



wwPDB EM Validation Summary Report ⓘ

Aug 8, 2026 – 02:59 PM JST

PDB ID : 9V7T / pdb_00009v7t
EMDB ID : EMD-64823
Title : PSI-LHCE supercomplex from Euglena gracilis.
Authors : Bai, T.Y.; Mao, Z.Y.; Tian, L.R.
Deposited on : 2025-05-28
Resolution : 2.23 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:

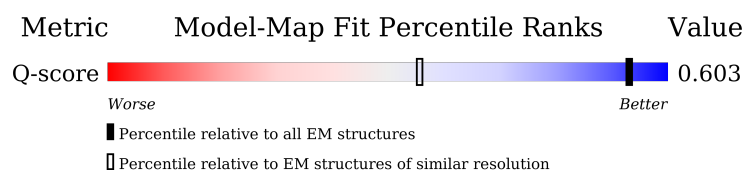
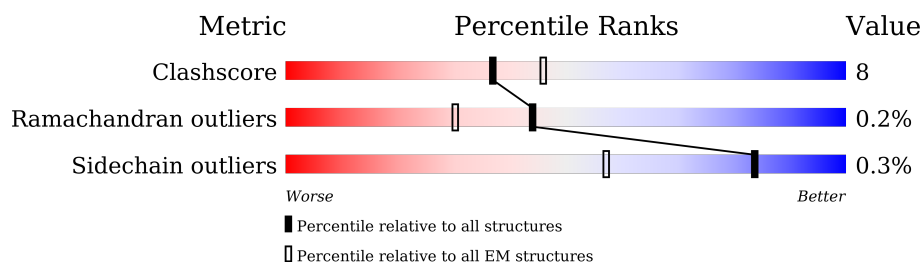
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

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 2.23 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	3335 (1.73 - 2.73)

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	751	
2	B	734	
3	C	81	
4	D	186	

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Mol	Chain	Length	Quality of chain
5	E	63	
6	F	168	
7	J	37	
8	M	31	
9	a	166	
10	b	169	
11	c	221	
12	d	220	
13	e	199	
14	h	174	
15	i	177	
16	j	183	
17	k	172	
18	l	167	
19	m	168	
20	f	174	
21	g	178	
22	n	184	
23	o	164	
24	p	148	

2 Entry composition

There are 35 unique types of molecules in this entry. The entry contains 55406 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Photosystem I P700 chlorophyll a apoprotein A1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	741	Total	C	N	O	S	0	0
			5878	3860	994	1003	21		

- Molecule 2 is a protein called Photosystem I P700 chlorophyll a apoprotein A2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	731	Total	C	N	O	S	0	0
			5861	3855	984	1007	15		

- Molecule 3 is a protein called Photosystem I iron-sulfur center.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	80	Total	C	N	O	S	0	0
			596	363	104	118	11		

- Molecule 4 is a protein called PsaD.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	186	Total	C	N	O	S	0	0
			1393	892	235	262	4		

- Molecule 5 is a protein called PsaE.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	63	Total	C	N	O	0	0
			481	311	81	89		

- Molecule 6 is a protein called PsaF.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	168	Total	C	N	O	S	0	0
			1250	801	206	239	4		

- Molecule 7 is a protein called Photosystem I reaction center subunit IX.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	J	37	Total	C	N	O	S	0	0
			305	209	43	52	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	M	31	Total	C	N	O	S	0	0
			243	162	37	43	1		

- Molecule 9 is a protein called Chloroplast light-harvesting complex I protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	a	166	Total	C	N	O	S	0	0
			1274	819	220	228	7		

- Molecule 10 is a protein called Chloroplast light-harvesting complex I protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	b	169	Total	C	N	O	S	0	0
			1302	842	213	243	4		

- Molecule 11 is a protein called LHCE 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	c	221	Total	C	N	O	S	0	0
			1676	1087	282	302	5		

- Molecule 12 is a protein called Light harvesting chlorophyll a /b binding protein of PSII.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	d	220	Total	C	N	O	S	0	0
			1669	1088	275	302	4		

- Molecule 13 is a protein called Chloroplast light-harvesting complex II protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	e	199	Total	C	N	O	S	0	0
			1517	981	256	275	5		

- Molecule 14 is a protein called LHCE 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	h	174	Total	C	N	O	S	0	0
			1350	865	233	247	5		

- Molecule 15 is a protein called LHCE 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	i	177	Total	C	N	O	S	0	0
			1355	865	242	244	4		

- Molecule 16 is a protein called Chloroplast light-harvesting complex I protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	j	183	Total	C	N	O	S	0	0
			1450	944	246	254	6		

- Molecule 17 is a protein called Chloroplast light-harvesting complex I protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	k	172	Total	C	N	O	S	0	0
			1338	860	232	241	5		

- Molecule 18 is a protein called Chloroplast light-harvesting complex I protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	l	167	Total	C	N	O	S	0	0
			1256	811	214	227	4		

- Molecule 19 is a protein called Chloroplast light-harvesting complex I protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	m	168	Total	C	N	O	S	0	0
			1260	813	215	228	4		

- Molecule 20 is a protein called Chloroplast light-harvesting complex I protein, Lhca7_2.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	f	174	Total	C	N	O	S	0	0
			1332	851	236	241	4		

- Molecule 21 is a protein called Chloroplast light-harvesting complex I protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	g	178	Total	C	N	O	S	0	0
			1406	914	240	246	6		

- Molecule 22 is a protein called Chloroplast light-harvesting complex II protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	n	184	Total	C	N	O	S	0	0
			1411	921	232	254	4		

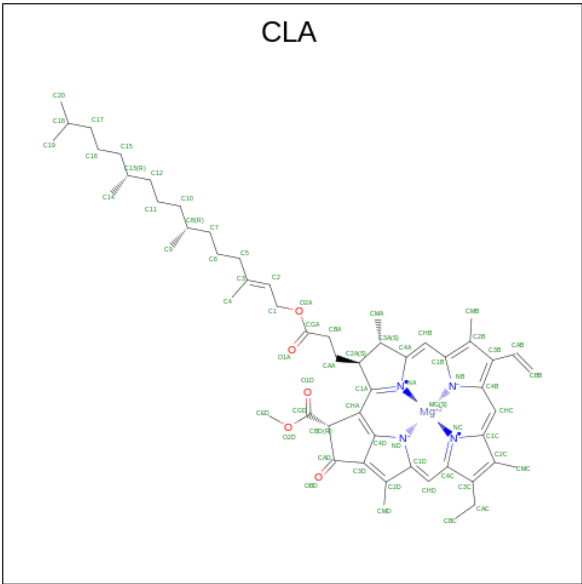
- Molecule 23 is a protein called Chloroplast light-harvesting complex I protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	o	164	Total	C	N	O	S	0	0
			1230	794	208	224	4		

- Molecule 24 is a protein called Chloroplast light-harvesting complex I protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	p	148	Total	C	N	O	S	0	0
			1126	727	188	207	4		

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



Mol	Chain	Residues	Atoms					AltConf
25	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
25	A	1	Total 63	C 53	Mg 1	N 4	O 5	0
25	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
25	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	A	1	Total 58	C 48	Mg 1	N 4	O 5	0
25	A	1	Total 59	C 49	Mg 1	N 4	O 5	0
25	A	1	Total 58	C 48	Mg 1	N 4	O 5	0
25	A	1	Total 43	C 35	Mg 1	N 4	O 3	0
25	A	1	Total 56	C 46	Mg 1	N 4	O 5	0
25	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	A	1	Total 57	C 47	Mg 1	N 4	O 5	0
25	A	1	Total 64	C 55	Mg 1	N 4	O 4	0
25	A	1	Total 53	C 43	Mg 1	N 4	O 5	0
25	A	1	Total 64	C 54	Mg 1	N 4	O 5	0
25	A	1	Total 58	C 48	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
25	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	A	1	Total 43	C 35	Mg 1	N 4	O 3	0
25	A	1	Total 43	C 35	Mg 1	N 4	O 3	0
25	A	1	Total 58	C 48	Mg 1	N 4	O 5	0
25	A	1	Total 52	C 42	Mg 1	N 4	O 5	0
25	A	1	Total 48	C 38	Mg 1	N 4	O 5	0
25	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	A	1	Total 63	C 53	Mg 1	N 4	O 5	0
25	A	1	Total 42	C 34	Mg 1	N 4	O 3	0
25	A	1	Total 57	C 47	Mg 1	N 4	O 5	0
25	A	1	Total 49	C 39	Mg 1	N 4	O 5	0
25	A	1	Total 52	C 42	Mg 1	N 4	O 5	0
25	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	A	1	Total 48	C 38	Mg 1	N 4	O 5	0
25	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	A	1	Total 43	C 35	Mg 1	N 4	O 3	0
25	A	1	Total 51	C 41	Mg 1	N 4	O 5	0
25	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
25	A	1	Total 55	C 45	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
25	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	A	1	Total 48	C 38	Mg 1	N 4	O 5	0
25	A	1	Total 53	C 43	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 42	C 34	Mg 1	N 4	O 3	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 43	C 35	Mg 1	N 4	O 3	0
25	B	1	Total 42	C 34	Mg 1	N 4	O 3	0
25	B	1	Total 43	C 35	Mg 1	N 4	O 3	0
25	B	1	Total 63	C 53	Mg 1	N 4	O 5	0
25	B	1	Total 64	C 54	Mg 1	N 4	O 5	0
25	B	1	Total 49	C 40	Mg 1	N 4	O 4	0
25	B	1	Total 59	C 49	Mg 1	N 4	O 5	0
25	B	1	Total 49	C 39	Mg 1	N 4	O 5	0
25	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	B	1	Total 50	C 40	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
25	B	1	Total 43	C 35	Mg 1	N 4	O 3	0
25	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 43	C 35	Mg 1	N 4	O 3	0
25	B	1	Total 43	C 35	Mg 1	N 4	O 3	0
25	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
25	B	1	Total 53	C 43	Mg 1	N 4	O 5	0
25	B	1	Total 53	C 43	Mg 1	N 4	O 5	0
25	B	1	Total 50	C 40	Mg 1	N 4	O 5	0
25	B	1	Total 61	C 51	Mg 1	N 4	O 5	0
25	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	B	1	Total 50	C 40	Mg 1	N 4	O 5	0
25	B	1	Total 59	C 49	Mg 1	N 4	O 5	0
25	B	1	Total 53	C 43	Mg 1	N 4	O 5	0
25	B	1	Total 63	C 53	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 53	C 43	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 50	C 40	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
25	B	1	Total 50	C 40	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	J	1	Total 50	C 40	Mg 1	N 4	O 5	0
25	a	1	Total 50	C 40	Mg 1	N 4	O 5	0
25	a	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	a	1	Total 53	C 43	Mg 1	N 4	O 5	0
25	a	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	a	1	Total 53	C 43	Mg 1	N 4	O 5	0
25	a	1	Total 50	C 40	Mg 1	N 4	O 5	0
25	a	1	Total 54	C 44	Mg 1	N 4	O 5	0
25	a	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	a	1	Total 43	C 35	Mg 1	N 4	O 3	0
25	a	1	Total 55	C 45	Mg 1	N 4	O 5	0
25	a	1	Total 63	C 53	Mg 1	N 4	O 5	0
25	b	1	Total 42	C 34	Mg 1	N 4	O 3	0
25	b	1	Total 53	C 43	Mg 1	N 4	O 5	0
25	b	1	Total 43	C 35	Mg 1	N 4	O 3	0
25	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	b	1	Total 41	C 33	Mg 1	N 4	O 3	0

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Mol	Chain	Residues	Atoms					AltConf
25	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	b	1	Total 42	C 34	Mg 1	N 4	O 3	0
25	b	1	Total 42	C 34	Mg 1	N 4	O 3	0
25	b	1	Total 52	C 42	Mg 1	N 4	O 5	0
25	b	1	Total 42	C 34	Mg 1	N 4	O 3	0
25	c	1	Total 42	C 34	Mg 1	N 4	O 3	0
25	c	1	Total 59	C 49	Mg 1	N 4	O 5	0
25	c	1	Total 53	C 43	Mg 1	N 4	O 5	0
25	c	1	Total 48	C 38	Mg 1	N 4	O 5	0
25	c	1	Total 43	C 35	Mg 1	N 4	O 3	0
25	c	1	Total 50	C 40	Mg 1	N 4	O 5	0
25	c	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	c	1	Total 55	C 45	Mg 1	N 4	O 5	0
25	c	1	Total 43	C 35	Mg 1	N 4	O 3	0
25	c	1	Total 43	C 35	Mg 1	N 4	O 3	0
25	c	1	Total 53	C 43	Mg 1	N 4	O 5	0
25	c	1	Total 42	C 34	Mg 1	N 4	O 3	0
25	c	1	Total 47	C 37	Mg 1	N 4	O 5	0
25	c	1	Total 41	C 33	Mg 1	N 4	O 3	0
25	d	1	Total 50	C 40	Mg 1	N 4	O 5	0
25	d	1	Total 57	C 47	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
25	d	1	Total 42	C 34	Mg 1	N 4	O 3	0
25	d	1	Total 52	C 42	Mg 1	N 4	O 5	0
25	d	1	Total 49	C 39	Mg 1	N 4	O 5	0
25	d	1	Total 59	C 49	Mg 1	N 4	O 5	0
25	d	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	d	1	Total 42	C 34	Mg 1	N 4	O 3	0
25	d	1	Total 42	C 34	Mg 1	N 4	O 3	0
25	d	1	Total 42	C 34	Mg 1	N 4	O 3	0
25	e	1	Total 41	C 33	Mg 1	N 4	O 3	0
25	e	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	e	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	e	1	Total 50	C 40	Mg 1	N 4	O 5	0
25	e	1	Total 42	C 34	Mg 1	N 4	O 3	0
25	e	1	Total 43	C 35	Mg 1	N 4	O 3	0
25	e	1	Total 48	C 38	Mg 1	N 4	O 5	0
25	e	1	Total 52	C 42	Mg 1	N 4	O 5	0
25	e	1	Total 55	C 45	Mg 1	N 4	O 5	0
25	e	1	Total 42	C 34	Mg 1	N 4	O 3	0
25	e	1	Total 43	C 35	Mg 1	N 4	O 3	0
25	e	1	Total 55	C 45	Mg 1	N 4	O 5	0
25	e	1	Total 42	C 34	Mg 1	N 4	O 3	0

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Mol	Chain	Residues	Atoms					AltConf
25	h	1	Total 50	C 40	Mg 1	N 4	O 5	0
25	h	1	Total 55	C 45	Mg 1	N 4	O 5	0
25	h	1	Total 43	C 35	Mg 1	N 4	O 3	0
25	h	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	h	1	Total 48	C 38	Mg 1	N 4	O 5	0
25	h	1	Total 50	C 40	Mg 1	N 4	O 5	0
25	h	1	Total 54	C 44	Mg 1	N 4	O 5	0
25	h	1	Total 43	C 35	Mg 1	N 4	O 3	0
25	h	1	Total 58	C 48	Mg 1	N 4	O 5	0
25	h	1	Total 53	C 43	Mg 1	N 4	O 5	0
25	h	1	Total 43	C 35	Mg 1	N 4	O 3	0
25	h	1	Total 42	C 34	Mg 1	N 4	O 3	0
25	h	1	Total 43	C 35	Mg 1	N 4	O 3	0
25	i	1	Total 53	C 43	Mg 1	N 4	O 5	0
25	i	1	Total 64	C 54	Mg 1	N 4	O 5	0
25	i	1	Total 43	C 35	Mg 1	N 4	O 3	0
25	i	1	Total 43	C 35	Mg 1	N 4	O 3	0
25	i	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	i	1	Total 43	C 35	Mg 1	N 4	O 3	0
25	i	1	Total 55	C 45	Mg 1	N 4	O 5	0
25	i	1	Total 43	C 35	Mg 1	N 4	O 3	0

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Mol	Chain	Residues	Atoms					AltConf
25	i	1	Total 43	C 35	Mg 1	N 4	O 3	0
25	i	1	Total 59	C 49	Mg 1	N 4	O 5	0
25	i	1	Total 42	C 34	Mg 1	N 4	O 3	0
25	i	1	Total 50	C 40	Mg 1	N 4	O 5	0
25	j	1	Total 50	C 40	Mg 1	N 4	O 5	0
25	j	1	Total 55	C 45	Mg 1	N 4	O 5	0
25	j	1	Total 42	C 34	Mg 1	N 4	O 3	0
25	j	1	Total 57	C 47	Mg 1	N 4	O 5	0
25	j	1	Total 47	C 37	Mg 1	N 4	O 5	0
25	j	1	Total 50	C 40	Mg 1	N 4	O 5	0
25	j	1	Total 64	C 54	Mg 1	N 4	O 5	0
25	j	1	Total 50	C 40	Mg 1	N 4	O 5	0
25	j	1	Total 55	C 45	Mg 1	N 4	O 5	0
25	j	1	Total 62	C 52	Mg 1	N 4	O 5	0
25	j	1	Total 42	C 34	Mg 1	N 4	O 3	0
25	j	1	Total 43	C 35	Mg 1	N 4	O 3	0
25	j	1	Total 50	C 40	Mg 1	N 4	O 5	0
25	k	1	Total 43	C 35	Mg 1	N 4	O 3	0
25	k	1	Total 53	C 43	Mg 1	N 4	O 5	0
25	k	1	Total 42	C 34	Mg 1	N 4	O 3	0
25	k	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
25	k	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
25	k	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
25	k	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
25	k	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
25	k	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
25	k	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
25	k	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
25	k	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
25	k	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
25	l	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
25	l	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
25	l	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
25	l	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
25	l	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
25	l	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
25	l	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
25	l	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
25	l	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
25	l	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
25	l	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
25	l	1	Total	C	Mg	N	O	0
			42	34	1	4	3	

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Mol	Chain	Residues	Atoms					AltConf
25	m	1	Total 42	C 34	Mg 1	N 4	O 3	0
25	m	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	m	1	Total 54	C 44	Mg 1	N 4	O 5	0
25	m	1	Total 43	C 35	Mg 1	N 4	O 3	0
25	m	1	Total 42	C 34	Mg 1	N 4	O 3	0
25	m	1	Total 50	C 40	Mg 1	N 4	O 5	0
25	m	1	Total 42	C 34	Mg 1	N 4	O 3	0
25	m	1	Total 43	C 35	Mg 1	N 4	O 3	0
25	m	1	Total 43	C 35	Mg 1	N 4	O 3	0
25	m	1	Total 42	C 34	Mg 1	N 4	O 3	0
25	f	1	Total 42	C 34	Mg 1	N 4	O 3	0
25	f	1	Total 59	C 49	Mg 1	N 4	O 5	0
25	f	1	Total 43	C 35	Mg 1	N 4	O 3	0
25	f	1	Total 42	C 34	Mg 1	N 4	O 3	0
25	f	1	Total 42	C 34	Mg 1	N 4	O 3	0
25	f	1	Total 55	C 45	Mg 1	N 4	O 5	0
25	f	1	Total 42	C 34	Mg 1	N 4	O 3	0
25	f	1	Total 42	C 34	Mg 1	N 4	O 3	0
25	f	1	Total 59	C 49	Mg 1	N 4	O 5	0
25	f	1	Total 42	C 34	Mg 1	N 4	O 3	0

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Mol	Chain	Residues	Atoms					AltConf
25	f	1	Total 43	C 35	Mg 1	N 4	O 3	0
25	g	1	Total 42	C 34	Mg 1	N 4	O 3	0
25	g	1	Total 53	C 43	Mg 1	N 4	O 5	0
25	g	1	Total 42	C 34	Mg 1	N 4	O 3	0
25	g	1	Total 43	C 35	Mg 1	N 4	O 3	0
25	g	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	g	1	Total 50	C 40	Mg 1	N 4	O 5	0
25	g	1	Total 55	C 45	Mg 1	N 4	O 5	0
25	g	1	Total 42	C 34	Mg 1	N 4	O 3	0
25	g	1	Total 42	C 34	Mg 1	N 4	O 3	0
25	g	1	Total 55	C 45	Mg 1	N 4	O 5	0
25	g	1	Total 42	C 34	Mg 1	N 4	O 3	0
25	g	1	Total 42	C 34	Mg 1	N 4	O 3	0
25	g	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	n	1	Total 59	C 49	Mg 1	N 4	O 5	0
25	n	1	Total 55	C 45	Mg 1	N 4	O 5	0
25	n	1	Total 48	C 38	Mg 1	N 4	O 5	0
25	n	1	Total 42	C 34	Mg 1	N 4	O 3	0
25	n	1	Total 42	C 34	Mg 1	N 4	O 3	0
25	n	1	Total 42	C 34	Mg 1	N 4	O 3	0
25	n	1	Total 41	C 33	Mg 1	N 4	O 3	0

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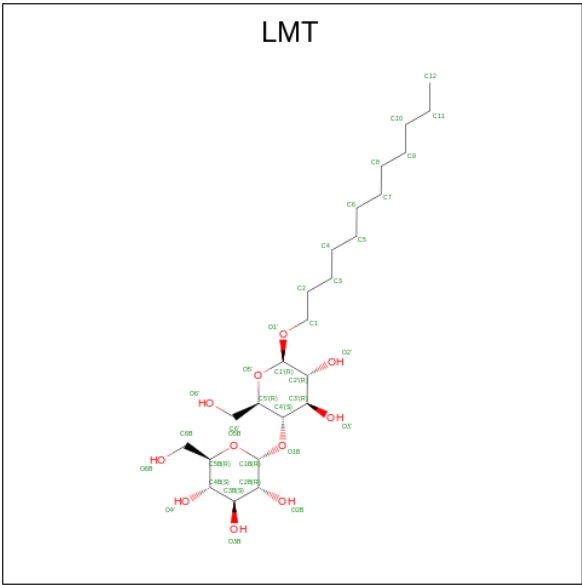
Mol	Chain	Residues	Atoms					AltConf
25	n	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	n	1	Total 41	C 33	Mg 1	N 4	O 3	0
25	n	1	Total 42	C 34	Mg 1	N 4	O 3	0
25	n	1	Total 42	C 34	Mg 1	N 4	O 3	0
25	o	1	Total 41	C 33	Mg 1	N 4	O 3	0
25	o	1	Total 47	C 37	Mg 1	N 4	O 5	0
25	o	1	Total 43	C 35	Mg 1	N 4	O 3	0
25	o	1	Total 42	C 34	Mg 1	N 4	O 3	0
25	o	1	Total 43	C 35	Mg 1	N 4	O 3	0
25	o	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	o	1	Total 41	C 33	Mg 1	N 4	O 3	0
25	o	1	Total 42	C 35	Mg 1	N 4	O 2	0
25	o	1	Total 42	C 34	Mg 1	N 4	O 3	0
25	o	1	Total 43	C 35	Mg 1	N 4	O 3	0
25	p	1	Total 42	C 34	Mg 1	N 4	O 3	0
25	p	1	Total 43	C 35	Mg 1	N 4	O 3	0
25	p	1	Total 42	C 34	Mg 1	N 4	O 3	0
25	p	1	Total 43	C 35	Mg 1	N 4	O 3	0
25	p	1	Total 42	C 34	Mg 1	N 4	O 3	0
25	p	1	Total 50	C 40	Mg 1	N 4	O 5	0
25	p	1	Total 45	C 35	Mg 1	N 4	O 5	0

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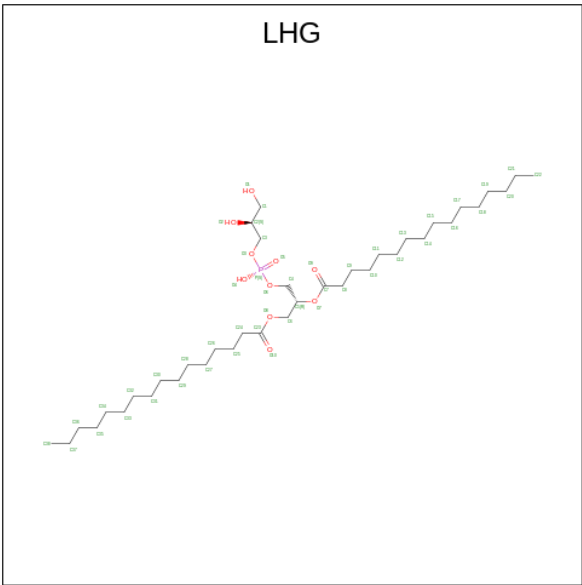
Mol	Chain	Residues	Atoms					AltConf
25	p	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
25	p	1	Total	C	Mg	N	O	0
			43	35	1	4	3	

- Molecule 26 is DODECYL-BETA-D-MALTOSE (CCD ID: LMT) (formula: C₂₄H₄₆O₁₁).



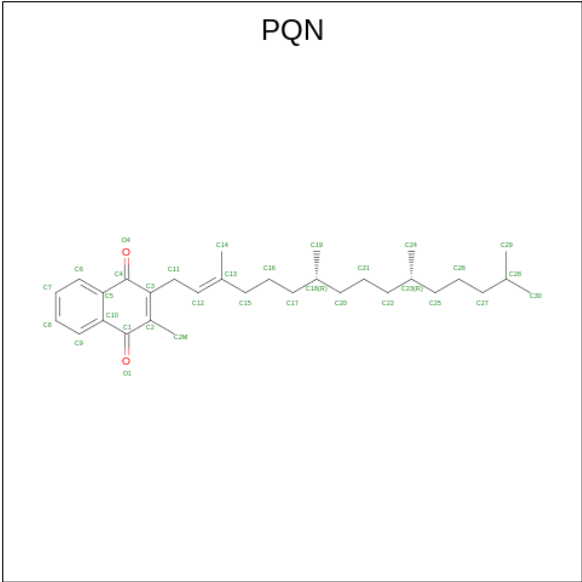
Mol	Chain	Residues	Atoms			AltConf
26	A	1	Total	C	O	0
			35	24	11	

- Molecule 27 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



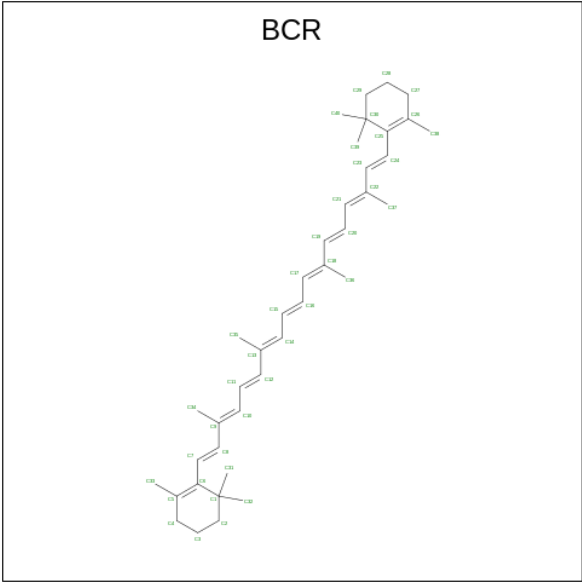
Mol	Chain	Residues	Atoms				AltConf
27	A	1	Total	C	O	P	0
			38	27	10	1	
27	A	1	Total	C	O	P	0
			49	38	10	1	
27	a	1	Total	C	O	P	0
			26	15	10	1	
27	b	1	Total	C	O	P	0
			31	20	10	1	
27	c	1	Total	C	O	P	0
			30	19	10	1	
27	d	1	Total	C	O	P	0
			29	18	10	1	
27	h	1	Total	C	O	P	0
			30	19	10	1	
27	h	1	Total	C	O	P	0
			31	20	10	1	
27	i	1	Total	C	O	P	0
			36	25	10	1	
27	j	1	Total	C	O	P	0
			37	26	10	1	
27	m	1	Total	C	O	P	0
			32	21	10	1	
27	g	1	Total	C	O	P	0
			35	24	10	1	

- Molecule 28 is PHYLLOQUINONE (CCD ID: PQN) (formula: C₃₁H₄₆O₂).



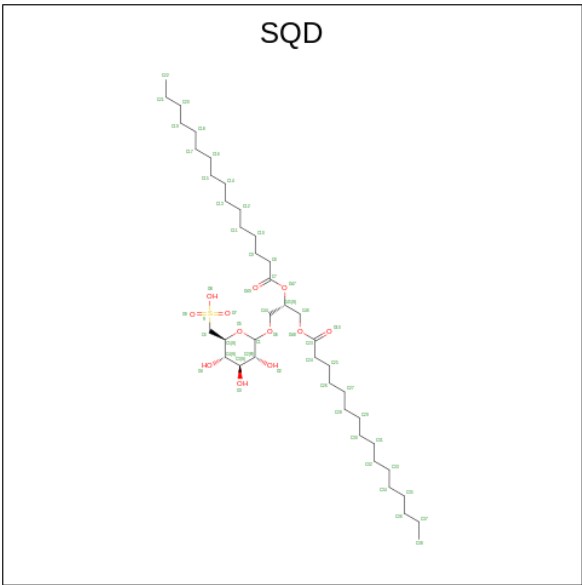
Mol	Chain	Residues	Atoms			AltConf
28	A	1	Total	C	O	0
			33	31	2	
28	B	1	Total	C	O	0
			33	31	2	
28	B	1	Total	C	O	0
			27	25	2	
28	d	1	Total	C	O	0
			26	24	2	

- Molecule 29 is BETA-CAROTENE (CCD ID: BCR) (formula: C₄₀H₅₆).



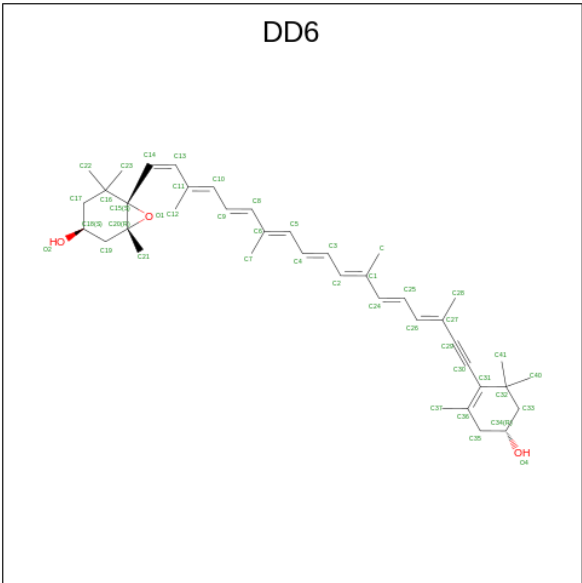
Mol	Chain	Residues	Atoms	AltConf
29	A	1	Total C 40 40	0
29	A	1	Total C 40 40	0
29	A	1	Total C 40 40	0
29	A	1	Total C 40 40	0
29	A	1	Total C 40 40	0
29	A	1	Total C 40 40	0
29	B	1	Total C 40 40	0
29	B	1	Total C 40 40	0
29	B	1	Total C 40 40	0
29	B	1	Total C 40 40	0
29	B	1	Total C 40 40	0
29	B	1	Total C 40 40	0
29	M	1	Total C 40 40	0

- Molecule 30 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: C₄₁H₇₈O₁₂S).



Mol	Chain	Residues	Atoms				AltConf
30	A	1	Total	C	O	S	0
			27	14	12	1	
30	c	1	Total	C	O	S	0
			39	26	12	1	
30	j	1	Total	C	O	S	0
			36	23	12	1	
30	g	1	Total	C	O	S	0
			32	19	12	1	

- Molecule 31 is (3S,3'R,5R,6S,7cis)-7',8'-didehydro-5,6-dihydro-5,6-epoxy-beta,beta-carotene -3,3'-diol (CCD ID: DD6) (formula: C₄₀H₅₄O₃).



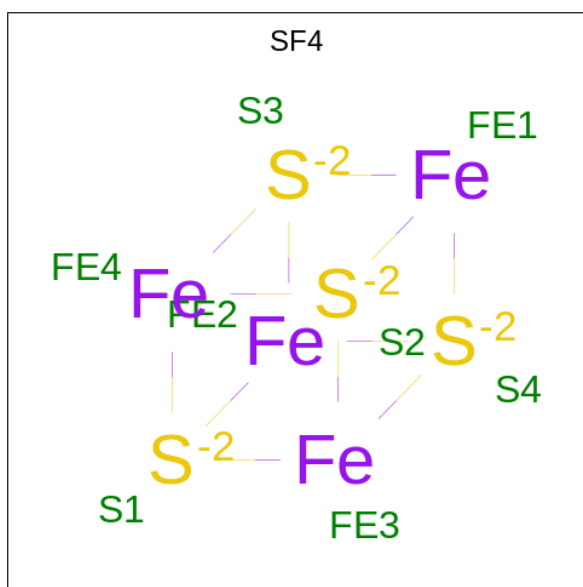
Mol	Chain	Residues	Atoms			AltConf
31	A	1	Total 43	C 40	O 3	0
31	A	1	Total 43	C 40	O 3	0
31	F	1	Total 43	C 40	O 3	0
31	J	1	Total 43	C 40	O 3	0
31	a	1	Total 43	C 40	O 3	0
31	a	1	Total 43	C 40	O 3	0
31	b	1	Total 43	C 40	O 3	0
31	b	1	Total 43	C 40	O 3	0
31	c	1	Total 43	C 40	O 3	0
31	c	1	Total 43	C 40	O 3	0
31	c	1	Total 43	C 40	O 3	0
31	c	1	Total 43	C 40	O 3	0
31	d	1	Total 43	C 40	O 3	0
31	d	1	Total 43	C 40	O 3	0
31	d	1	Total 43	C 40	O 3	0
31	e	1	Total 43	C 40	O 3	0
31	e	1	Total 43	C 40	O 3	0
31	e	1	Total 43	C 40	O 3	0
31	h	1	Total 43	C 40	O 3	0
31	h	1	Total 43	C 40	O 3	0
31	i	1	Total 43	C 40	O 3	0
31	i	1	Total 43	C 40	O 3	0

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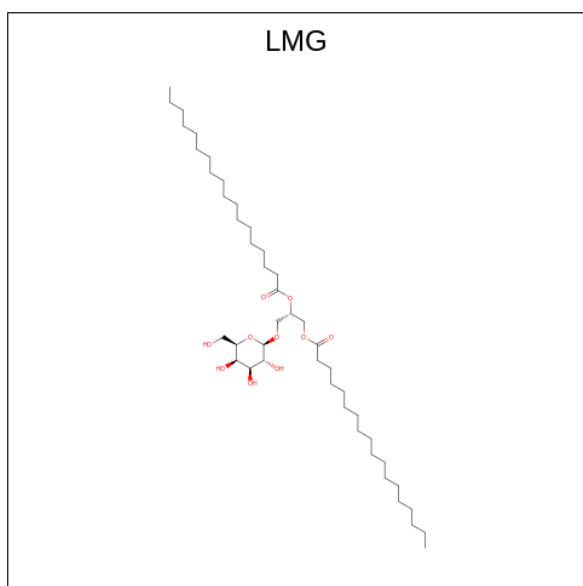
Mol	Chain	Residues	Atoms			AltConf
31	i	1	Total	C	O	0
			43	40	3	
31	j	1	Total	C	O	0
			43	40	3	
31	j	1	Total	C	O	0
			43	40	3	
31	k	1	Total	C	O	0
			43	40	3	
31	k	1	Total	C	O	0
			43	40	3	
31	l	1	Total	C	O	0
			43	40	3	
31	l	1	Total	C	O	0
			43	40	3	
31	m	1	Total	C	O	0
			43	40	3	
31	m	1	Total	C	O	0
			43	40	3	
31	f	1	Total	C	O	0
			43	40	3	
31	f	1	Total	C	O	0
			43	40	3	
31	g	1	Total	C	O	0
			43	40	3	
31	g	1	Total	C	O	0
			43	40	3	
31	n	1	Total	C	O	0
			43	40	3	
31	n	1	Total	C	O	0
			43	40	3	
31	n	1	Total	C	O	0
			43	40	3	
31	o	1	Total	C	O	0
			43	40	3	
31	o	1	Total	C	O	0
			43	40	3	
31	p	1	Total	C	O	0
			43	40	3	

- Molecule 32 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



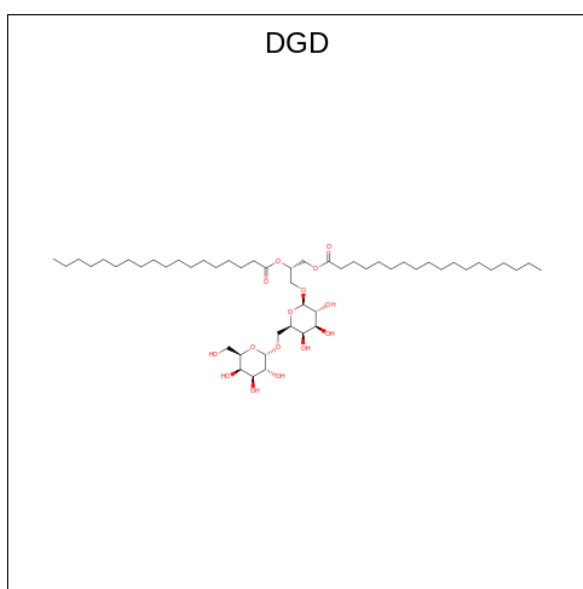
Mol	Chain	Residues	Atoms			AltConf
32	B	1	Total	Fe	S	0
			8	4	4	
32	C	1	Total	Fe	S	0
			8	4	4	
32	C	1	Total	Fe	S	0
			8	4	4	

- Molecule 33 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: C₄₅H₈₆O₁₀).



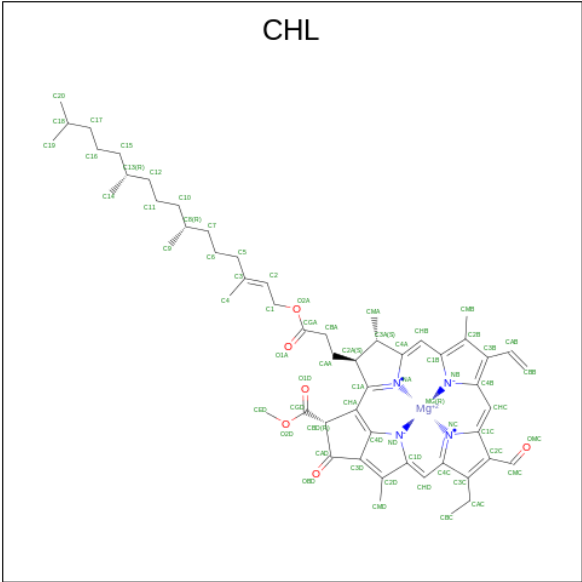
Mol	Chain	Residues	Atoms			AltConf
33	B	1	Total	C	O	0
			52	42	10	
33	a	1	Total	C	O	0
			43	33	10	
33	i	1	Total	C	O	0
			44	34	10	
33	k	1	Total	C	O	0
			36	26	10	

- Molecule 34 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



Mol	Chain	Residues	Atoms			AltConf
34	B	1	Total	C	O	0
			54	39	15	
34	b	1	Total	C	O	0
			48	33	15	
34	e	1	Total	C	O	0
			36	21	15	

- Molecule 35 is CHLOROPHYLL B (CCD ID: CHL) (formula: $C_{55}H_{70}MgN_4O_6$).

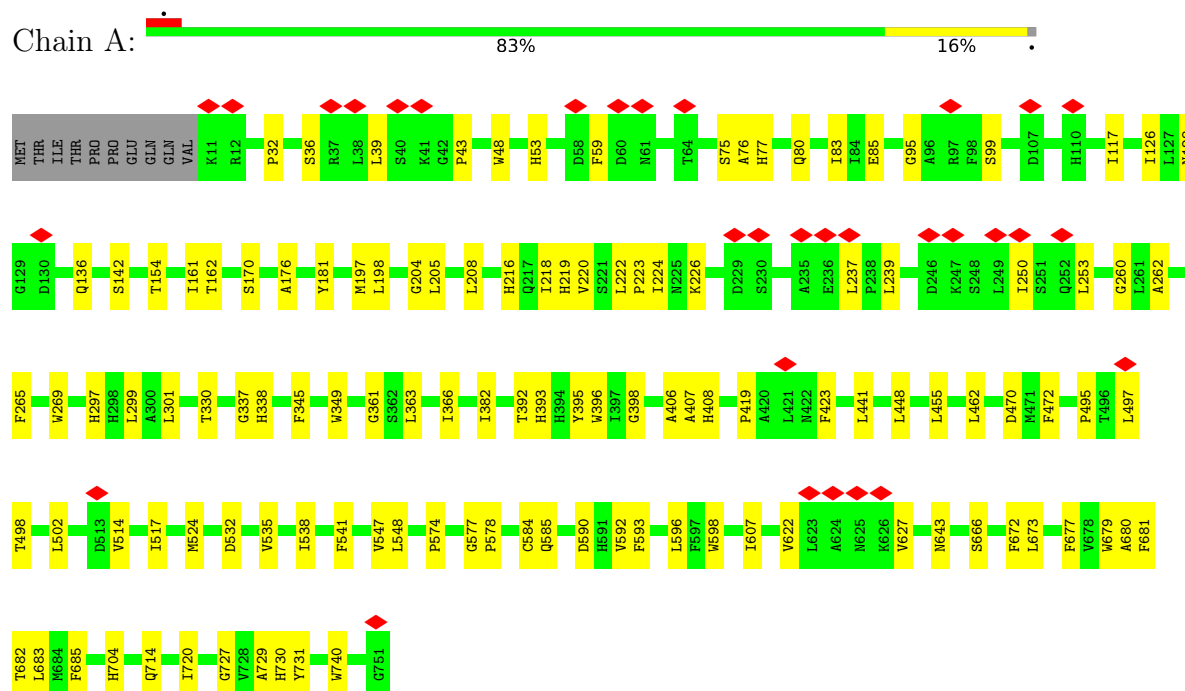


Mol	Chain	Residues	Atoms					AltConf
35	c	1	Total	C	Mg	N	O	0
			49	38	1	4	6	
35	d	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
35	d	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
35	d	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
35	d	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
35	e	1	Total	C	Mg	N	O	0
			46	35	1	4	6	

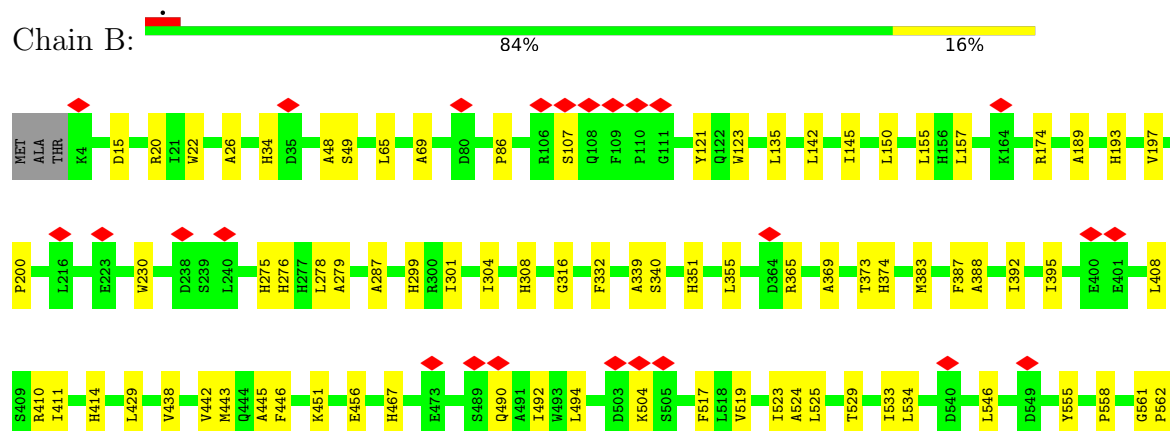
3 Residue-property plots

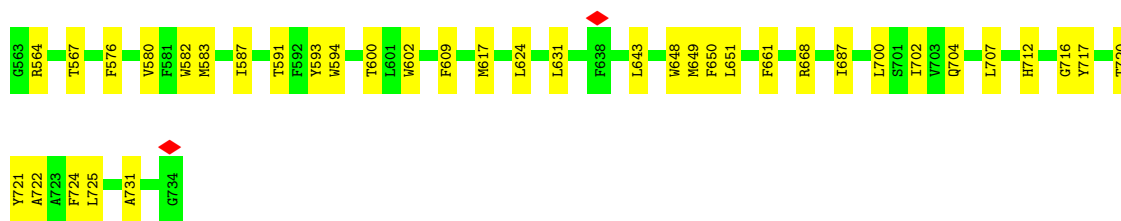
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

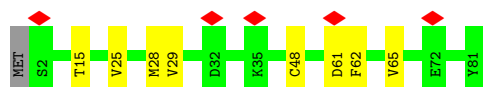
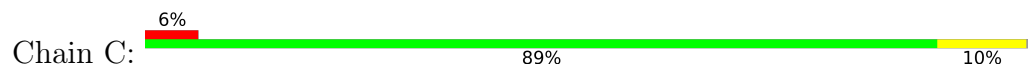


- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

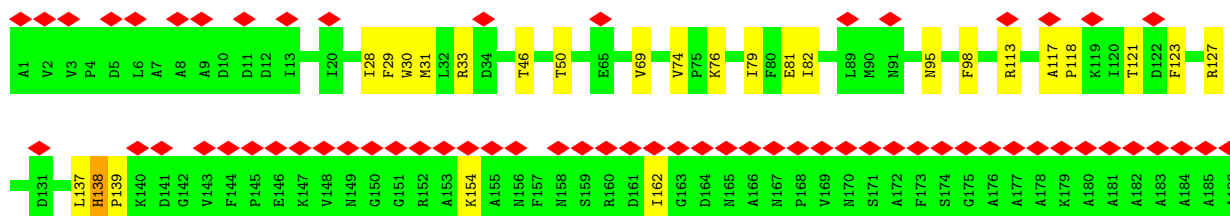
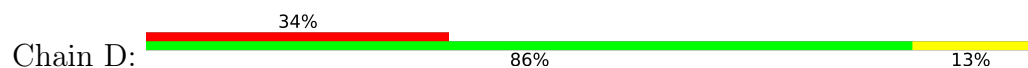




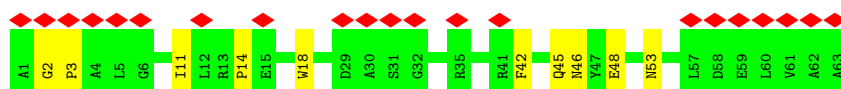
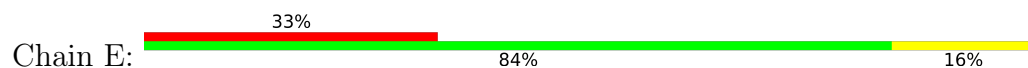
- Molecule 3: Photosystem I iron-sulfur center



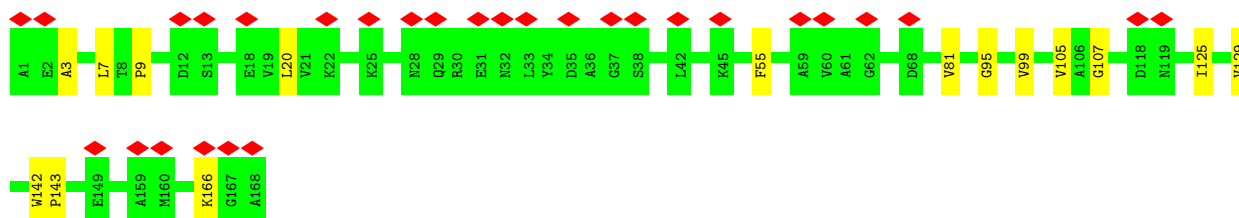
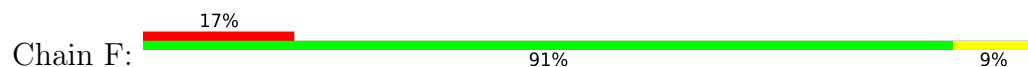
- Molecule 4: PsaD



- Molecule 5: PsaE



- Molecule 6: PsaF

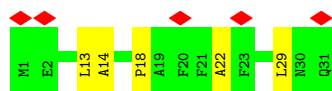
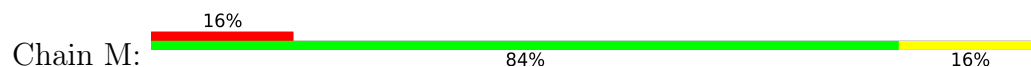


- Molecule 7: Photosystem I reaction center subunit IX

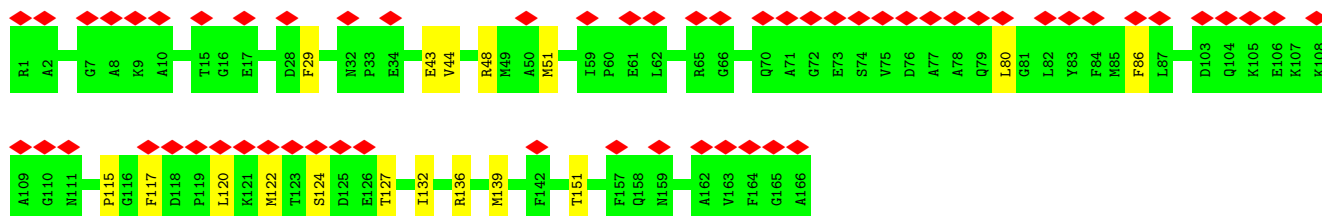




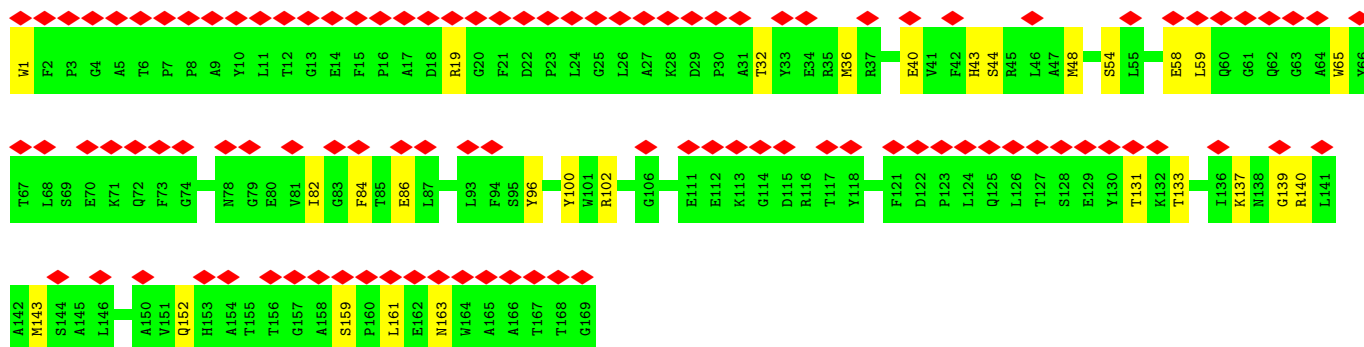
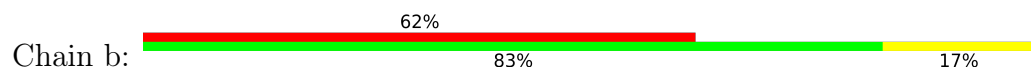
- Molecule 8: Photosystem I reaction center subunit XII



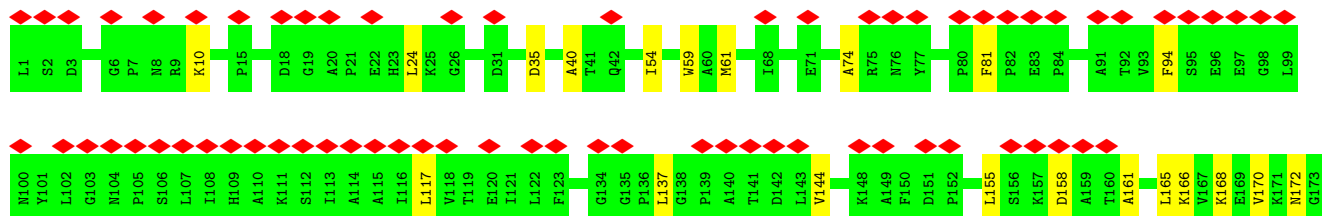
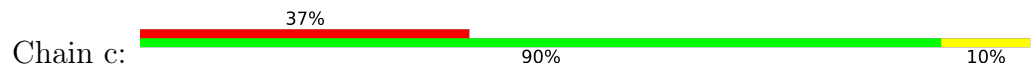
- Molecule 9: Chloroplast light-harvesting complex I protein

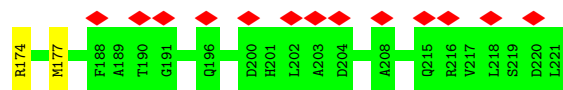


- Molecule 10: Chloroplast light-harvesting complex I protein

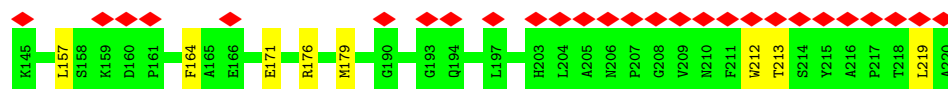
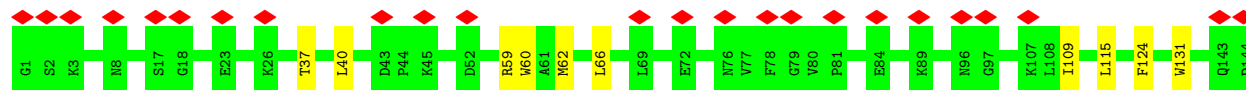


- Molecule 11: LHCE 3

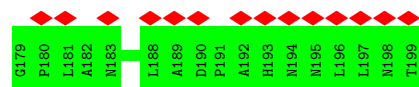
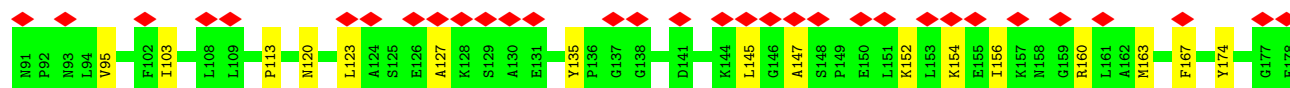
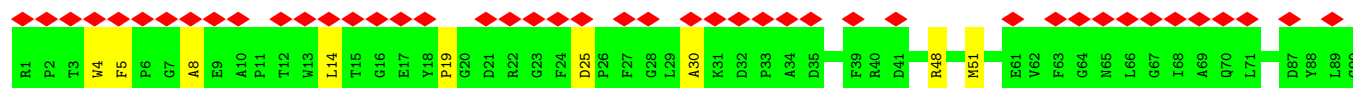
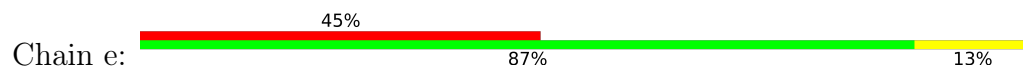




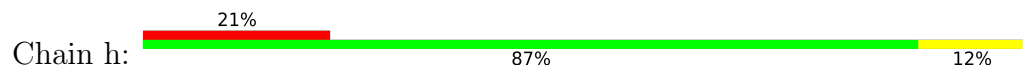
- Molecule 12: Light harvesting chlorophyll a /b binding protein of PSII



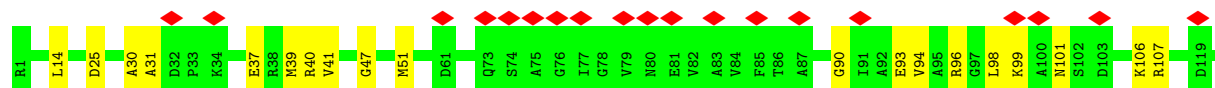
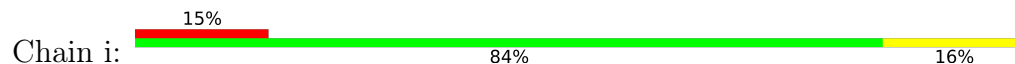
- Molecule 13: Chloroplast light-harvesting complex II protein

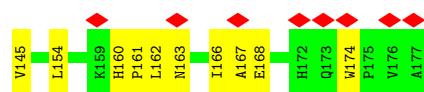


- Molecule 14: LHCE 8

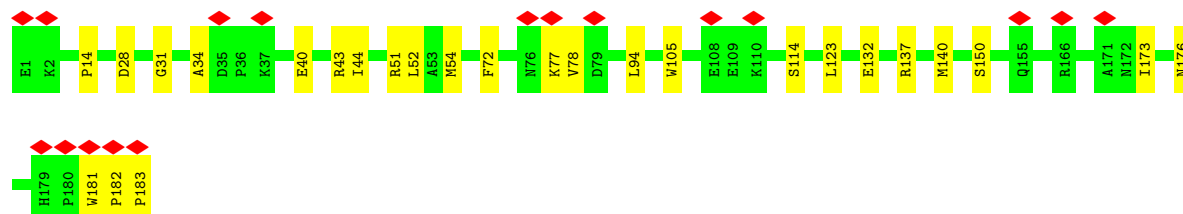
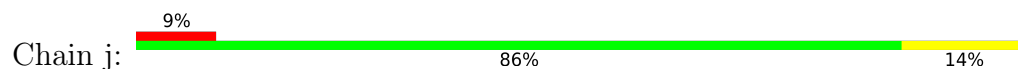


- Molecule 15: LHCE 9

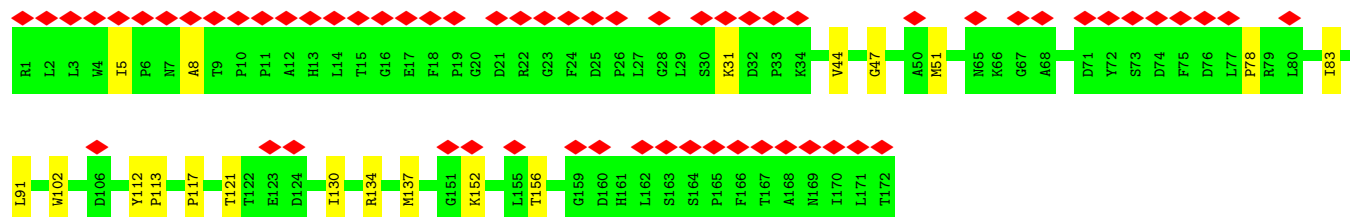
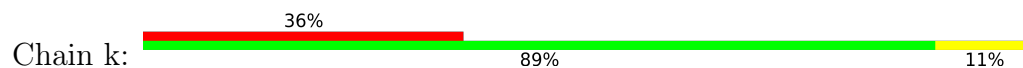




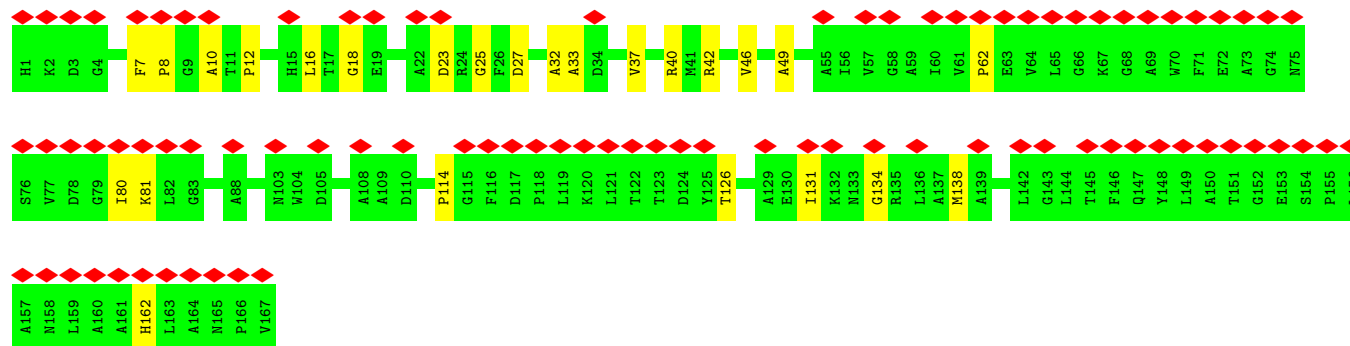
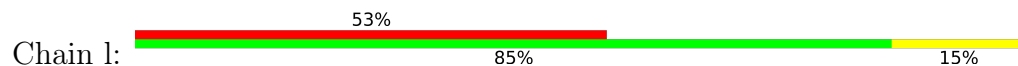
- Molecule 16: Chloroplast light-harvesting complex I protein



