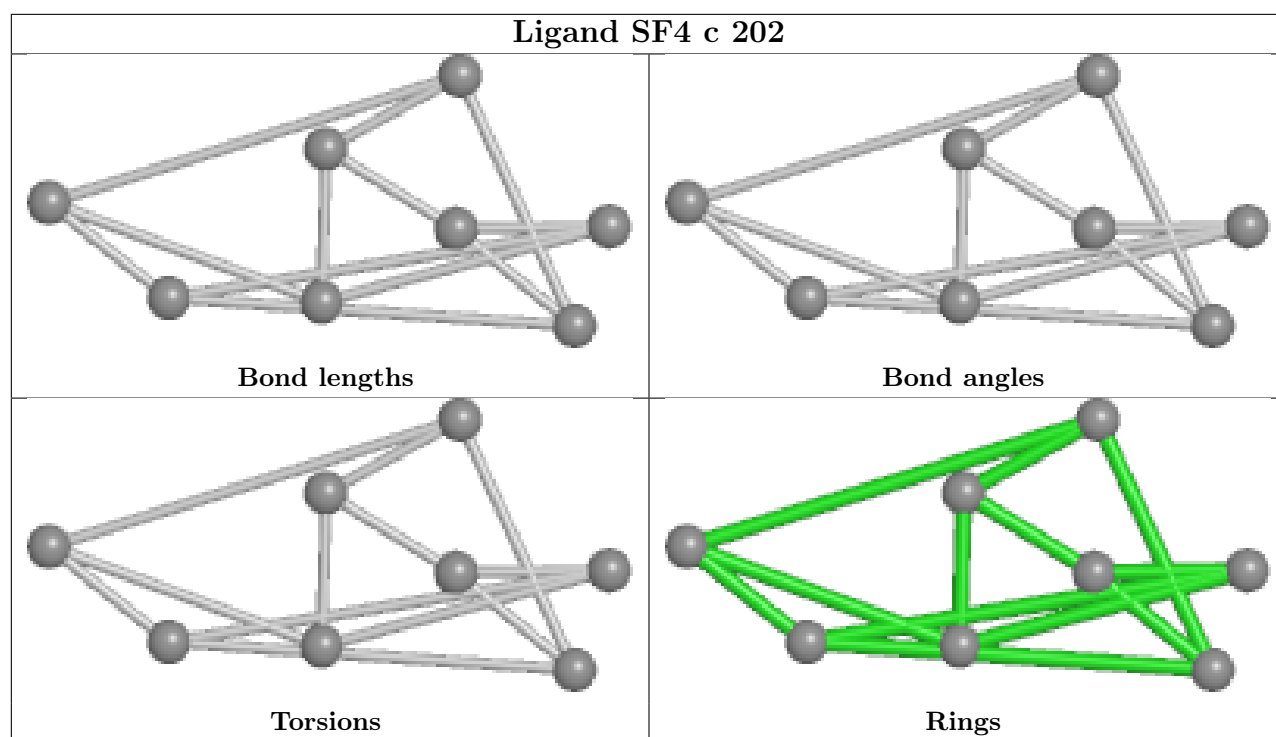


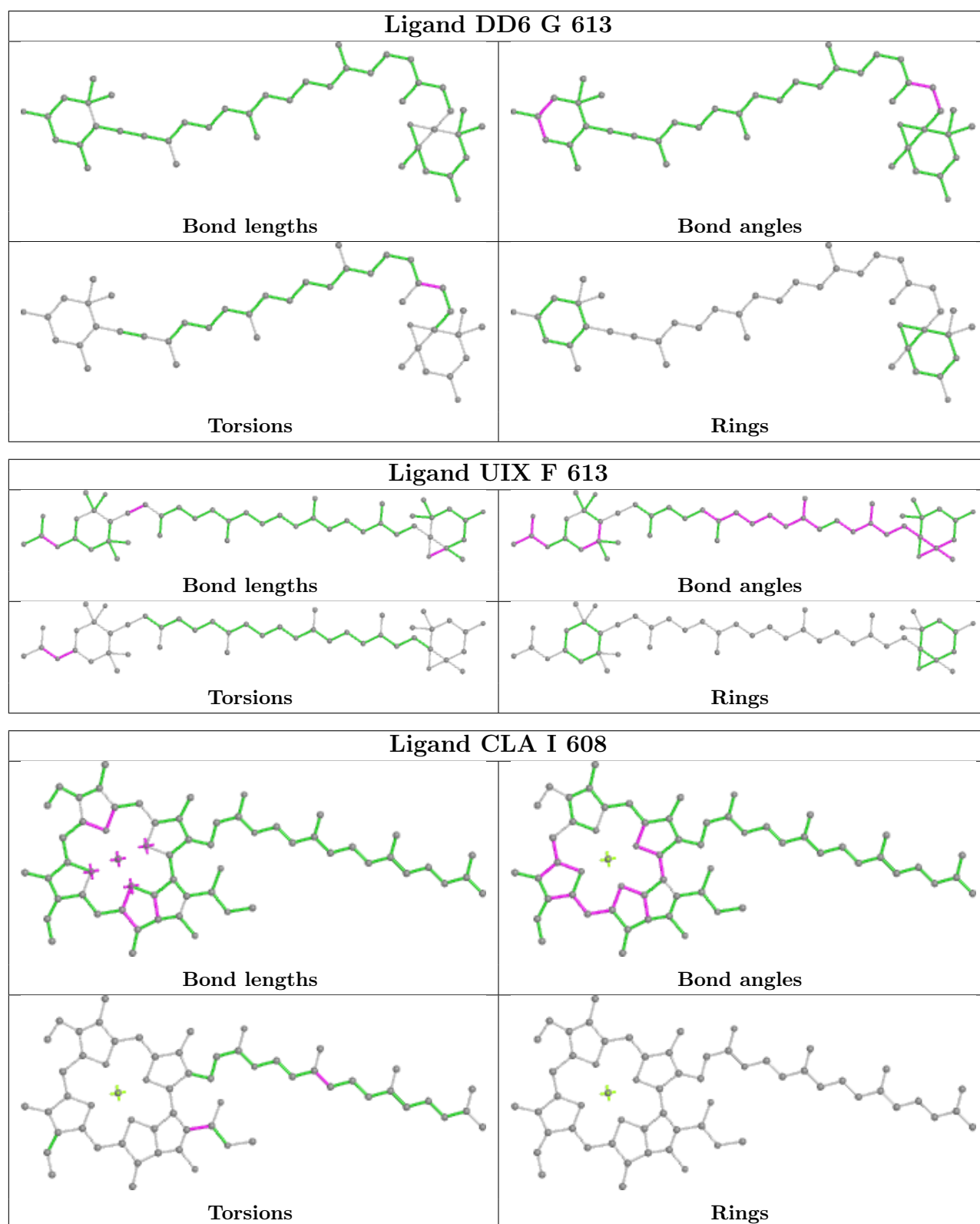


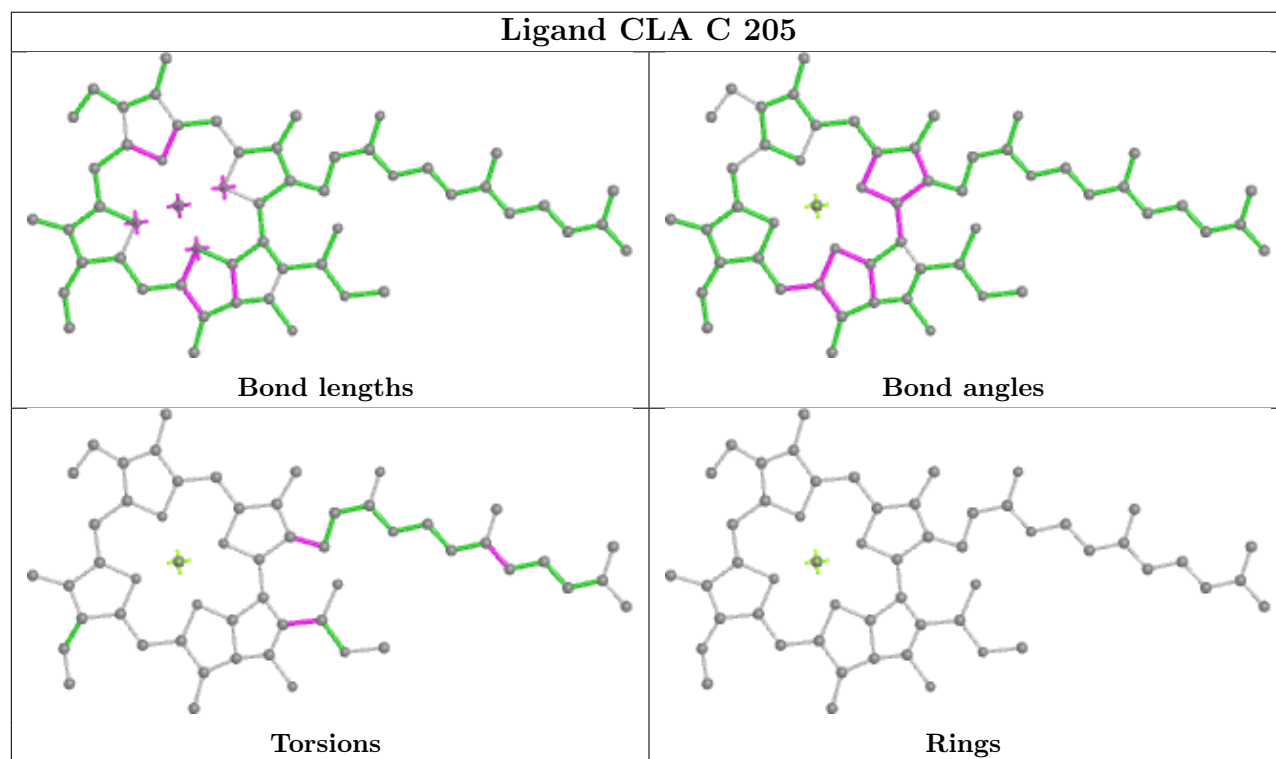
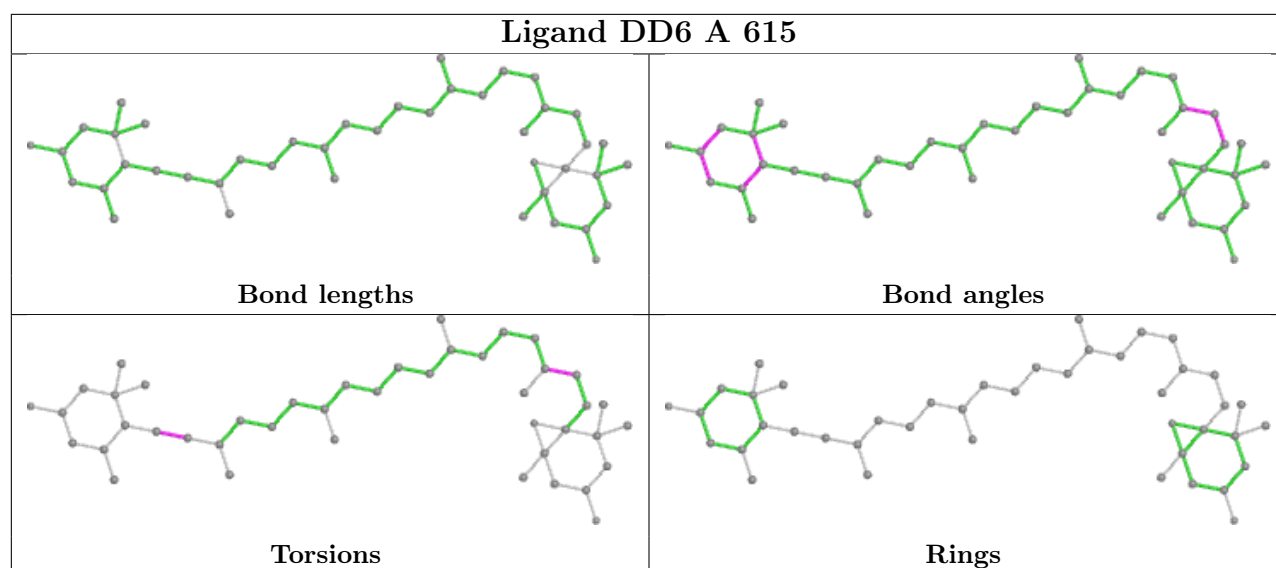


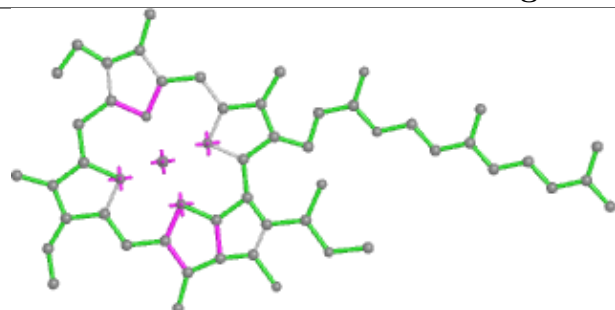
Ligand CLA I 609



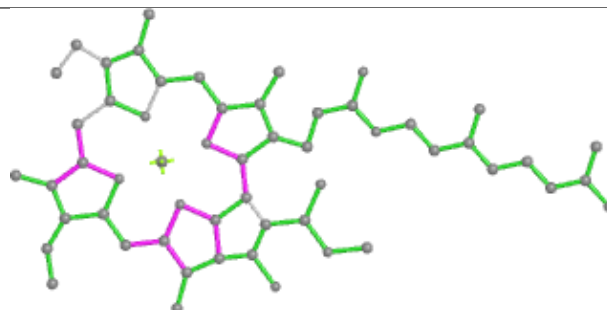




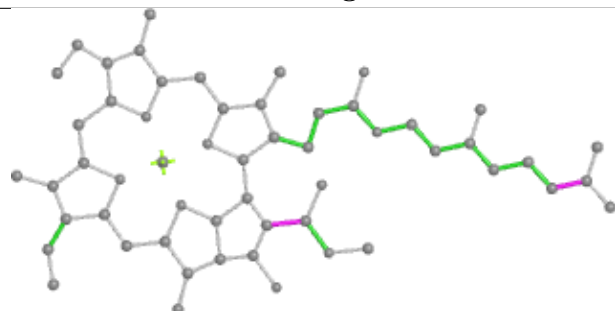


Ligand CLA a 802

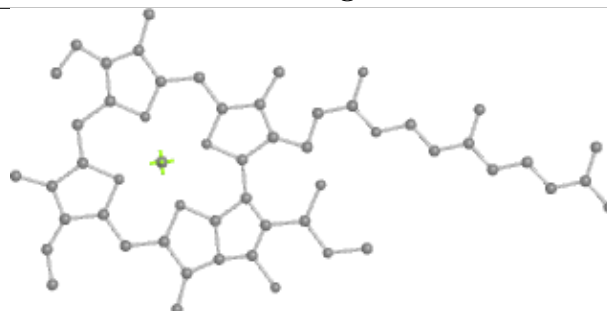
Bond lengths



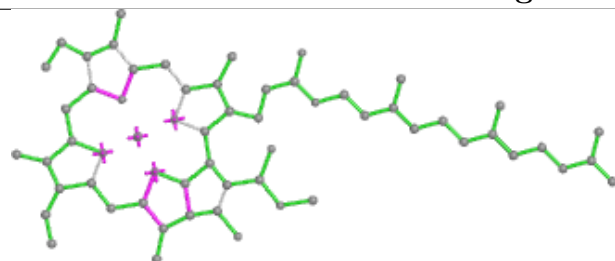
Bond angles



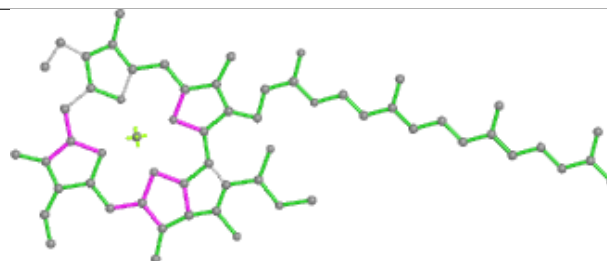
Torsions



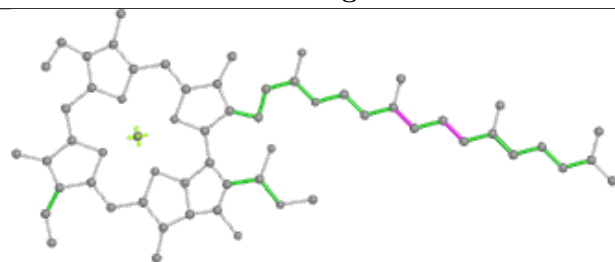
Rings

Ligand CLA D 607

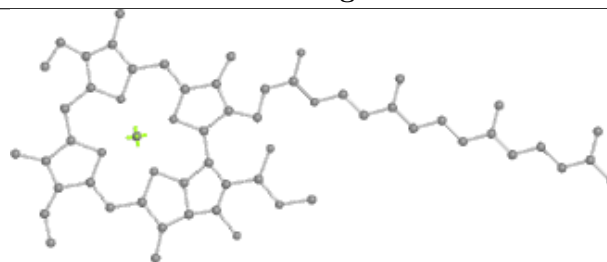
Bond lengths



Bond angles

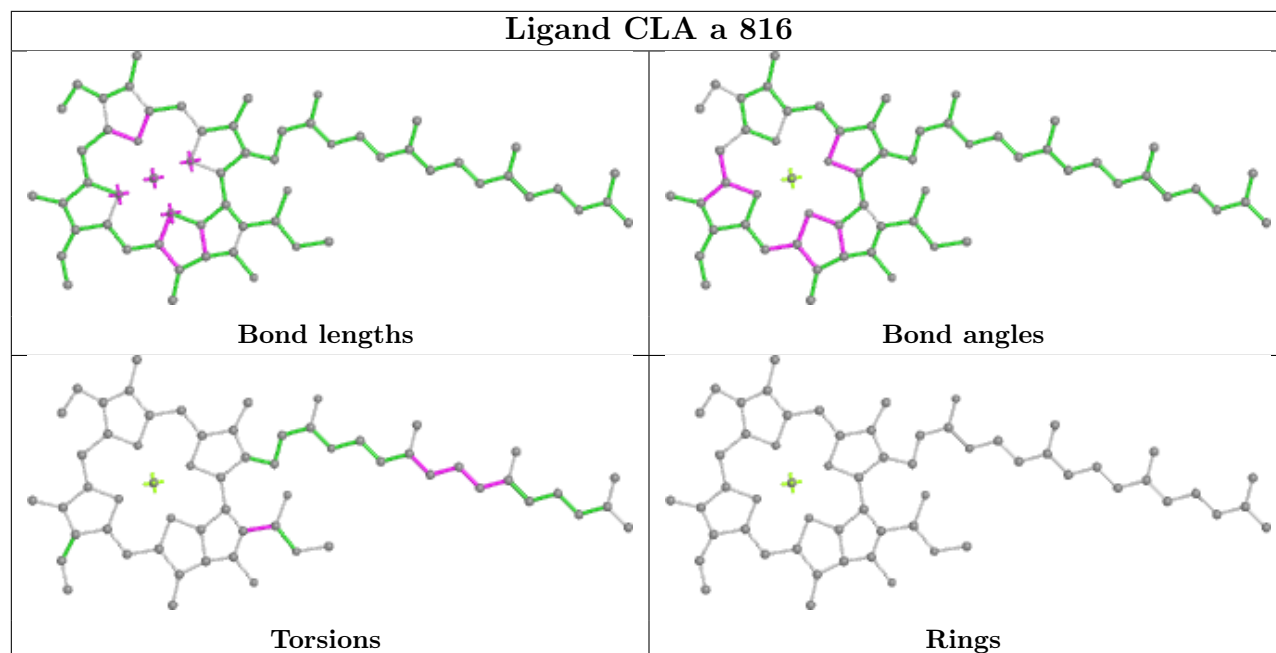


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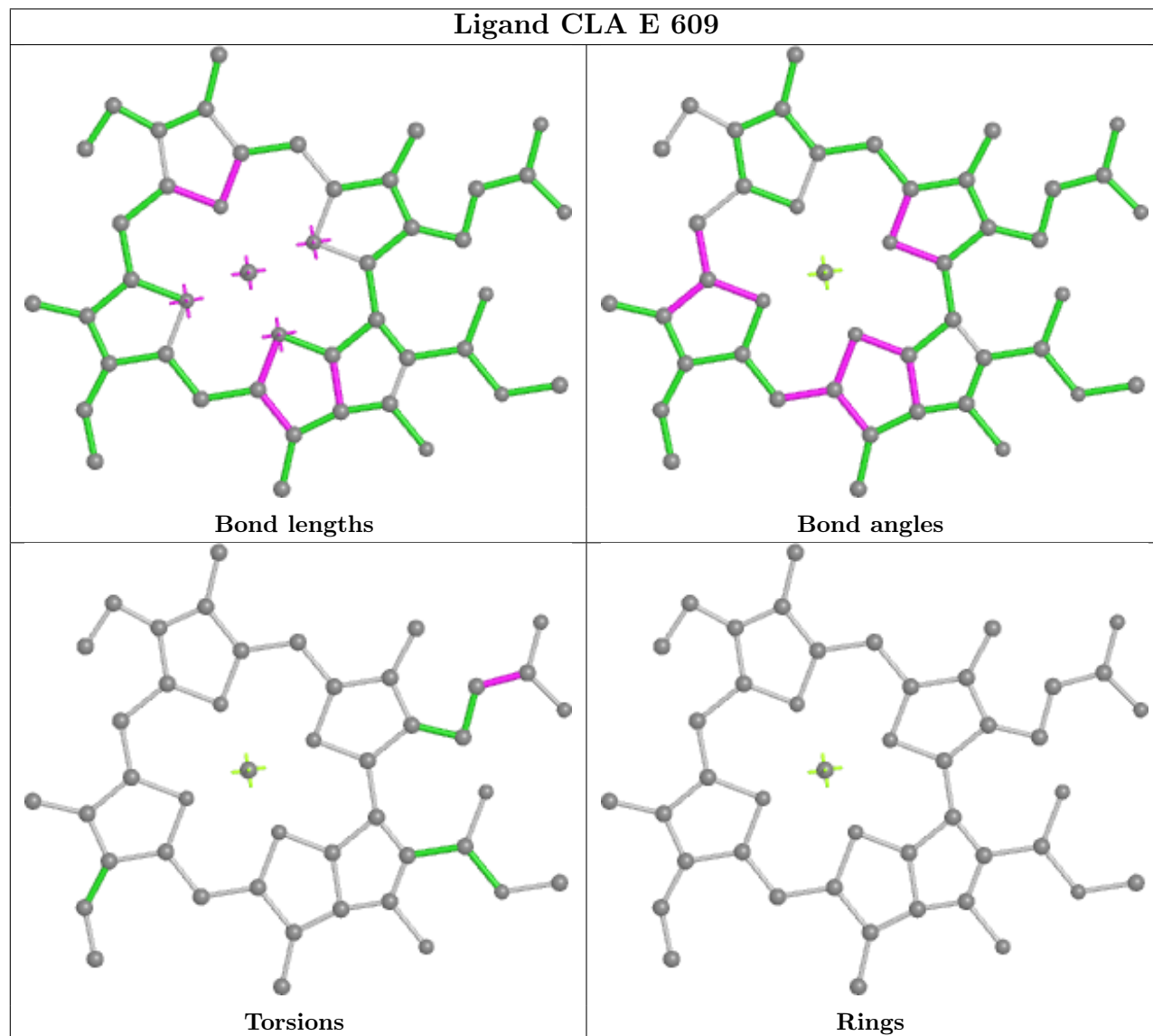


Rings

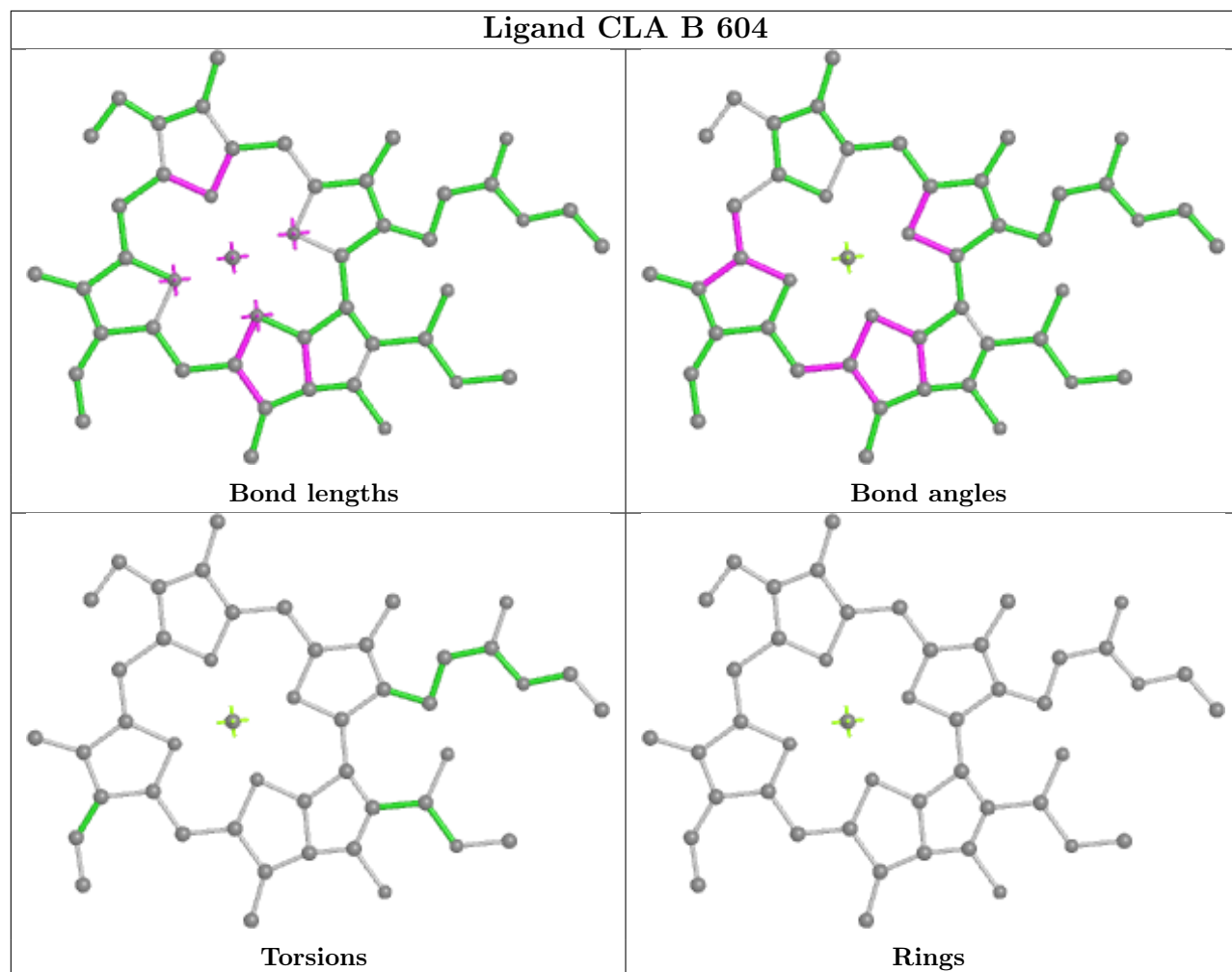
Ligand CLA a 816



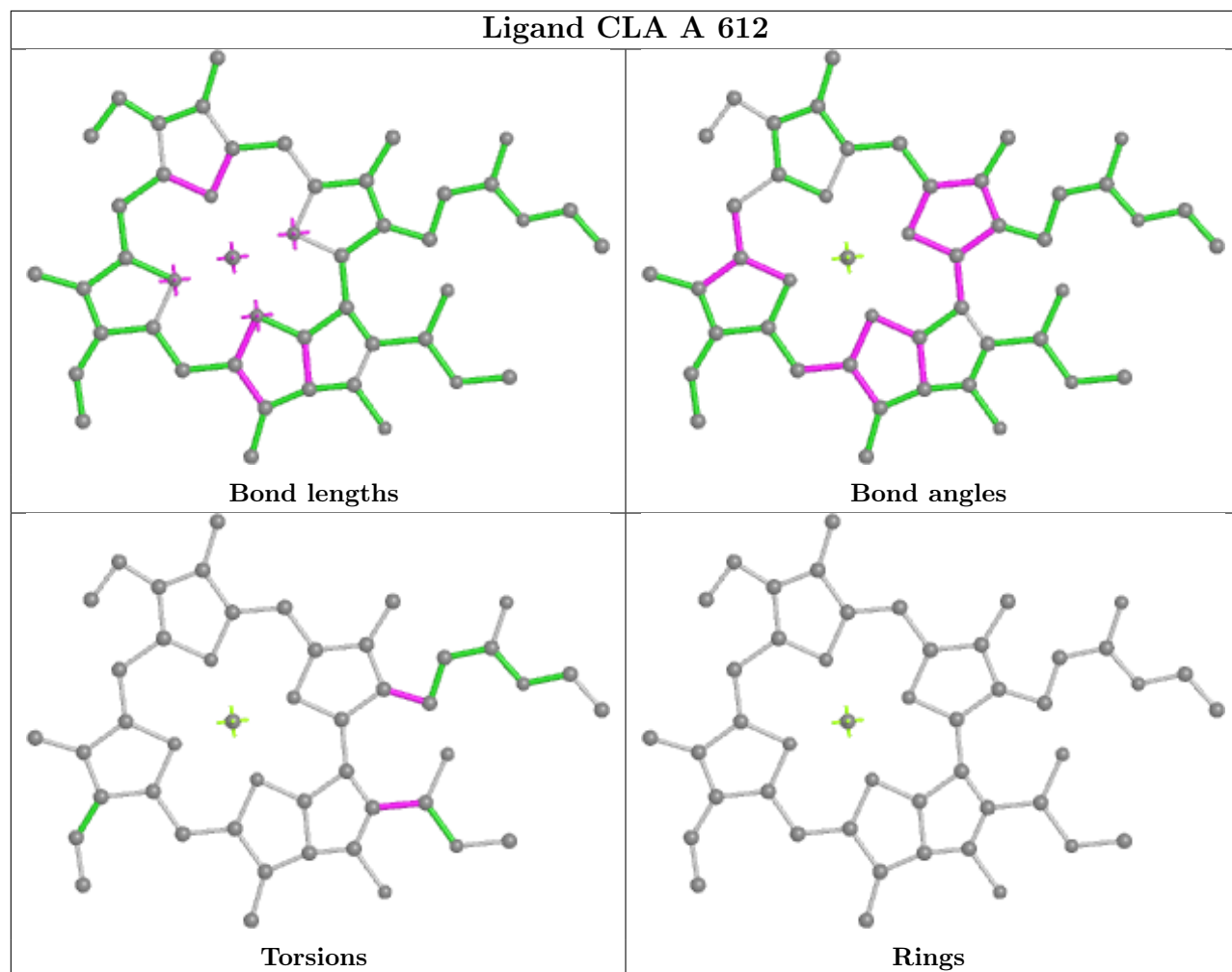
Ligand CLA E 609



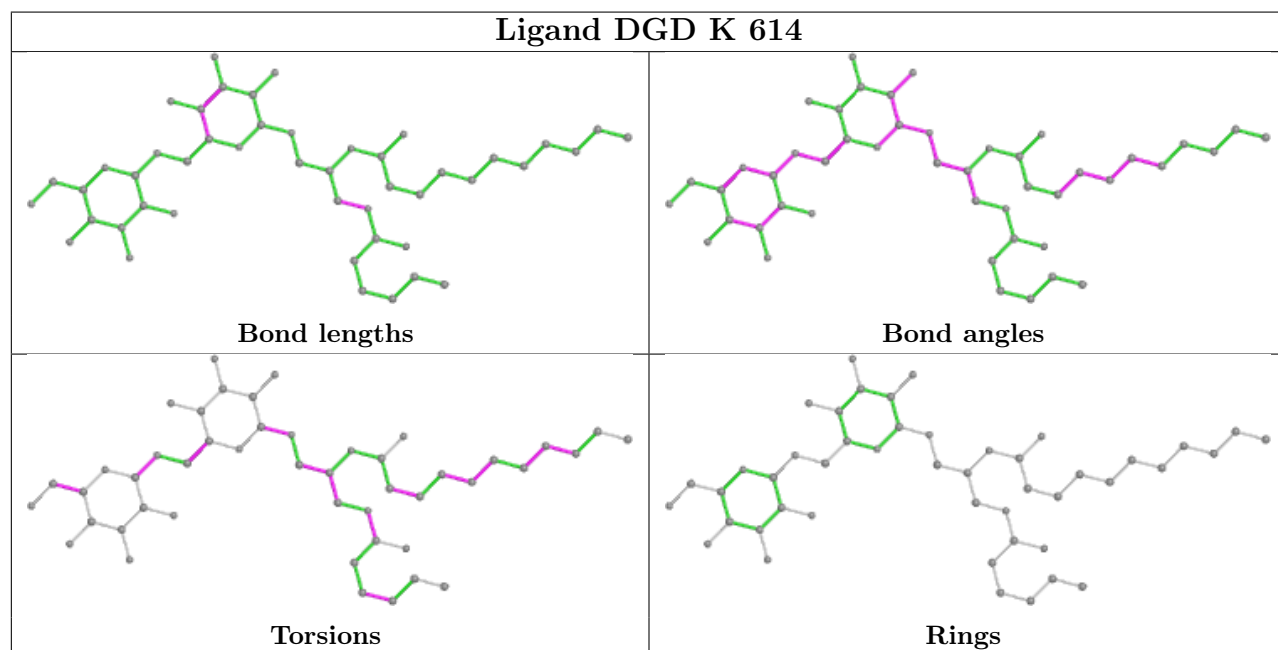
Ligand CLA B 604



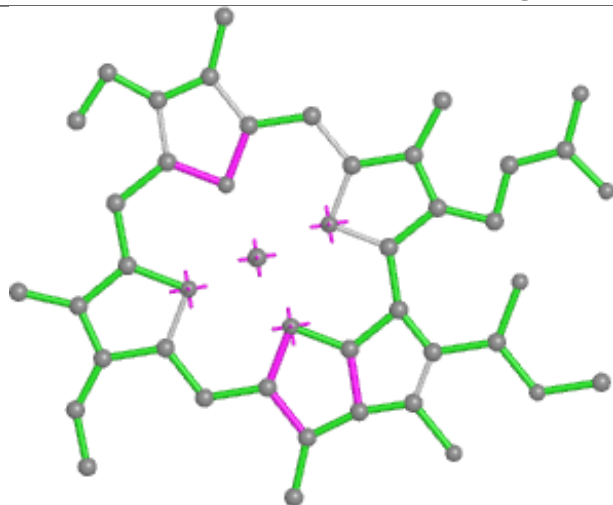
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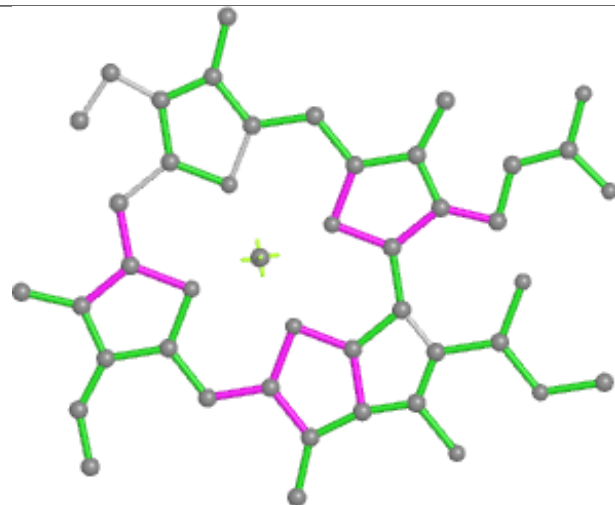
Ligand DGD K 614



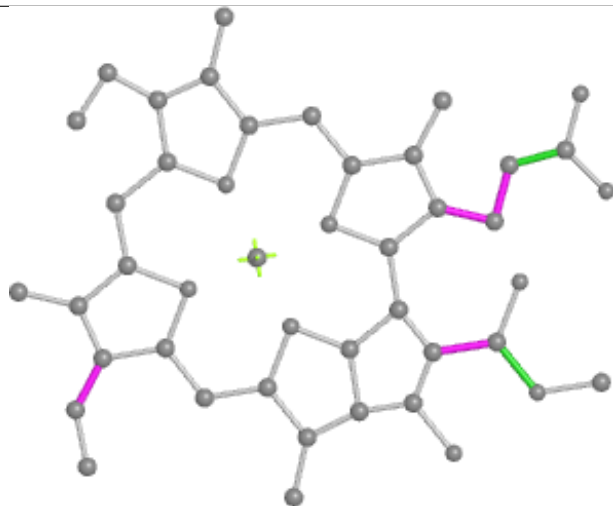
Ligand CLA F 605



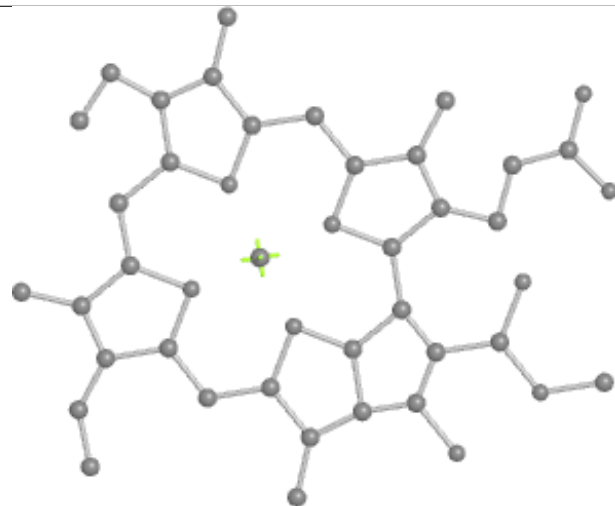
Bond lengths



Bond angles

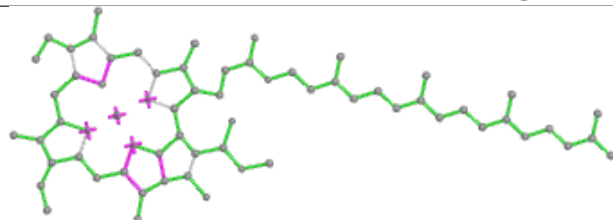


Torsions

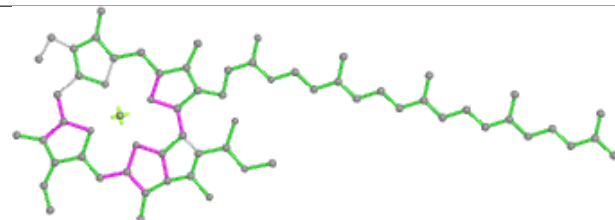


Rings

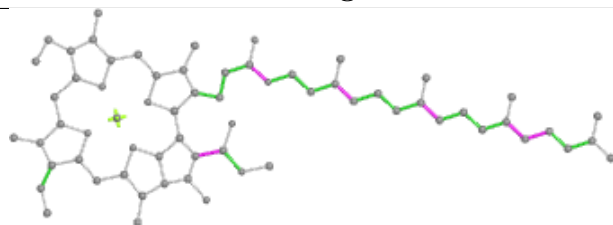
Ligand CLA E 607



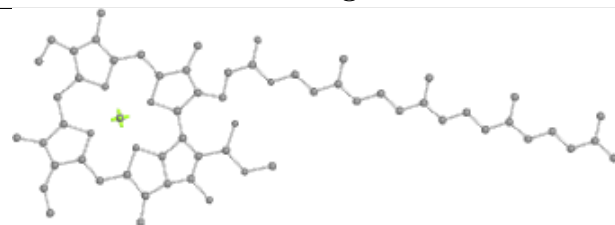
Bond lengths



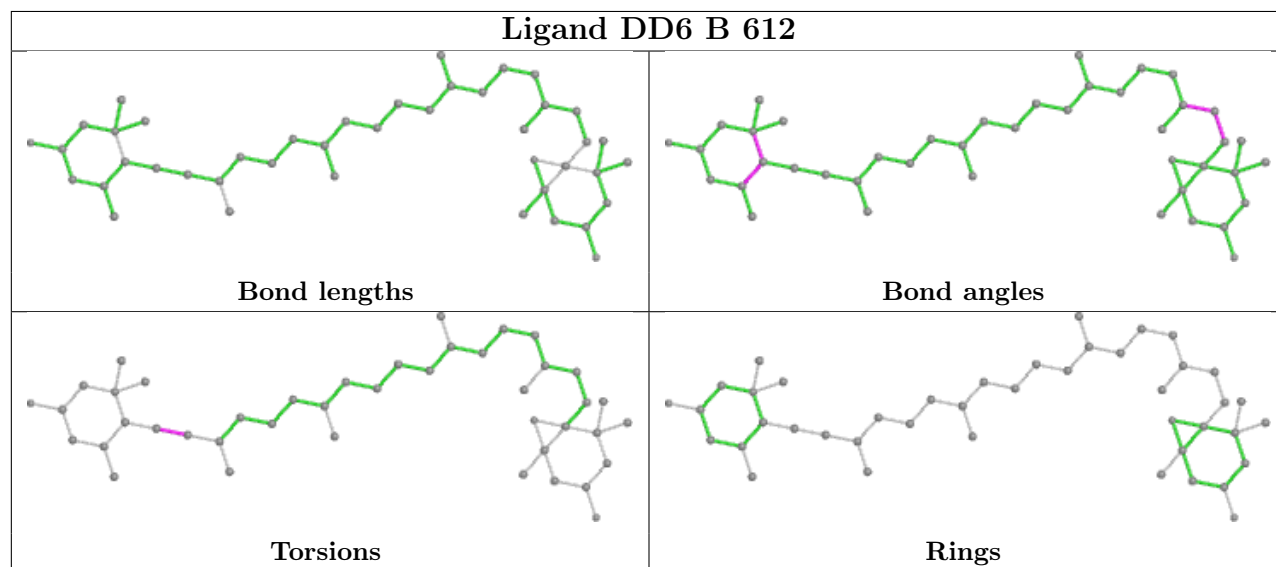
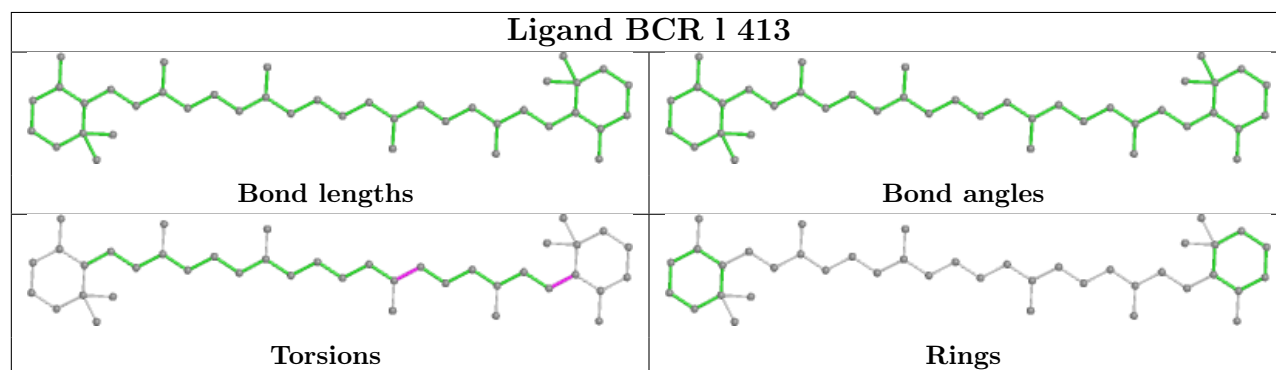
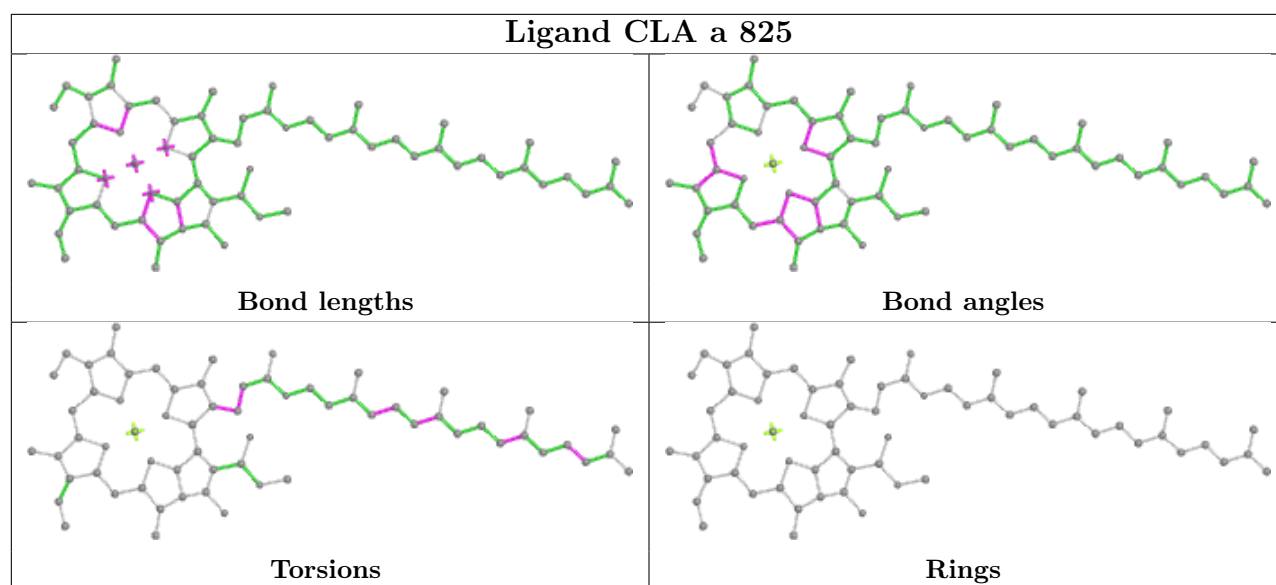
Bond angles

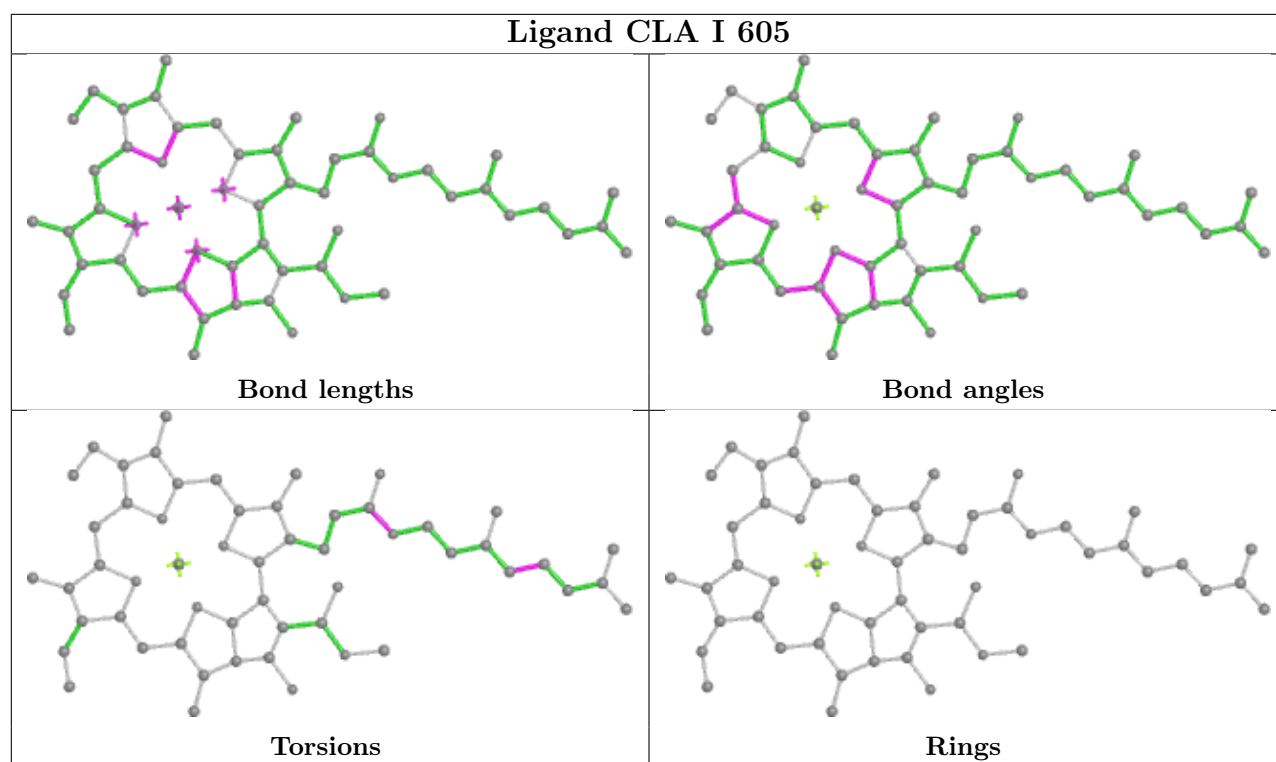


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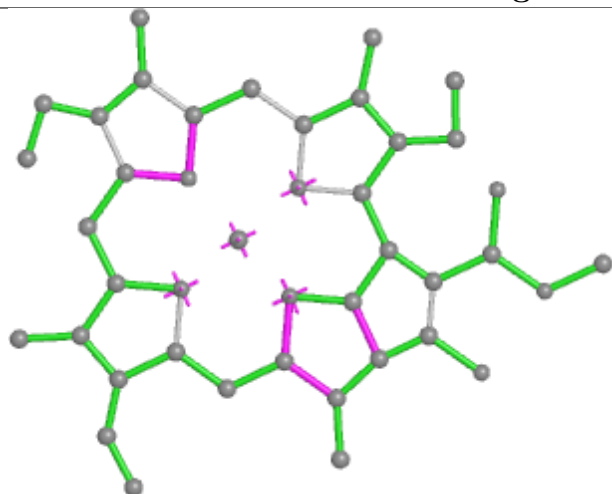


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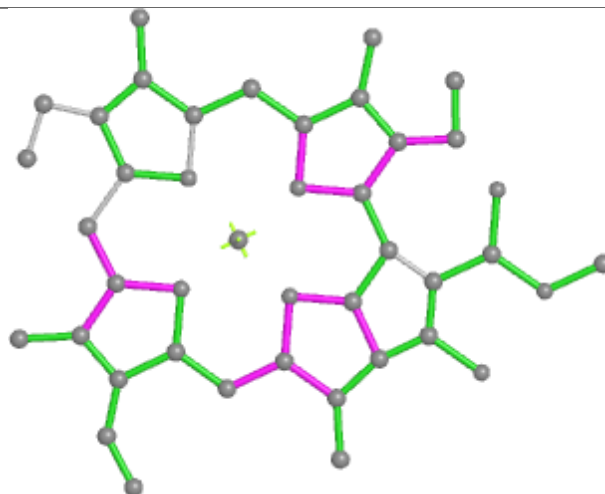




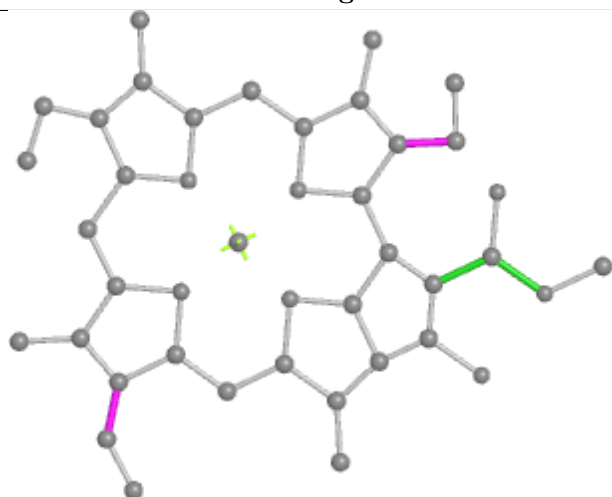
Ligand CLA A 601



Bond lengths



Bond angles

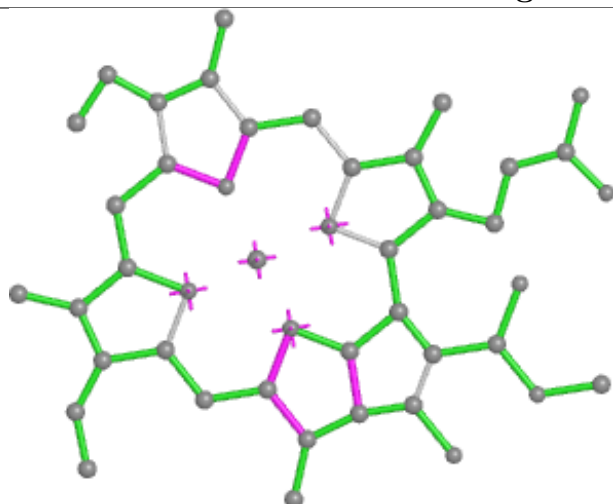


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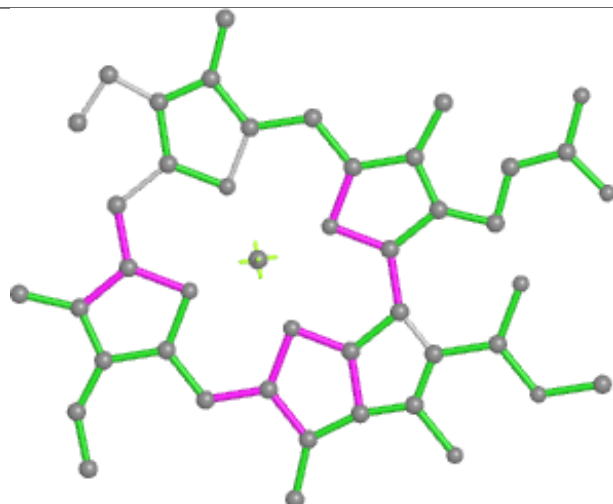