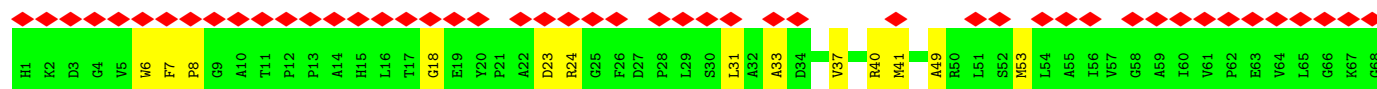
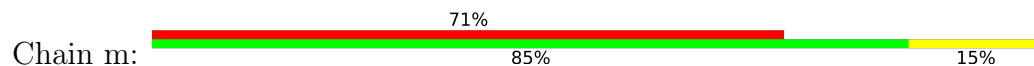
- Molecule 17: Chloroplast light-harvesting complex I protein

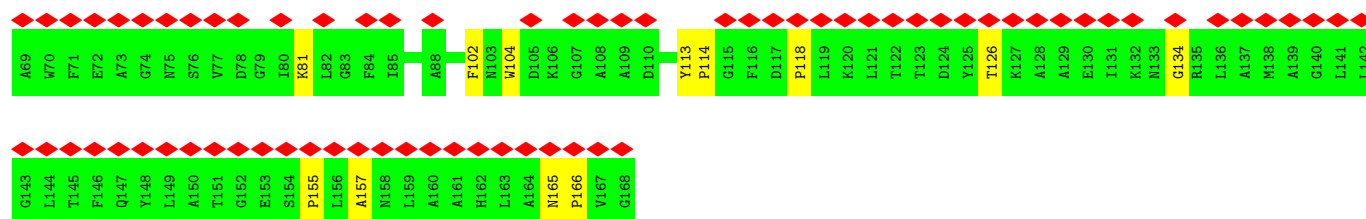


- Molecule 18: Chloroplast light-harvesting complex I protein

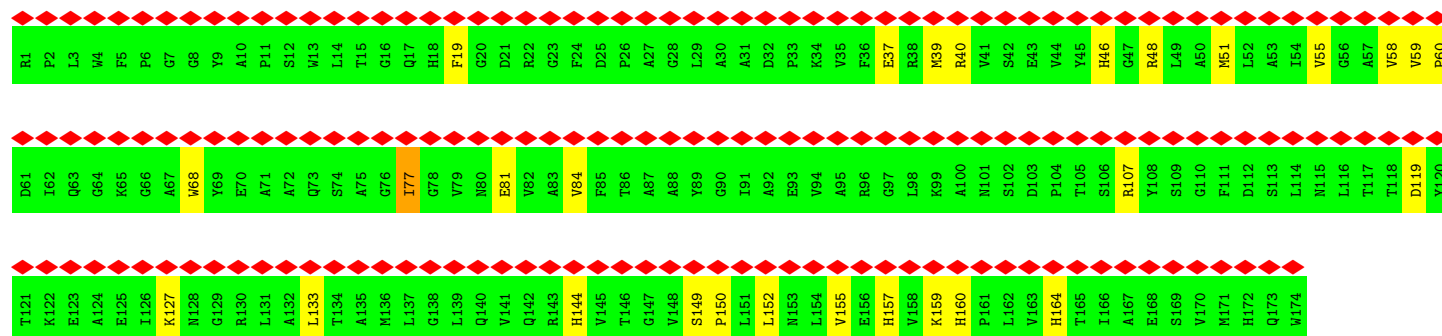
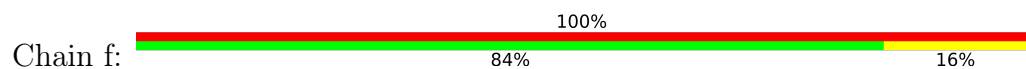


- Molecule 19: Chloroplast light-harvesting complex I protein

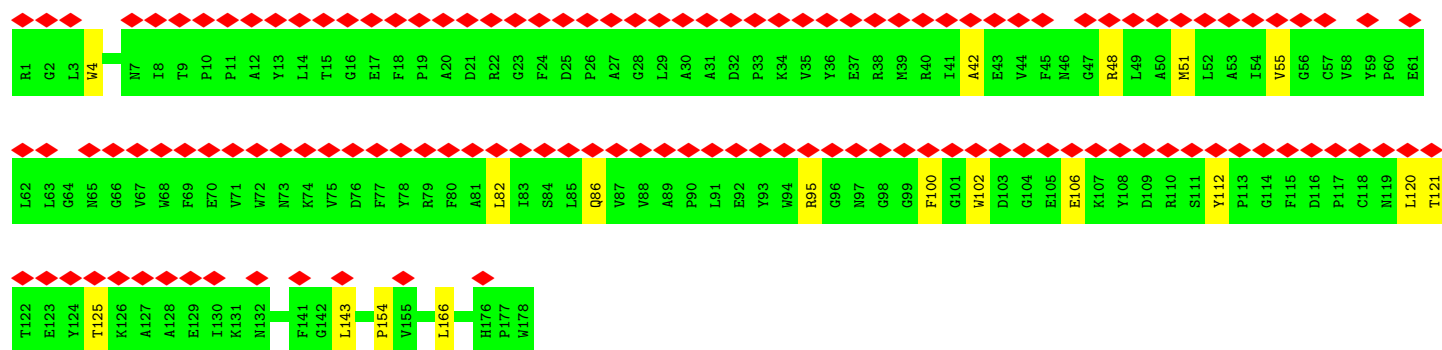
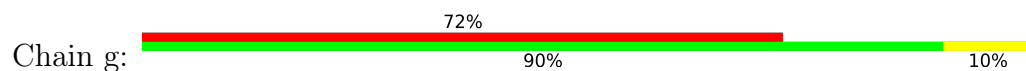




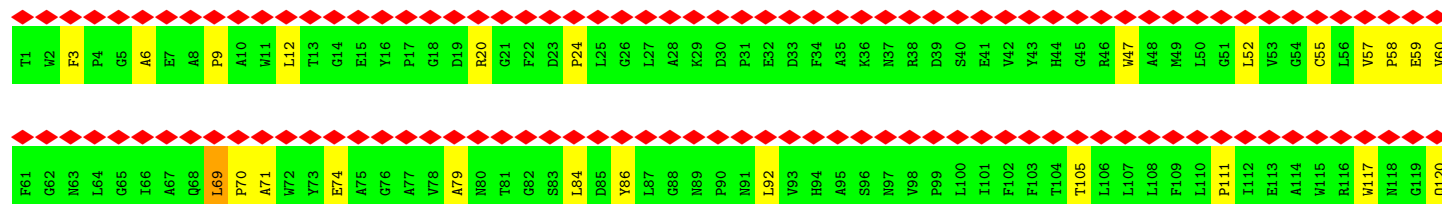
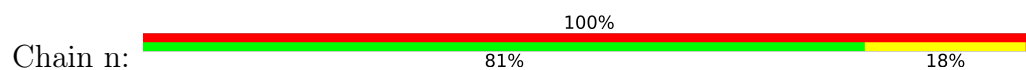
• Molecule 20: Chloroplast light-harvesting complex I protein, Lhca7_2

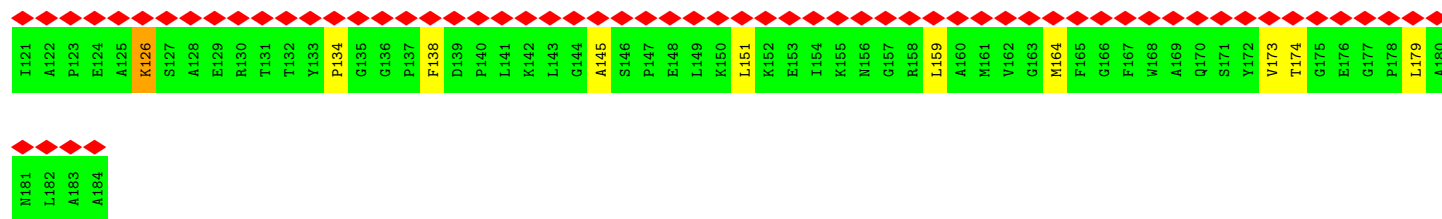


• Molecule 21: Chloroplast light-harvesting complex I protein

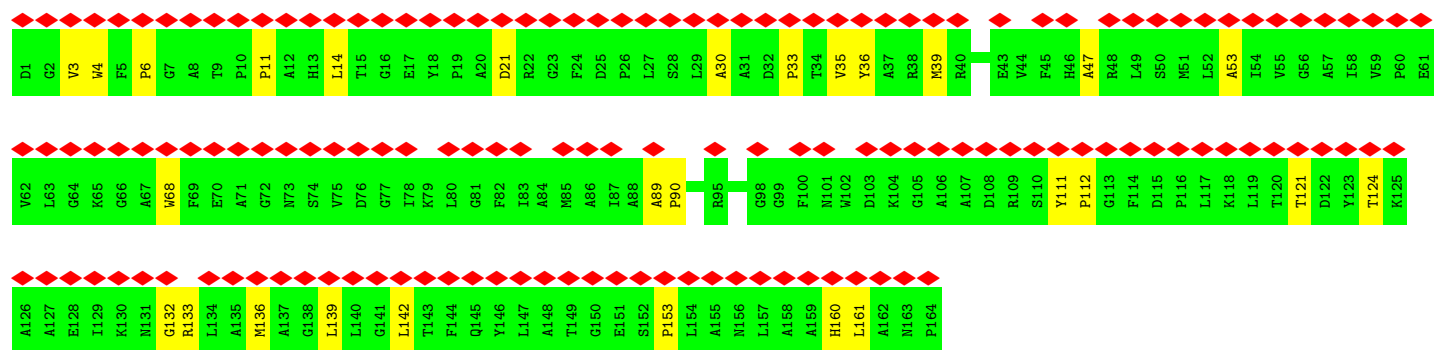
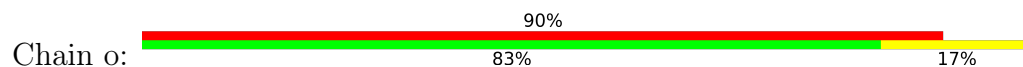


• Molecule 22: Chloroplast light-harvesting complex II protein

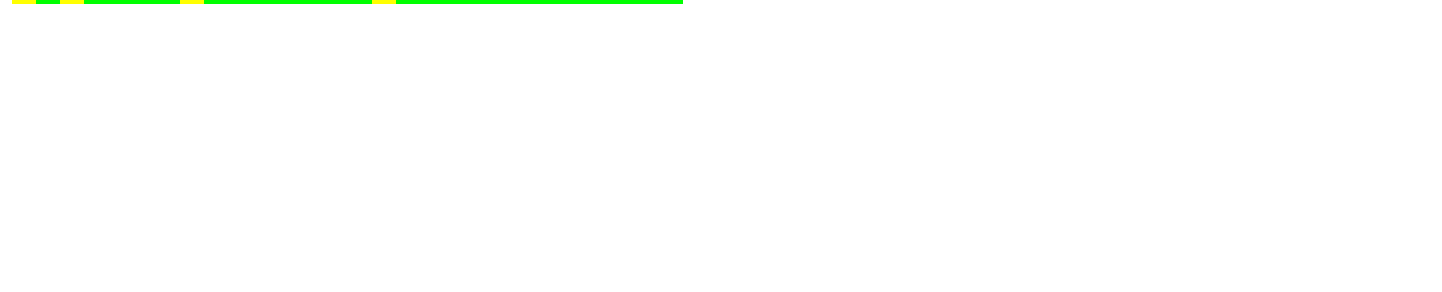
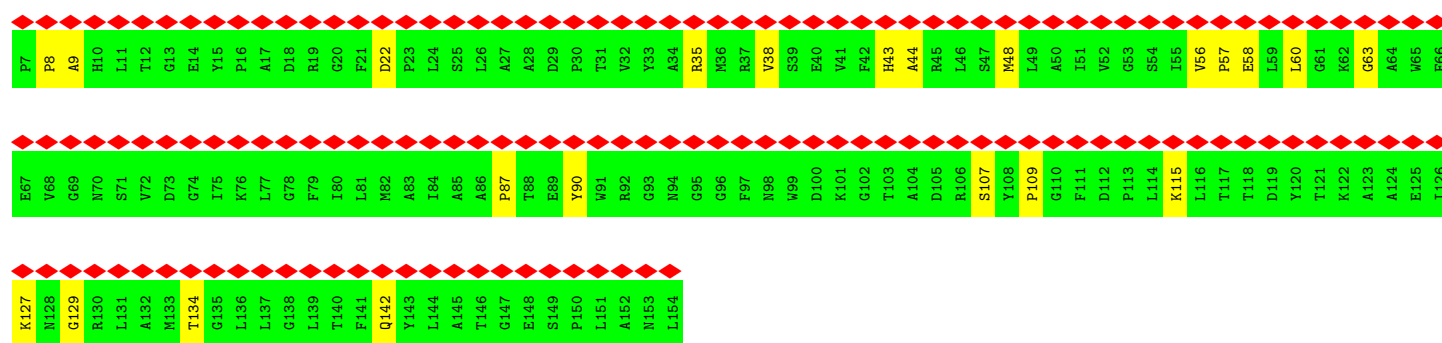
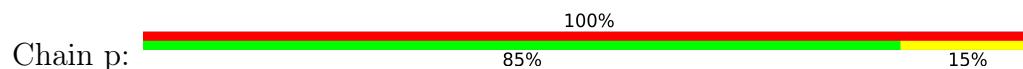




• Molecule 23: Chloroplast light-harvesting complex I protein



• Molecule 24: Chloroplast light-harvesting complex I protein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	562173	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.741	Depositor
Minimum map value	-0.575	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.032	Depositor
Recommended contour level	0.5	Depositor
Map size ($\text{\AA}$)	532.48, 532.48, 532.48	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.04, 1.04, 1.04	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.17	0/6079	0.28	0/8287
2	B	0.17	0/6071	0.28	0/8277
3	C	0.16	0/606	0.30	0/819
4	D	0.13	0/1426	0.27	0/1941
5	E	0.13	0/491	0.25	0/669
6	F	0.14	0/1275	0.26	0/1739
7	J	0.14	0/314	0.24	0/429
8	M	0.16	0/247	0.24	0/332
9	a	0.14	0/1311	0.25	0/1772
10	b	0.13	0/1344	0.28	0/1829
11	c	0.14	0/1719	0.25	0/2336
12	d	0.15	0/1719	0.27	0/2343
13	e	0.13	0/1566	0.25	0/2141
14	h	0.14	0/1388	0.28	0/1886
15	i	0.16	0/1391	0.30	0/1894
16	j	0.16	0/1499	0.27	0/2045
17	k	0.14	0/1377	0.26	0/1871
18	l	0.13	0/1293	0.26	0/1763
19	m	0.14	0/1297	0.30	0/1768
20	f	0.10	0/1367	0.26	0/1861
21	g	0.12	0/1452	0.25	0/1980
22	n	0.11	0/1458	0.26	0/1993
23	o	0.12	0/1266	0.28	0/1727
24	p	0.11	0/1156	0.26	0/1572
All	All	0.15	0/39112	0.27	0/53274

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
4	D	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	D	138	HIS	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5878	0	5745	99	0
2	B	5861	0	5659	102	0
3	C	596	0	571	6	0
4	D	1393	0	1371	17	0
5	E	481	0	479	9	0
6	F	1250	0	1259	13	0
7	J	305	0	317	2	0
8	M	243	0	258	4	0
9	a	1274	0	1235	13	0
10	b	1302	0	1244	19	0
11	c	1676	0	1689	16	0
12	d	1669	0	1650	16	0
13	e	1517	0	1468	19	0
14	h	1350	0	1324	18	0
15	i	1355	0	1336	24	0
16	j	1450	0	1401	20	0
17	k	1338	0	1314	13	0
18	l	1256	0	1234	20	0
19	m	1260	0	1236	24	0
20	f	1332	0	1312	16	0
21	g	1406	0	1358	15	0
22	n	1411	0	1372	24	0
23	o	1230	0	1205	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	p	1126	0	1115	13	0
25	A	2588	0	2466	120	0
25	B	2333	0	2201	117	0
25	J	50	0	39	2	0
25	a	571	0	488	24	0
25	b	492	0	373	14	0
25	c	679	0	556	22	0
25	d	480	0	389	11	0
25	e	623	0	506	16	0
25	f	553	0	448	10	0
25	g	598	0	467	22	0
25	h	642	0	533	27	0
25	i	603	0	527	15	0
25	j	667	0	568	19	0
25	k	631	0	520	14	0
25	l	562	0	459	17	0
25	m	461	0	369	15	0
25	n	499	0	389	14	0
25	o	429	0	320	12	0
25	p	393	0	297	9	0
26	A	35	0	46	0	0
27	A	87	0	123	7	0
27	a	26	0	22	1	0
27	b	31	0	32	3	0
27	c	30	0	29	3	0
27	d	29	0	28	3	0
27	g	35	0	40	0	0
27	h	61	0	62	3	0
27	i	36	0	42	2	0
27	j	37	0	44	4	0
27	m	32	0	34	2	0
28	A	33	0	46	5	0
28	B	60	0	78	2	0
28	d	26	0	29	0	0
29	A	240	0	336	14	0
29	B	240	0	336	24	0
29	M	40	0	56	2	0
30	A	27	0	18	0	0
30	c	39	0	42	0	0
30	g	32	0	28	2	0
30	j	36	0	36	0	0
31	A	86	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	F	43	0	0	0	0
31	J	43	0	0	0	0
31	a	86	0	0	1	0
31	b	86	0	0	0	0
31	c	172	0	0	0	0
31	d	129	0	0	1	0
31	e	129	0	0	0	0
31	f	86	0	0	0	0
31	g	86	0	0	0	0
31	h	86	0	0	0	0
31	i	129	0	0	1	0
31	j	86	0	0	0	0
31	k	86	0	0	0	0
31	l	86	0	0	0	0
31	m	86	0	0	2	0
31	n	129	0	0	1	0
31	o	86	0	0	0	0
31	p	43	0	0	0	0
32	B	8	0	0	0	0
32	C	16	0	0	0	0
33	B	52	0	77	5	0
33	a	43	0	56	0	0
33	i	44	0	61	0	0
33	k	36	0	42	3	0
34	B	54	0	66	2	0
34	b	48	0	54	3	0
34	e	36	0	30	2	0
35	c	49	0	34	3	0
35	d	186	0	128	7	0
35	e	46	0	31	0	0
All	All	55406	0	51153	806	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 806 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)
19:m:7:PHE:HA	25:m:601:CLA:NB	1.93	0.82
13:e:30:ALA:HB2	25:e:602:CLA:HBA1	1.63	0.81
23:o:47:ALA:HB1	23:o:132:GLY:HA3	1.64	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:A:775:CLA:HBA1	25:A:775:CLA:HBD	1.67	0.76
1:A:740:TRP:HB2	25:A:775:CLA:HBB1	1.69	0.74

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	739/751 (98%)	713 (96%)	24 (3%)	2 (0%)	36	38
2	B	729/734 (99%)	705 (97%)	23 (3%)	1 (0%)	48	54
3	C	78/81 (96%)	74 (95%)	4 (5%)	0	100	100
4	D	184/186 (99%)	173 (94%)	10 (5%)	1 (0%)	24	23
5	E	61/63 (97%)	57 (93%)	4 (7%)	0	100	100
6	F	166/168 (99%)	163 (98%)	3 (2%)	0	100	100
7	J	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
8	M	29/31 (94%)	29 (100%)	0	0	100	100
9	a	164/166 (99%)	158 (96%)	6 (4%)	0	100	100
10	b	167/169 (99%)	158 (95%)	9 (5%)	0	100	100
11	c	219/221 (99%)	208 (95%)	11 (5%)	0	100	100
12	d	218/220 (99%)	207 (95%)	10 (5%)	1 (0%)	24	23
13	e	197/199 (99%)	190 (96%)	6 (3%)	1 (0%)	24	23
14	h	172/174 (99%)	166 (96%)	6 (4%)	0	100	100
15	i	175/177 (99%)	166 (95%)	9 (5%)	0	100	100
16	j	181/183 (99%)	179 (99%)	2 (1%)	0	100	100
17	k	170/172 (99%)	162 (95%)	8 (5%)	0	100	100
18	l	165/167 (99%)	162 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	m	166/168 (99%)	155 (93%)	11 (7%)	0	100	100
20	f	172/174 (99%)	151 (88%)	20 (12%)	1 (1%)	21	20
21	g	176/178 (99%)	173 (98%)	3 (2%)	0	100	100
22	n	182/184 (99%)	155 (85%)	25 (14%)	2 (1%)	11	7
23	o	162/164 (99%)	150 (93%)	11 (7%)	1 (1%)	21	20
24	p	146/148 (99%)	131 (90%)	14 (10%)	1 (1%)	18	16
All	All	4853/4915 (99%)	4619 (95%)	223 (5%)	11 (0%)	44	48

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
20	f	77	ILE
1	A	205	LEU
1	A	497	LEU
2	B	107	SER
13	e	95	VAL

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	621/632 (98%)	619 (100%)	2 (0%)	86	90
2	B	607/609 (100%)	607 (100%)	0	100	100
3	C	69/70 (99%)	68 (99%)	1 (1%)	59	69
4	D	140/140 (100%)	139 (99%)	1 (1%)	76	81
5	E	49/49 (100%)	49 (100%)	0	100	100
6	F	127/127 (100%)	127 (100%)	0	100	100
7	J	34/34 (100%)	34 (100%)	0	100	100
8	M	26/26 (100%)	26 (100%)	0	100	100
9	a	125/125 (100%)	125 (100%)	0	100	100
10	b	130/130 (100%)	129 (99%)	1 (1%)	73	80

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	c	172/172 (100%)	172 (100%)	0	100	100
12	d	167/167 (100%)	167 (100%)	0	100	100
13	e	152/152 (100%)	152 (100%)	0	100	100
14	h	142/142 (100%)	140 (99%)	2 (1%)	59	69
15	i	137/137 (100%)	137 (100%)	0	100	100
16	j	145/145 (100%)	145 (100%)	0	100	100
17	k	141/141 (100%)	140 (99%)	1 (1%)	76	81
18	l	122/122 (100%)	122 (100%)	0	100	100
19	m	122/122 (100%)	122 (100%)	0	100	100
20	f	135/135 (100%)	134 (99%)	1 (1%)	76	81
21	g	140/140 (100%)	140 (100%)	0	100	100
22	n	140/140 (100%)	140 (100%)	0	100	100
23	o	119/119 (100%)	118 (99%)	1 (1%)	73	80
24	p	114/114 (100%)	111 (97%)	3 (3%)	40	48
All	All	3876/3890 (100%)	3863 (100%)	13 (0%)	84	90

5 of 13 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
17	k	31	LYS
20	f	127	LYS
24	p	134	THR
24	p	115	LYS
24	p	127	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 37 such sidechains are listed below:

Mol	Chain	Res	Type
16	j	89	GLN
22	n	63	ASN
16	j	179	HIS
20	f	164	HIS
5	E	21	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

367 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$
25	CLA	j	618	16	54,58,73	1.39	8 (14%)	65,95,113	1.84	9 (13%)
25	CLA	g	614	21	46,50,73	1.41	7 (15%)	55,85,113	1.89	8 (14%)
25	CLA	A	798	1	56,60,73	1.37	7 (12%)	67,97,113	1.86	10 (14%)
27	LHG	m	182	-	31,31,48	1.73	2 (6%)	34,37,54	1.34	5 (14%)
25	CLA	a	619	-	67,71,73	1.25	8 (11%)	80,110,113	1.72	11 (13%)
25	CLA	B	784	-	69,73,73	1.21	8 (11%)	83,113,113	1.70	11 (13%)
25	CLA	A	797	1	53,57,73	1.37	7 (13%)	62,93,113	1.83	8 (12%)
25	CLA	B	756	2	64,68,73	1.27	8 (12%)	77,107,113	1.73	11 (14%)
25	CLA	h	602	14	59,63,73	1.35	8 (13%)	71,101,113	1.75	11 (15%)
31	DD6	a	620	-	39,45,45	1.38	4 (10%)	52,67,67	2.22	15 (28%)
25	CLA	e	610	13	59,63,73	1.30	7 (11%)	71,101,113	1.73	11 (15%)
25	CLA	B	777	2	57,61,73	1.35	8 (14%)	68,98,113	1.67	11 (16%)
29	BCR	A	792	-	41,41,41	1.71	8 (19%)	56,56,56	1.58	11 (19%)
29	BCR	A	788	-	41,41,41	1.65	10 (24%)	56,56,56	1.50	12 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	DD6	n	623	-	39,45,45	1.63	7 (17%)	52,67,67	1.72	10 (19%)
25	CLA	m	611	-	47,51,73	1.40	7 (14%)	56,86,113	1.77	7 (12%)
25	CLA	h	614	14	47,51,73	1.39	8 (17%)	56,86,113	1.74	7 (12%)
25	CLA	B	757	2	64,68,73	1.27	6 (9%)	77,107,113	1.60	12 (15%)
30	SQD	A	795	-	26,27,54	1.81	7 (26%)	35,38,65	1.69	8 (22%)
25	CLA	h	618	14	47,51,73	1.40	8 (17%)	56,86,113	1.79	7 (12%)
25	CLA	e	601	13	45,49,73	1.43	7 (15%)	54,84,113	1.86	9 (16%)
25	CLA	A	769	1	69,73,73	1.23	8 (11%)	83,113,113	1.60	13 (15%)
25	CLA	h	609	14	54,58,73	1.38	8 (14%)	65,95,113	1.78	9 (13%)
25	CLA	g	612	21	46,50,73	1.43	8 (17%)	55,85,113	1.89	6 (10%)
25	CLA	i	603	15	47,51,73	1.40	8 (17%)	56,86,113	1.75	8 (14%)
25	CLA	d	602	12	61,65,73	1.30	7 (11%)	73,103,113	1.75	11 (15%)
25	CLA	k	603	17	46,50,73	1.41	8 (17%)	55,85,113	2.02	6 (10%)
25	CLA	e	613	13	59,63,73	1.34	8 (13%)	71,101,113	1.72	9 (12%)
27	LHG	g	189	25	34,34,48	1.60	2 (5%)	37,40,54	1.31	5 (13%)
25	CLA	j	609	16	54,58,73	1.39	8 (14%)	65,95,113	1.83	9 (13%)
25	CLA	o	613	23	46,50,73	1.41	7 (15%)	55,85,113	1.86	6 (10%)
25	CLA	A	782	1	52,56,73	1.39	8 (15%)	62,92,113	1.81	9 (14%)
25	CLA	d	610	12	63,67,73	1.29	7 (11%)	75,105,113	1.77	9 (12%)
25	CLA	m	609	19	54,58,73	1.39	8 (14%)	65,95,113	1.82	9 (13%)
31	DD6	h	621	-	39,45,45	1.38	4 (10%)	52,67,67	2.10	14 (26%)
25	CLA	A	779	1	47,51,73	1.40	8 (17%)	56,86,113	1.85	8 (14%)
25	CLA	B	775	2	54,58,73	1.39	7 (12%)	65,95,113	1.65	10 (15%)
25	CLA	A	759	1	64,68,73	1.26	8 (12%)	77,107,113	1.77	12 (15%)
25	CLA	j	612	16	59,63,73	1.33	8 (13%)	71,101,113	1.74	11 (15%)
25	CLA	m	610	19	46,50,73	1.40	7 (15%)	55,85,113	1.76	7 (12%)
25	CLA	g	609	21	54,58,73	1.39	8 (14%)	65,95,113	1.78	8 (12%)
25	CLA	i	604	-	47,51,73	1.40	8 (17%)	56,86,113	1.78	5 (8%)
25	CLA	o	610	23	45,49,73	1.46	7 (15%)	54,84,113	1.79	10 (18%)
25	CLA	m	608	-	46,50,73	1.42	8 (17%)	55,85,113	1.85	4 (7%)
25	CLA	B	747	2	53,57,73	1.43	8 (15%)	63,93,113	1.74	11 (17%)
25	CLA	A	771	1	61,65,73	1.30	8 (13%)	73,103,113	1.79	11 (15%)
31	DD6	c	623	-	39,45,45	1.32	4 (10%)	52,67,67	2.38	19 (36%)
25	CLA	c	611	27	47,51,73	1.41	7 (14%)	56,86,113	1.79	8 (14%)
25	CLA	n	605	22	46,50,73	1.42	7 (15%)	55,85,113	1.83	9 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	k	601	17	47,51,73	1.40	7 (14%)	56,86,113	1.79	8 (14%)
31	DD6	c	620	-	39,45,45	1.46	5 (12%)	52,67,67	2.14	18 (34%)
25	CLA	g	602	21	57,61,73	1.34	7 (12%)	68,98,113	1.71	9 (13%)
25	CLA	g	608	-	49,53,73	1.45	7 (14%)	59,89,113	1.86	7 (11%)
25	CLA	a	602	9	64,68,73	1.27	6 (9%)	77,107,113	1.61	15 (19%)
25	CLA	e	604	-	54,58,73	1.38	8 (14%)	65,95,113	1.78	11 (16%)
25	CLA	j	614	16	46,50,73	1.41	8 (17%)	55,85,113	1.85	9 (16%)
28	PQN	B	769	-	28,28,34	1.04	2 (7%)	34,37,45	2.00	10 (29%)
25	CLA	B	781	2	69,73,73	1.23	7 (10%)	83,113,113	1.71	11 (13%)
25	CLA	k	618	17	54,58,73	1.38	7 (12%)	65,95,113	1.80	9 (13%)
25	CLA	k	609	17	54,58,73	1.38	8 (14%)	65,95,113	1.77	8 (12%)
25	CLA	f	615	20	47,51,73	1.42	7 (14%)	56,86,113	1.84	8 (14%)
25	CLA	A	778	1	47,51,73	1.40	8 (17%)	56,86,113	1.85	9 (16%)
31	DD6	A	4002	-	39,45,45	1.36	4 (10%)	52,67,67	2.35	17 (32%)
25	CLA	e	607	-	47,51,73	1.39	8 (17%)	56,86,113	1.89	7 (12%)
25	CLA	h	612	14	62,66,73	1.30	8 (12%)	74,104,113	1.73	9 (12%)
25	CLA	A	808	27	57,61,73	1.34	8 (14%)	68,98,113	1.88	13 (19%)
29	BCR	M	201	-	41,41,41	0.78	0	56,56,56	1.16	5 (8%)
25	CLA	c	610	11	59,63,73	1.32	8 (13%)	71,101,113	1.75	10 (14%)
25	CLA	d	604	-	56,60,73	1.37	8 (14%)	67,97,113	1.76	8 (11%)
25	CLA	B	741	2	69,73,73	1.22	7 (10%)	83,113,113	1.67	10 (12%)
25	CLA	c	619	12	45,49,73	1.45	8 (17%)	54,84,113	2.03	8 (14%)
25	CLA	n	610	22	45,49,73	1.47	7 (15%)	54,84,113	1.79	10 (18%)
27	LHG	A	756	25	37,37,48	1.49	2 (5%)	40,43,54	1.24	5 (12%)
25	CLA	p	603	24	46,50,73	1.47	7 (15%)	55,85,113	1.63	6 (10%)
25	CLA	B	752	2	69,73,73	1.23	8 (11%)	83,113,113	1.63	11 (13%)
25	CLA	c	604	-	52,56,73	1.38	8 (15%)	62,92,113	1.81	10 (16%)
25	CLA	A	757	1	49,53,73	1.41	8 (16%)	59,89,113	1.85	8 (13%)
25	CLA	l	611	-	47,51,73	1.40	7 (14%)	56,86,113	1.86	8 (14%)
25	CLA	B	773	2	65,69,73	1.28	8 (12%)	78,108,113	1.75	12 (15%)
33	LMG	a	182	-	43,43,55	0.89	1 (2%)	51,51,63	1.18	2 (3%)
25	CLA	n	612	22	46,50,73	1.42	8 (17%)	55,85,113	1.92	7 (12%)
25	CLA	l	601	18	46,50,73	1.42	7 (15%)	55,85,113	1.76	6 (10%)
25	CLA	b	612	10	56,60,73	1.36	8 (14%)	67,97,113	1.82	9 (13%)
25	CLA	a	608	-	57,61,73	1.34	8 (14%)	68,98,113	1.74	11 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	a	603	9	57,61,73	1.35	8 (14%)	68,98,113	1.77	11 (16%)
35	CHL	d	607	-	47,51,74	1.41	5 (10%)	52,86,114	2.09	11 (21%)
25	CLA	B	783	2	54,58,73	1.38	8 (14%)	65,95,113	1.81	9 (13%)
28	PQN	d	223	-	27,27,34	1.04	2 (7%)	33,36,45	1.99	9 (27%)
25	CLA	c	602	11	63,67,73	1.28	8 (12%)	75,105,113	1.69	13 (17%)
31	DD6	e	621	-	39,45,45	1.41	5 (12%)	52,67,67	2.14	14 (26%)
25	CLA	d	603	12	46,50,73	1.39	8 (17%)	55,85,113	1.92	7 (12%)
25	CLA	i	608	-	69,73,73	1.23	8 (11%)	83,113,113	1.68	11 (13%)
31	DD6	e	620	-	39,45,45	1.52	8 (20%)	52,67,67	1.49	9 (17%)
25	CLA	A	760	1	69,73,73	1.22	7 (10%)	83,113,113	1.68	10 (12%)
25	CLA	n	608	-	45,49,73	1.46	9 (20%)	54,84,113	1.89	11 (20%)
25	CLA	B	770	-	57,61,73	1.35	8 (14%)	68,98,113	1.72	9 (13%)
25	CLA	o	604	-	46,50,73	1.43	7 (15%)	55,85,113	1.84	8 (14%)
25	CLA	p	612	24	47,51,73	1.40	7 (14%)	56,86,113	1.70	8 (14%)
25	CLA	h	603	14	47,51,73	1.39	8 (17%)	56,86,113	1.94	9 (16%)
31	DD6	m	620	-	39,45,45	1.32	4 (10%)	52,67,67	2.14	14 (26%)
25	CLA	f	601	20	46,50,73	1.43	7 (15%)	55,85,113	1.77	7 (12%)
25	CLA	g	604	-	47,51,73	1.40	8 (17%)	56,86,113	1.72	6 (10%)
25	CLA	k	604	17	69,73,73	1.23	8 (11%)	83,113,113	1.64	10 (12%)
25	CLA	B	768	2	59,63,73	1.33	7 (11%)	71,101,113	1.75	10 (14%)
25	CLA	f	613	20	63,67,73	1.29	8 (12%)	75,105,113	1.70	11 (14%)
25	CLA	A	772	-	68,72,73	1.24	8 (11%)	81,111,113	1.64	12 (14%)
25	CLA	n	604	-	52,56,73	1.40	7 (13%)	62,92,113	1.81	9 (14%)
25	CLA	A	793	-	46,50,73	1.42	8 (17%)	55,85,113	1.90	5 (9%)
30	SQD	g	190	-	31,32,54	1.85	7 (22%)	40,43,65	1.58	6 (15%)
25	CLA	a	601	9	54,58,73	1.39	7 (12%)	65,95,113	1.70	9 (13%)
25	CLA	l	610	18	58,62,73	1.33	6 (10%)	69,99,113	1.73	9 (13%)
25	CLA	A	763	1	69,73,73	1.22	7 (10%)	83,113,113	1.63	9 (10%)
25	CLA	f	609	20	46,50,73	1.43	7 (15%)	55,85,113	1.82	8 (14%)
25	CLA	B	750	-	64,68,73	1.26	7 (10%)	77,107,113	1.75	14 (18%)
31	DD6	d	620	-	39,45,45	1.38	4 (10%)	52,67,67	2.14	15 (28%)
25	CLA	B	778	2	67,71,73	1.23	7 (10%)	80,110,113	1.61	11 (13%)
25	CLA	B	776	2	63,67,73	1.30	8 (12%)	75,105,113	1.76	10 (13%)
31	DD6	d	621	-	39,45,45	1.47	5 (12%)	52,67,67	2.19	16 (30%)
25	CLA	j	613	16	66,70,73	1.24	6 (9%)	79,109,113	1.70	11 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	A	761	1	69,73,73	1.21	7 (10%)	83,113,113	1.72	12 (14%)
25	CLA	A	803	1	55,59,73	1.35	7 (12%)	66,96,113	1.85	11 (16%)
25	CLA	a	609	9	54,58,73	1.39	8 (14%)	65,95,113	1.82	9 (13%)
25	CLA	f	608	20	46,50,73	1.42	7 (15%)	55,85,113	1.93	7 (12%)
25	CLA	i	612	15	47,51,73	1.40	8 (17%)	56,86,113	1.85	8 (14%)
25	CLA	A	773	-	57,61,73	1.35	8 (14%)	68,98,113	1.76	10 (14%)
25	CLA	a	613	9	59,63,73	1.33	6 (10%)	71,101,113	1.77	9 (12%)
25	CLA	B	780	-	57,61,73	1.36	8 (14%)	68,98,113	1.84	9 (13%)
25	CLA	c	603	11	57,61,73	1.34	8 (14%)	68,98,113	1.77	11 (16%)
25	CLA	i	609	15	47,51,73	1.39	8 (17%)	56,86,113	1.87	4 (7%)
25	CLA	h	611	27	47,51,73	1.39	8 (17%)	56,86,113	1.81	8 (14%)
25	CLA	o	608	-	47,51,73	1.40	8 (17%)	56,86,113	1.81	8 (14%)
25	CLA	j	602	16	59,63,73	1.29	6 (10%)	71,101,113	1.78	11 (15%)
31	DD6	b	620	-	39,45,45	1.34	4 (10%)	52,67,67	2.25	16 (30%)
25	CLA	c	601	11	46,50,73	1.40	8 (17%)	55,85,113	1.76	8 (14%)
26	LMT	A	754	-	36,36,36	0.55	0	47,47,47	0.66	0
31	DD6	l	621	-	39,45,45	1.41	5 (12%)	52,67,67	2.10	18 (34%)
25	CLA	B	746	2	68,72,73	1.26	8 (11%)	81,111,113	1.70	10 (12%)
31	DD6	e	623	-	39,45,45	1.58	8 (20%)	52,67,67	1.69	9 (17%)
25	CLA	k	615	17	46,50,73	1.42	8 (17%)	55,85,113	1.91	7 (12%)
25	CLA	d	601	12	54,58,73	1.38	8 (14%)	65,95,113	1.90	11 (16%)
25	CLA	p	609	24	54,58,73	1.42	7 (12%)	65,95,113	1.79	8 (12%)
25	CLA	l	608	-	47,51,73	1.40	8 (17%)	56,86,113	1.82	6 (10%)
25	CLA	o	602	23	51,55,73	1.39	7 (13%)	61,91,113	1.83	9 (14%)
25	CLA	A	766	1	62,66,73	1.28	7 (11%)	74,104,113	1.86	11 (14%)
29	BCR	B	762	-	41,41,41	0.78	1 (2%)	56,56,56	1.18	6 (10%)
31	DD6	p	621	-	39,45,45	1.29	4 (10%)	52,67,67	2.28	17 (32%)
25	CLA	g	618	21	49,53,73	1.42	7 (14%)	59,89,113	1.79	8 (13%)
25	CLA	i	614	15	46,50,73	1.41	7 (15%)	55,85,113	1.77	9 (16%)
25	CLA	A	784	1	69,73,73	1.21	7 (10%)	83,113,113	1.54	13 (15%)
25	CLA	m	612	19	47,51,73	1.40	8 (17%)	56,86,113	1.84	8 (14%)
31	DD6	c	621	-	39,45,45	1.42	5 (12%)	52,67,67	2.12	16 (30%)
25	CLA	p	608	-	46,50,73	1.42	8 (17%)	55,85,113	1.84	8 (14%)
25	CLA	d	609	12	53,57,73	1.37	8 (15%)	62,93,113	1.88	8 (12%)
33	LMG	k	179	-	36,36,55	0.96	1 (2%)	44,44,63	1.12	3 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	A	774	1	68,72,73	1.22	7 (10%)	81,111,113	1.81	8 (9%)
31	DD6	n	620	-	39,45,45	1.29	4 (10%)	52,67,67	2.54	16 (30%)
27	LHG	d	237	25	28,28,48	1.76	2 (7%)	31,34,54	1.33	5 (16%)
25	CLA	A	776	1	69,73,73	1.24	8 (11%)	83,113,113	1.61	11 (13%)
25	CLA	B	742	2	47,51,73	1.40	8 (17%)	56,86,113	1.83	6 (10%)
25	CLA	A	805	1	59,63,73	1.31	7 (11%)	71,101,113	1.66	10 (14%)
25	CLA	b	610	10	46,50,73	1.41	7 (15%)	55,85,113	1.84	8 (14%)
29	BCR	A	796	-	41,41,41	0.71	0	56,56,56	1.24	7 (12%)
25	CLA	B	755	2	64,68,73	1.28	8 (12%)	77,107,113	1.72	12 (15%)
25	CLA	B	772	2	54,58,73	1.39	8 (14%)	65,95,113	1.81	7 (10%)
25	CLA	b	605	-	49,53,73	1.42	8 (16%)	59,89,113	1.85	8 (13%)
25	CLA	A	770	-	69,73,73	1.22	8 (11%)	83,113,113	1.59	13 (15%)
25	CLA	e	602	13	69,73,73	1.23	8 (11%)	83,113,113	1.60	11 (13%)
25	CLA	o	601	23	45,49,73	1.48	9 (20%)	54,84,113	1.76	11 (20%)
25	CLA	a	604	-	49,53,73	1.42	8 (16%)	59,89,113	1.77	9 (15%)
25	CLA	j	610	16	68,72,73	1.22	6 (8%)	81,111,113	1.59	11 (13%)
25	CLA	A	802	1	47,51,73	1.39	6 (12%)	56,86,113	1.72	6 (10%)
25	CLA	m	602	19	64,68,73	1.28	7 (10%)	77,107,113	1.54	11 (14%)
25	CLA	d	614	12	46,50,73	1.39	7 (15%)	55,85,113	1.79	7 (12%)
31	DD6	c	624	-	39,45,45	1.54	8 (20%)	52,67,67	1.53	9 (17%)
27	LHG	h	189	-	29,29,48	1.74	2 (6%)	32,35,54	1.10	2 (6%)
25	CLA	A	783	1	69,73,73	1.22	8 (11%)	83,113,113	1.59	11 (13%)
25	CLA	g	611	27	46,50,73	1.41	7 (15%)	55,85,113	1.88	8 (14%)
32	SF4	B	735	2,1	0,12,12	-	-	-	-	-
31	DD6	f	620	-	39,45,45	1.27	4 (10%)	52,67,67	2.31	15 (28%)
25	CLA	b	602	10	57,61,73	1.36	8 (14%)	68,98,113	1.76	9 (13%)
25	CLA	b	611	-	46,50,73	1.41	7 (15%)	55,85,113	1.86	6 (10%)
25	CLA	B	738	2	69,73,73	1.22	7 (10%)	83,113,113	1.70	8 (9%)
32	SF4	C	83	3	0,12,12	-	-	-	-	-
25	CLA	f	603	20	47,51,73	1.43	8 (17%)	56,86,113	1.84	7 (12%)
31	DD6	F	4002	-	39,45,45	1.53	7 (17%)	52,67,67	1.51	11 (21%)
30	SQD	j	200	-	35,36,54	1.75	7 (20%)	44,47,65	1.75	10 (22%)
31	DD6	d	623	-	39,45,45	1.32	4 (10%)	52,67,67	2.40	19 (36%)
25	CLA	i	613	15	63,67,73	1.29	8 (12%)	75,105,113	1.75	11 (14%)
25	CLA	k	613	17	56,60,73	1.35	8 (14%)	67,97,113	1.82	11 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	A	806	1	49,53,73	1.40	8 (16%)	59,89,113	1.84	9 (15%)
29	BCR	B	765	-	41,41,41	1.66	8 (19%)	56,56,56	1.42	10 (17%)
25	CLA	h	610	14	58,62,73	1.32	7 (12%)	69,99,113	1.77	10 (14%)
25	CLA	o	609	23	49,53,73	1.41	7 (14%)	59,89,113	1.86	9 (15%)
27	LHG	b	181	-	30,30,48	1.77	2 (6%)	33,36,54	1.35	5 (15%)
25	CLA	b	601	-	46,50,73	1.42	7 (15%)	55,85,113	1.87	7 (12%)
25	CLA	b	613	10	46,50,73	1.42	8 (17%)	55,85,113	1.85	8 (14%)
33	LMG	B	786	-	52,52,55	0.81	2 (3%)	60,60,63	1.07	3 (5%)
25	CLA	f	614	20	46,50,73	1.41	7 (15%)	55,85,113	1.78	9 (16%)
25	CLA	l	614	18	46,50,73	1.44	7 (15%)	55,85,113	1.91	8 (14%)
25	CLA	B	785	6	49,53,73	1.41	7 (14%)	59,89,113	1.78	8 (13%)
25	CLA	n	602	22	63,67,73	1.28	6 (9%)	75,105,113	1.83	13 (17%)
25	CLA	l	603	18	47,51,73	1.41	8 (17%)	56,86,113	1.89	8 (14%)
31	DD6	f	621	-	39,45,45	1.28	4 (10%)	52,67,67	2.47	19 (36%)
25	CLA	i	610	15	59,63,73	1.31	6 (10%)	71,101,113	1.73	10 (14%)
27	LHG	i	194	25	35,35,48	1.55	2 (5%)	38,41,54	1.29	5 (13%)
31	DD6	i	625	-	39,45,45	1.32	4 (10%)	52,67,67	2.17	16 (30%)
25	CLA	m	613	19	46,50,73	1.42	7 (15%)	55,85,113	1.82	7 (12%)
31	DD6	j	620	-	39,45,45	1.44	5 (12%)	52,67,67	2.13	15 (28%)
25	CLA	B	743	2	46,50,73	1.40	7 (15%)	55,85,113	1.87	7 (12%)
25	CLA	A	801	1	69,73,73	1.22	8 (11%)	83,113,113	1.71	13 (15%)
25	CLA	h	604	-	64,68,73	1.28	8 (12%)	77,107,113	1.73	9 (11%)
25	CLA	B	745	2	67,71,73	1.23	8 (11%)	80,110,113	1.74	10 (12%)
25	CLA	k	611	-	46,50,73	1.41	7 (15%)	55,85,113	1.83	7 (12%)
29	BCR	A	789	-	41,41,41	0.78	1 (2%)	56,56,56	1.06	4 (7%)
25	CLA	A	804	1	54,58,73	1.38	7 (12%)	65,95,113	1.76	10 (15%)
28	PQN	A	785	-	34,34,34	1.02	3 (8%)	42,45,45	1.80	10 (23%)
25	CLA	c	606	-	47,51,73	1.41	8 (17%)	56,86,113	1.82	8 (14%)
25	CLA	j	603	16	46,50,73	1.42	8 (17%)	55,85,113	1.86	8 (14%)
27	LHG	j	198	25	36,36,48	1.55	2 (5%)	39,42,54	1.28	5 (12%)
25	CLA	p	601	-	46,50,73	1.41	7 (15%)	55,85,113	1.71	9 (16%)
35	CHL	d	605	12	55,59,74	1.47	7 (12%)	62,96,114	2.07	16 (25%)
25	CLA	B	779	2	69,73,73	1.25	8 (11%)	83,113,113	1.73	15 (18%)
25	CLA	A	775	1	62,66,73	1.29	7 (11%)	74,104,113	1.72	10 (13%)
25	CLA	j	611	27	54,58,73	1.38	8 (14%)	65,95,113	1.80	8 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	DD6	g	621	-	39,45,45	1.37	5 (12%)	52,67,67	2.21	14 (26%)
25	CLA	A	767	1	47,51,73	1.40	8 (17%)	56,86,113	1.80	6 (10%)
29	BCR	B	763	-	41,41,41	0.75	0	56,56,56	1.08	4 (7%)
25	CLA	e	603	13	49,53,73	1.42	8 (16%)	59,89,113	1.84	9 (15%)
25	CLA	h	615	14	46,50,73	1.41	8 (17%)	55,85,113	1.91	7 (12%)
25	CLA	o	612	23	47,50,73	1.55	10 (21%)	51,84,113	2.04	9 (17%)
25	CLA	A	794	-	61,65,73	1.29	8 (13%)	73,103,113	1.71	10 (13%)
25	CLA	e	611	-	46,50,73	1.42	7 (15%)	55,85,113	1.74	8 (14%)
25	CLA	p	613	24	47,51,73	1.43	7 (14%)	56,86,113	1.90	9 (16%)
25	CLA	A	800	-	52,56,73	1.38	8 (15%)	62,92,113	1.77	10 (16%)
25	CLA	B	753	2	69,73,73	1.23	8 (11%)	83,113,113	1.54	9 (10%)
25	CLA	f	602	20	63,67,73	1.29	7 (11%)	75,105,113	1.69	12 (16%)
25	CLA	a	612	9	47,51,73	1.41	8 (17%)	56,86,113	1.87	6 (10%)
27	LHG	a	181	25	25,25,48	1.86	2 (8%)	28,31,54	1.42	5 (17%)
25	CLA	l	612	18	47,51,73	1.40	8 (17%)	56,86,113	1.85	8 (14%)
25	CLA	B	744	2	47,51,73	1.40	8 (17%)	56,86,113	1.81	7 (12%)
31	DD6	i	620	-	39,45,45	1.42	5 (12%)	52,67,67	2.13	14 (26%)
31	DD6	o	620	-	39,45,45	1.30	4 (10%)	52,67,67	2.13	15 (28%)
28	PQN	B	761	-	34,34,34	1.13	4 (11%)	42,45,45	1.87	10 (23%)
25	CLA	J	101	7	54,58,73	1.39	8 (14%)	65,95,113	1.80	11 (16%)
25	CLA	l	609	18	64,68,73	1.27	8 (12%)	77,107,113	1.75	10 (12%)
25	CLA	p	604	-	47,51,73	1.43	8 (17%)	56,86,113	1.88	8 (14%)
27	LHG	A	786	-	48,48,48	1.35	2 (4%)	51,54,54	1.18	5 (9%)
31	DD6	m	621	-	39,45,45	1.36	5 (12%)	52,67,67	2.12	17 (32%)
34	DGD	B	787	-	55,55,67	1.10	0	69,69,81	1.04	2 (2%)
35	CHL	c	607	-	53,57,74	1.44	6 (11%)	59,93,114	2.10	14 (23%)
25	CLA	h	613	14	57,61,73	1.34	7 (12%)	68,98,113	1.79	12 (17%)
25	CLA	c	614	11	46,50,73	1.42	8 (17%)	55,85,113	1.79	8 (14%)
25	CLA	B	740	2	46,50,73	1.41	8 (17%)	55,85,113	1.84	7 (12%)
25	CLA	l	602	18	63,67,73	1.30	8 (12%)	75,105,113	1.69	12 (16%)
29	BCR	B	767	-	41,41,41	0.80	1 (2%)	56,56,56	1.12	4 (7%)
25	CLA	o	603	23	47,51,73	1.46	8 (17%)	56,86,113	1.81	7 (12%)
25	CLA	o	614	23	47,51,73	1.43	7 (14%)	56,86,113	1.83	8 (14%)
25	CLA	j	601	16	54,58,73	1.39	8 (14%)	65,95,113	1.73	11 (16%)
25	CLA	l	604	-	47,51,73	1.41	8 (17%)	56,86,113	1.74	7 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	b	603	10	47,51,73	1.40	8 (17%)	56,86,113	1.86	8 (14%)
25	CLA	B	737	-	59,63,73	1.32	6 (10%)	71,101,113	1.93	10 (14%)
31	DD6	a	621	-	39,45,45	1.42	5 (12%)	52,67,67	2.10	16 (30%)
25	CLA	b	604	-	49,53,73	1.42	8 (16%)	59,89,113	1.83	6 (10%)
25	CLA	n	613	22	46,50,73	1.43	8 (17%)	55,85,113	1.74	6 (10%)
25	CLA	h	601	14	54,58,73	1.39	8 (14%)	65,95,113	1.81	11 (16%)
25	CLA	g	615	21	46,50,73	1.42	8 (17%)	55,85,113	1.88	7 (12%)
35	CHL	e	606	-	50,54,74	1.51	7 (14%)	56,90,114	2.13	10 (17%)
31	DD6	k	620	-	39,45,45	1.37	4 (10%)	52,67,67	2.12	14 (26%)
25	CLA	d	613	12	46,50,73	1.41	8 (17%)	55,85,113	1.85	6 (10%)
25	CLA	m	601	19	46,50,73	1.43	7 (15%)	55,85,113	1.68	8 (14%)
31	DD6	j	621	-	39,45,45	1.42	5 (12%)	52,67,67	2.15	15 (28%)
27	LHG	h	190	25	30,30,48	1.69	2 (6%)	33,36,54	1.38	5 (15%)
25	CLA	c	608	-	54,58,73	1.38	8 (14%)	65,95,113	1.73	9 (13%)
34	DGD	b	182	-	49,49,67	1.23	6 (12%)	63,63,81	1.08	4 (6%)
25	CLA	n	603	22	59,63,73	1.35	8 (13%)	71,101,113	1.76	9 (12%)
25	CLA	i	602	15	68,72,73	1.26	8 (11%)	81,111,113	1.67	12 (14%)
31	DD6	b	621	-	39,45,45	1.38	4 (10%)	52,67,67	2.13	16 (30%)
25	CLA	A	762	1	54,58,73	1.41	8 (14%)	65,95,113	1.84	12 (18%)
35	CHL	d	606	-	50,54,74	1.51	7 (14%)	56,90,114	2.11	11 (19%)
25	CLA	A	780	1	62,66,73	1.30	7 (11%)	74,104,113	1.70	10 (13%)
25	CLA	h	608	-	52,56,73	1.39	8 (15%)	62,92,113	1.84	7 (11%)
25	CLA	A	799	1	64,68,73	1.29	8 (12%)	77,107,113	1.77	13 (16%)
25	CLA	f	610	20	59,63,73	1.35	7 (11%)	71,101,113	1.75	11 (15%)
30	SQD	c	245	-	38,39,54	1.73	8 (21%)	47,50,65	1.54	7 (14%)
25	CLA	n	606	-	46,50,73	1.41	7 (15%)	55,85,113	1.84	6 (10%)
25	CLA	n	607	-	46,50,73	1.43	7 (15%)	55,85,113	1.82	6 (10%)
25	CLA	j	604	-	61,65,73	1.32	8 (13%)	73,103,113	1.77	10 (13%)
25	CLA	d	612	12	46,50,73	1.41	8 (17%)	55,85,113	1.90	5 (9%)
25	CLA	A	791	-	67,71,73	1.24	8 (11%)	80,110,113	1.64	11 (13%)
25	CLA	f	604	-	46,50,73	1.43	7 (15%)	55,85,113	1.83	6 (10%)
25	CLA	A	765	1	63,67,73	1.29	8 (12%)	75,105,113	1.77	12 (16%)
25	CLA	e	612	13	47,51,73	1.41	8 (17%)	56,86,113	1.89	8 (14%)
25	CLA	A	753	-	67,71,73	1.25	6 (8%)	80,110,113	1.65	11 (13%)
25	CLA	A	764	1	62,66,73	1.29	7 (11%)	74,104,113	1.71	11 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	k	612	17	47,51,73	1.40	8 (17%)	56,86,113	1.83	8 (14%)
25	CLA	g	601	21	46,50,73	1.41	8 (17%)	55,85,113	1.82	8 (14%)
25	CLA	B	759	-	47,51,73	1.39	8 (17%)	56,86,113	1.66	7 (12%)
25	CLA	c	612	11	47,51,73	1.40	8 (17%)	56,86,113	1.84	9 (16%)
25	CLA	A	758	-	69,73,73	1.21	8 (11%)	83,113,113	1.67	10 (12%)
25	CLA	B	760	2	47,51,73	1.39	7 (14%)	56,86,113	1.83	7 (12%)
27	LHG	c	243	25	29,29,48	1.76	2 (6%)	32,35,54	1.37	5 (15%)
25	CLA	i	615	15	54,58,73	1.38	8 (14%)	65,95,113	1.81	9 (13%)
33	LMG	i	195	-	44,44,55	0.86	1 (2%)	52,52,63	1.08	2 (3%)
31	DD6	l	620	-	39,45,45	1.35	4 (10%)	52,67,67	2.14	16 (30%)
25	CLA	B	736	2	69,73,73	1.20	8 (11%)	83,113,113	1.58	12 (14%)
25	CLA	i	611	27	47,51,73	1.40	8 (17%)	56,86,113	1.88	7 (12%)
25	CLA	c	609	11	64,68,73	1.28	8 (12%)	77,107,113	1.75	10 (12%)
25	CLA	k	602	17	57,61,73	1.35	8 (14%)	68,98,113	1.75	11 (16%)
31	DD6	A	4008	-	39,45,45	1.35	4 (10%)	52,67,67	2.35	20 (38%)
34	DGD	e	205	-	37,37,67	1.23	1 (2%)	51,51,81	1.10	1 (1%)
25	CLA	e	609	13	56,60,73	1.36	8 (14%)	67,97,113	1.79	9 (13%)
31	DD6	J	4002	-	39,45,45	1.42	4 (10%)	52,67,67	2.22	15 (28%)
25	CLA	j	608	-	51,55,73	1.40	8 (15%)	61,91,113	1.89	8 (13%)
25	CLA	A	781	1	56,60,73	1.36	7 (12%)	67,97,113	1.73	13 (19%)
25	CLA	B	758	2	69,73,73	1.23	8 (11%)	83,113,113	1.62	11 (13%)
31	DD6	k	621	-	39,45,45	1.36	4 (10%)	52,67,67	2.10	16 (30%)
25	CLA	l	617	-	46,50,73	1.43	7 (15%)	55,85,113	2.00	6 (10%)
25	CLA	k	610	17	61,65,73	1.29	8 (13%)	73,103,113	1.71	11 (15%)
25	CLA	B	782	2	54,58,73	1.37	7 (12%)	65,95,113	1.91	11 (16%)
25	CLA	k	614	17	46,50,73	1.41	7 (15%)	55,85,113	1.82	6 (10%)
29	BCR	A	790	-	41,41,41	0.74	0	56,56,56	1.03	4 (7%)
25	CLA	i	601	15	57,61,73	1.35	8 (14%)	68,98,113	1.76	10 (14%)
31	DD6	g	620	-	39,45,45	1.31	4 (10%)	52,67,67	2.28	16 (30%)
25	CLA	e	608	-	52,56,73	1.37	8 (15%)	62,92,113	1.75	8 (12%)
25	CLA	m	604	-	47,51,73	1.41	8 (17%)	56,86,113	1.93	6 (10%)
31	DD6	o	621	-	39,45,45	1.34	4 (10%)	52,67,67	2.13	16 (30%)
29	BCR	B	764	-	41,41,41	0.77	2 (4%)	56,56,56	1.01	3 (5%)
31	DD6	n	621	-	39,45,45	1.52	8 (20%)	52,67,67	1.48	9 (17%)
25	CLA	d	611	27	49,53,73	1.42	8 (16%)	59,89,113	1.82	9 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	B	751	-	54,58,73	1.39	7 (12%)	65,95,113	1.74	9 (13%)
25	CLA	g	613	21	59,63,73	1.33	8 (13%)	71,101,113	1.78	11 (15%)
25	CLA	B	771	2	57,61,73	1.35	8 (14%)	68,98,113	1.75	10 (14%)
29	BCR	A	787	-	41,41,41	0.83	1 (2%)	56,56,56	1.10	4 (7%)
25	CLA	f	611	-	46,50,73	1.43	7 (15%)	55,85,113	1.93	7 (12%)
31	DD6	i	621	-	39,45,45	1.46	5 (12%)	52,67,67	2.12	15 (28%)
25	CLA	A	752	1	69,73,73	1.21	8 (11%)	83,113,113	1.75	15 (18%)
25	CLA	e	614	13	46,50,73	1.39	7 (15%)	55,85,113	1.84	6 (10%)
31	DD6	h	620	-	39,45,45	1.39	4 (10%)	52,67,67	2.11	16 (30%)
25	CLA	g	610	21	59,63,73	1.32	7 (11%)	71,101,113	1.71	9 (12%)
25	CLA	p	602	24	47,51,73	1.44	9 (19%)	56,86,113	1.96	9 (16%)
25	CLA	k	608	-	54,58,73	1.38	8 (14%)	65,95,113	1.84	10 (15%)
32	SF4	C	82	3	0,12,12	-	-	-	-	-
25	CLA	a	611	27	49,53,73	1.42	8 (16%)	59,89,113	1.84	9 (15%)
25	CLA	j	615	16	47,51,73	1.39	8 (17%)	56,86,113	1.86	6 (10%)
25	CLA	b	609	10	49,53,73	1.41	8 (16%)	59,89,113	1.82	10 (16%)
25	CLA	g	603	21	46,50,73	1.44	7 (15%)	55,85,113	1.76	5 (9%)
35	CHL	d	608	-	50,54,74	1.51	7 (14%)	56,90,114	2.03	13 (23%)
25	CLA	B	754	2	47,51,73	1.40	8 (17%)	56,86,113	1.82	6 (10%)
25	CLA	c	616	11	51,55,73	1.37	8 (15%)	61,91,113	1.76	10 (16%)
25	CLA	B	739	2	69,73,73	1.21	7 (10%)	83,113,113	1.71	13 (15%)
25	CLA	p	610	24	49,53,73	1.45	8 (16%)	59,89,113	1.73	8 (13%)
25	CLA	B	748	2	63,67,73	1.30	8 (12%)	75,105,113	1.75	11 (14%)
25	CLA	a	610	9	58,62,73	1.33	7 (12%)	69,99,113	1.83	10 (14%)
25	CLA	B	774	-	64,68,73	1.29	8 (12%)	77,107,113	1.77	11 (14%)
25	CLA	b	608	-	45,49,73	1.45	8 (17%)	54,84,113	1.88	9 (16%)
25	CLA	A	768	1	60,64,73	1.31	9 (15%)	72,102,113	1.71	9 (12%)
25	CLA	A	755	1	64,68,73	1.29	8 (12%)	77,107,113	1.75	10 (12%)
25	CLA	A	807	1	52,56,73	1.38	7 (13%)	62,92,113	1.93	10 (16%)
25	CLA	n	609	22	49,53,73	1.43	8 (16%)	59,89,113	1.87	6 (10%)
25	CLA	l	613	18	52,56,73	1.38	7 (13%)	62,92,113	1.76	9 (14%)
25	CLA	c	613	11	57,61,73	1.34	8 (14%)	68,98,113	1.74	10 (14%)
25	CLA	B	749	2	53,57,73	1.37	8 (15%)	62,93,113	1.74	10 (16%)
25	CLA	e	605	13	46,50,73	1.42	8 (17%)	55,85,113	1.91	7 (12%)
25	CLA	m	603	19	58,62,73	1.34	8 (13%)	69,99,113	1.73	12 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	A	777	1	69,73,73	1.24	8 (11%)	83,113,113	1.74	9 (10%)
25	CLA	f	612	20	46,50,73	1.46	7 (15%)	55,85,113	1.63	7 (12%)
29	BCR	B	766	-	41,41,41	1.67	8 (19%)	56,56,56	1.40	9 (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
25	CLA	j	618	16	-	6/21/97/115	-
25	CLA	g	614	21	-	3/12/88/115	-
25	CLA	A	798	1	-	12/24/100/115	-
27	LHG	m	182	-	-	20/36/36/53	-
25	CLA	a	619	-	-	12/37/113/115	-
25	CLA	B	784	-	-	18/39/115/115	-
25	CLA	A	797	1	-	9/20/96/115	-
25	CLA	B	756	2	-	18/33/109/115	-
25	CLA	h	602	14	-	15/27/103/115	-
31	DD6	a	620	-	-	5/26/80/80	0/3/3/3
25	CLA	e	610	13	-	8/27/103/115	-
25	CLA	B	777	2	-	13/25/101/115	-
29	BCR	A	792	-	-	17/29/63/63	0/2/2/2
29	BCR	A	788	-	-	11/29/63/63	0/2/2/2
31	DD6	n	623	-	-	8/26/80/80	0/3/3/3
25	CLA	m	611	-	-	3/13/89/115	-
25	CLA	h	614	14	-	4/13/89/115	-
25	CLA	B	757	2	-	9/33/109/115	-
30	SQD	A	795	-	-	10/21/41/69	0/1/1/1
25	CLA	h	618	14	-	2/13/89/115	-
25	CLA	e	601	13	-	5/10/86/115	-
25	CLA	A	769	1	-	15/39/115/115	-
25	CLA	h	609	14	-	8/21/97/115	-
25	CLA	g	612	21	-	4/12/88/115	-
25	CLA	i	603	15	-	8/13/89/115	-
25	CLA	d	602	12	-	5/30/106/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	k	603	17	-	5/12/88/115	-
25	CLA	e	613	13	-	4/27/103/115	-
27	LHG	g	189	25	-	25/39/39/53	-
25	CLA	j	609	16	-	5/21/97/115	-
25	CLA	o	613	23	-	8/12/88/115	-
25	CLA	A	782	1	-	4/19/95/115	-
25	CLA	d	610	12	-	14/32/108/115	-
25	CLA	m	609	19	-	4/21/97/115	-
31	DD6	h	621	-	-	0/26/80/80	0/3/3/3
25	CLA	A	779	1	-	7/13/89/115	-
25	CLA	B	775	2	-	8/21/97/115	-
25	CLA	A	759	1	-	11/33/109/115	-
25	CLA	j	612	16	-	11/27/103/115	-
25	CLA	m	610	19	-	6/12/88/115	-
25	CLA	g	609	21	-	5/21/97/115	-
25	CLA	i	604	-	-	3/13/89/115	-
25	CLA	o	610	23	-	2/10/86/115	-
25	CLA	m	608	-	-	2/12/88/115	-
25	CLA	B	747	2	-	5/19/95/115	-
25	CLA	A	771	1	-	10/30/106/115	-
31	DD6	c	623	-	-	8/26/80/80	0/3/3/3
25	CLA	c	611	27	-	1/13/89/115	-
25	CLA	n	605	22	-	6/12/88/115	-
25	CLA	k	601	17	-	3/13/89/115	-
31	DD6	c	620	-	-	4/26/80/80	0/3/3/3
25	CLA	g	602	21	-	16/25/101/115	-
25	CLA	g	608	-	-	7/15/91/115	-
25	CLA	a	602	9	-	17/33/109/115	-
25	CLA	e	604	-	-	4/21/97/115	-
25	CLA	j	614	16	-	3/12/88/115	-
28	PQN	B	769	-	-	5/16/36/43	0/2/2/2
25	CLA	B	781	2	-	11/39/115/115	-
25	CLA	k	618	17	-	3/21/97/115	-
25	CLA	k	609	17	-	2/21/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	f	615	20	-	9/13/89/115	-
25	CLA	A	778	1	-	3/13/89/115	-
31	DD6	A	4002	-	-	3/26/80/80	0/3/3/3
25	CLA	e	607	-	-	7/13/89/115	-
25	CLA	h	612	14	-	8/31/107/115	-
25	CLA	A	808	27	-	12/25/101/115	-
29	BCR	M	201	-	-	6/29/63/63	0/2/2/2
25	CLA	c	610	11	-	13/27/103/115	-
25	CLA	d	604	-	-	7/24/100/115	-
25	CLA	B	741	2	-	15/39/115/115	-
25	CLA	c	619	12	-	5/10/86/115	-
25	CLA	n	610	22	-	3/10/86/115	-
27	LHG	A	756	25	-	19/42/42/53	-
25	CLA	p	603	24	-	4/12/88/115	-
25	CLA	B	752	2	-	13/39/115/115	-
25	CLA	c	604	-	-	6/19/95/115	-
25	CLA	A	757	1	-	7/15/91/115	-
25	CLA	l	611	-	-	3/13/89/115	-
25	CLA	B	773	2	-	6/35/111/115	-
33	LMG	a	182	-	-	18/38/58/70	0/1/1/1
25	CLA	n	612	22	-	4/12/88/115	-
25	CLA	l	601	18	-	4/12/88/115	-
25	CLA	b	612	10	-	11/24/100/115	-
25	CLA	a	608	-	-	13/25/101/115	-
25	CLA	a	603	9	-	8/25/101/115	-
35	CHL	d	607	-	-	4/14/90/117	-
25	CLA	B	783	2	-	3/21/97/115	-
28	PQN	d	223	-	-	5/15/35/43	0/2/2/2
25	CLA	c	602	11	-	14/32/108/115	-
31	DD6	e	621	-	-	5/26/80/80	0/3/3/3
25	CLA	d	603	12	-	5/12/88/115	-
25	CLA	i	608	-	-	13/39/115/115	-
31	DD6	e	620	-	-	9/26/80/80	0/3/3/3
25	CLA	A	760	1	-	23/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	n	608	-	-	2/10/86/115	-
25	CLA	B	770	-	-	8/25/101/115	-
25	CLA	o	604	-	-	3/12/88/115	-
25	CLA	p	612	24	-	5/13/89/115	-
25	CLA	h	603	14	-	5/13/89/115	-
31	DD6	m	620	-	-	5/26/80/80	0/3/3/3
25	CLA	f	601	20	-	7/12/88/115	-
25	CLA	g	604	-	-	5/13/89/115	-
25	CLA	k	604	17	-	20/39/115/115	-
25	CLA	B	768	2	-	6/27/103/115	-
25	CLA	f	613	20	-	14/32/108/115	-
25	CLA	A	772	-	-	13/37/113/115	-
25	CLA	n	604	-	-	8/19/95/115	-
25	CLA	A	793	-	-	0/12/88/115	-
30	SQD	g	190	-	-	13/27/47/69	0/1/1/1
25	CLA	a	601	9	-	6/21/97/115	-
25	CLA	l	610	18	-	14/26/102/115	-
25	CLA	A	763	1	-	16/39/115/115	-
25	CLA	f	609	20	-	4/12/88/115	-
25	CLA	B	750	-	-	10/33/109/115	-
31	DD6	d	620	-	-	2/26/80/80	0/3/3/3
25	CLA	B	778	2	-	14/37/113/115	-
25	CLA	B	776	2	-	10/32/108/115	-
31	DD6	d	621	-	-	3/26/80/80	0/3/3/3
25	CLA	j	613	16	-	10/36/112/115	-
25	CLA	A	761	1	-	14/39/115/115	-
25	CLA	A	803	1	-	8/23/99/115	-
25	CLA	a	609	9	-	5/21/97/115	-
25	CLA	f	608	20	-	2/12/88/115	-
25	CLA	i	612	15	-	5/13/89/115	-
25	CLA	A	773	-	-	8/25/101/115	-
25	CLA	a	613	9	-	14/27/103/115	-
25	CLA	B	780	-	-	7/25/101/115	-
25	CLA	c	603	11	-	6/25/101/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	i	609	15	-	4/13/89/115	-
25	CLA	h	611	27	-	5/13/89/115	-
25	CLA	o	608	-	-	5/13/89/115	-
25	CLA	j	602	16	-	4/27/103/115	-
31	DD6	b	620	-	-	5/26/80/80	0/3/3/3
25	CLA	c	601	11	-	6/12/88/115	-
26	LMT	A	754	-	-	7/21/61/61	0/2/2/2
31	DD6	l	621	-	-	3/26/80/80	0/3/3/3
25	CLA	B	746	2	-	13/38/114/115	-
31	DD6	e	623	-	-	15/26/80/80	0/3/3/3
25	CLA	k	615	17	-	5/12/88/115	-
25	CLA	d	601	12	-	6/21/97/115	-
25	CLA	p	609	24	-	10/21/97/115	-
25	CLA	l	608	-	-	6/13/89/115	-
25	CLA	o	602	23	-	10/18/94/115	-
25	CLA	A	766	1	-	18/31/107/115	-
29	BCR	B	762	-	-	7/29/63/63	0/2/2/2
31	DD6	p	621	-	-	3/26/80/80	0/3/3/3
25	CLA	g	618	21	-	4/15/91/115	-
25	CLA	i	614	15	-	3/12/88/115	-
25	CLA	A	784	1	-	15/39/115/115	-
25	CLA	m	612	19	-	3/13/89/115	-
31	DD6	c	621	-	-	0/26/80/80	0/3/3/3
25	CLA	p	608	-	-	6/12/88/115	-
25	CLA	d	609	12	-	5/20/96/115	-
33	LMG	k	179	-	-	16/31/51/70	0/1/1/1
25	CLA	A	774	1	-	16/38/114/115	-
31	DD6	n	620	-	-	5/26/80/80	0/3/3/3
27	LHG	d	237	25	-	14/33/33/53	-
25	CLA	A	776	1	-	8/39/115/115	-
25	CLA	B	742	2	-	3/13/89/115	-
25	CLA	A	805	1	-	8/27/103/115	-
25	CLA	b	610	10	-	4/12/88/115	-
29	BCR	A	796	-	-	9/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	B	755	2	-	17/33/109/115	-
25	CLA	B	772	2	-	12/21/97/115	-
25	CLA	b	605	-	-	6/15/91/115	-
25	CLA	A	770	-	-	12/39/115/115	-
25	CLA	e	602	13	-	20/39/115/115	-
25	CLA	o	601	23	-	2/10/86/115	-
25	CLA	a	604	-	-	7/15/91/115	-
25	CLA	j	610	16	-	20/38/114/115	-
25	CLA	A	802	1	-	6/13/89/115	-
25	CLA	m	602	19	-	16/33/109/115	-
25	CLA	d	614	12	-	4/12/88/115	-
31	DD6	c	624	-	-	15/26/80/80	0/3/3/3
27	LHG	h	189	-	-	14/33/33/53	-
25	CLA	A	783	1	-	12/39/115/115	-
25	CLA	g	611	27	-	3/12/88/115	-
32	SF4	B	735	2,1	-	-	0/6/5/5
31	DD6	f	620	-	-	5/26/80/80	0/3/3/3
25	CLA	b	602	10	-	11/25/101/115	-
25	CLA	b	611	-	-	4/12/88/115	-
25	CLA	B	738	2	-	18/39/115/115	-
32	SF4	C	83	3	-	-	0/6/5/5
25	CLA	f	603	20	-	1/13/89/115	-
31	DD6	F	4002	-	-	18/26/80/80	0/3/3/3
30	SQD	j	200	-	-	12/31/51/69	0/1/1/1
31	DD6	d	623	-	-	4/26/80/80	0/3/3/3
25	CLA	i	613	15	-	10/32/108/115	-
25	CLA	k	613	17	-	10/24/100/115	-
25	CLA	A	806	1	-	2/15/91/115	-
29	BCR	B	765	-	-	11/29/63/63	0/2/2/2
25	CLA	h	610	14	-	10/26/102/115	-
25	CLA	o	609	23	-	5/15/91/115	-
27	LHG	b	181	-	-	24/35/35/53	-
25	CLA	b	601	-	-	4/12/88/115	-
25	CLA	b	613	10	-	5/12/88/115	-
33	LMG	B	786	-	-	19/47/67/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	f	614	20	-	6/12/88/115	-
25	CLA	l	614	18	-	5/12/88/115	-
25	CLA	B	785	6	-	9/15/91/115	-
25	CLA	n	602	22	-	14/32/108/115	-
25	CLA	l	603	18	-	2/13/89/115	-
31	DD6	f	621	-	-	7/26/80/80	0/3/3/3
25	CLA	i	610	15	-	12/27/103/115	-
27	LHG	i	194	25	-	19/40/40/53	-
31	DD6	i	625	-	-	1/26/80/80	0/3/3/3
25	CLA	m	613	19	-	5/12/88/115	-
31	DD6	j	620	-	-	4/26/80/80	0/3/3/3
25	CLA	B	743	2	-	4/12/88/115	-
25	CLA	A	801	1	-	18/39/115/115	-
25	CLA	h	604	-	-	8/33/109/115	-
25	CLA	B	745	2	-	19/37/113/115	-
25	CLA	k	611	-	-	5/12/88/115	-
29	BCR	A	789	-	-	5/29/63/63	0/2/2/2
25	CLA	A	804	1	-	10/21/97/115	-
28	PQN	A	785	-	-	8/23/43/43	0/2/2/2
25	CLA	c	606	-	-	4/13/89/115	-
25	CLA	j	603	16	-	2/12/88/115	-
27	LHG	j	198	25	-	24/41/41/53	-
25	CLA	p	601	-	-	3/12/88/115	-
35	CHL	d	605	12	-	8/23/99/117	-
25	CLA	B	779	2	-	15/39/115/115	-
25	CLA	A	775	1	-	16/31/107/115	-
25	CLA	j	611	27	-	8/21/97/115	-
31	DD6	g	621	-	-	4/26/80/80	0/3/3/3
25	CLA	A	767	1	-	6/13/89/115	-
29	BCR	B	763	-	-	2/29/63/63	0/2/2/2
25	CLA	e	603	13	-	5/15/91/115	-
25	CLA	h	615	14	-	6/12/88/115	-
25	CLA	o	612	23	-	4/13/85/115	-
25	CLA	A	794	-	-	8/30/106/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	e	611	-	-	3/12/88/115	-
25	CLA	p	613	24	-	5/13/89/115	-
25	CLA	A	800	-	-	5/19/95/115	-
25	CLA	B	753	2	-	15/39/115/115	-
25	CLA	f	602	20	-	14/32/108/115	-
25	CLA	a	612	9	-	5/13/89/115	-
27	LHG	a	181	25	-	9/30/30/53	-
25	CLA	l	612	18	-	6/13/89/115	-
25	CLA	B	744	2	-	3/13/89/115	-
31	DD6	i	620	-	-	2/26/80/80	0/3/3/3
31	DD6	o	620	-	-	5/26/80/80	0/3/3/3
28	PQN	B	761	-	-	7/23/43/43	0/2/2/2
25	CLA	J	101	7	-	14/21/97/115	-
25	CLA	l	609	18	-	13/33/109/115	-
25	CLA	p	604	-	-	5/13/89/115	-
27	LHG	A	786	-	-	22/53/53/53	-
31	DD6	m	621	-	-	6/26/80/80	0/3/3/3
34	DGD	B	787	-	-	19/43/83/95	0/2/2/2
35	CHL	c	607	-	-	6/21/97/117	-
25	CLA	h	613	14	-	10/25/101/115	-
25	CLA	c	614	11	-	6/12/88/115	-
25	CLA	B	740	2	-	2/12/88/115	-
25	CLA	l	602	18	-	12/32/108/115	-
29	BCR	B	767	-	-	5/29/63/63	0/2/2/2
25	CLA	o	603	23	-	6/13/89/115	-
25	CLA	o	614	23	-	5/13/89/115	-
25	CLA	j	601	16	-	8/21/97/115	-
25	CLA	l	604	-	-	4/13/89/115	-
25	CLA	b	603	10	-	6/13/89/115	-
25	CLA	B	737	-	-	9/27/103/115	-
31	DD6	a	621	-	-	0/26/80/80	0/3/3/3
25	CLA	b	604	-	-	5/15/91/115	-
25	CLA	n	613	22	-	4/12/88/115	-
25	CLA	h	601	14	-	9/21/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	g	615	21	-	0/12/88/115	-
35	CHL	e	606	-	-	10/17/93/117	-
31	DD6	k	620	-	-	2/26/80/80	0/3/3/3
25	CLA	d	613	12	-	4/12/88/115	-
25	CLA	m	601	19	-	5/12/88/115	-
31	DD6	j	621	-	-	3/26/80/80	0/3/3/3
27	LHG	h	190	25	-	11/35/35/53	-
25	CLA	c	608	-	-	11/21/97/115	-
34	DGD	b	182	-	-	18/37/77/95	0/2/2/2
25	CLA	n	603	22	-	14/27/103/115	-
25	CLA	i	602	15	-	11/38/114/115	-
31	DD6	b	621	-	-	1/26/80/80	0/3/3/3
25	CLA	A	762	1	-	2/21/97/115	-
35	CHL	d	606	-	-	8/17/93/117	-
25	CLA	A	780	1	-	14/31/107/115	-
25	CLA	h	608	-	-	7/19/95/115	-
25	CLA	A	799	1	-	17/33/109/115	-
25	CLA	f	610	20	-	15/27/103/115	-
30	SQD	c	245	-	-	21/34/54/69	0/1/1/1
25	CLA	n	606	-	-	6/12/88/115	-
25	CLA	n	607	-	-	3/12/88/115	-
25	CLA	j	604	-	-	11/30/106/115	-
25	CLA	d	612	12	-	3/12/88/115	-
25	CLA	A	791	-	-	12/37/113/115	-
25	CLA	f	604	-	-	5/12/88/115	-
25	CLA	A	765	1	-	10/32/108/115	-
25	CLA	e	612	13	-	2/13/89/115	-
25	CLA	A	753	-	-	10/37/113/115	-
25	CLA	A	764	1	-	11/31/107/115	-
25	CLA	k	612	17	-	2/13/89/115	-
25	CLA	g	601	21	-	6/12/88/115	-
25	CLA	B	759	-	-	5/13/89/115	-
25	CLA	c	612	11	-	4/13/89/115	-
25	CLA	A	758	-	-	10/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	B	760	2	-	4/13/89/115	-
27	LHG	c	243	25	-	11/34/34/53	-
25	CLA	i	615	15	-	4/21/97/115	-
33	LMG	i	195	-	-	11/39/59/70	0/1/1/1
31	DD6	l	620	-	-	2/26/80/80	0/3/3/3
25	CLA	B	736	2	-	10/39/115/115	-
25	CLA	i	611	27	-	4/13/89/115	-
25	CLA	c	609	11	-	16/33/109/115	-
25	CLA	k	602	17	-	10/25/101/115	-
31	DD6	A	4008	-	-	9/26/80/80	0/3/3/3
34	DGD	e	205	-	-	6/24/64/95	0/2/2/2
25	CLA	e	609	13	-	8/24/100/115	-
31	DD6	J	4002	-	-	2/26/80/80	0/3/3/3
25	CLA	j	608	-	-	5/18/94/115	-
25	CLA	A	781	1	-	8/24/100/115	-
25	CLA	B	758	2	-	22/39/115/115	-
31	DD6	k	621	-	-	3/26/80/80	0/3/3/3
25	CLA	l	617	-	-	6/12/88/115	-
25	CLA	k	610	17	-	14/30/106/115	-
25	CLA	B	782	2	-	6/21/97/115	-
25	CLA	k	614	17	-	4/12/88/115	-
29	BCR	A	790	-	-	12/29/63/63	0/2/2/2
25	CLA	i	601	15	-	14/25/101/115	-
31	DD6	g	620	-	-	4/26/80/80	0/3/3/3
25	CLA	e	608	-	-	6/19/95/115	-
25	CLA	m	604	-	-	5/13/89/115	-
31	DD6	o	621	-	-	3/26/80/80	0/3/3/3
29	BCR	B	764	-	-	7/29/63/63	0/2/2/2
31	DD6	n	621	-	-	13/26/80/80	0/3/3/3
25	CLA	d	611	27	-	5/15/91/115	-
25	CLA	B	751	-	-	8/21/97/115	-
25	CLA	g	613	21	-	12/27/103/115	-
25	CLA	B	771	2	-	9/25/101/115	-
29	BCR	A	787	-	-	5/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	f	611	-	-	2/12/88/115	-
31	DD6	i	621	-	-	3/26/80/80	0/3/3/3
25	CLA	A	752	1	-	18/39/115/115	-
25	CLA	e	614	13	-	4/12/88/115	-
31	DD6	h	620	-	-	3/26/80/80	0/3/3/3
25	CLA	g	610	21	-	10/27/103/115	-
25	CLA	p	602	24	-	9/13/89/115	-
25	CLA	k	608	-	-	2/21/97/115	-
32	SF4	C	82	3	-	-	0/6/5/5
25	CLA	a	611	27	-	6/15/91/115	-
25	CLA	j	615	16	-	5/13/89/115	-
25	CLA	b	609	10	-	3/15/91/115	-
25	CLA	g	603	21	-	4/12/88/115	-
35	CHL	d	608	-	-	8/17/93/117	-
25	CLA	B	754	2	-	7/13/89/115	-
25	CLA	c	616	11	-	5/18/94/115	-
25	CLA	B	739	2	-	13/39/115/115	-
25	CLA	p	610	24	-	11/15/91/115	-
25	CLA	B	748	2	-	12/32/108/115	-
25	CLA	a	610	9	-	10/26/102/115	-
25	CLA	B	774	-	-	15/33/109/115	-
25	CLA	b	608	-	-	2/10/86/115	-
25	CLA	A	768	1	-	10/29/105/115	-
25	CLA	A	755	1	-	8/33/109/115	-
25	CLA	A	807	1	-	5/19/95/115	-
25	CLA	n	609	22	-	7/15/91/115	-
25	CLA	l	613	18	-	7/19/95/115	-
25	CLA	c	613	11	-	8/25/101/115	-
25	CLA	B	749	2	-	8/20/96/115	-
25	CLA	e	605	13	-	3/12/88/115	-
25	CLA	m	603	19	-	10/26/102/115	-
25	CLA	A	777	1	-	13/39/115/115	-
25	CLA	f	612	20	-	4/12/88/115	-
29	BCR	B	766	-	-	14/29/63/63	0/2/2/2

The worst 5 of 2451 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	b	181	LHG	P-O3	6.37	1.85	1.59
27	m	182	LHG	P-O3	6.32	1.84	1.59
27	c	243	LHG	P-O3	6.28	1.84	1.59
27	d	237	LHG	P-O3	6.22	1.84	1.59
27	h	189	LHG	P-O3	6.19	1.84	1.59

The worst 5 of 3426 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	774	CLA	C4A-NA-C1A	11.56	111.90	106.71
25	k	603	CLA	C4A-NA-C1A	11.50	111.88	106.71
25	B	737	CLA	C4A-NA-C1A	11.20	111.74	106.71
25	o	612	CLA	C4A-NA-C1A	11.17	111.73	106.71
25	A	777	CLA	C4A-NA-C1A	11.10	111.70	106.71

There are no chirality outliers.

5 of 2949 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
25	A	752	CLA	CHA-CBD-CGD-O2D
25	A	753	CLA	C1-C2-C3-C4
25	A	753	CLA	C1-C2-C3-C5
25	A	757	CLA	C2B-C3B-CAB-CBB
25	A	757	CLA	C4B-C3B-CAB-CBB

There are no ring outliers.

259 monomers are involved in 540 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	j	618	CLA	1	0
25	A	798	CLA	3	0
27	m	182	LHG	2	0
25	a	619	CLA	5	0
25	B	784	CLA	2	0
25	A	797	CLA	2	0
25	B	756	CLA	4	0
25	h	602	CLA	1	0
25	e	610	CLA	4	0
25	B	777	CLA	5	0
29	A	792	BCR	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	A	788	BCR	3	0
25	B	757	CLA	2	0
25	A	769	CLA	5	0
25	h	609	CLA	2	0
25	g	612	CLA	1	0
25	i	603	CLA	2	0
25	d	602	CLA	1	0
25	k	603	CLA	1	0
25	e	613	CLA	1	0
25	j	609	CLA	2	0
25	A	782	CLA	2	0
25	d	610	CLA	4	0
25	B	775	CLA	5	0
25	m	610	CLA	3	0
25	g	609	CLA	3	0
25	i	604	CLA	1	0
25	o	610	CLA	3	0
25	m	608	CLA	1	0
25	B	747	CLA	4	0
25	A	771	CLA	2	0
25	c	611	CLA	3	0
25	g	602	CLA	3	0
25	g	608	CLA	4	0
25	a	602	CLA	7	0
25	e	604	CLA	1	0
25	B	781	CLA	9	0
25	k	618	CLA	2	0
25	k	609	CLA	1	0
25	f	615	CLA	1	0
25	h	612	CLA	2	0
25	A	808	CLA	2	0
29	M	201	BCR	2	0
25	c	610	CLA	3	0
25	d	604	CLA	2	0
25	B	741	CLA	3	0
25	n	610	CLA	1	0
27	A	756	LHG	2	0
25	p	603	CLA	4	0
25	B	752	CLA	6	0
25	A	757	CLA	1	0
25	B	773	CLA	5	0
25	n	612	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	b	612	CLA	4	0
25	a	608	CLA	3	0
25	a	603	CLA	1	0
35	d	607	CHL	2	0
25	B	783	CLA	3	0
25	c	602	CLA	2	0
25	d	603	CLA	2	0
25	i	608	CLA	2	0
25	A	760	CLA	6	0
25	n	608	CLA	3	0
25	B	770	CLA	1	0
25	p	612	CLA	1	0
25	h	603	CLA	1	0
31	m	620	DD6	1	0
25	k	604	CLA	1	0
25	f	613	CLA	3	0
25	A	772	CLA	4	0
25	n	604	CLA	2	0
25	A	793	CLA	3	0
30	g	190	SQD	2	0
25	a	601	CLA	1	0
25	l	610	CLA	4	0
25	A	763	CLA	3	0
25	B	750	CLA	4	0
25	B	778	CLA	7	0
25	B	776	CLA	4	0
25	j	613	CLA	4	0
25	A	761	CLA	3	0
25	a	609	CLA	1	0
25	f	608	CLA	1	0
25	i	612	CLA	1	0
25	A	773	CLA	3	0
25	a	613	CLA	2	0
25	B	780	CLA	2	0
25	c	603	CLA	4	0
25	i	609	CLA	1	0
25	h	611	CLA	1	0
25	o	608	CLA	1	0
25	c	601	CLA	1	0
25	B	746	CLA	3	0
25	d	601	CLA	1	0
25	p	609	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	l	608	CLA	1	0
25	o	602	CLA	2	0
25	A	766	CLA	5	0
29	B	762	BCR	2	0
25	i	614	CLA	1	0
25	A	784	CLA	7	0
25	p	608	CLA	1	0
33	k	179	LMG	3	0
25	A	774	CLA	3	0
27	d	237	LHG	3	0
25	A	776	CLA	3	0
25	B	742	CLA	1	0
25	A	805	CLA	2	0
25	b	610	CLA	2	0
29	A	796	BCR	2	0
25	B	755	CLA	2	0
25	B	772	CLA	3	0
25	b	605	CLA	1	0
25	A	770	CLA	4	0
25	e	602	CLA	4	0
25	o	601	CLA	1	0
25	a	604	CLA	1	0
25	j	610	CLA	3	0
25	m	602	CLA	5	0
25	d	614	CLA	1	0
27	h	189	LHG	1	0
25	A	783	CLA	5	0
25	b	602	CLA	1	0
25	B	738	CLA	3	0
31	d	623	DD6	1	0
25	i	613	CLA	2	0
25	k	613	CLA	2	0
29	B	765	BCR	4	0
25	h	610	CLA	9	0
25	o	609	CLA	1	0
27	b	181	LHG	3	0
25	b	601	CLA	1	0
33	B	786	LMG	5	0
25	f	614	CLA	1	0
25	l	614	CLA	3	0
25	B	785	CLA	3	0
25	n	602	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	l	603	CLA	1	0
25	i	610	CLA	3	0
27	i	194	LHG	2	0
25	m	613	CLA	1	0
25	A	801	CLA	1	0
25	h	604	CLA	2	0
25	B	745	CLA	3	0
29	A	789	BCR	1	0
25	A	804	CLA	2	0
28	A	785	PQN	5	0
25	c	606	CLA	1	0
27	j	198	LHG	4	0
35	d	605	CHL	1	0
25	B	779	CLA	2	0
25	A	775	CLA	7	0
25	j	611	CLA	2	0
25	A	767	CLA	3	0
29	B	763	BCR	2	0
25	e	603	CLA	1	0
25	h	615	CLA	2	0
25	o	612	CLA	1	0
25	A	794	CLA	3	0
25	e	611	CLA	1	0
25	p	613	CLA	1	0
25	A	800	CLA	2	0
25	B	753	CLA	6	0
25	f	602	CLA	2	0
27	a	181	LHG	1	0
25	B	744	CLA	1	0
28	B	761	PQN	2	0
25	J	101	CLA	2	0
25	l	609	CLA	3	0
27	A	786	LHG	5	0
31	m	621	DD6	1	0
34	B	787	DGD	2	0
35	c	607	CHL	3	0
25	h	613	CLA	3	0
25	c	614	CLA	1	0
25	l	602	CLA	4	0
29	B	767	BCR	3	0
25	o	614	CLA	4	0
25	j	601	CLA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	l	604	CLA	1	0
25	B	737	CLA	4	0
31	a	621	DD6	1	0
25	b	604	CLA	3	0
25	h	601	CLA	3	0
25	g	615	CLA	1	0
25	d	613	CLA	1	0
25	m	601	CLA	5	0
27	h	190	LHG	2	0
25	c	608	CLA	3	0
34	b	182	DGD	3	0
25	n	603	CLA	3	0
25	i	602	CLA	2	0
35	d	606	CHL	2	0
25	A	780	CLA	3	0
25	h	608	CLA	3	0
25	A	799	CLA	5	0
25	f	610	CLA	1	0
25	n	606	CLA	2	0
25	n	607	CLA	1	0
25	j	604	CLA	2	0
25	A	791	CLA	6	0
25	f	604	CLA	1	0
25	A	765	CLA	3	0
25	e	612	CLA	3	0
25	A	753	CLA	7	0
25	A	764	CLA	1	0
25	k	612	CLA	1	0
25	g	601	CLA	2	0
25	B	759	CLA	1	0
25	c	612	CLA	3	0
25	A	758	CLA	6	0
25	B	760	CLA	3	0
27	c	243	LHG	3	0
25	i	615	CLA	2	0
25	B	736	CLA	9	0
25	c	609	CLA	2	0
25	k	602	CLA	1	0
34	e	205	DGD	2	0
25	j	608	CLA	1	0
25	A	781	CLA	2	0
25	B	758	CLA	5	0

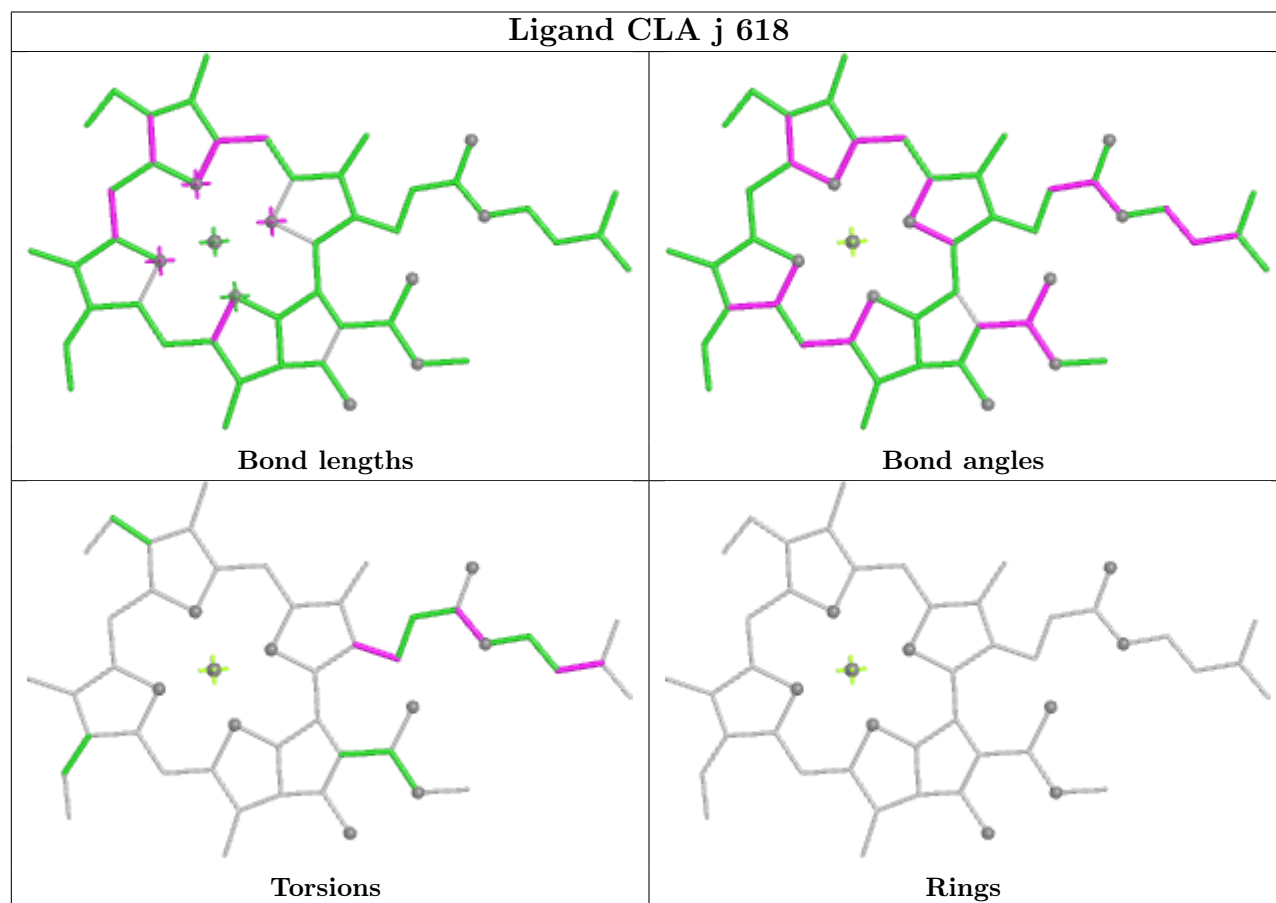
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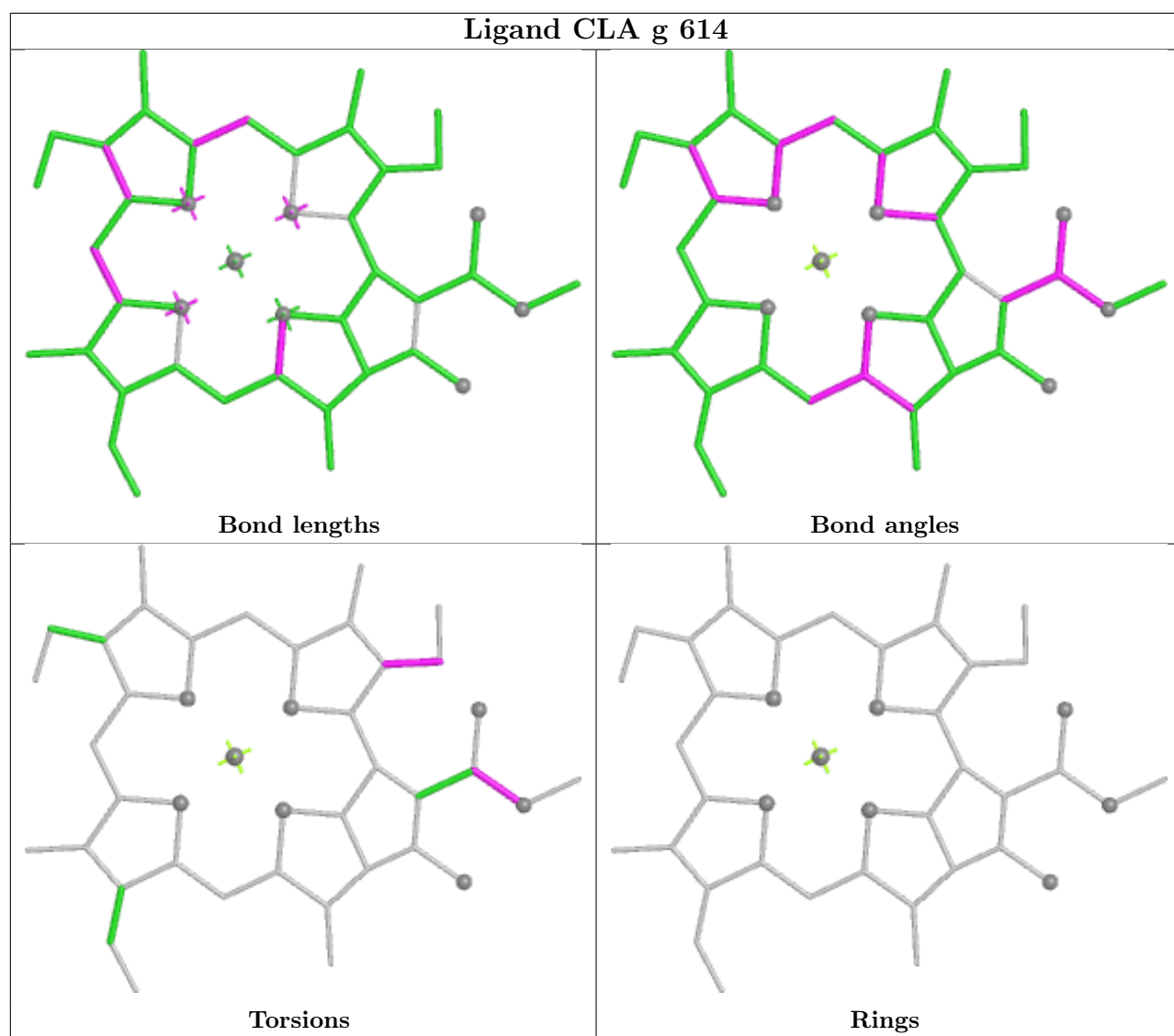
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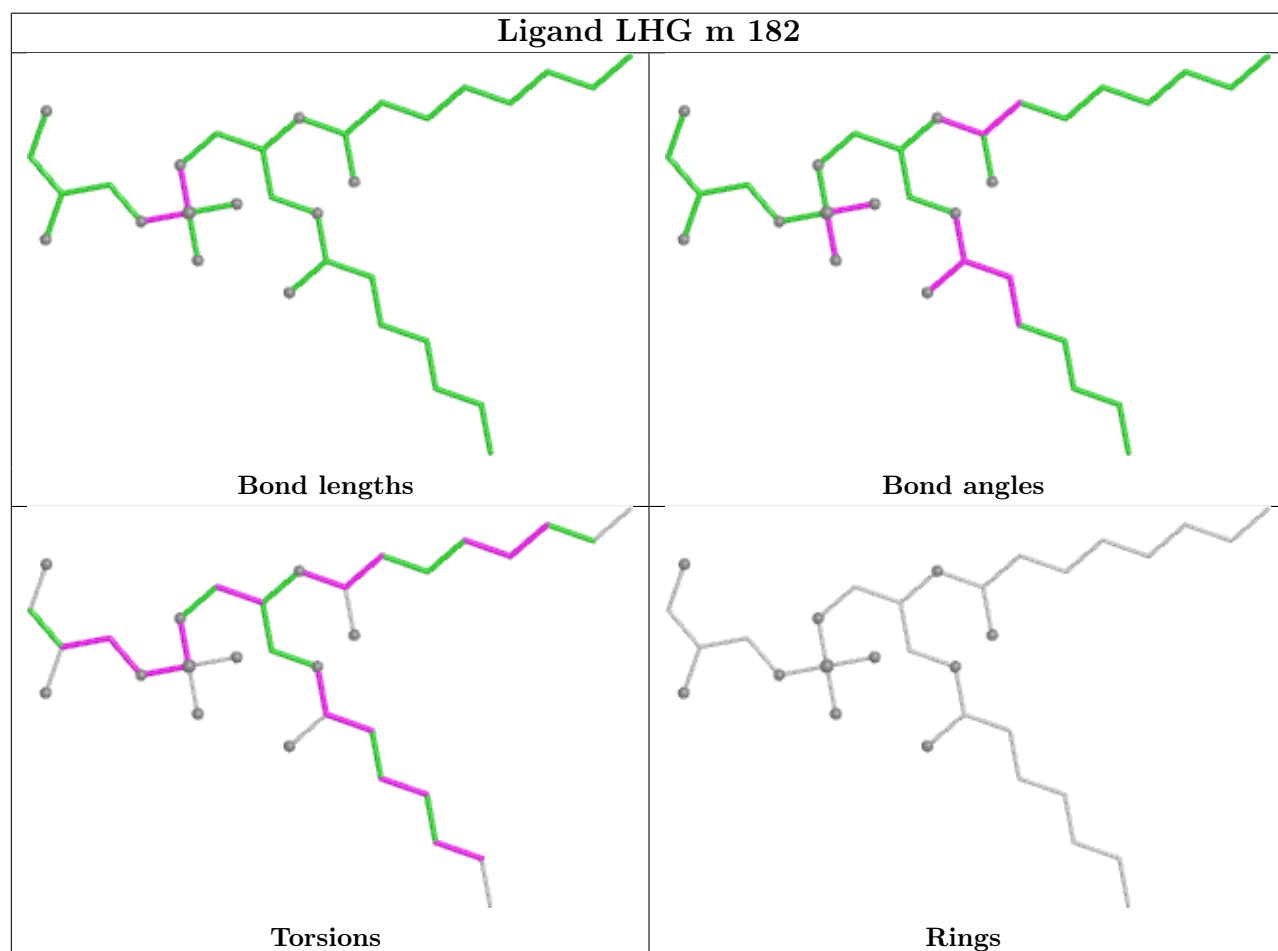
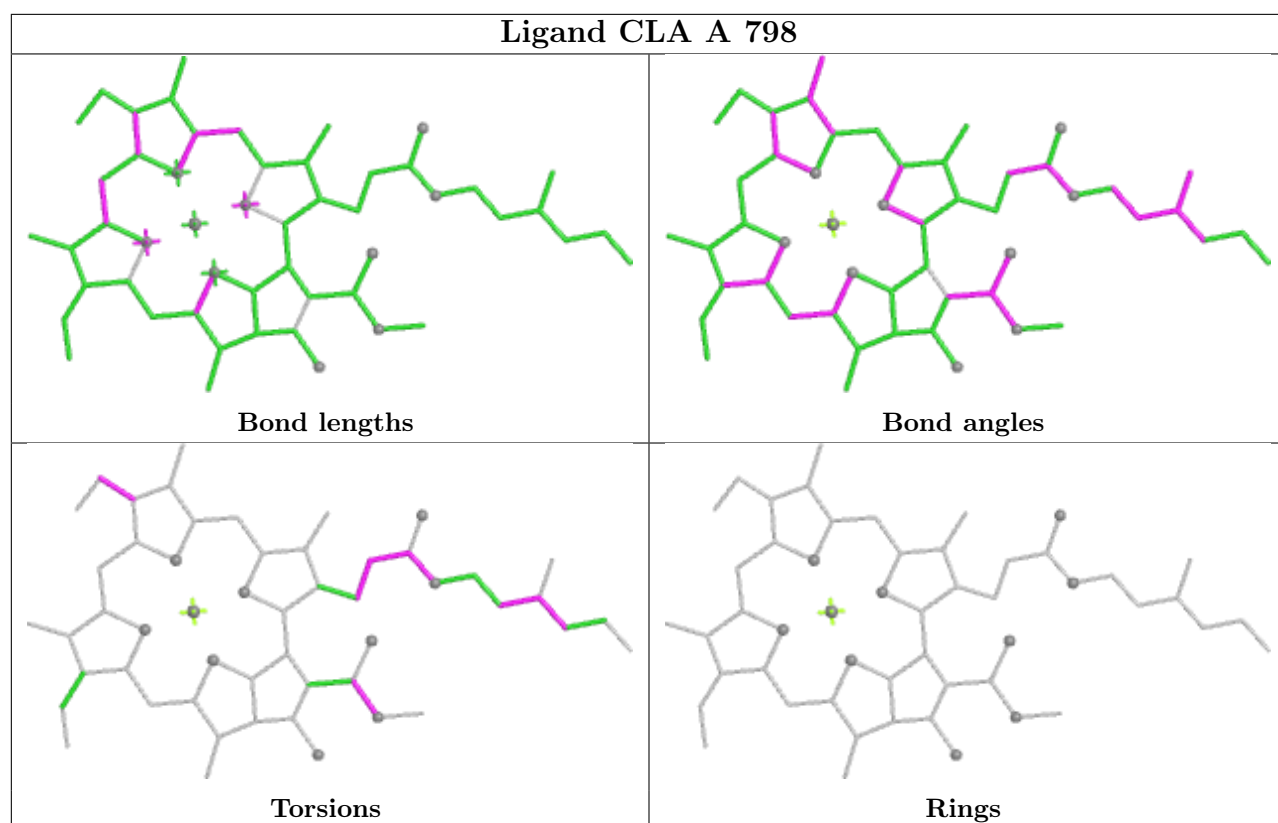
Mol	Chain	Res	Type	Clashes	Symm-Clashes
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25	k	610	CLA	4	0
25	B	782	CLA	4	0
29	A	790	BCR	2	0
25	i	601	CLA	2	0
25	e	608	CLA	3	0
29	B	764	BCR	5	0
31	n	621	DD6	1	0
25	d	611	CLA	1	0
25	B	751	CLA	4	0
25	g	613	CLA	3	0
25	B	771	CLA	3	0
29	A	787	BCR	3	0
31	i	621	DD6	1	0
25	A	752	CLA	7	0
25	g	610	CLA	7	0
25	p	602	CLA	3	0
25	k	608	CLA	3	0
25	a	611	CLA	1	0
25	b	609	CLA	2	0
25	g	603	CLA	1	0
35	d	608	CHL	2	0
25	B	739	CLA	5	0
25	p	610	CLA	1	0
25	B	748	CLA	1	0
25	a	610	CLA	3	0
25	B	774	CLA	5	0
25	b	608	CLA	1	0
25	A	768	CLA	3	0
25	A	755	CLA	2	0
25	n	609	CLA	1	0
25	l	613	CLA	1	0
25	c	613	CLA	2	0
25	B	749	CLA	1	0
25	e	605	CLA	1	0
25	m	603	CLA	1	0
25	A	777	CLA	4	0
29	B	766	BCR	8	0

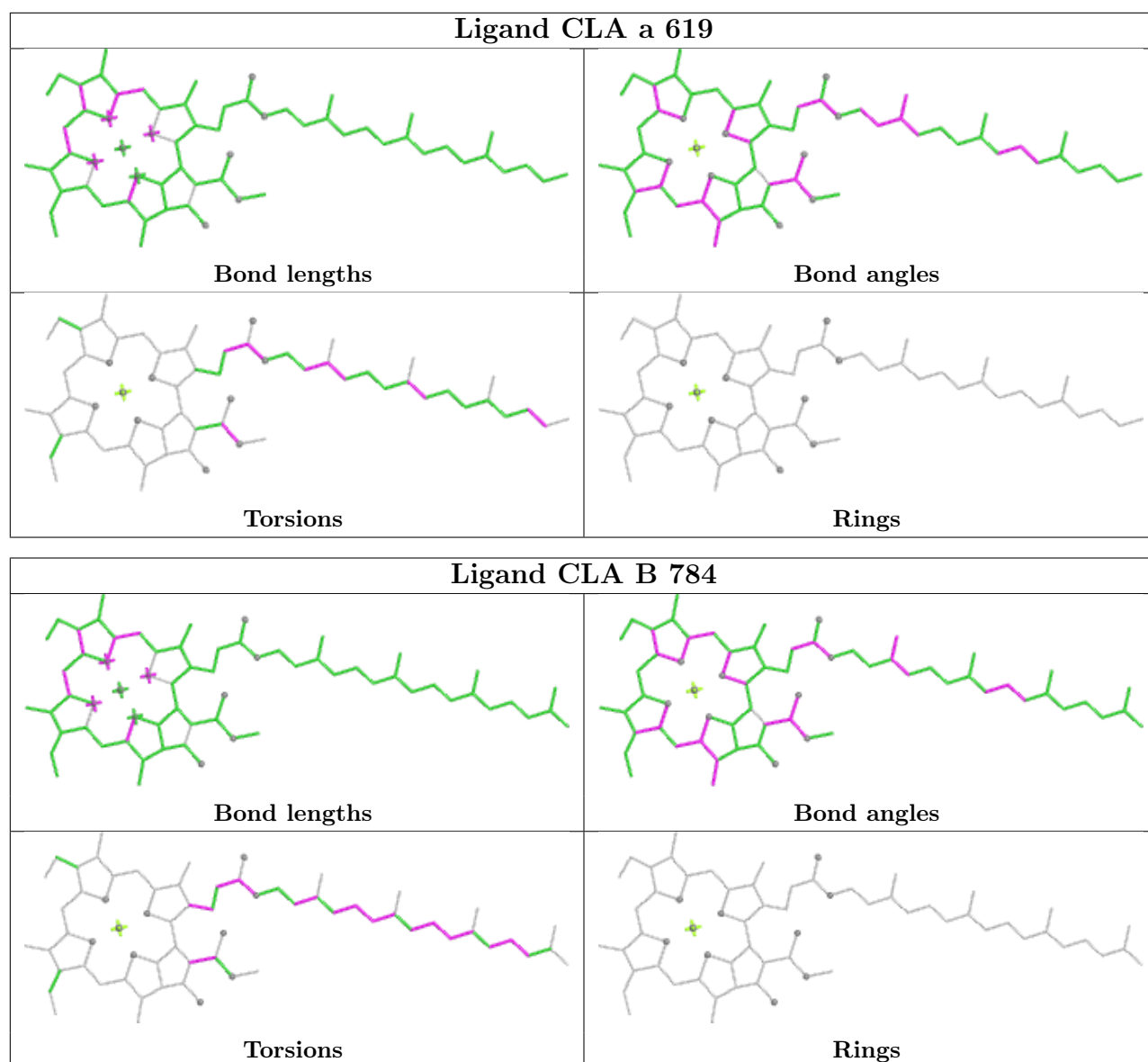
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