Rings

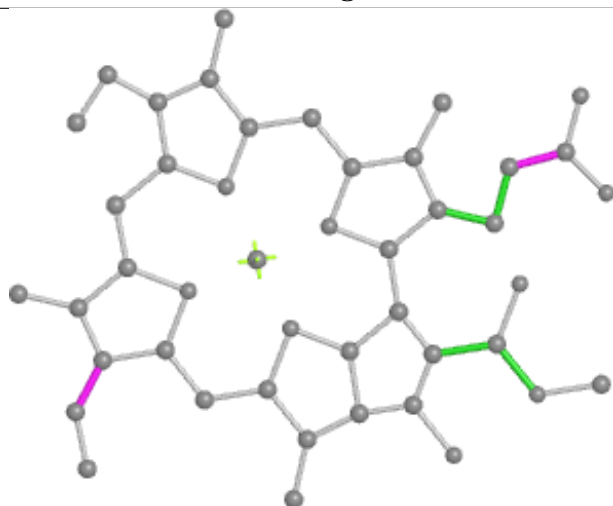
Ligand CLA F 604



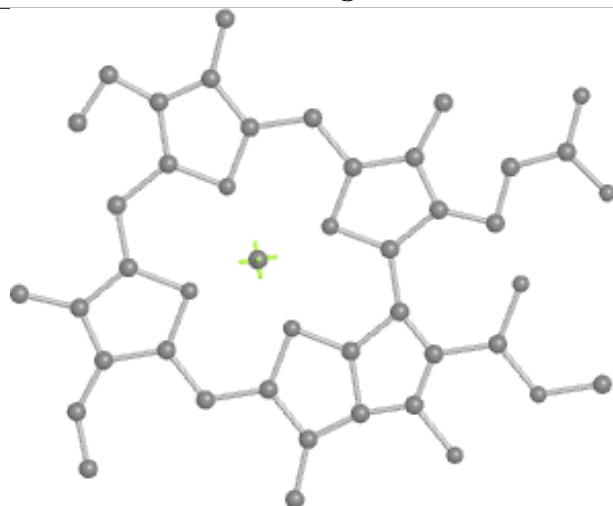
Bond lengths



Bond angles

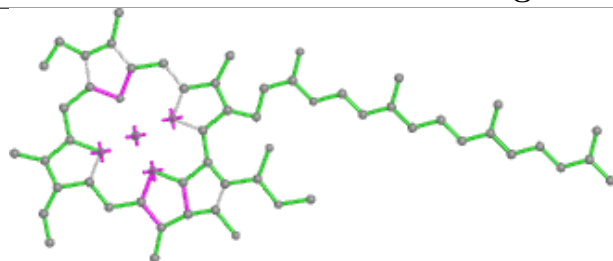


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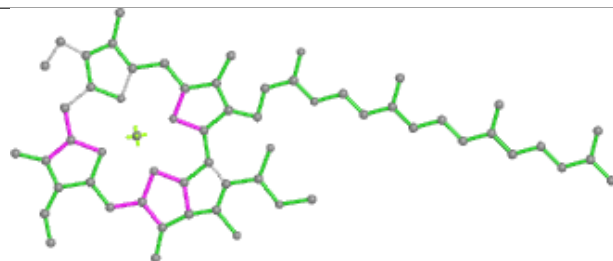


Rings

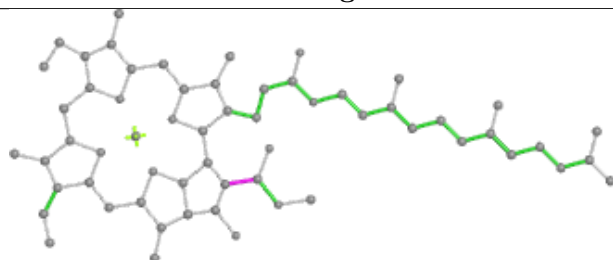
Ligand CLA A 602



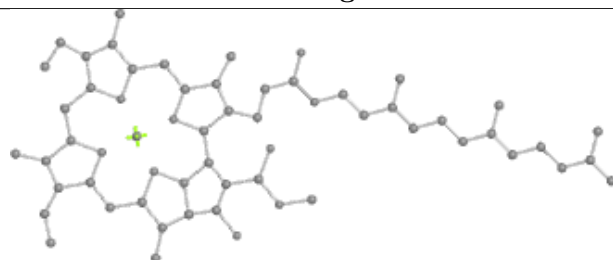
Bond lengths



Bond angles

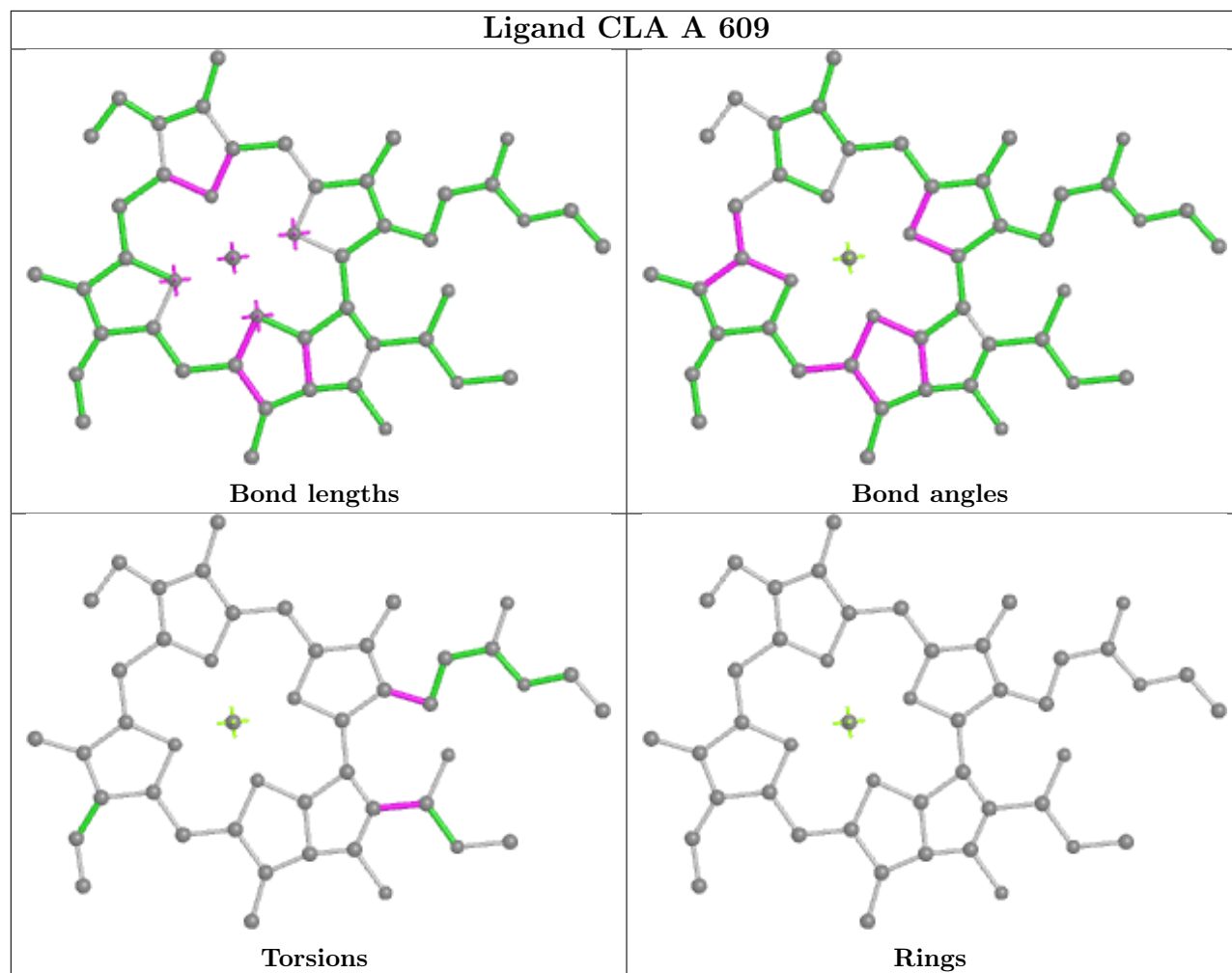


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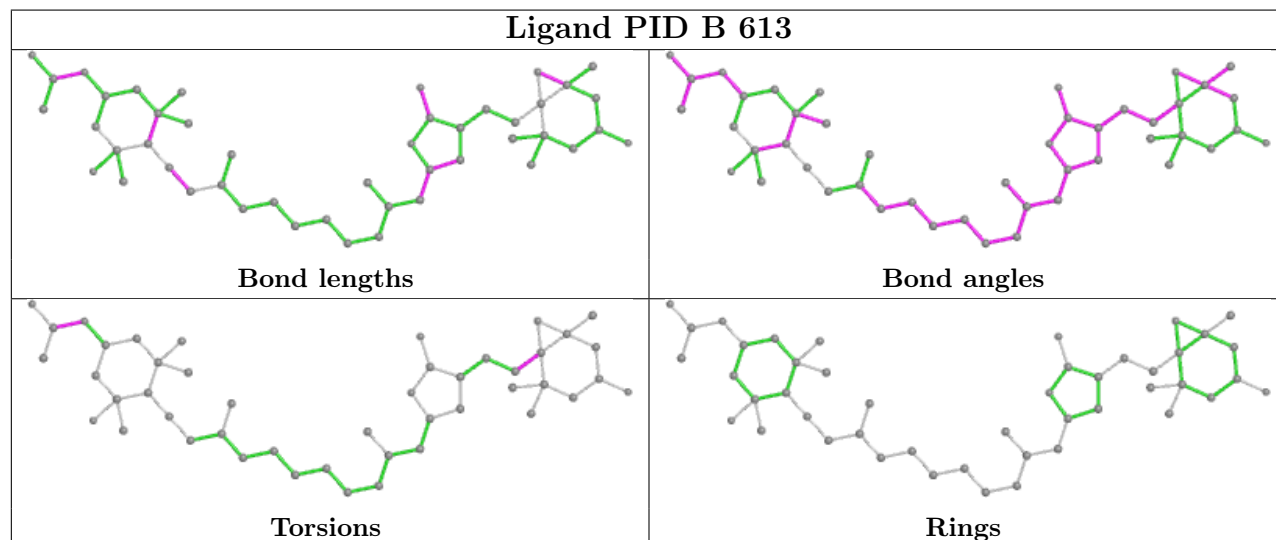


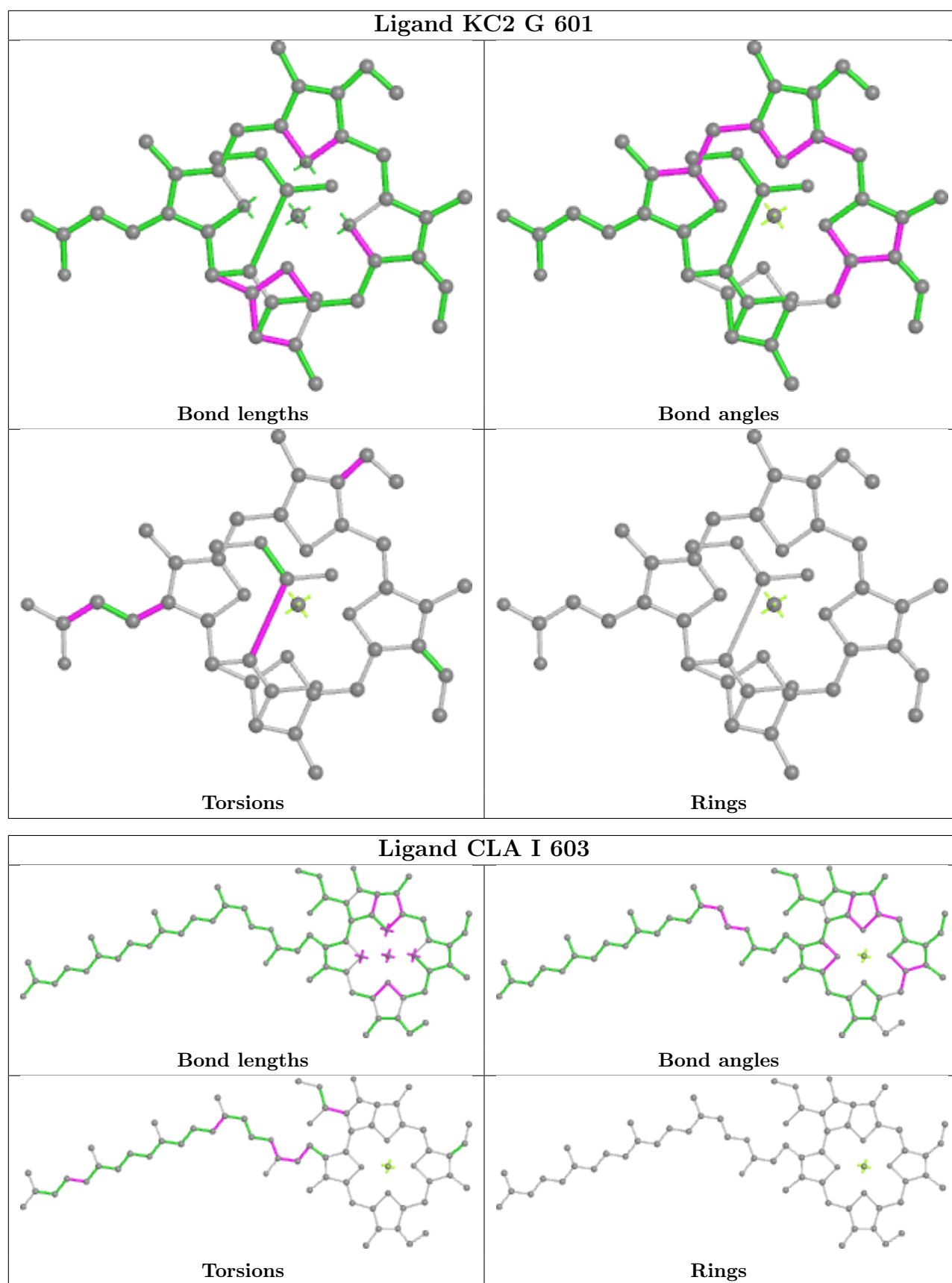
Rings

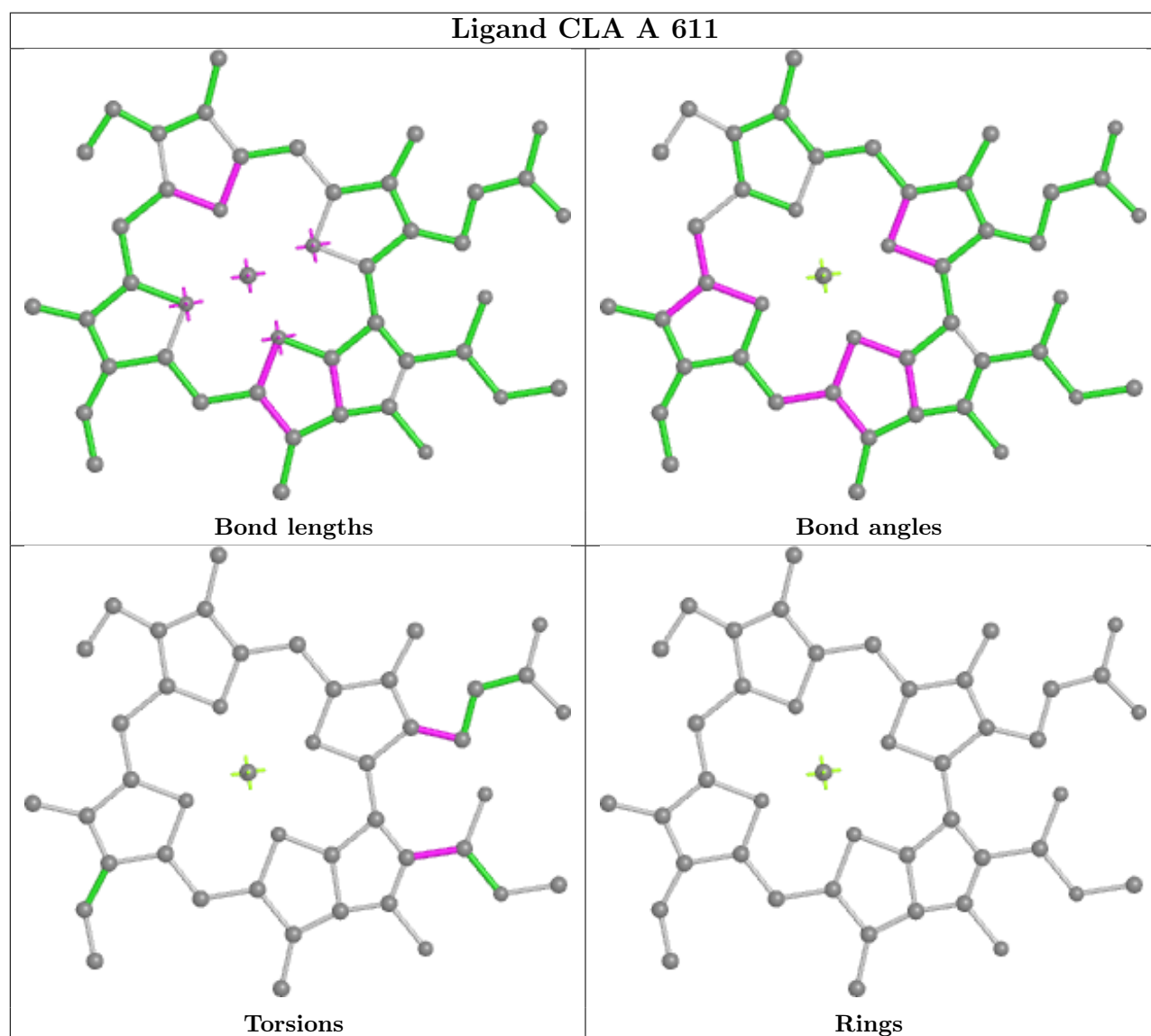
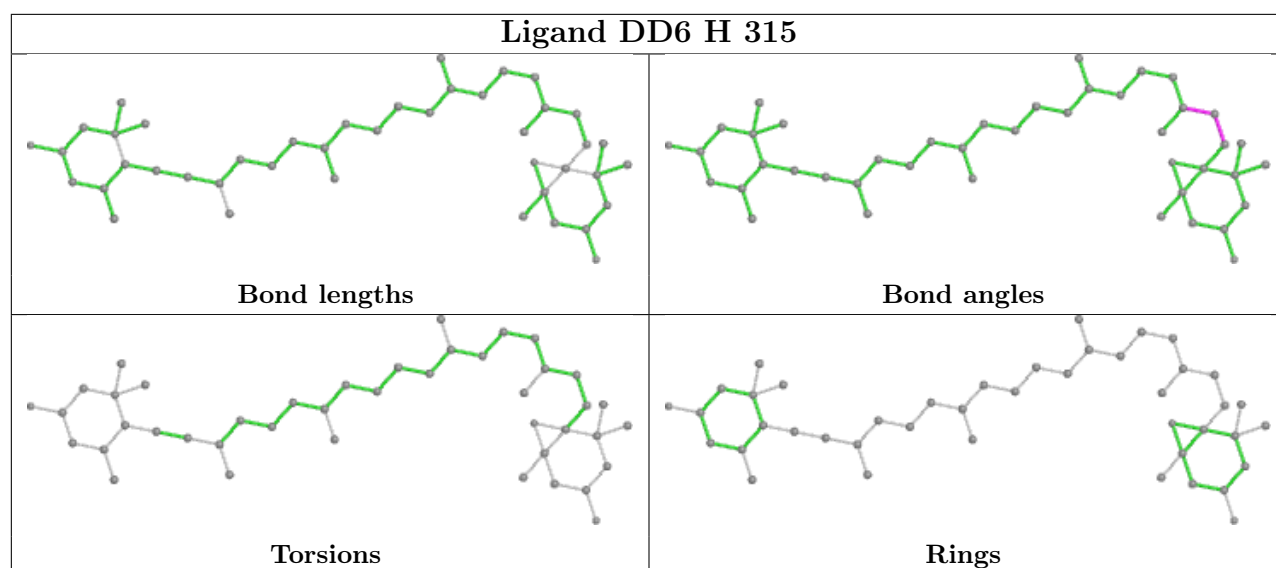
Ligand CLA A 609



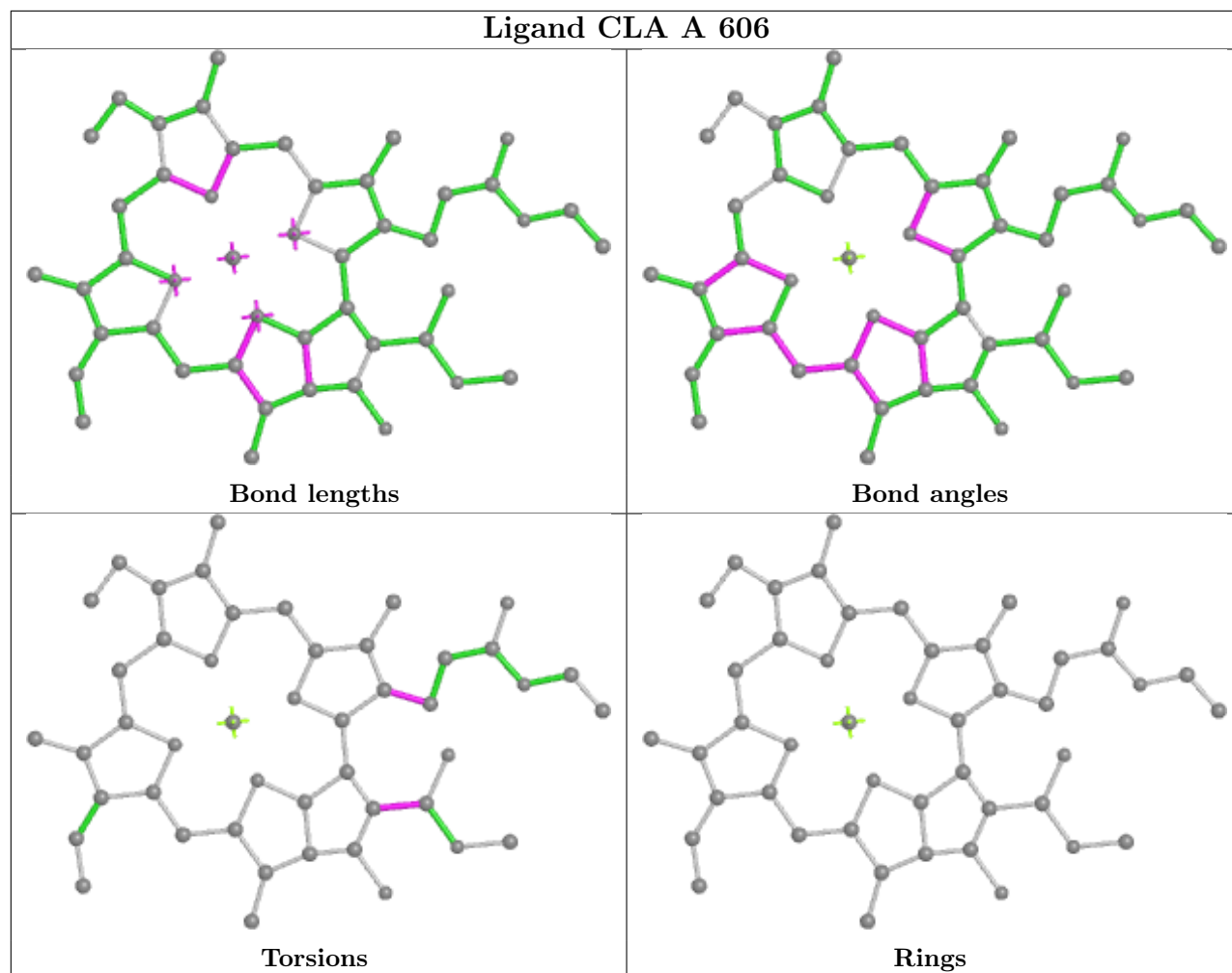
Ligand PID B 613



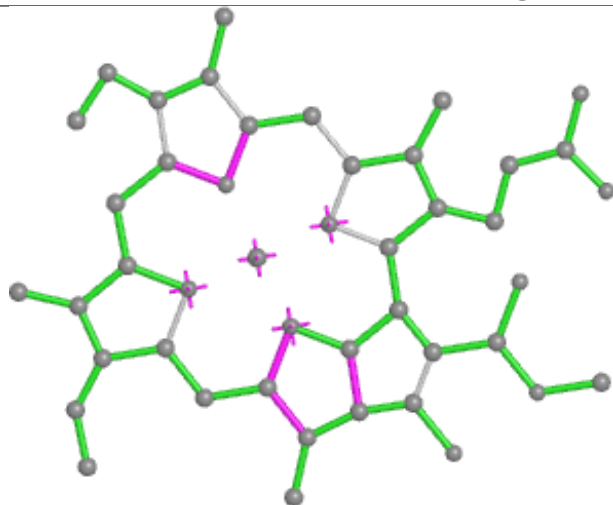




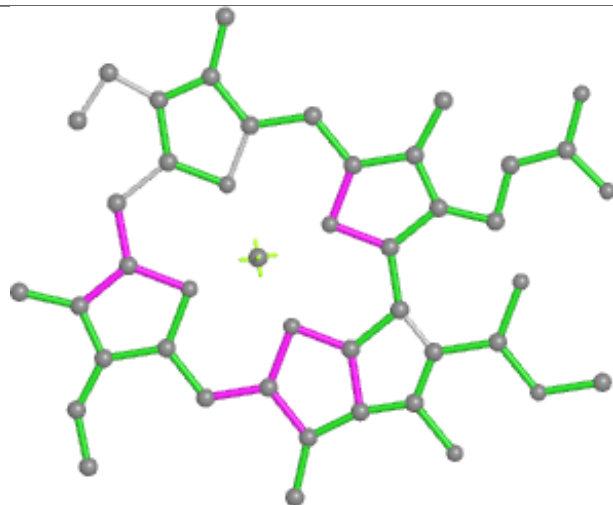
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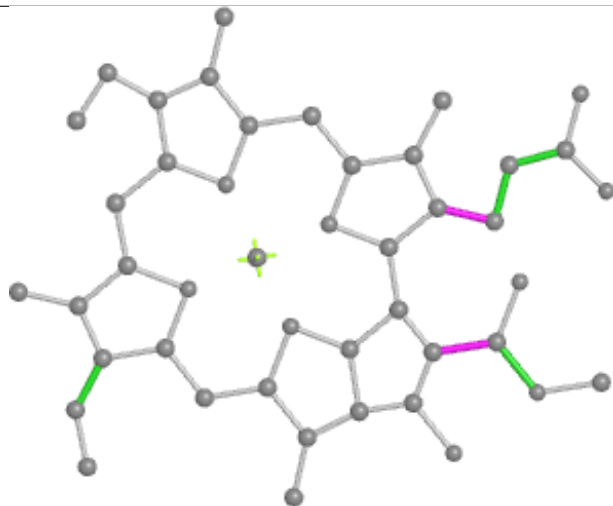
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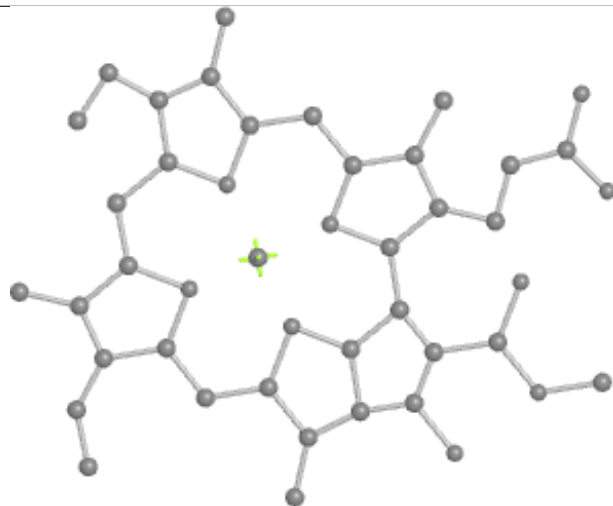
Bond lengths



Bond angles

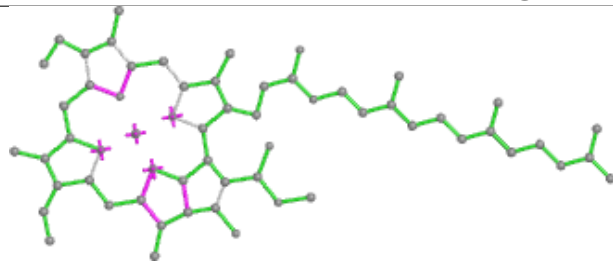


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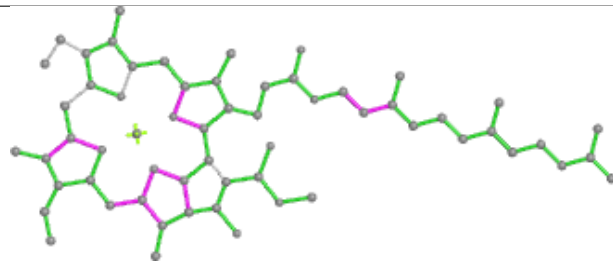


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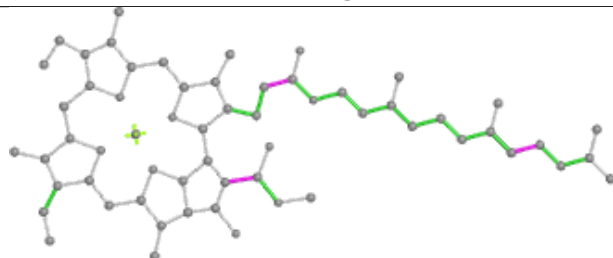
Ligand CLA F 601



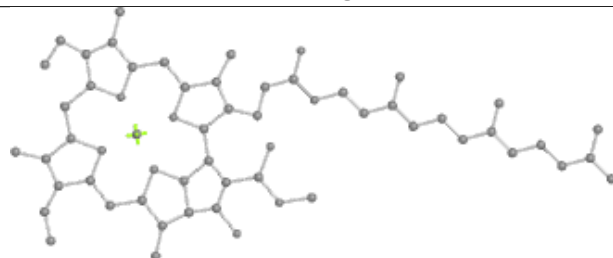
Bond lengths



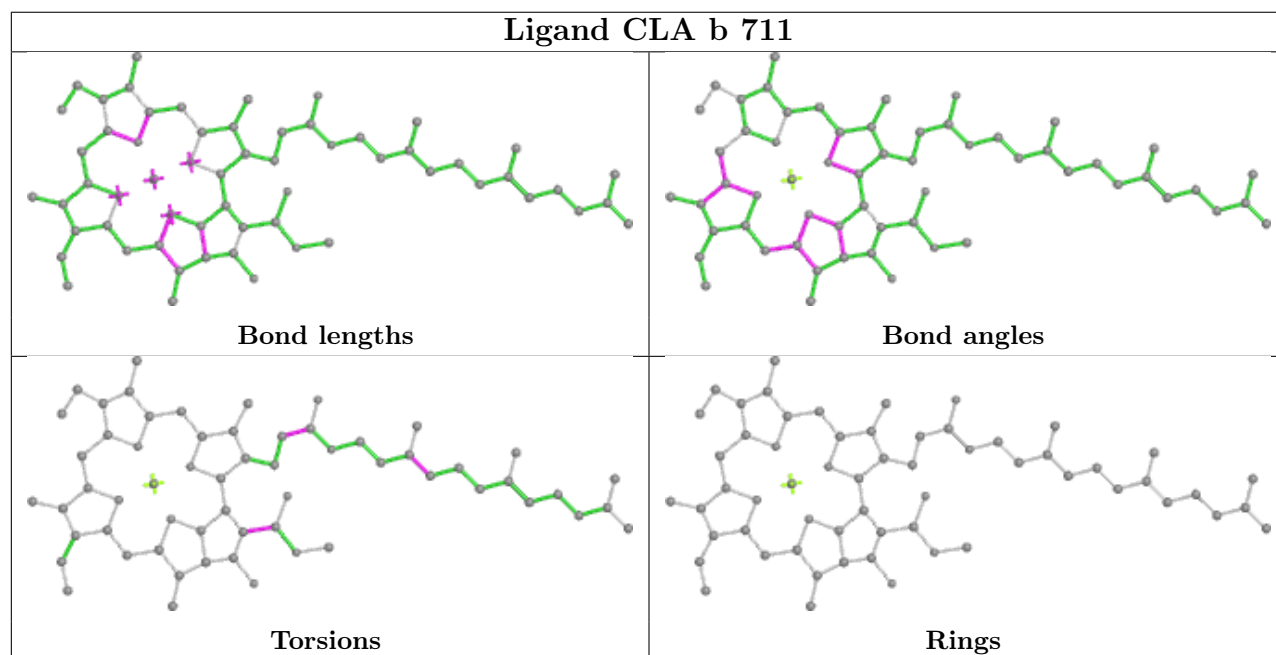
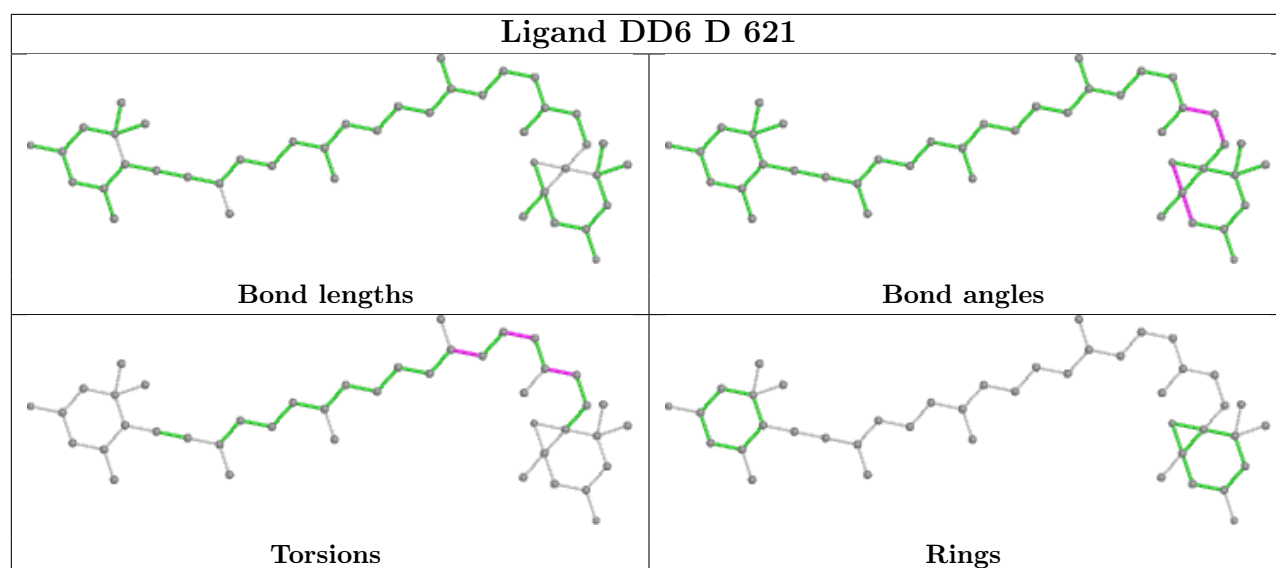
Bond angles



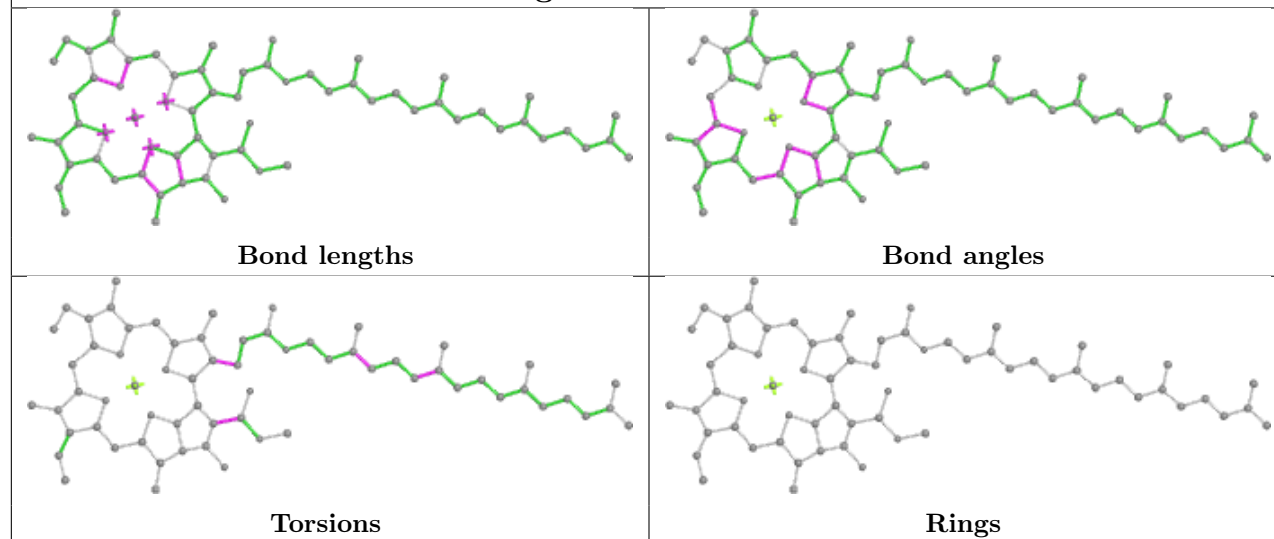
Torsions



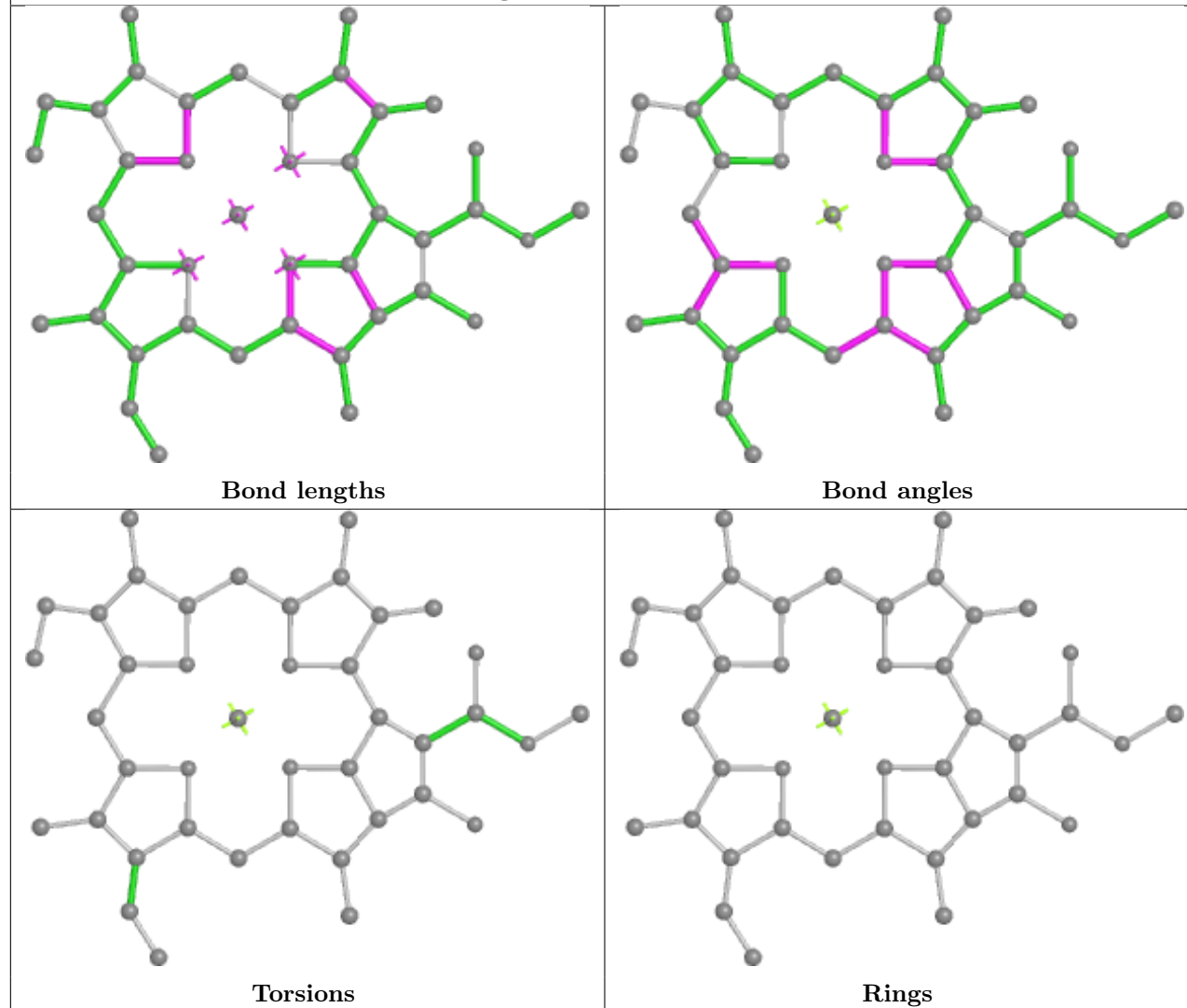
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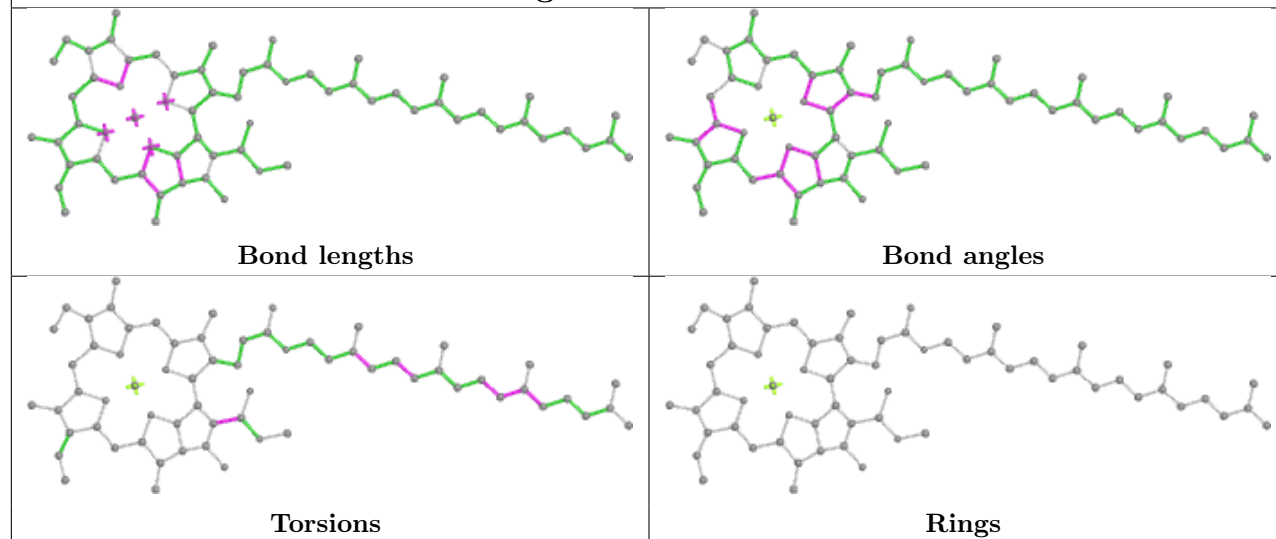
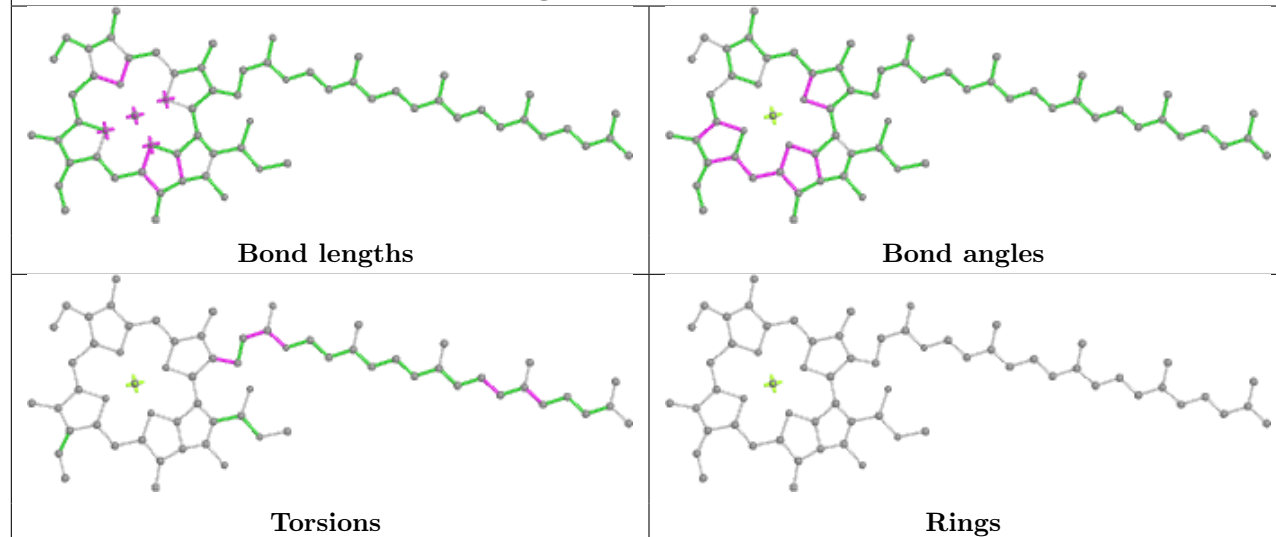


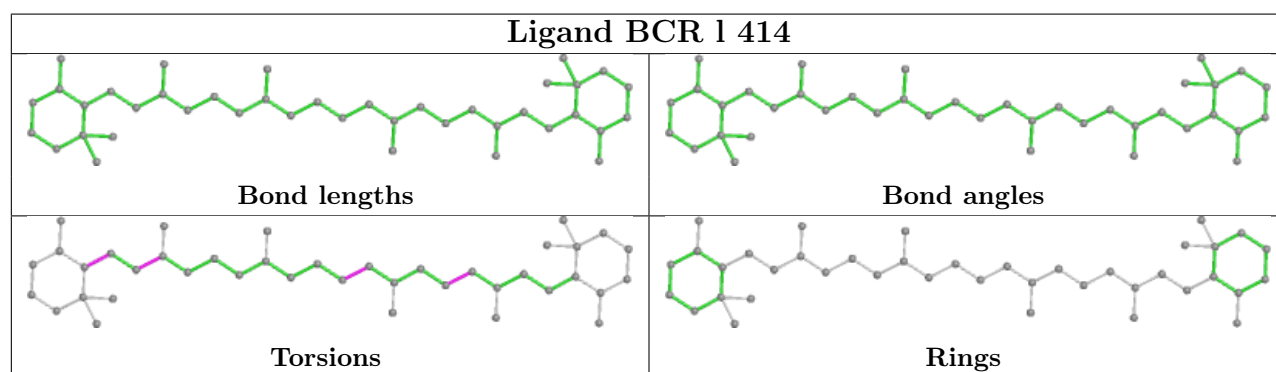
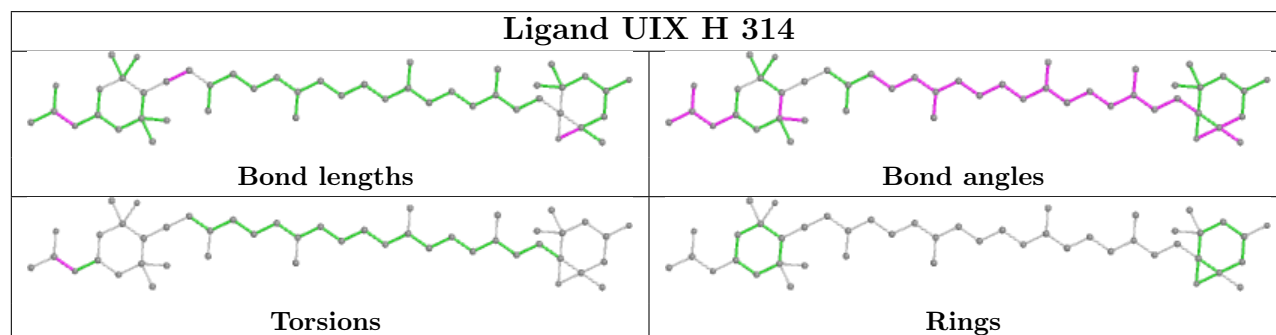
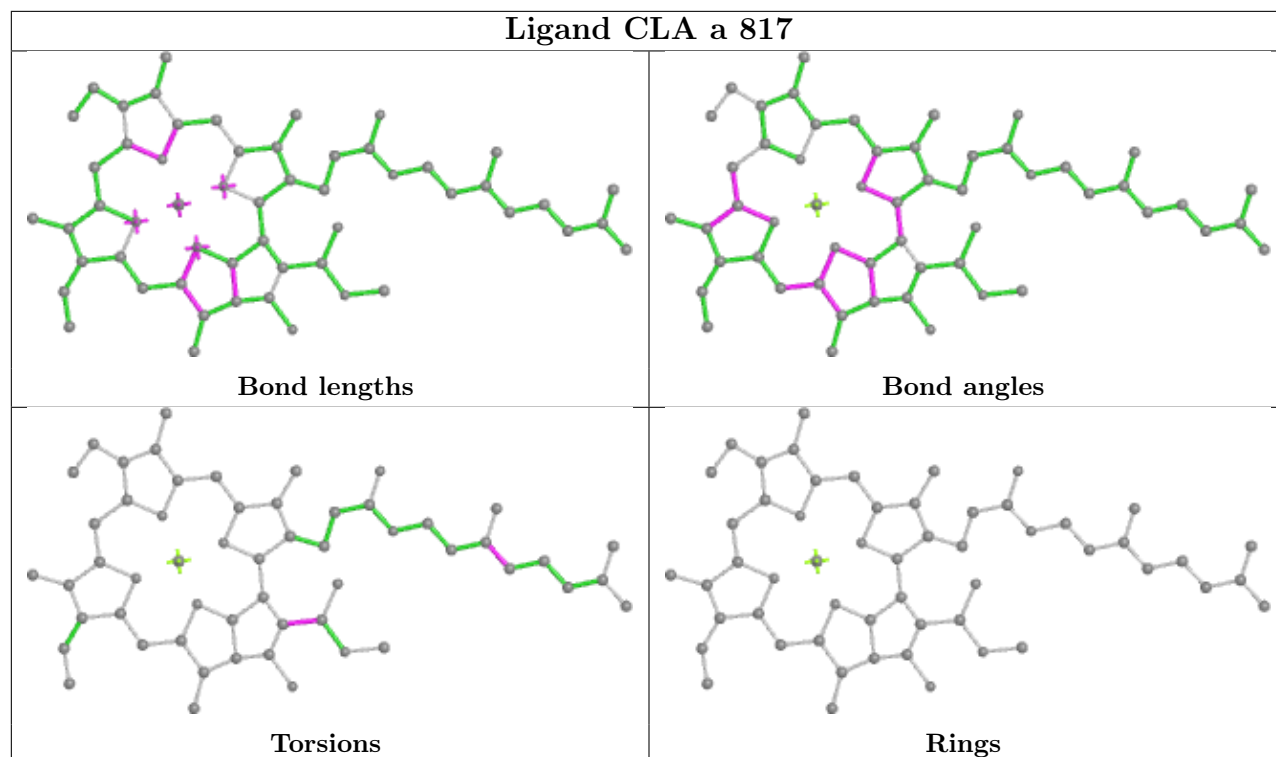
Ligand CLA b 708

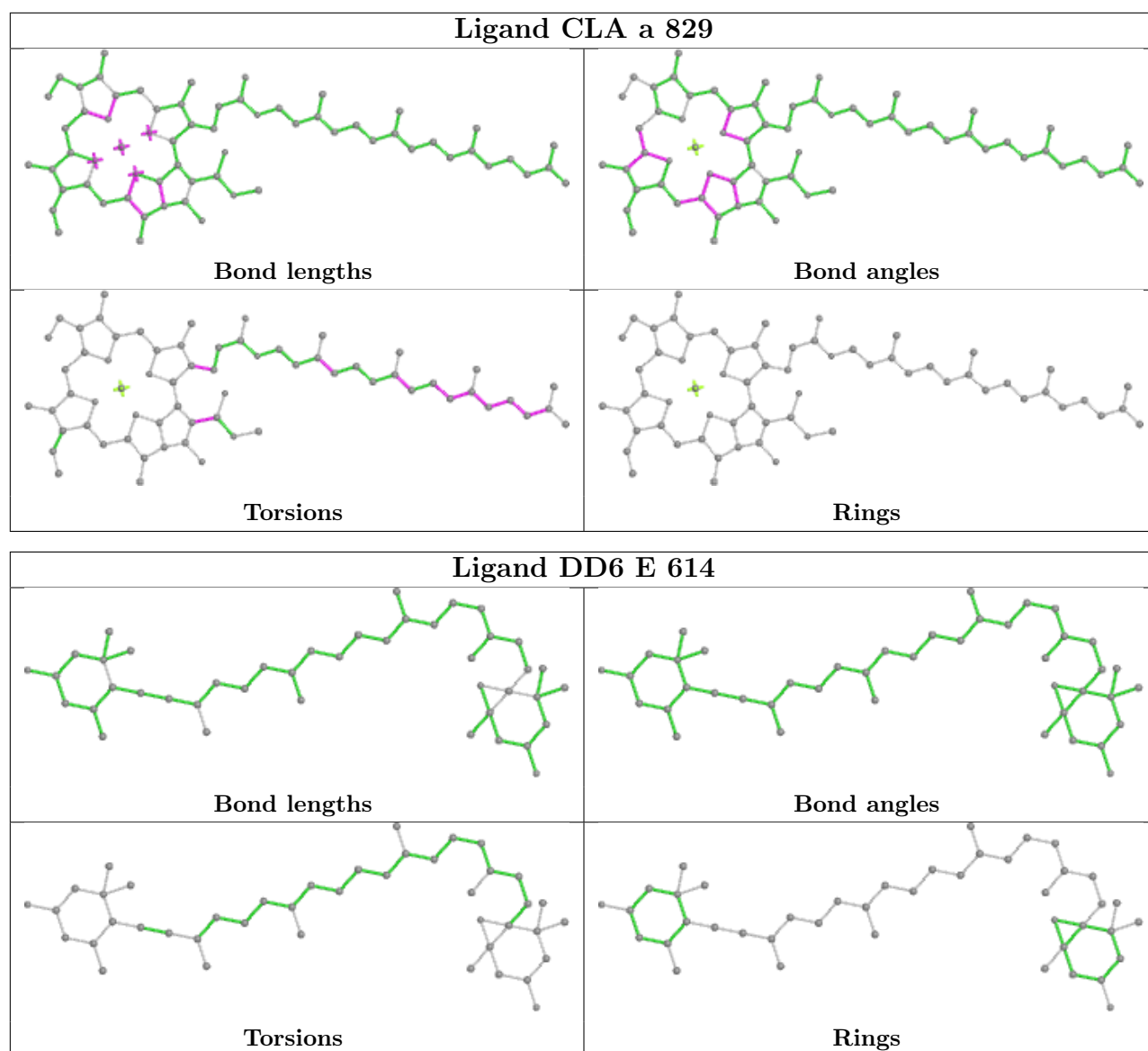


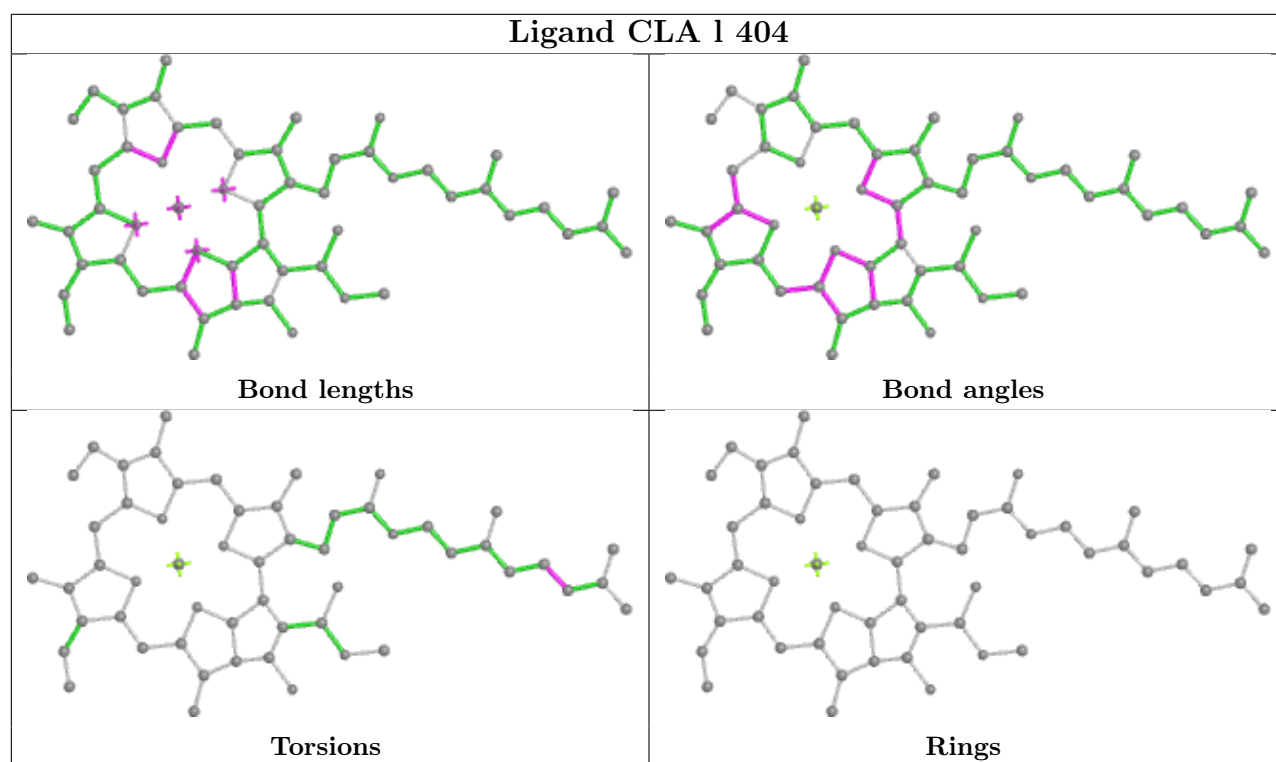
Ligand CLA T 604



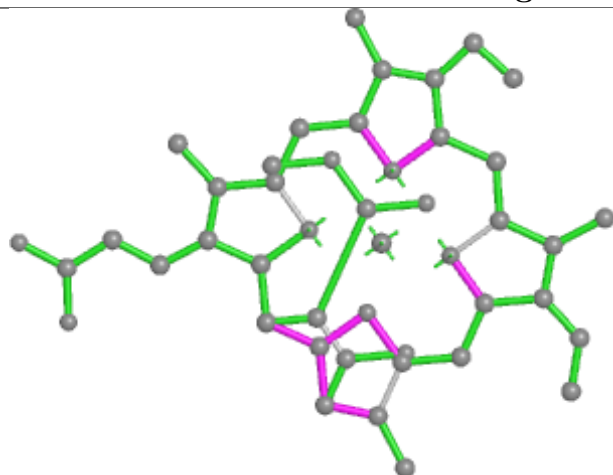
Ligand CLA a 824**Ligand CLA b 717**



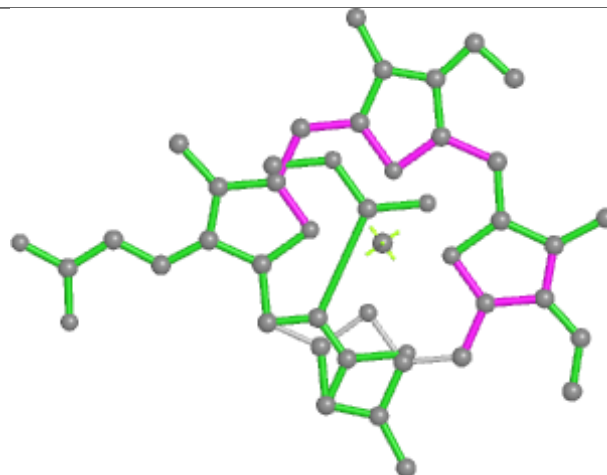




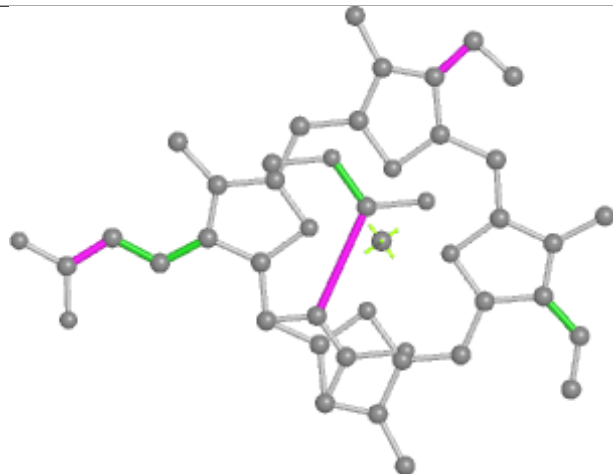
Ligand KC2 U 602



Bond lengths



Bond angles

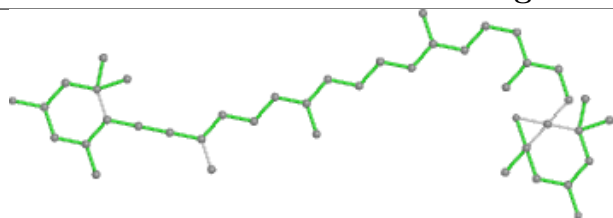


Torsions

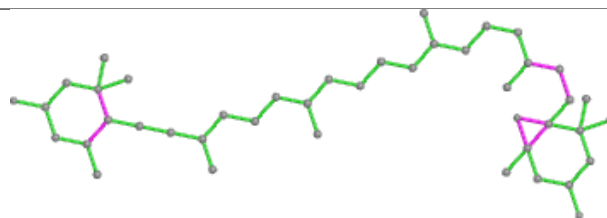


Rings

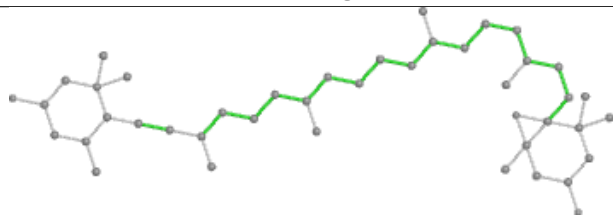
Ligand DD6 D 617



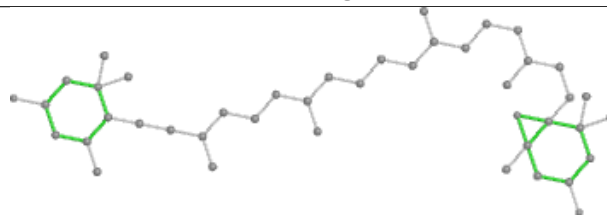
Bond lengths



Bond angles

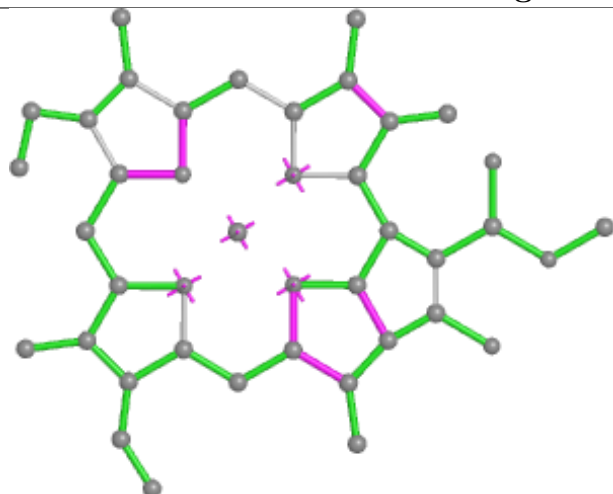


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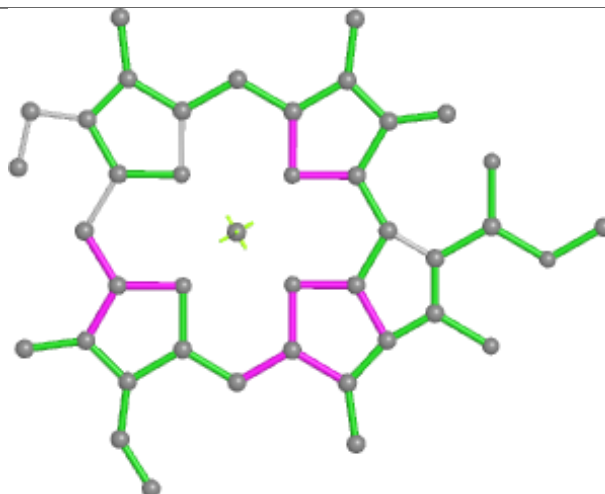


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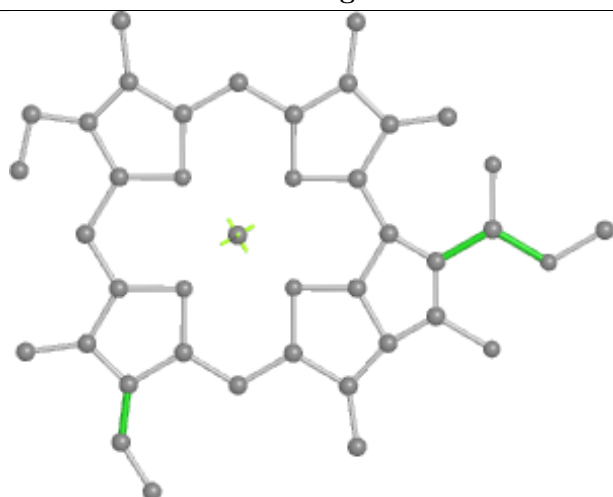
Ligand CLA T 609



Bond lengths



Bond angles

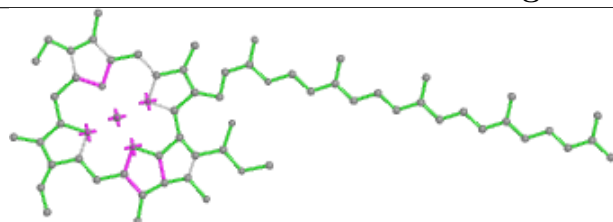


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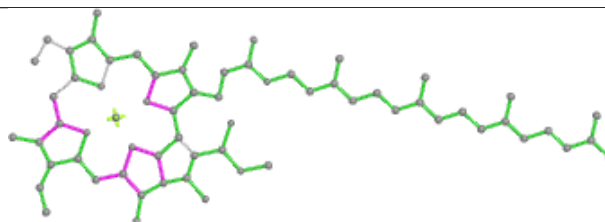


Rings

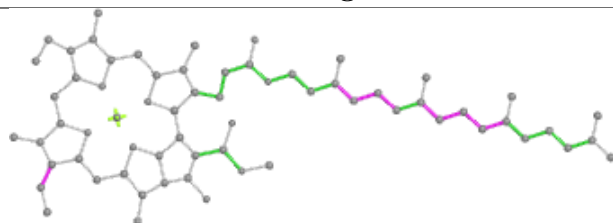
Ligand CLA 1 409



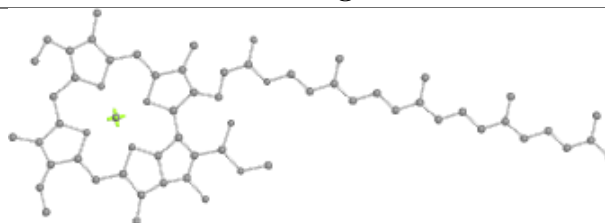
Bond lengths



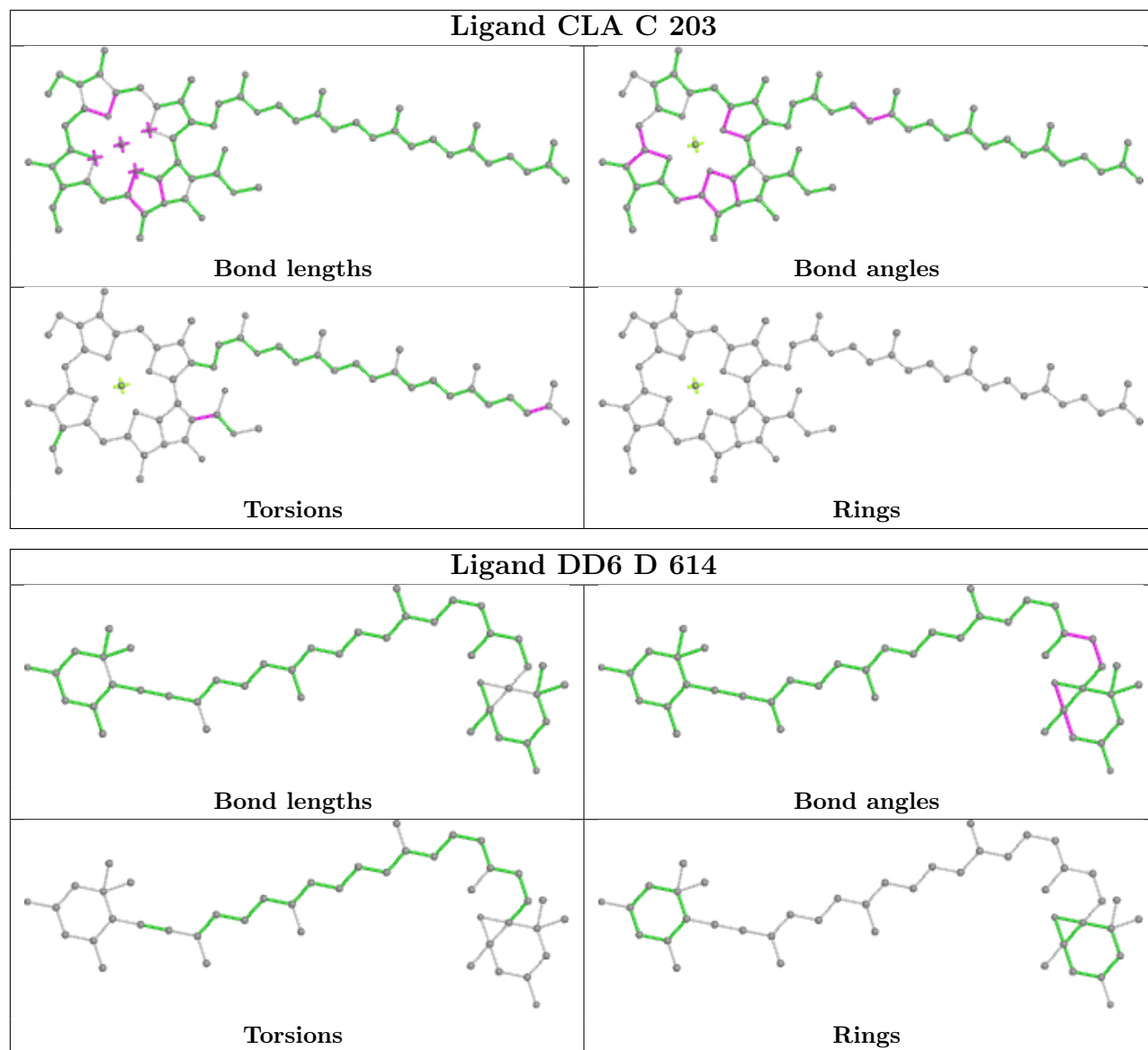
Bond angles



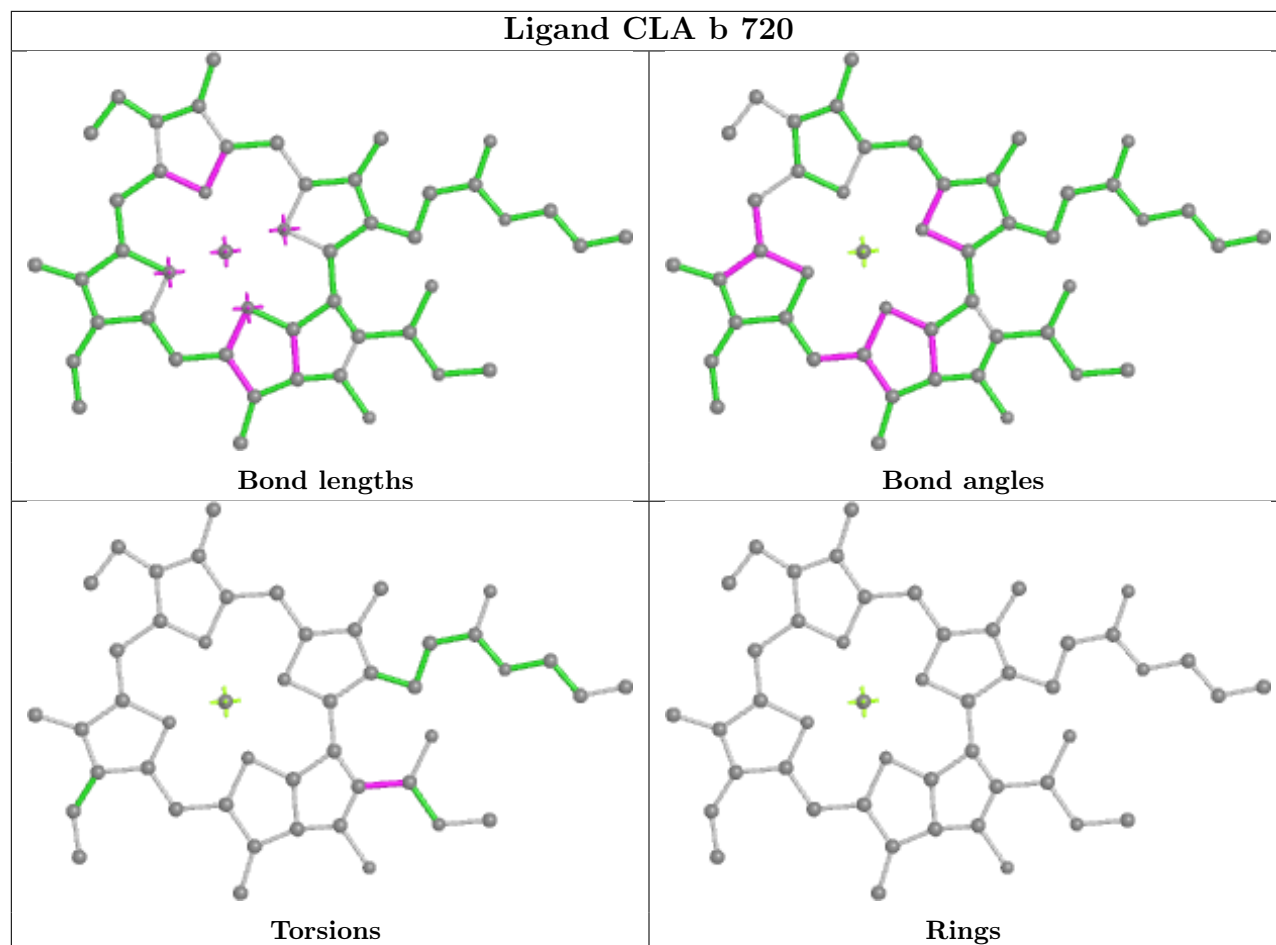
Torsions



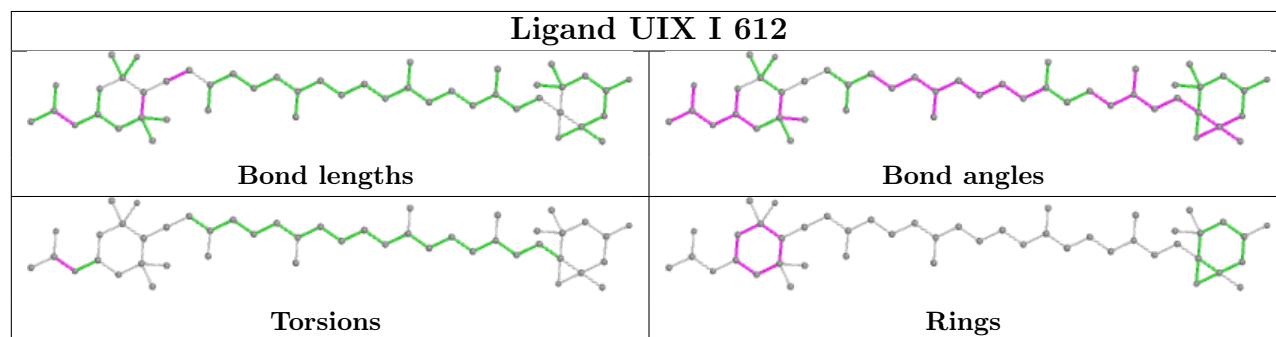
Rings



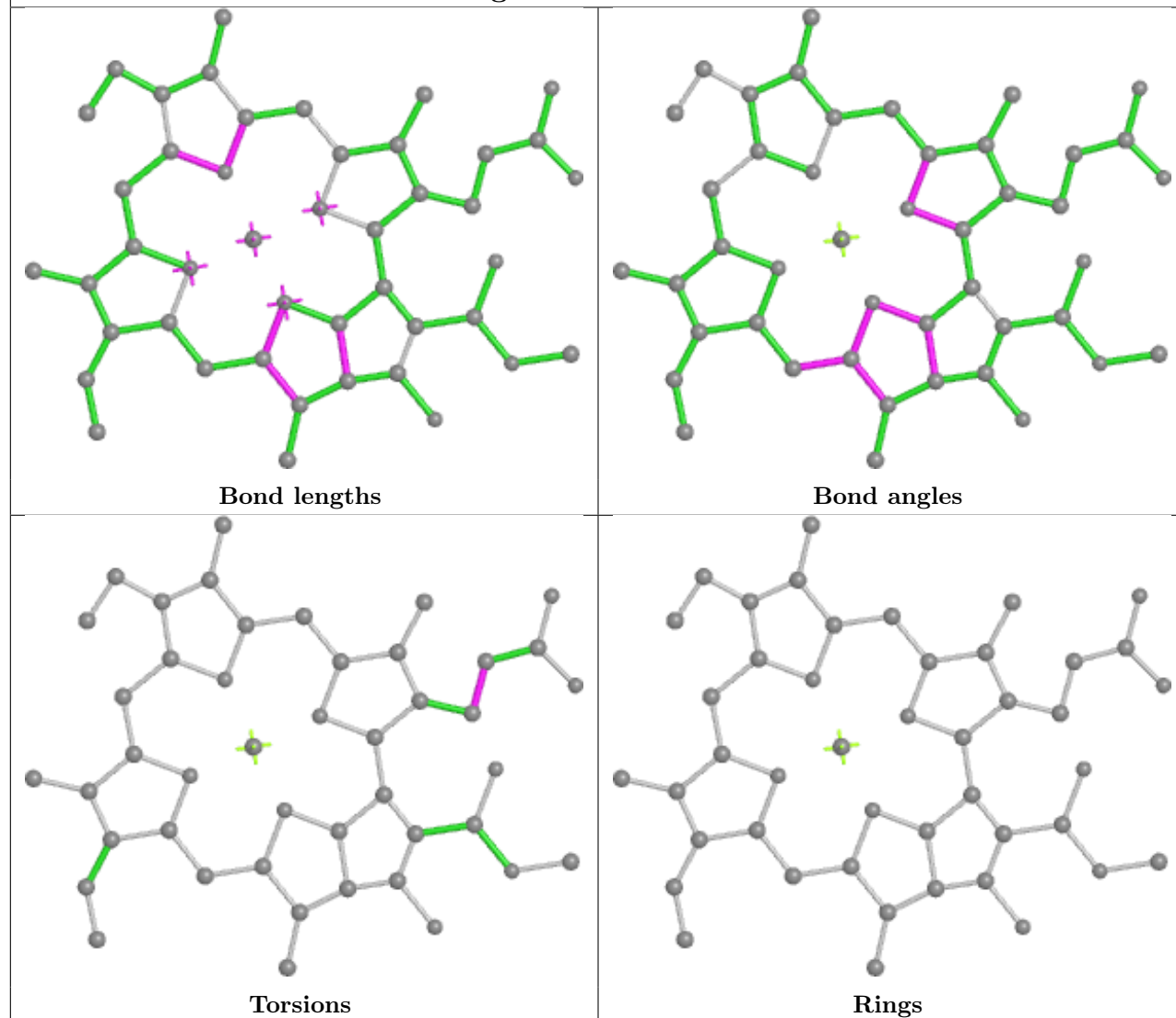
Ligand CLA b 720



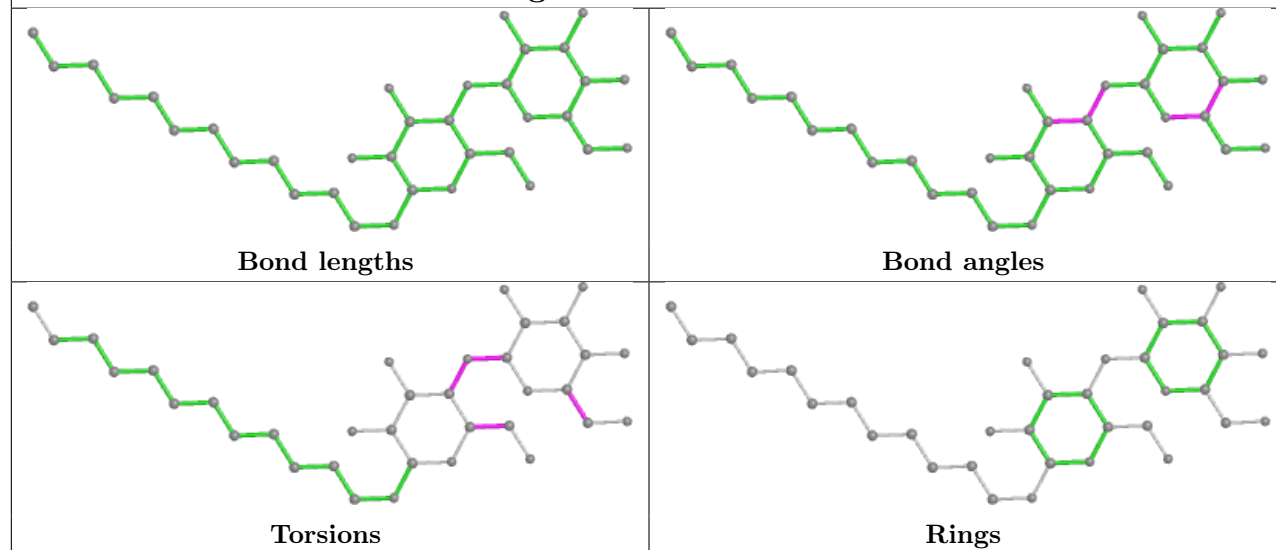
Ligand UIX I 612



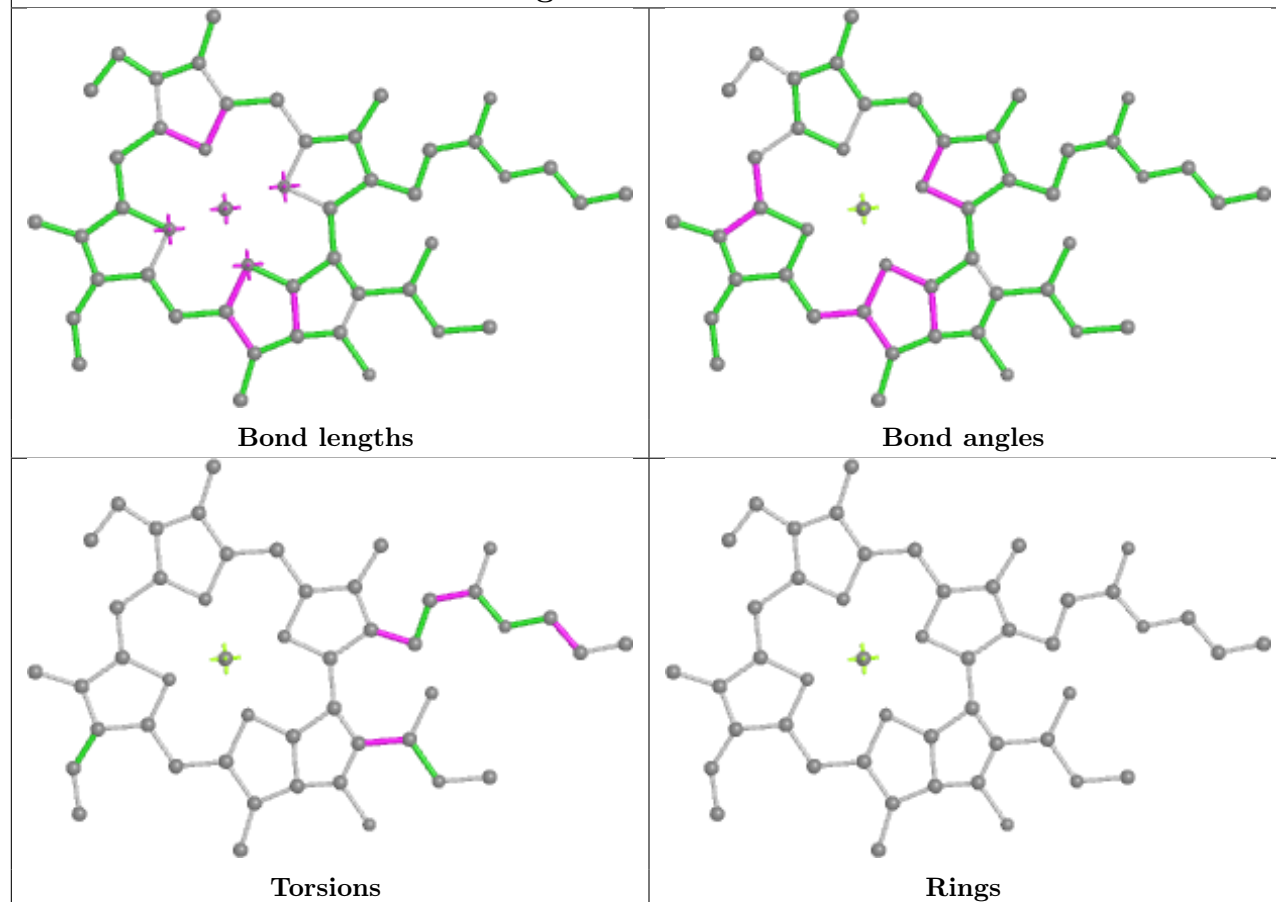
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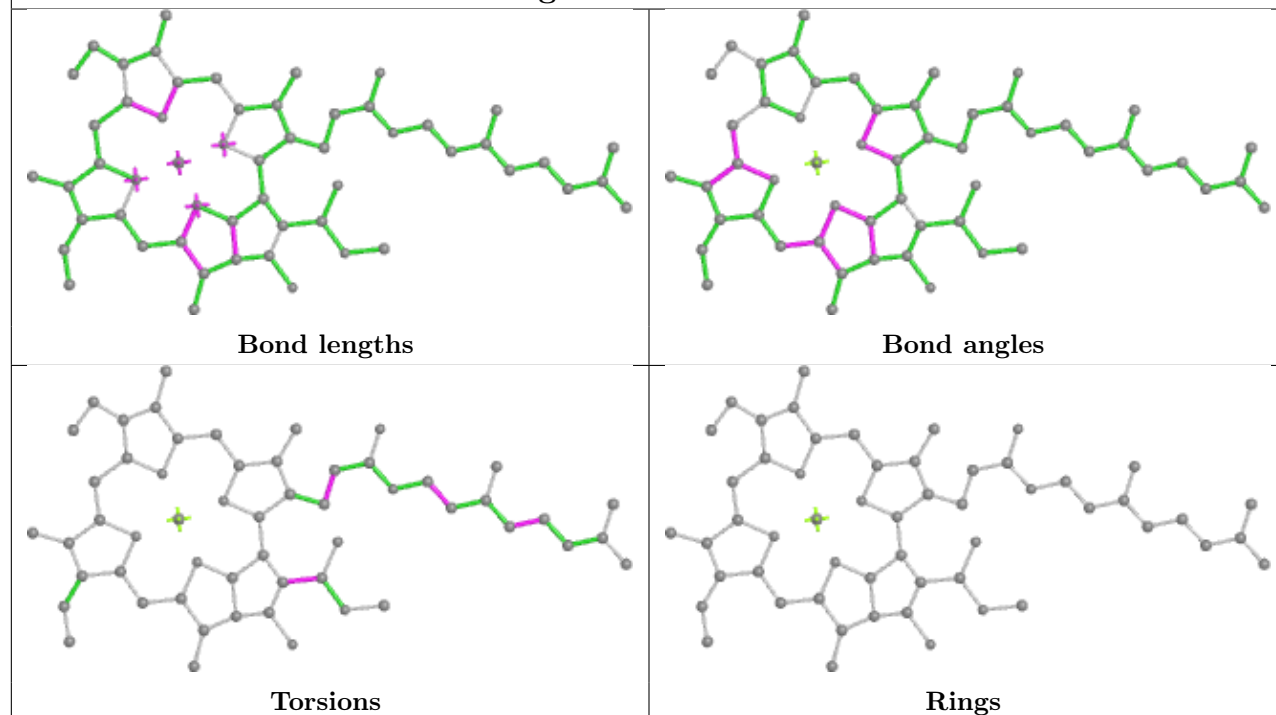
Ligand LMU T 613

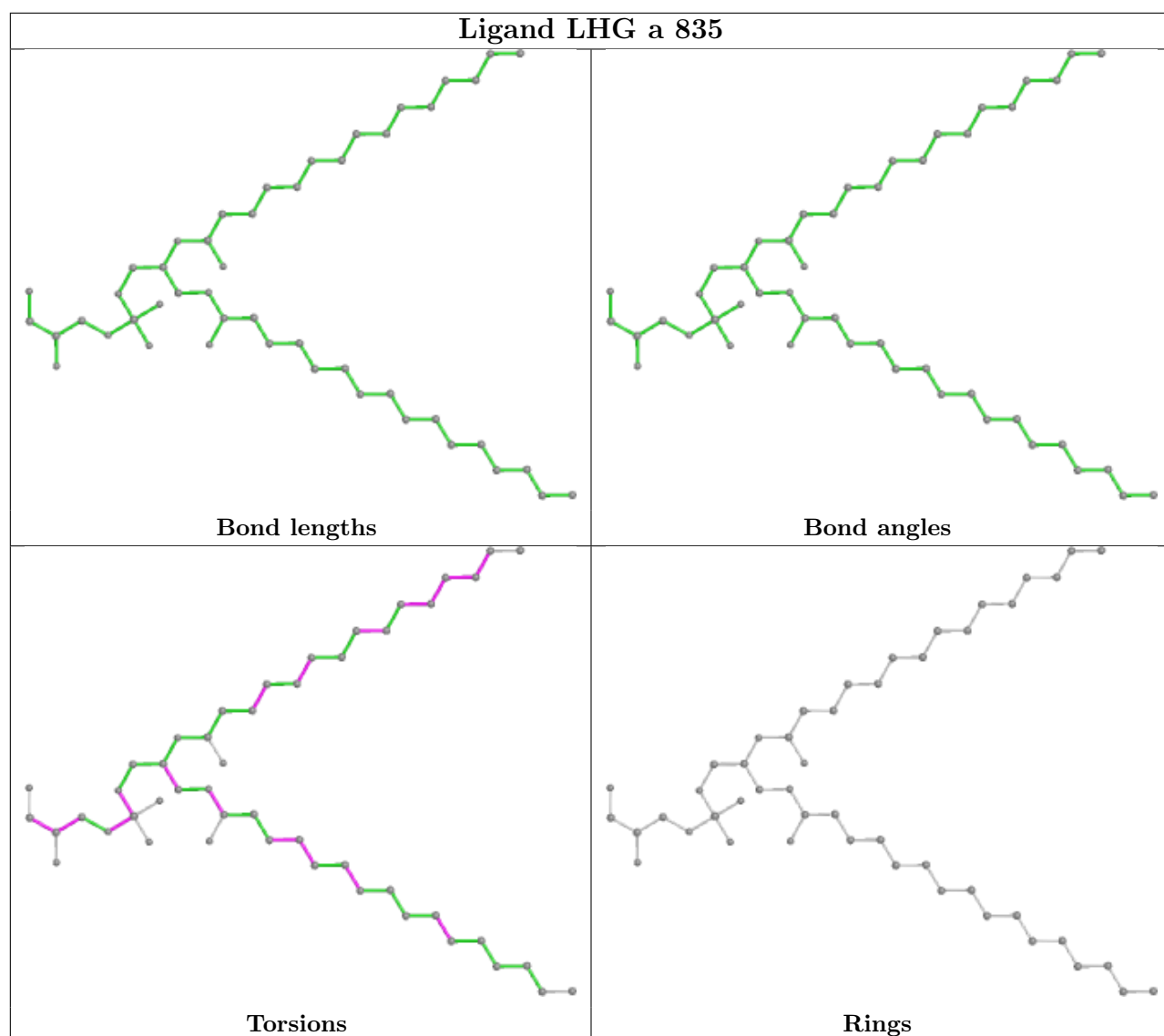


Ligand CLA a 828

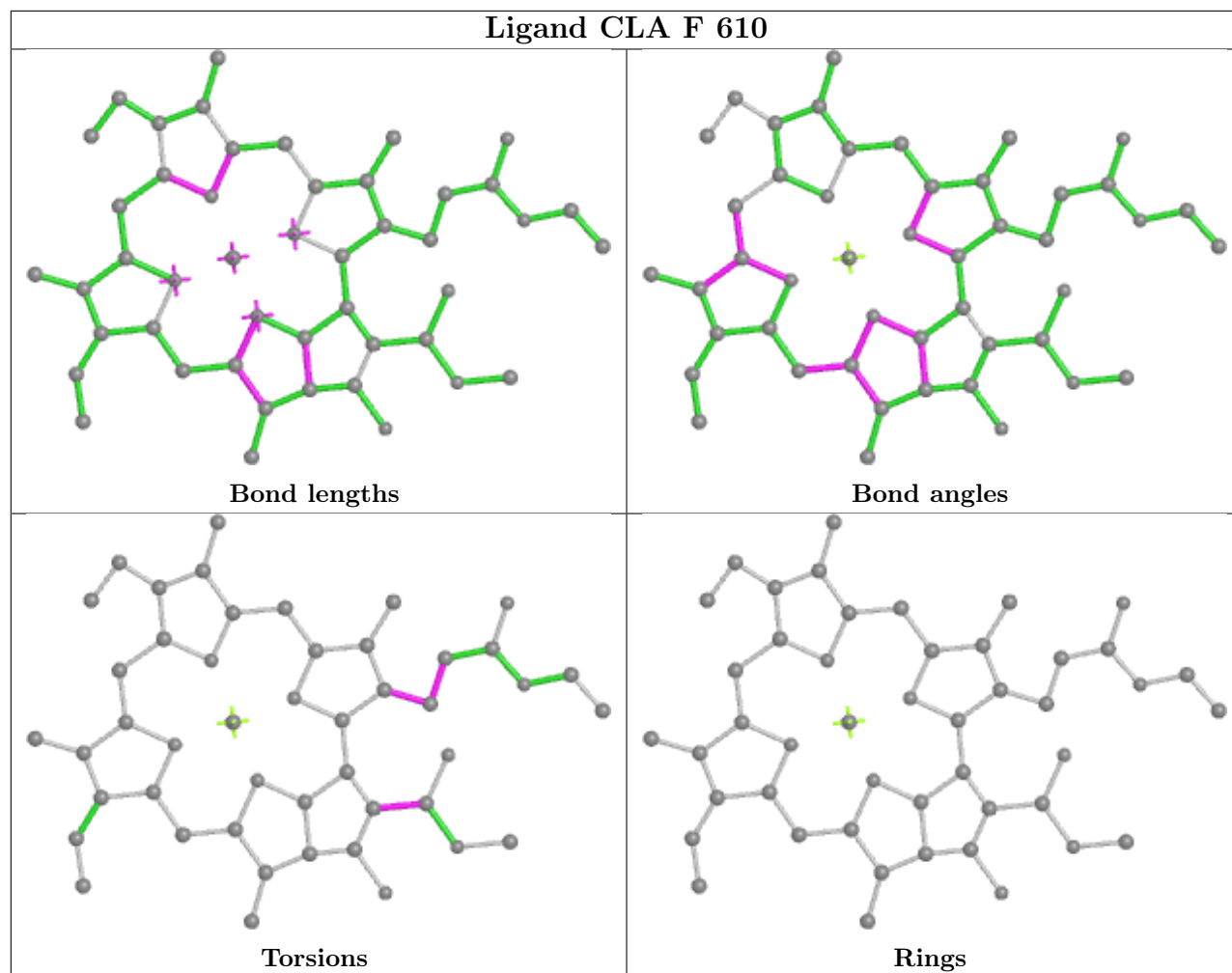


Ligand CLA I 602

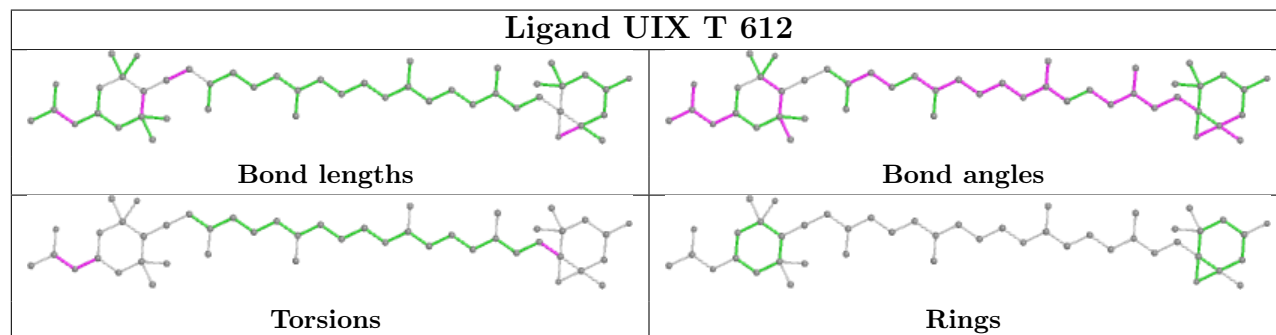


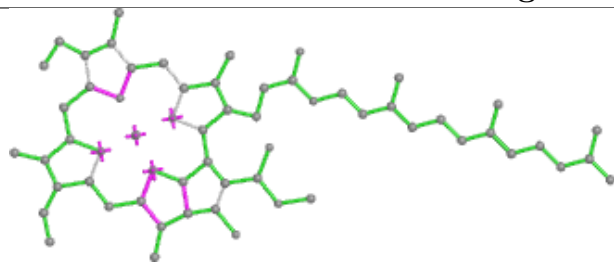


Ligand CLA F 610

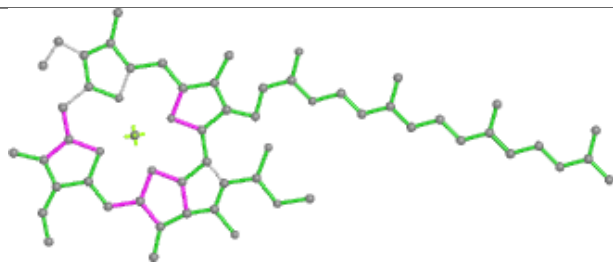


Ligand UIX T 612

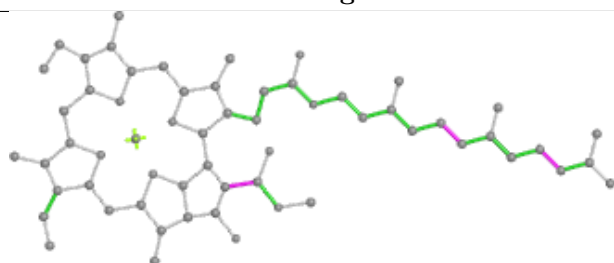


Ligand CLA J 603

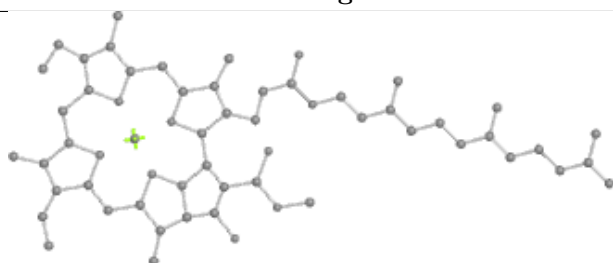
Bond lengths



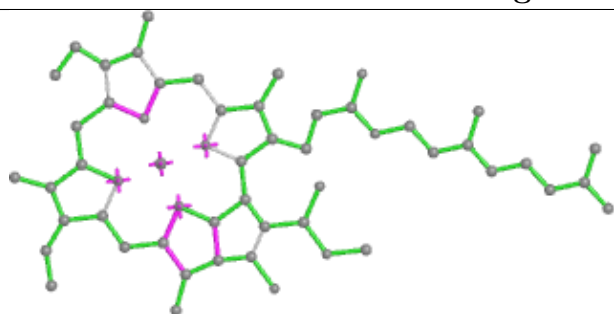
Bond angles



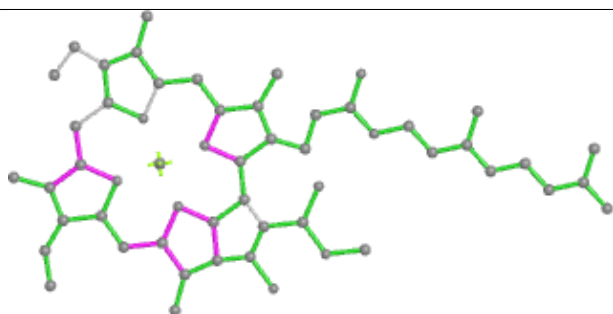
Torsions



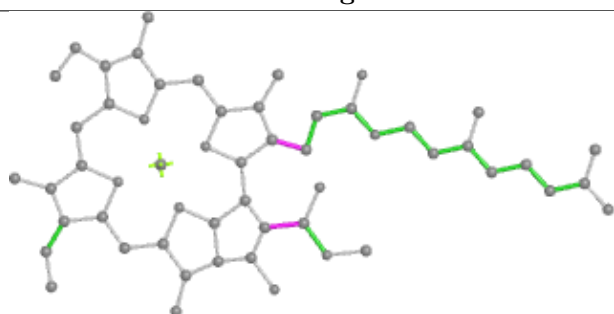
Rings

Ligand CLA A 610

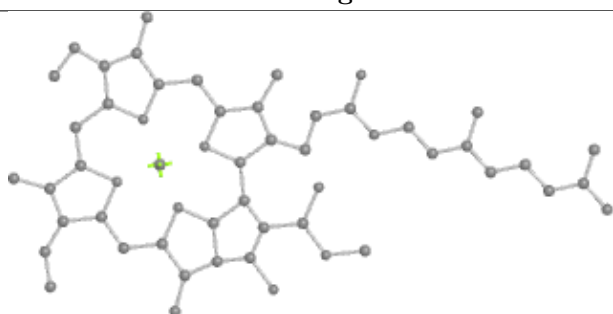
Bond lengths



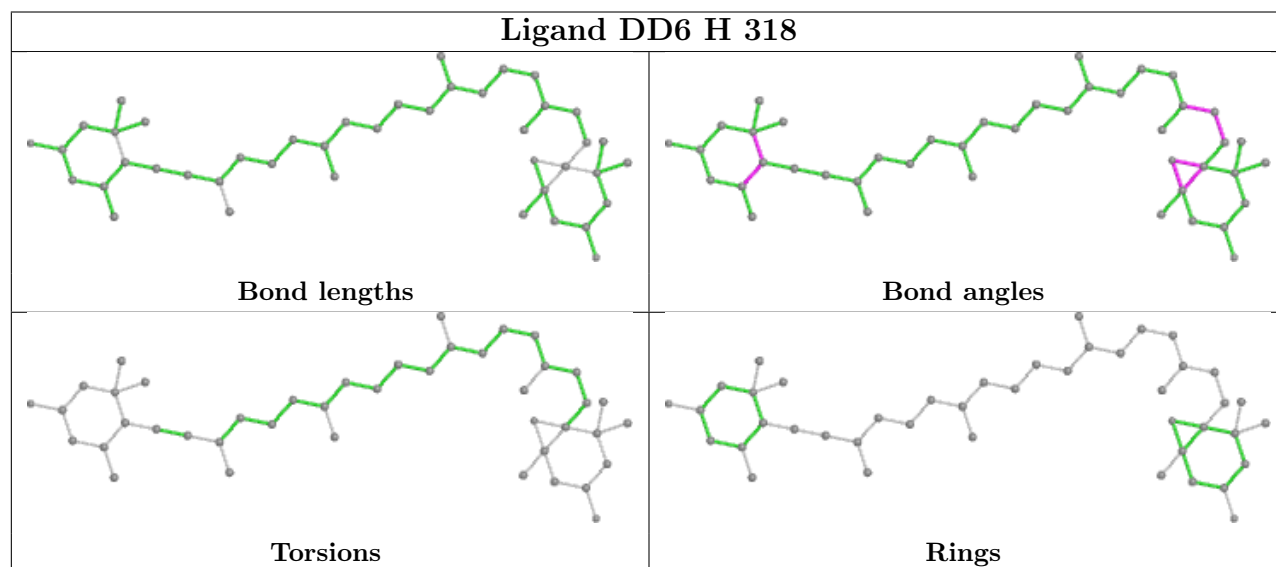
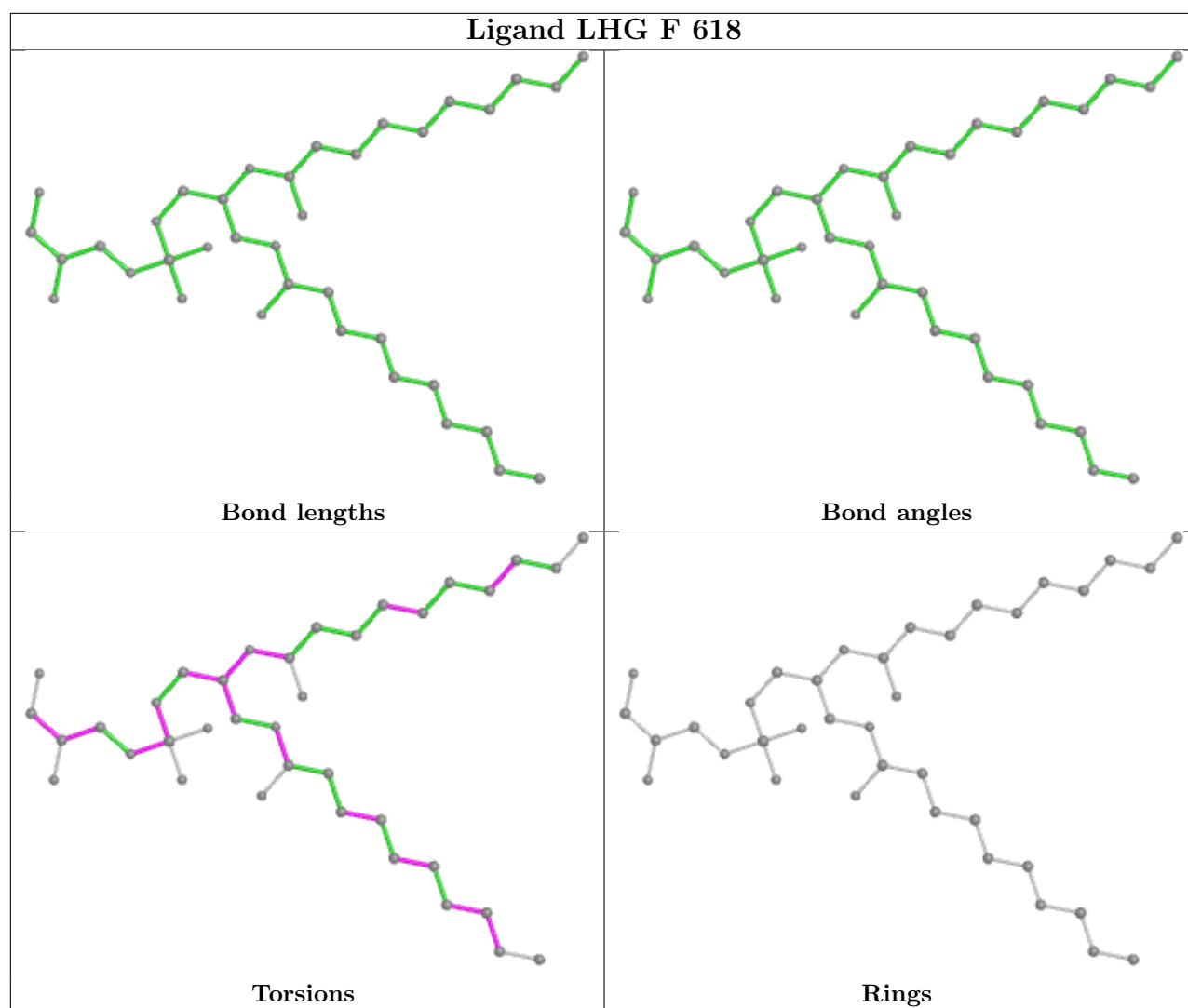
Bond angles