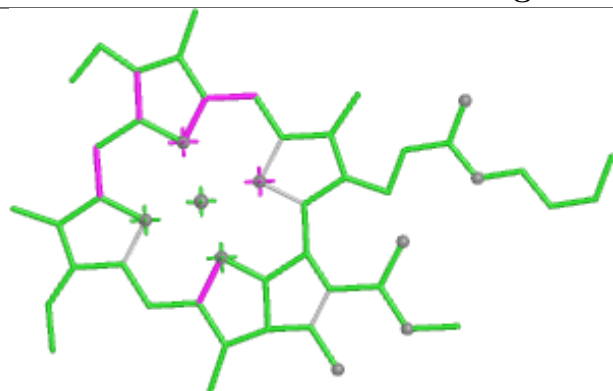




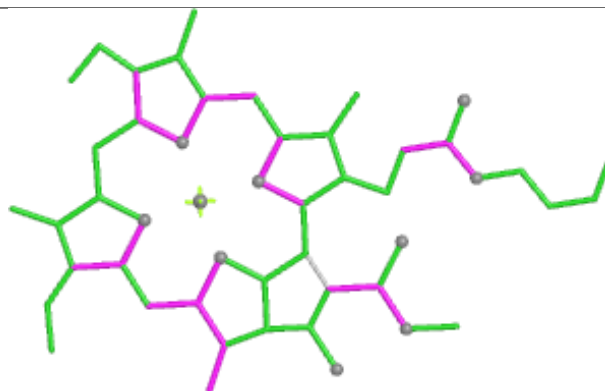




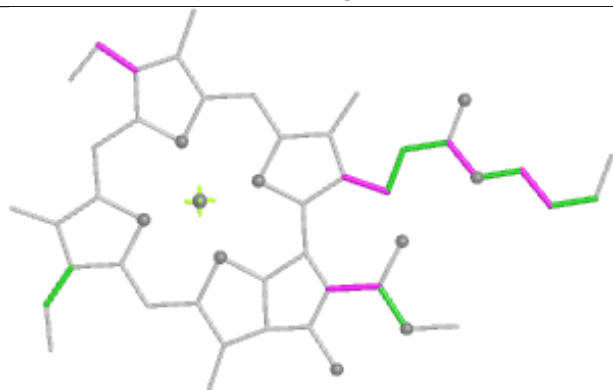
Ligand CLA A 797



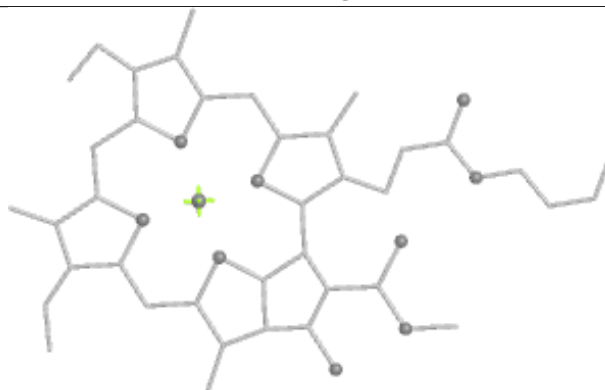
Bond lengths



Bond angles

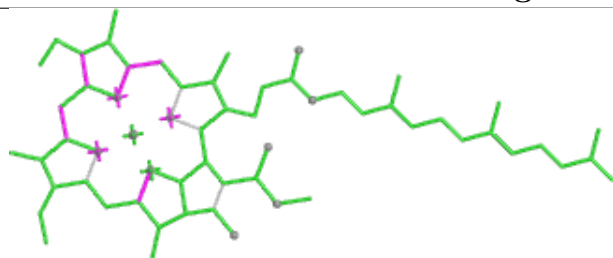


Torsions

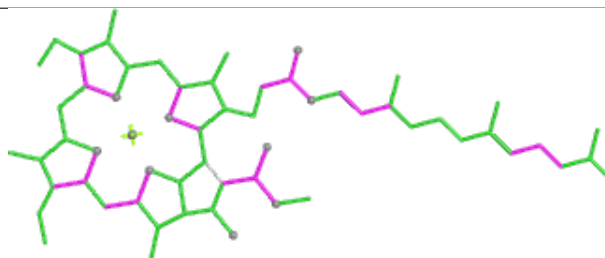


Rings

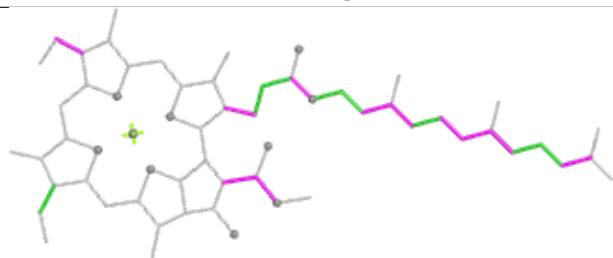
Ligand CLA B 756



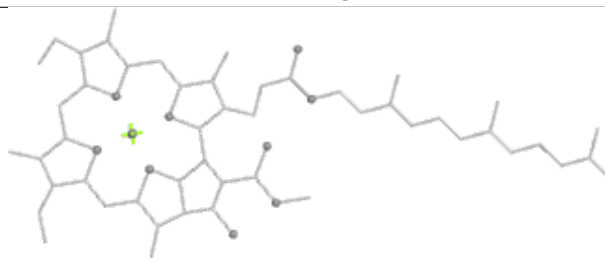
Bond lengths



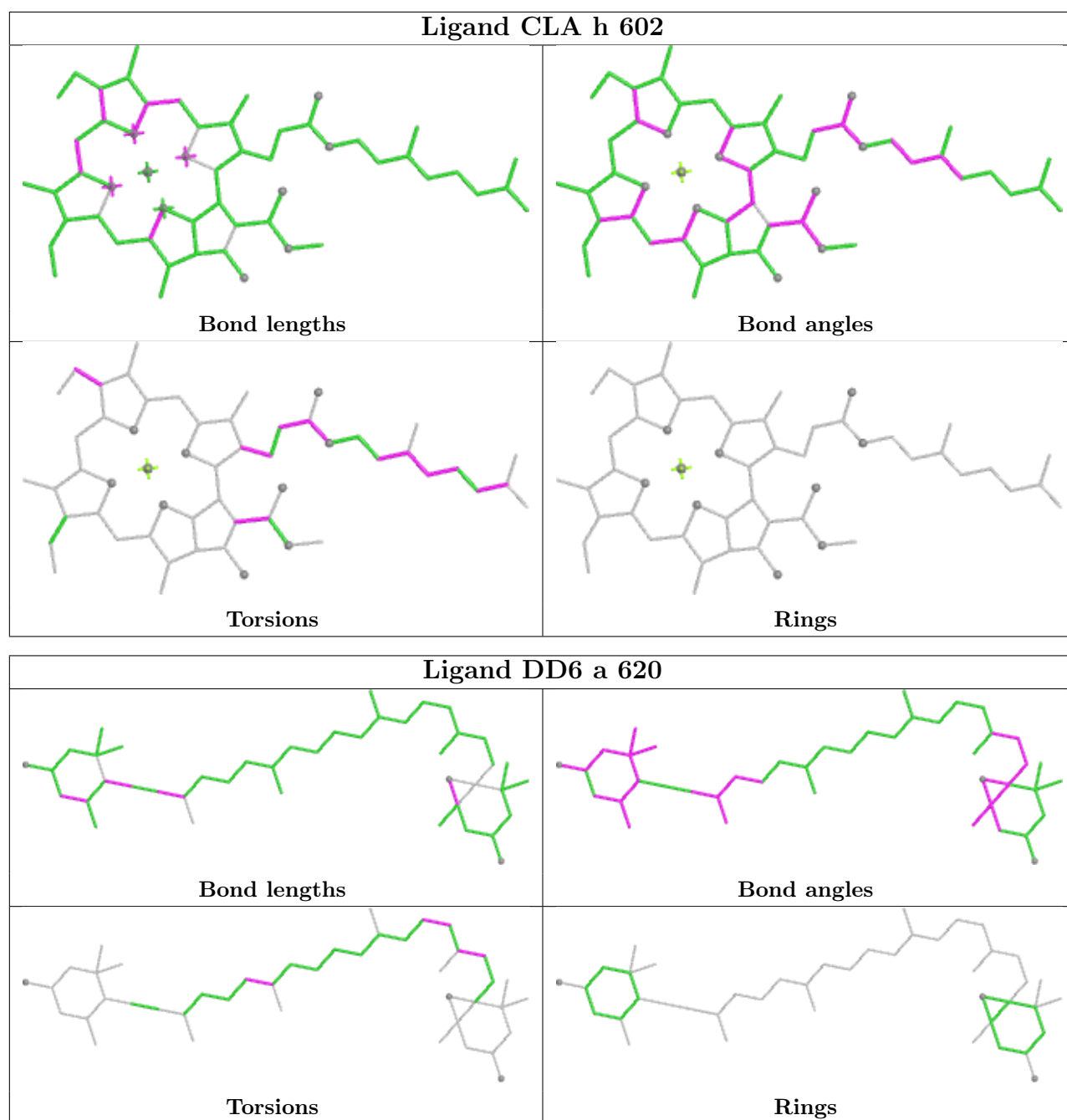
Bond angles

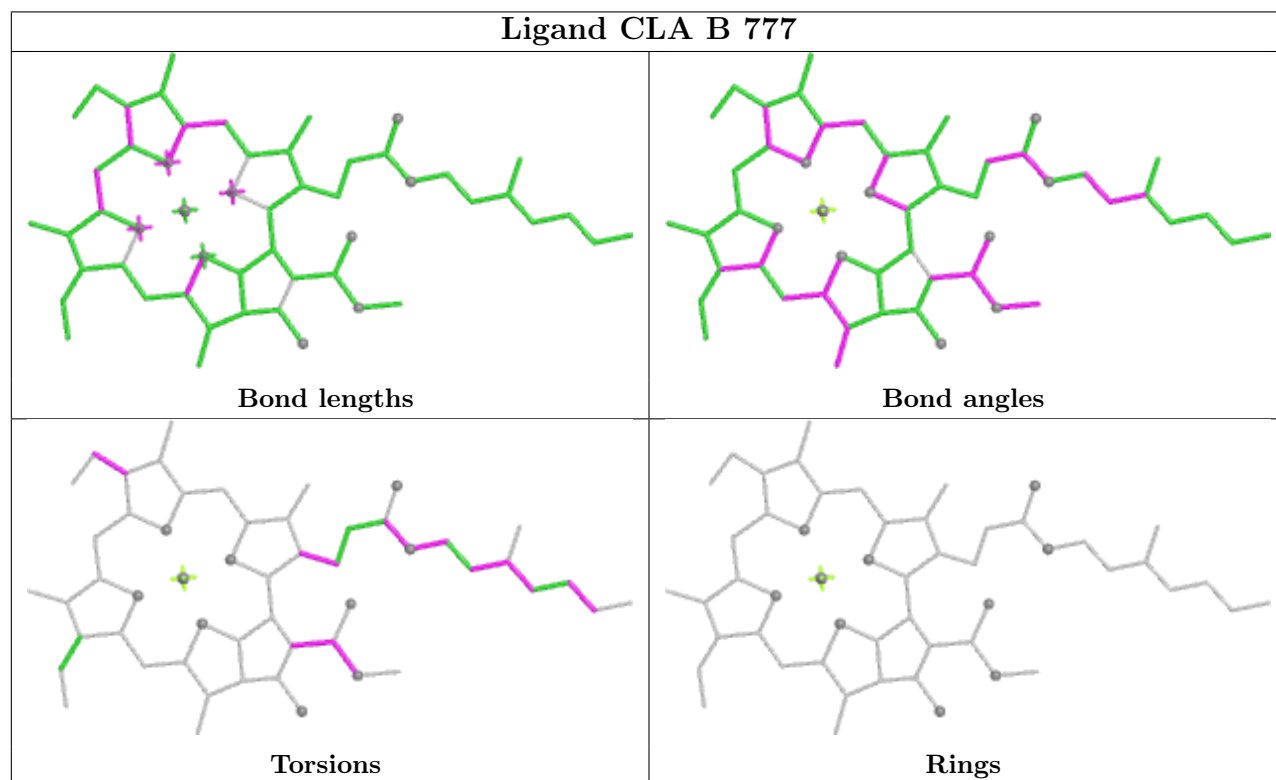
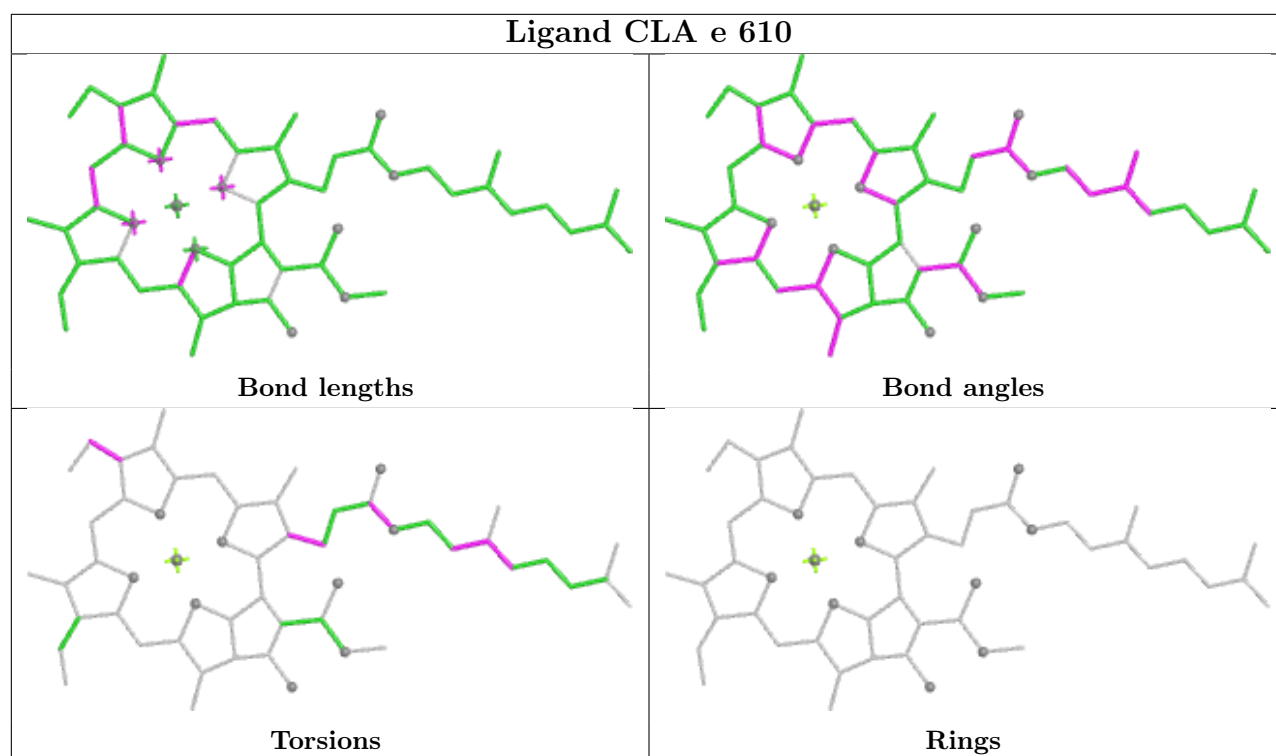


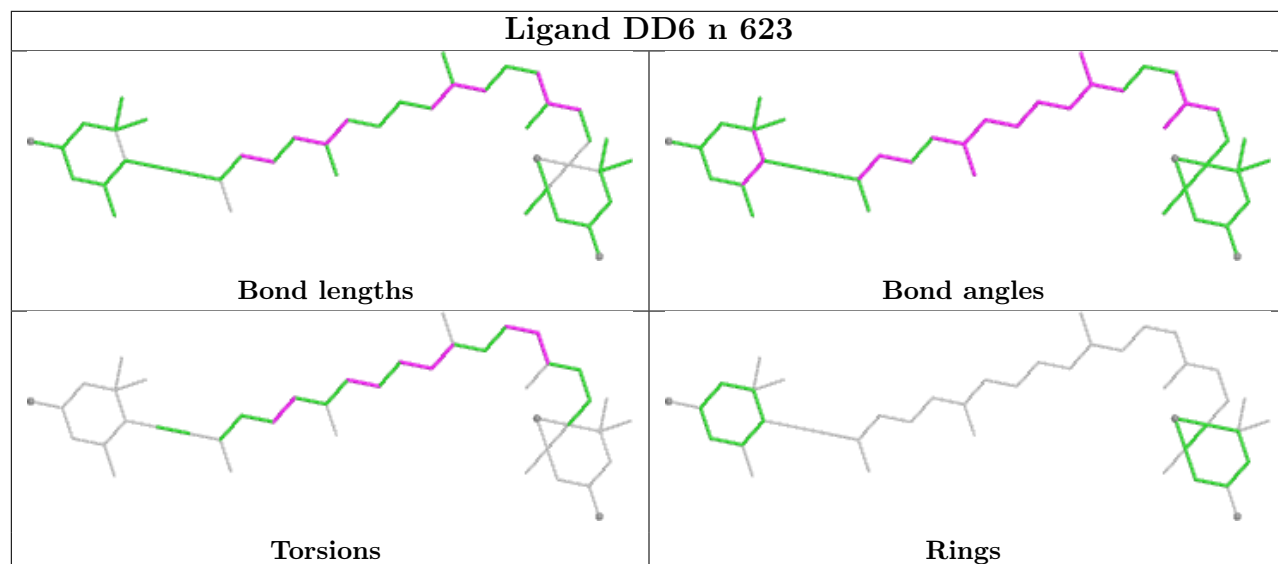
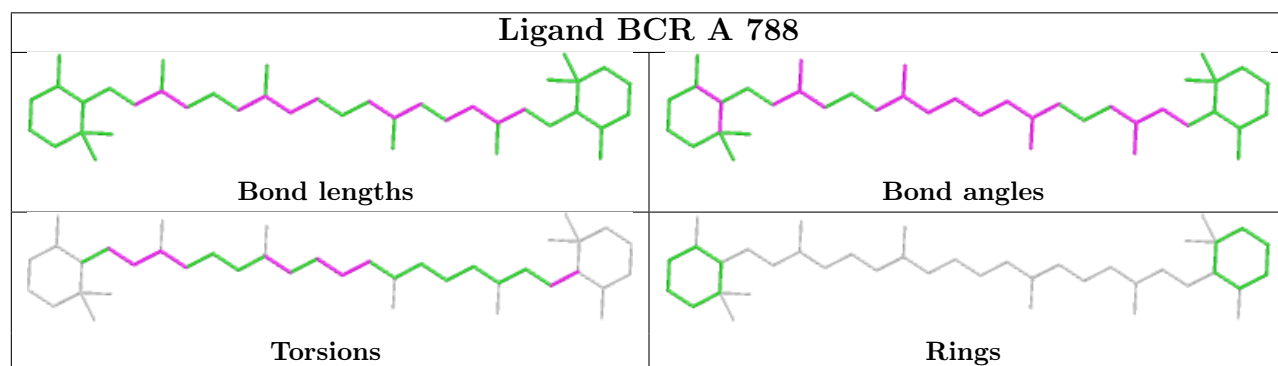
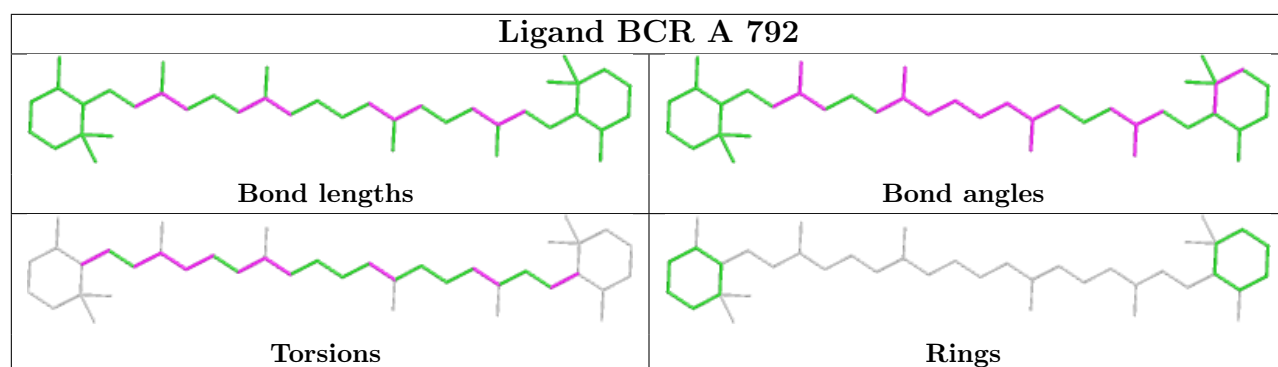
Torsions