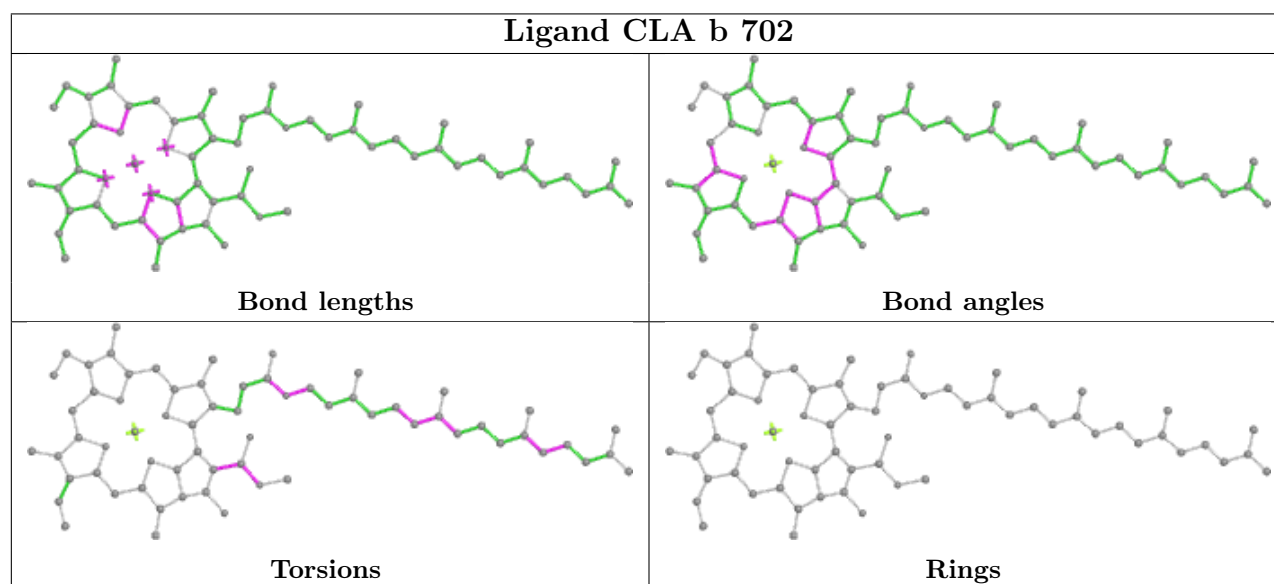
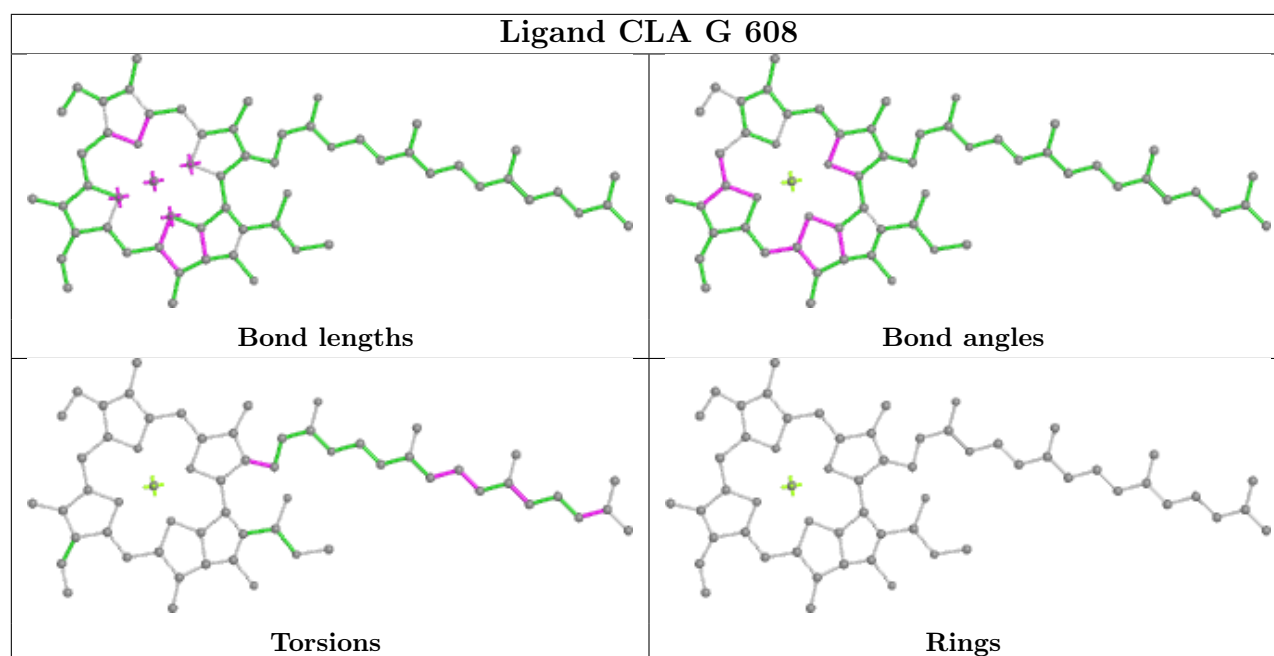


Torsions

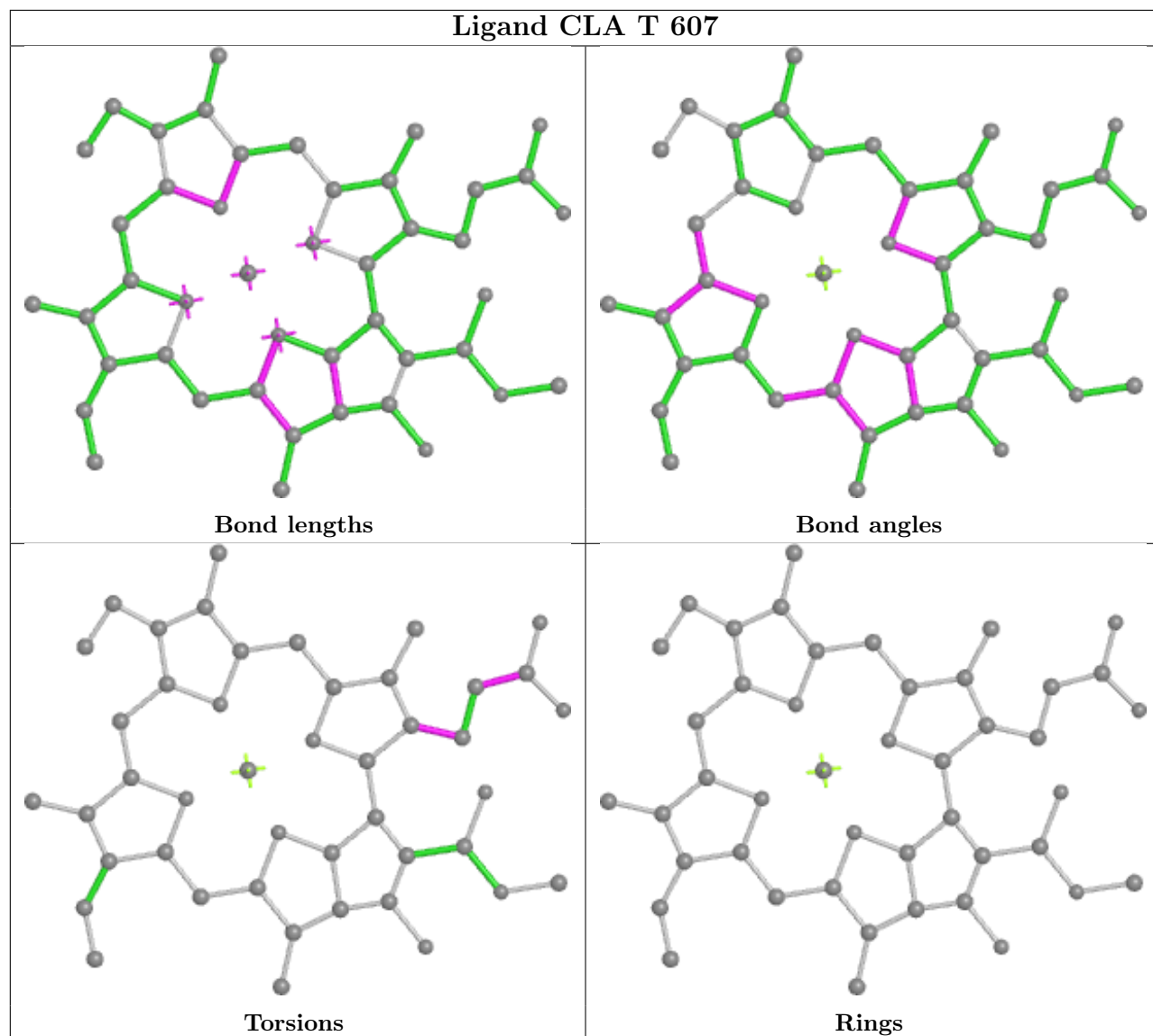


Rings

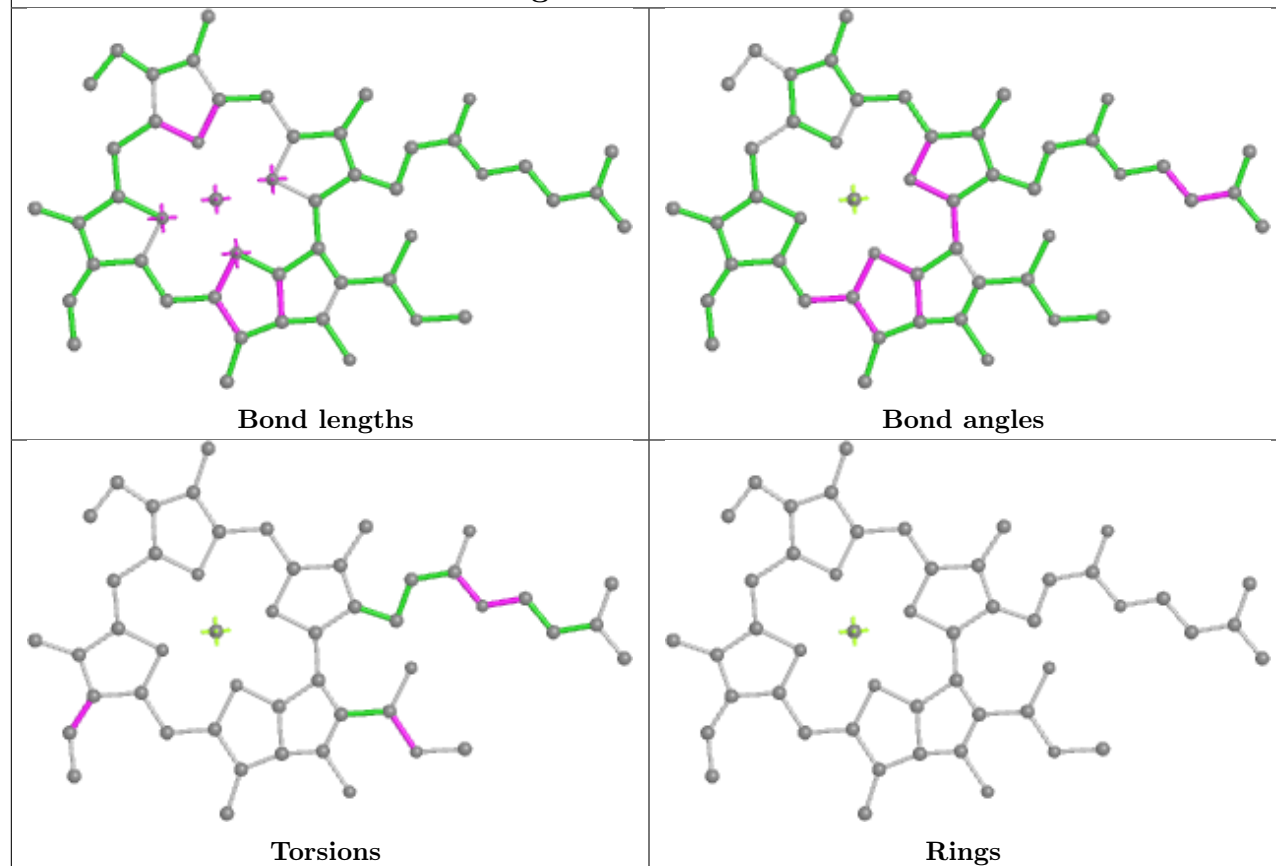




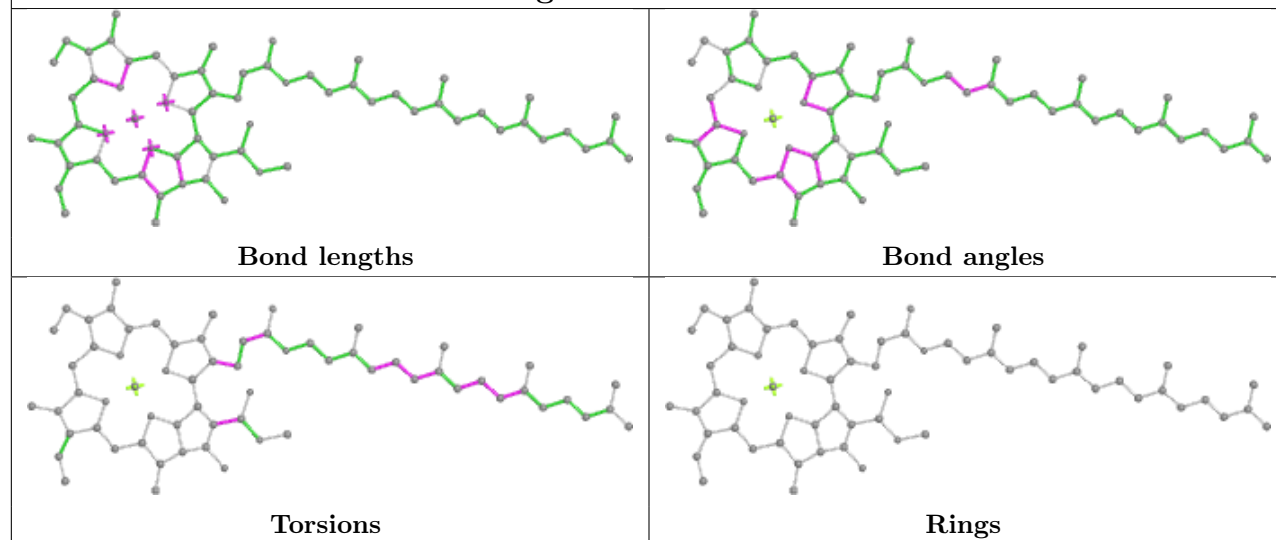
Ligand CLA T 607

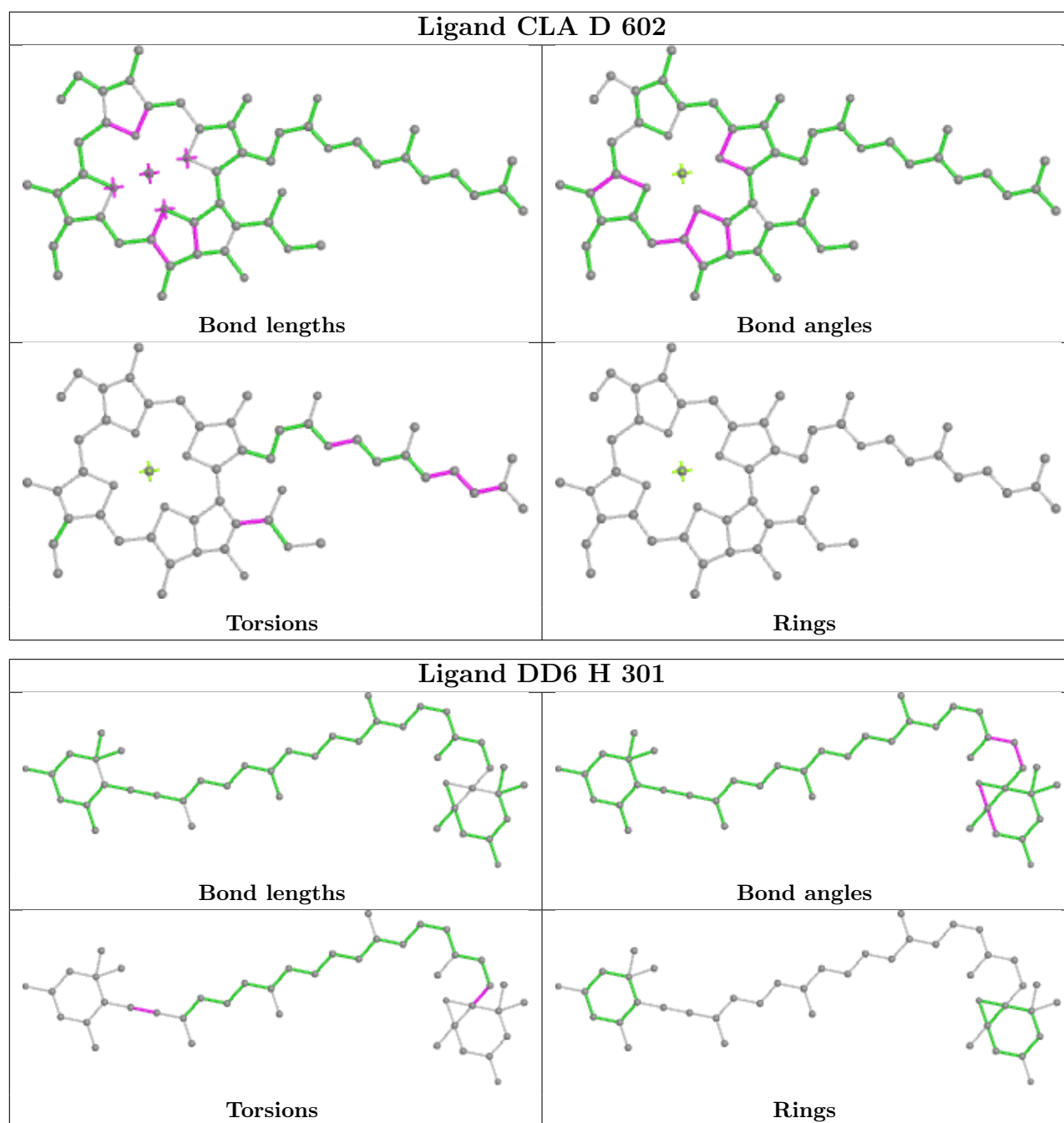


Ligand CLA U 603

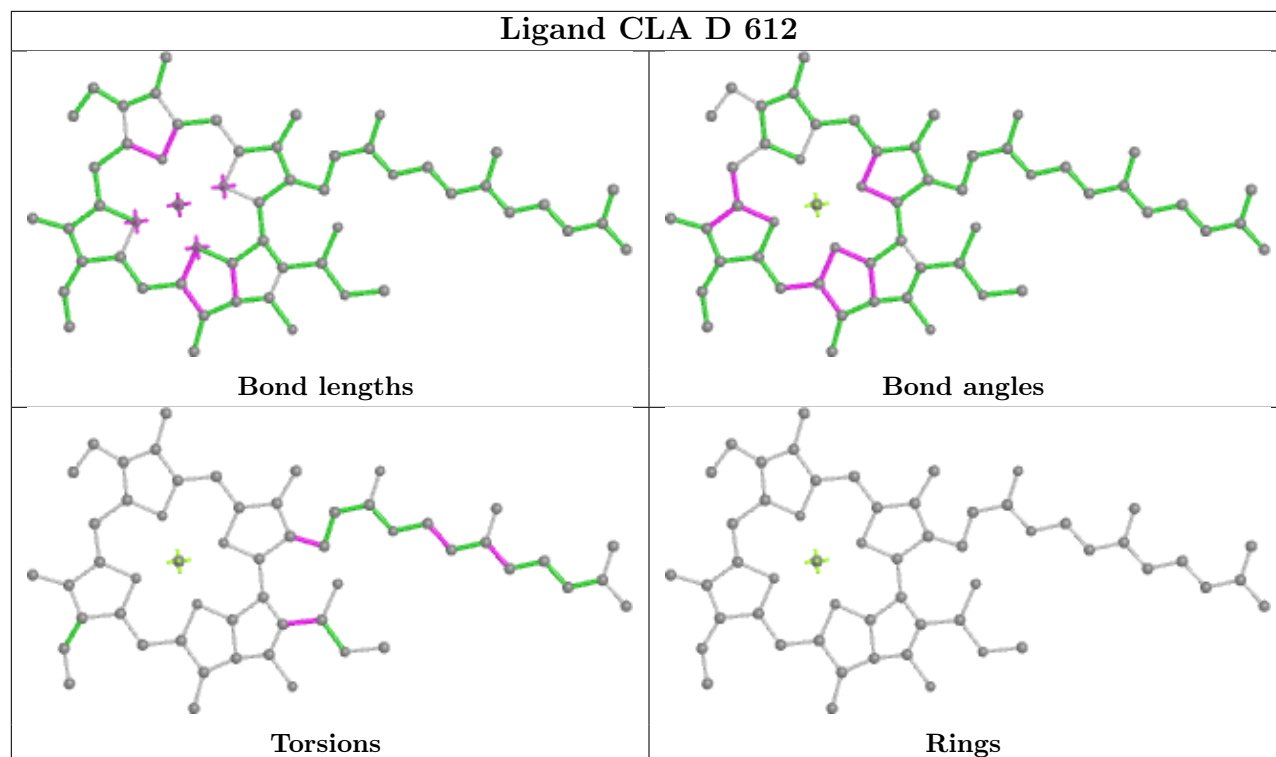


Ligand CLA a 823

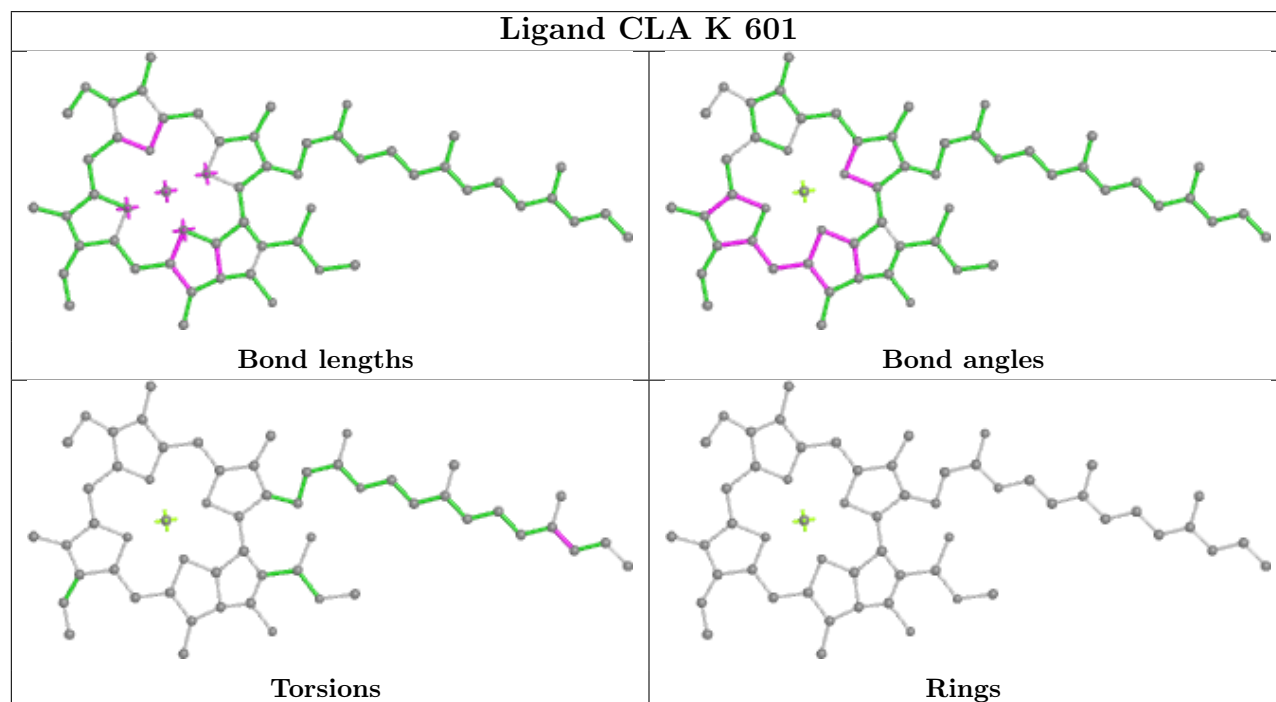


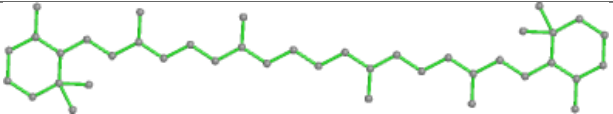
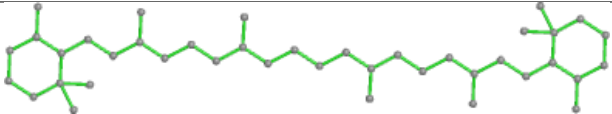
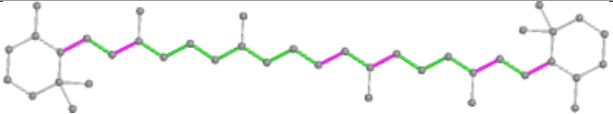
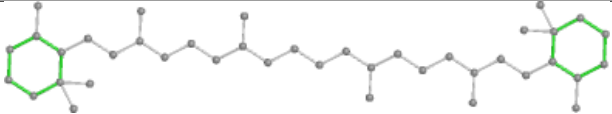






Ligand CLA D 612

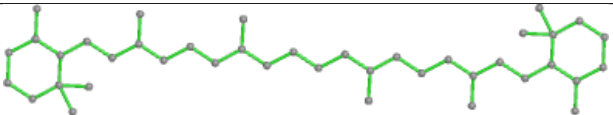
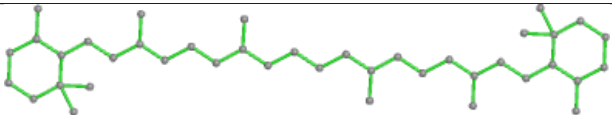
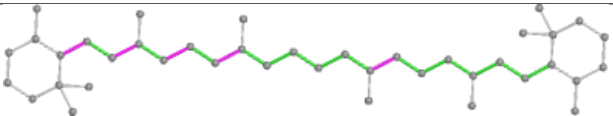
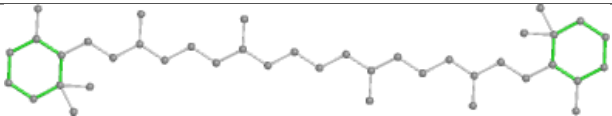


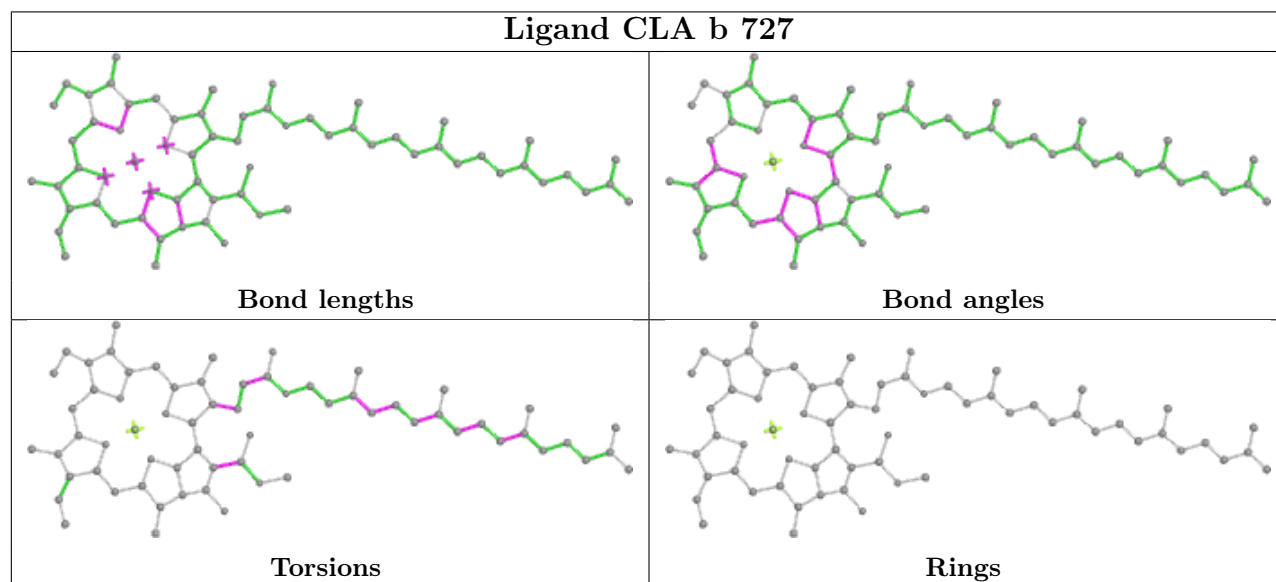
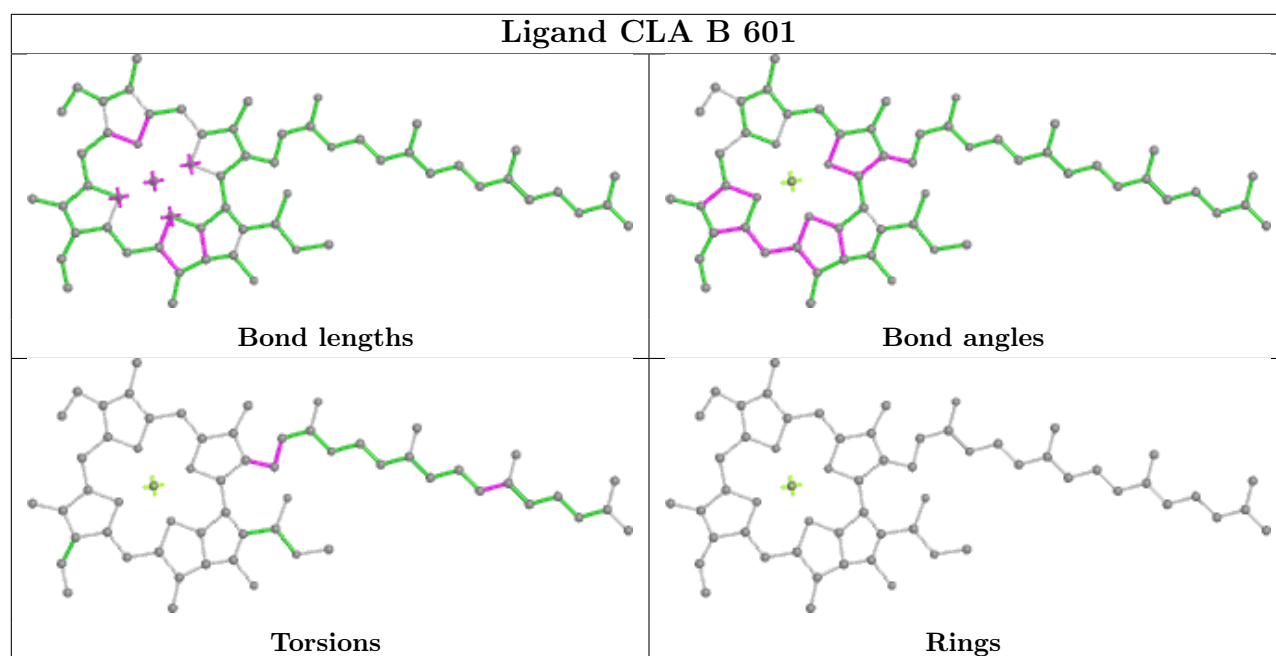
Ligand CLA K 601

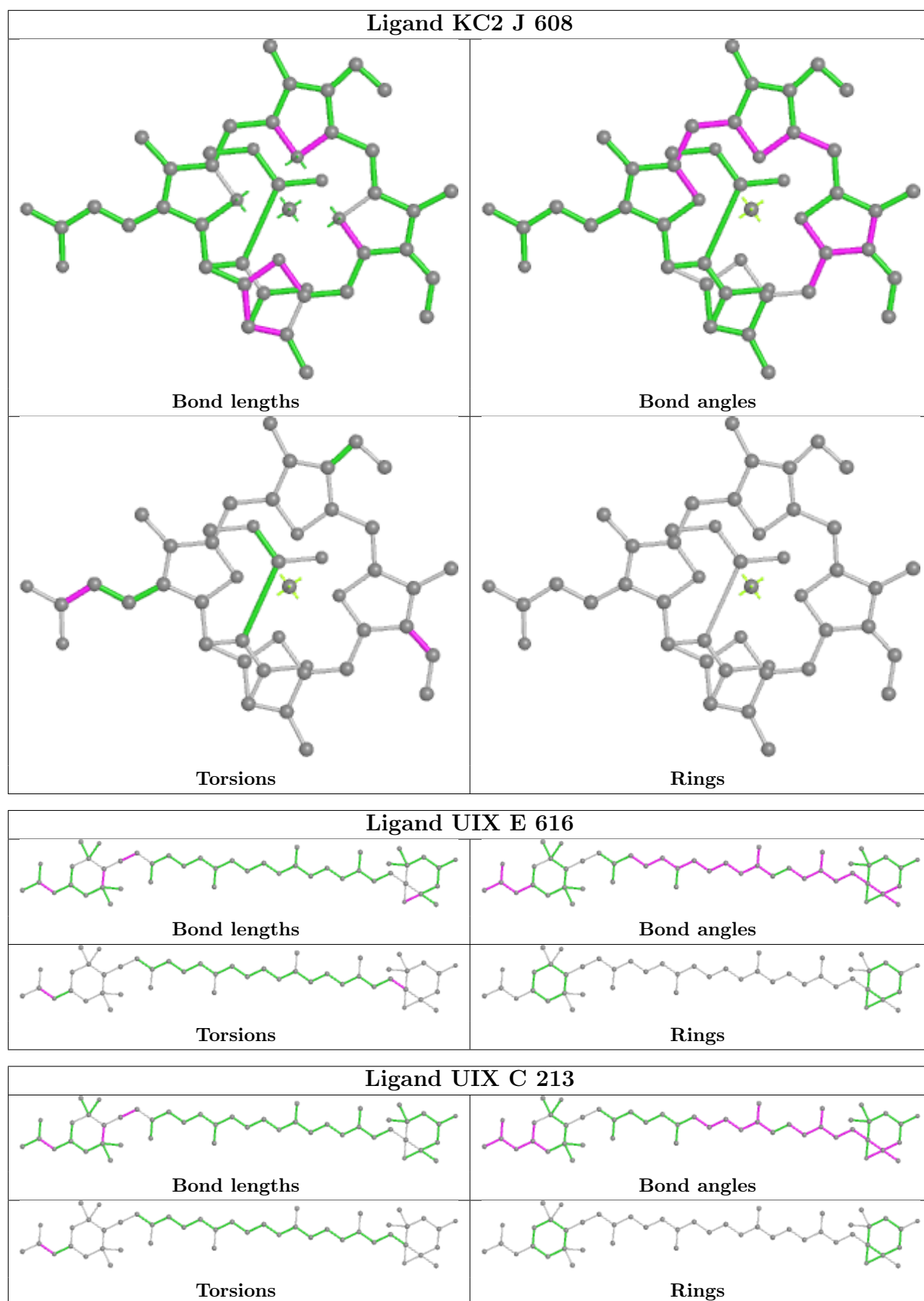


Ligand BCR j 203	
	
Bond lengths	Bond angles
	
Torsions	Rings

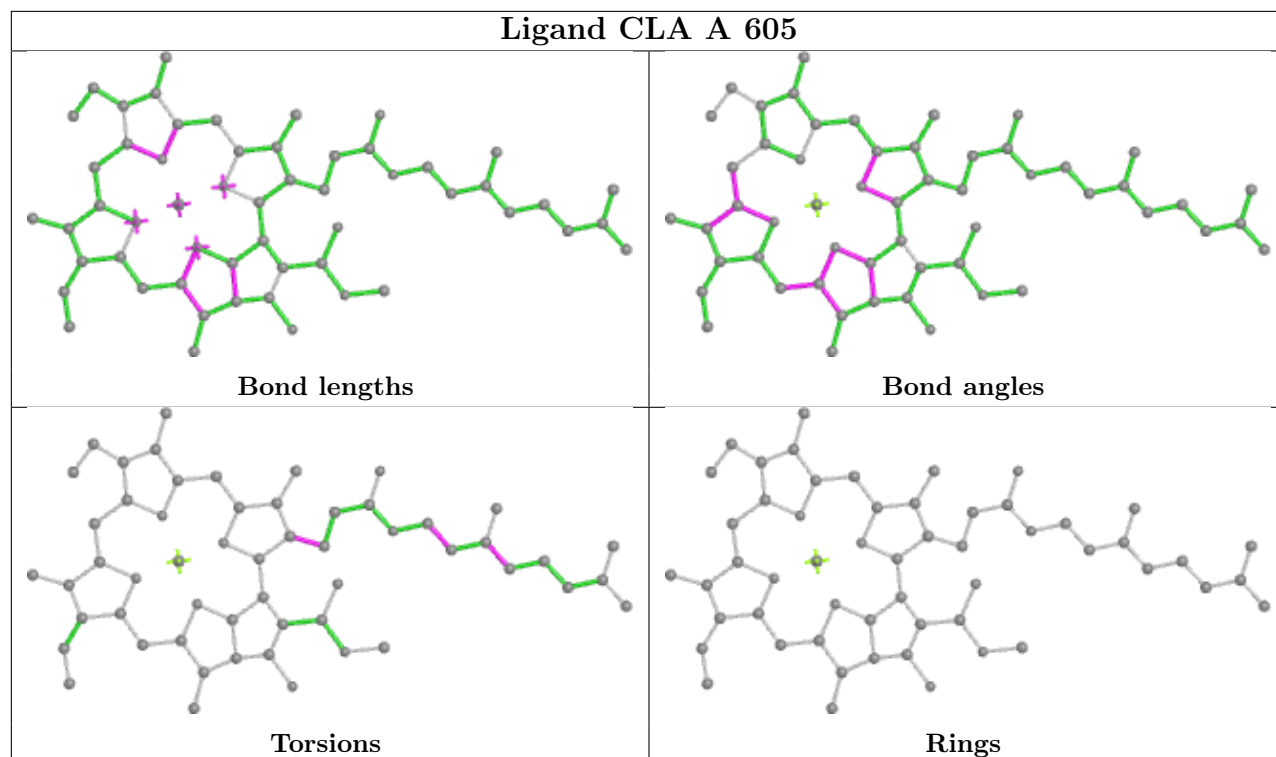
Ligand PID U 608	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR f 301	
	
Bond lengths	Bond angles
	
Torsions	Rings

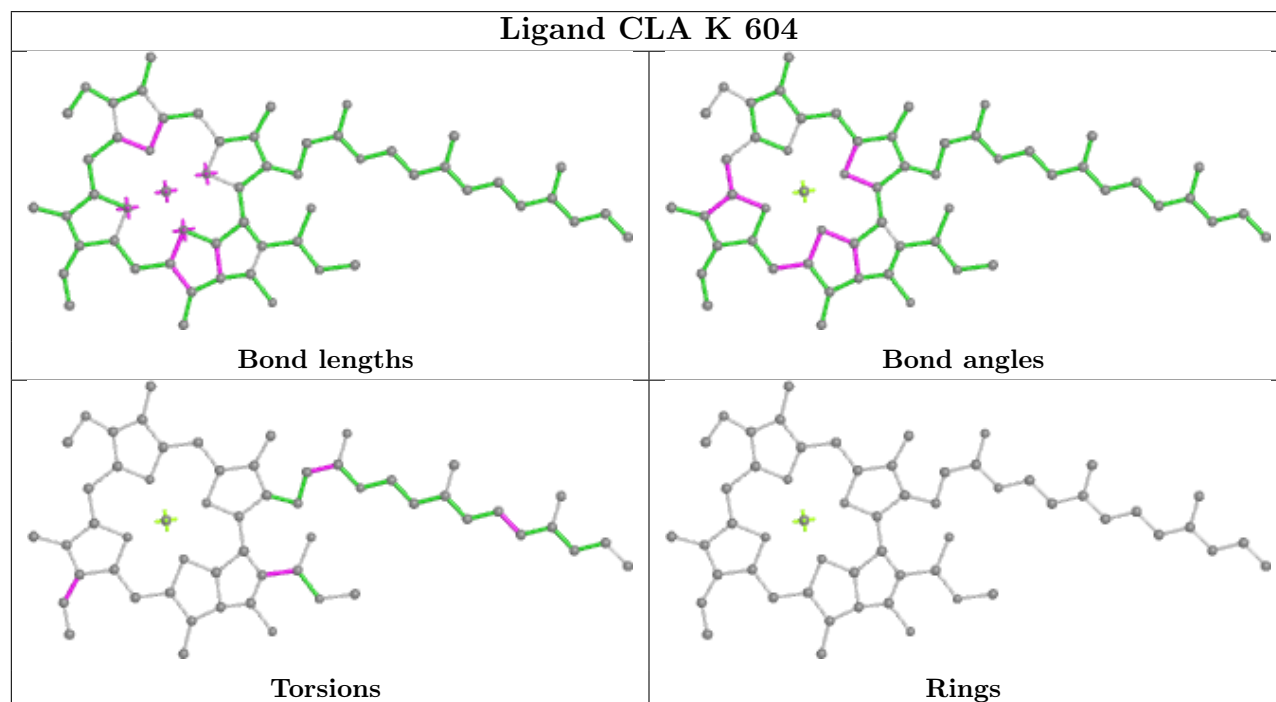


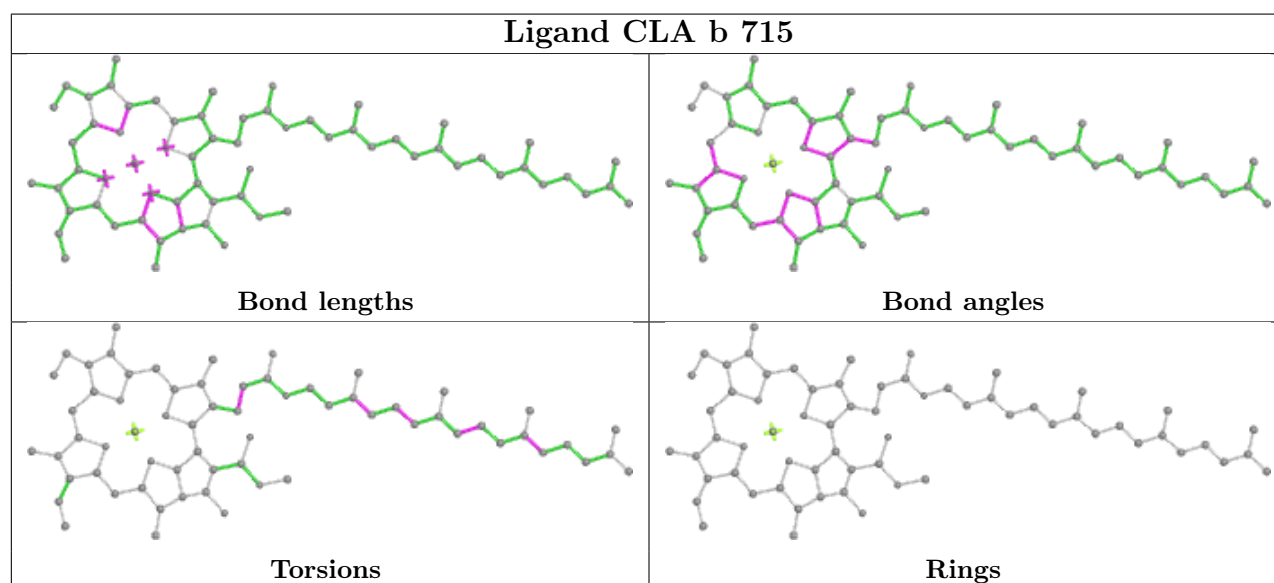
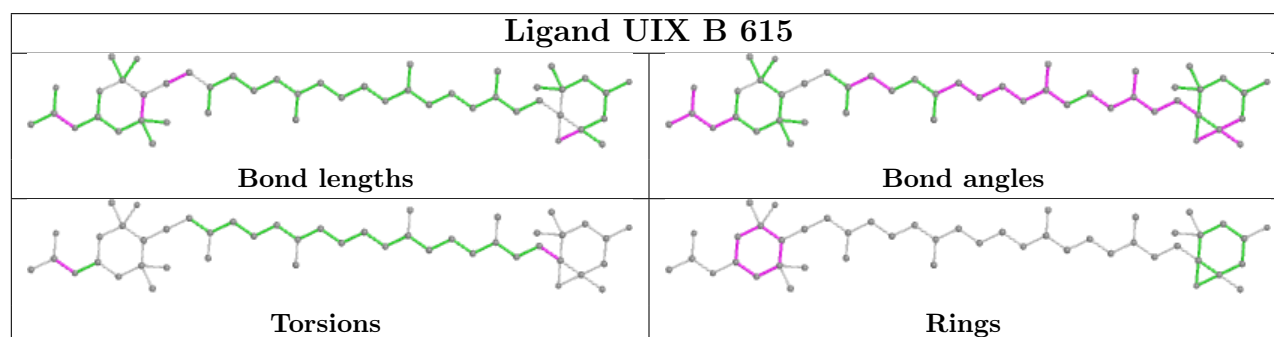
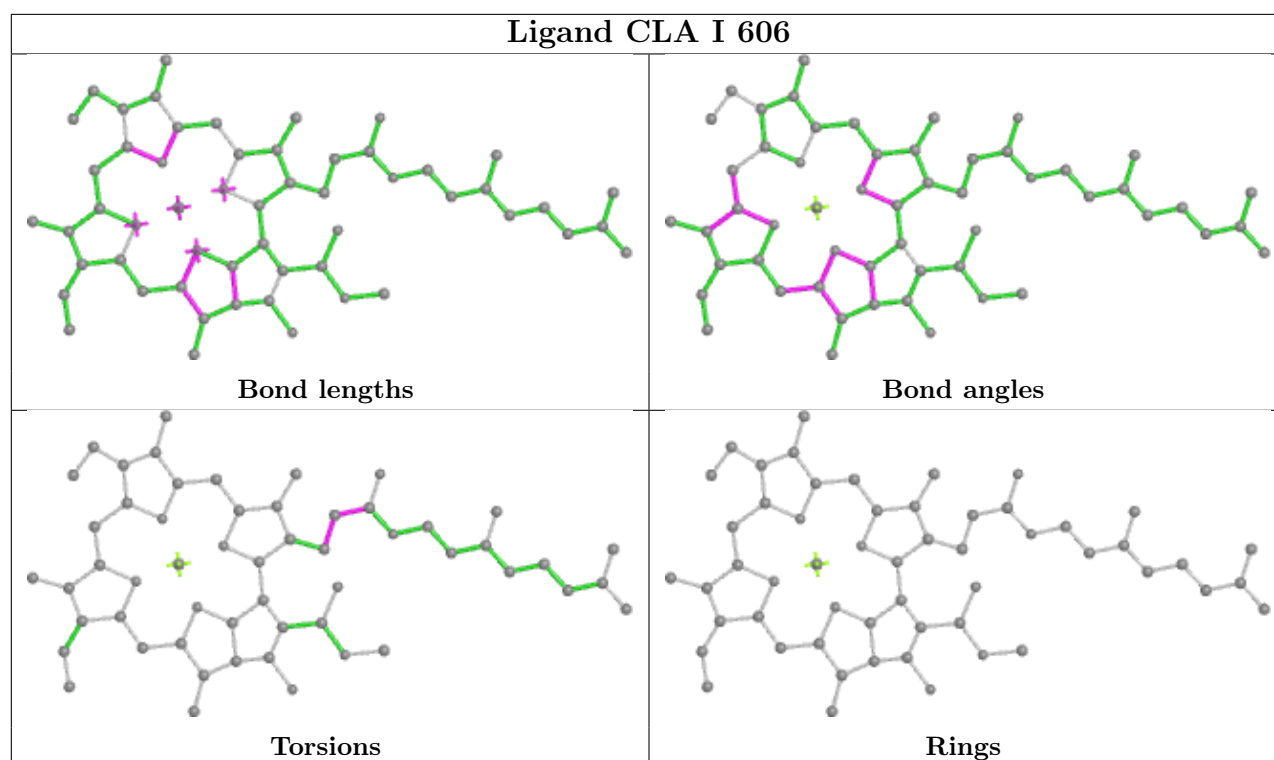


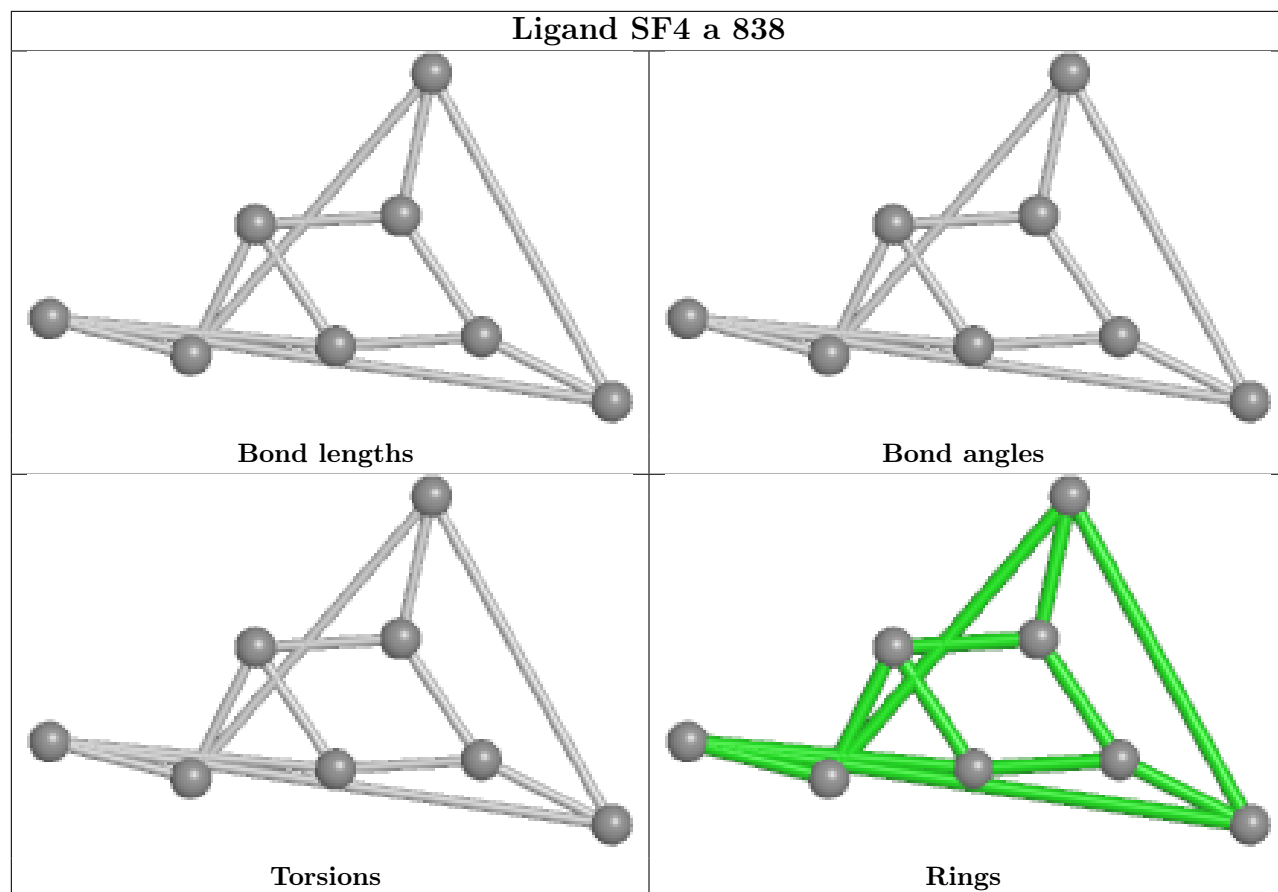
Ligand CLA A 605



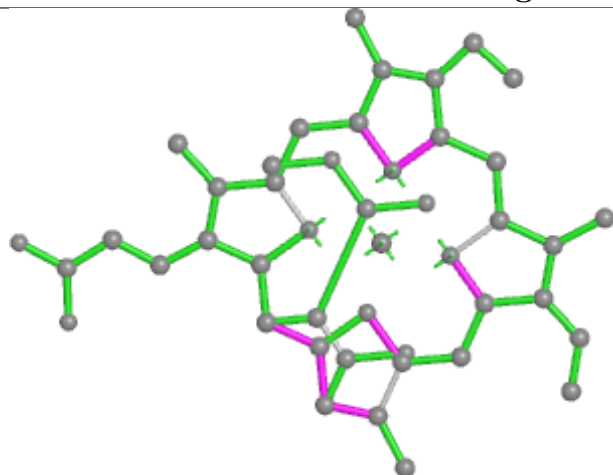
Ligand CLA K 604



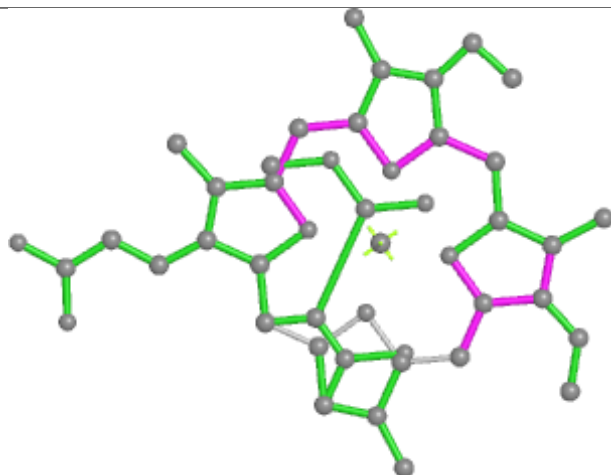




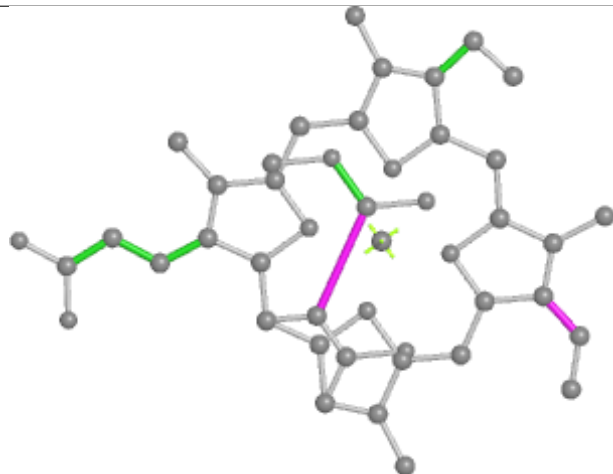
Ligand KC2 K 607



Bond lengths



Bond angles

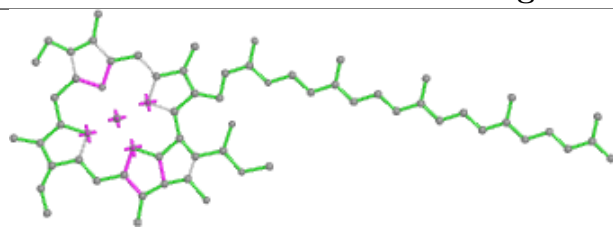


Torsions

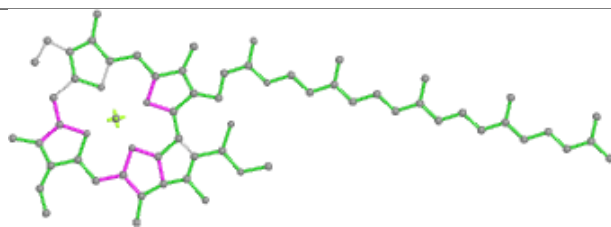


Rings

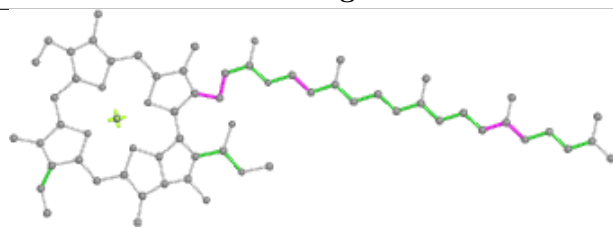
Ligand CLA b 724



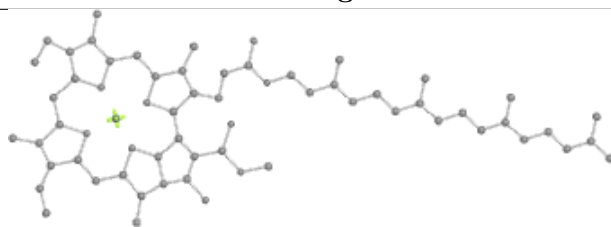
Bond lengths



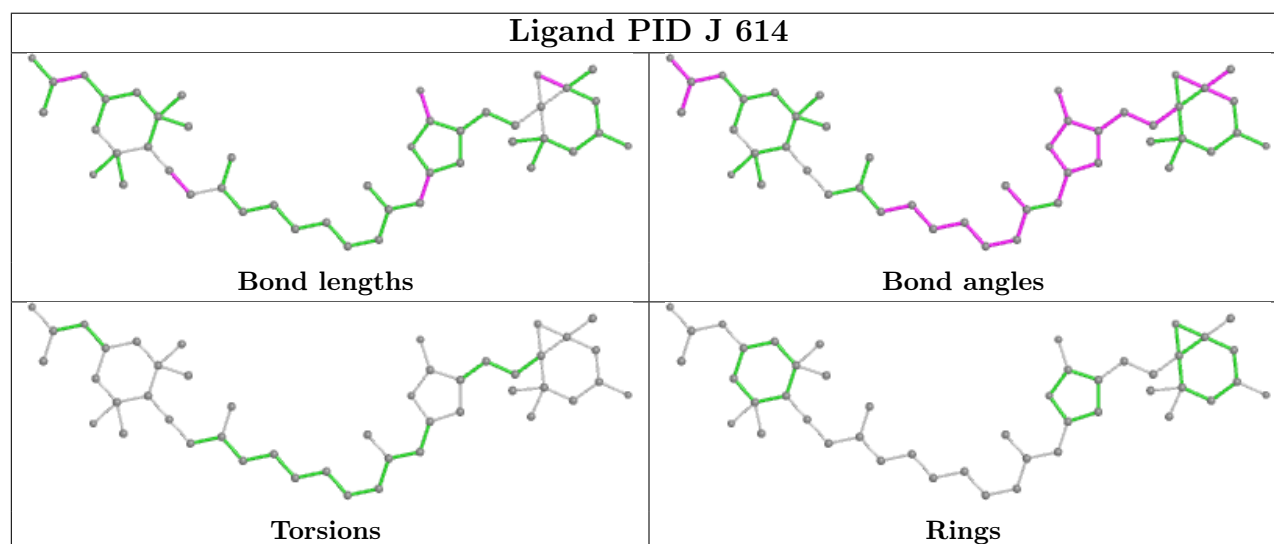
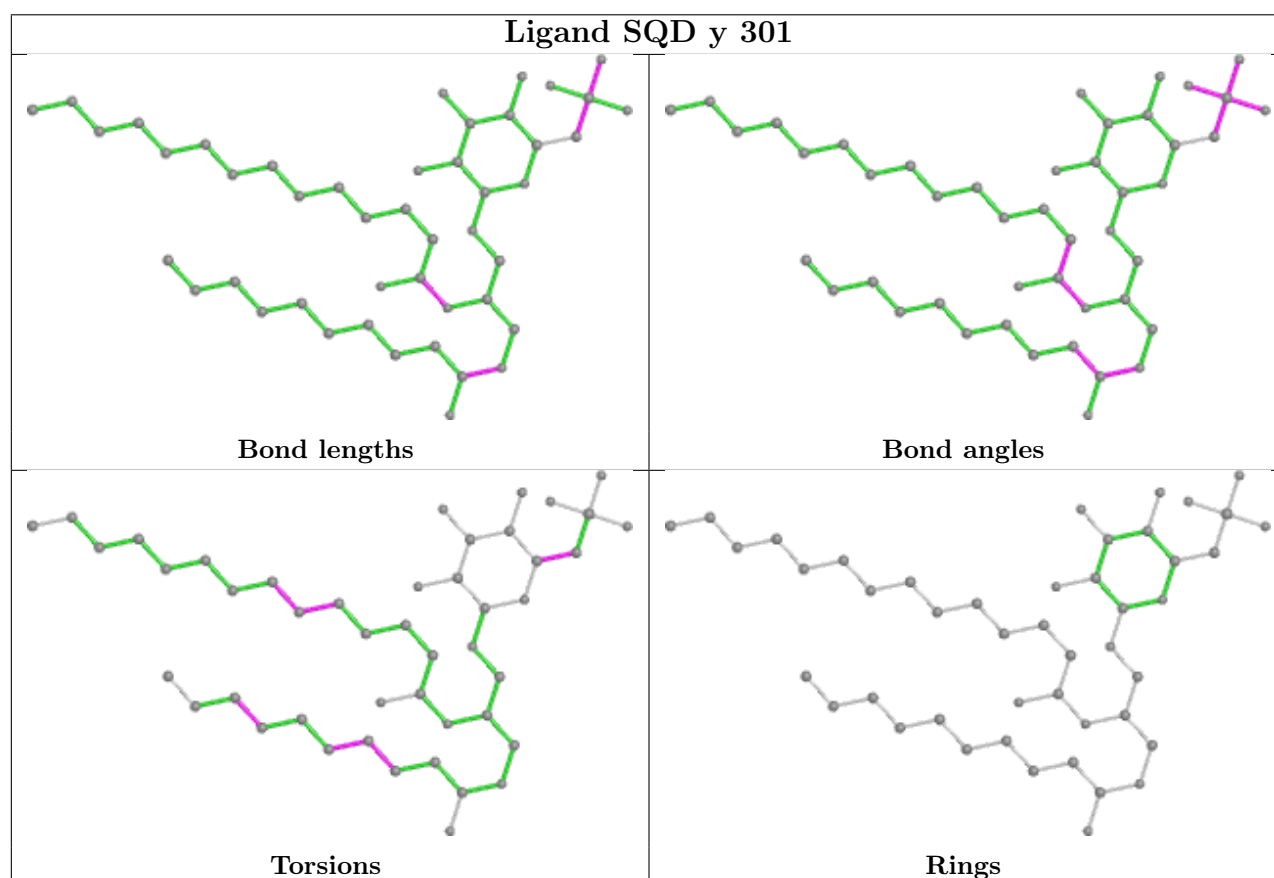
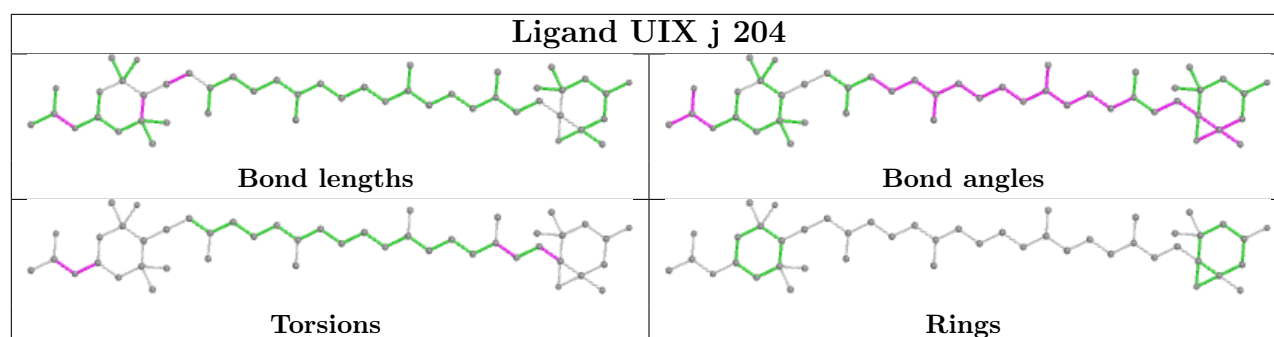
Bond angles

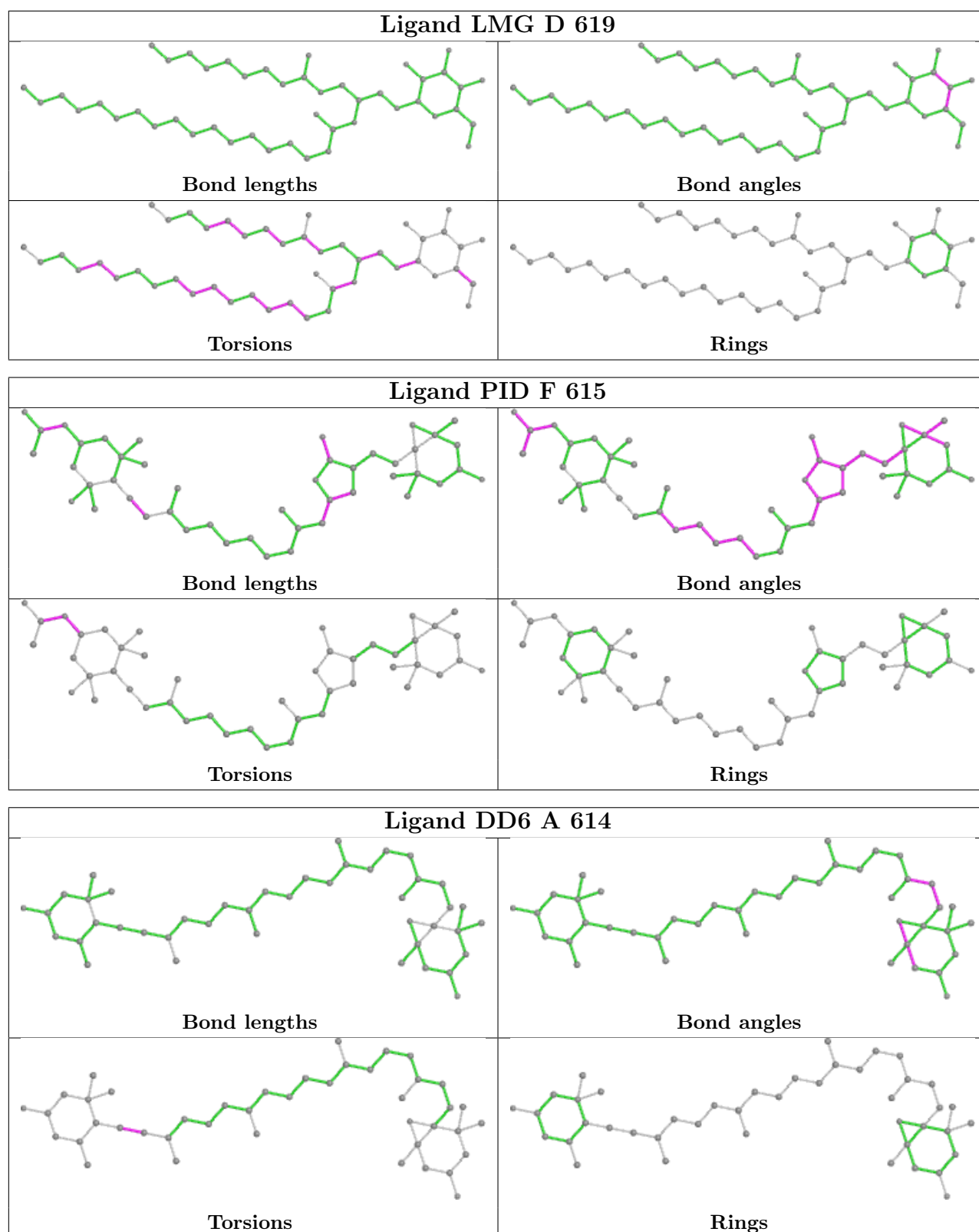


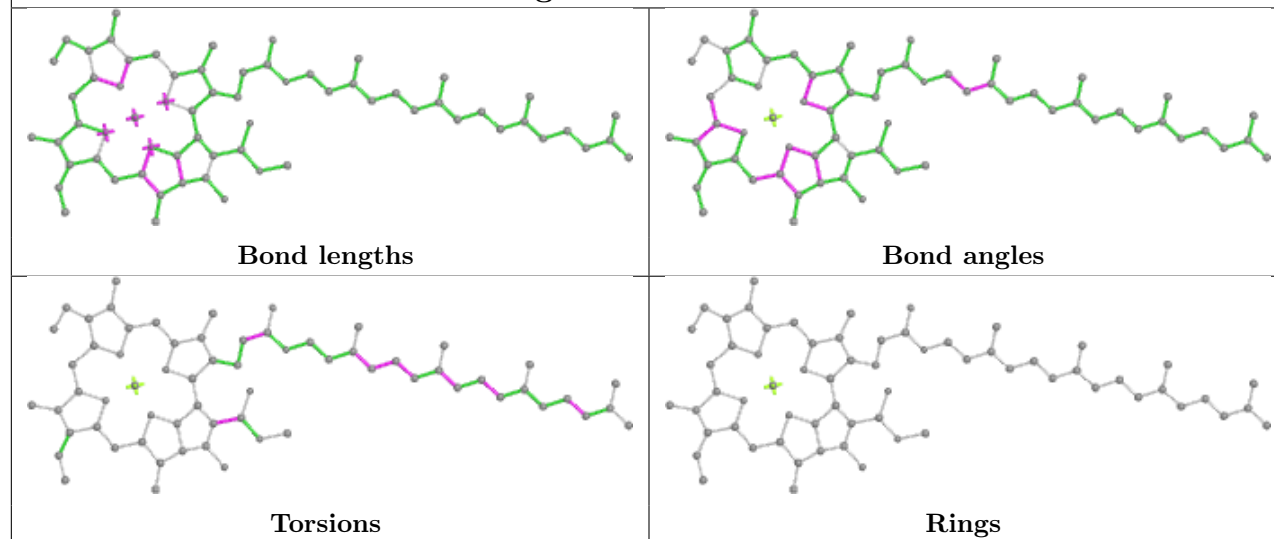
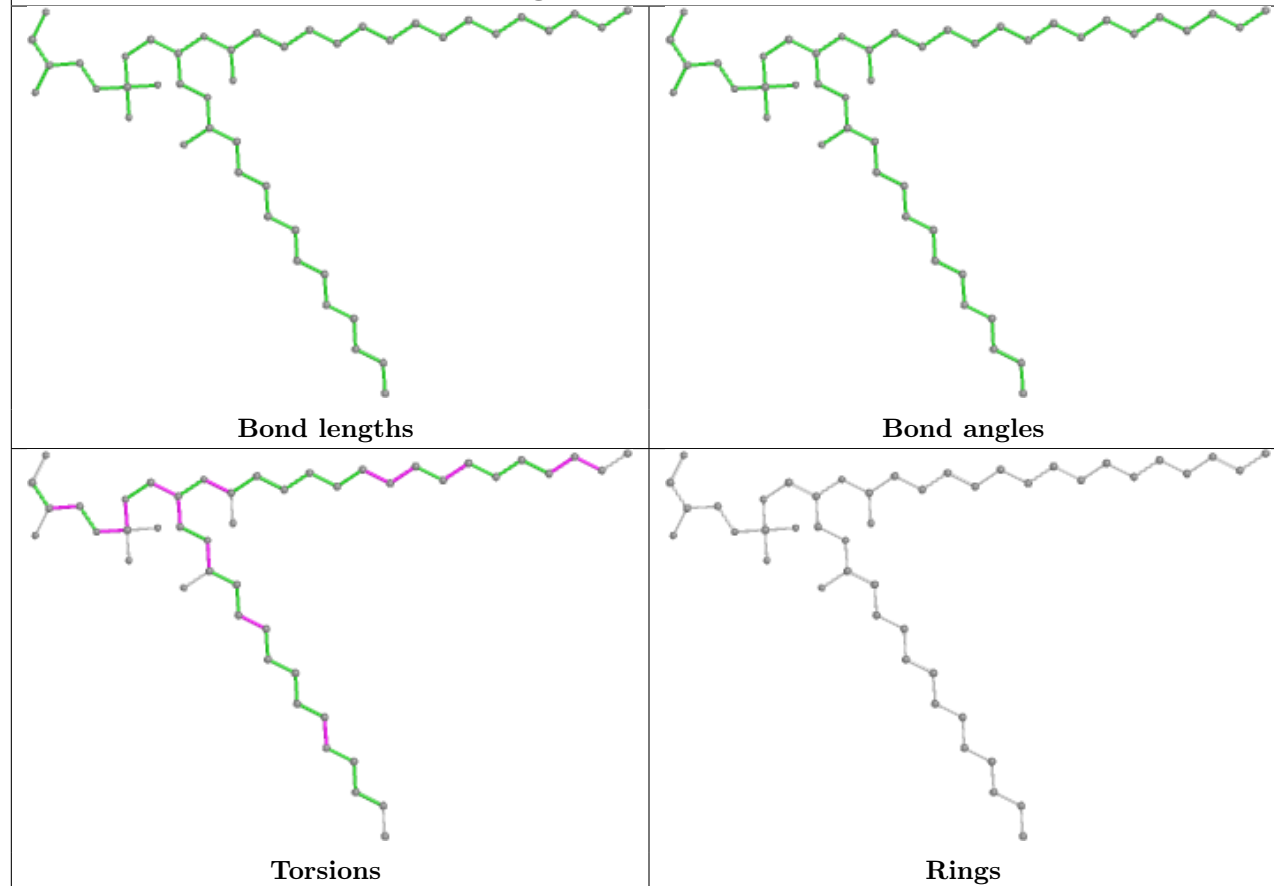
Torsions