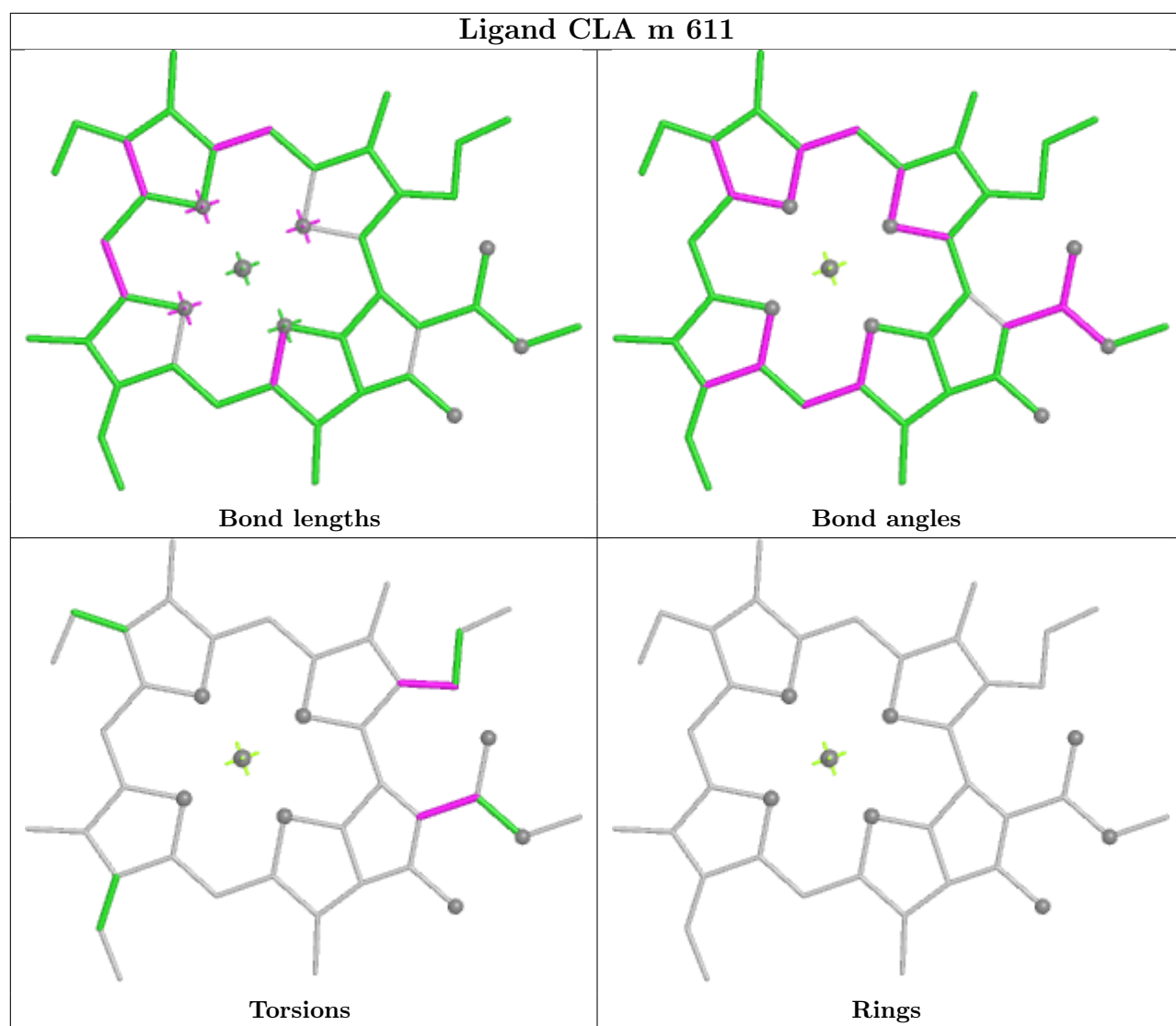


Rings

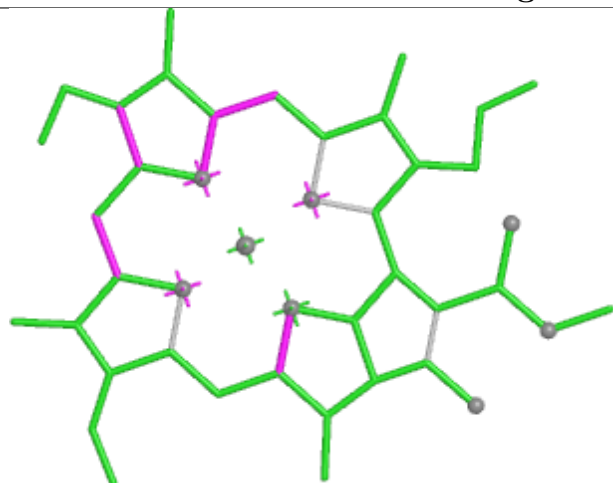




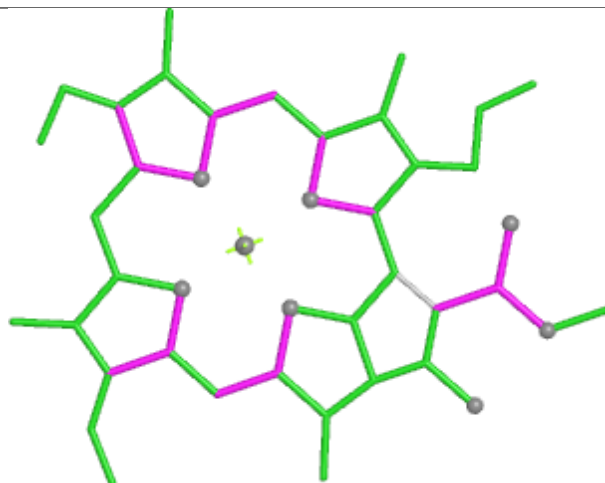




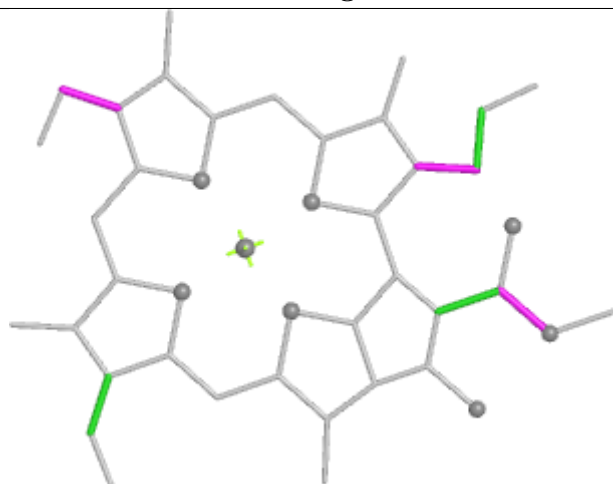
Ligand CLA h 614



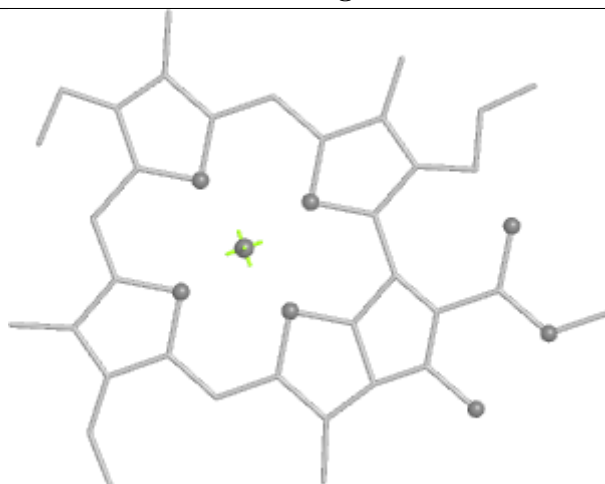
Bond lengths



Bond angles

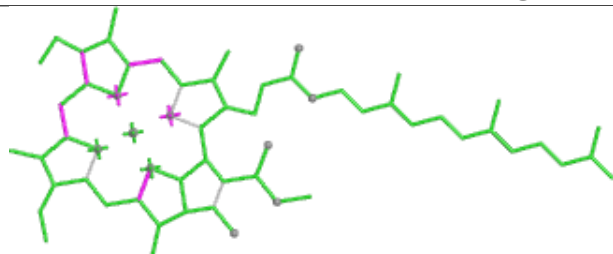


Torsions

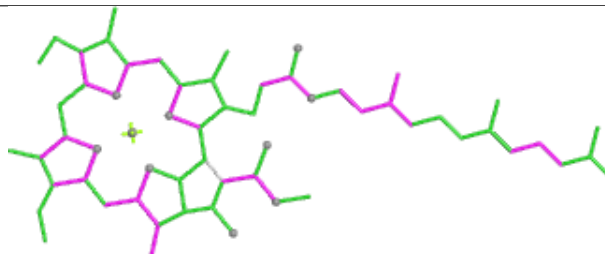


Rings

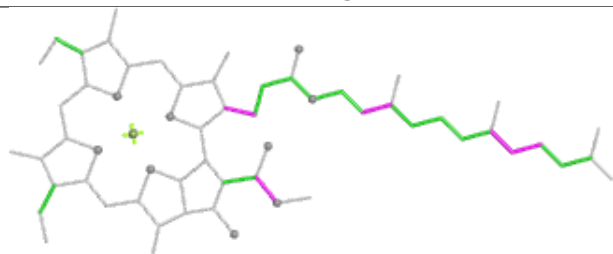
Ligand CLA B 757



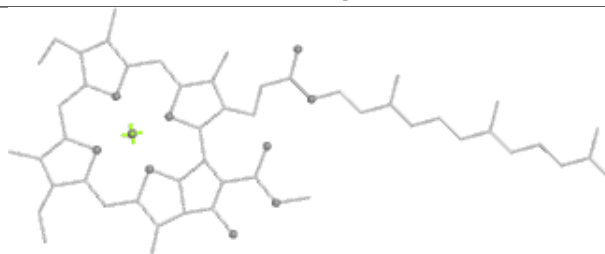
Bond lengths



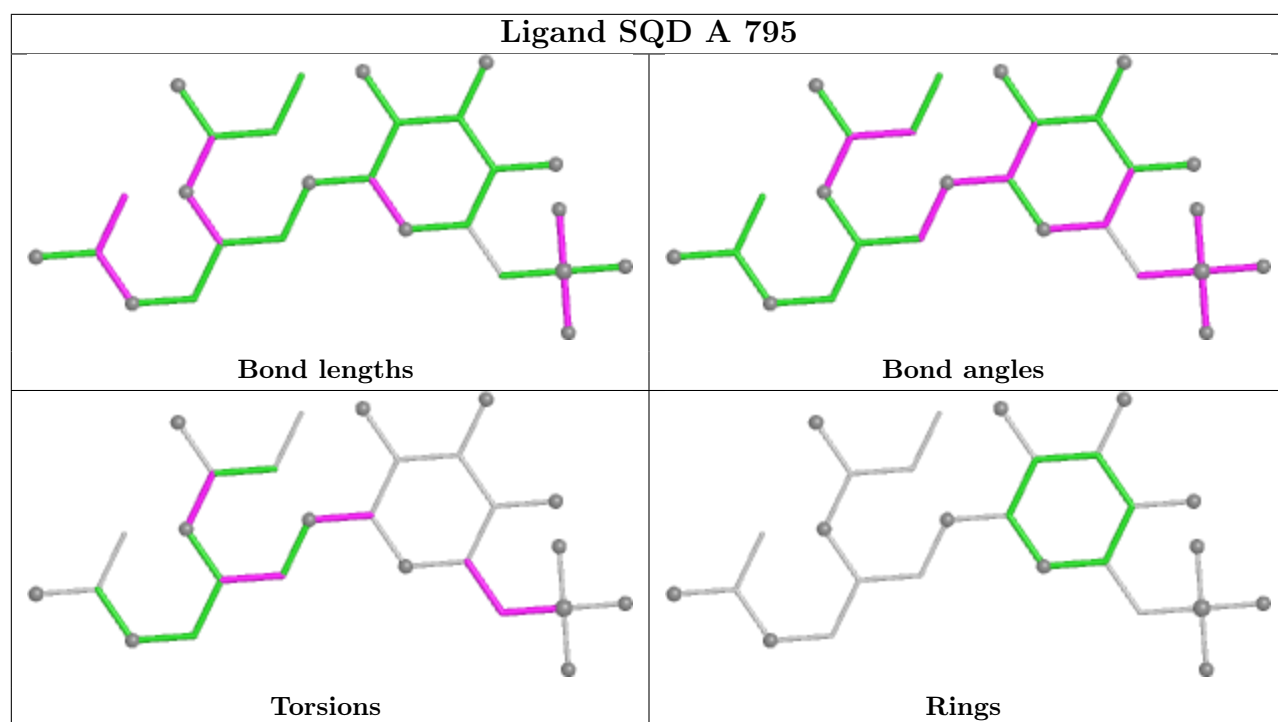
Bond angles



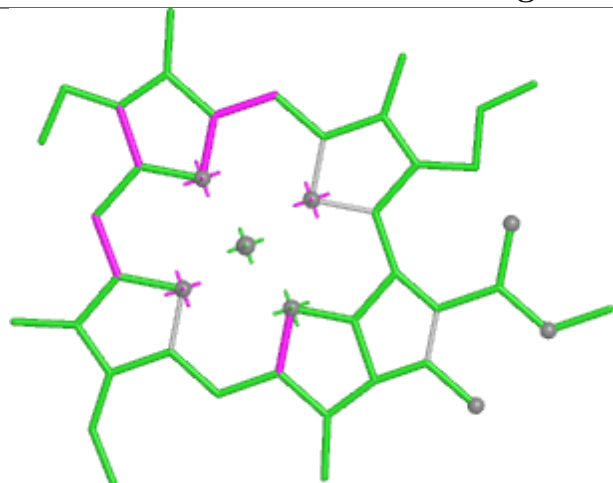
Torsions



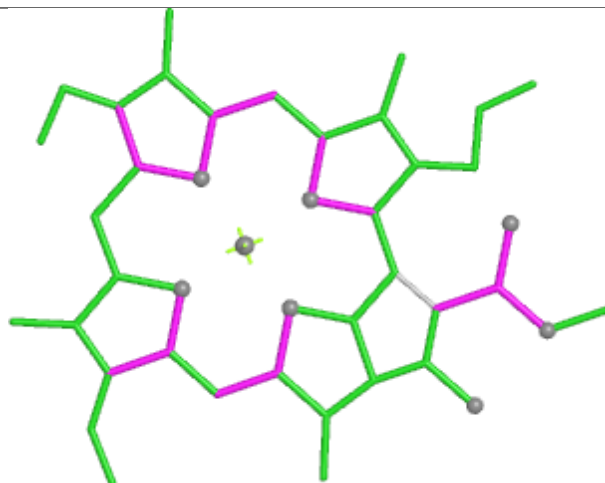
Rings



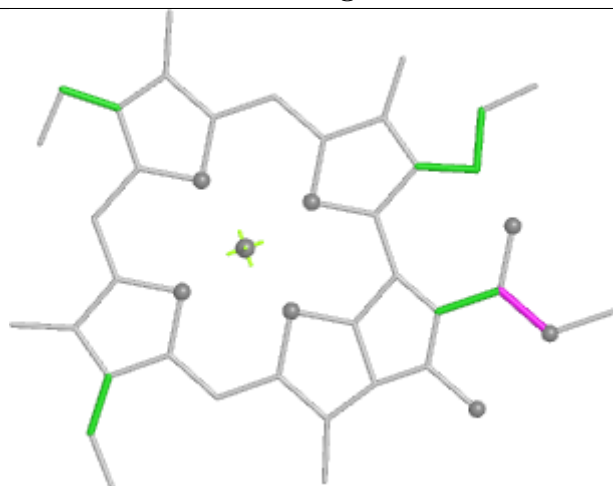
Ligand CLA h 618



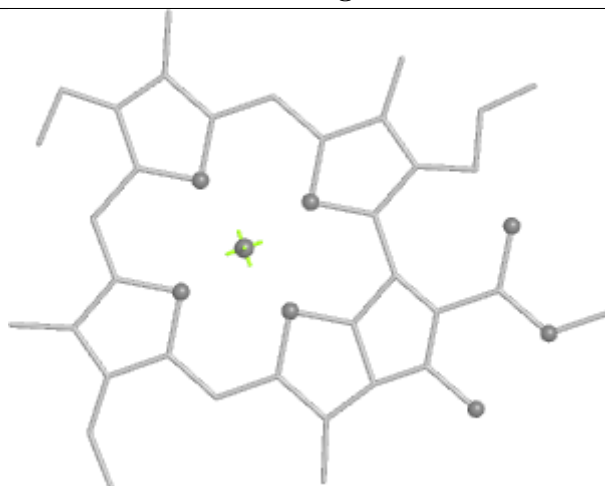
Bond lengths



Bond angles

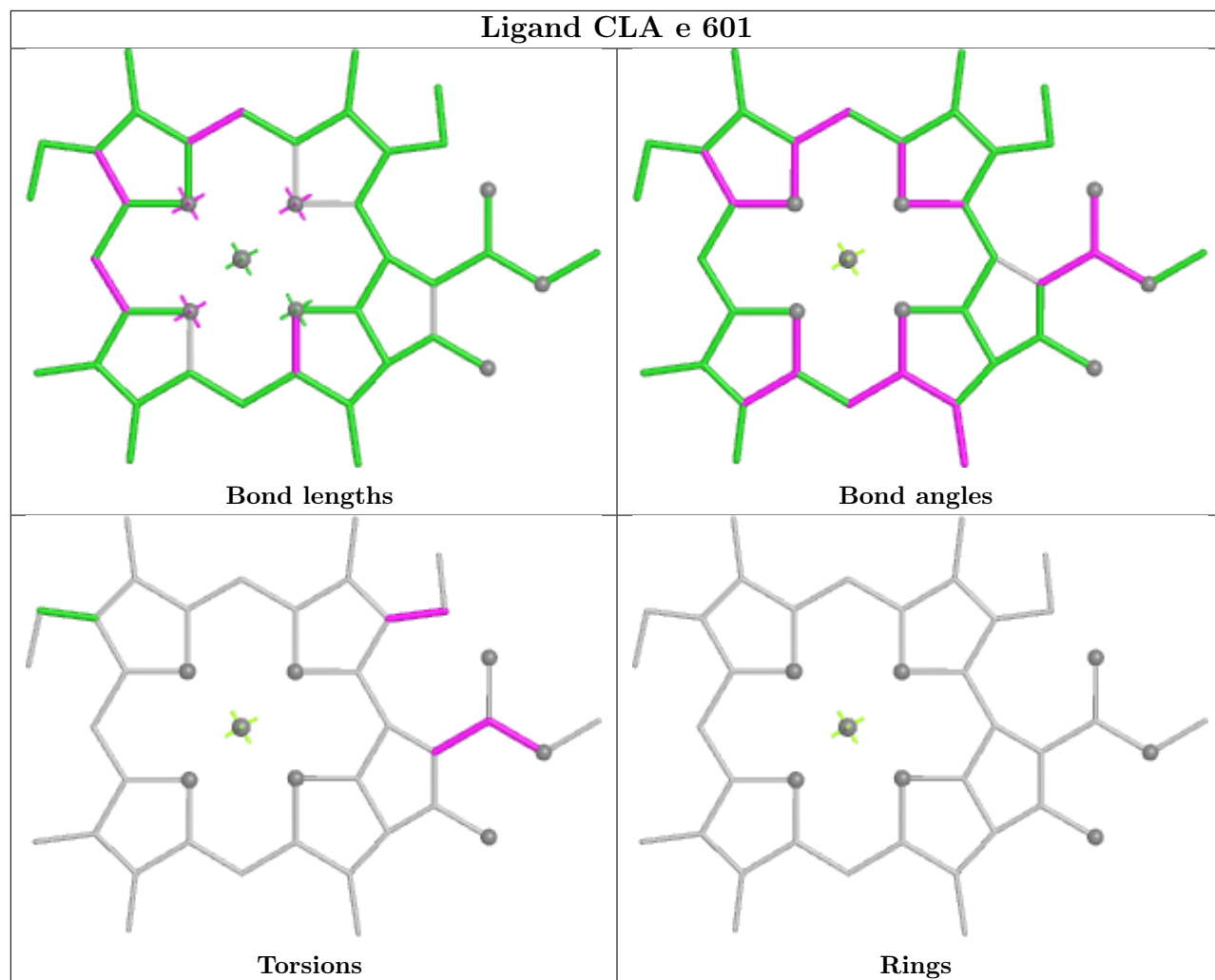


Torsions

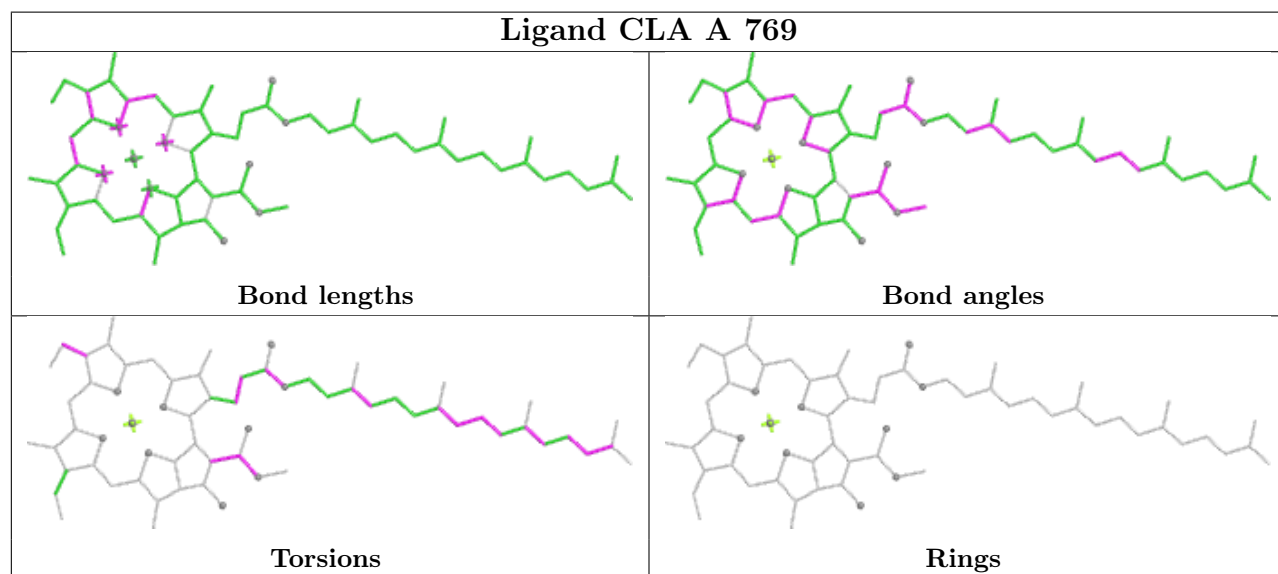


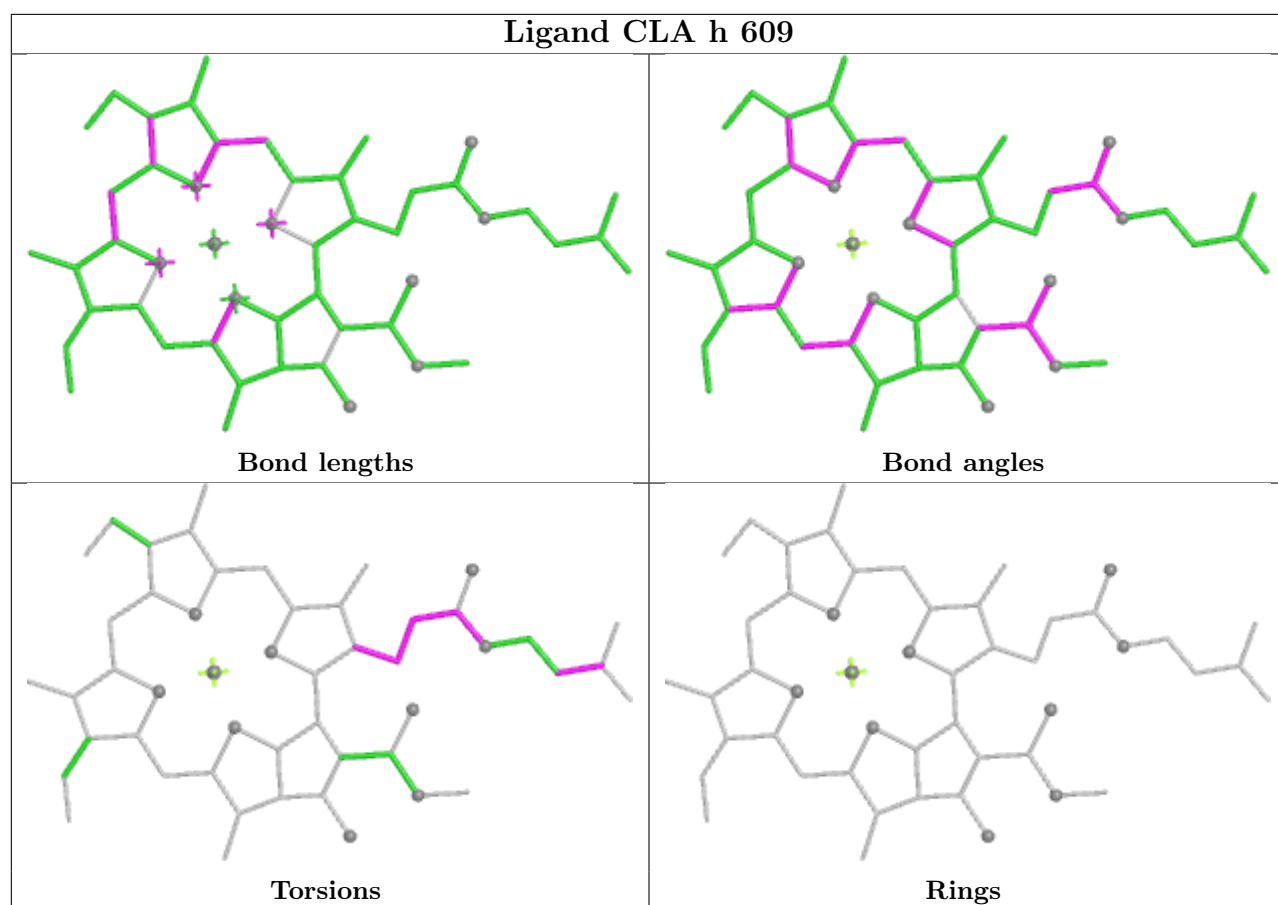
Rings

Ligand CLA e 601

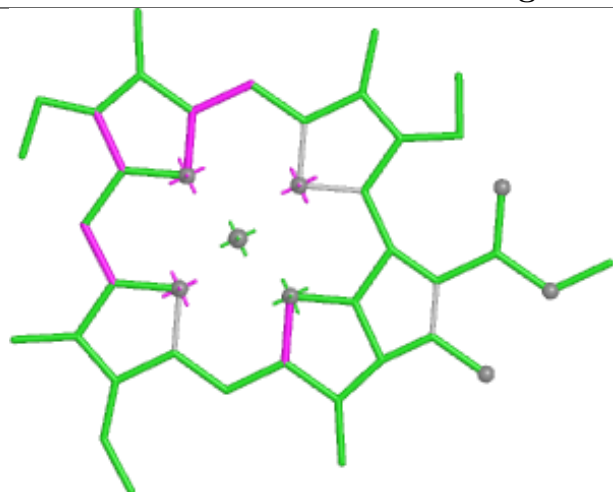


Ligand CLA A 769

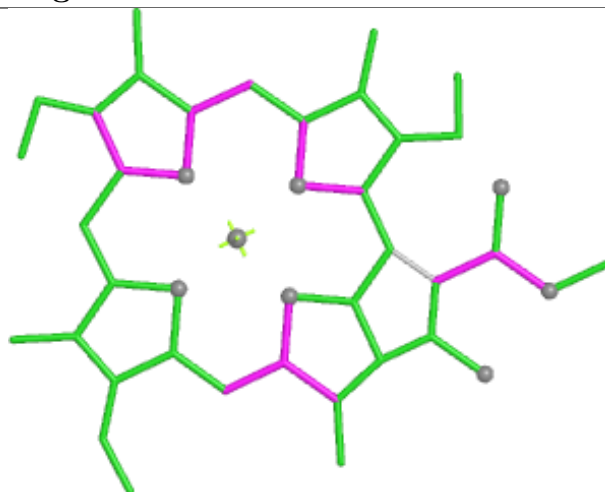




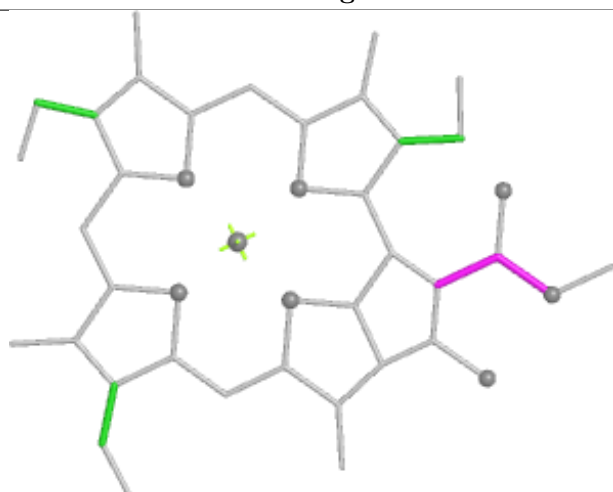
Ligand CLA g 612



Bond lengths



Bond angles

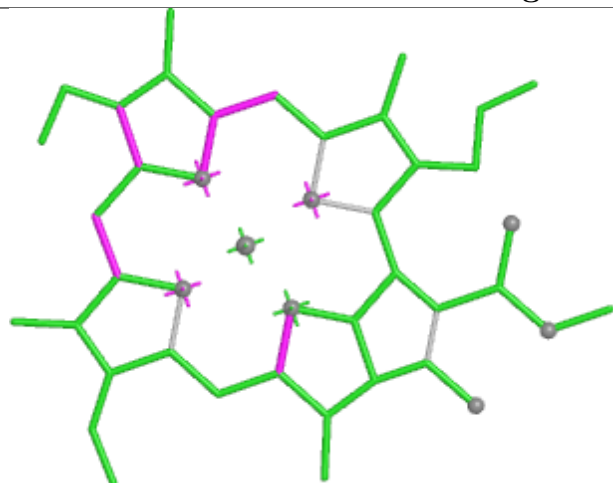


Torsions

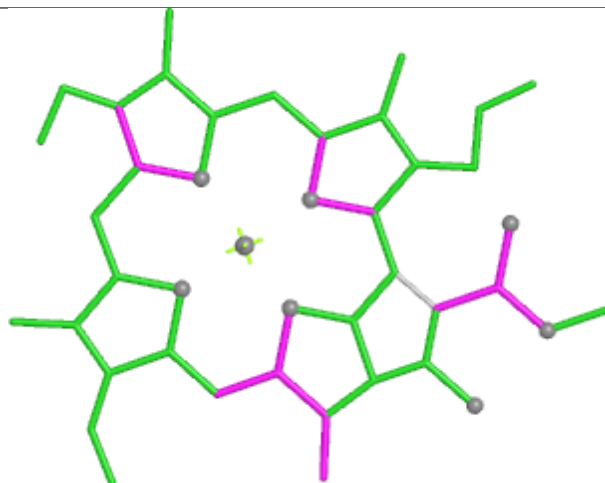


Rings

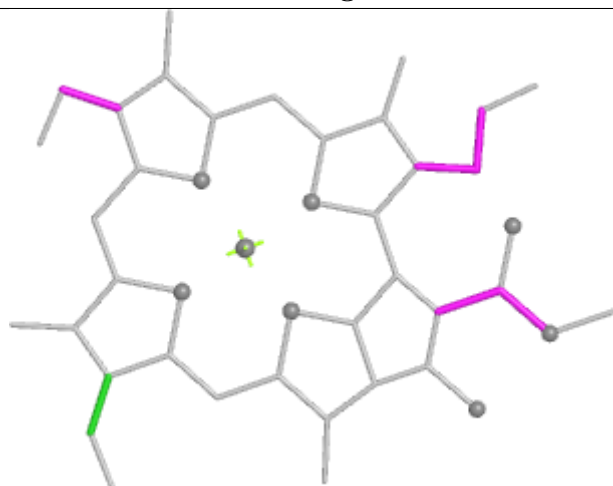
Ligand CLA i 603



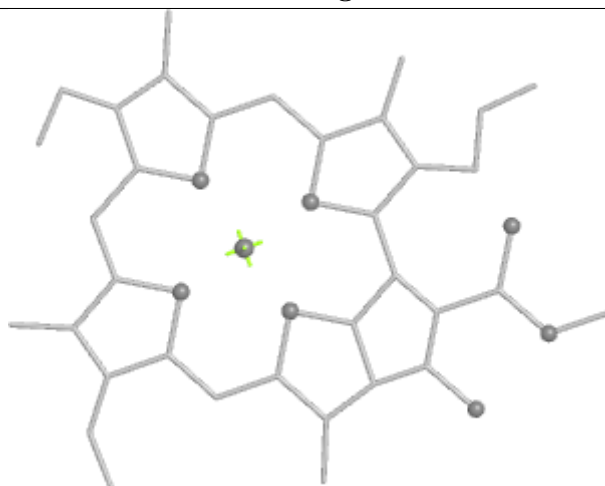
Bond lengths



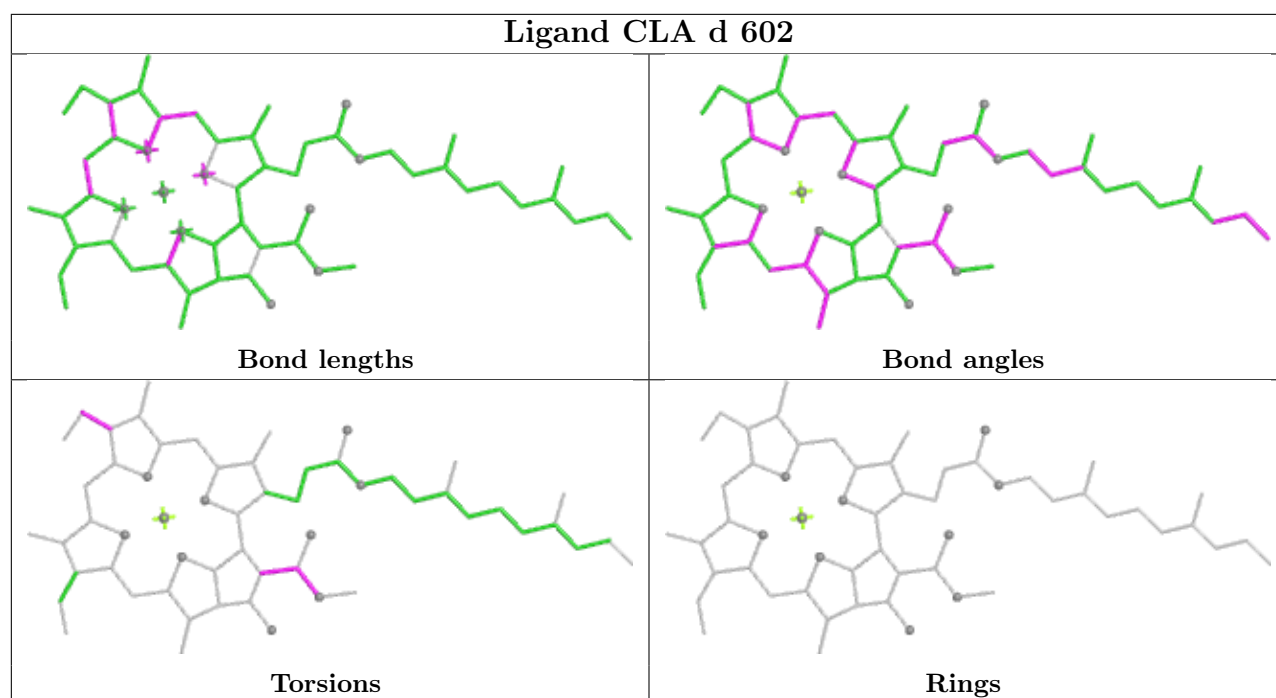
Bond angles



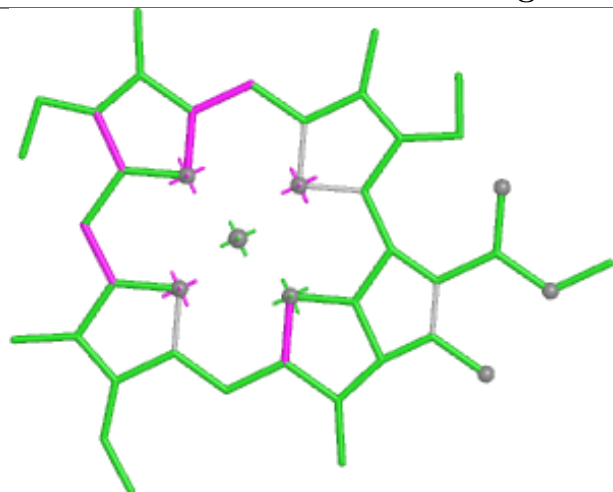
Torsions



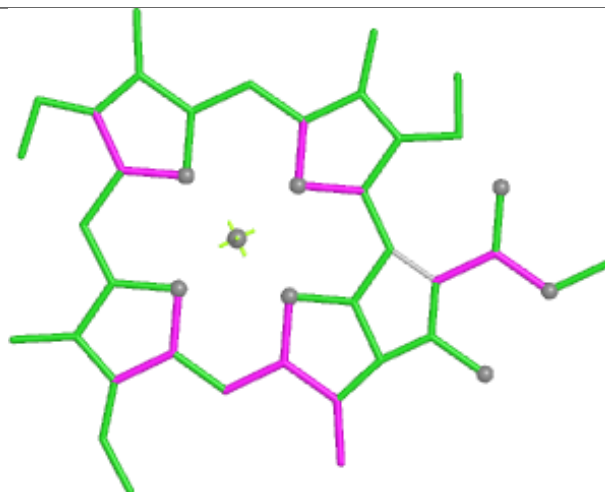
Rings



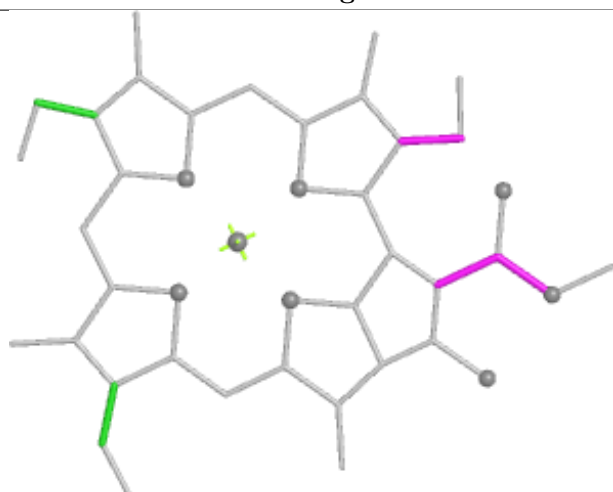
Ligand CLA k 603



Bond lengths



Bond angles

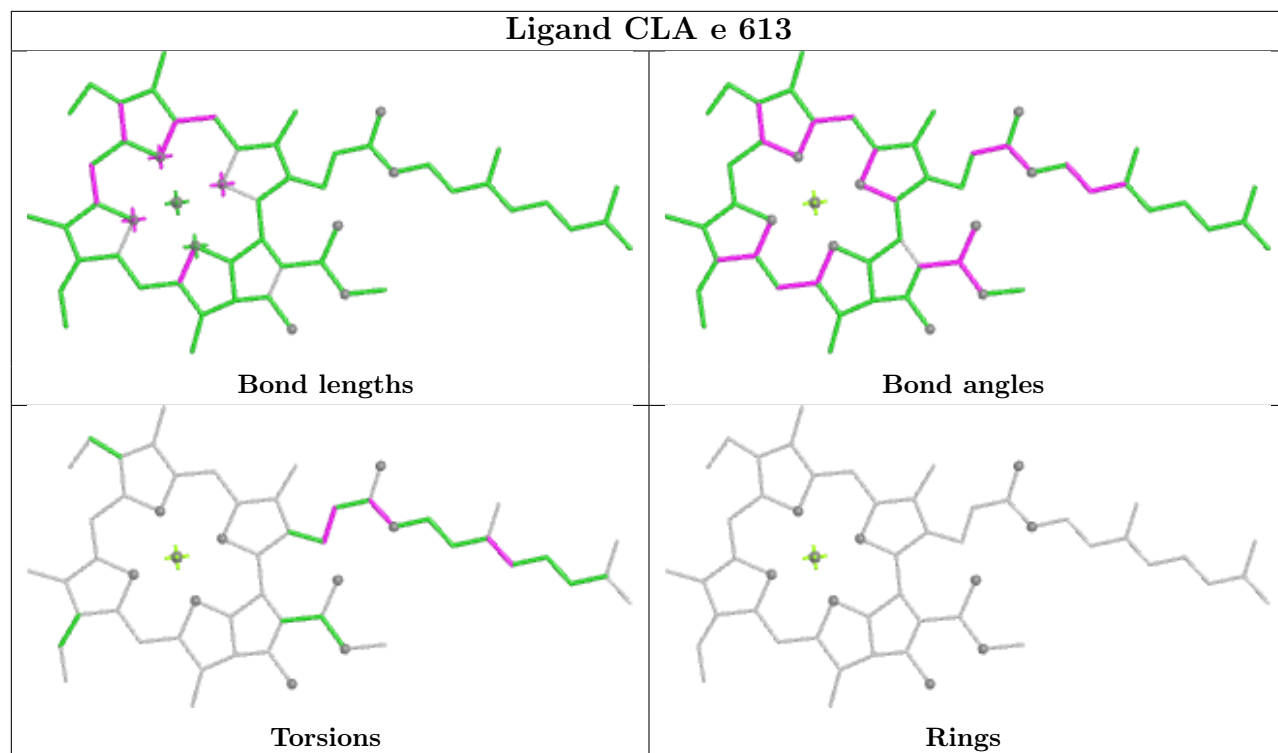


Torsions

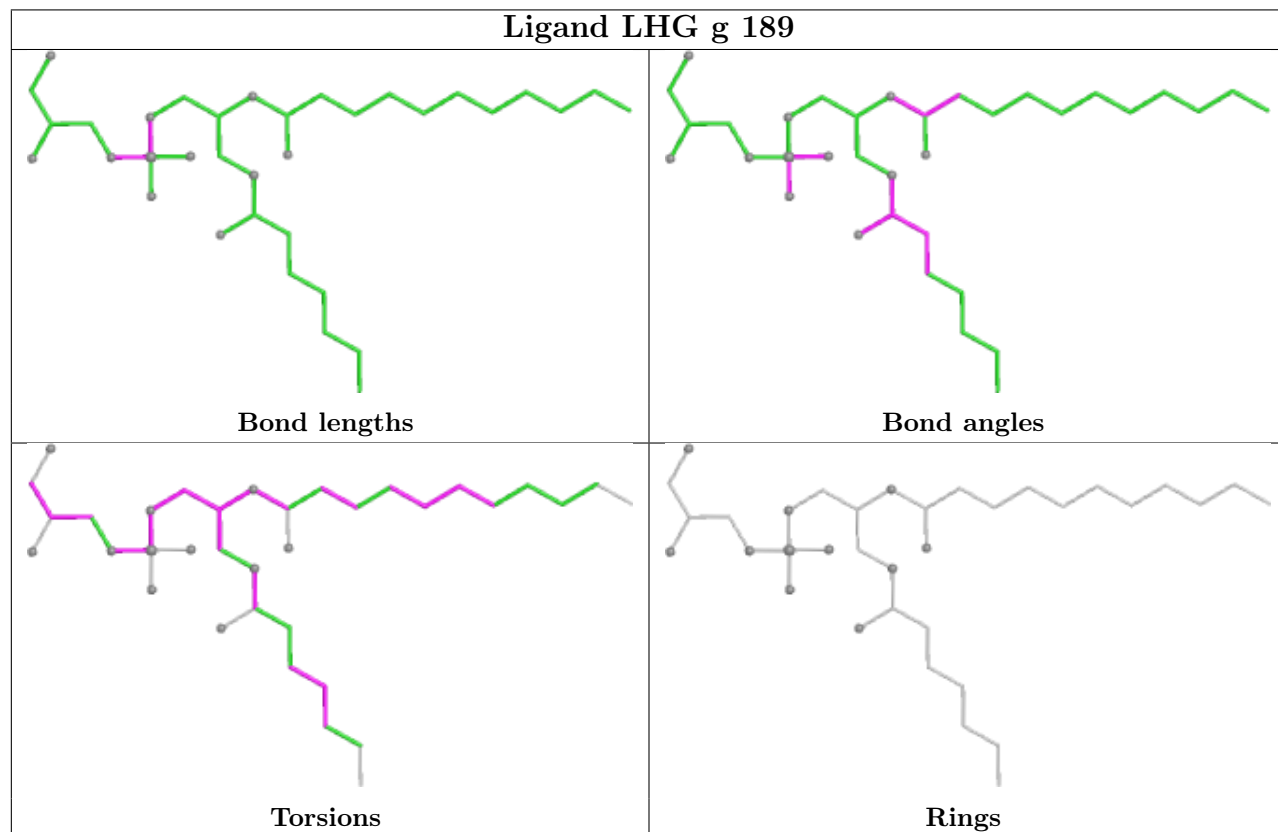


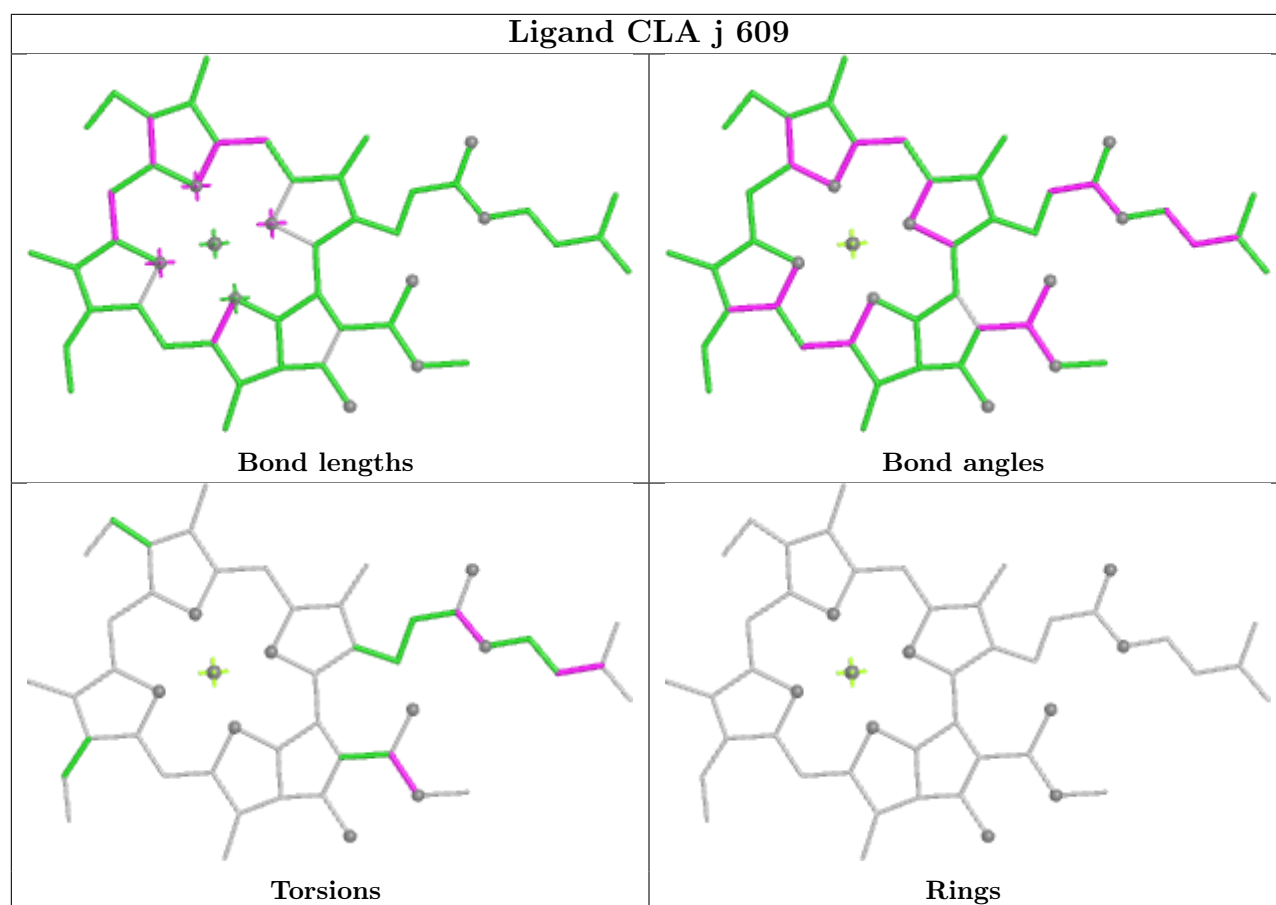
Rings

Ligand CLA e 613

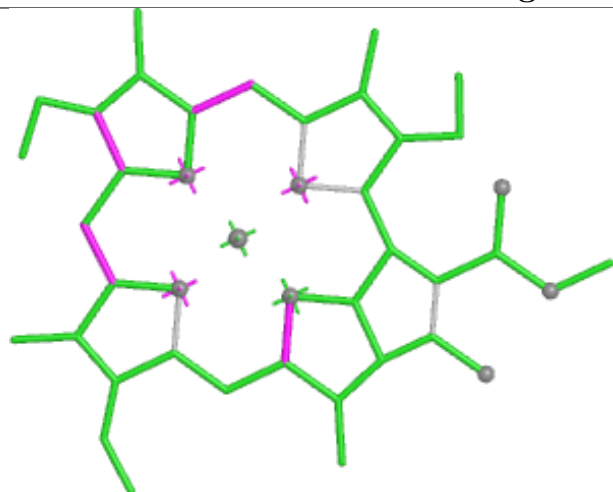


Ligand LHG g 189

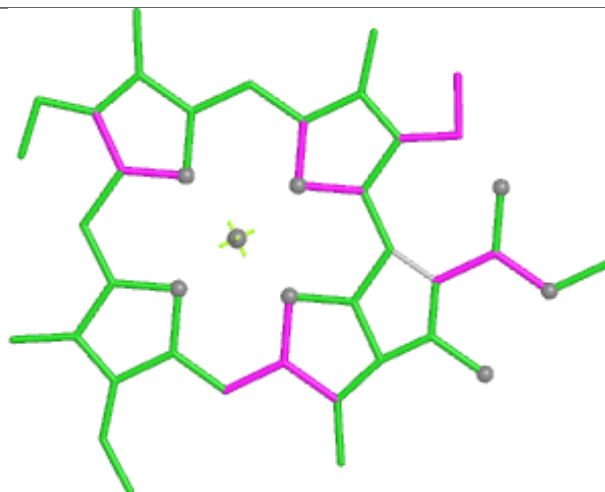




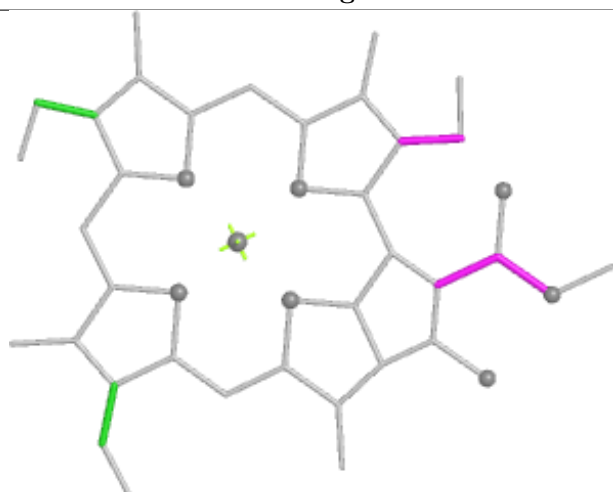
Ligand CLA o 613



Bond lengths



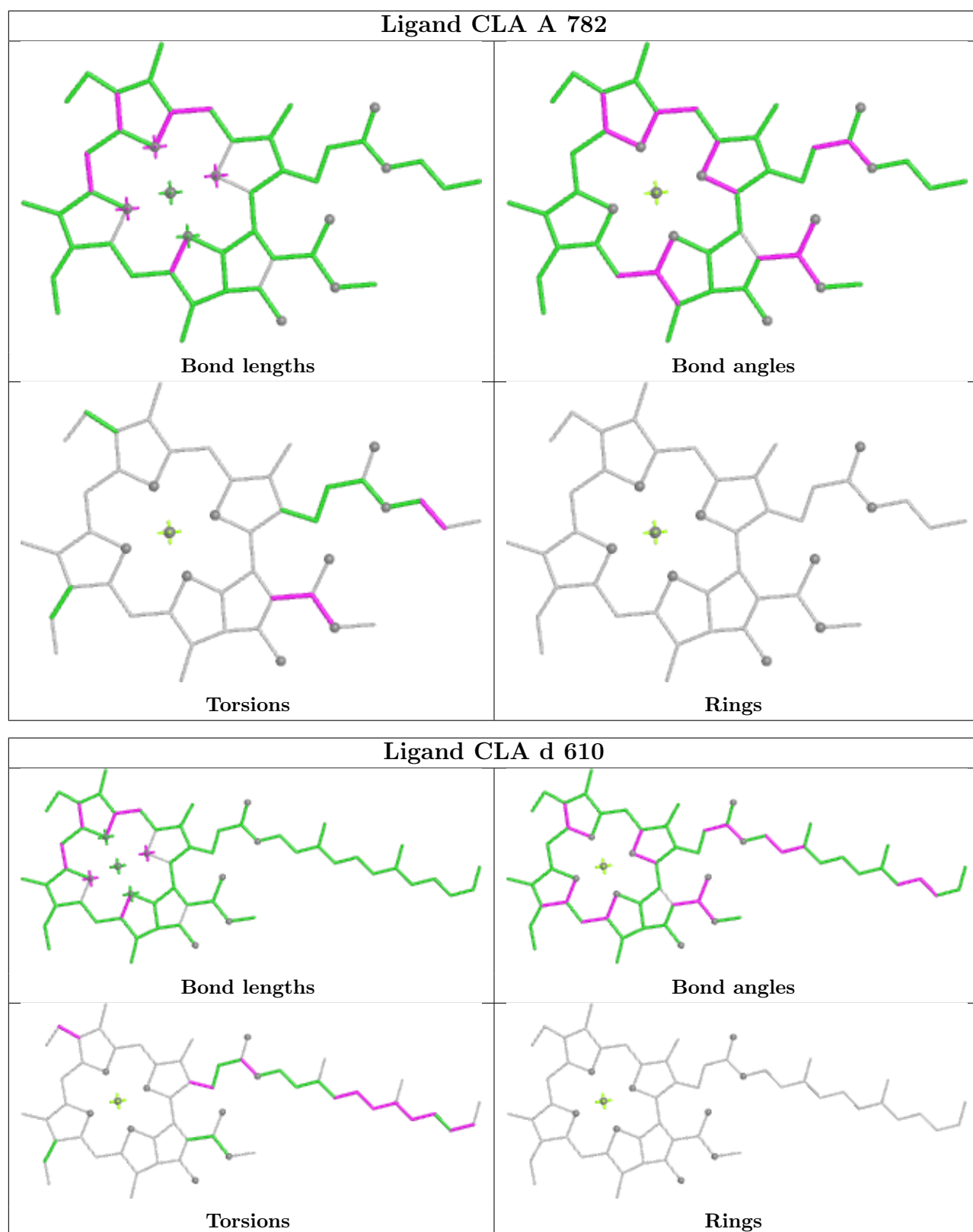
Bond angles

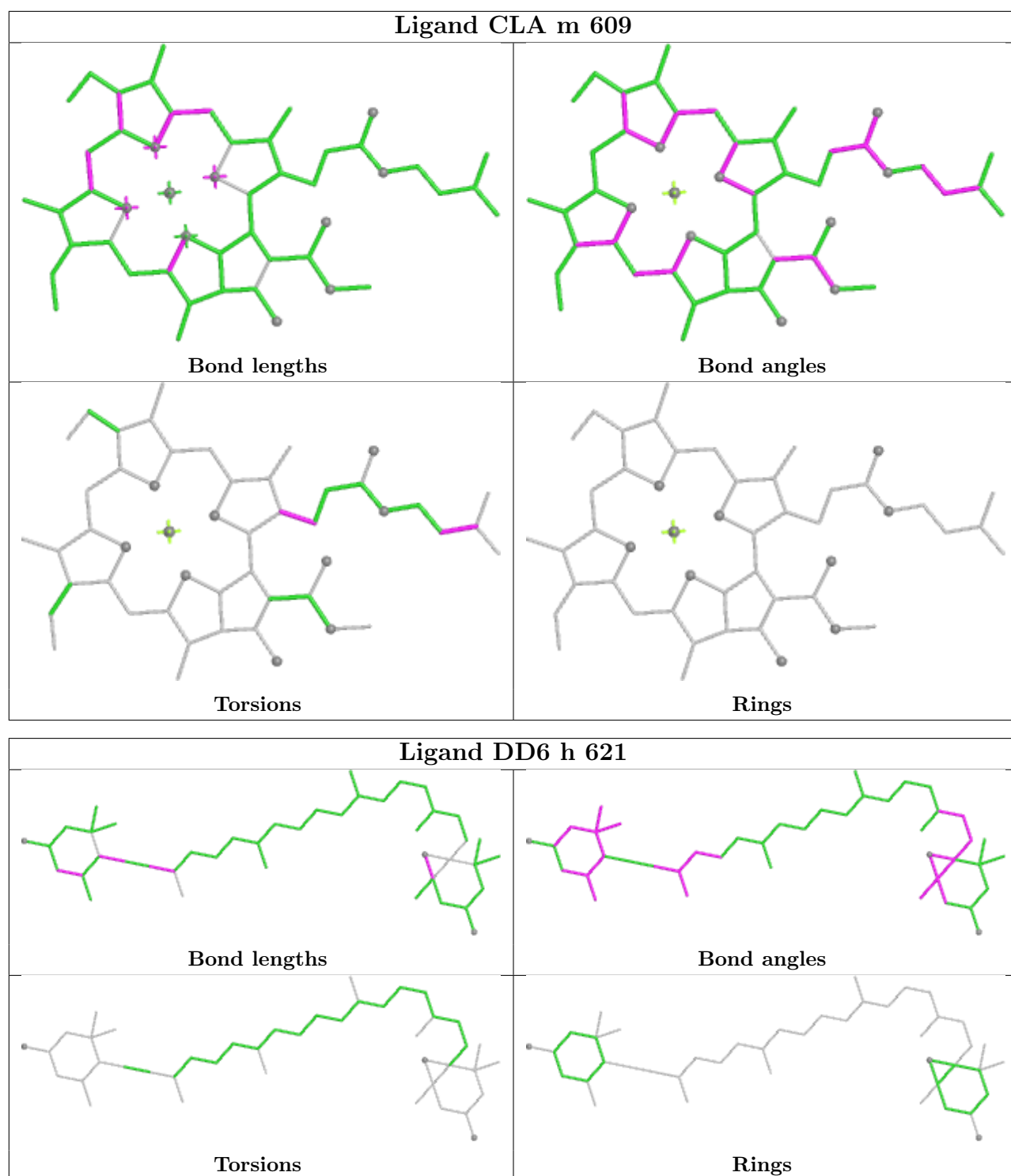


Torsions

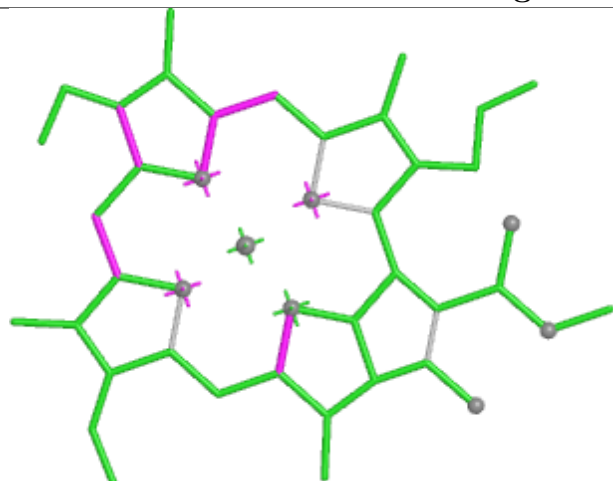


Rings

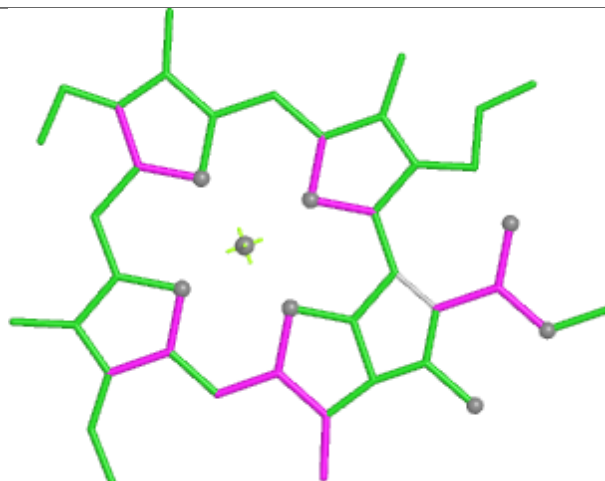




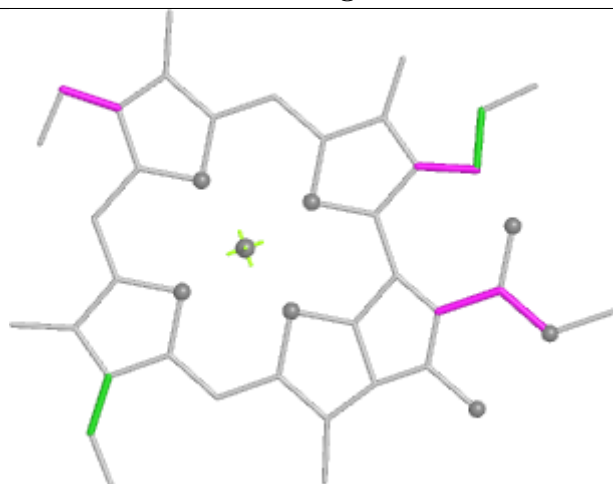
Ligand CLA A 779



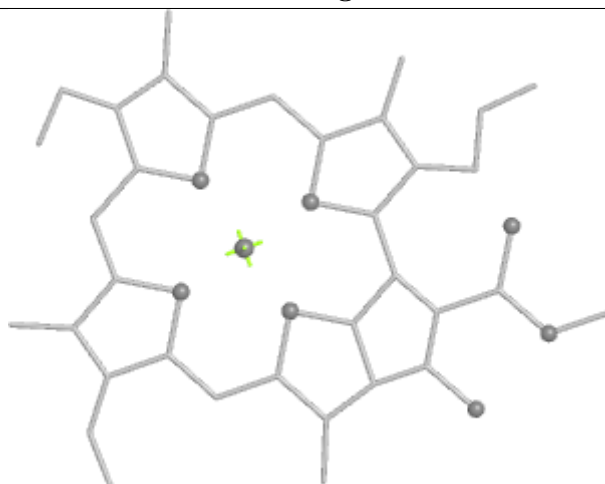
Bond lengths



Bond angles

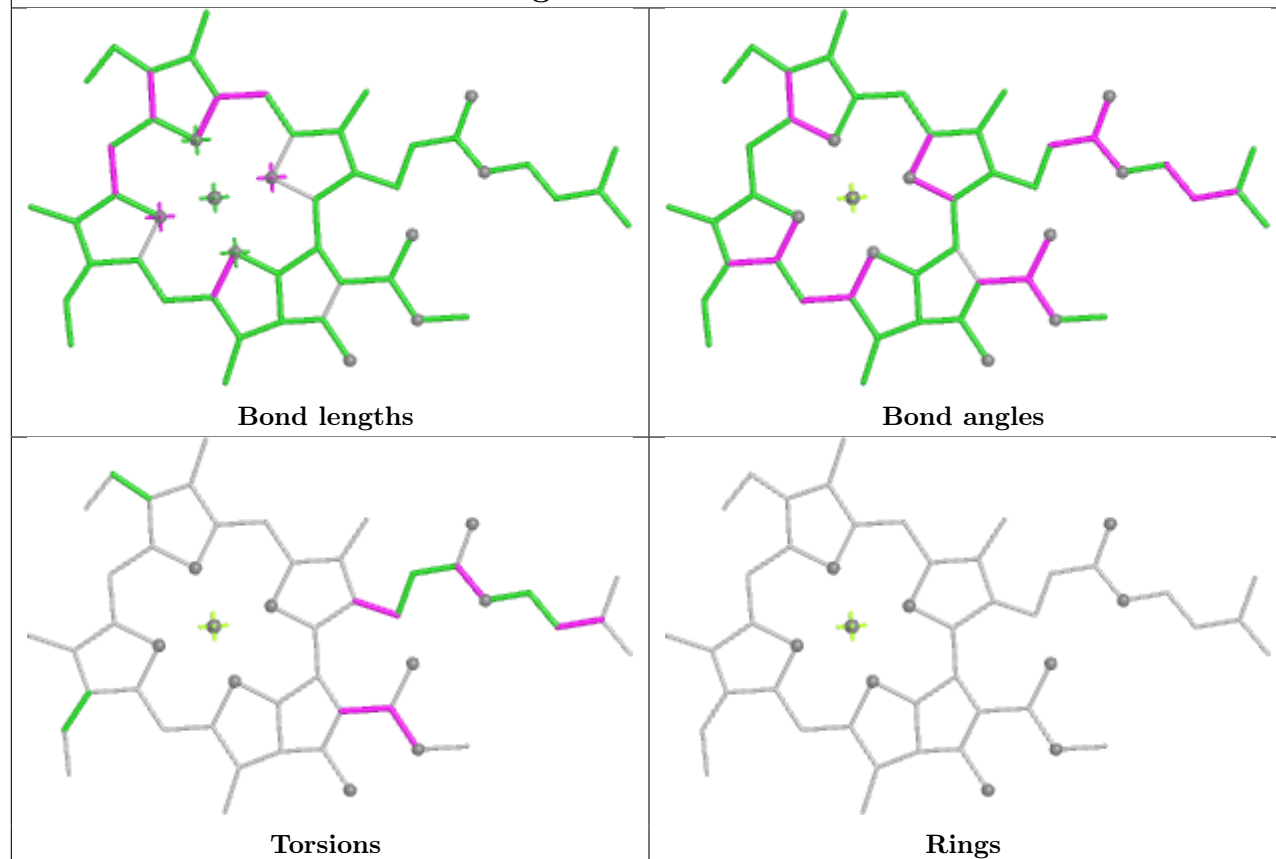


Torsions

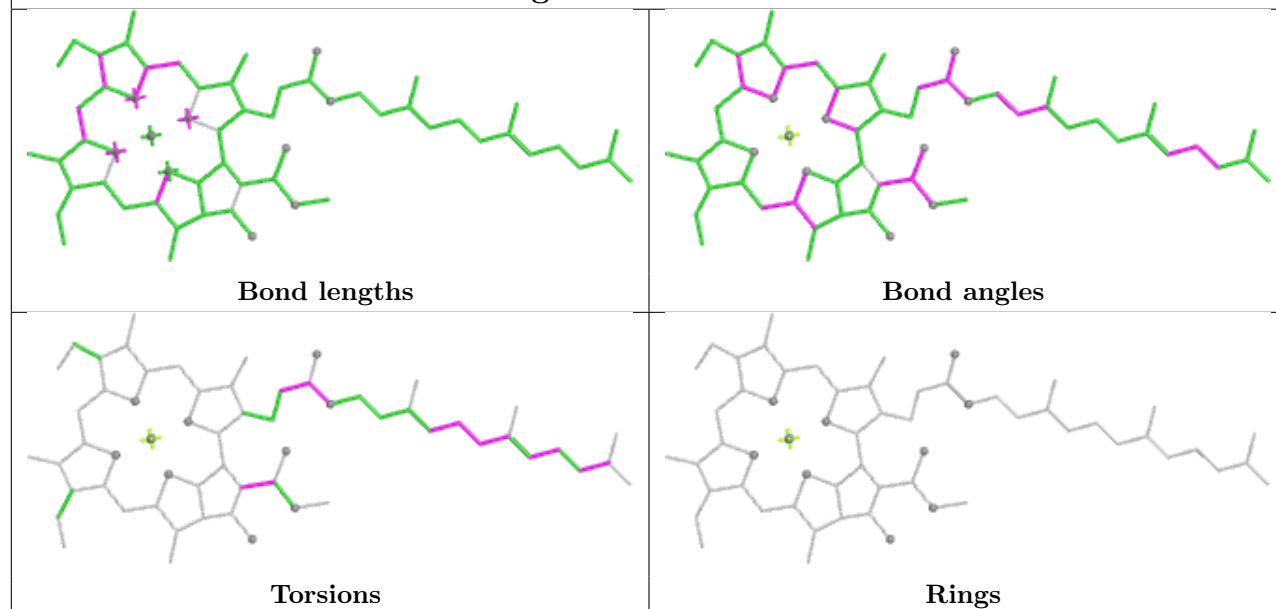


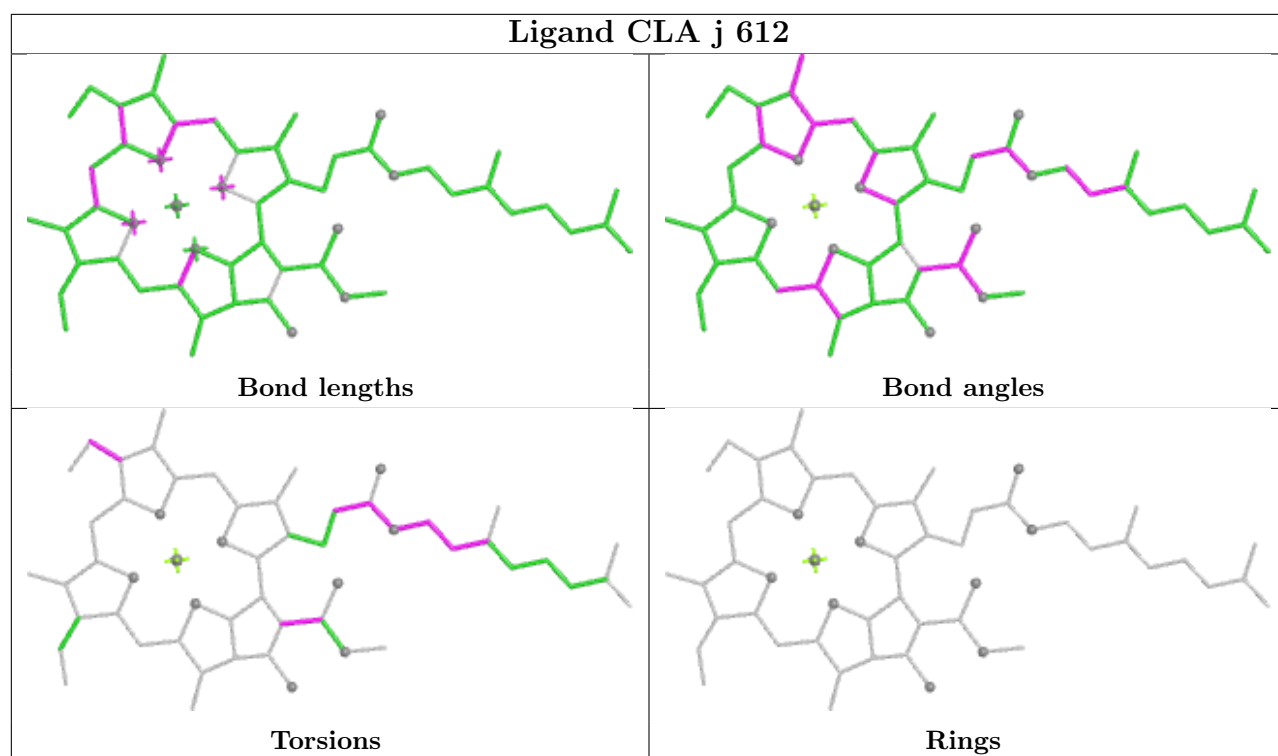
Rings

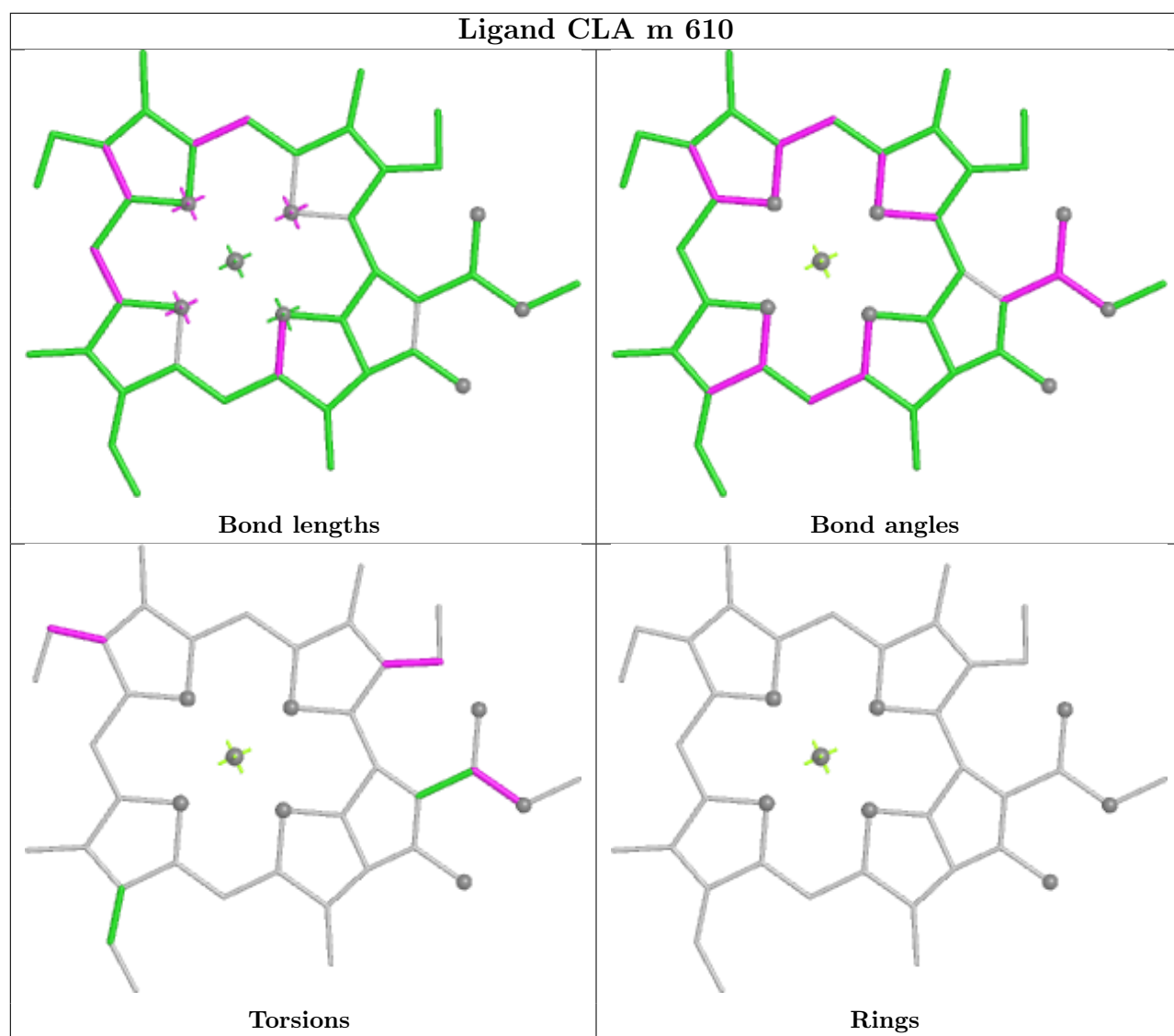
Ligand CLA B 775

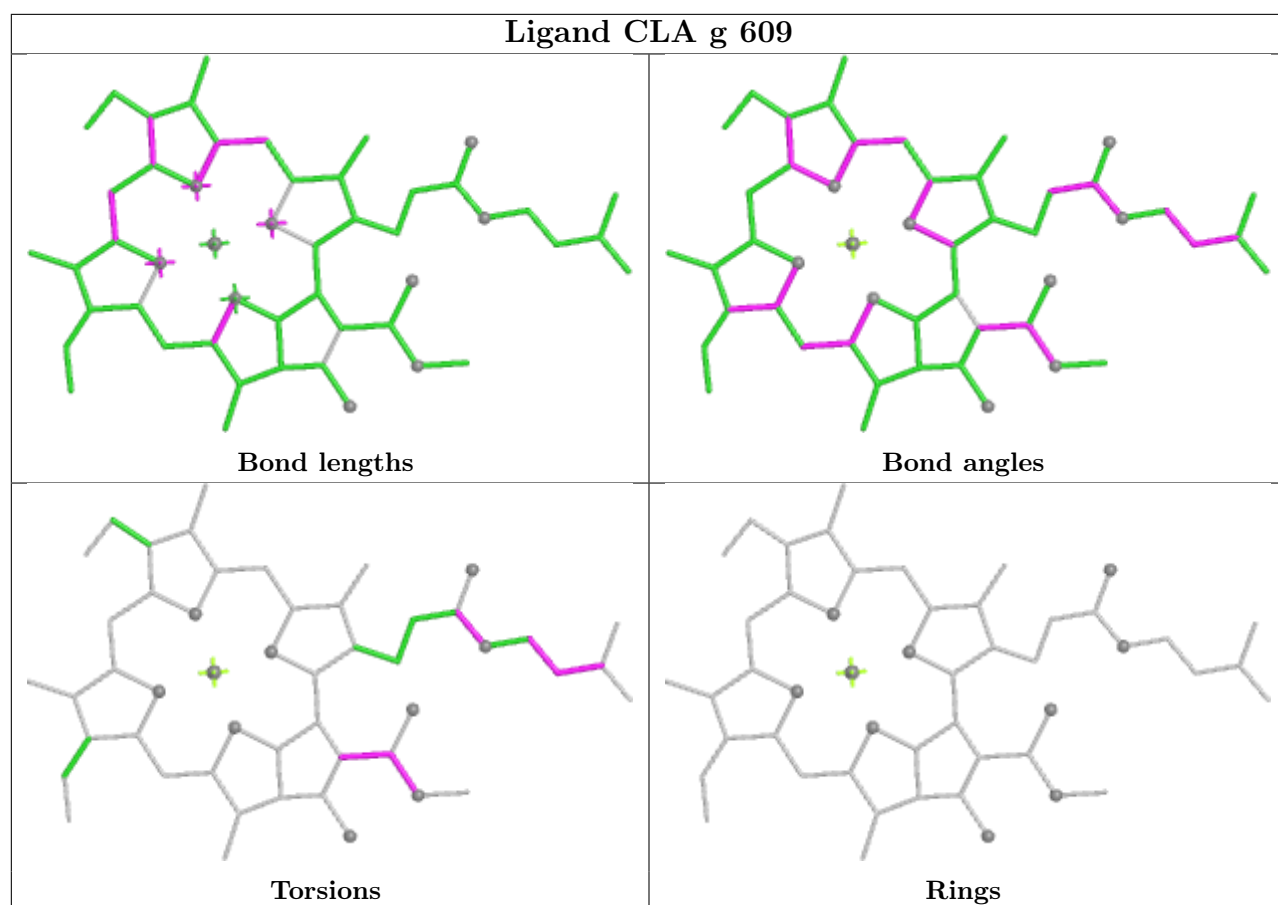


Ligand CLA A 759

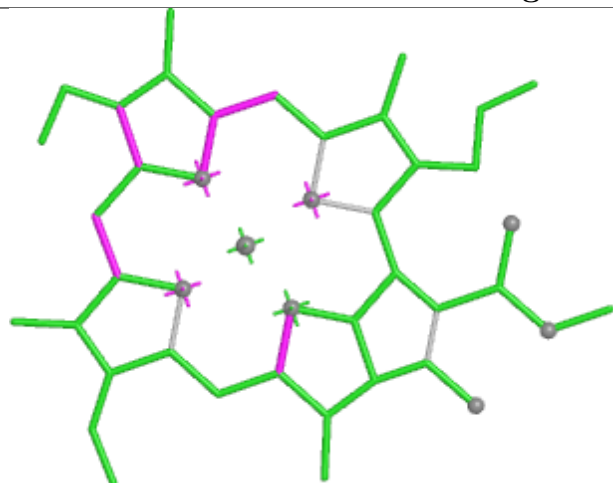




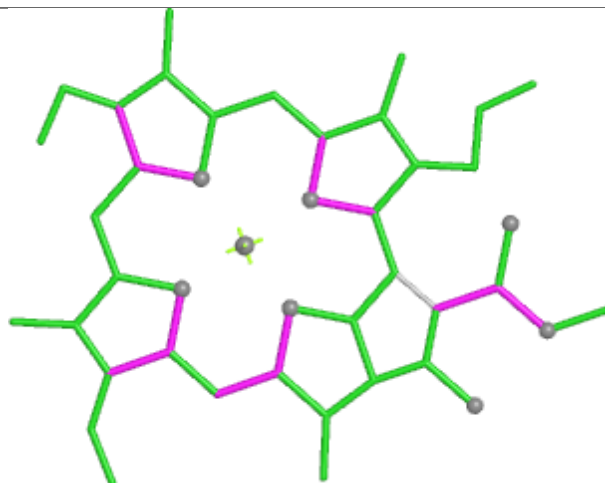




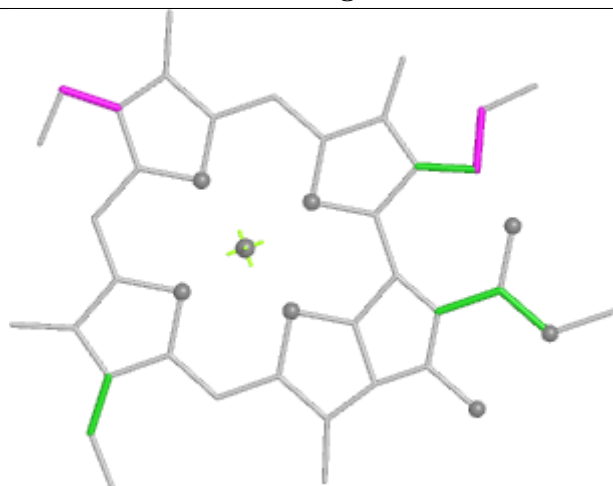
Ligand CLA i 604



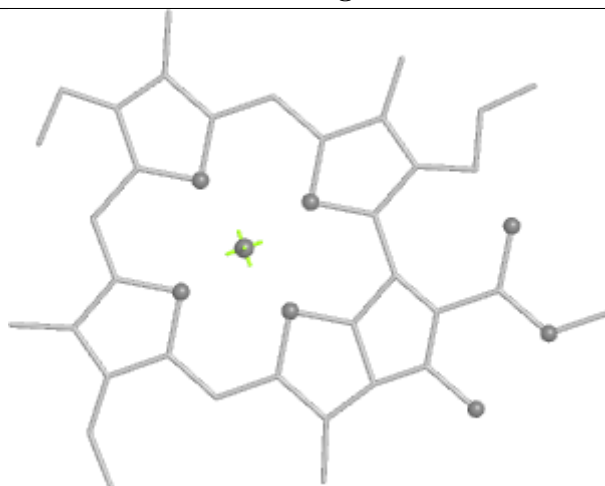
Bond lengths



Bond angles

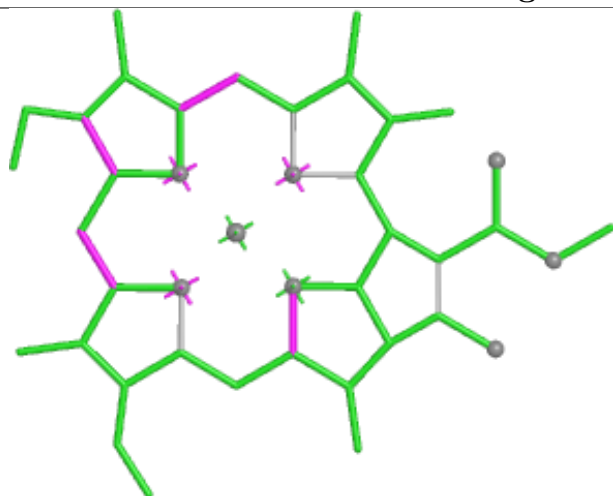


Torsions



Rings

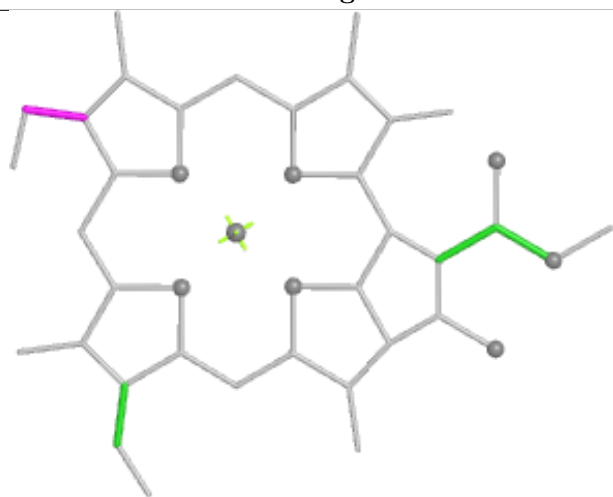
Ligand CLA o 610



Bond lengths



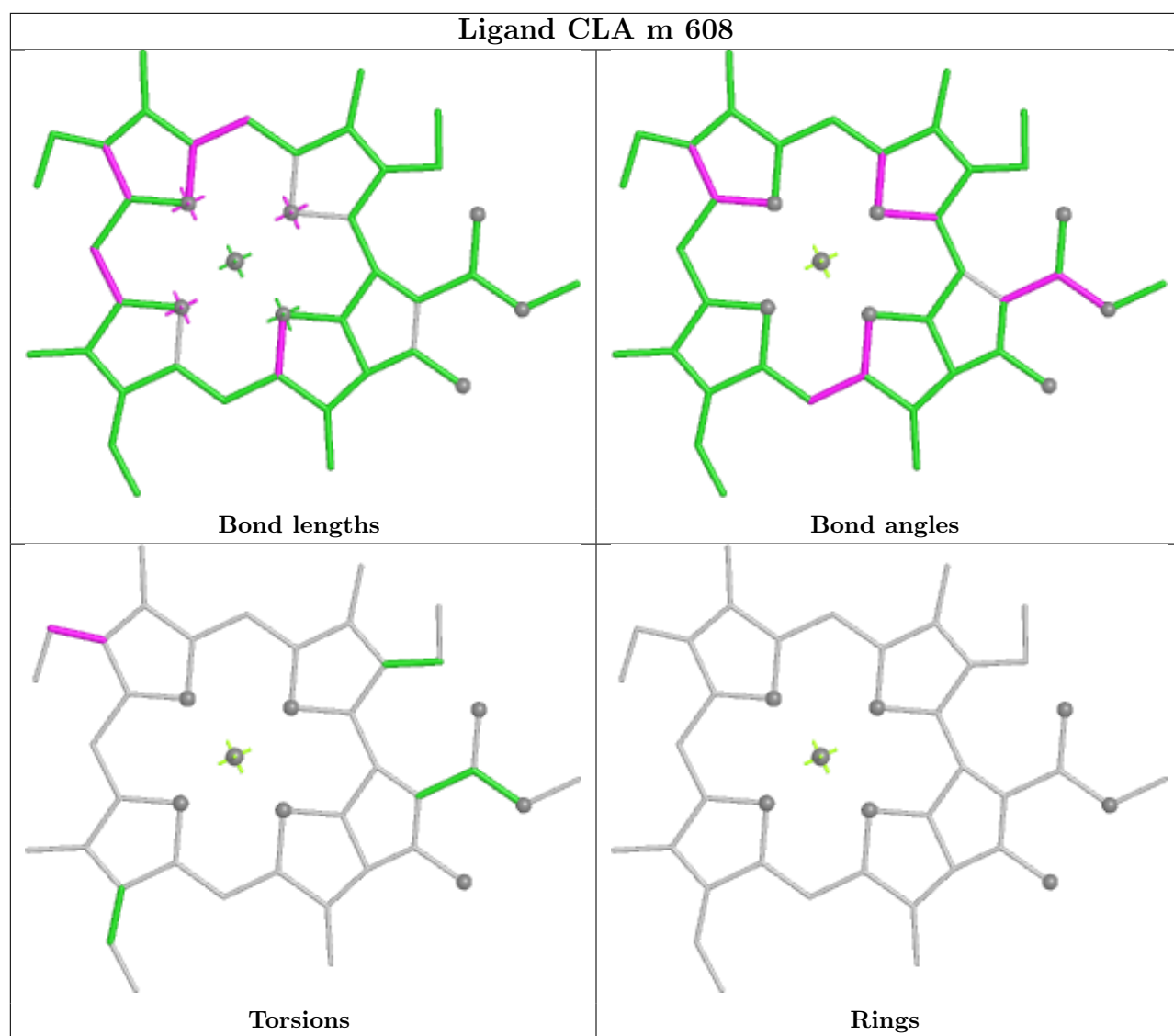
Bond angles



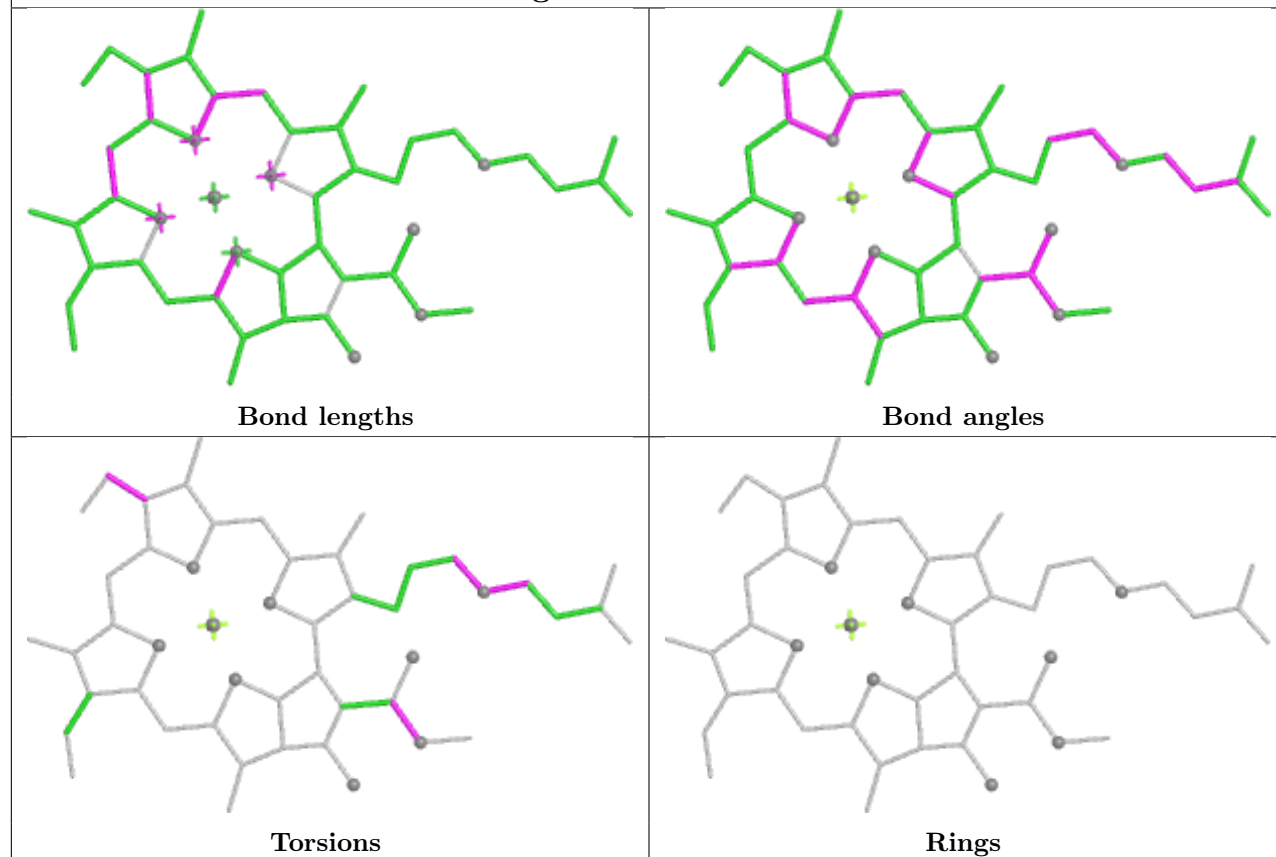
Torsions



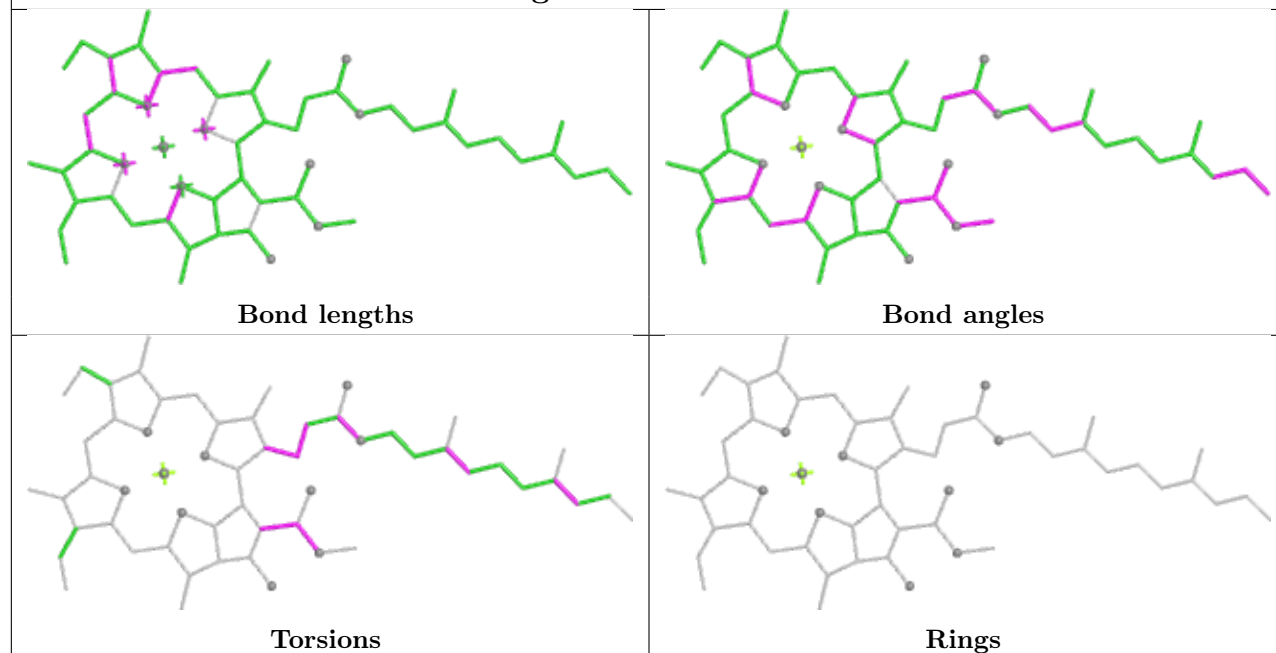
Rings

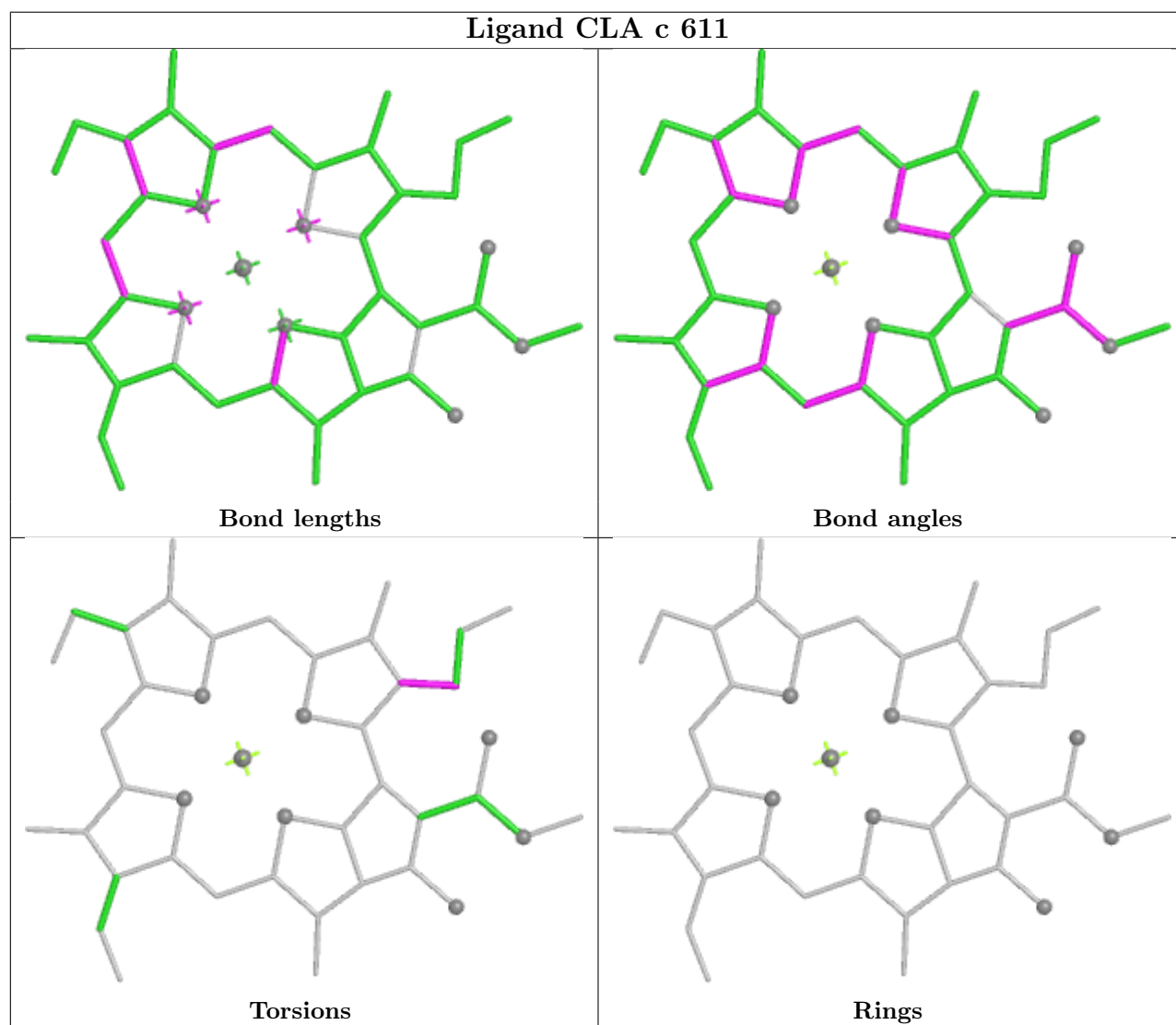
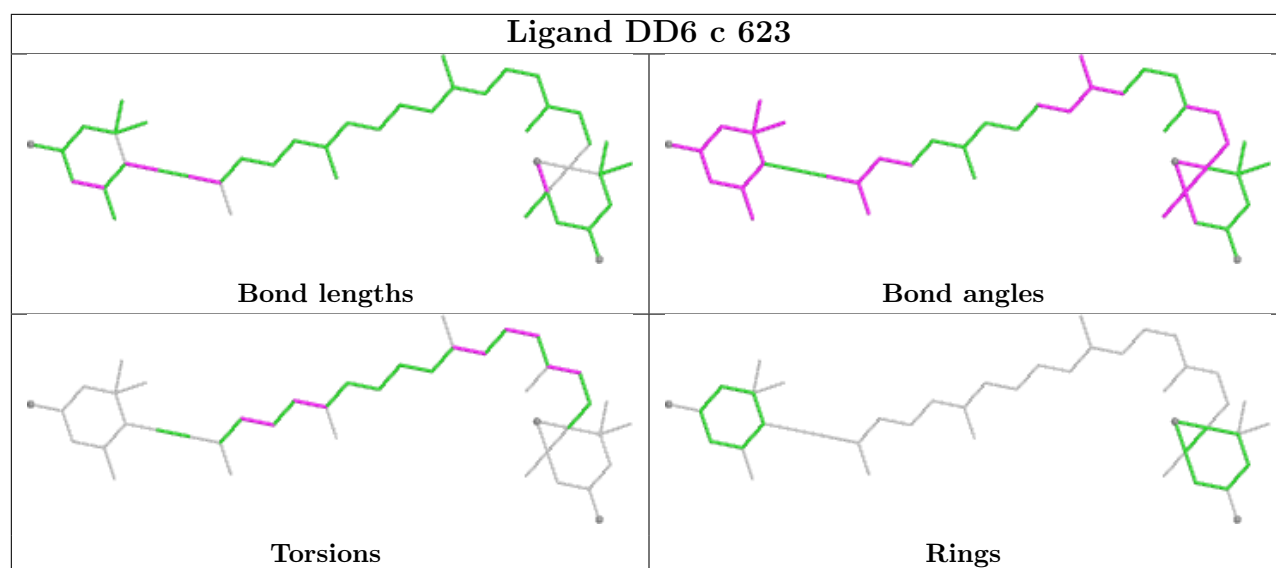