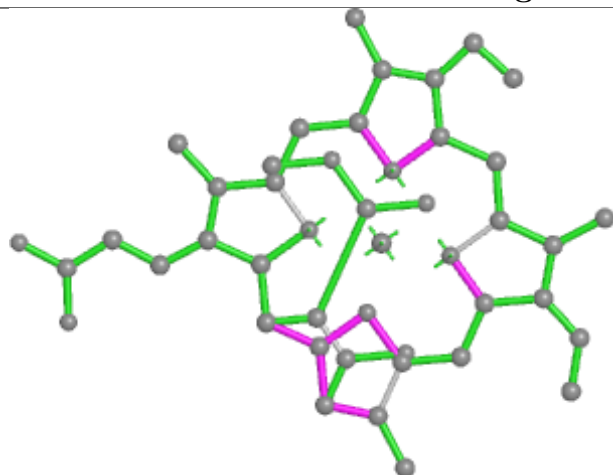
Rings



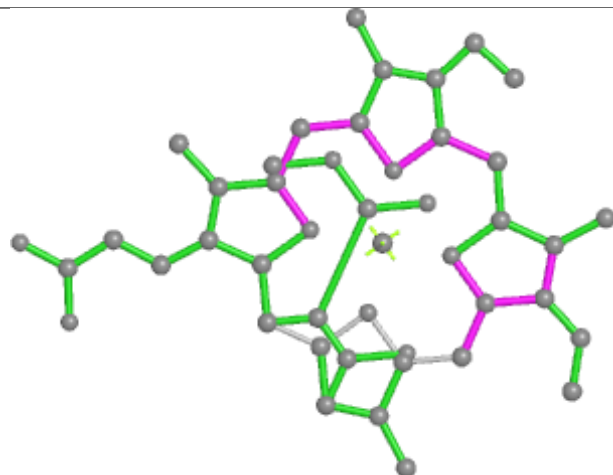


Ligand CLA b 706**Ligand LHG D 620**

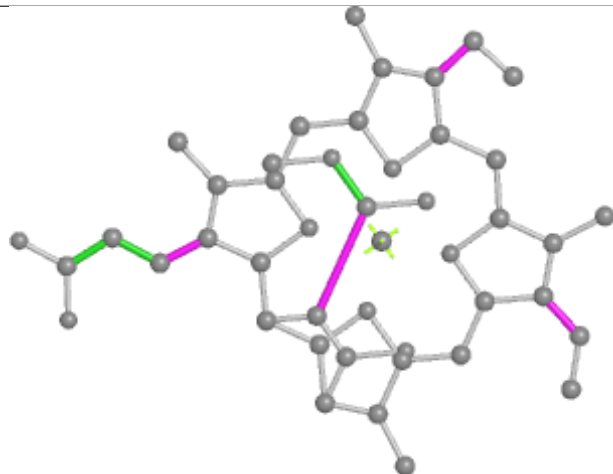
Ligand KC2 H 302



Bond lengths



Bond angles

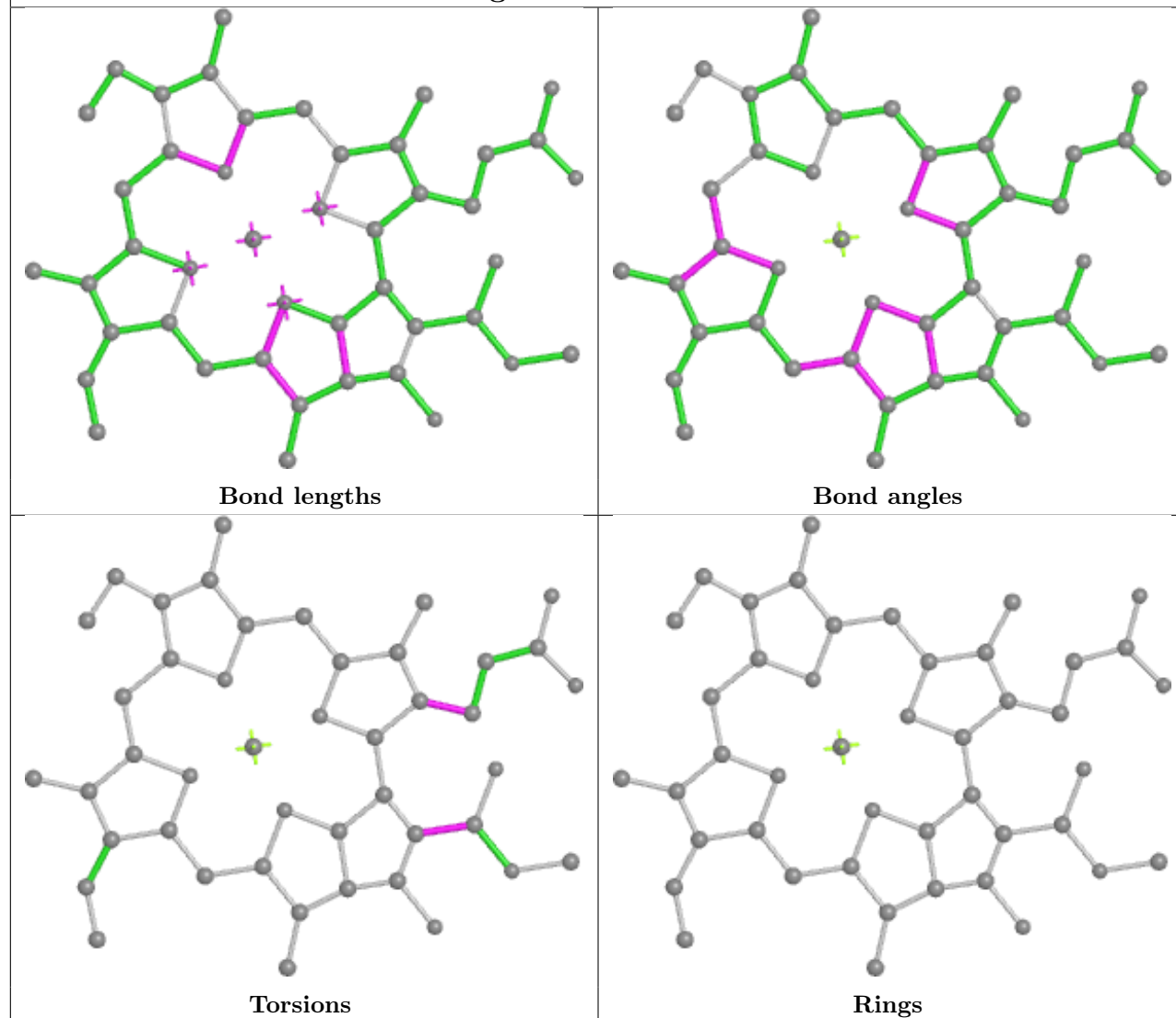


Torsions

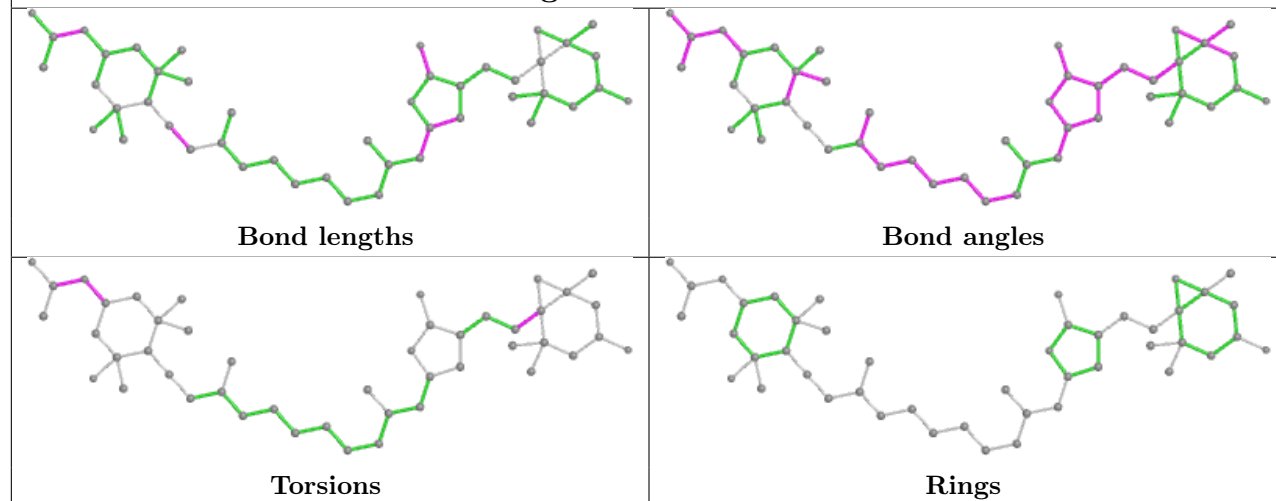


Rings

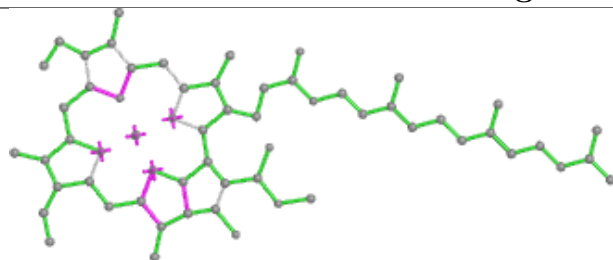
Ligand CLA D 601



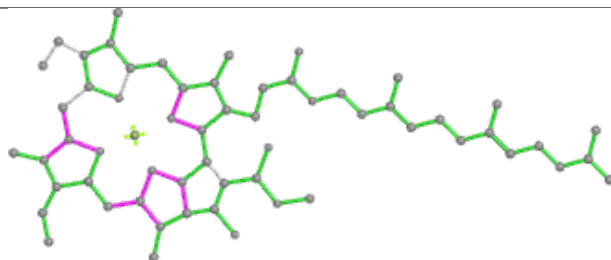
Ligand PID J 615



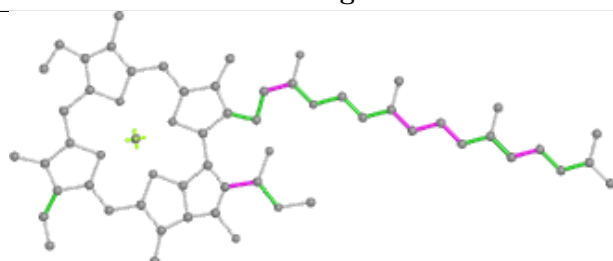
Ligand CLA E 606



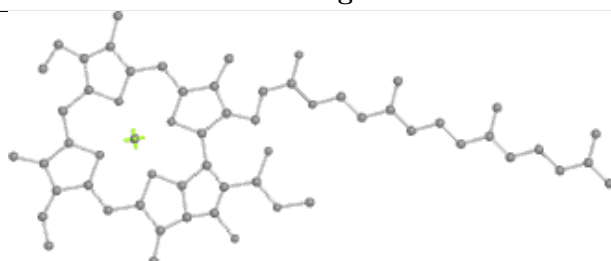
Bond lengths



Bond angles

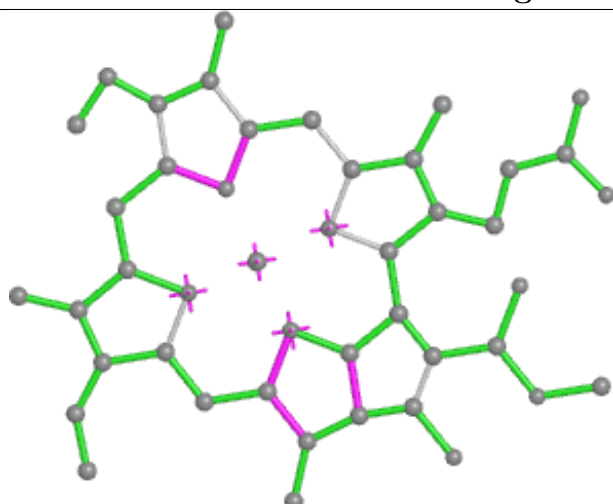


Torsions

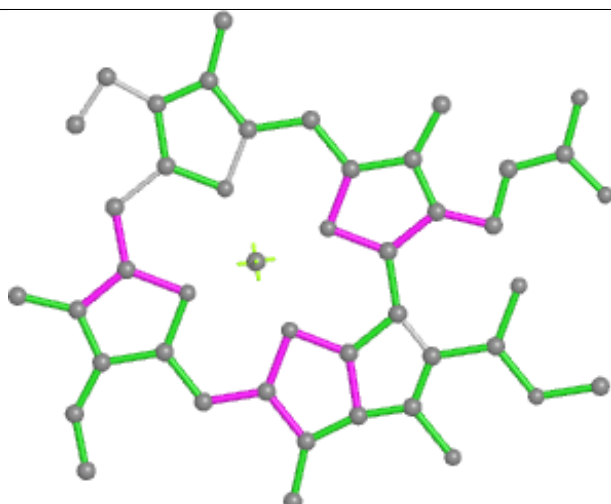


Rings

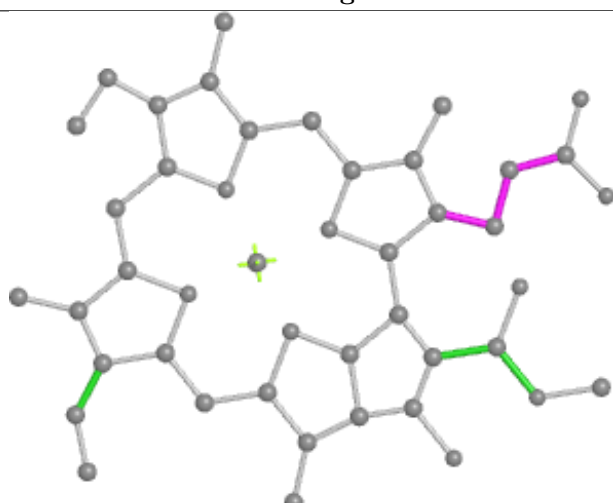
Ligand CLA B 605



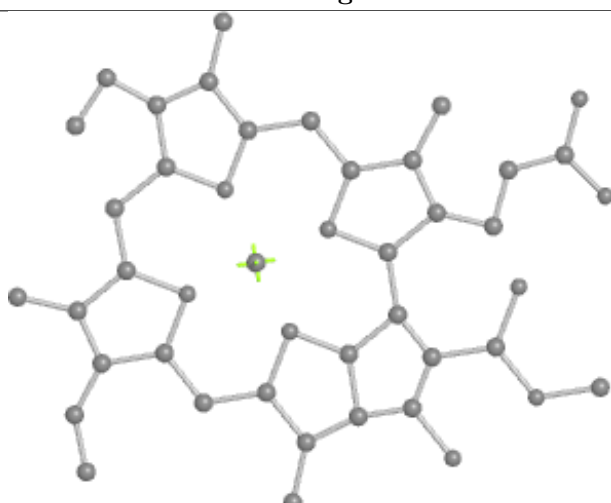
Bond lengths



Bond angles

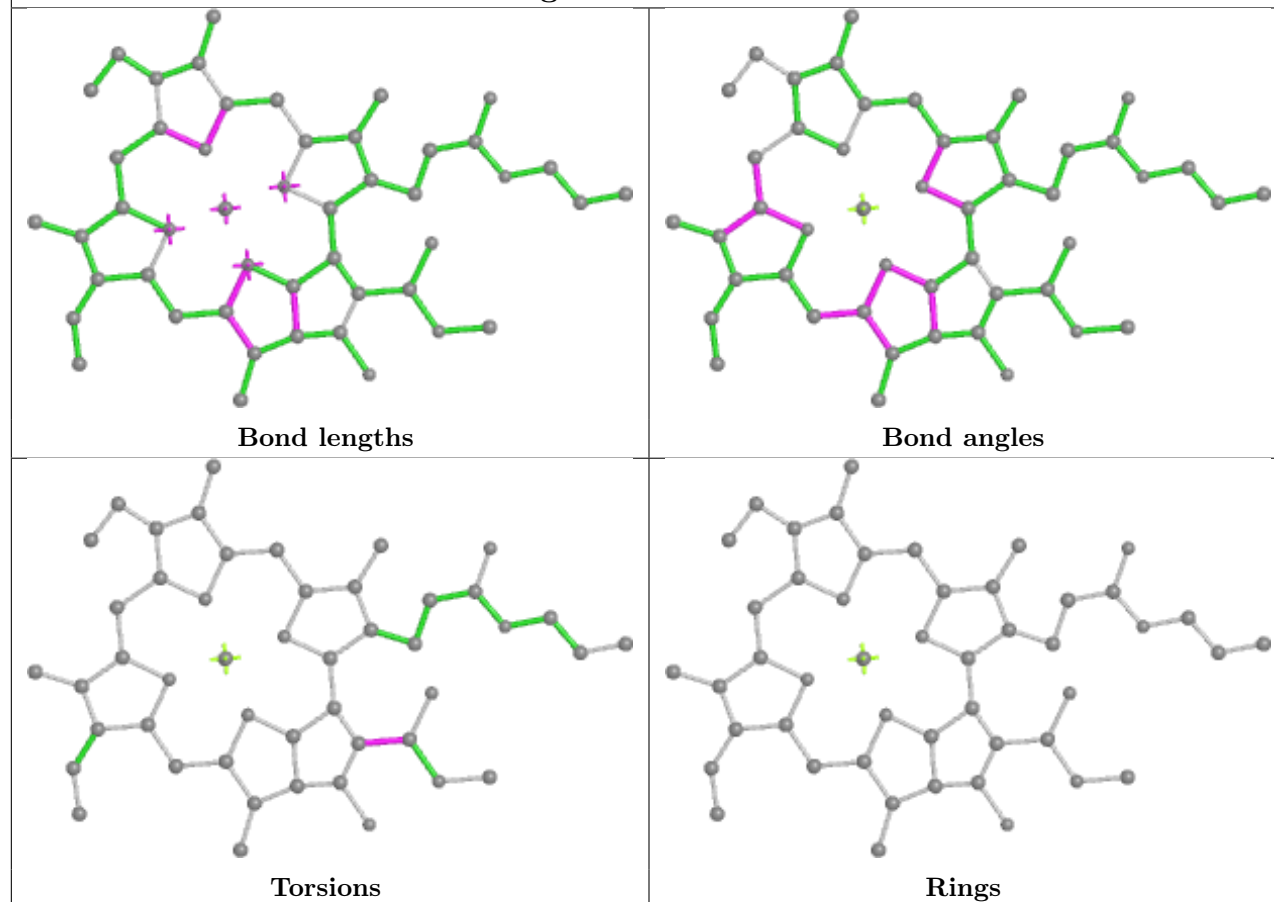


Torsions

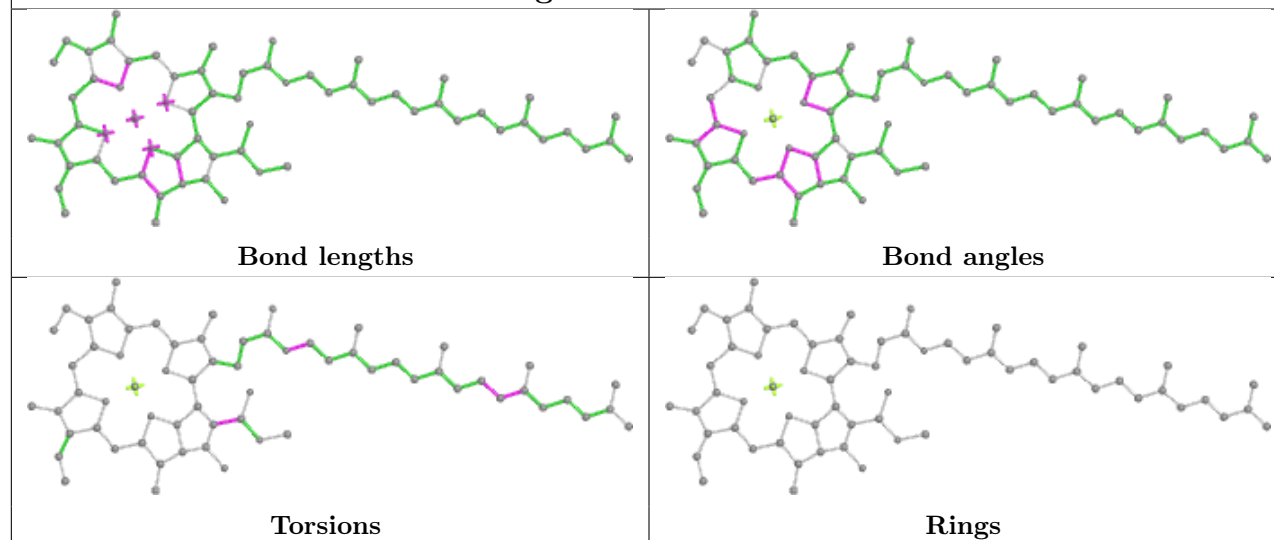


Rings

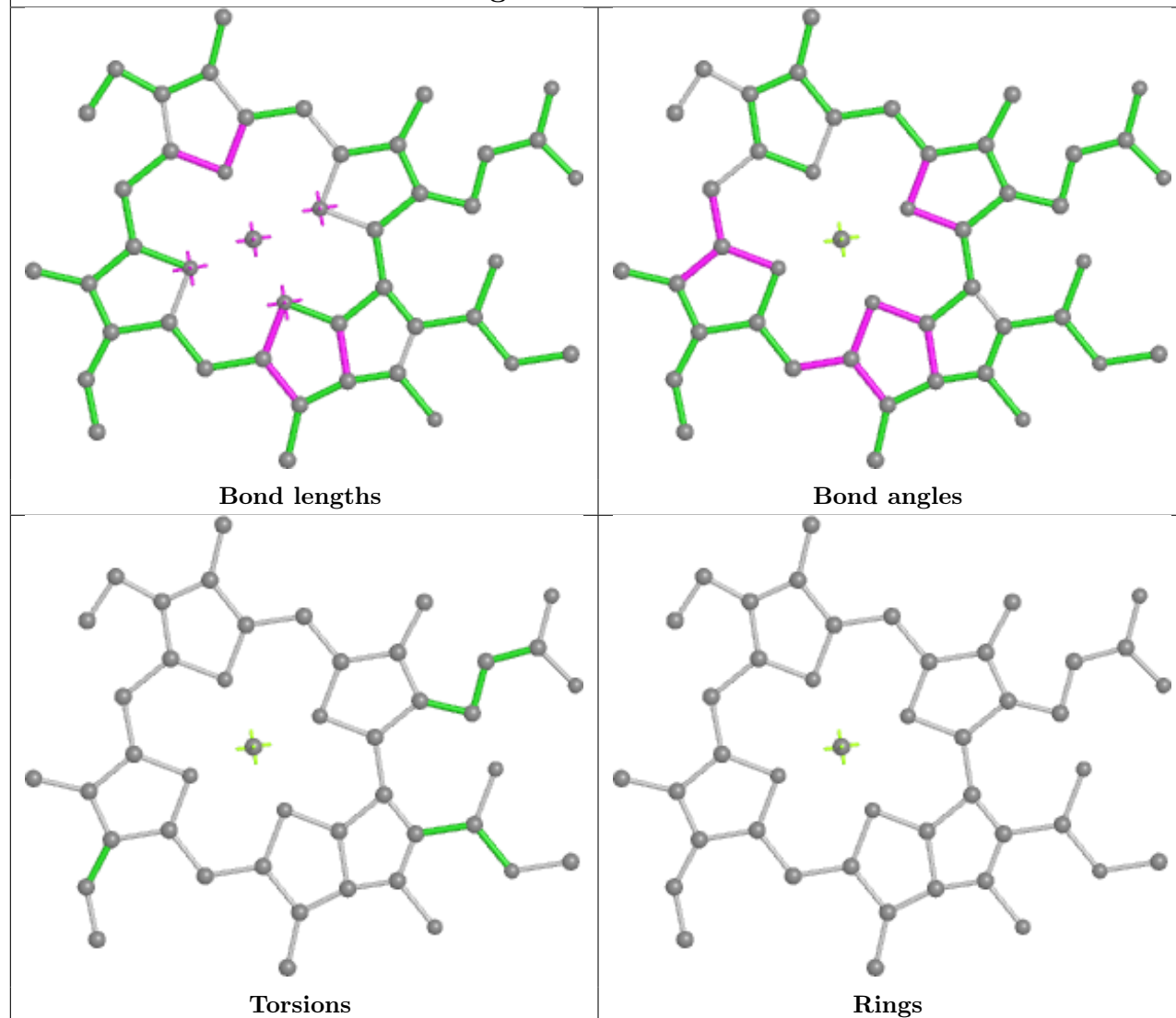
Ligand CLA l 411



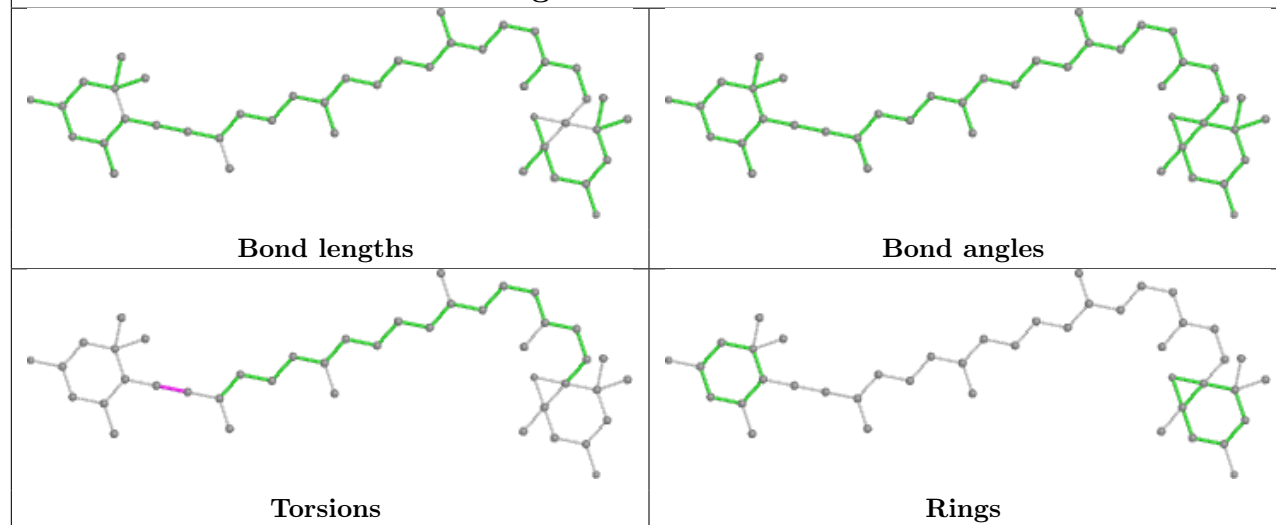
Ligand CLA b 709

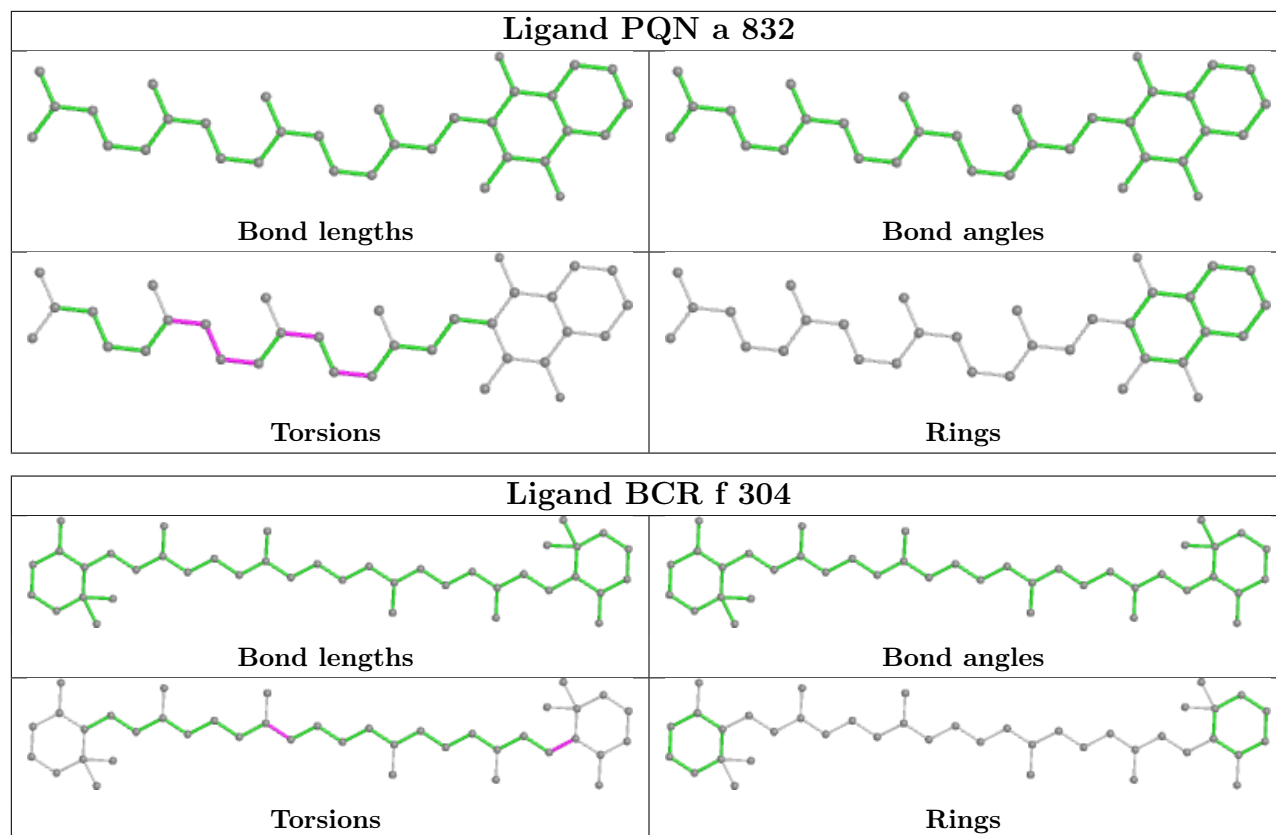


Ligand CLA A 607

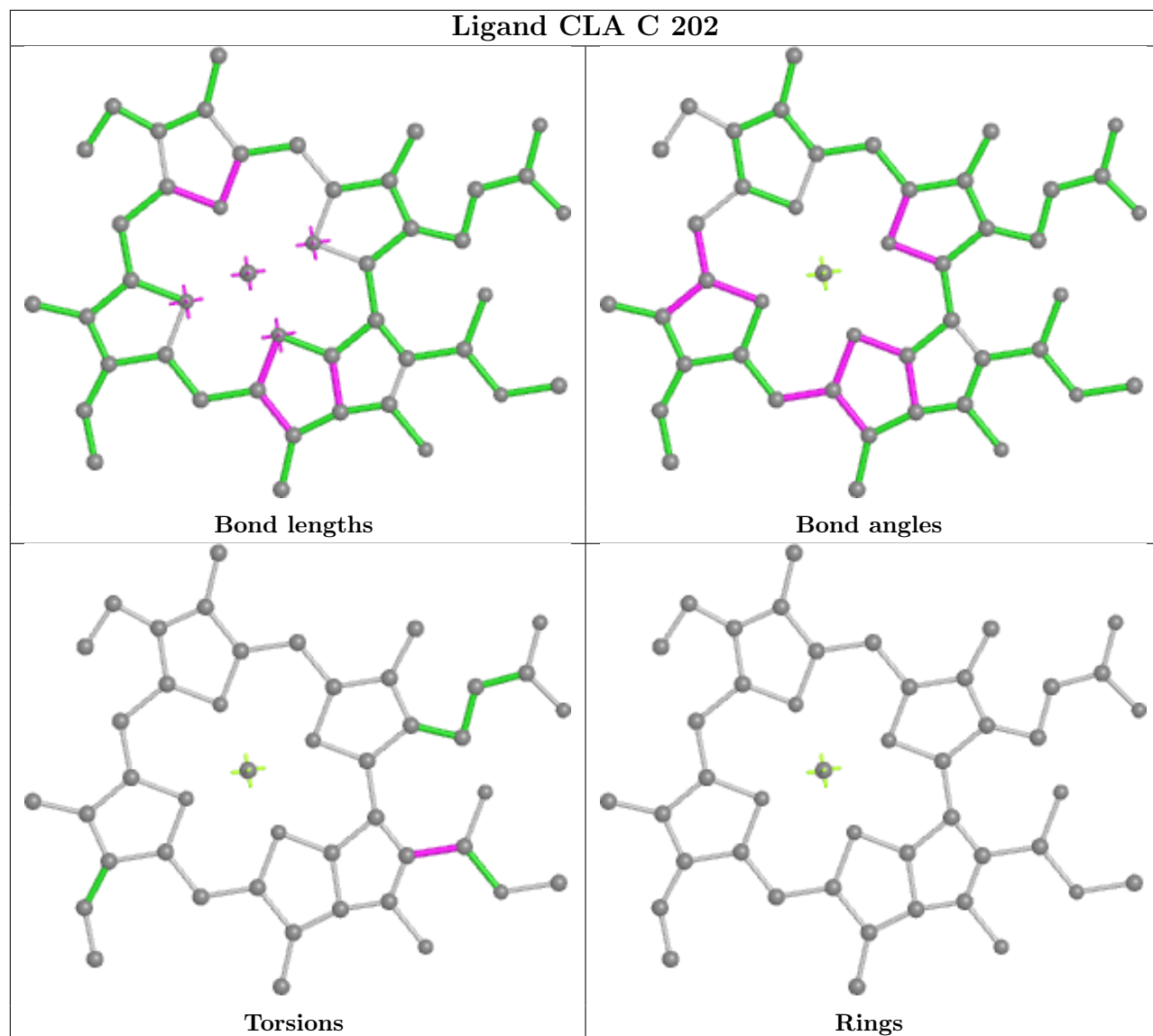


Ligand DD6 G 616

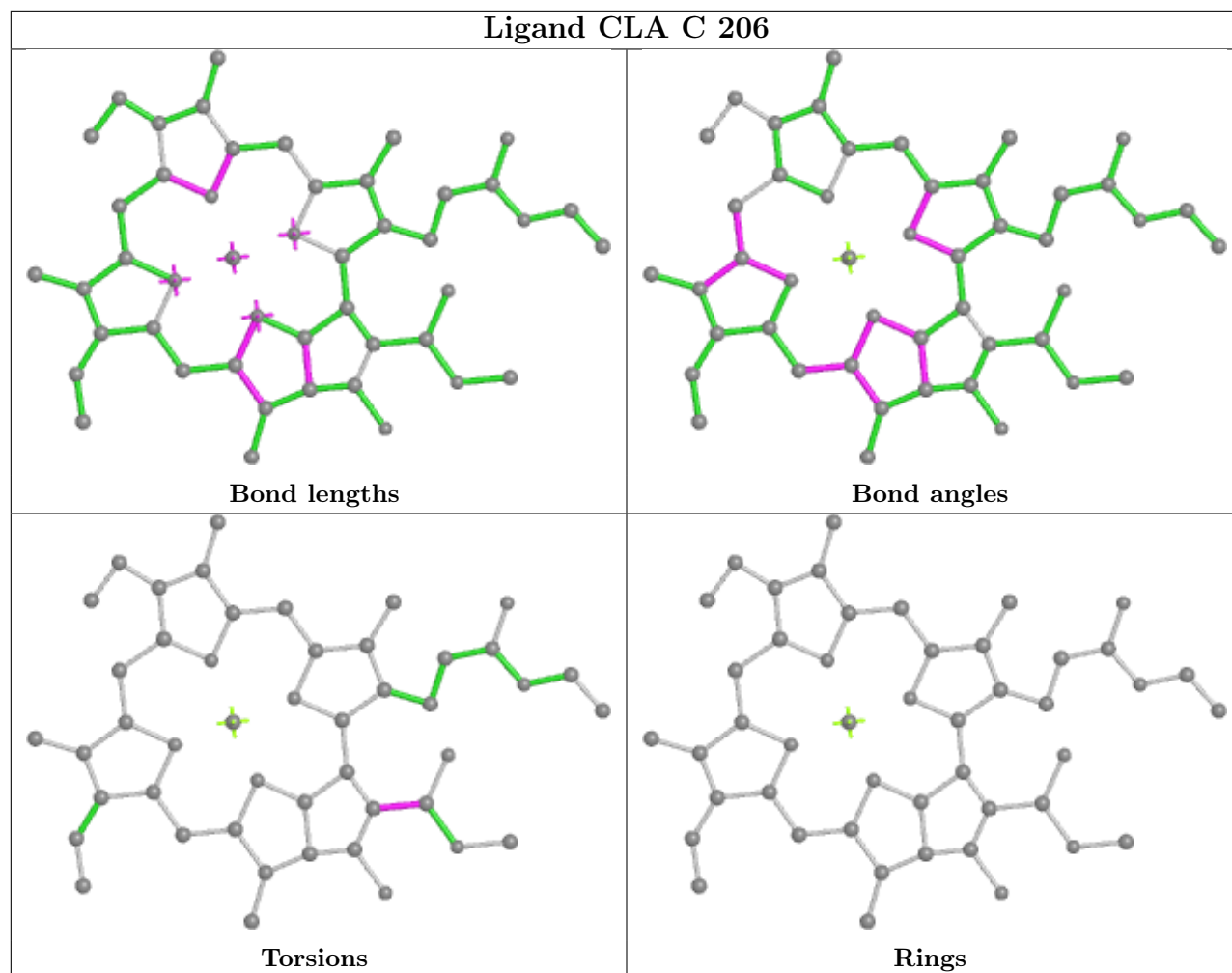




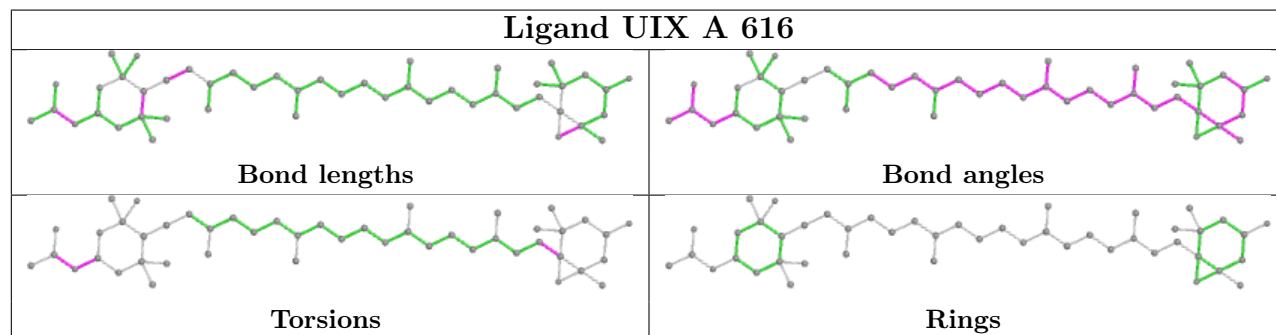
Ligand CLA C 202



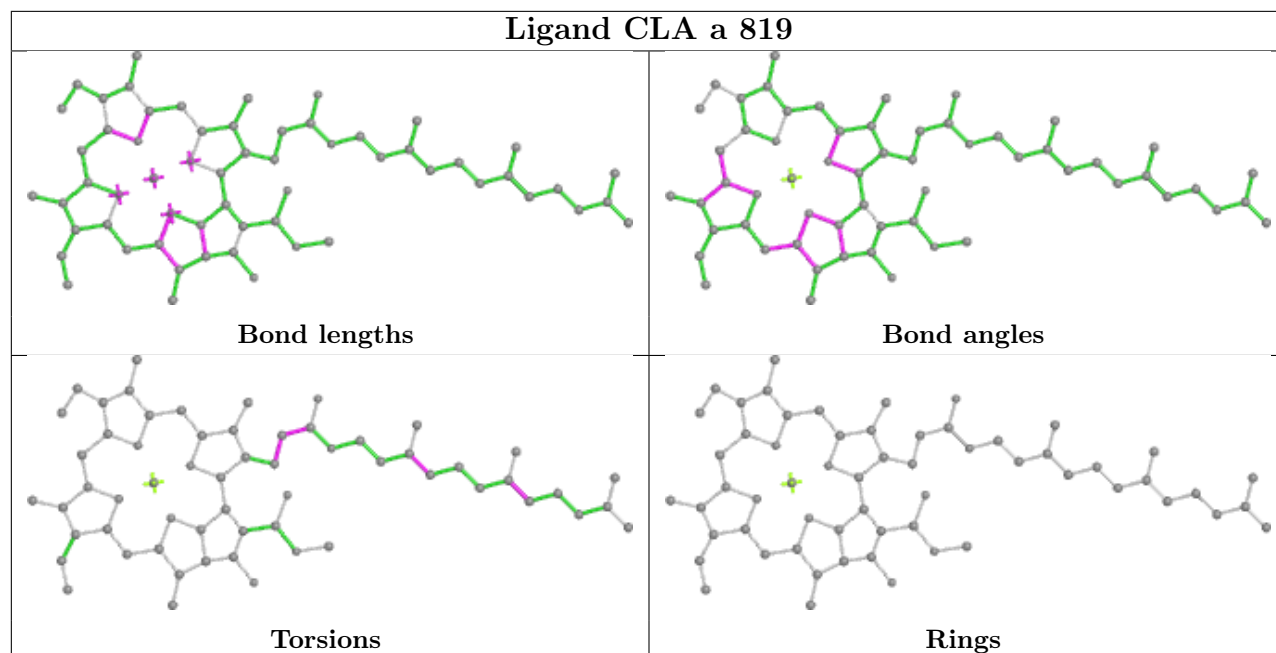
Ligand CLA C 206



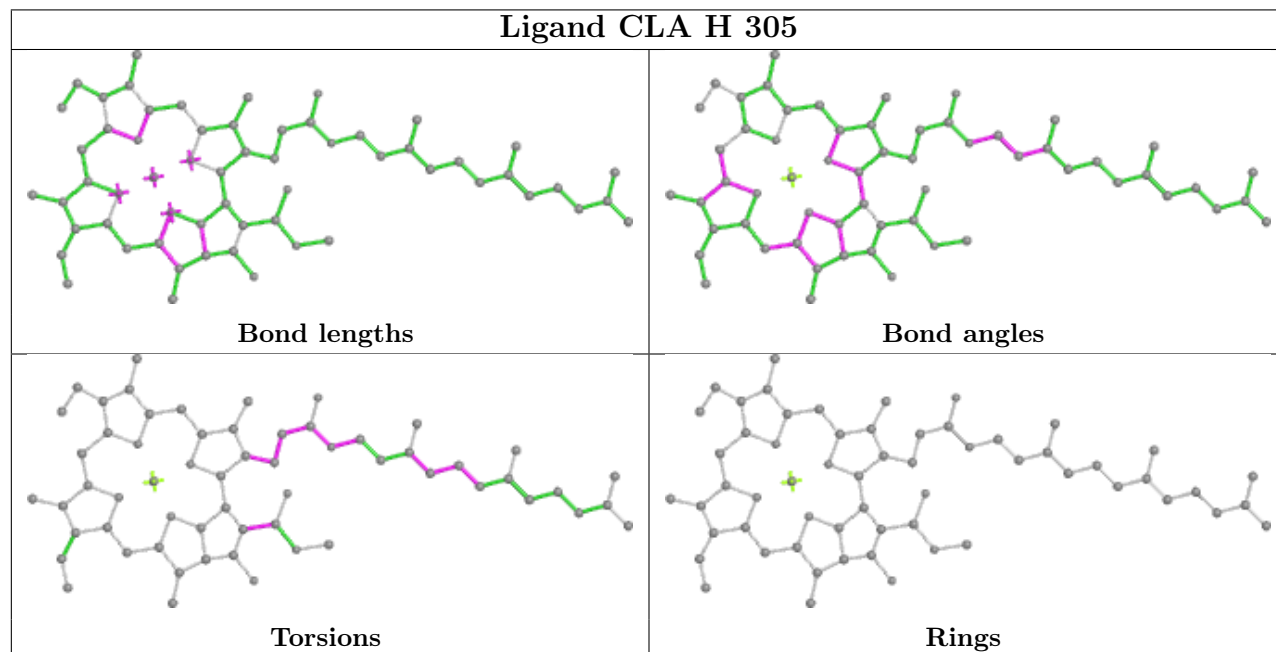
Ligand UIX A 616

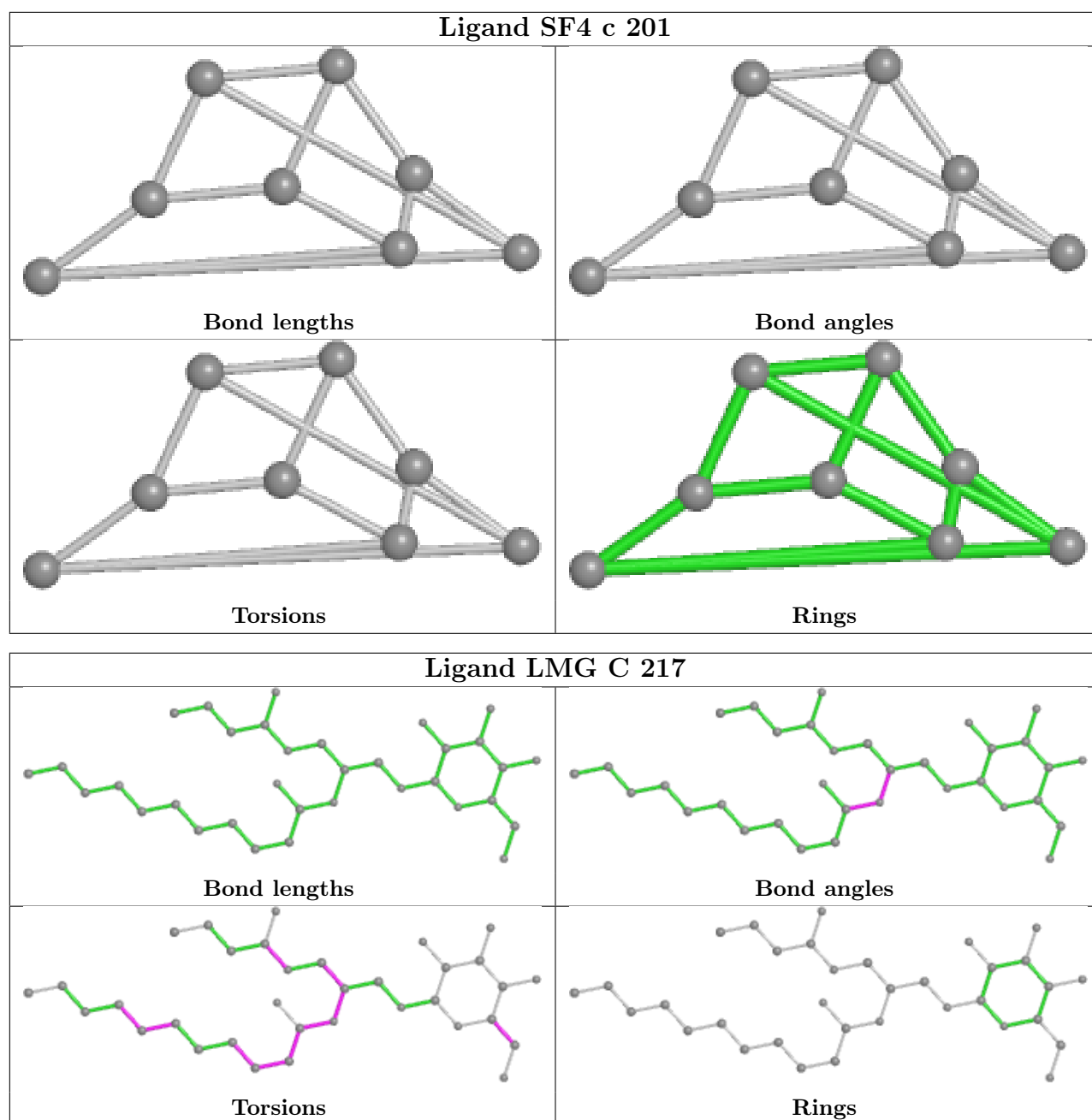


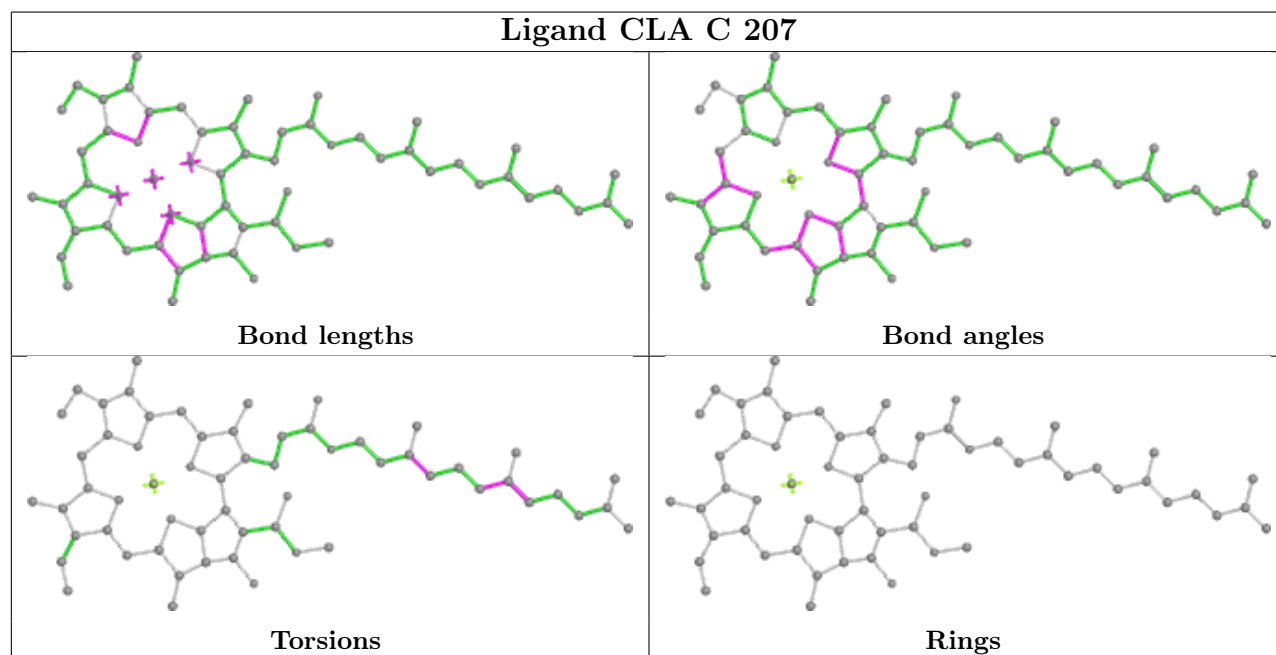
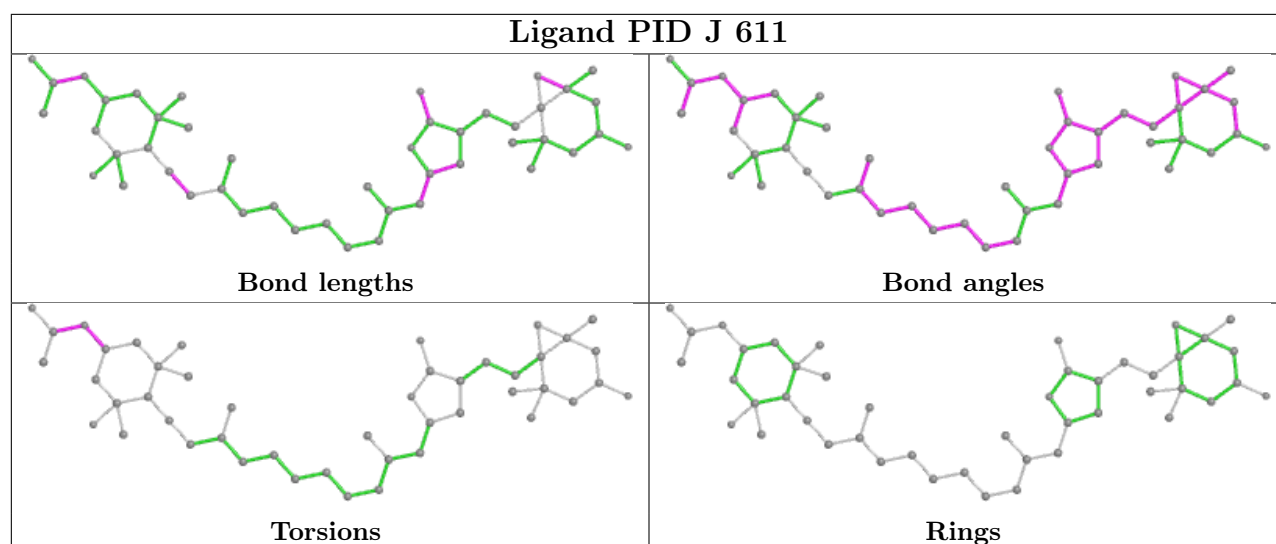
Ligand CLA a 819



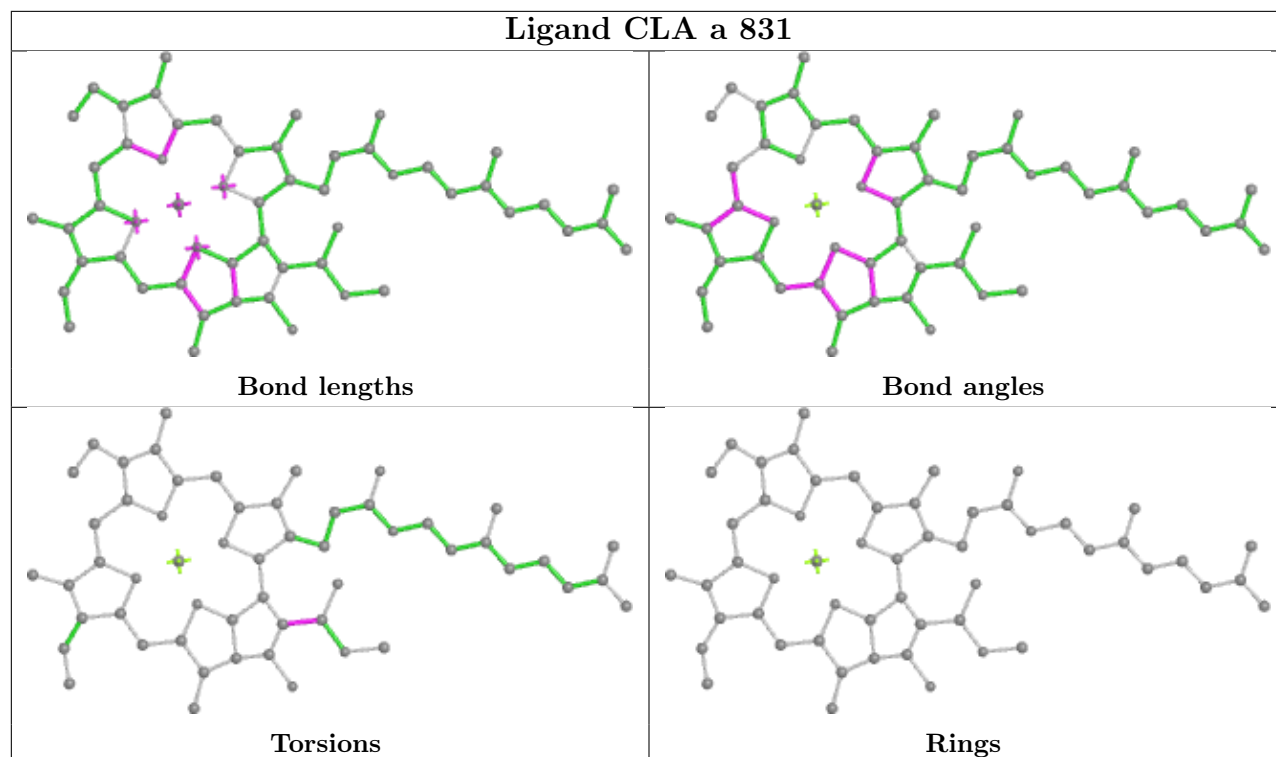
Ligand CLA H 305



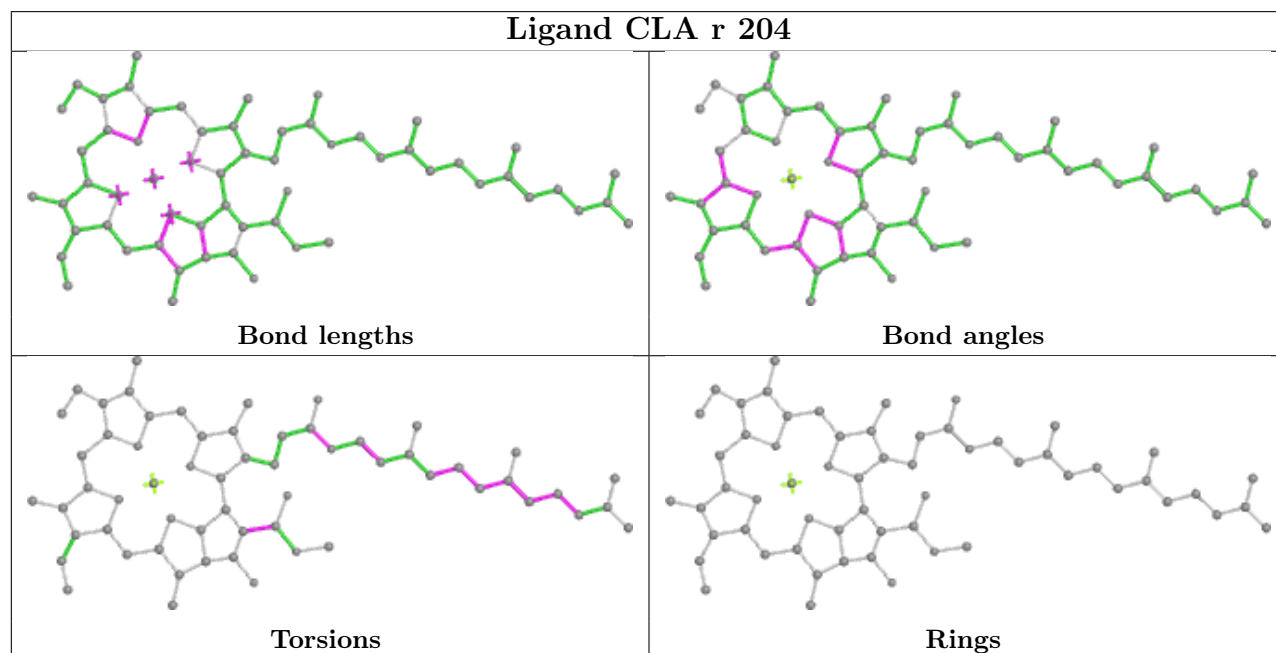


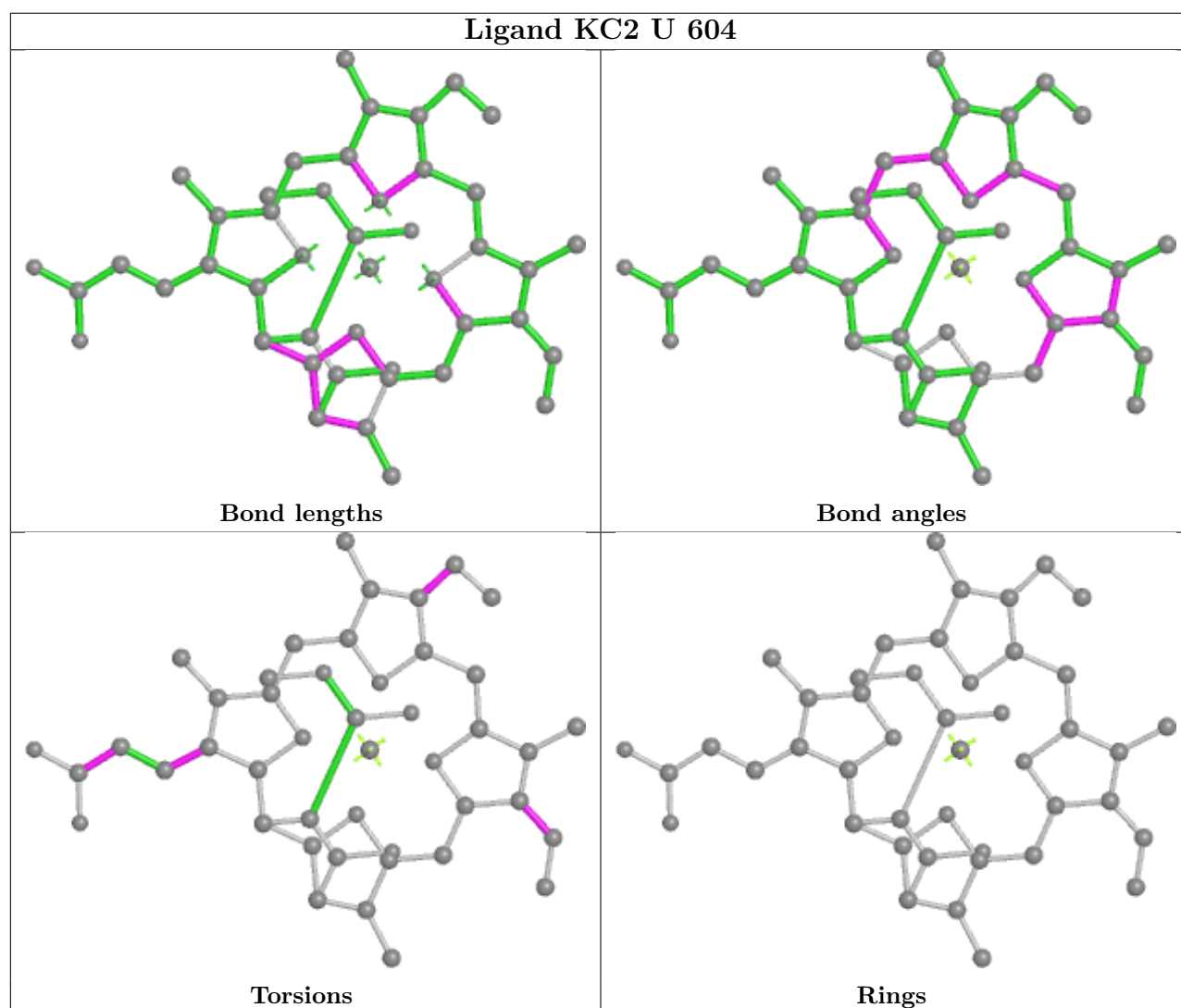
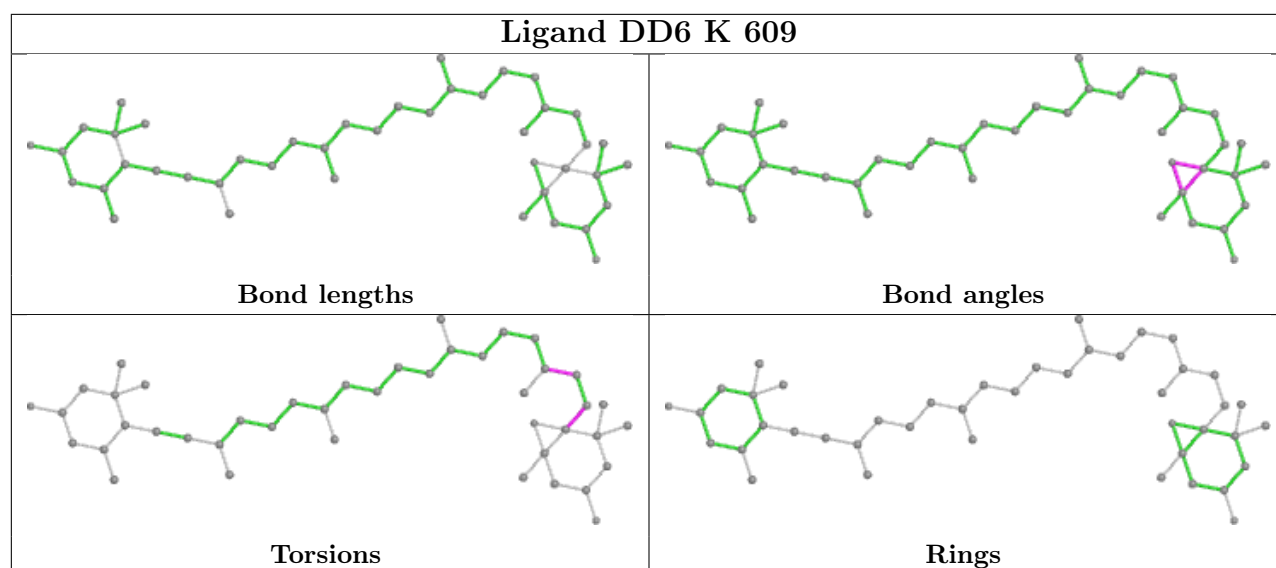


Ligand CLA a 831

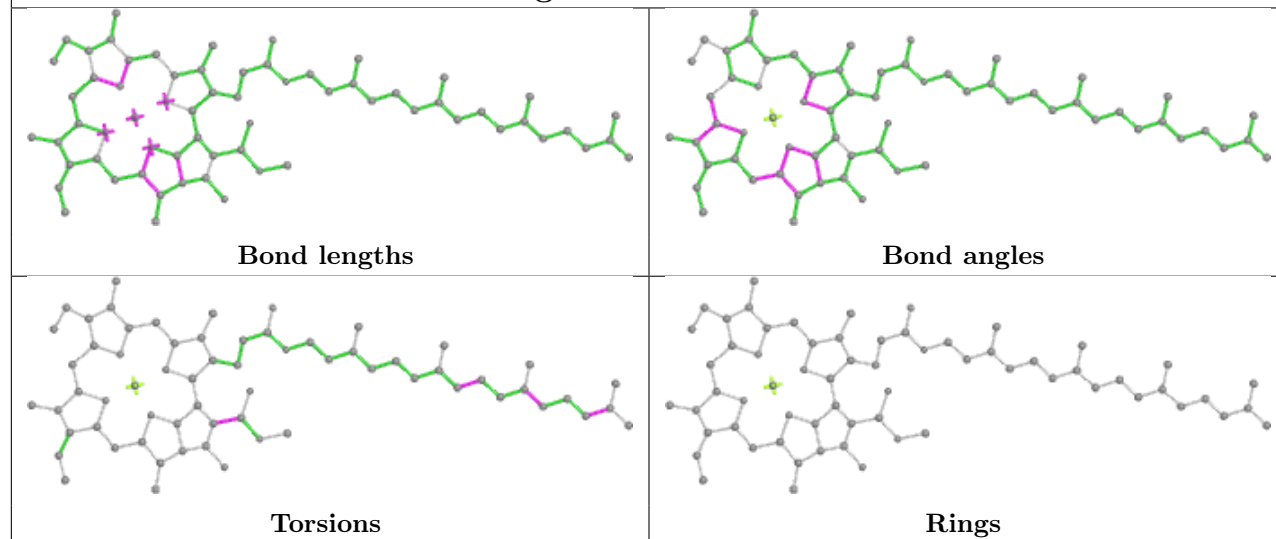


Ligand CLA r 204

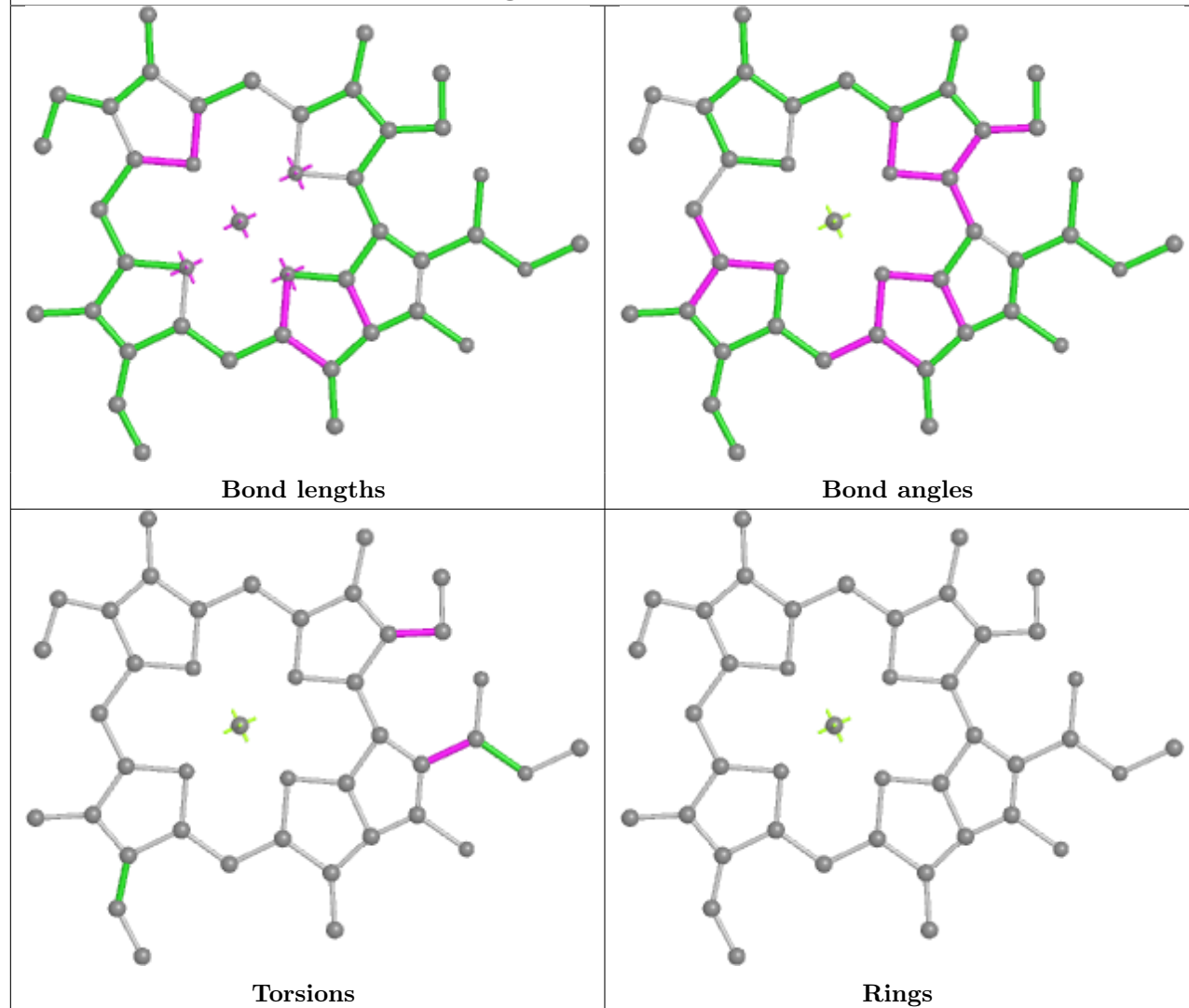


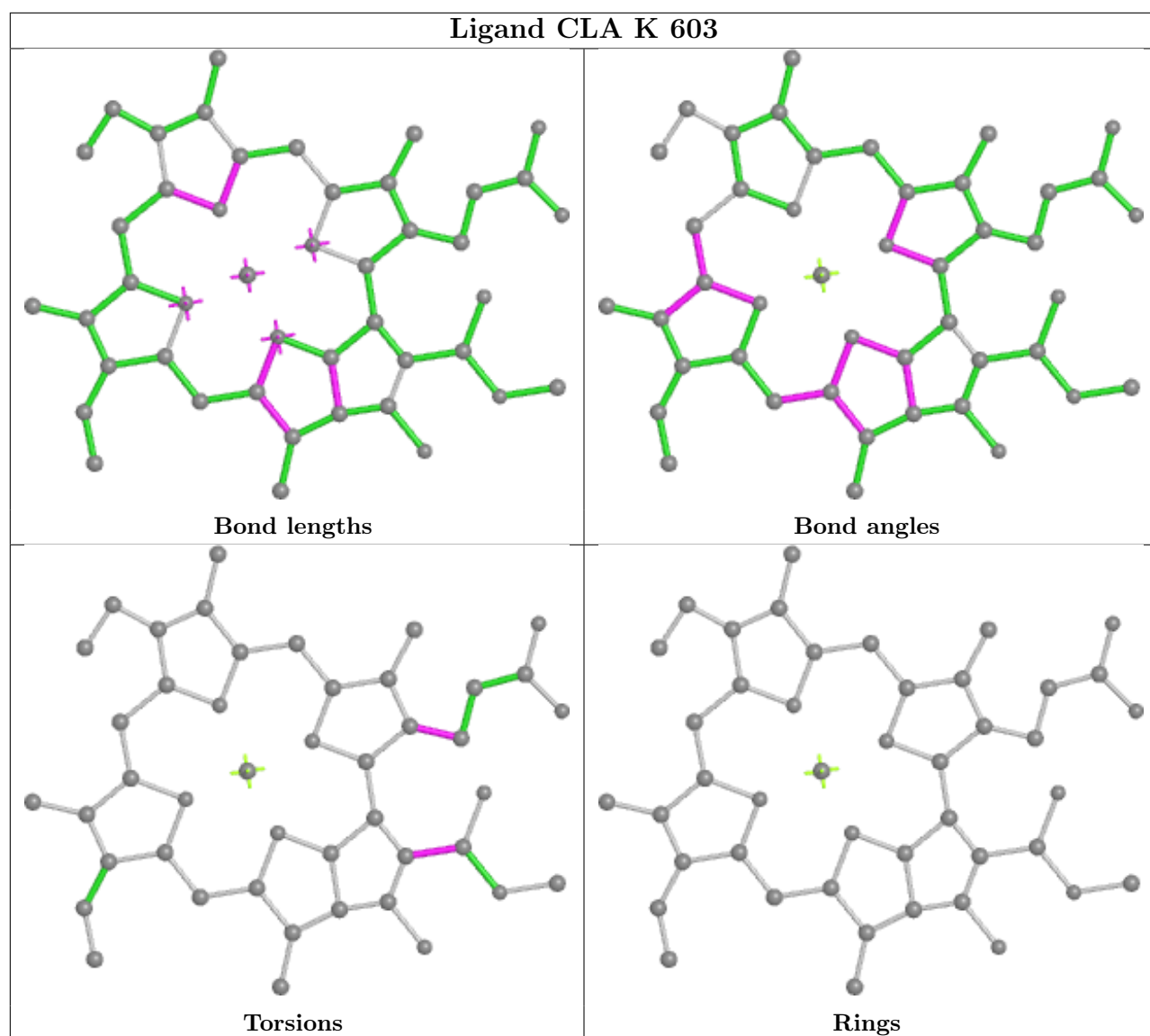


Ligand CLA b 716

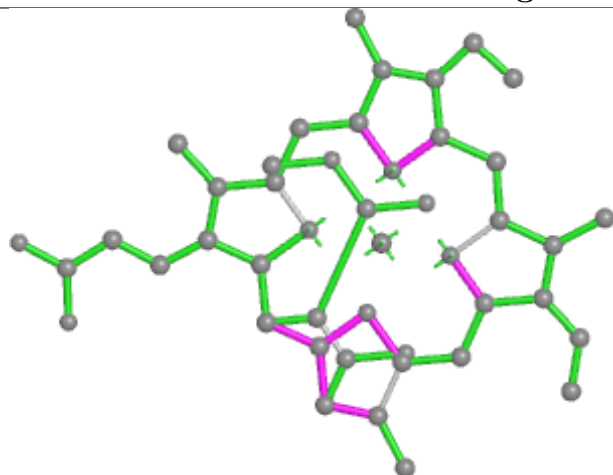


Ligand CLA I 611

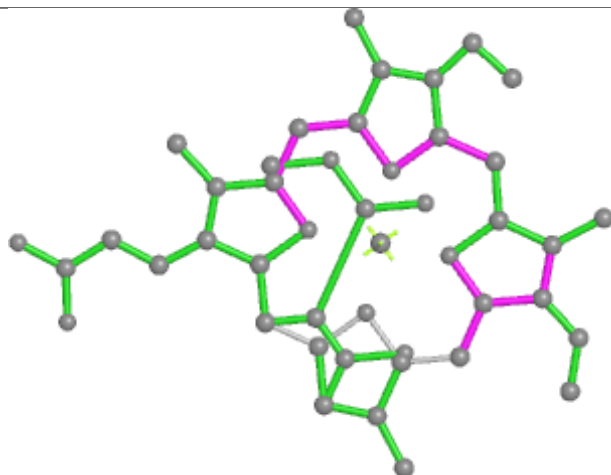




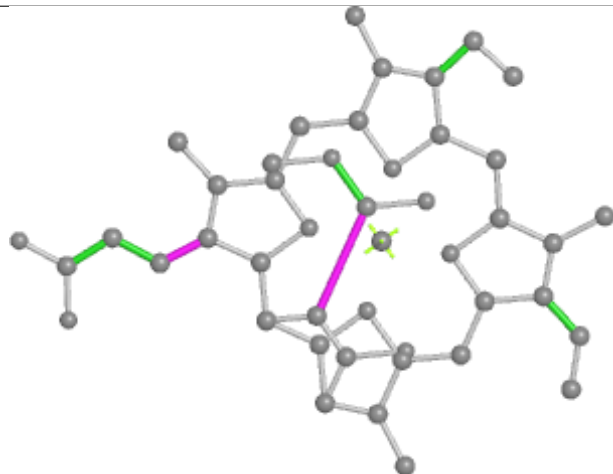
Ligand KC2 B 608



Bond lengths



Bond angles

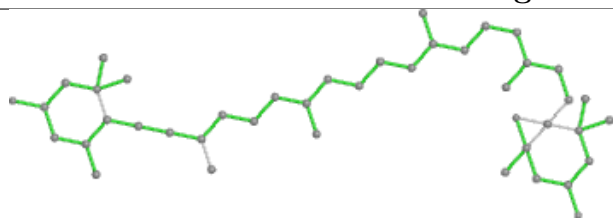


Torsions

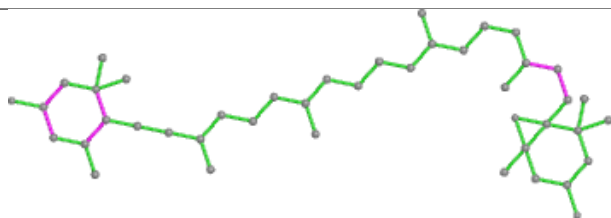


Rings

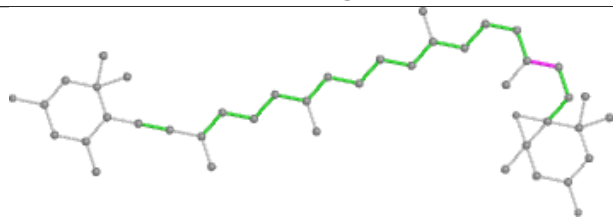
Ligand DD6 G 614



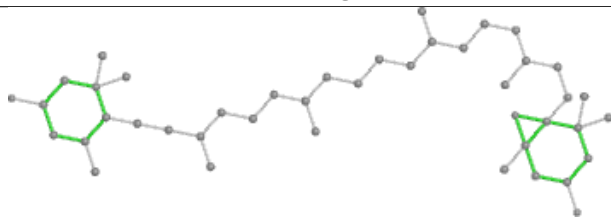
Bond lengths



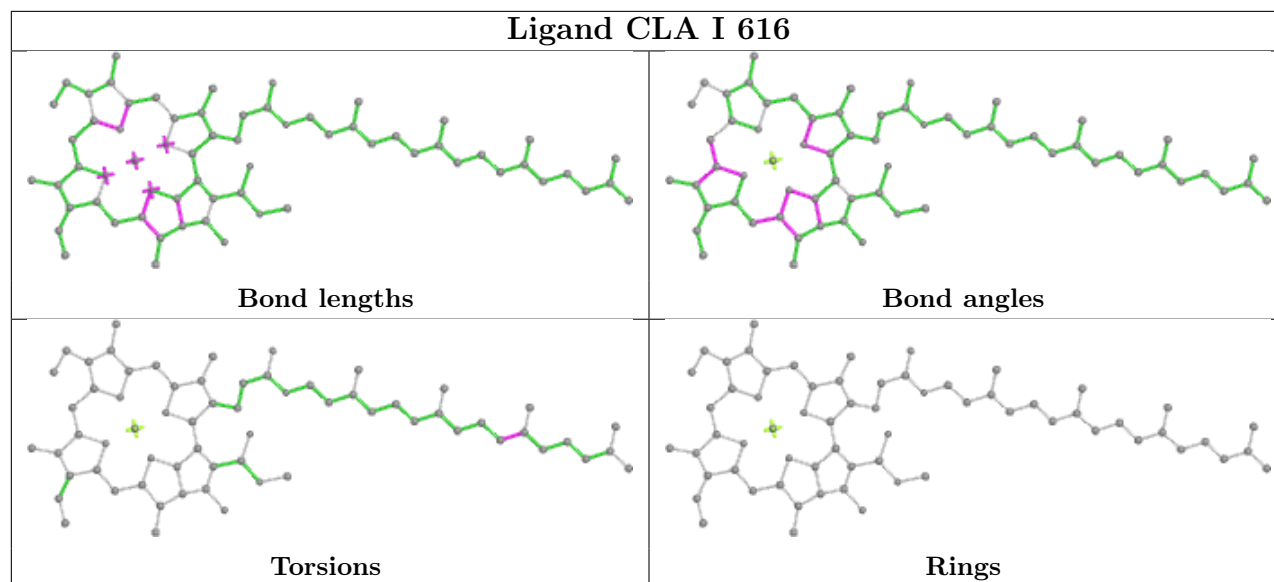
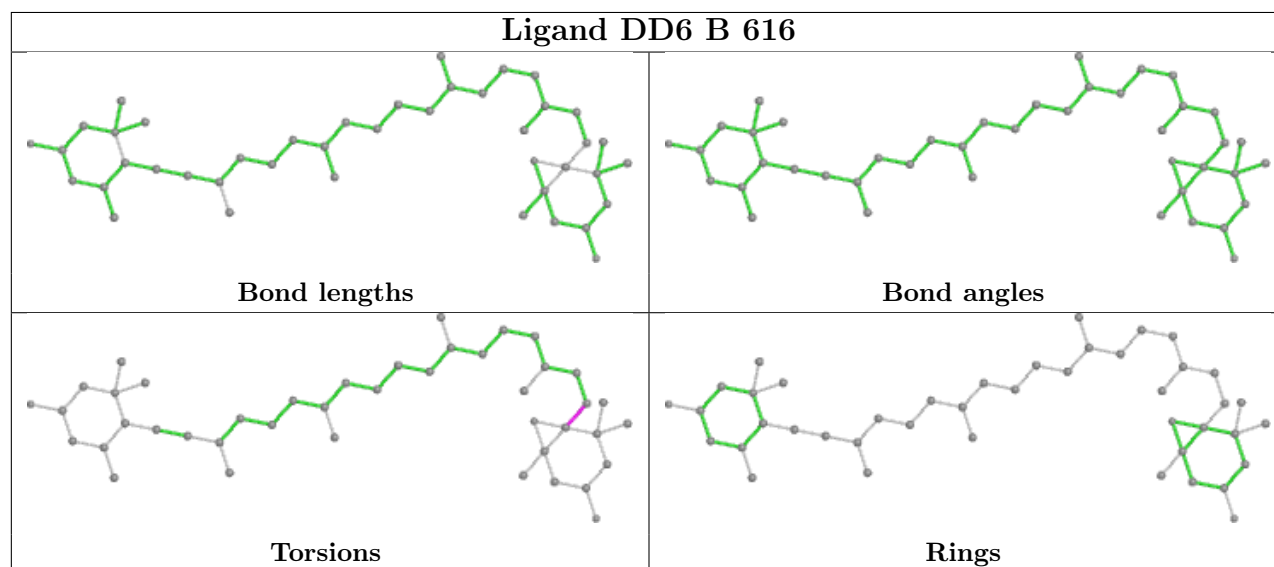
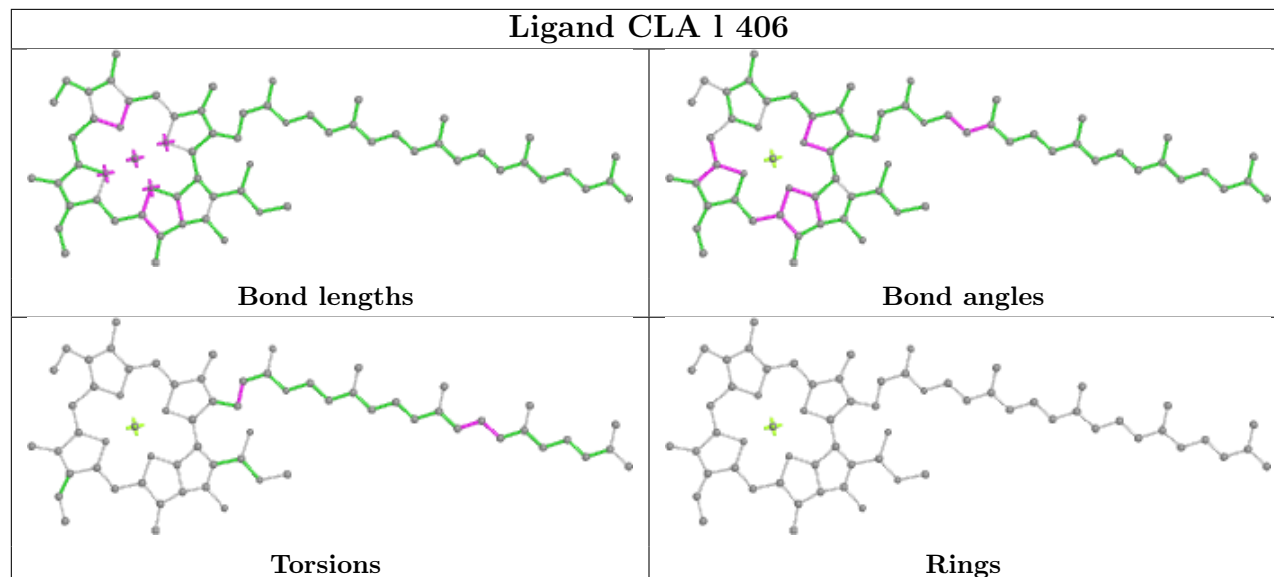
Bond angles

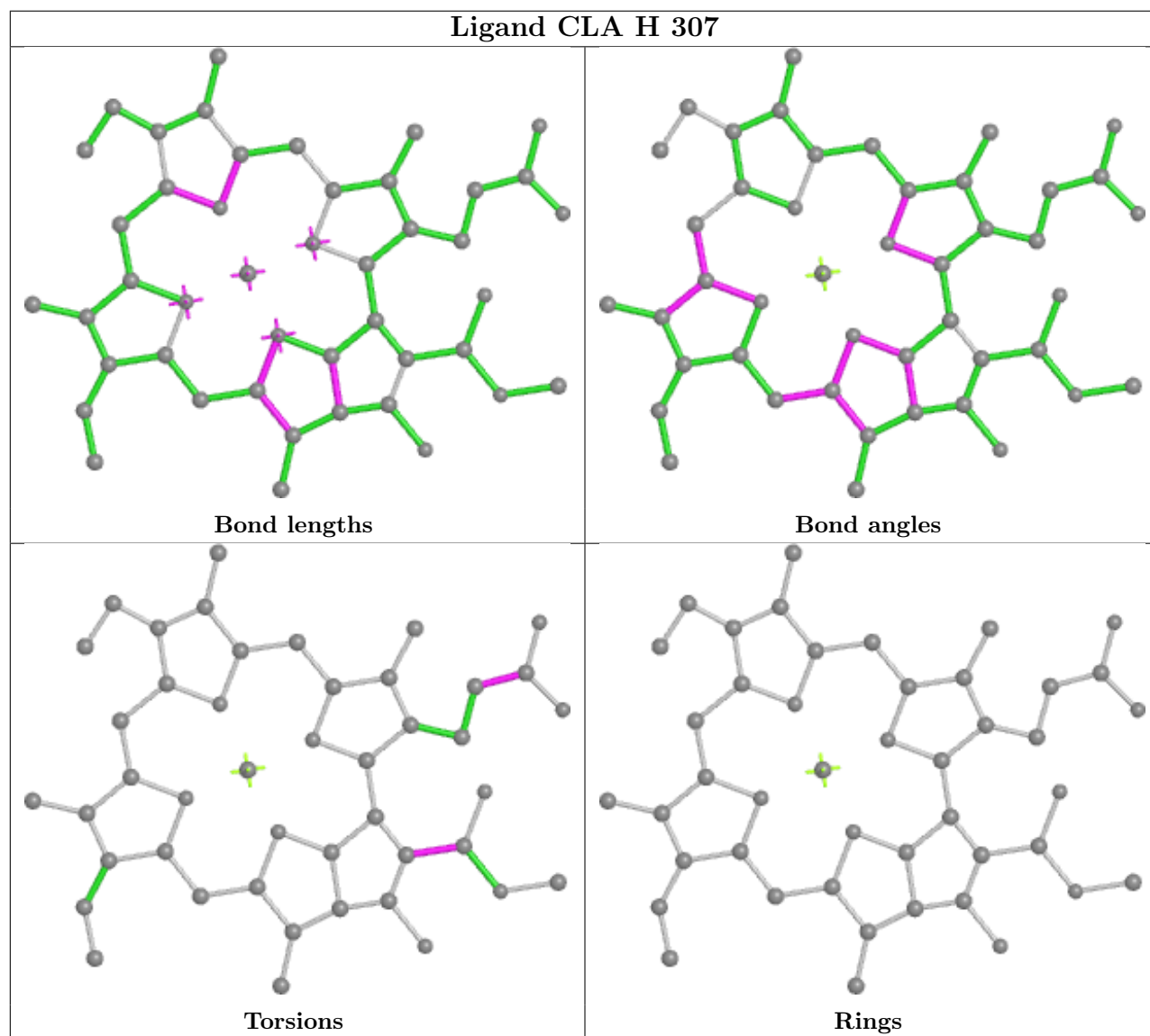
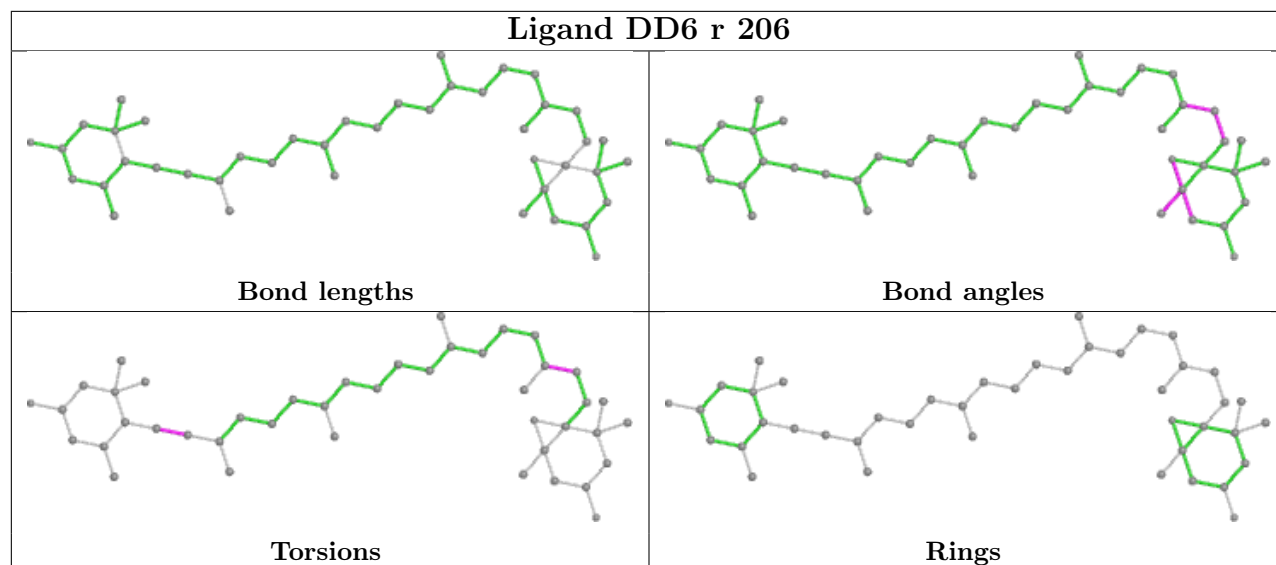


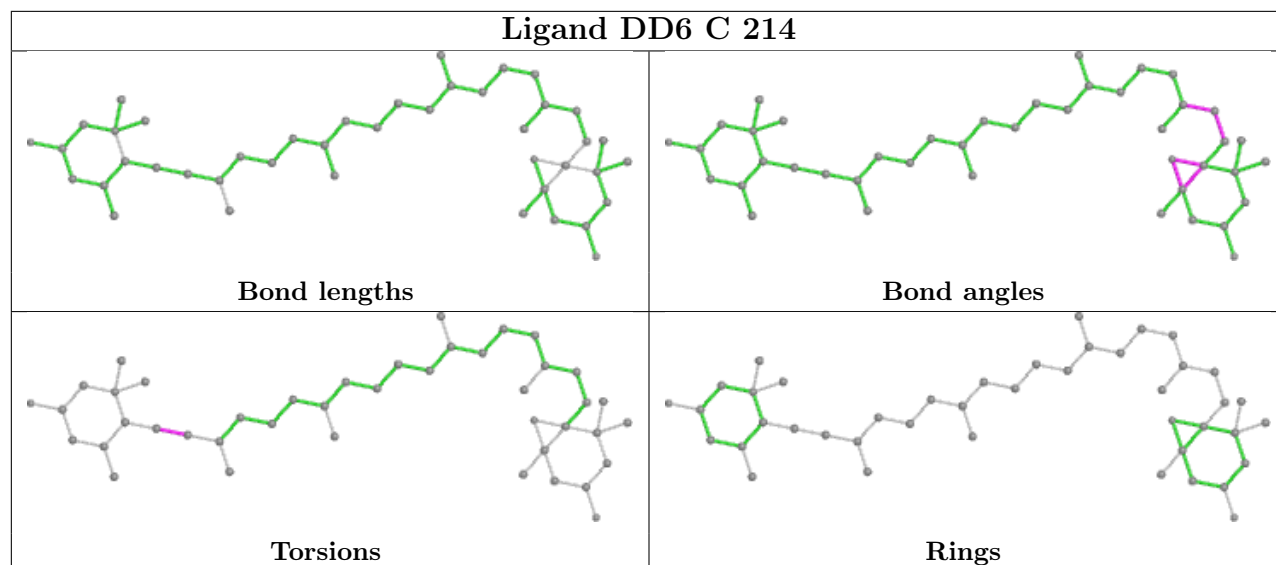
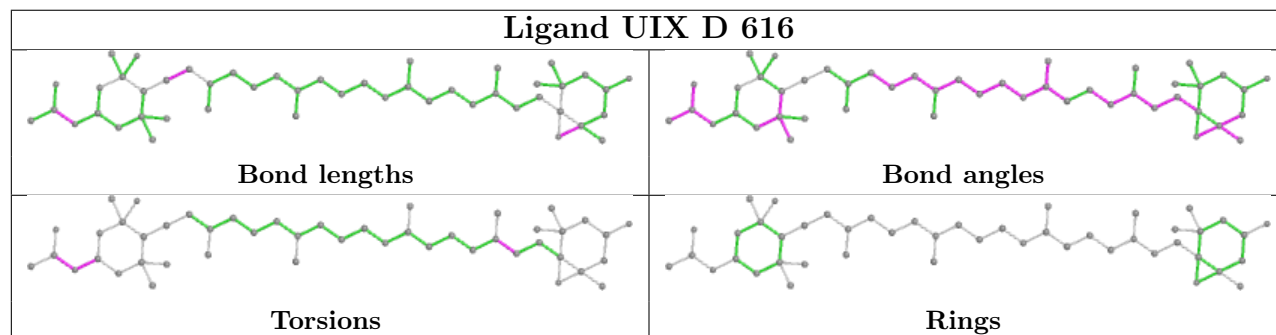
Torsions



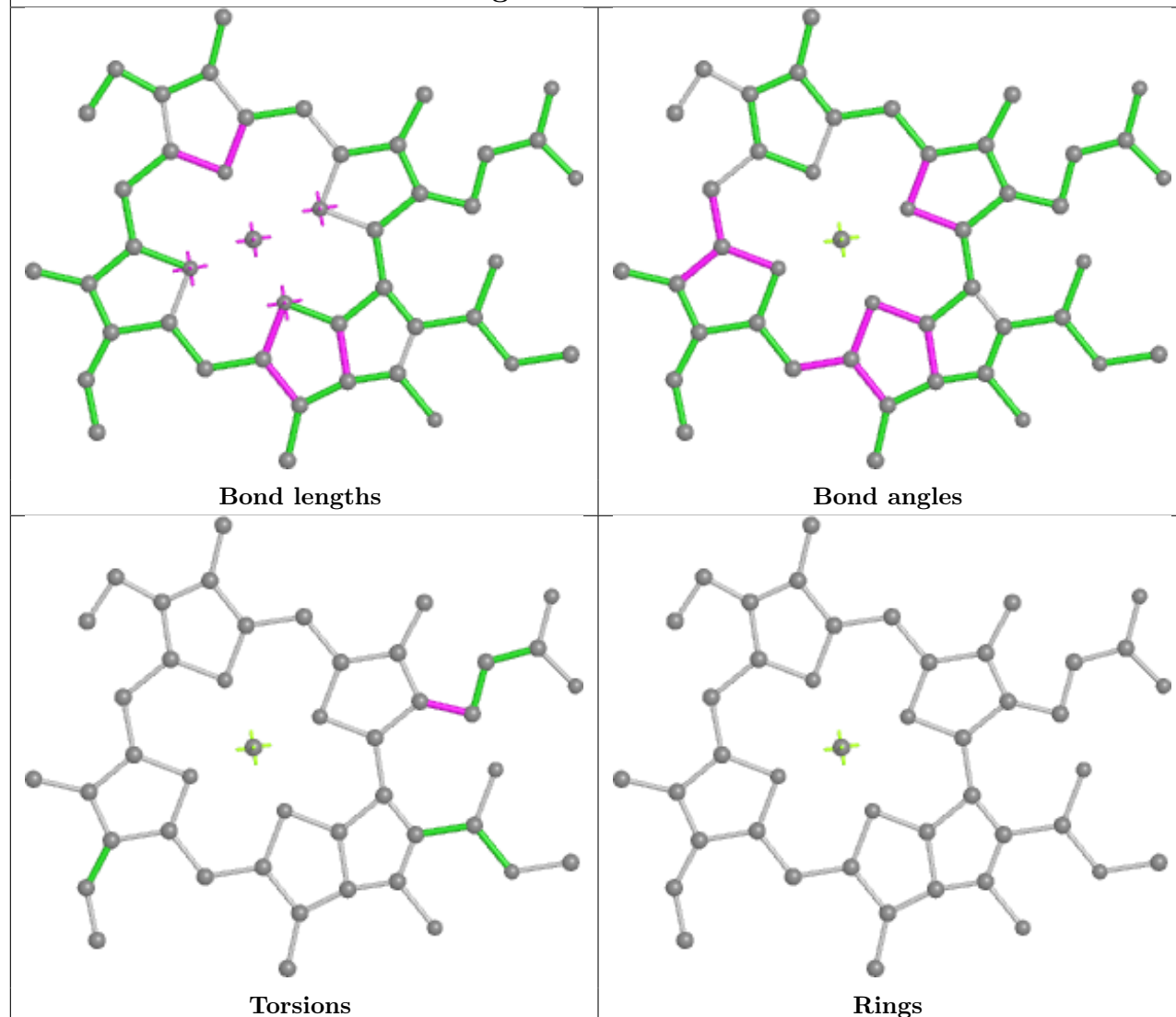
Rings

Ligand CLA I 616**Ligand DD6 B 616****Ligand CLA I 406**

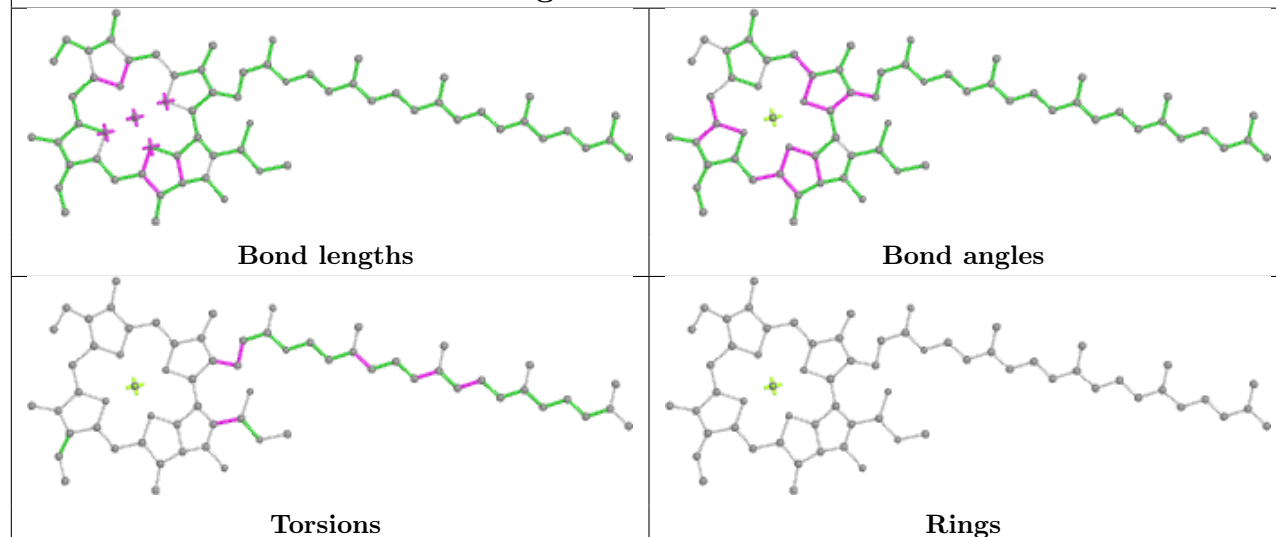


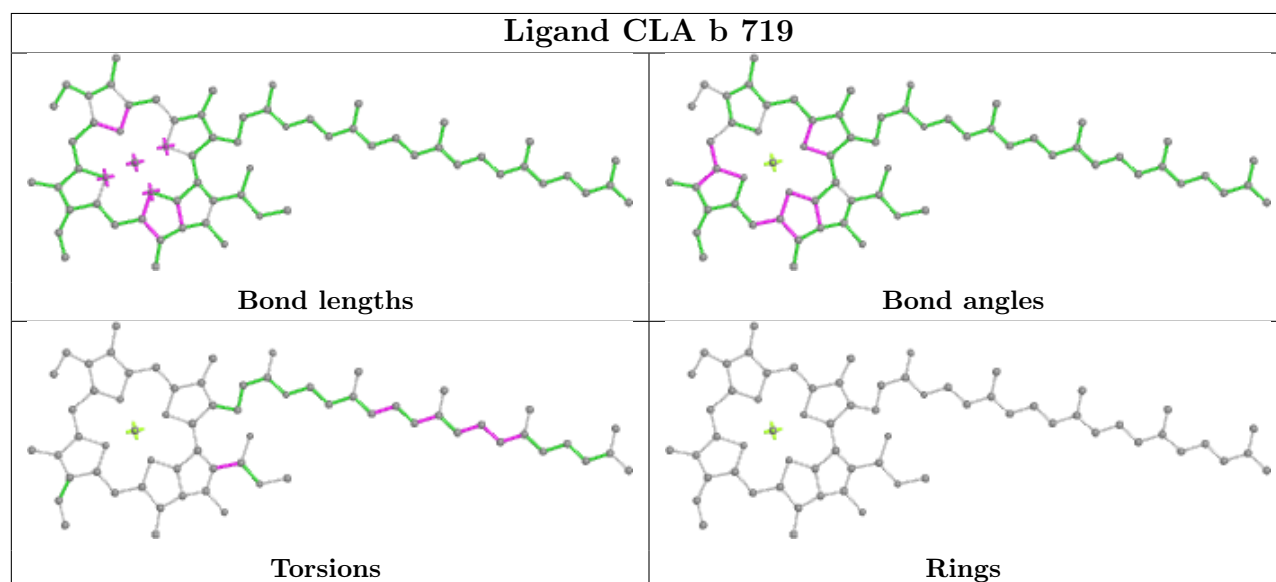
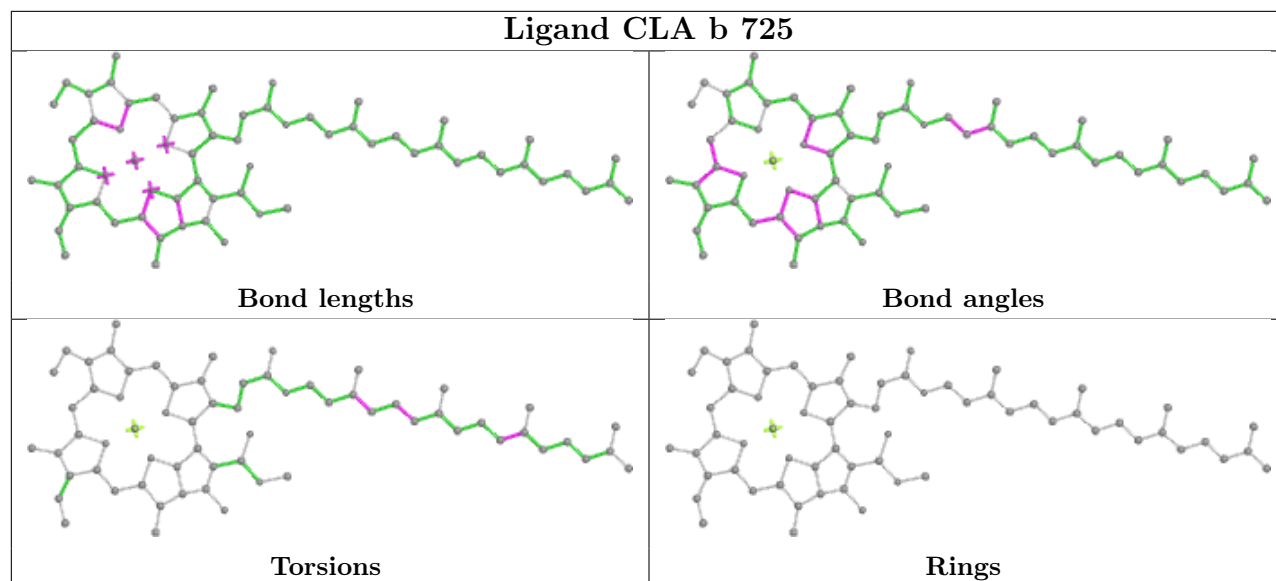
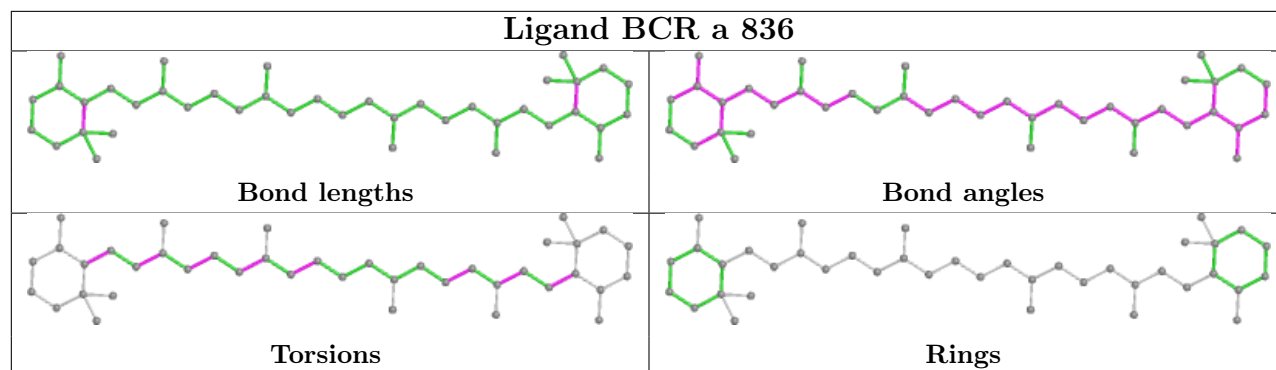
Ligand DD6 C 214**Ligand UIX D 616**

Ligand CLA F 608

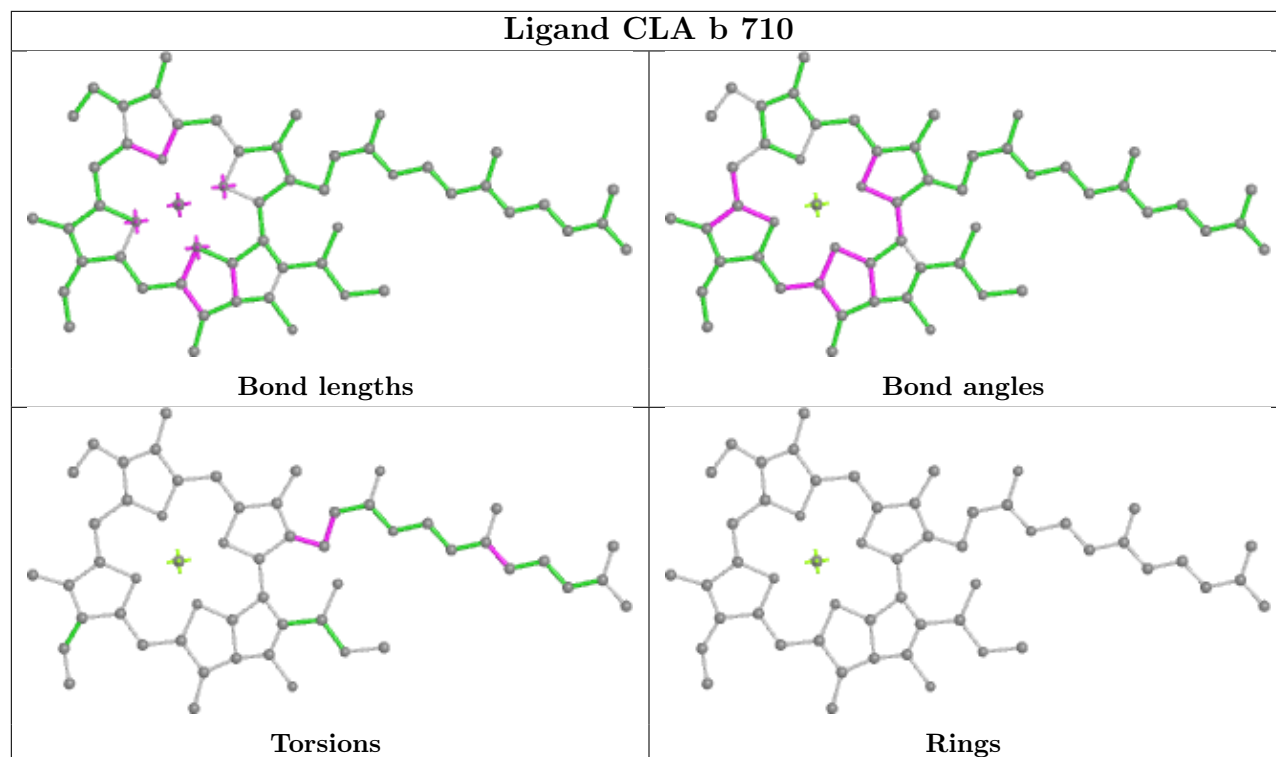


Ligand CLA a 807

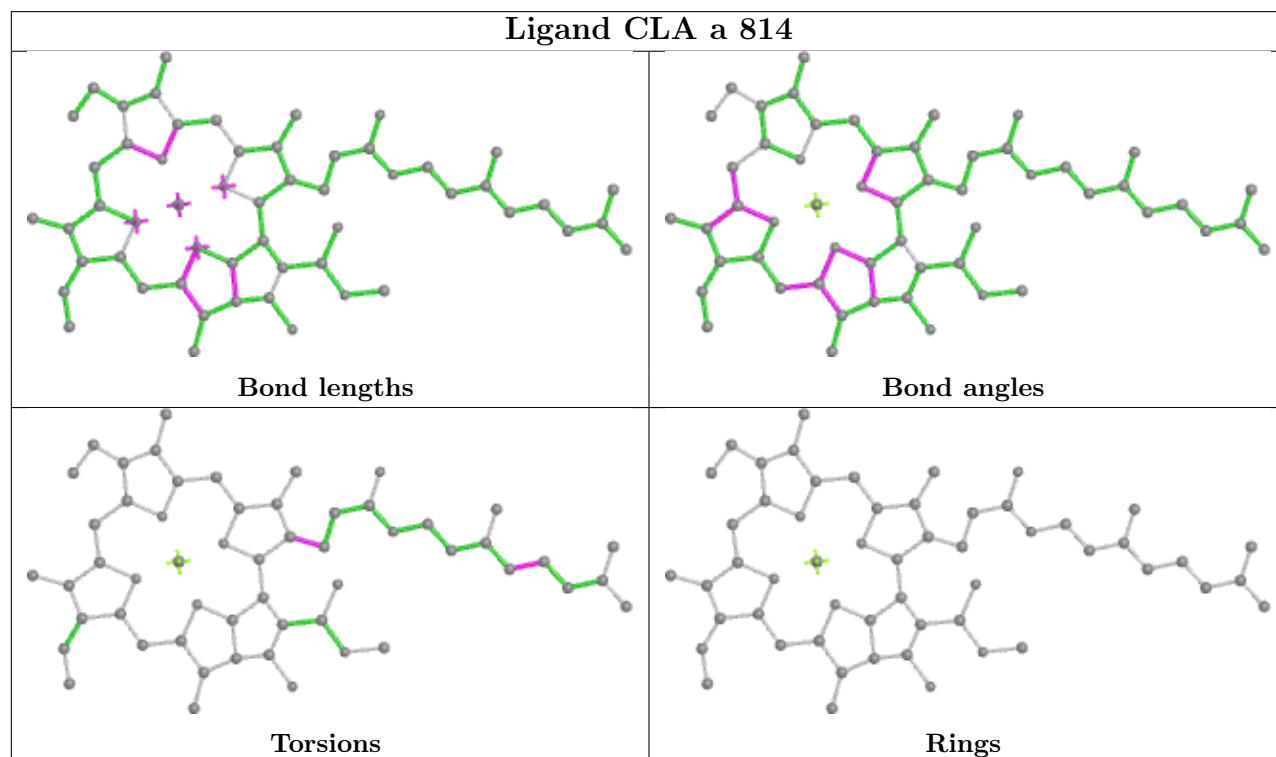




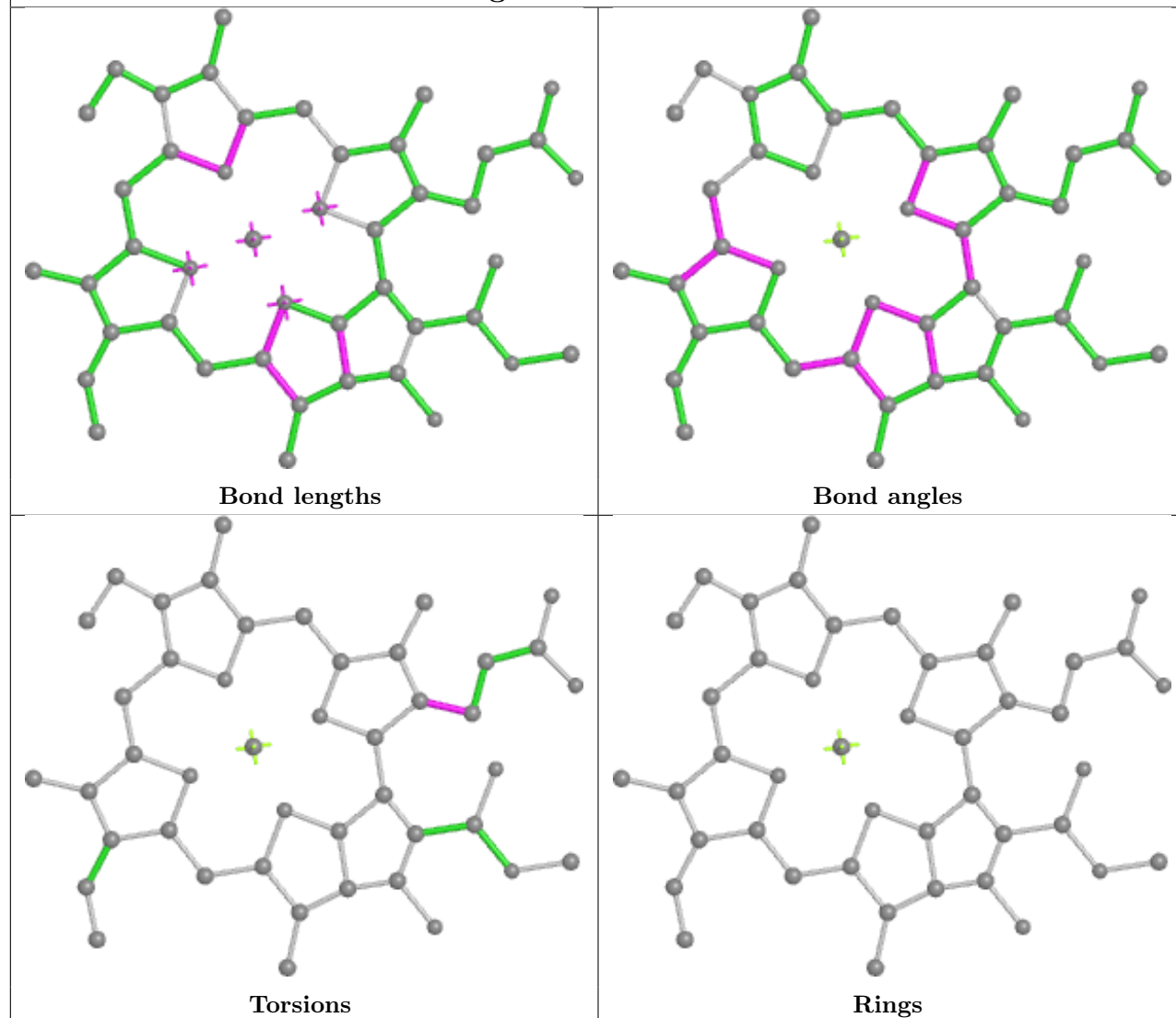
Ligand CLA b 710



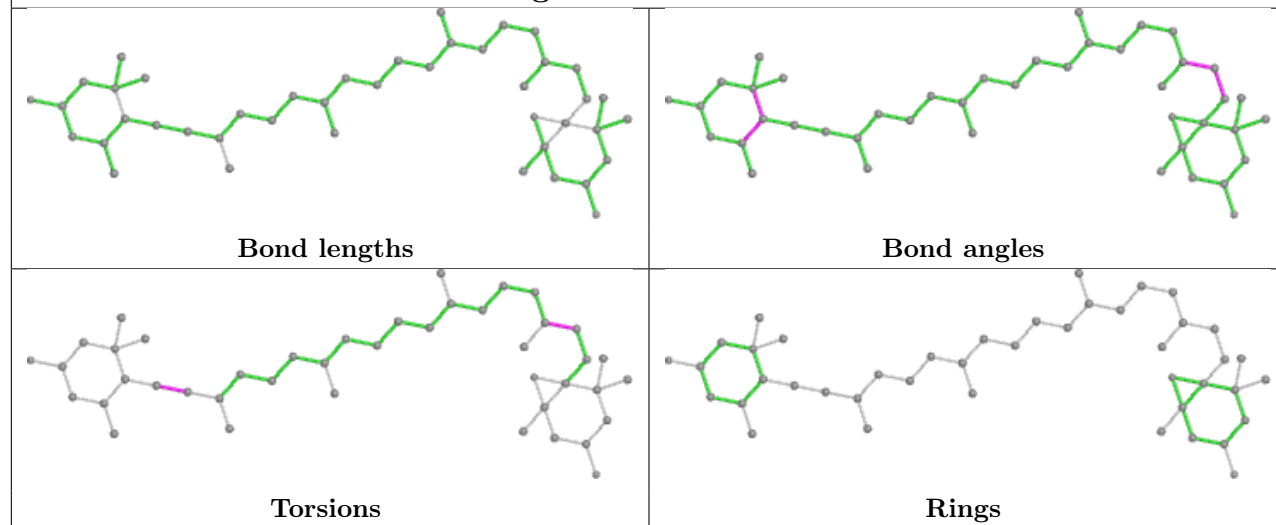
Ligand CLA a 814

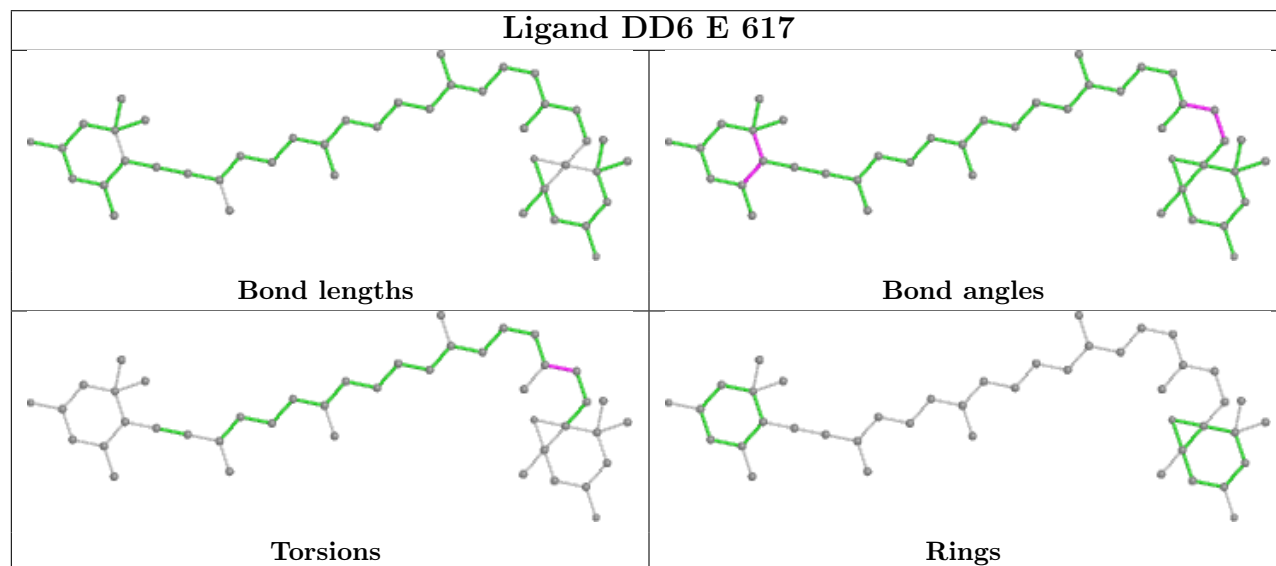
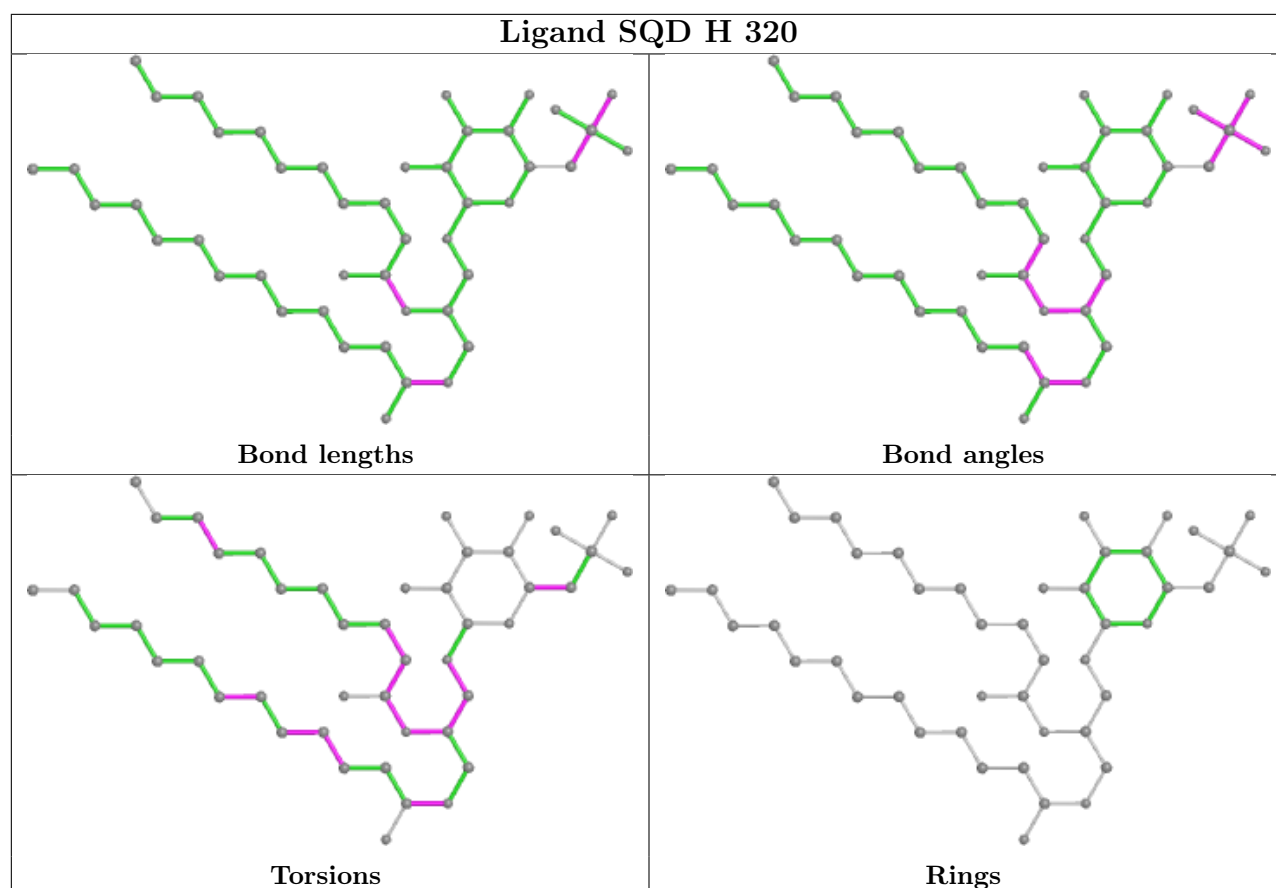