Ligand CLA B 747

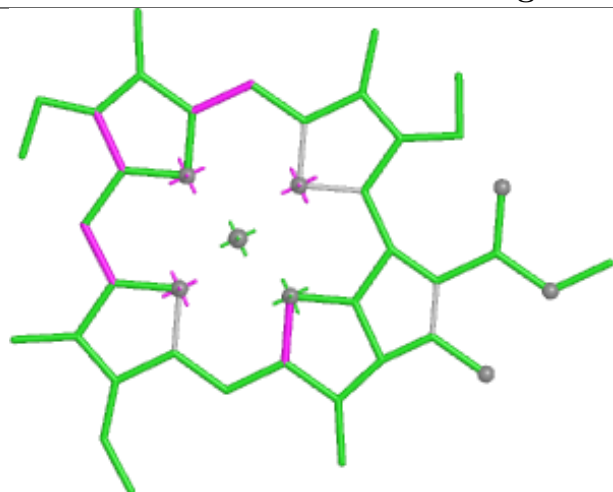


Ligand CLA A 771

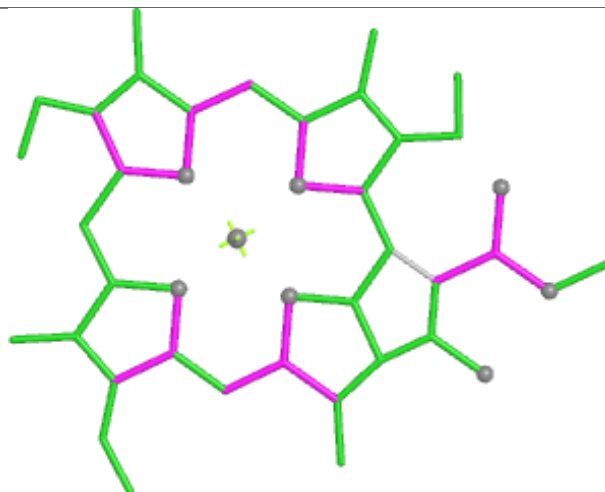




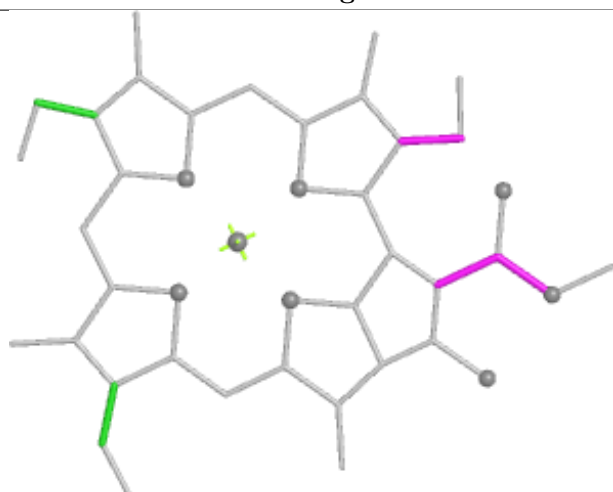
Ligand CLA n 605



Bond lengths



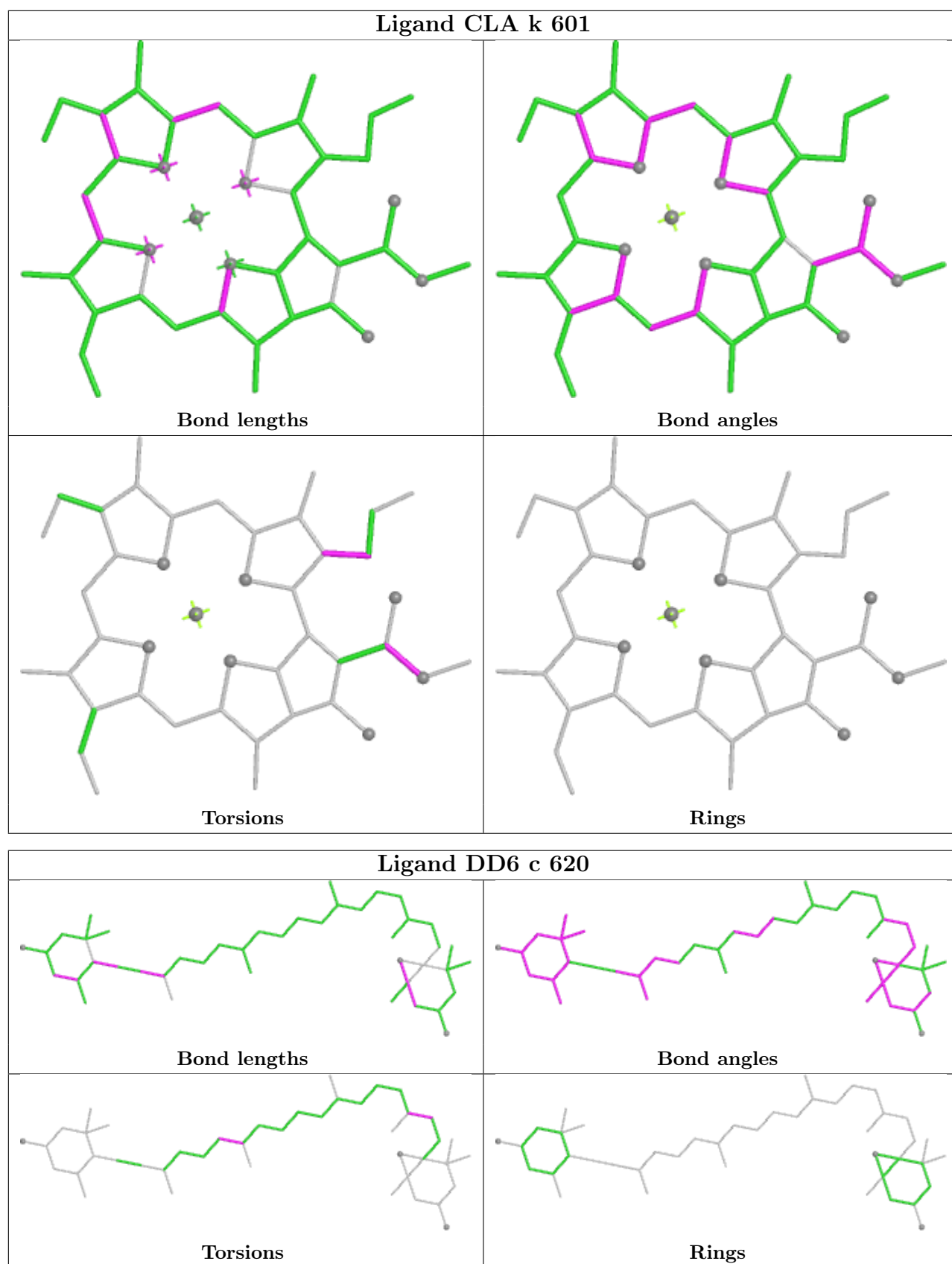
Bond angles

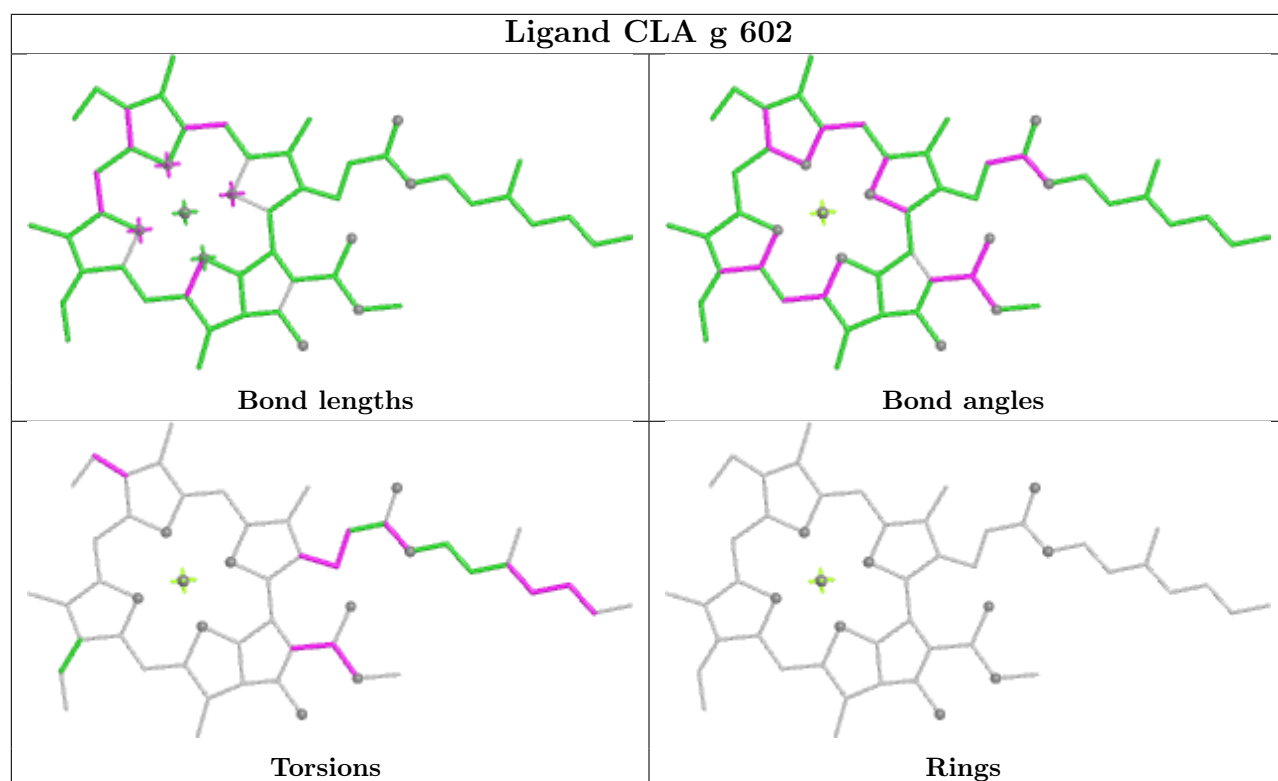


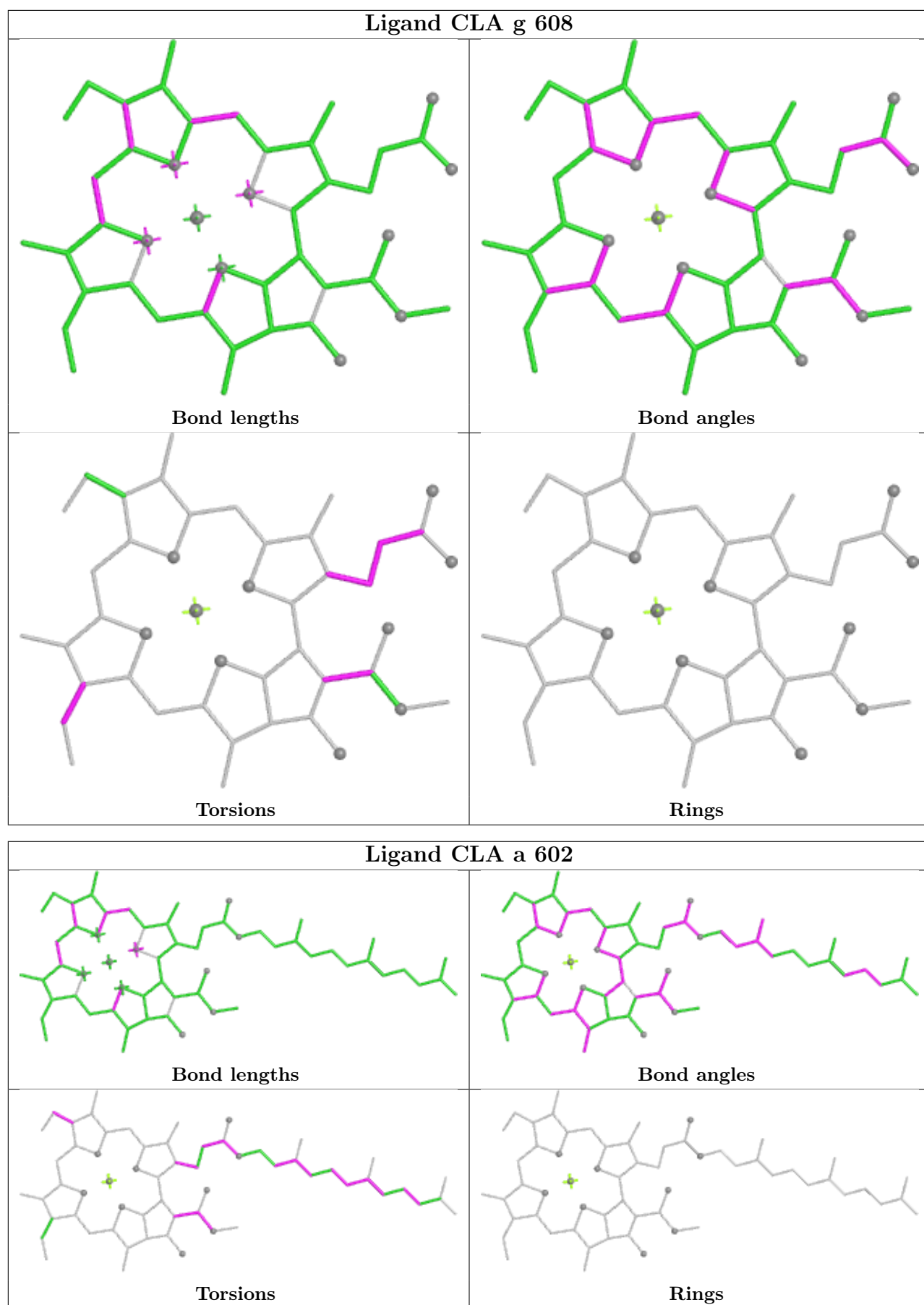
Torsions

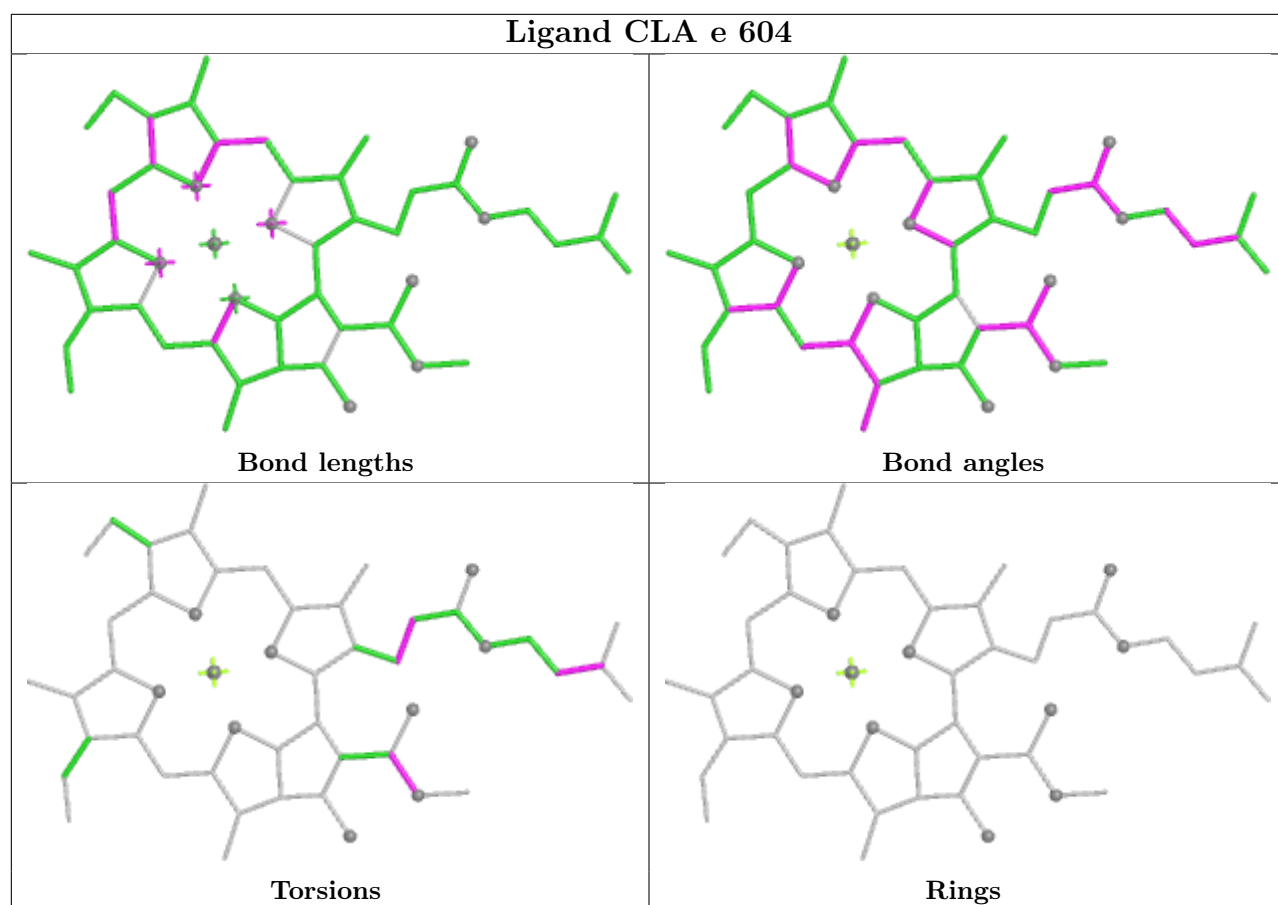


Rings

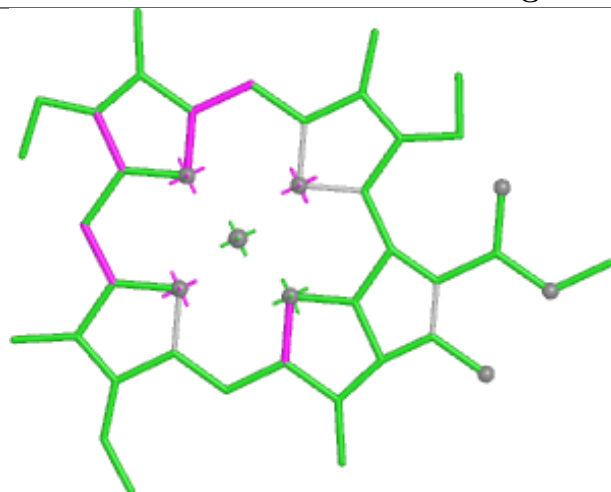




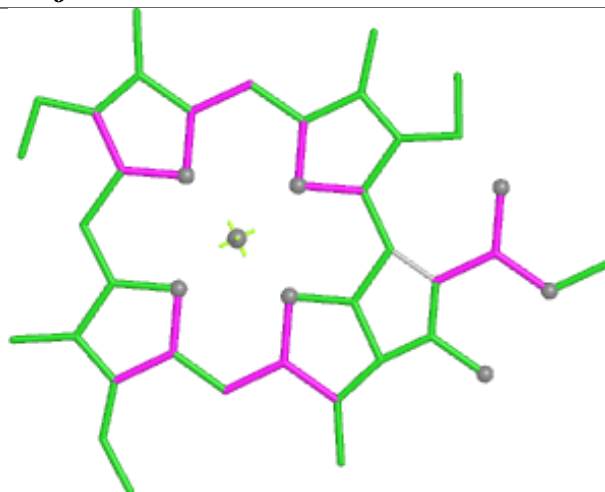




Ligand CLA j 614



Bond lengths



Bond angles

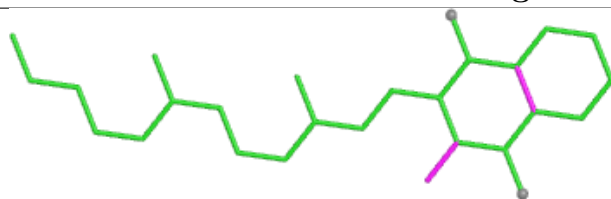


Torsions

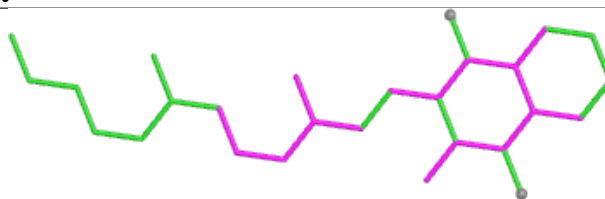


Rings

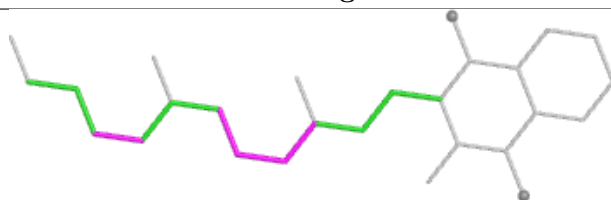
Ligand PQN B 769



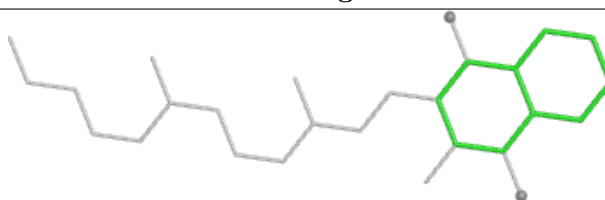
Bond lengths



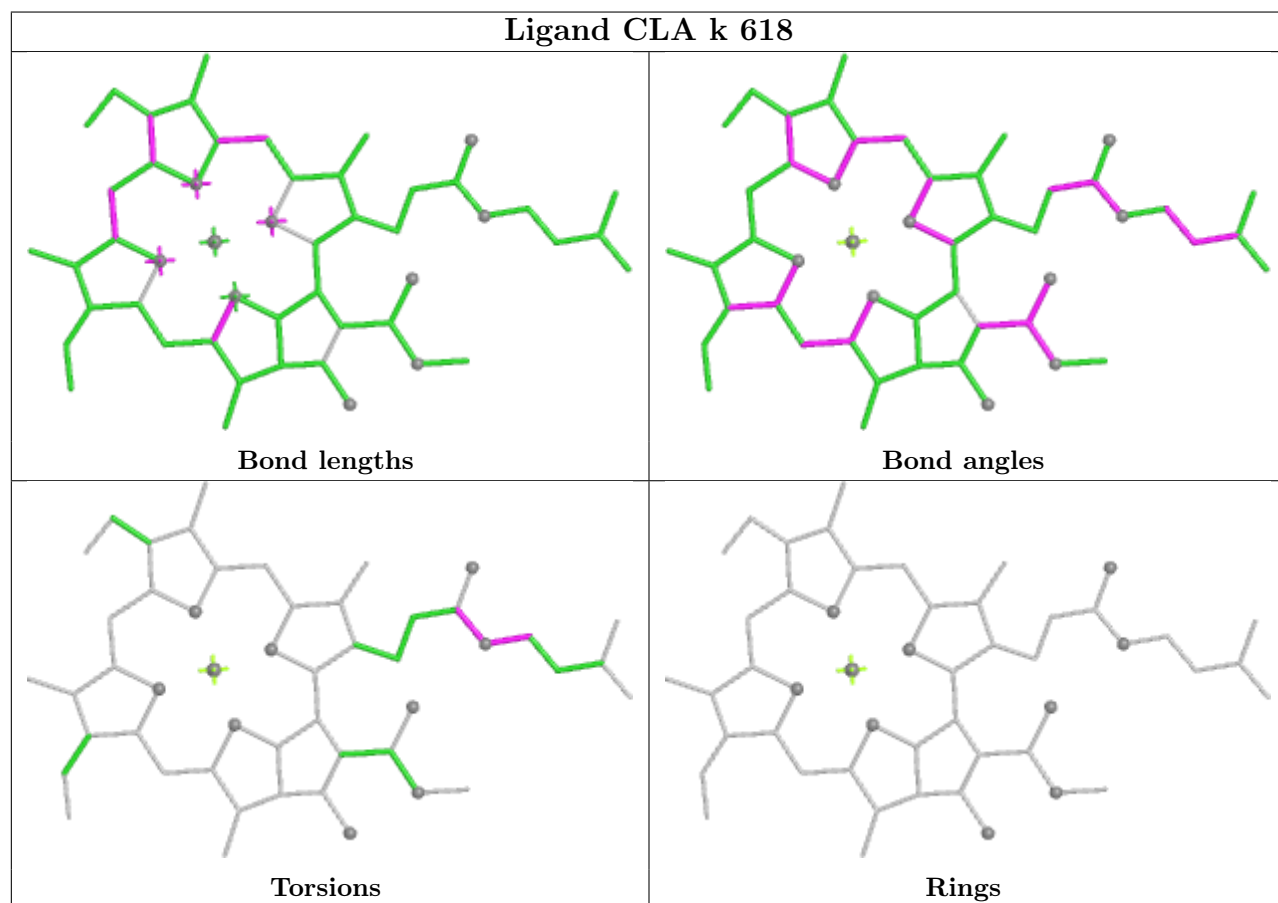
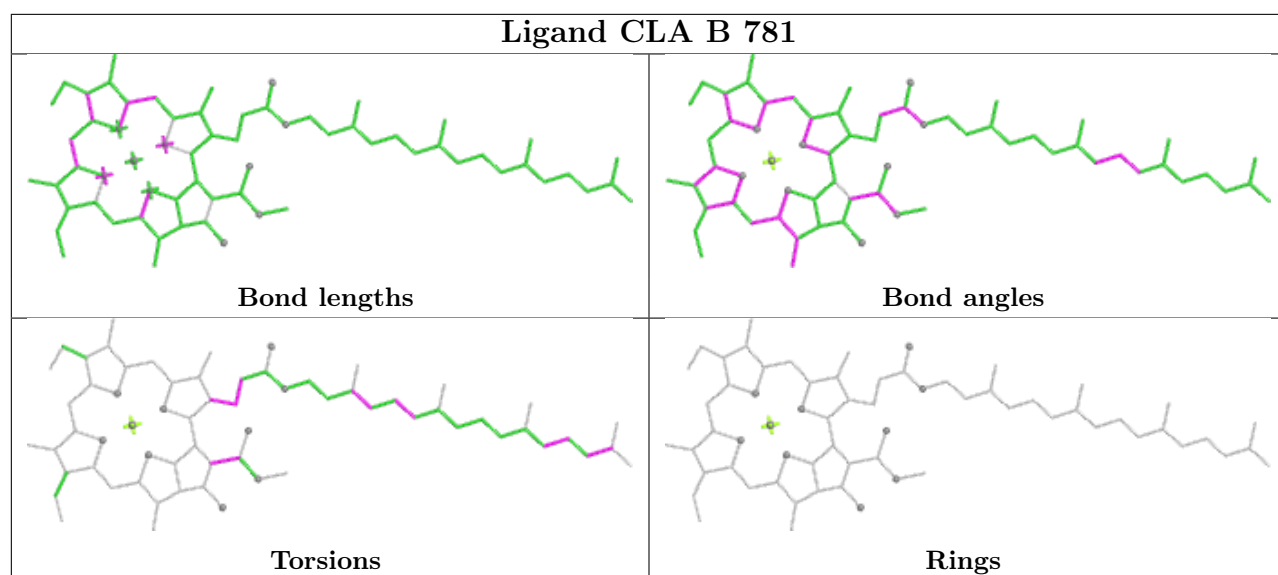
Bond angles

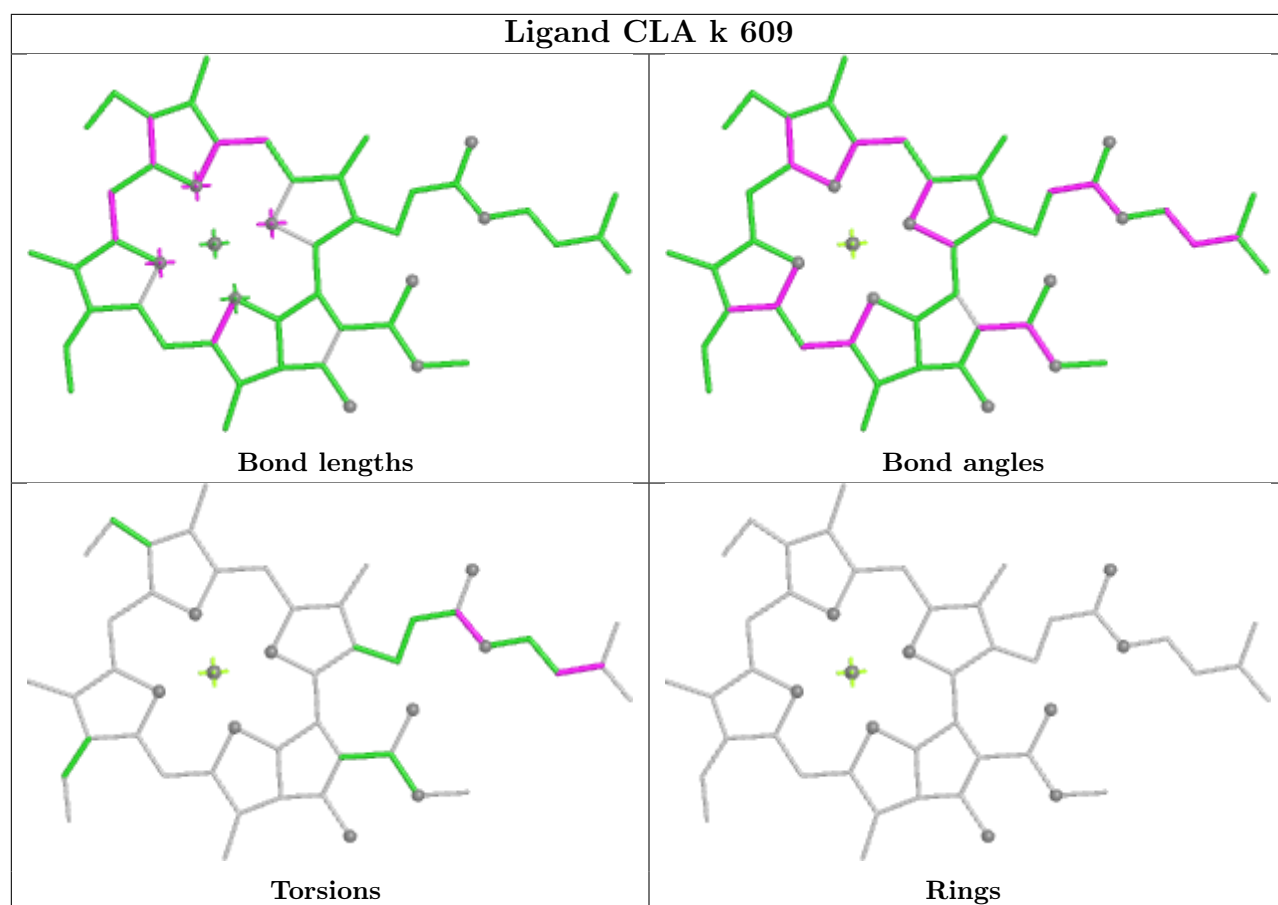


Torsions

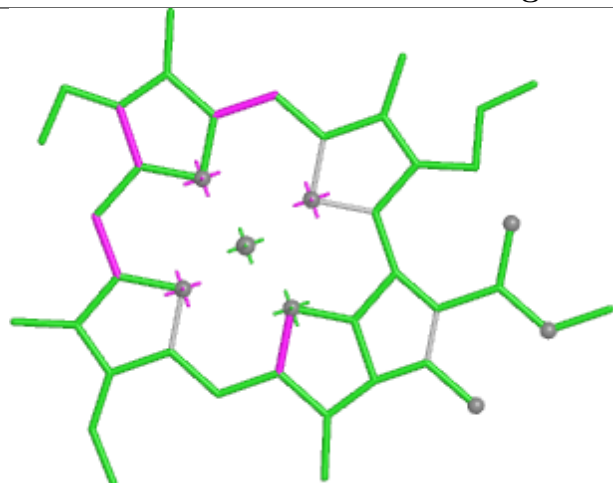


Rings

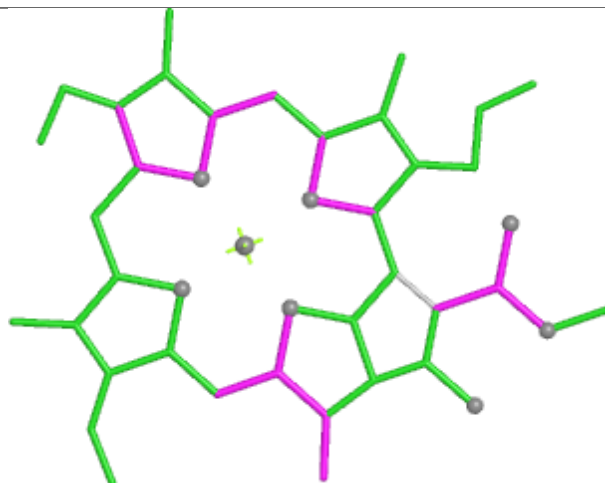




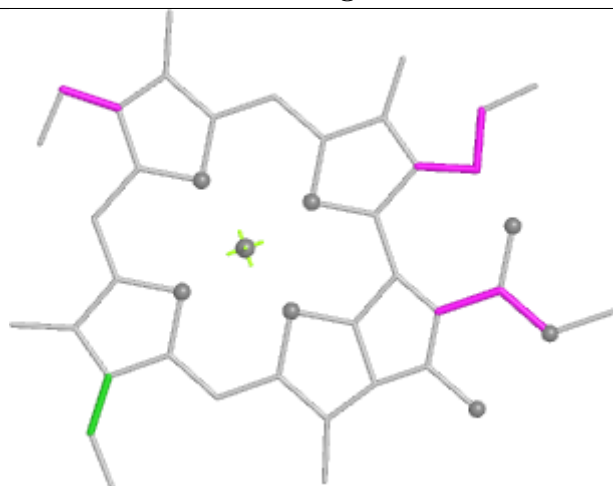
Ligand CLA f 615



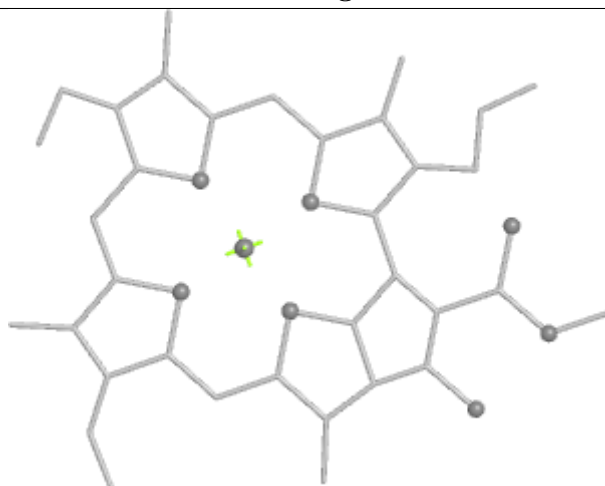
Bond lengths



Bond angles

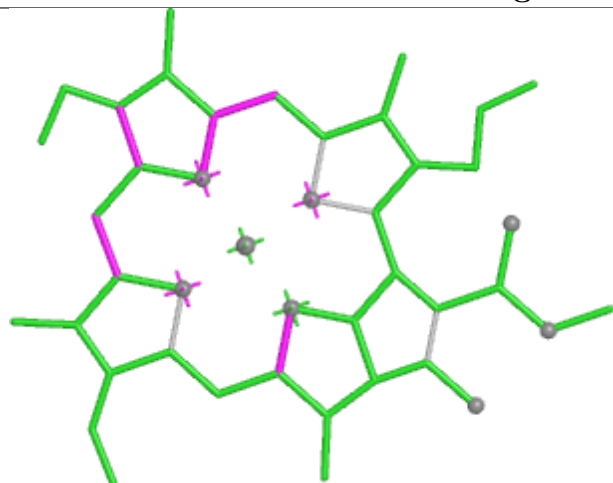


Torsions

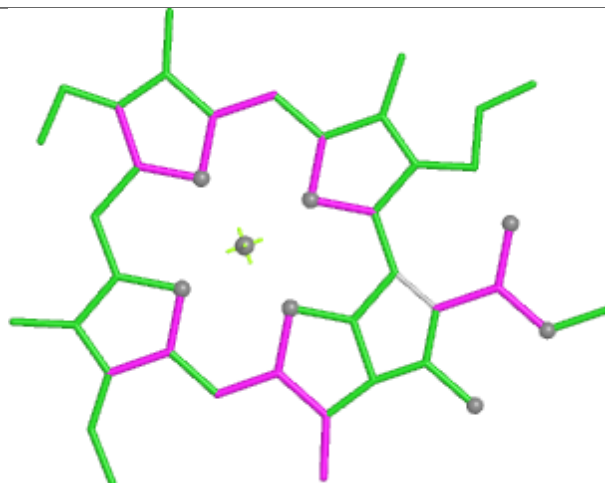


Rings

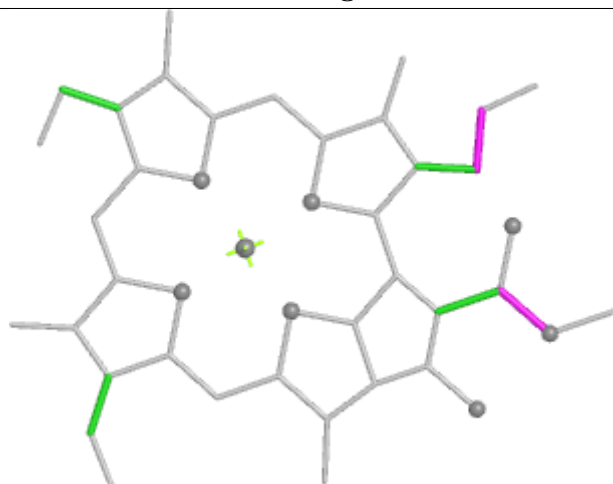
Ligand CLA A 778



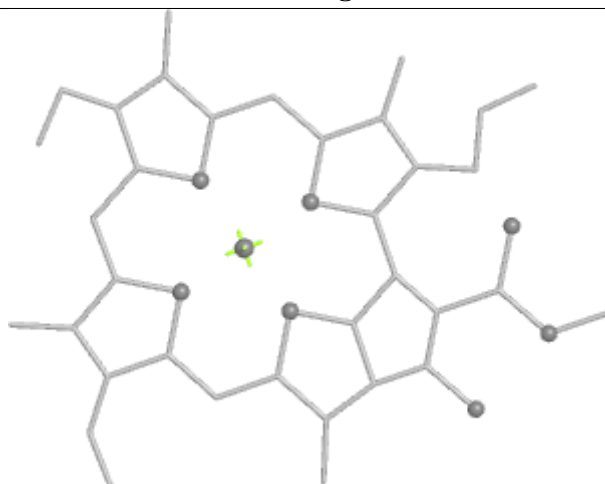
Bond lengths



Bond angles

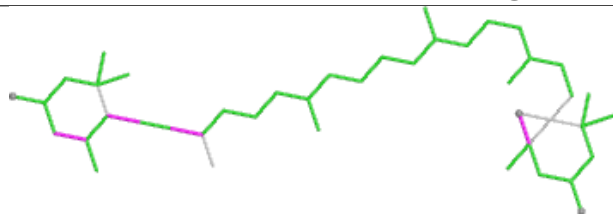


Torsions

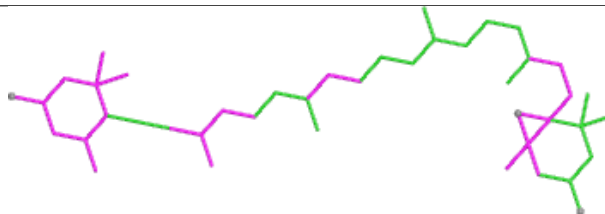


Rings

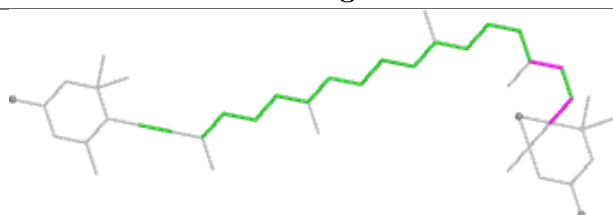
Ligand DD6 A 4002



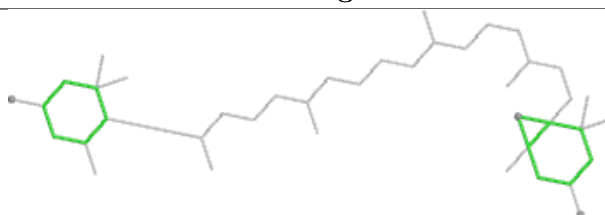
Bond lengths



Bond angles

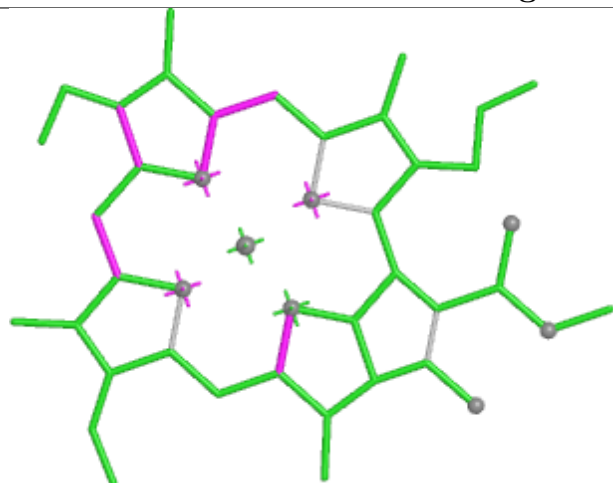


Torsions

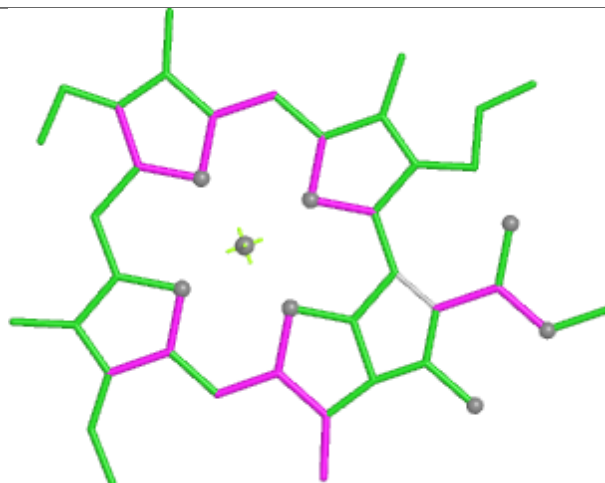


Rings

Ligand CLA e 607



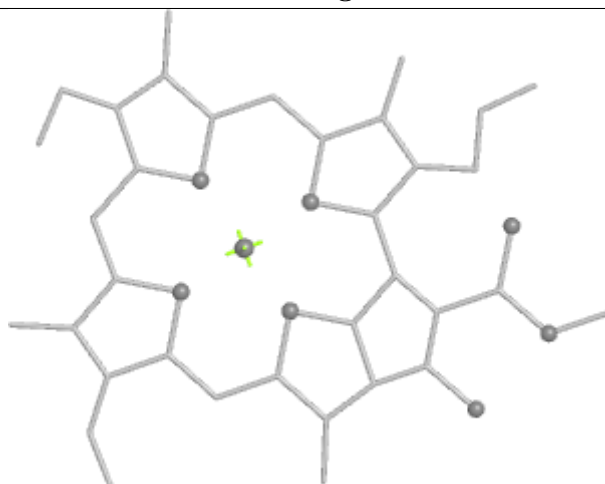
Bond lengths



Bond angles

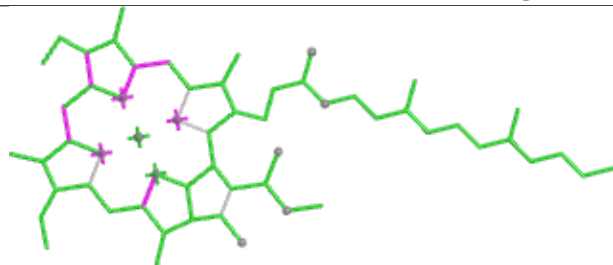


Torsions

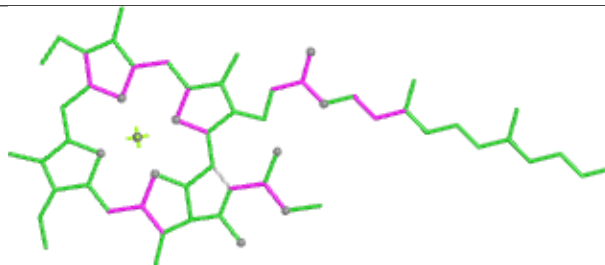


Rings

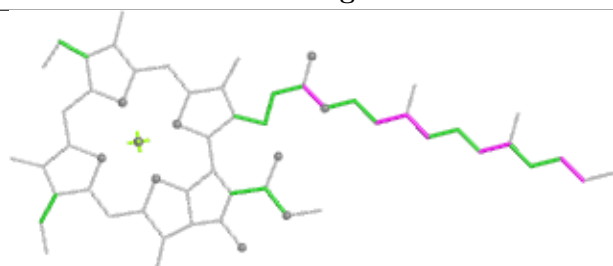
Ligand CLA h 612



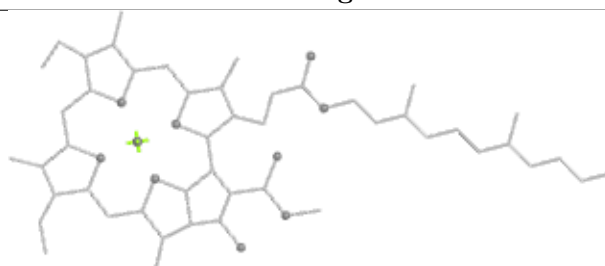
Bond lengths



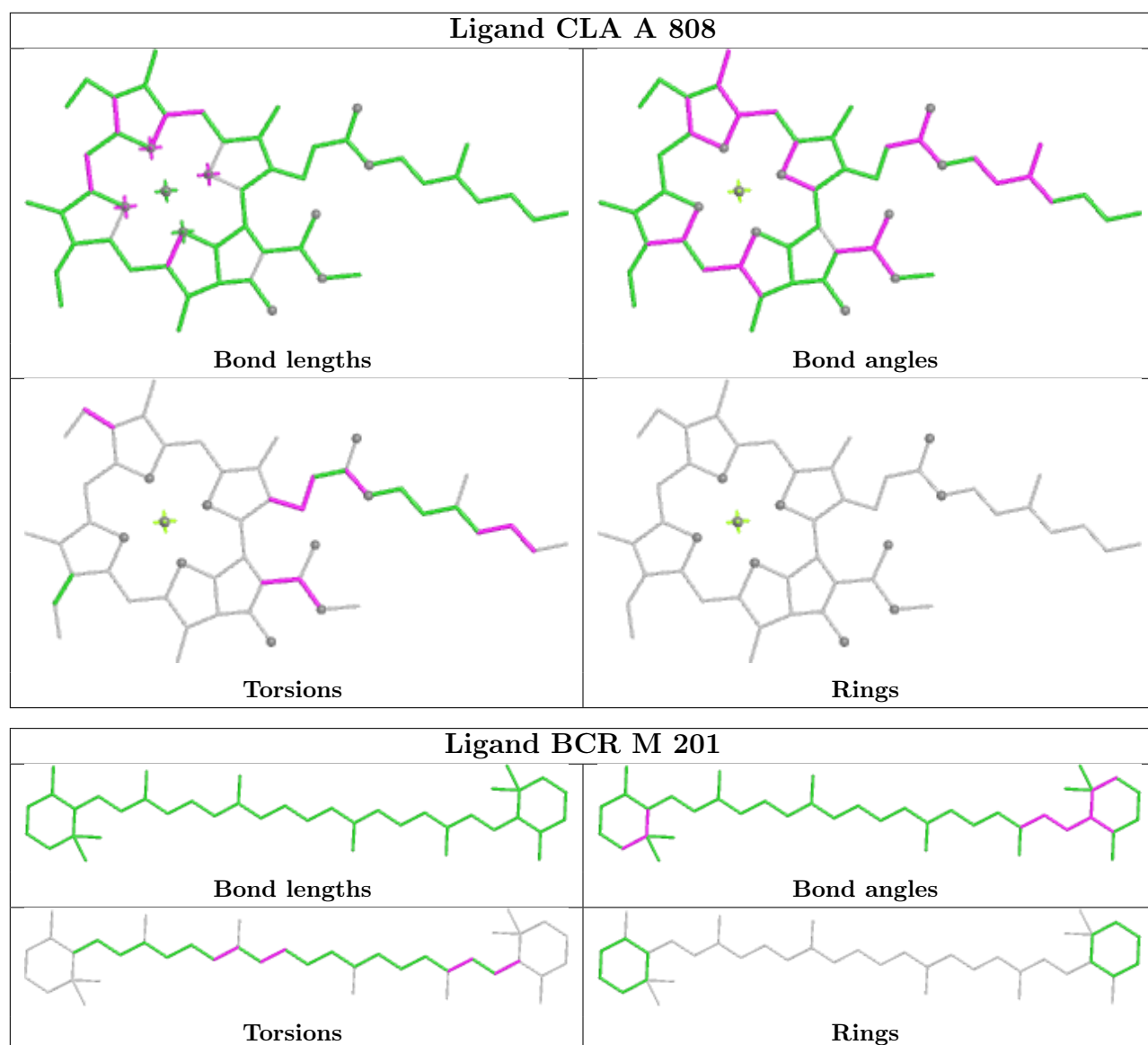
Bond angles



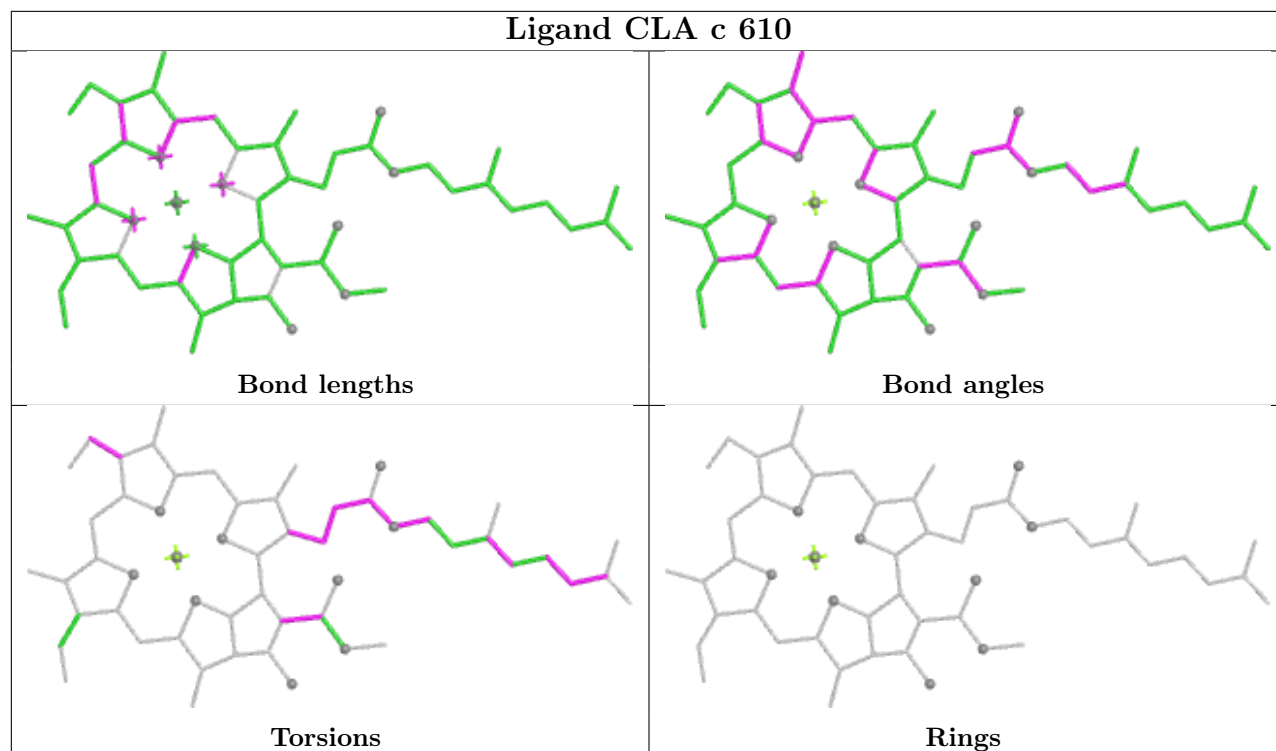
Torsions



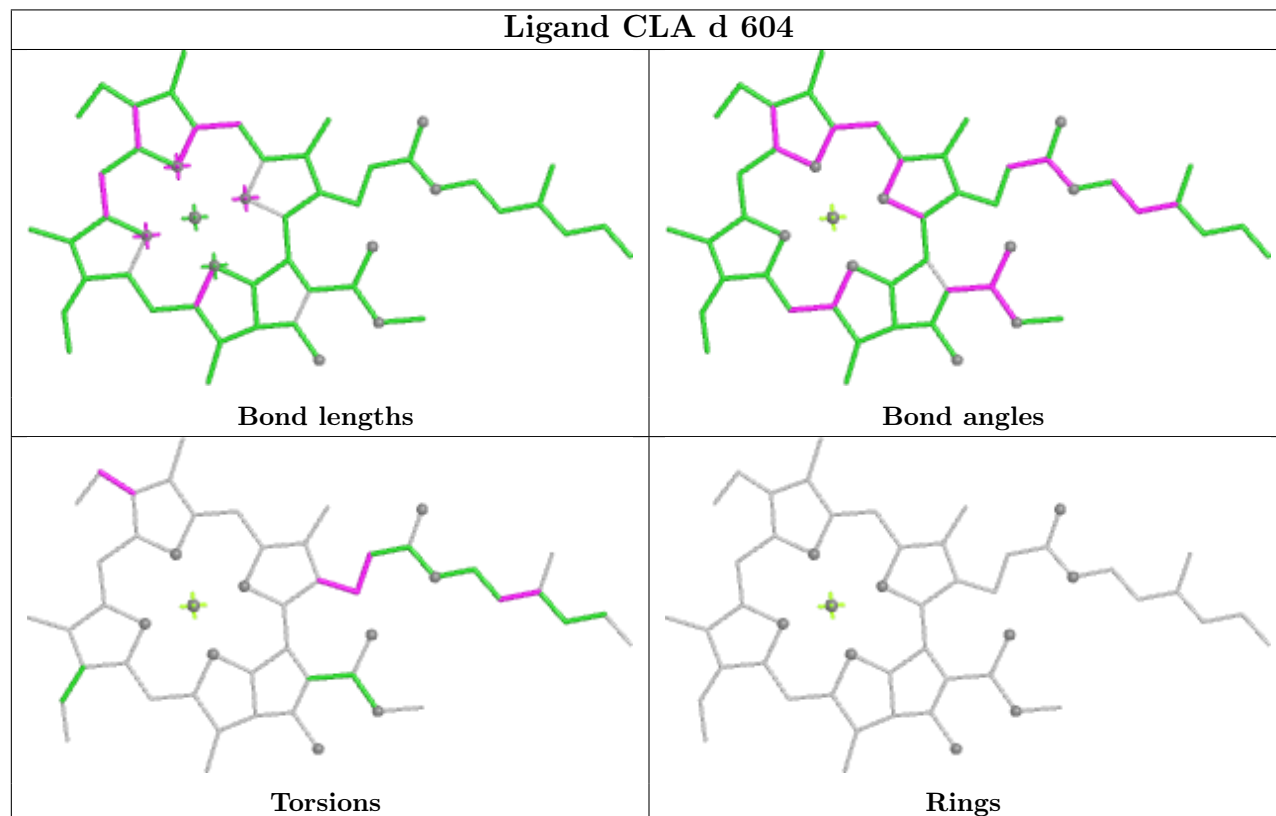
Rings

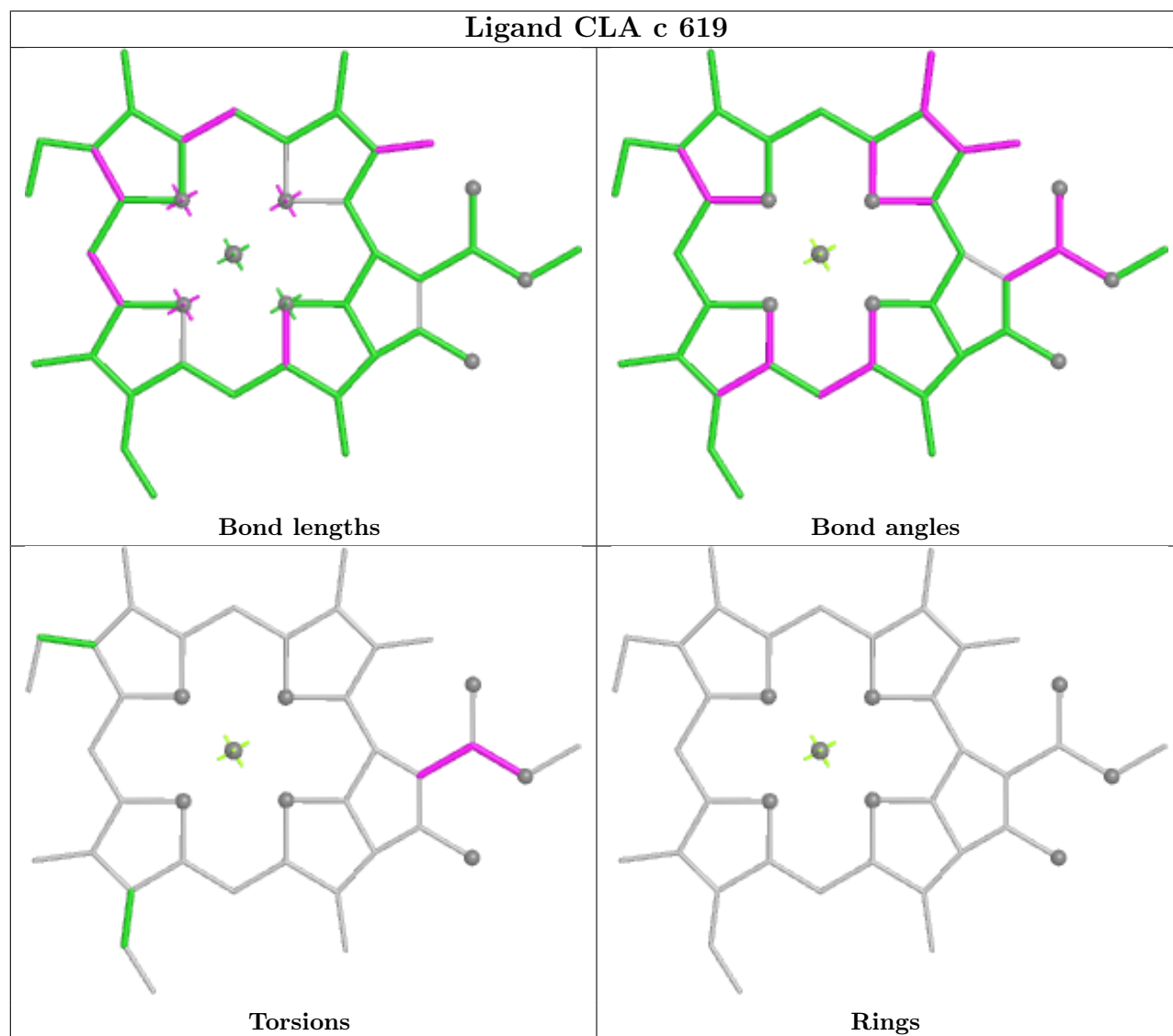
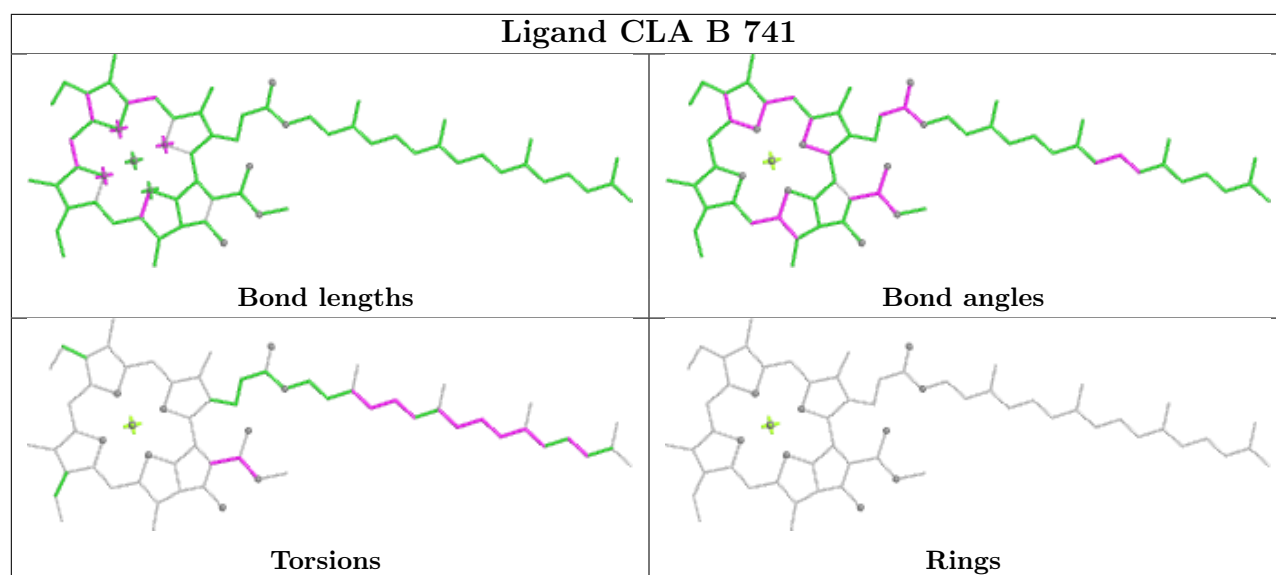


Ligand CLA c 610

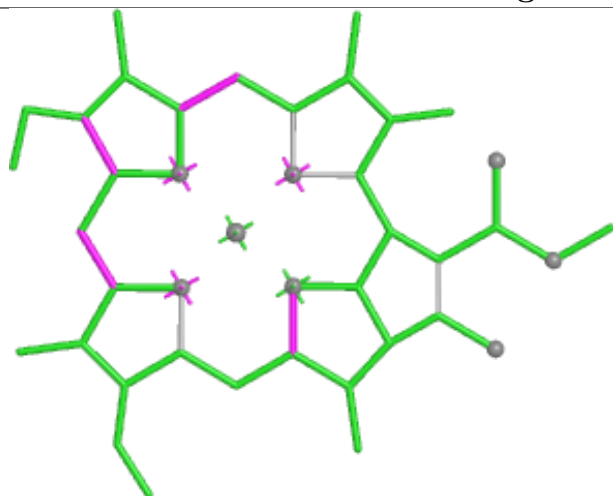


Ligand CLA d 604





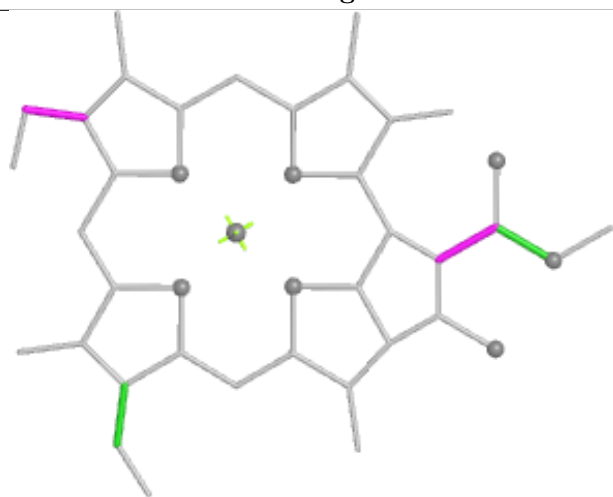
Ligand CLA n 610



Bond lengths



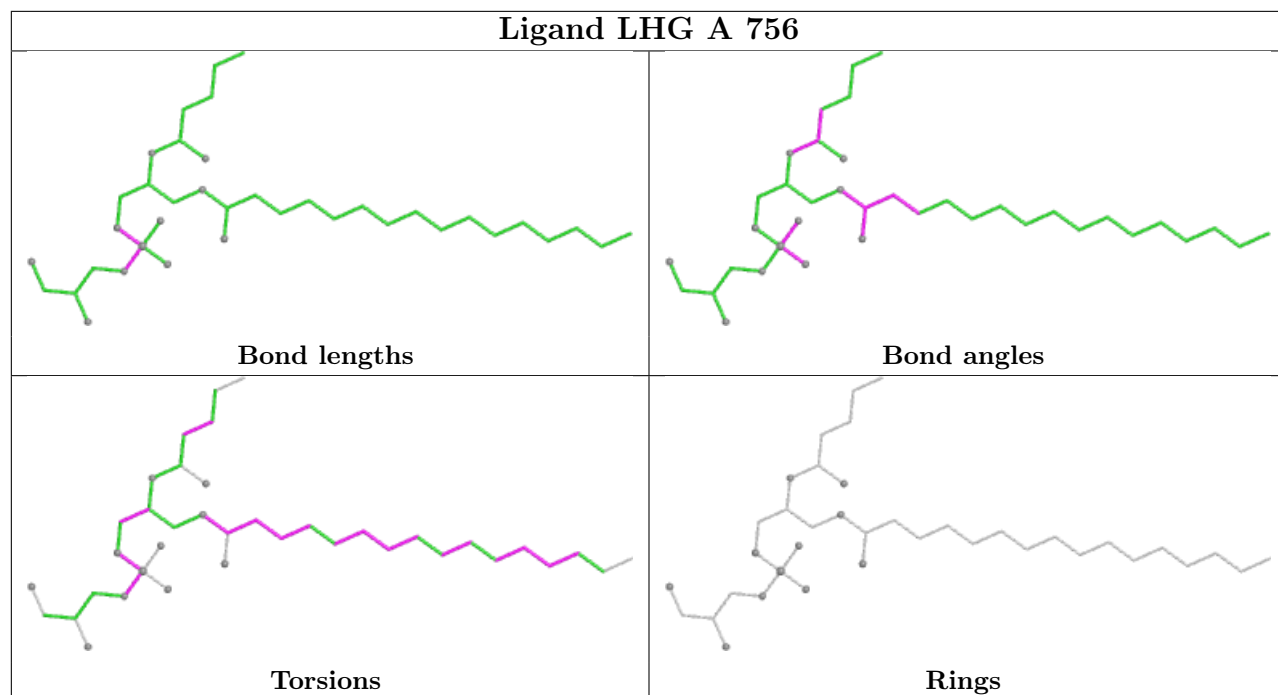
Bond angles



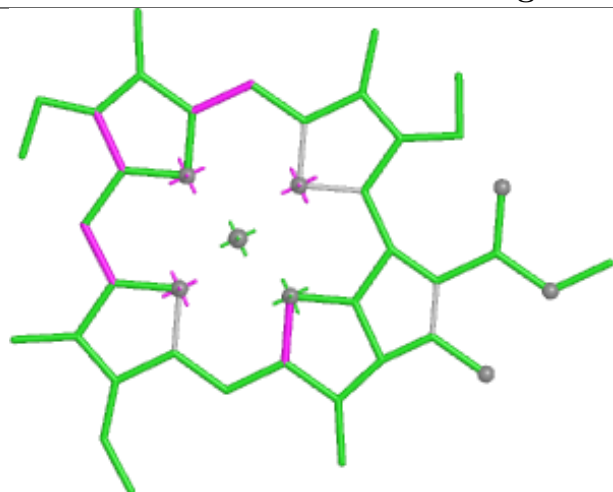
Torsions



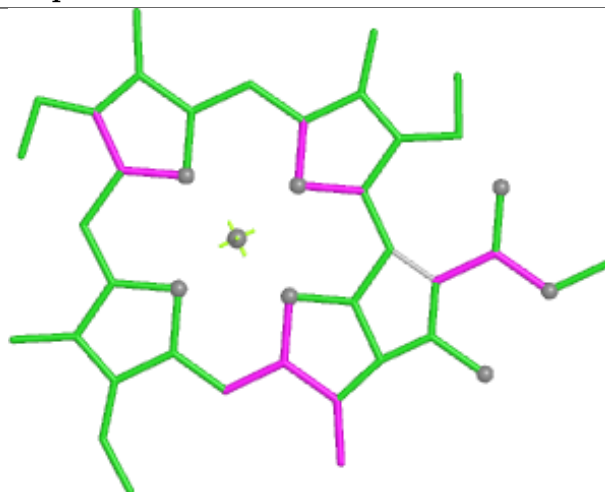
Rings



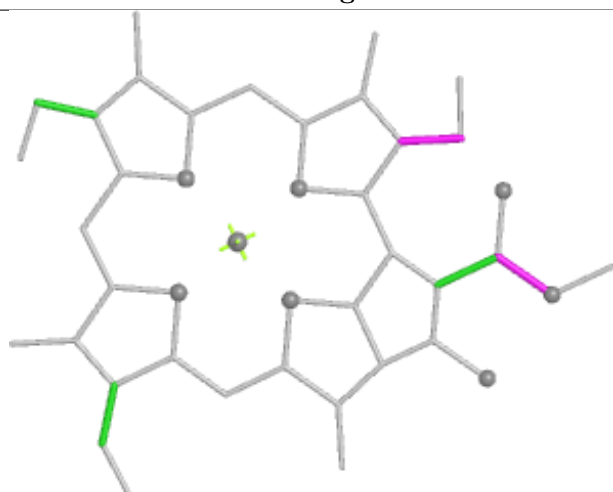
Ligand CLA p 603



Bond lengths



Bond angles

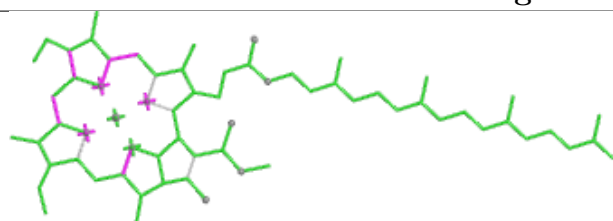


Torsions

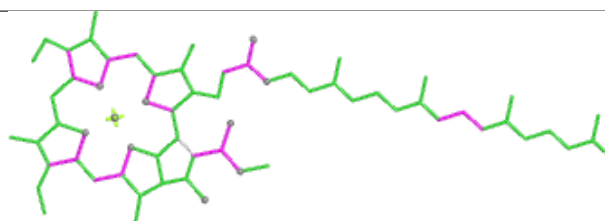


Rings

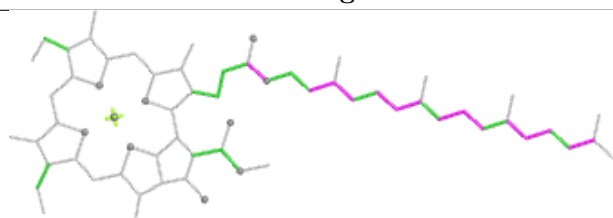
Ligand CLA B 752



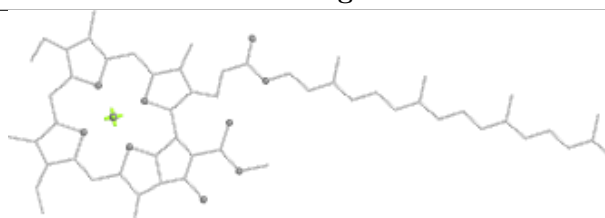
Bond lengths



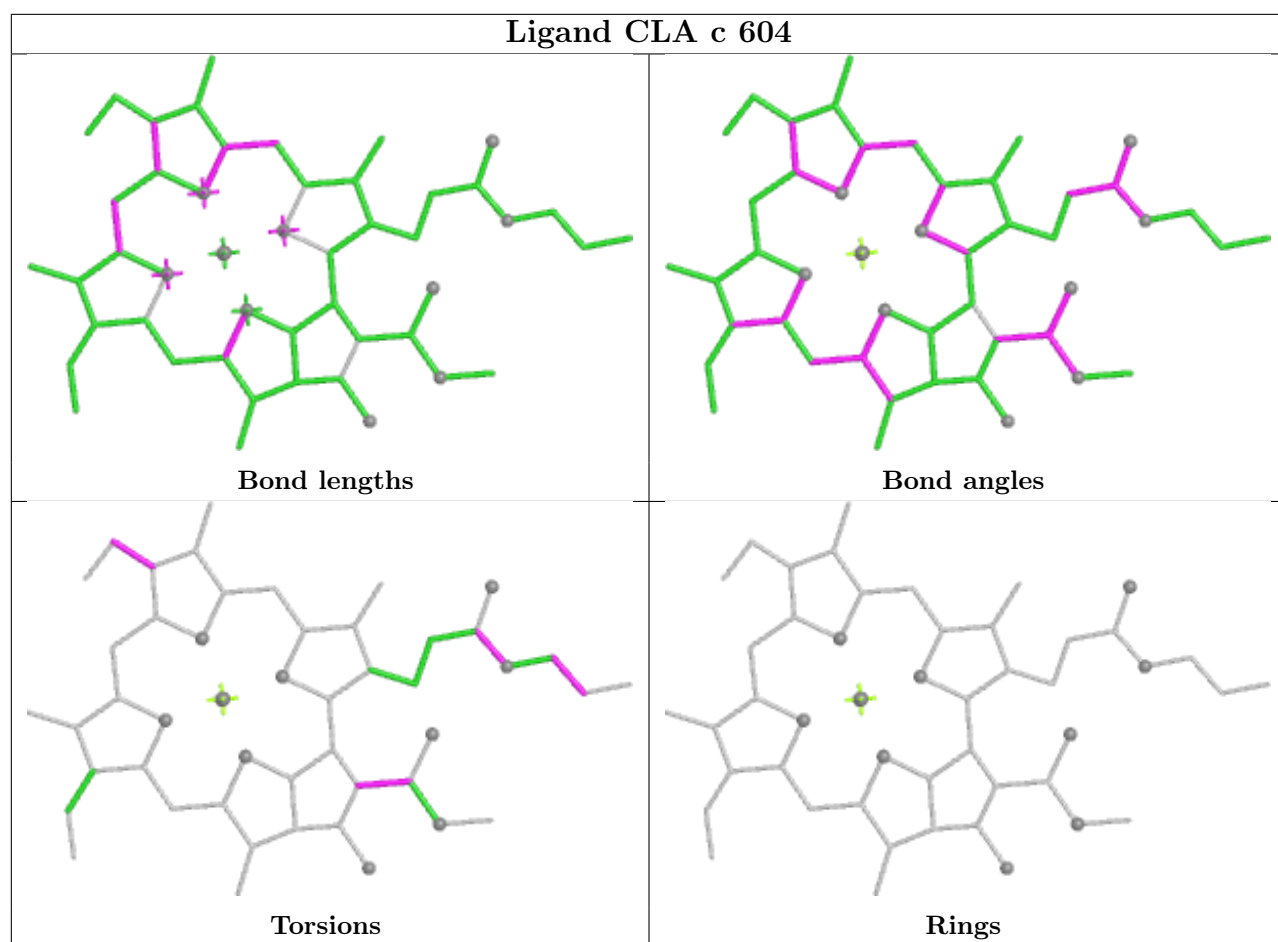
Bond angles



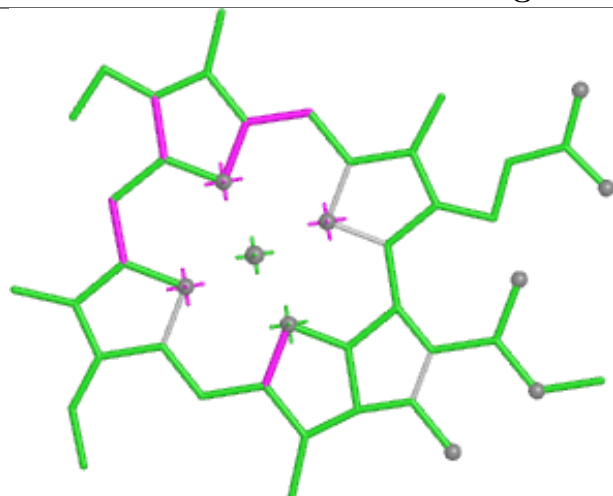
Torsions



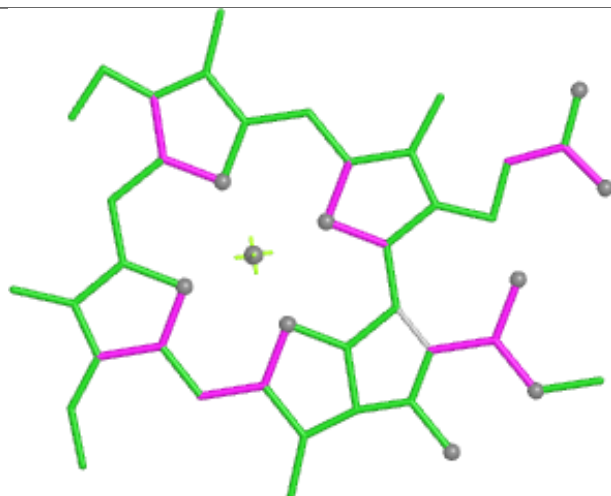
Rings



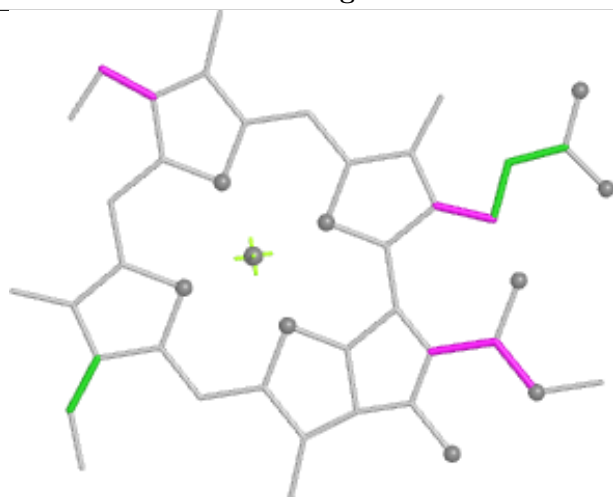
Ligand CLA A 757



Bond lengths



Bond angles

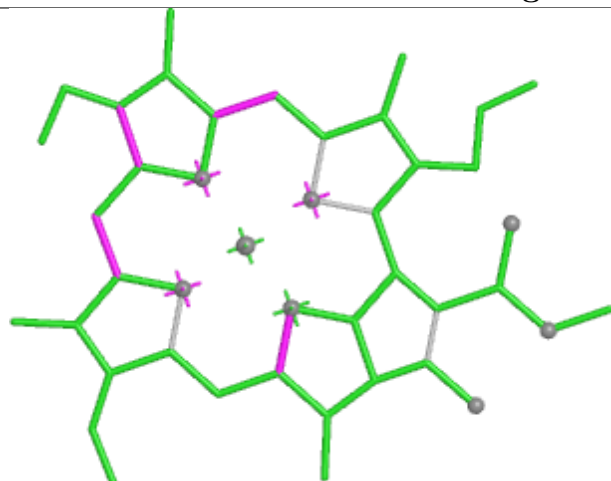


Torsions

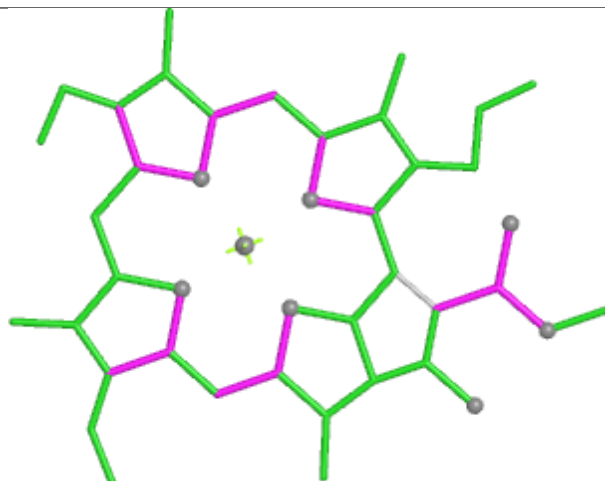


Rings

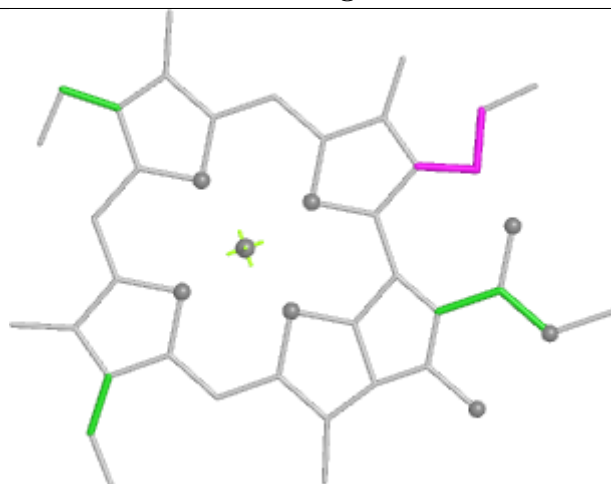
Ligand CLA 1 611



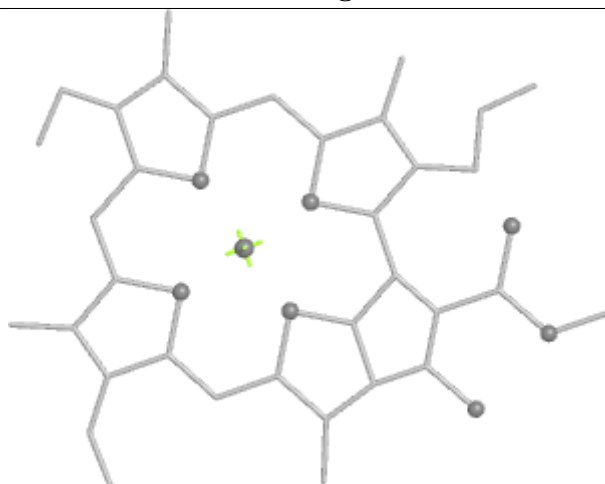
Bond lengths



Bond angles

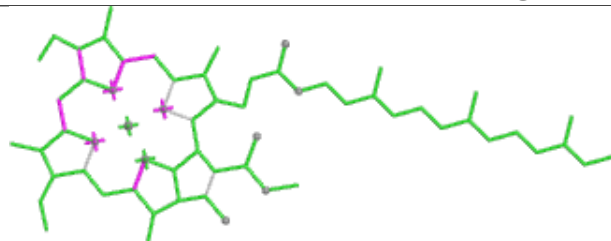


Torsions

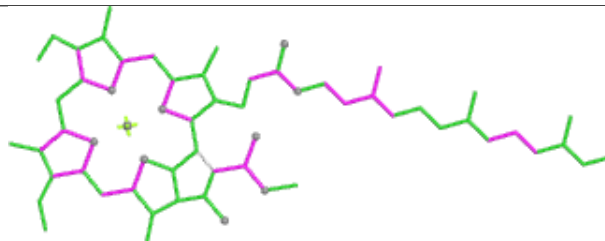


Rings

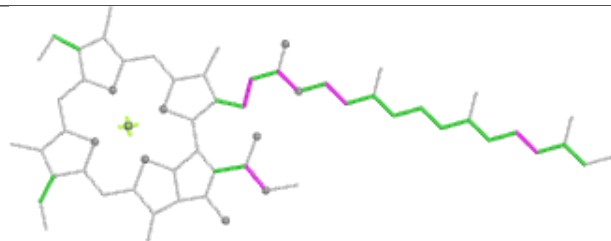
Ligand CLA B 773



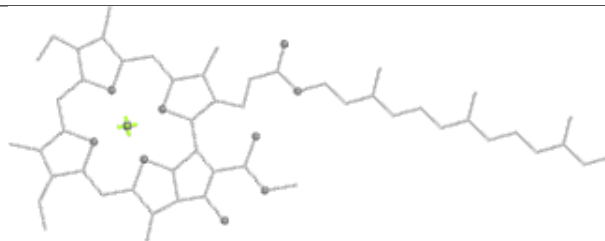
Bond lengths



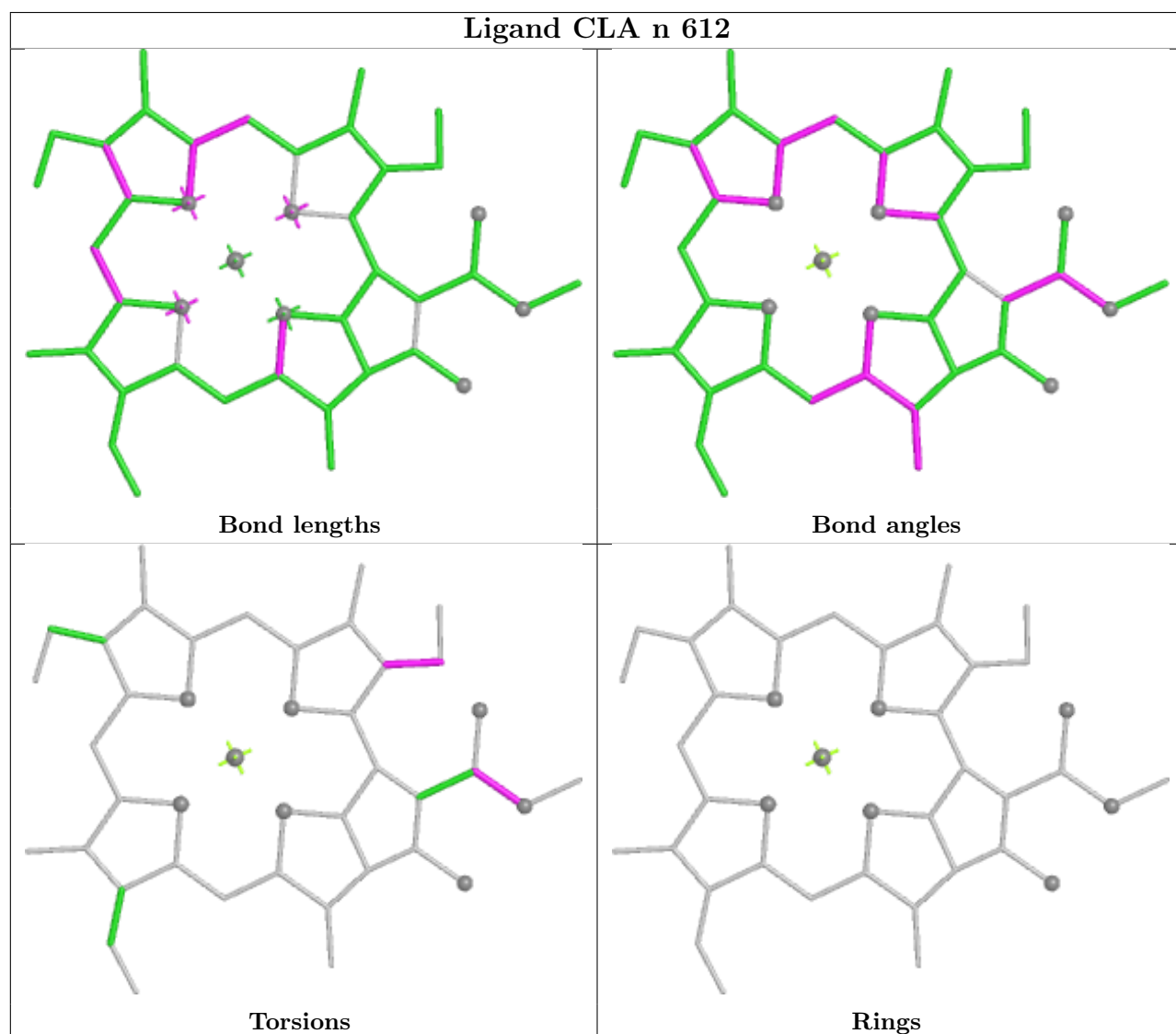
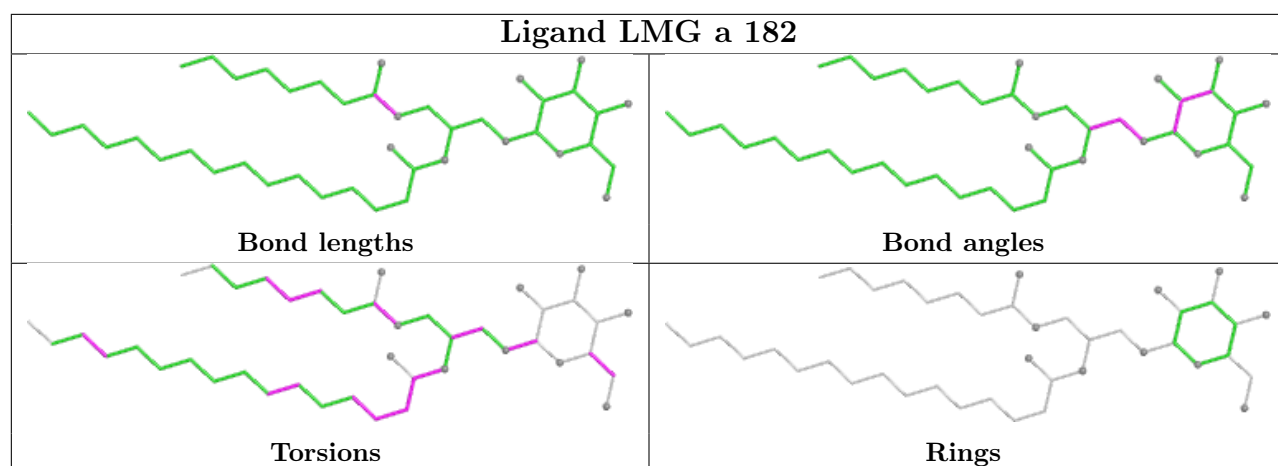
Bond angles



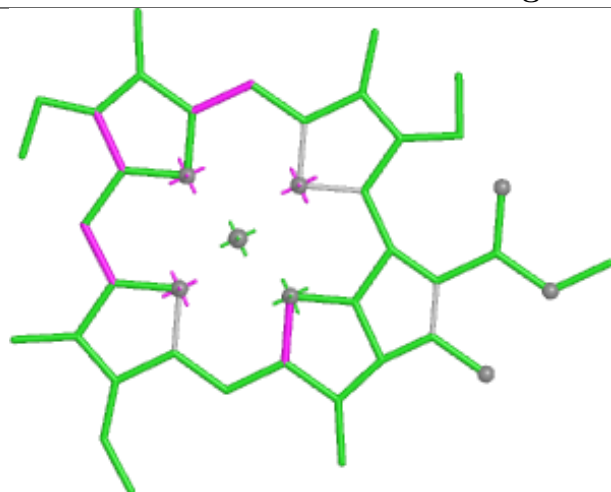
Torsions



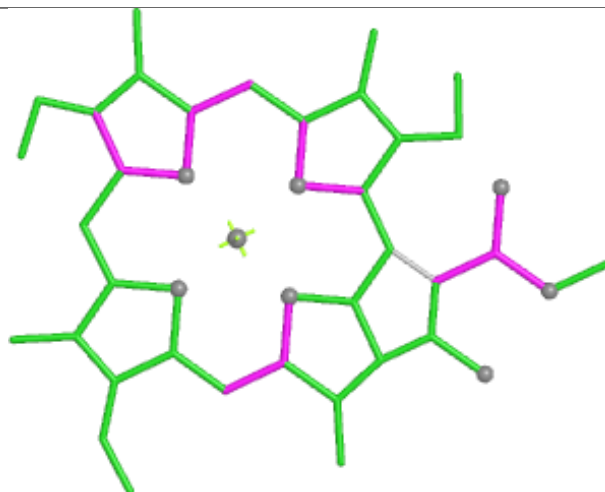
Rings



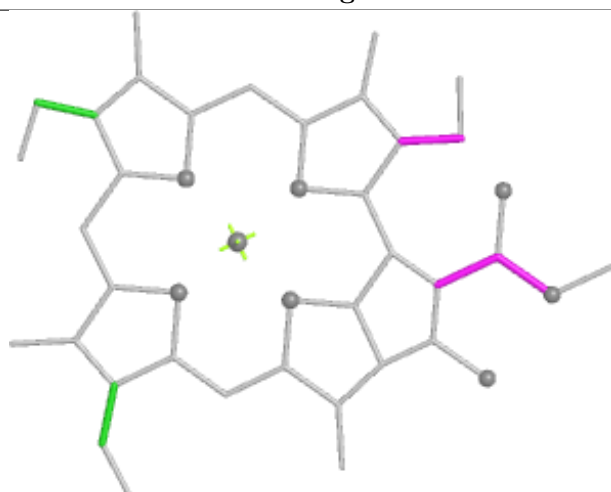
Ligand CLA 1 601



Bond lengths



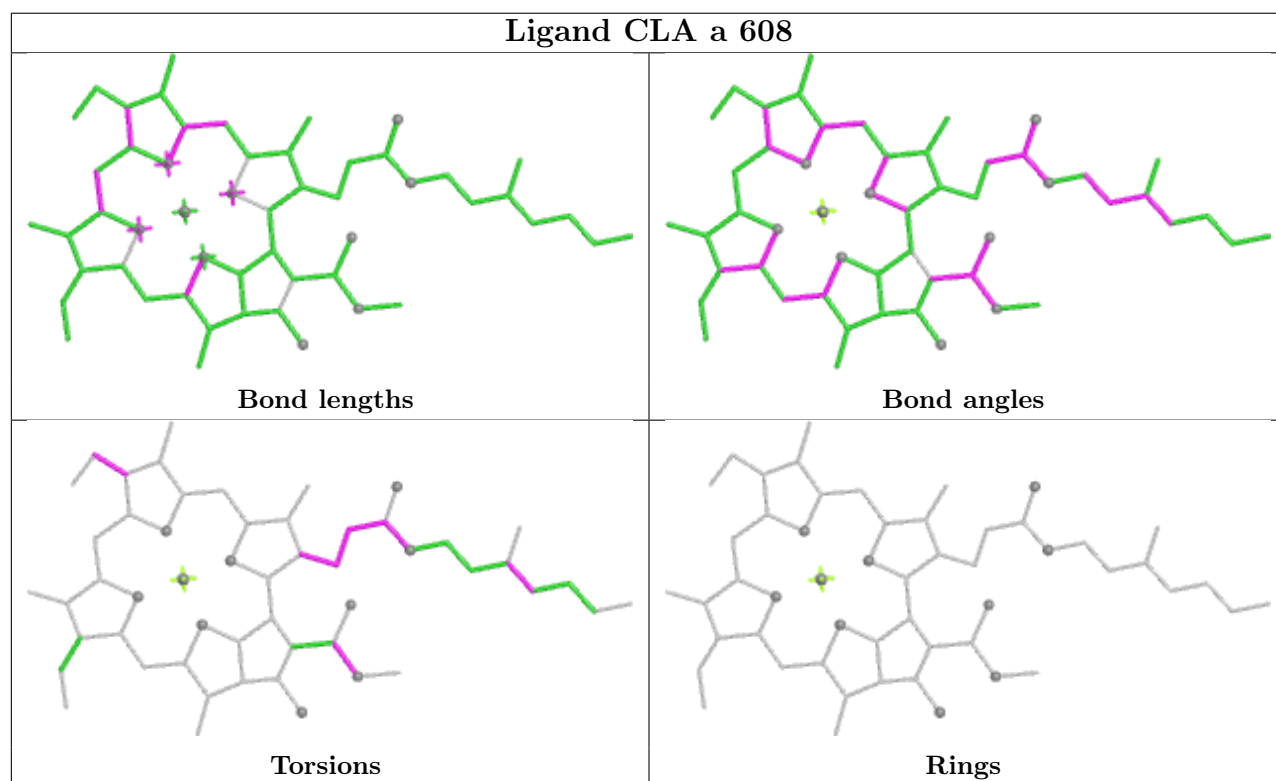
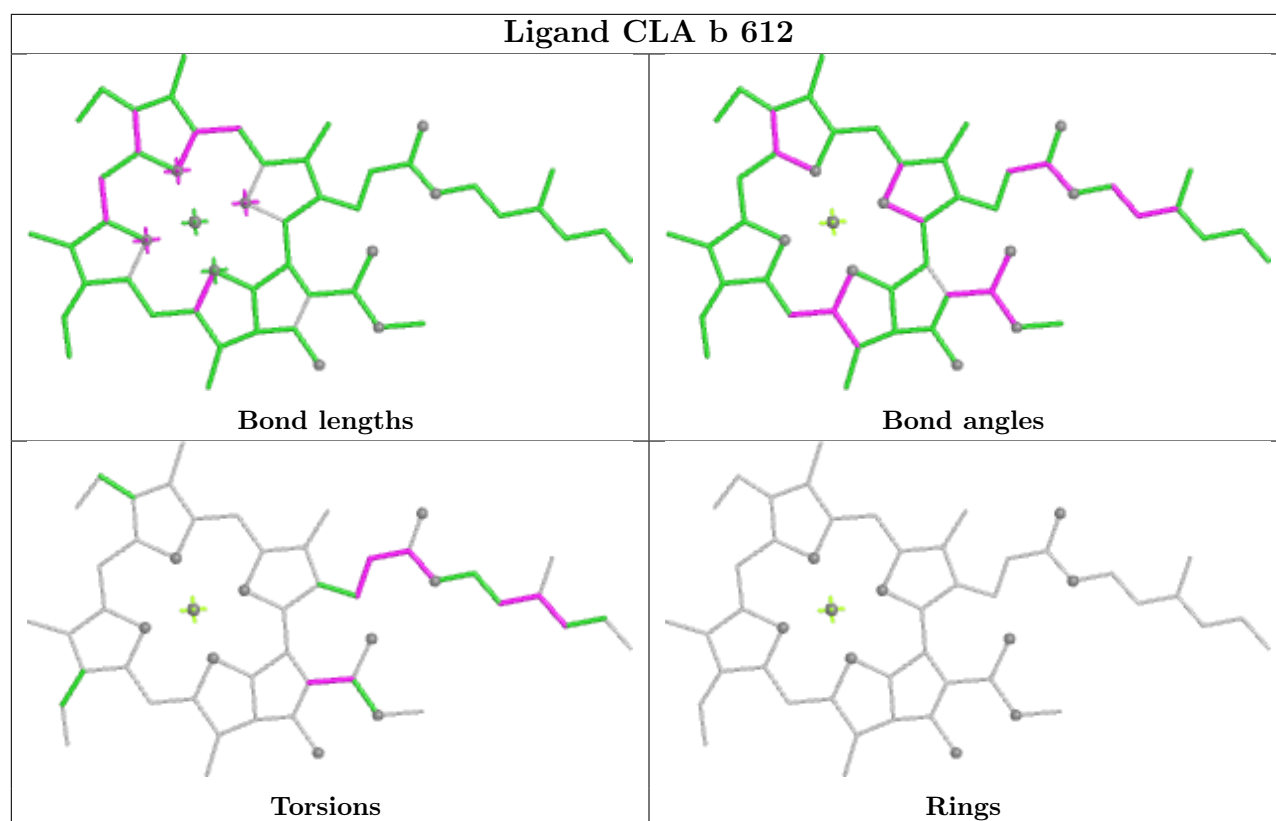
Bond angles