Ligand CLA K 608

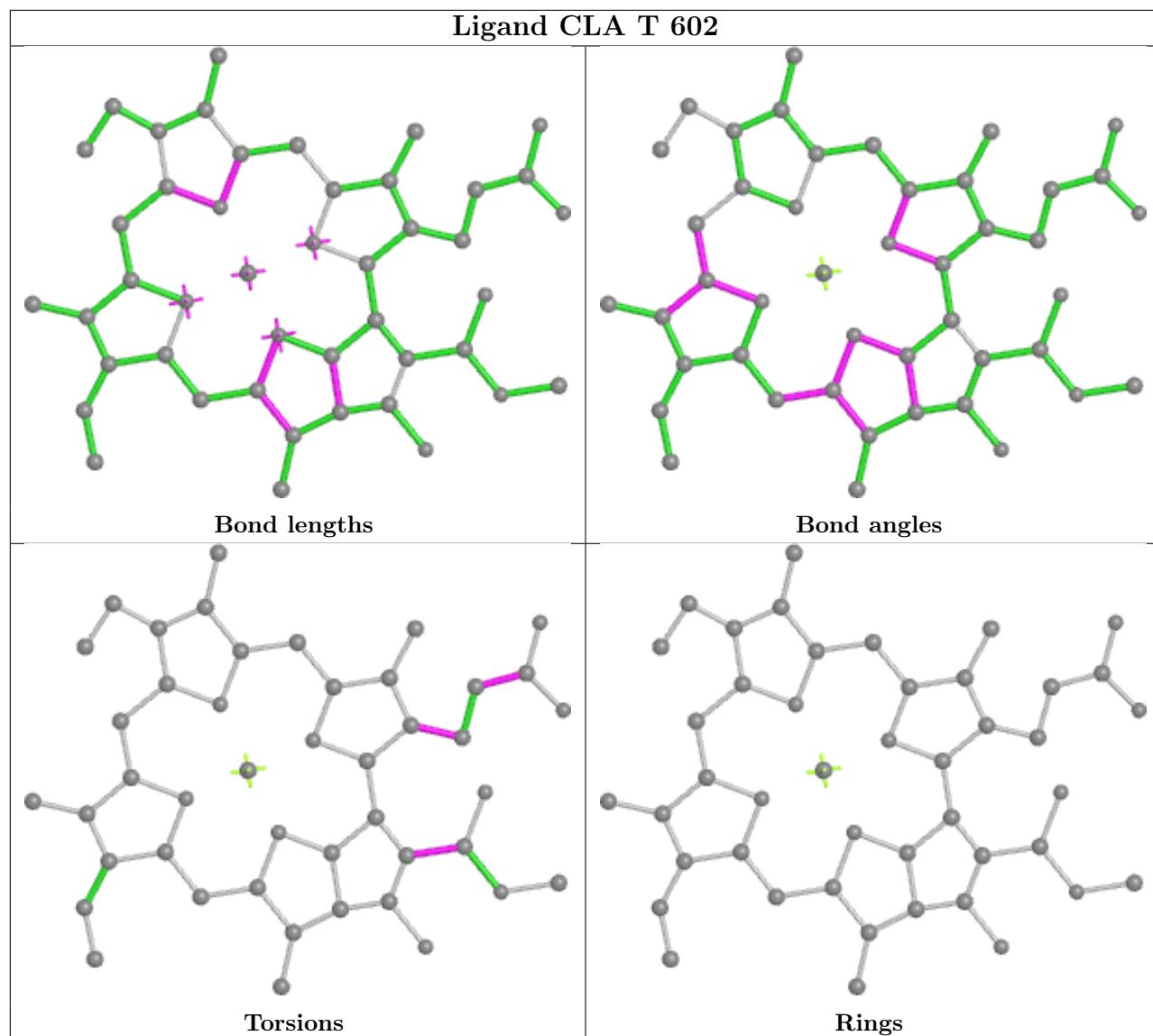


Ligand DD6 K 610

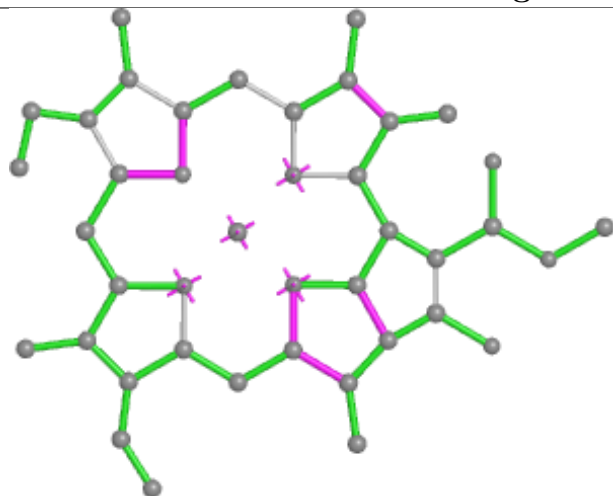




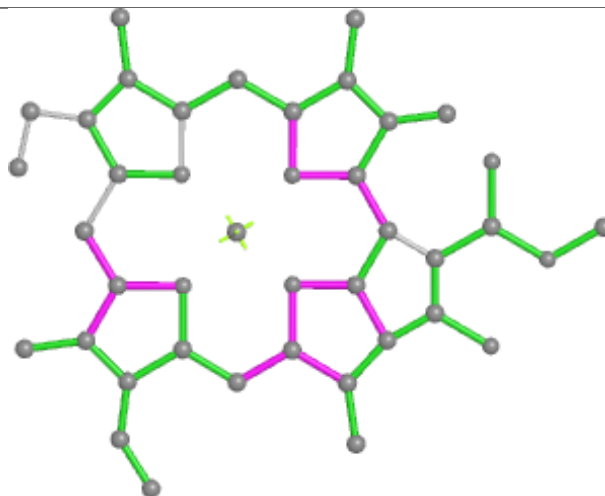
Ligand CLA T 602



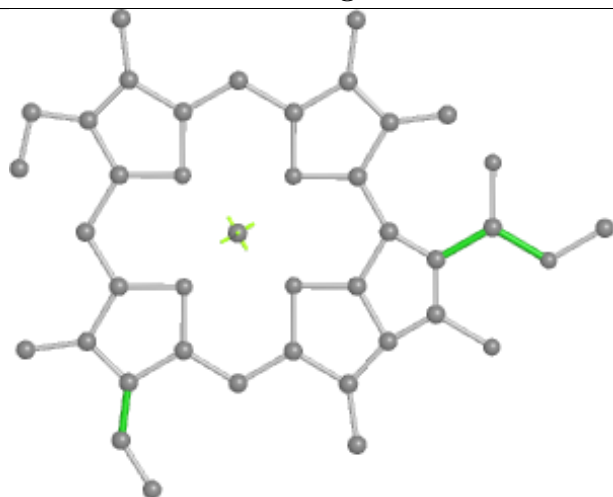
Ligand CLA K 606



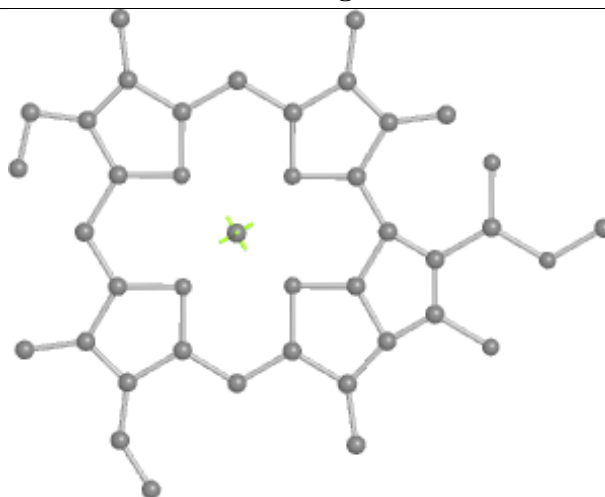
Bond lengths



Bond angles

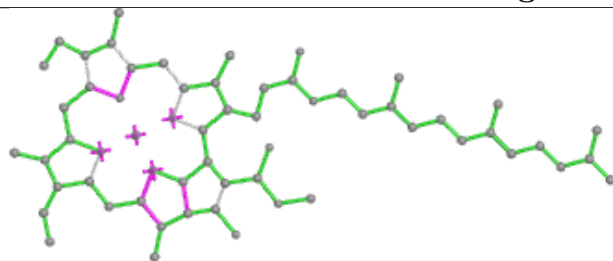


Torsions

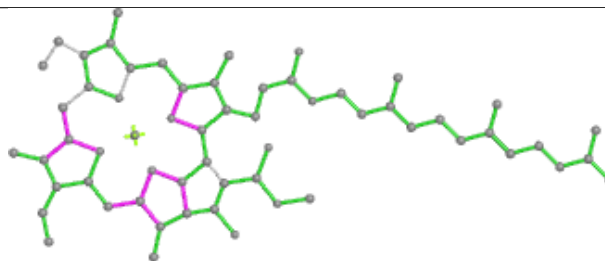


Rings

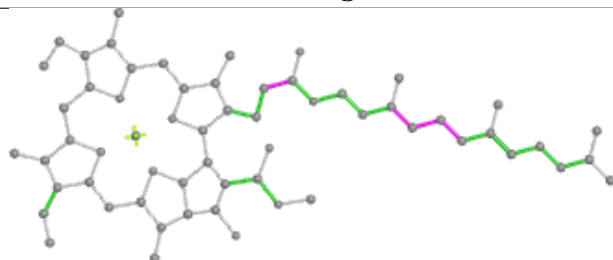
Ligand CLA J 605



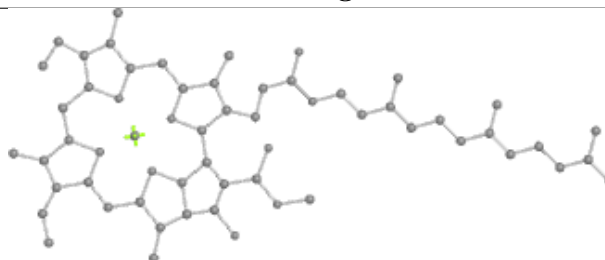
Bond lengths



Bond angles

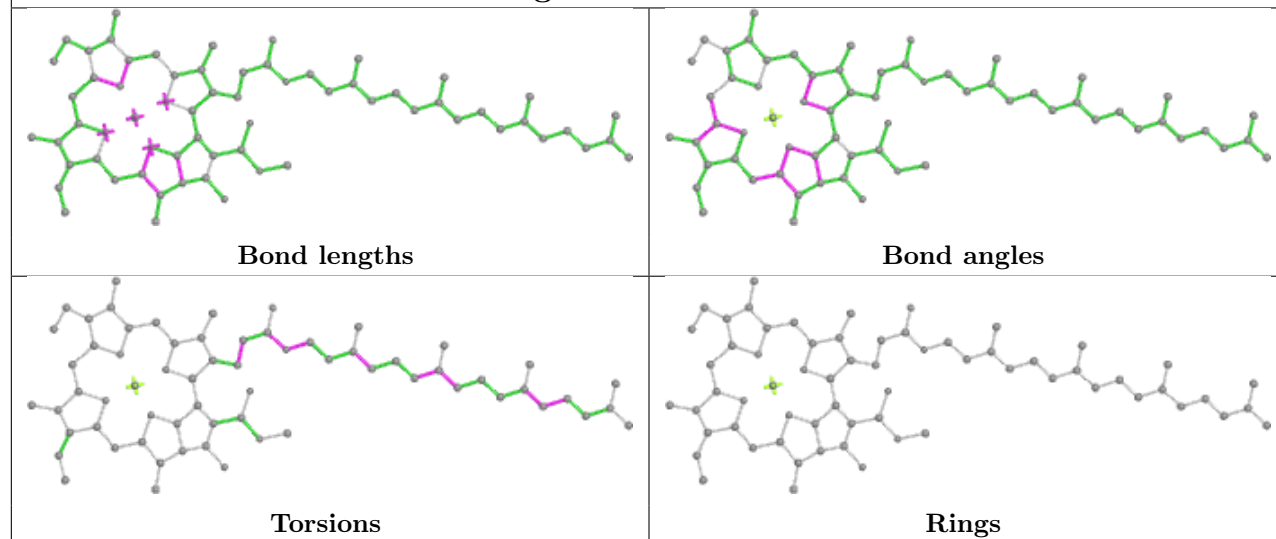


Torsions

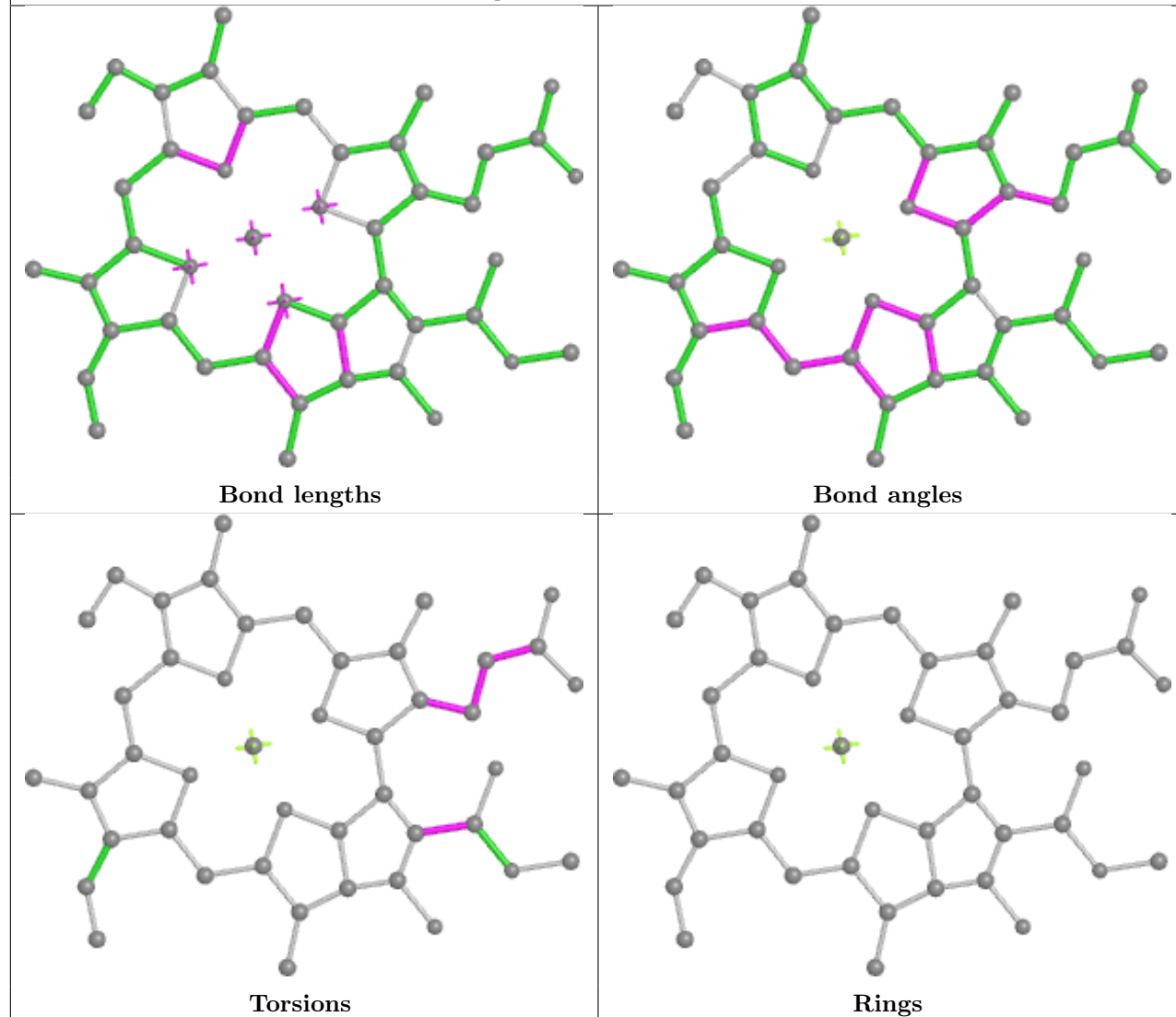


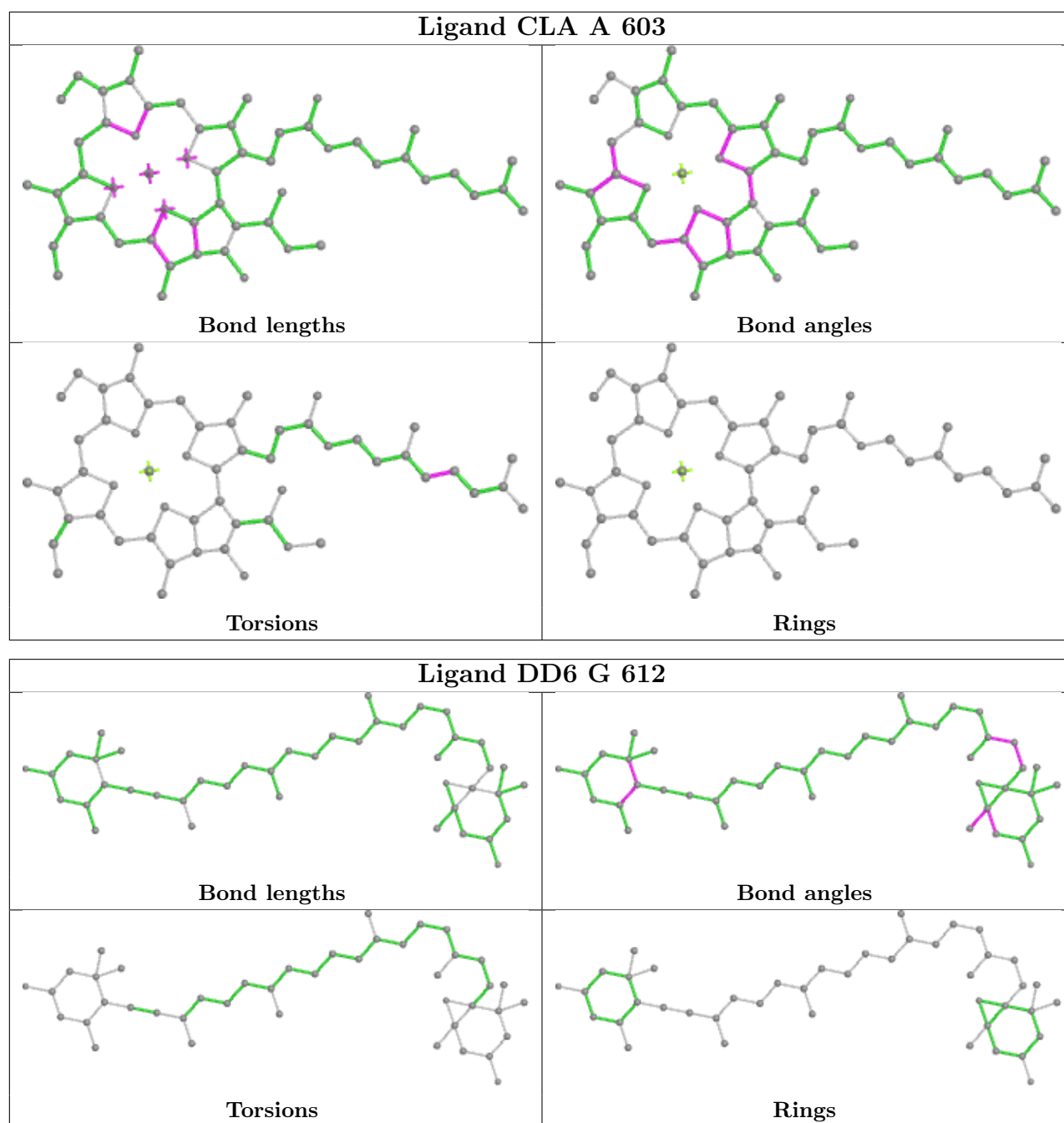
Rings

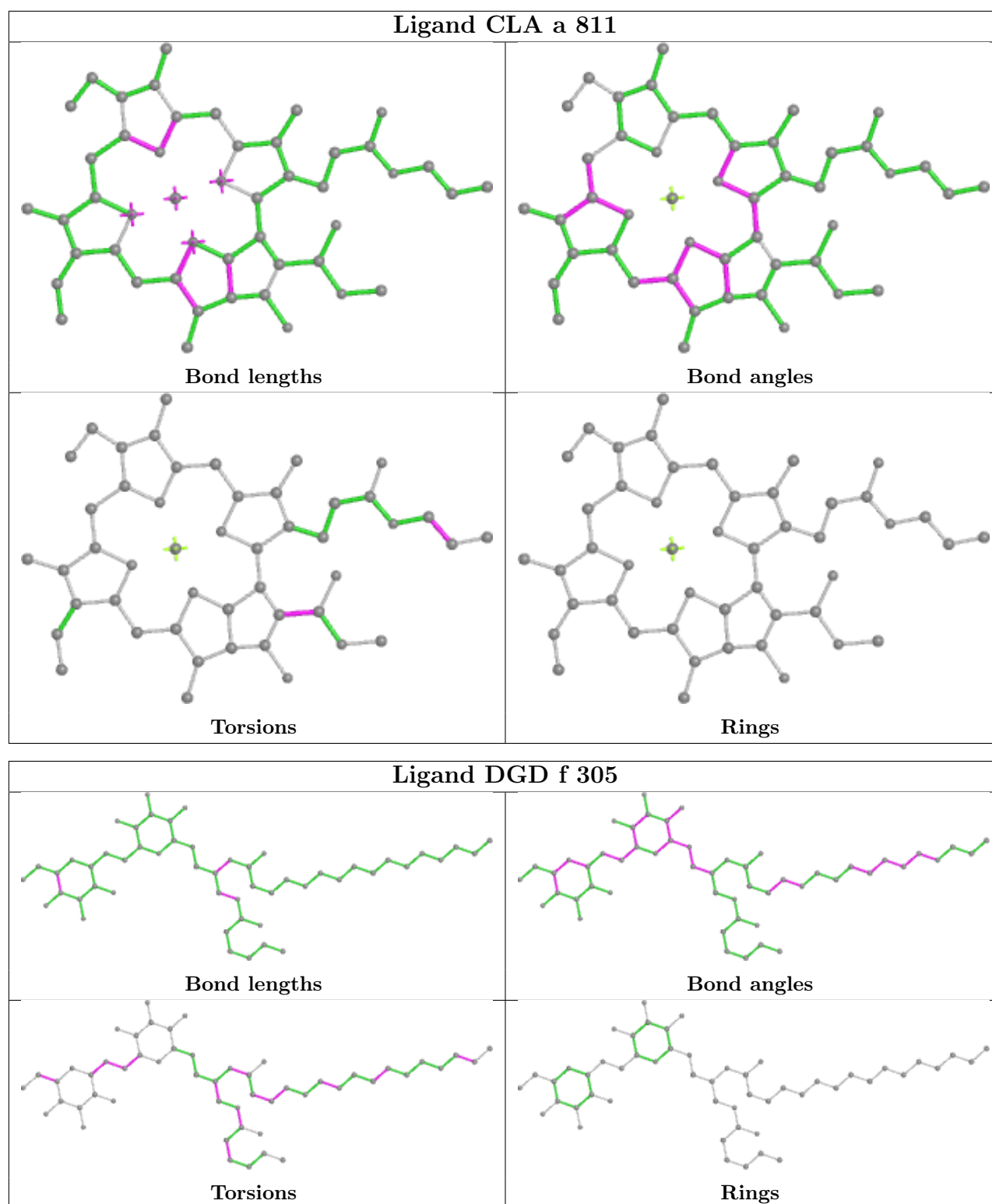
Ligand CLA F 606



Ligand CLA G 607







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

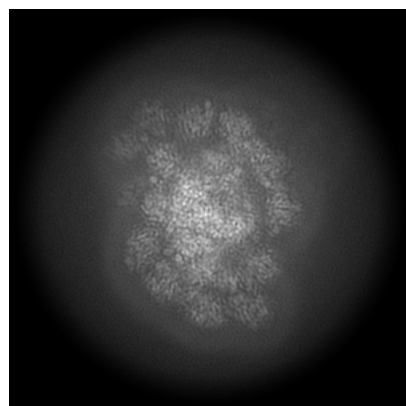
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-36366. These allow visual inspection of the internal detail of the map and identification of artifacts.

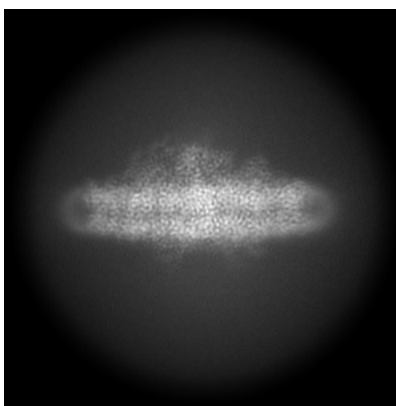
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

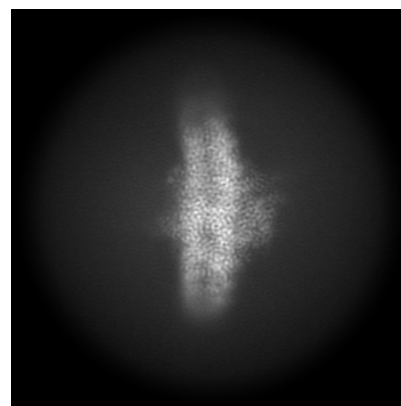
6.1.1 Primary map



X

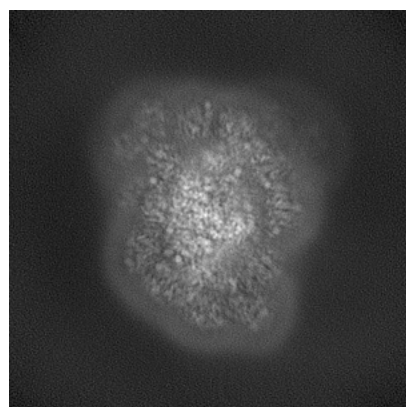


Y

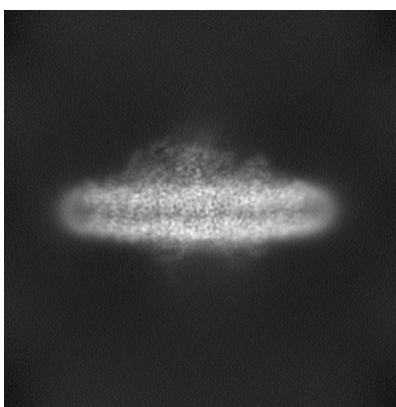


Z

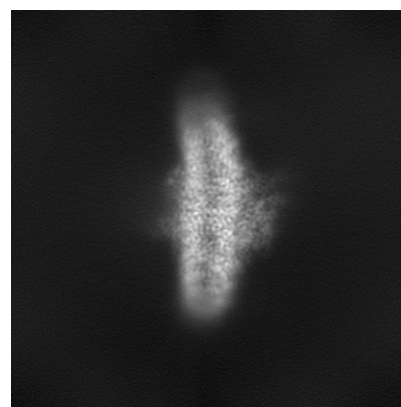
6.1.2 Raw map



X



Y

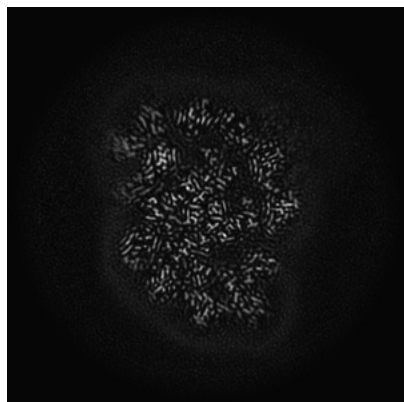


Z

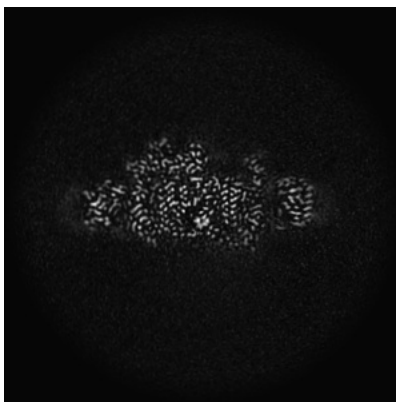
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

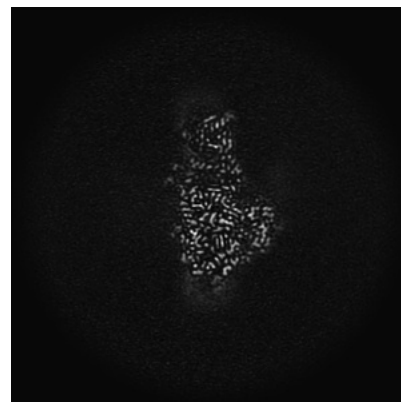
6.2.1 Primary map



X Index: 160

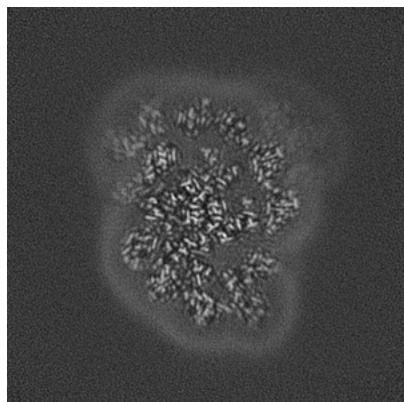


Y Index: 160

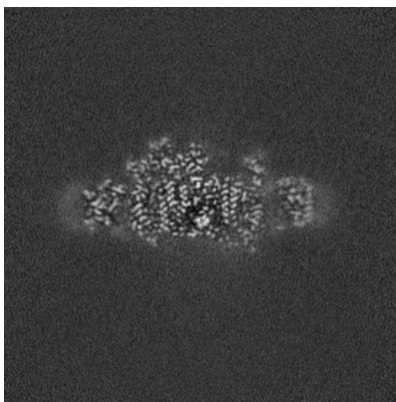


Z Index: 160

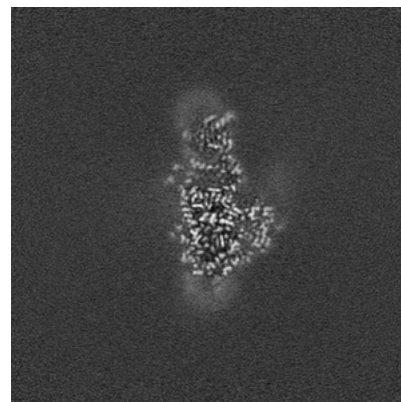
6.2.2 Raw map



X Index: 160



Y Index: 160

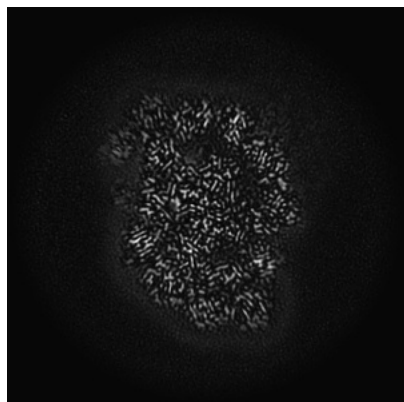


Z Index: 160

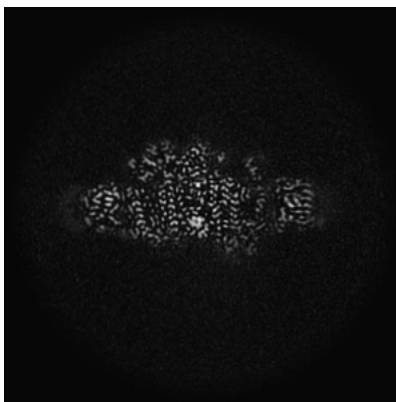
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

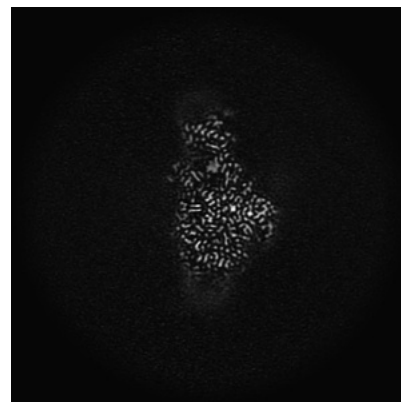
6.3.1 Primary map



X Index: 167

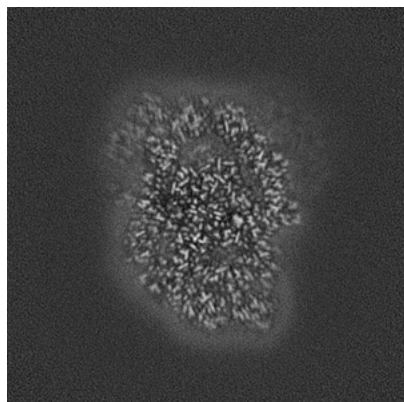


Y Index: 157

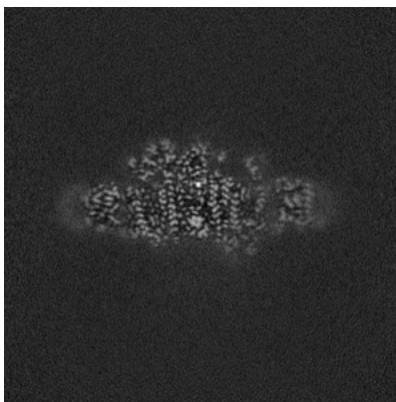


Z Index: 155

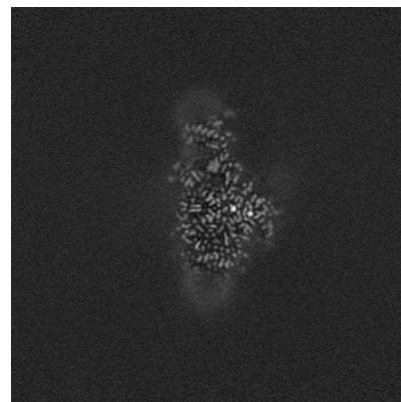
6.3.2 Raw map



X Index: 170



Y Index: 157

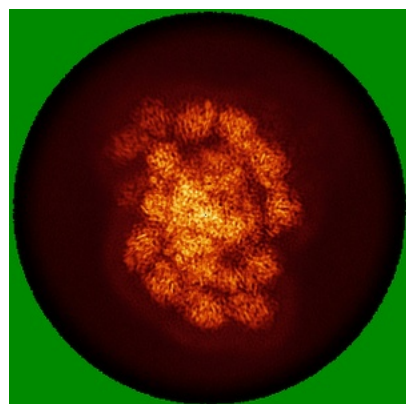


Z Index: 155

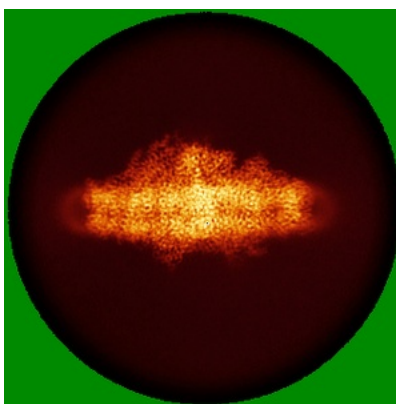
The images above show the largest variance slices of the map in three orthogonal directions.

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

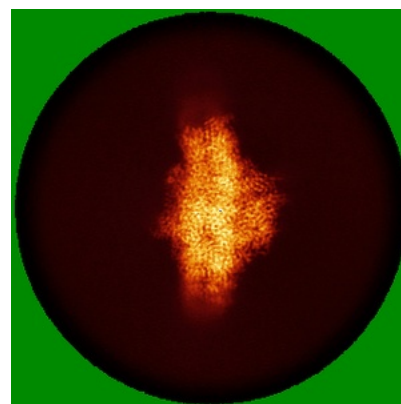
6.4.1 Primary map



X

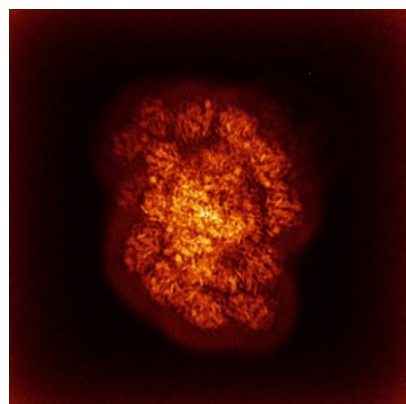


Y

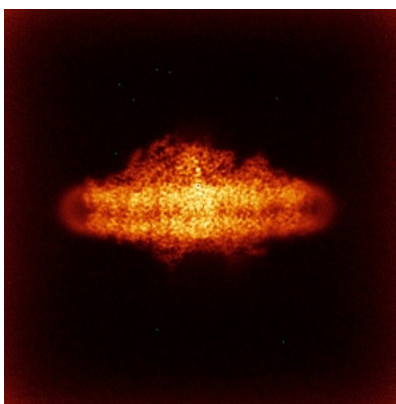


Z

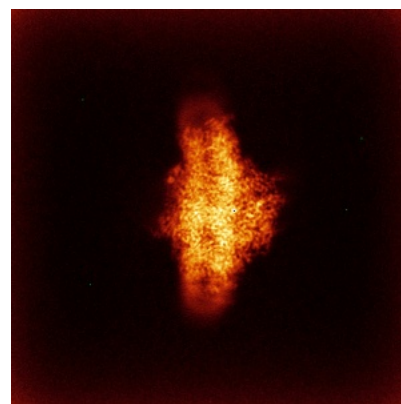
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



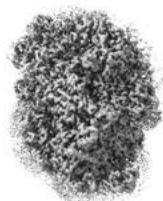
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.35. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X



Y



Z

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

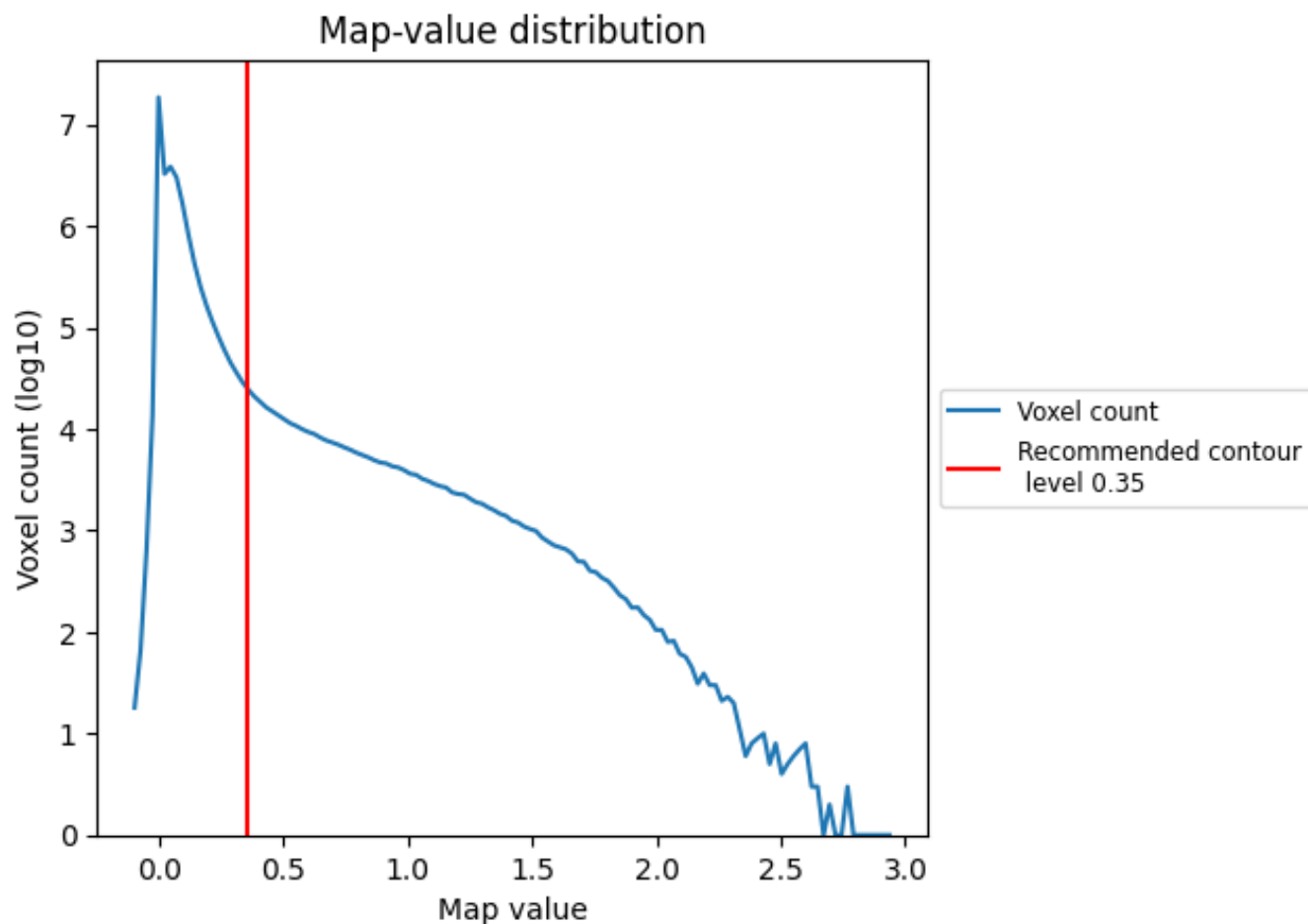
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

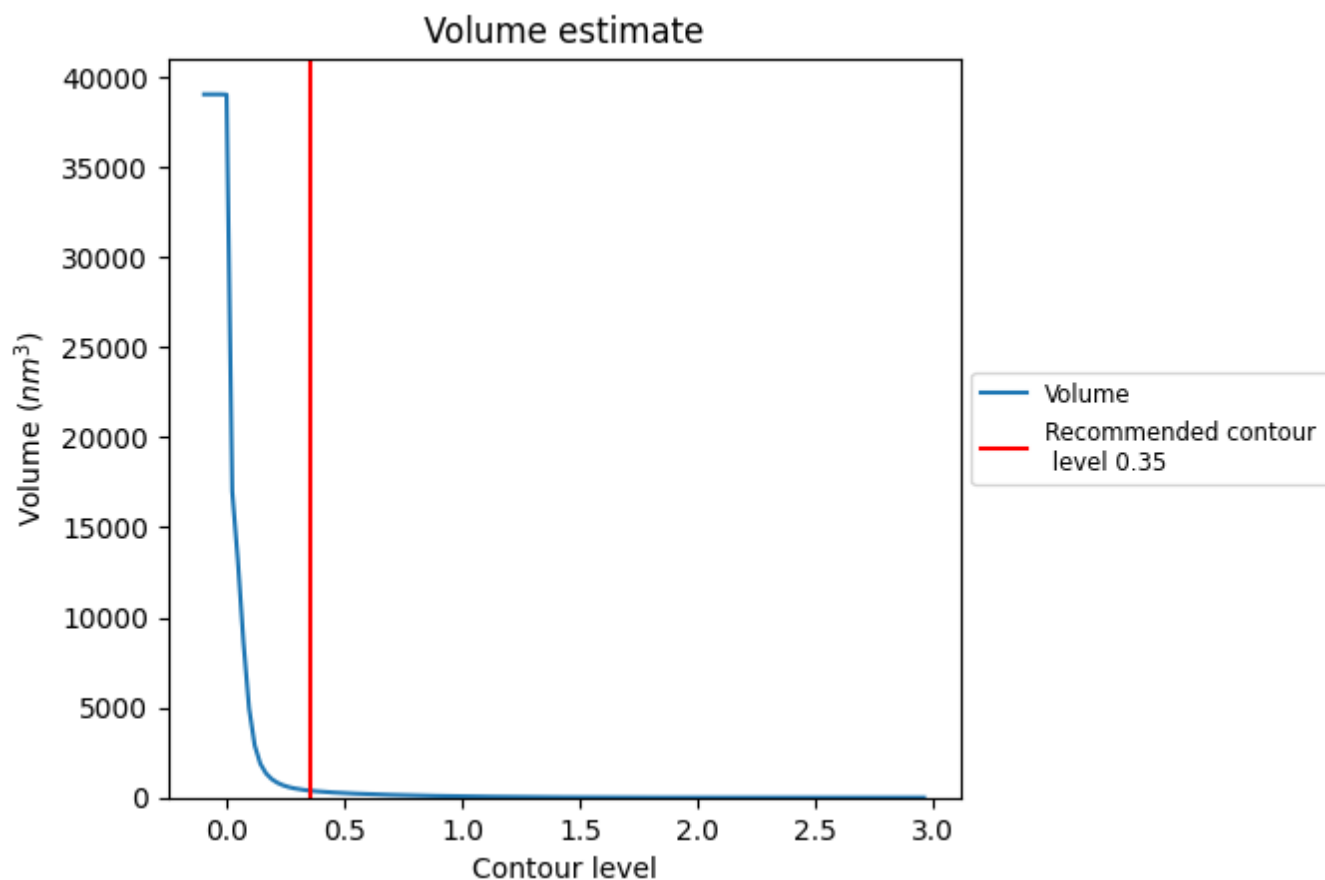
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

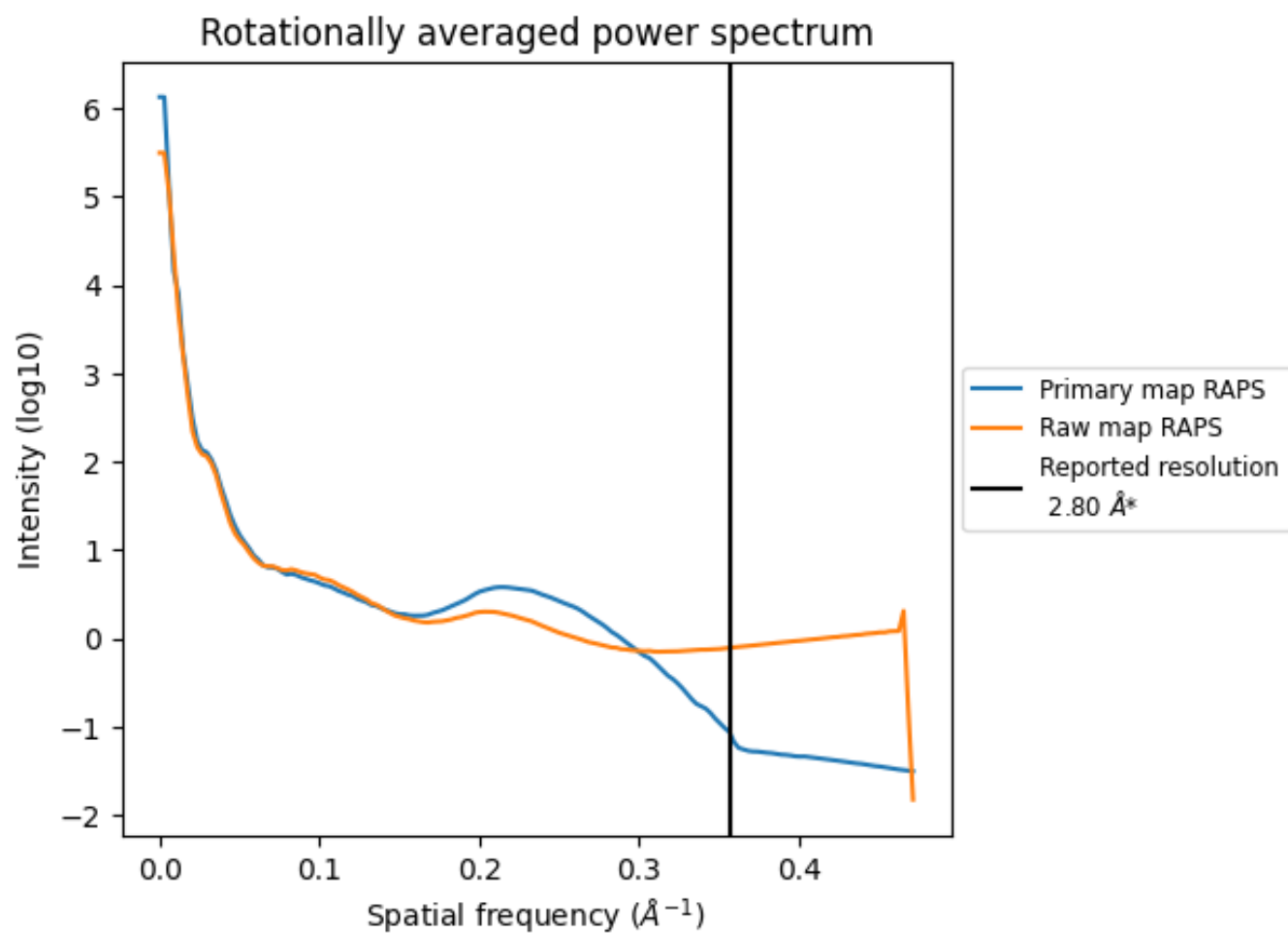
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 386 nm^3 ; this corresponds to an approximate mass of 349 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 ⓘ

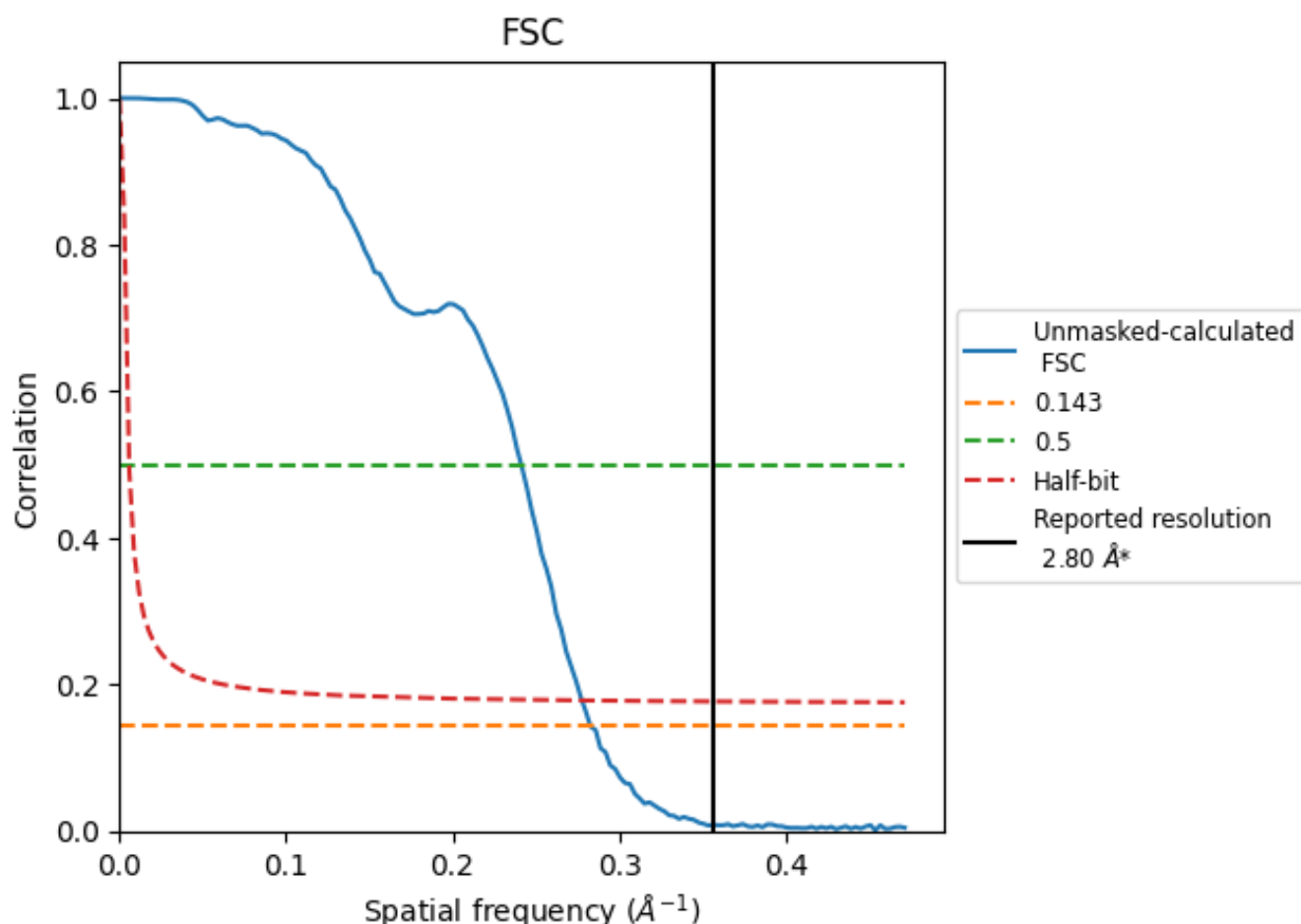


*Reported resolution corresponds to spatial frequency of 0.357 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.357 Å⁻¹

8.2 Resolution estimates [i](#)

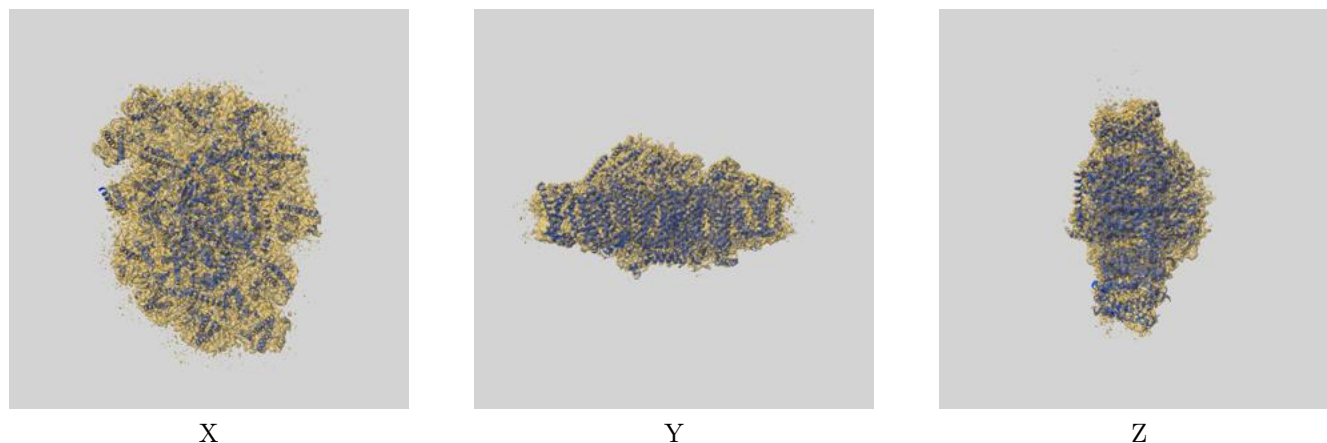
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.80	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.53	4.14	3.60

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.53 differs from the reported value 2.8 by more than 10 %

9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-36366 and PDB model 8JJR. Per-residue inclusion information can be found in [section 3](#) on [page 36](#).

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.35 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



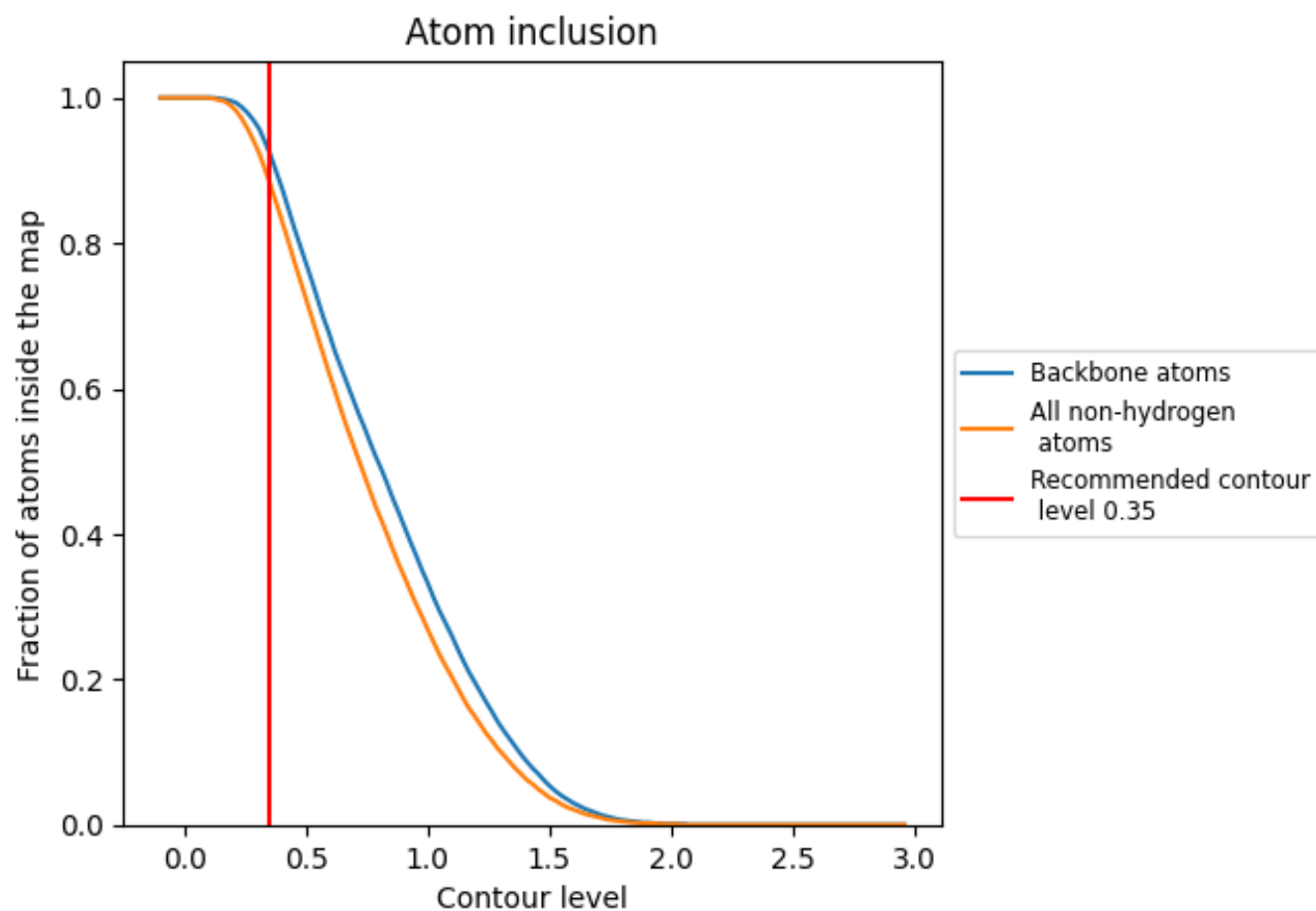
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.35).























































9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 88% 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 (0.35) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8830	 0.5750
A	 0.8810	 0.5710
B	 0.9160	 0.5810
C	 0.8970	 0.5880
D	 0.9220	 0.6000
E	 0.9190	 0.5760
F	 0.8660	 0.5680
G	 0.8660	 0.5410
H	 0.9040	 0.5730
I	 0.8900	 0.5700
J	 0.8410	 0.5450
K	 0.6670	 0.4810
T	 0.6320	 0.4260
U	 0.6680	 0.4840
a	 0.9250	 0.6020
b	 0.9490	 0.6130
c	 0.9760	 0.6000
d	 0.9020	 0.5800
e	 0.9500	 0.6090
f	 0.8320	 0.5850
i	 0.8890	 0.5790
j	 0.8380	 0.5740
l	 0.9350	 0.6010
m	 0.9130	 0.6000
r	 0.9290	 0.5780
x	 0.9140	 0.5860
y	 0.7230	 0.5400