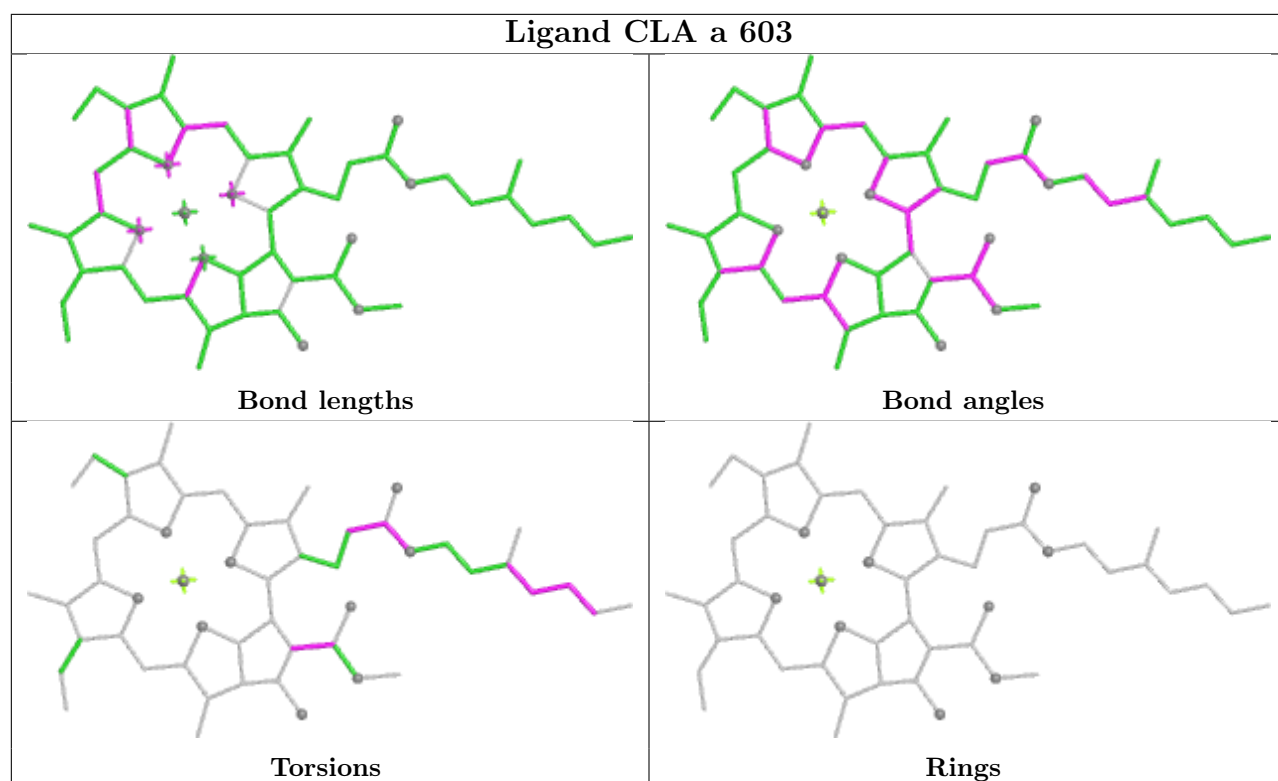


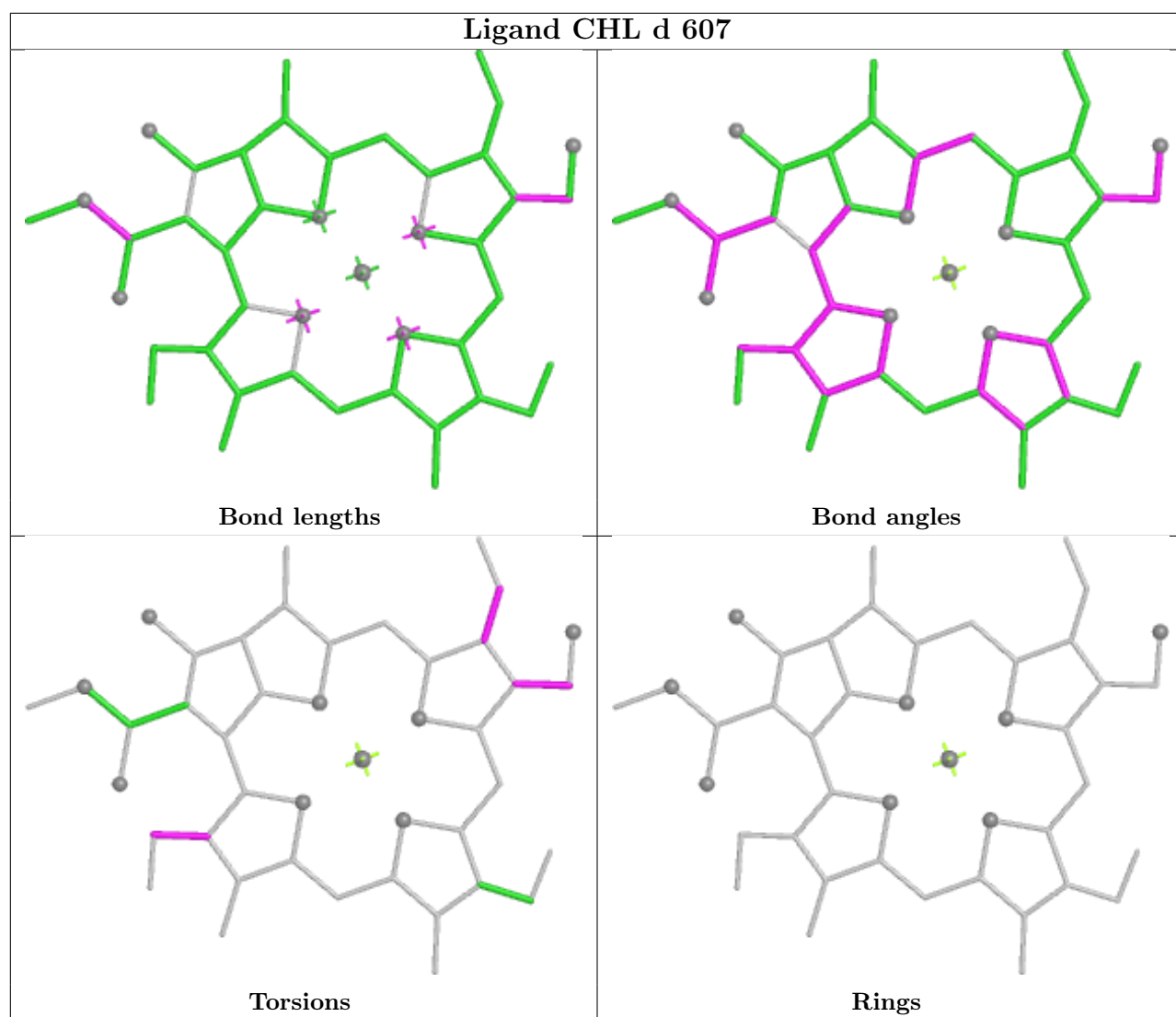
Torsions



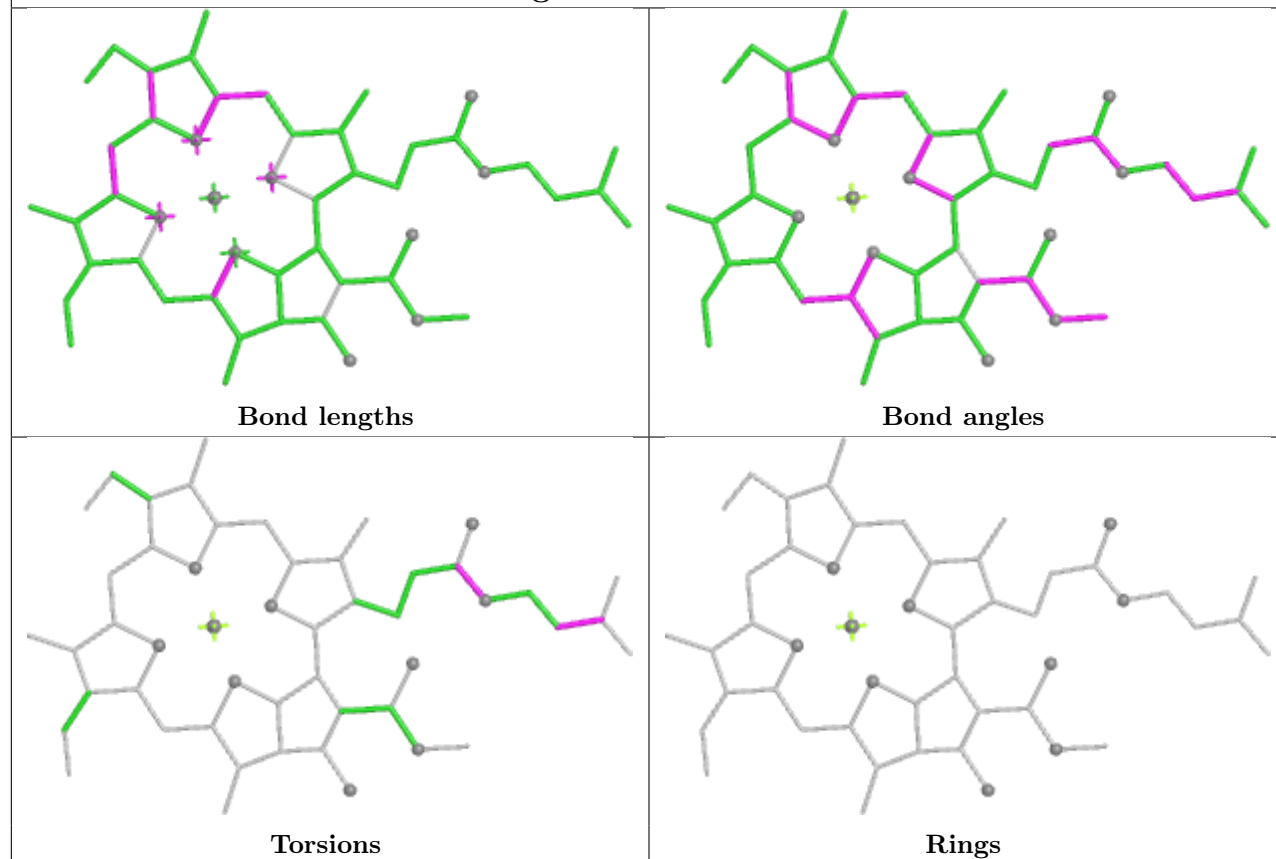
Rings



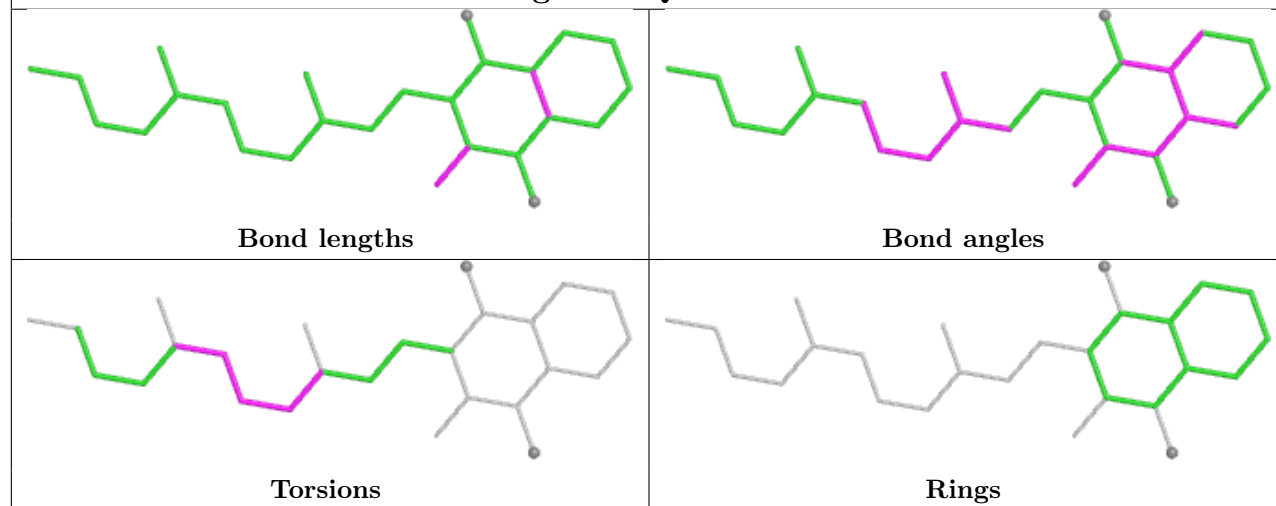


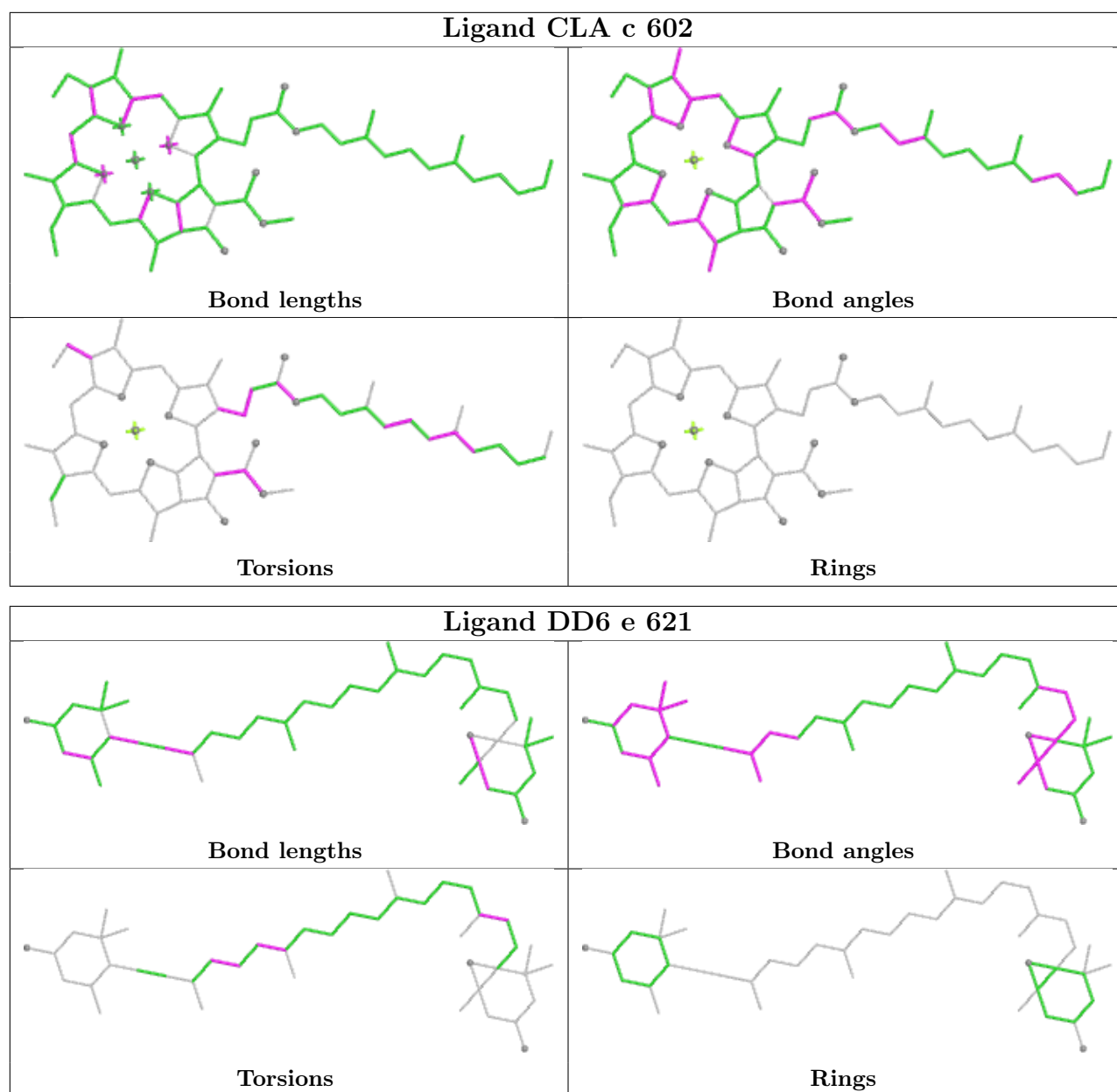


Ligand CLA B 783

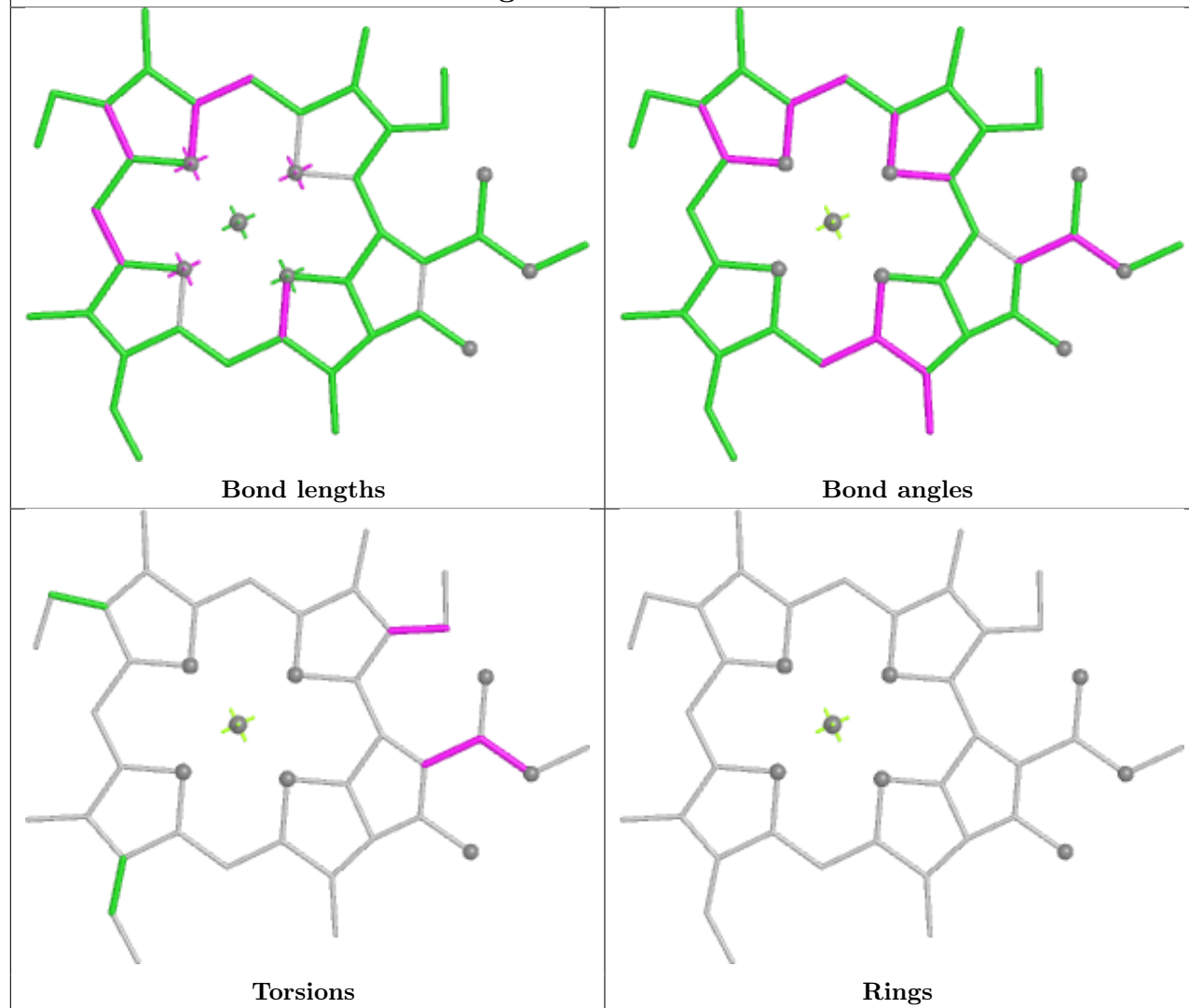


Ligand PQN d 223

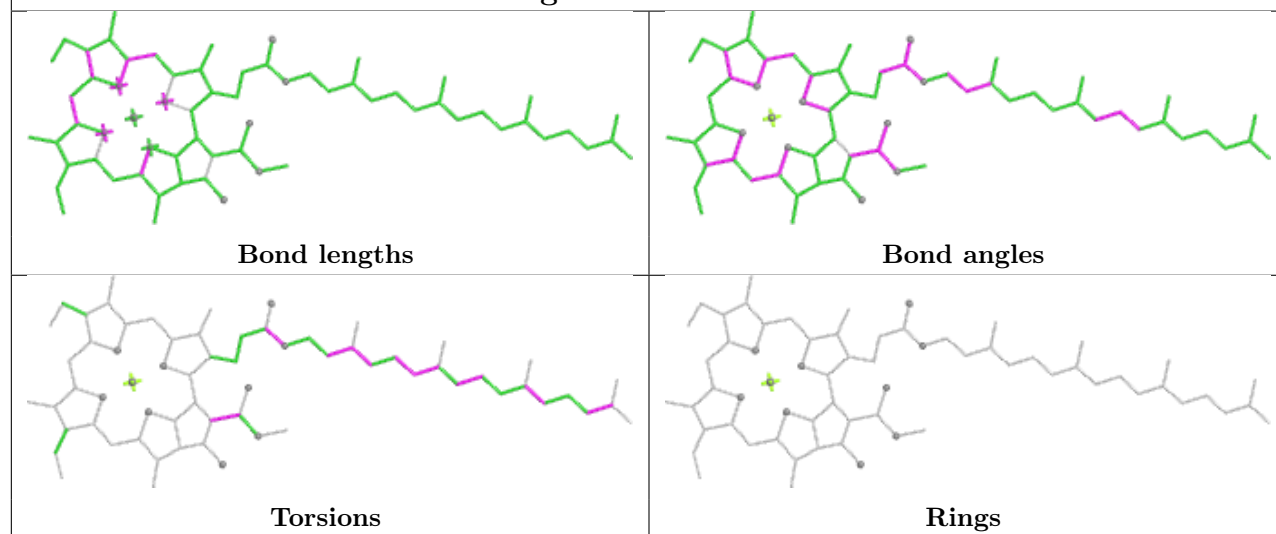


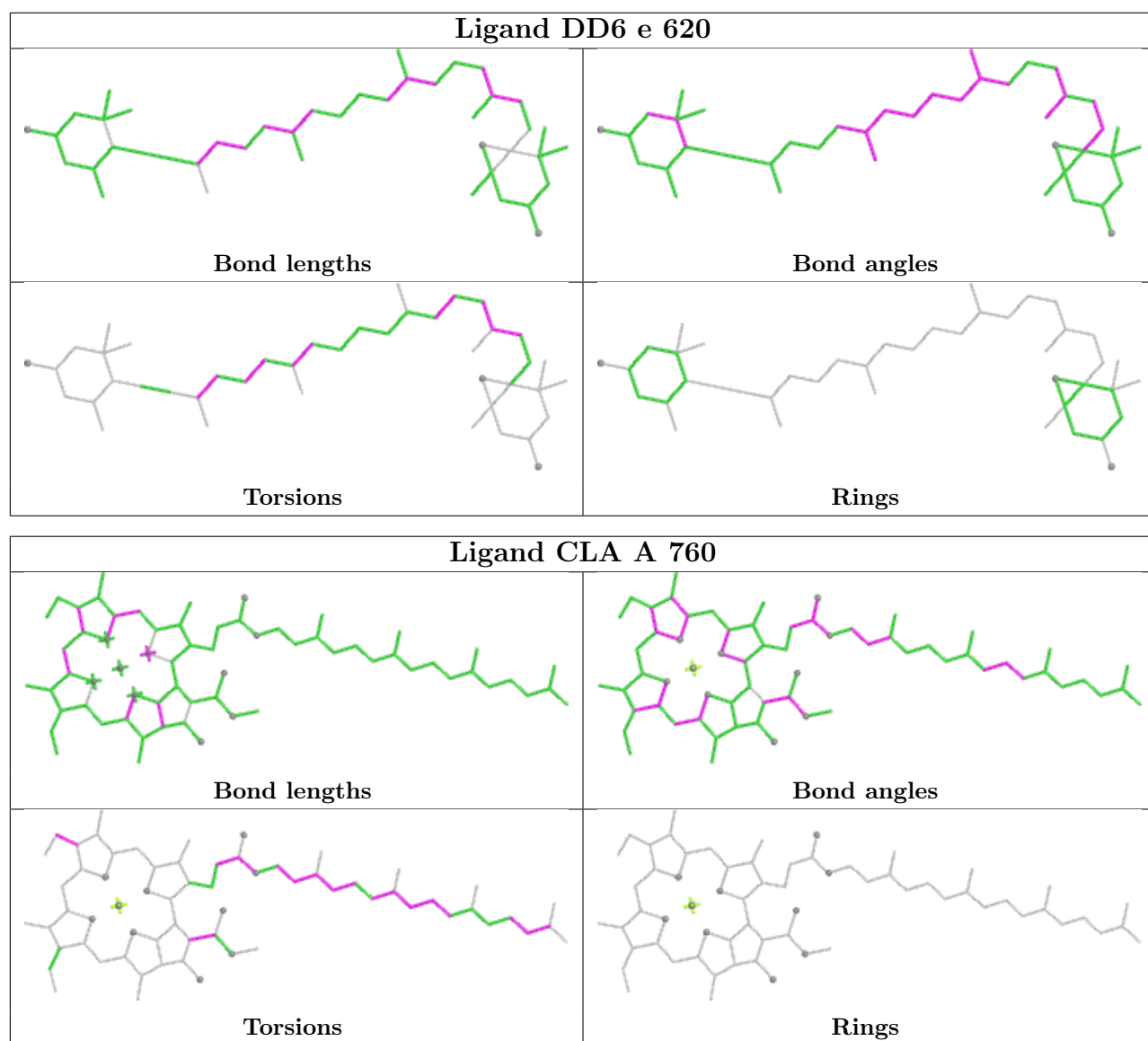


Ligand CLA d 603

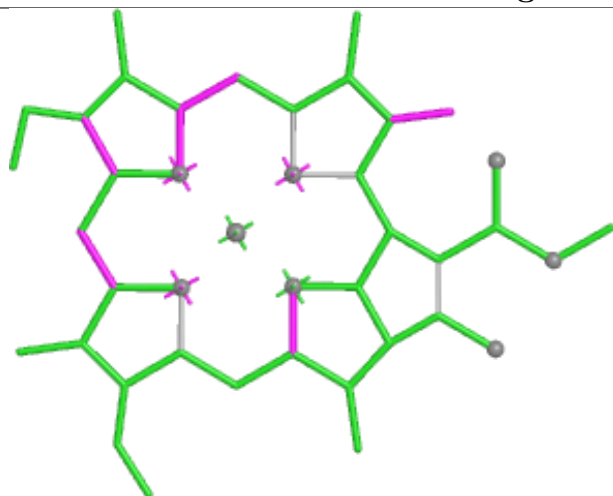


Ligand CLA i 608





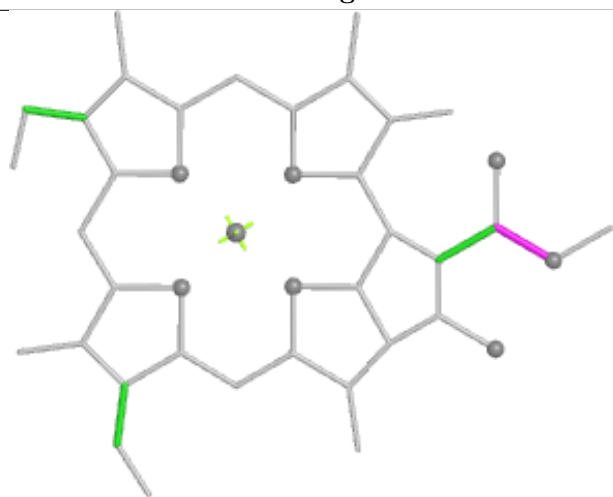
Ligand CLA n 608



Bond lengths



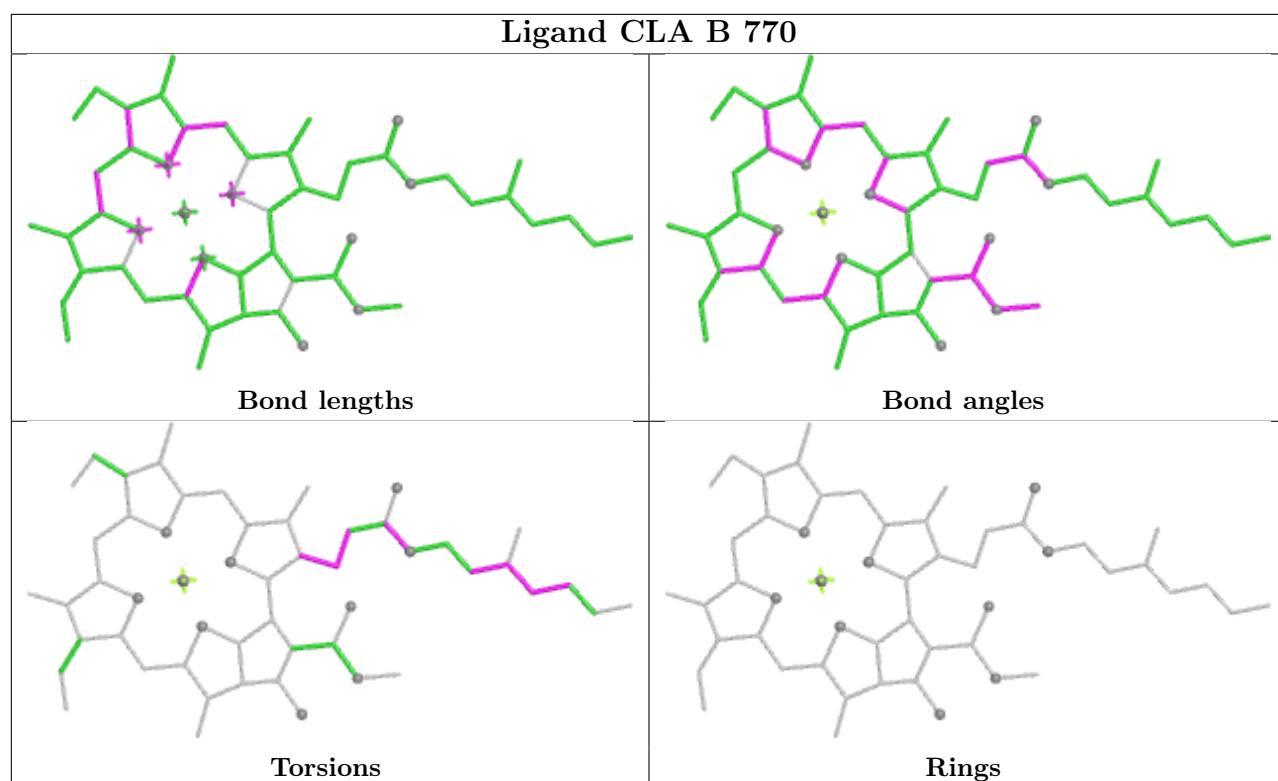
Bond angles



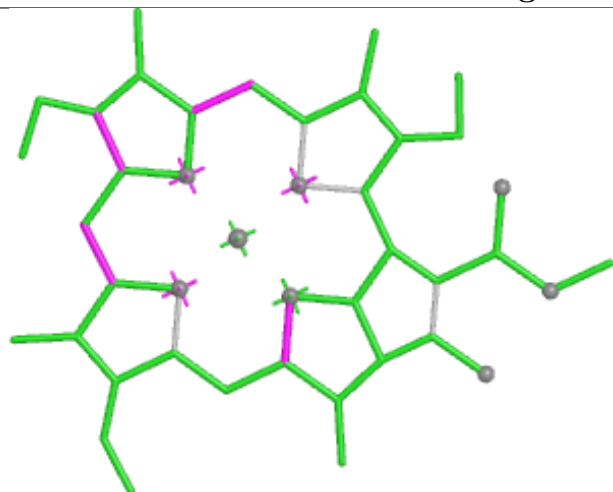
Torsions



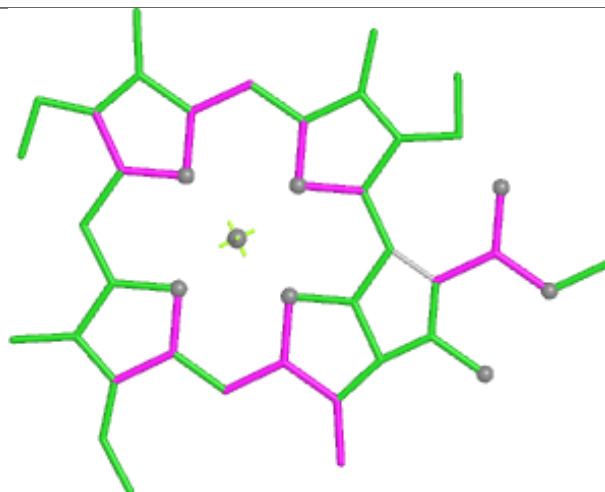
Rings



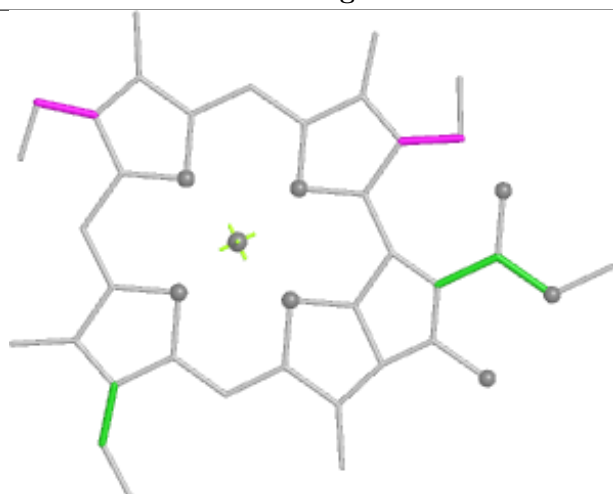
Ligand CLA o 604



Bond lengths



Bond angles

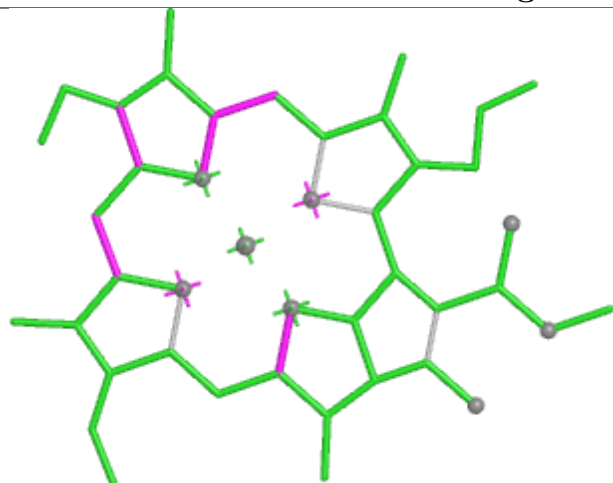


Torsions

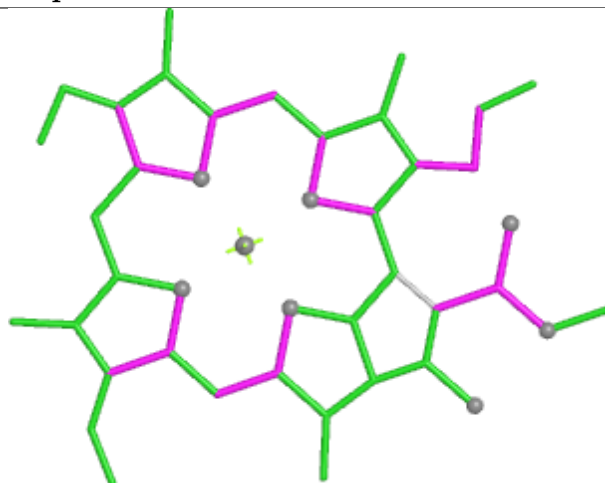


Rings

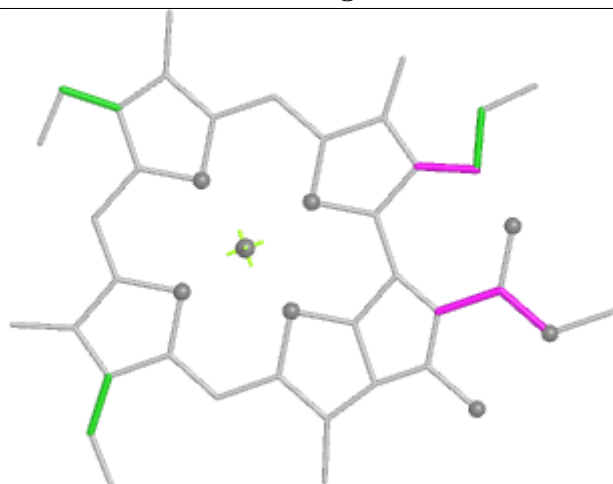
Ligand CLA p 612



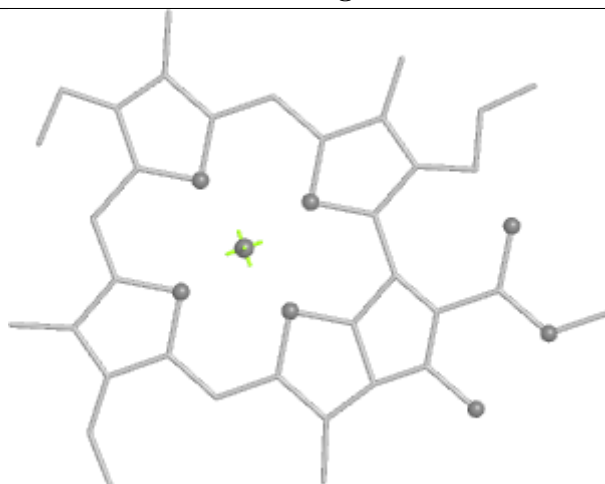
Bond lengths



Bond angles

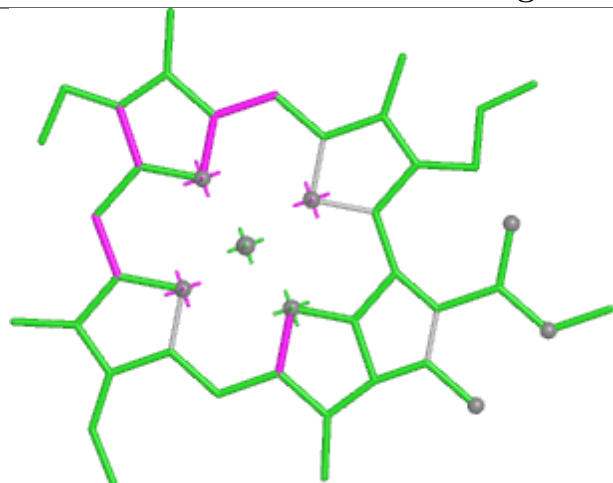


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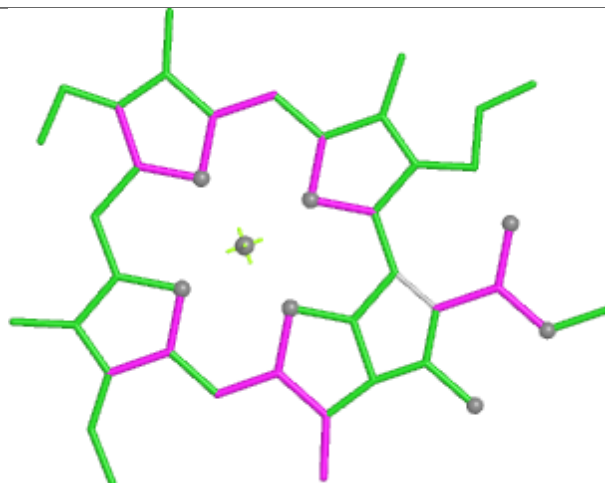


Rings

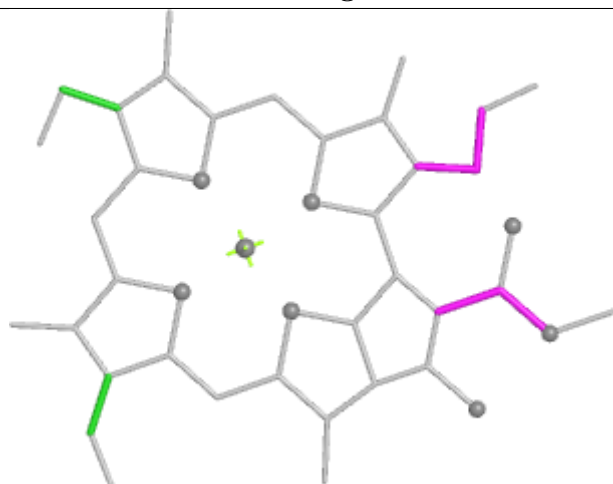
Ligand CLA h 603



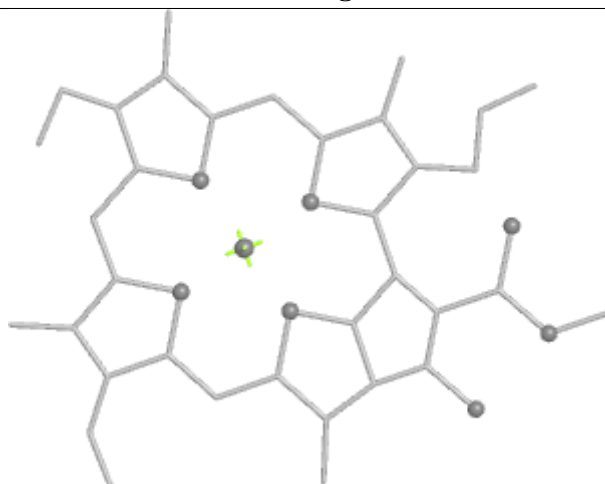
Bond lengths



Bond angles

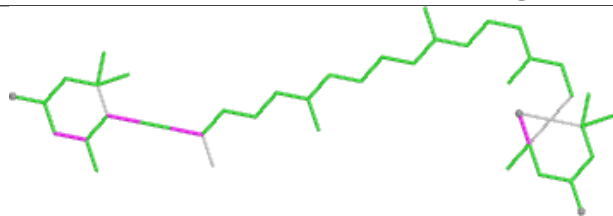


Torsions

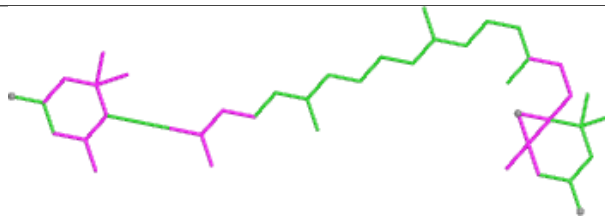


Rings

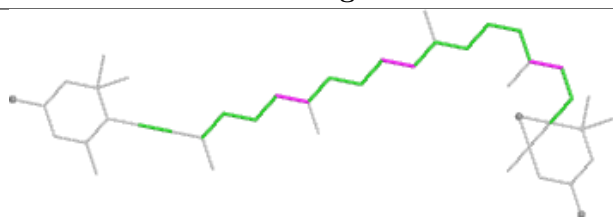
Ligand DD6 m 620



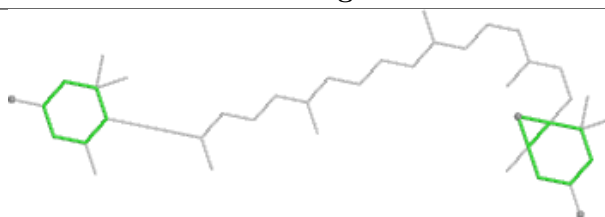
Bond lengths



Bond angles

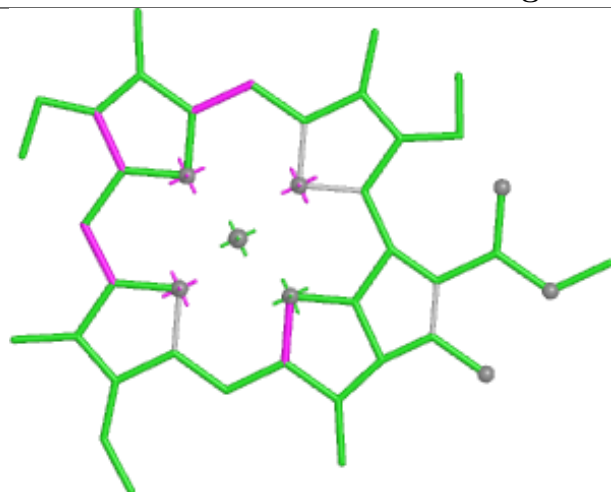


Torsions

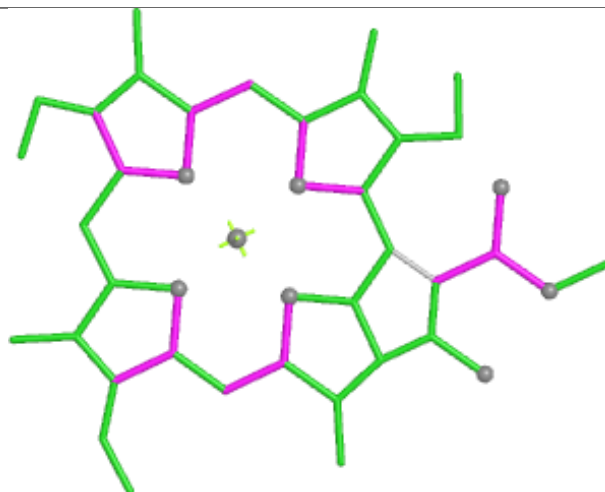


Rings

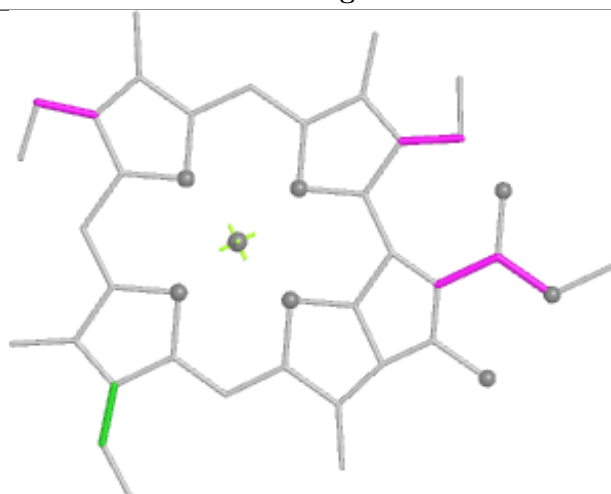
Ligand CLA f 601



Bond lengths



Bond angles

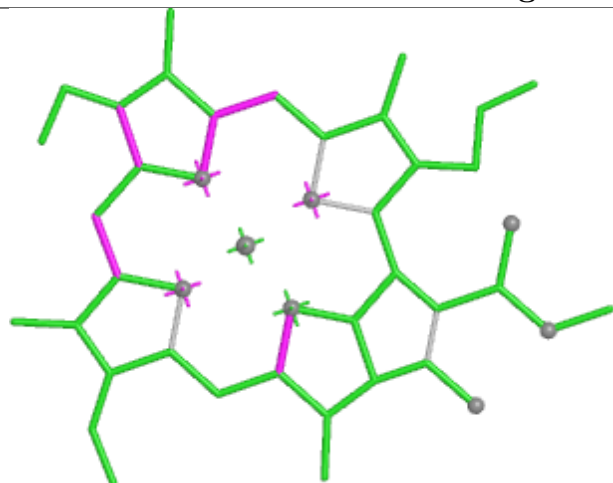


Torsions

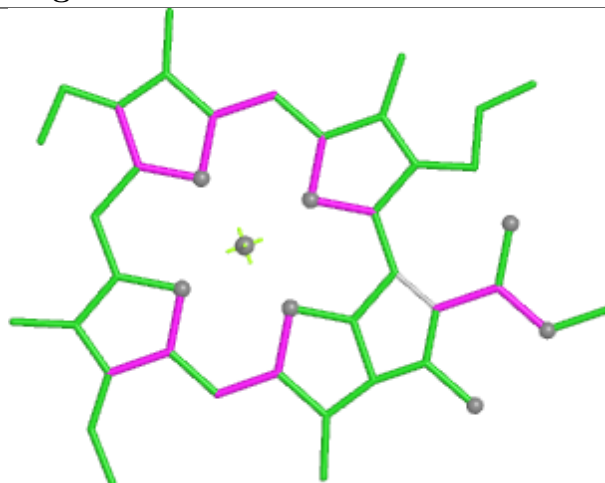


Rings

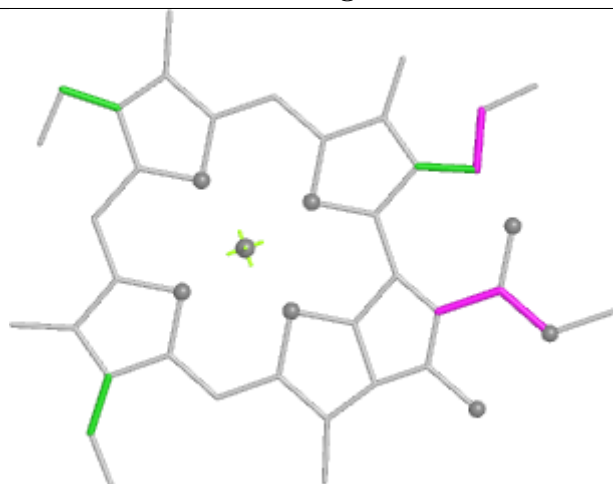
Ligand CLA g 604



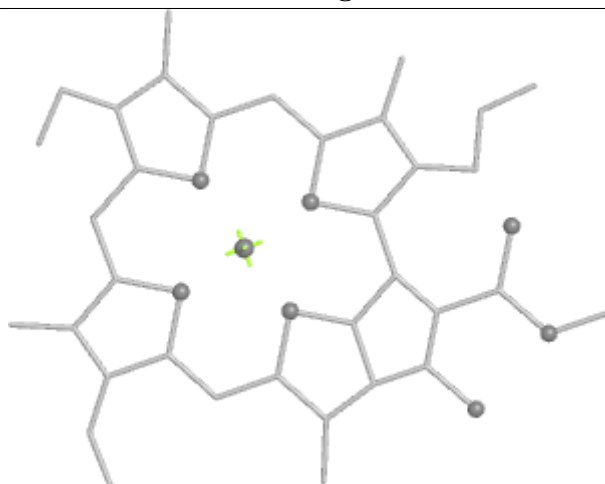
Bond lengths



Bond angles

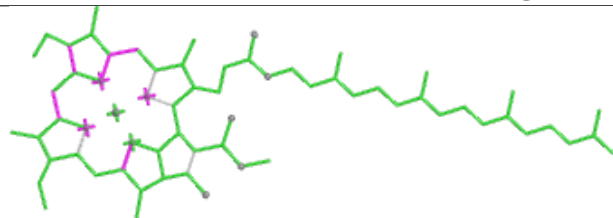


Torsions

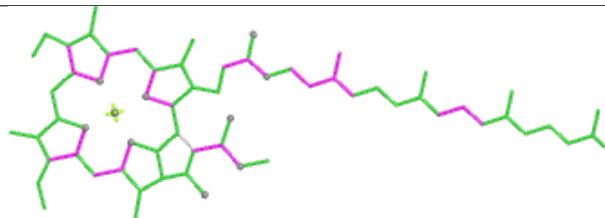


Rings

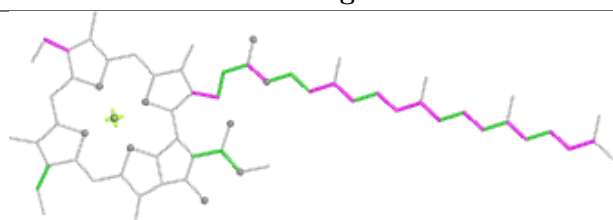
Ligand CLA k 604



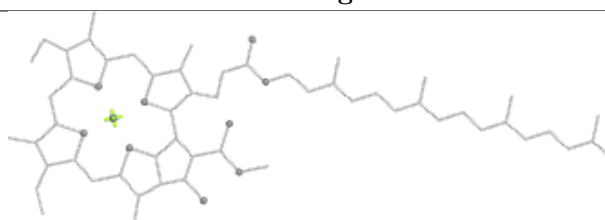
Bond lengths



Bond angles

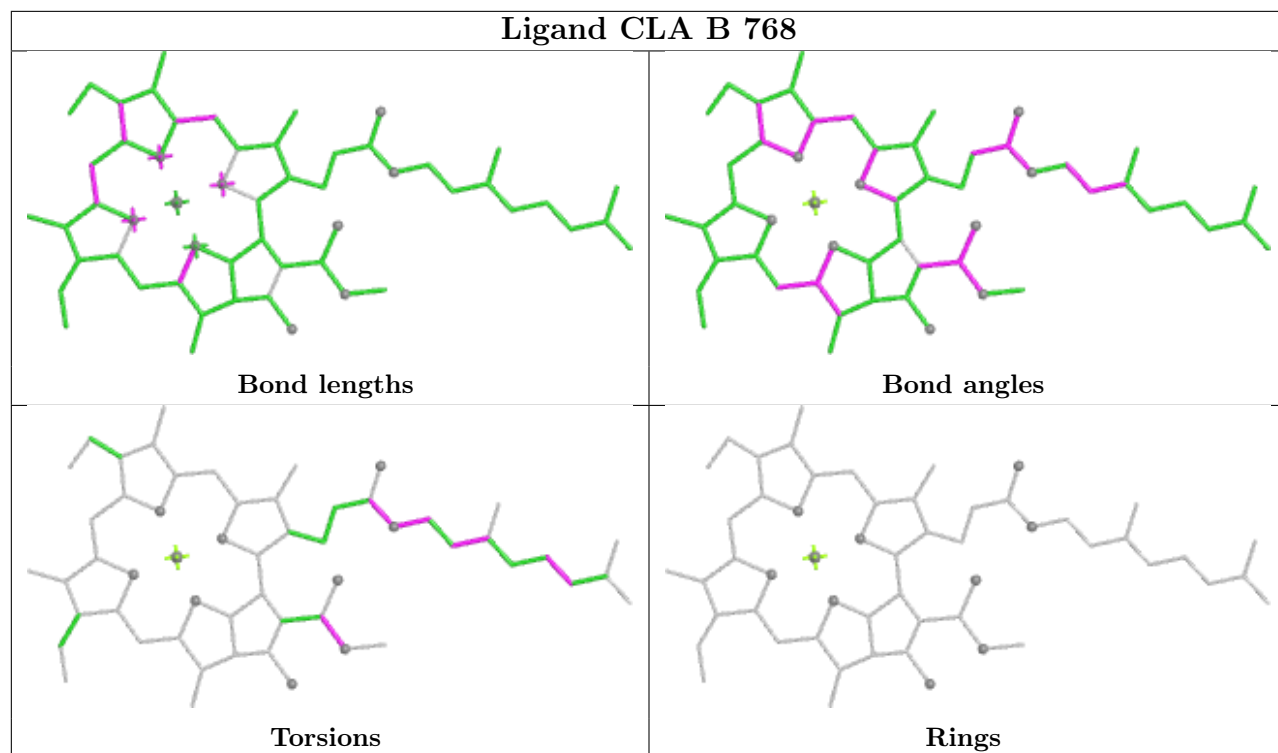


Torsions

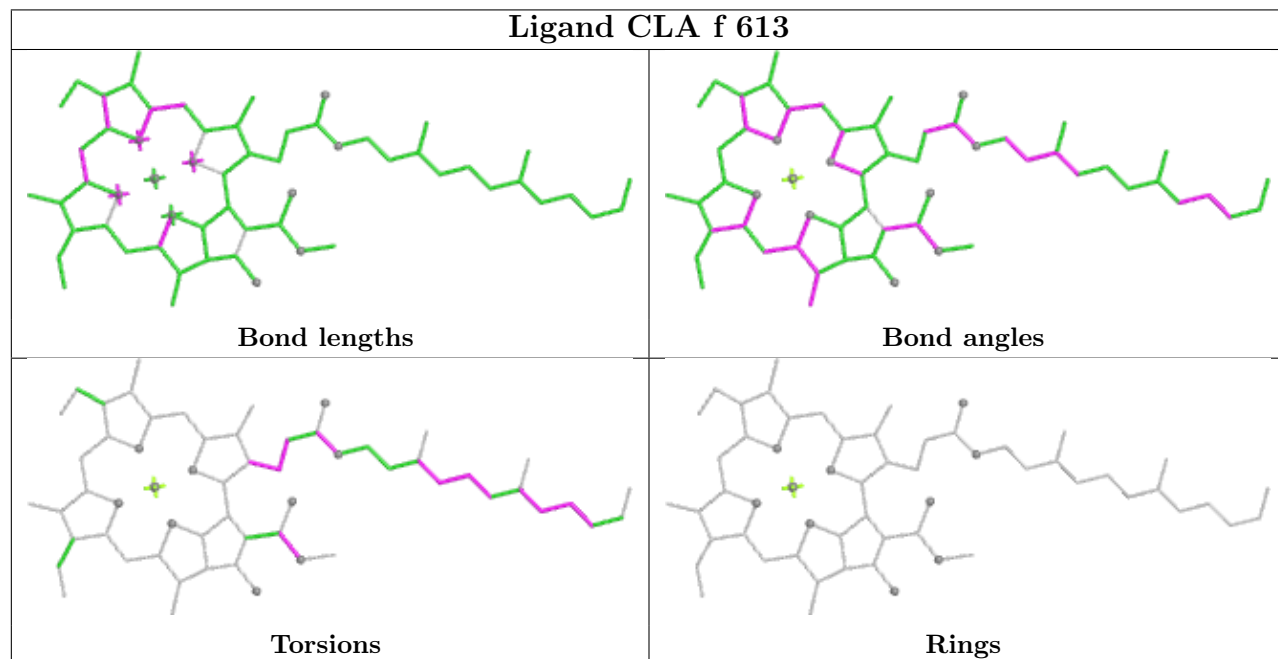


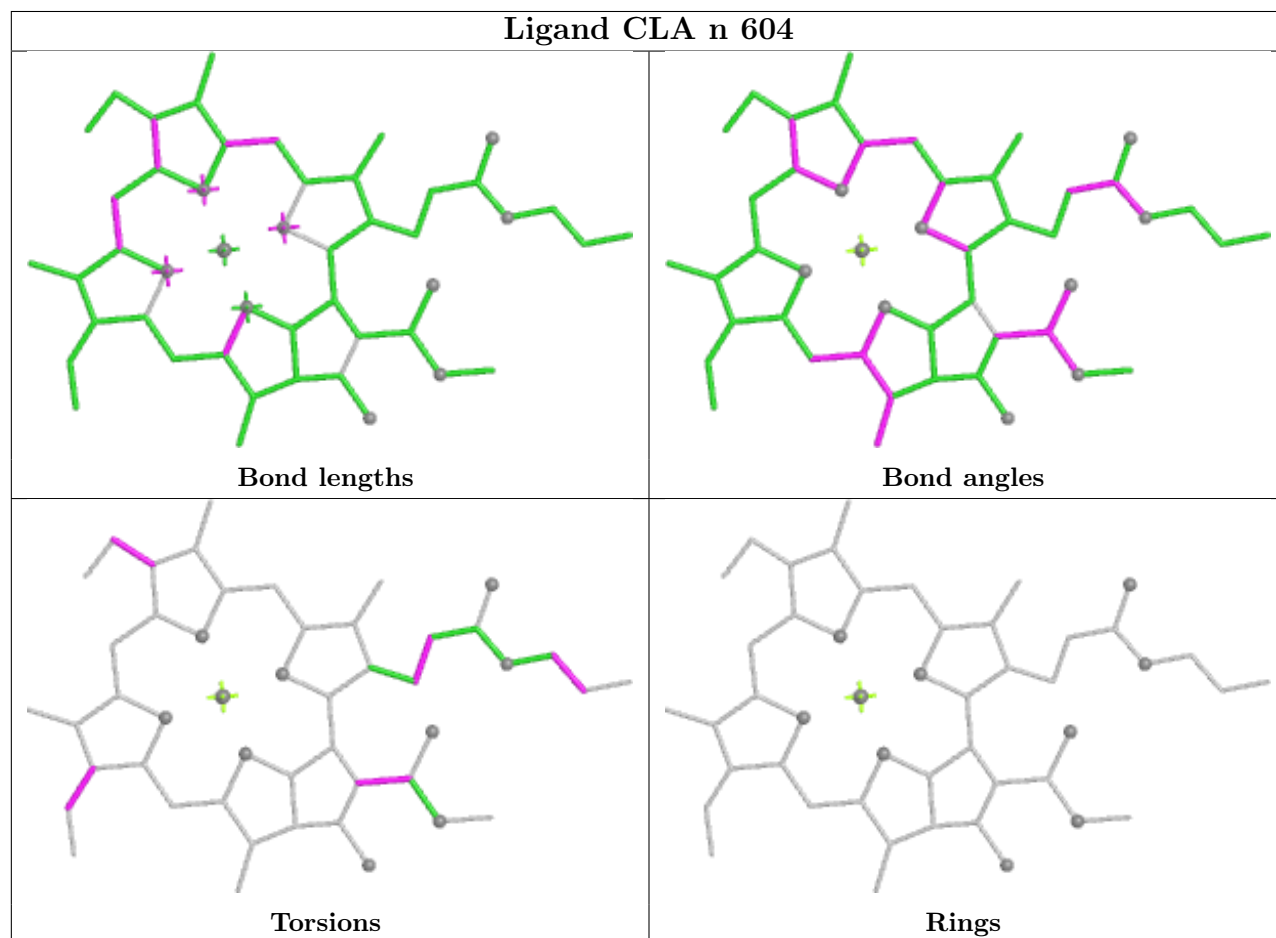
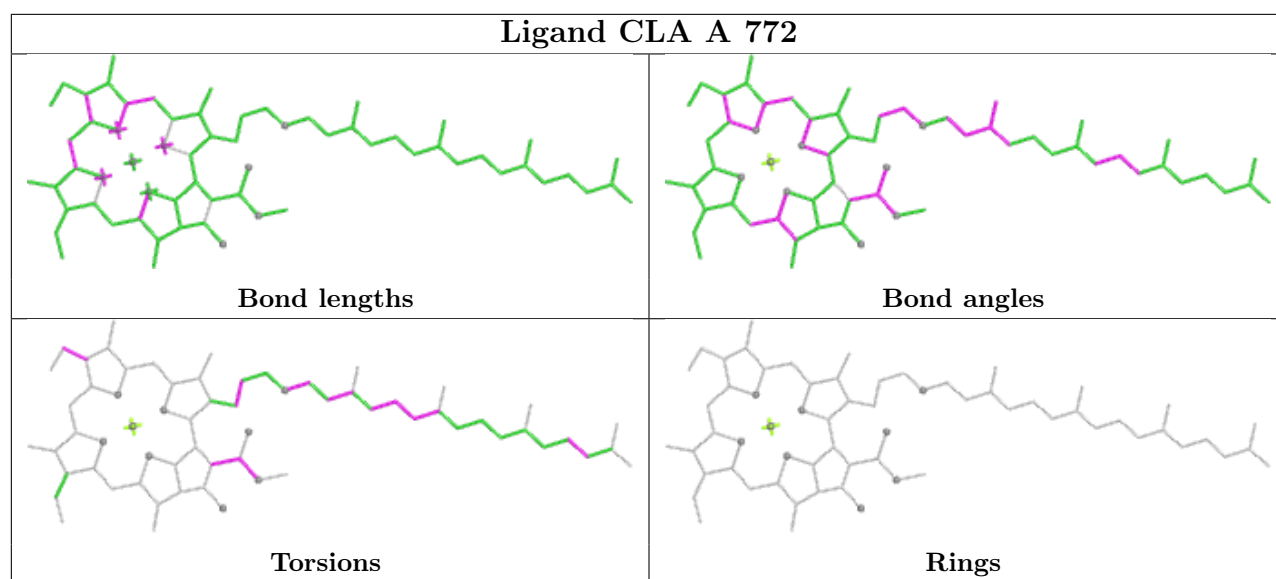
Rings

Ligand CLA B 768

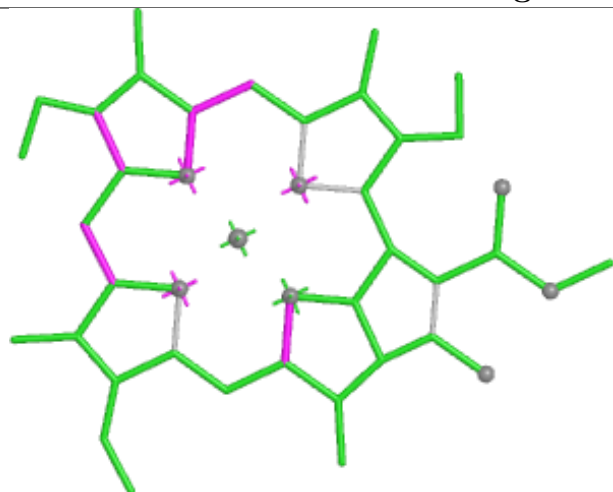


Ligand CLA f 613

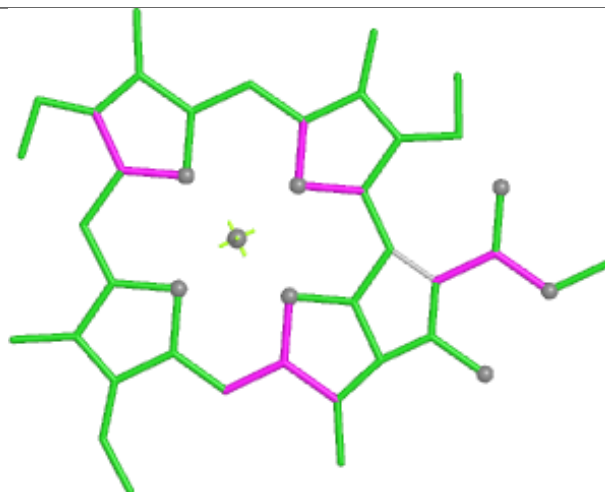




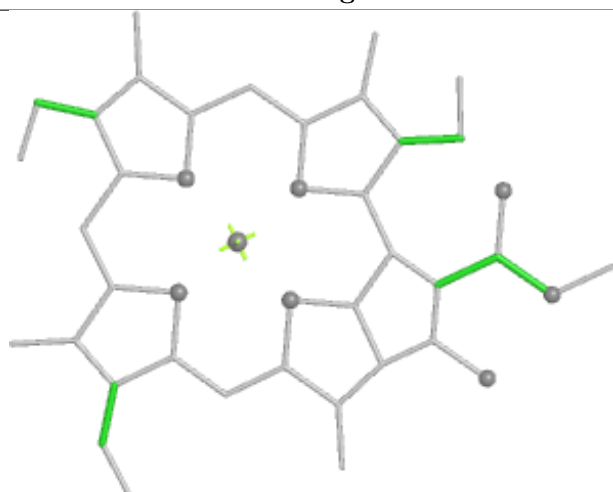
Ligand CLA A 793



Bond lengths



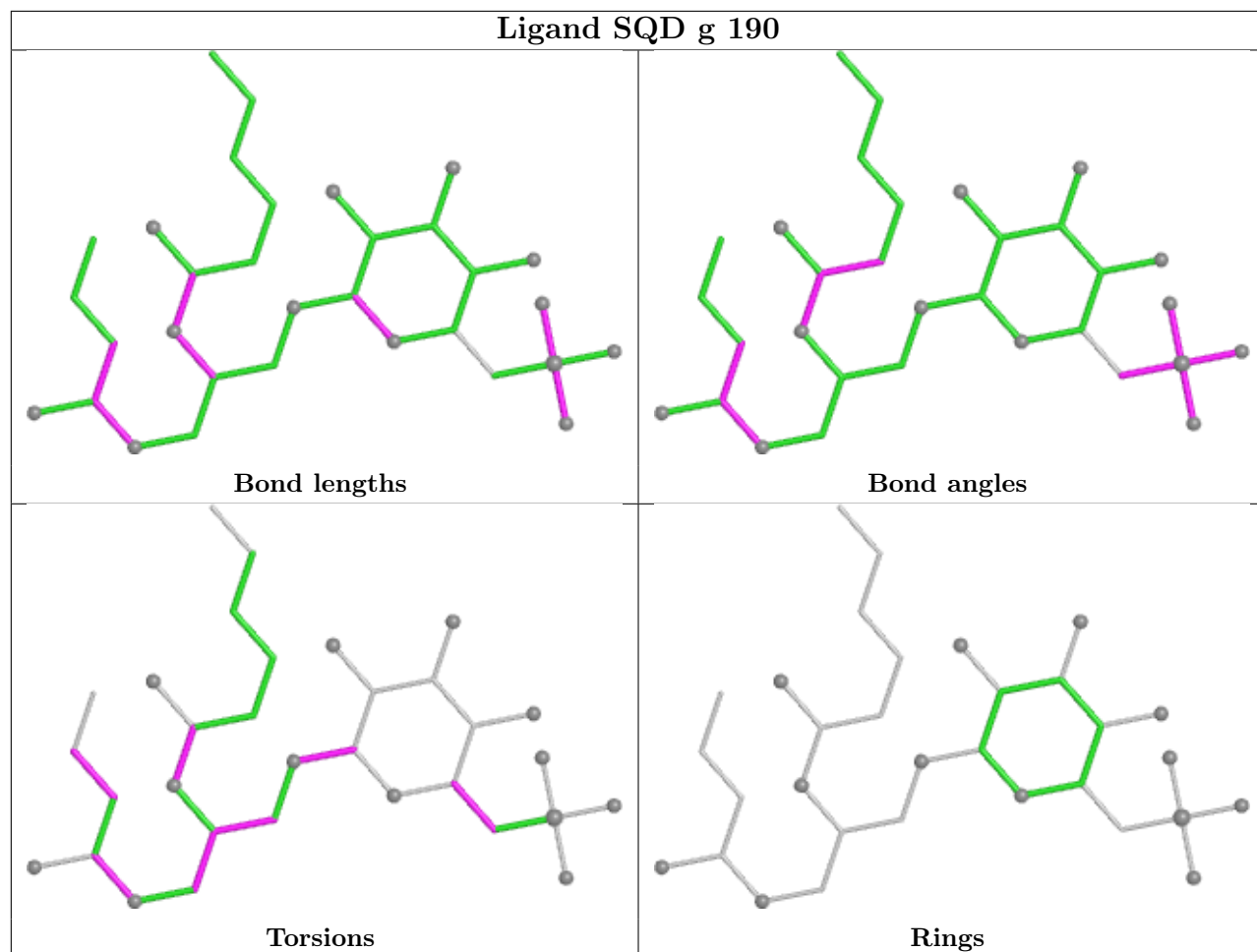
Bond angles



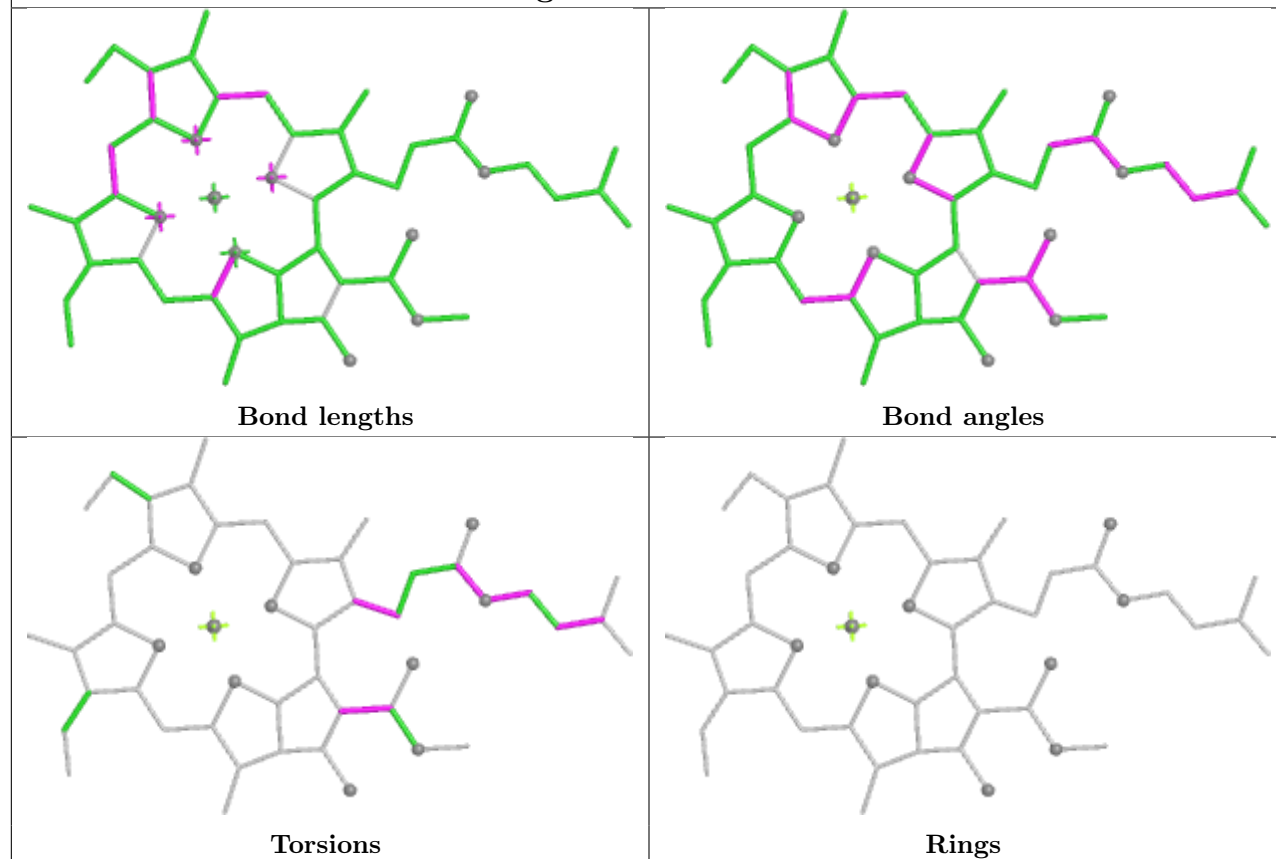
Torsions



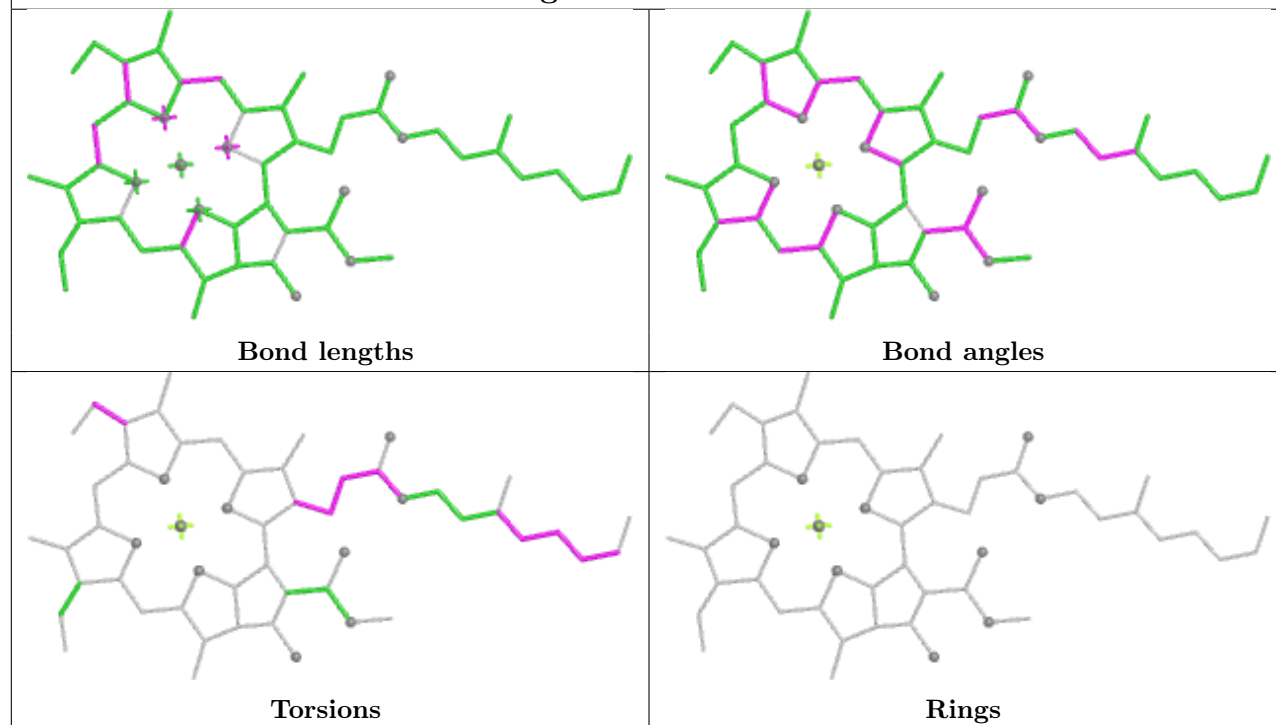
Rings

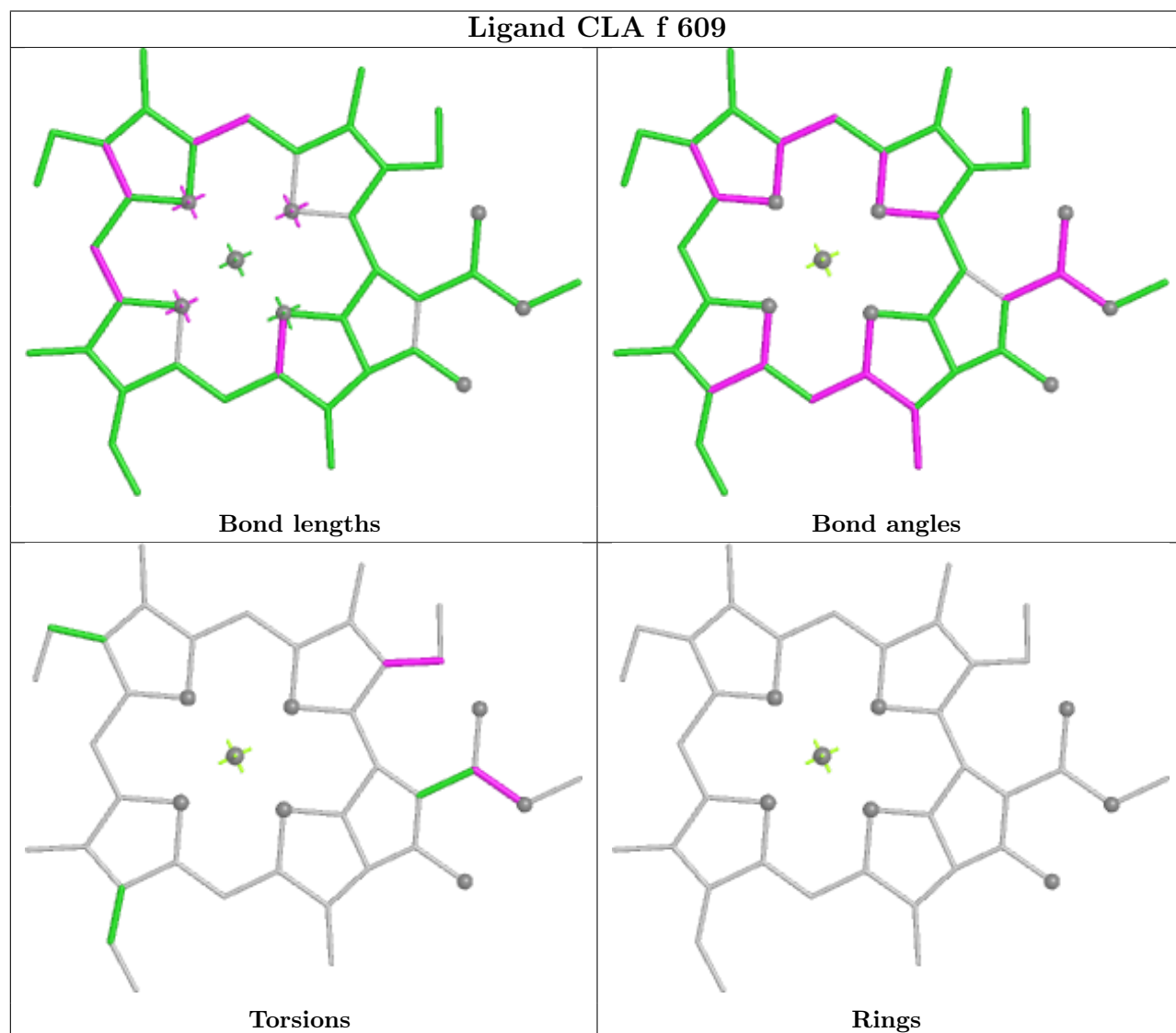
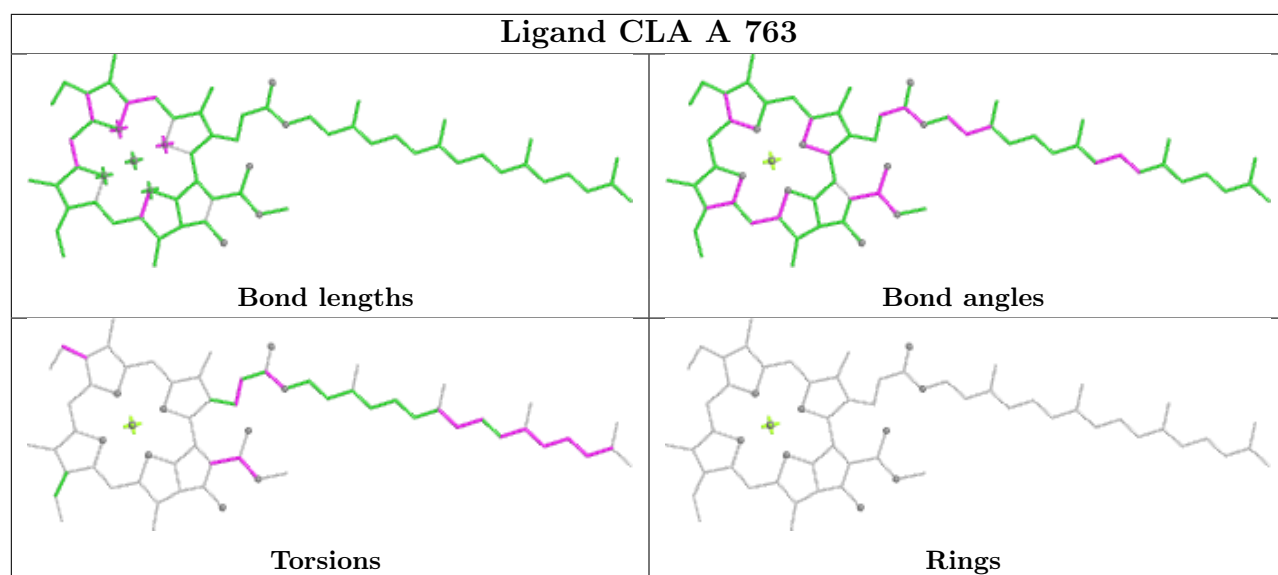


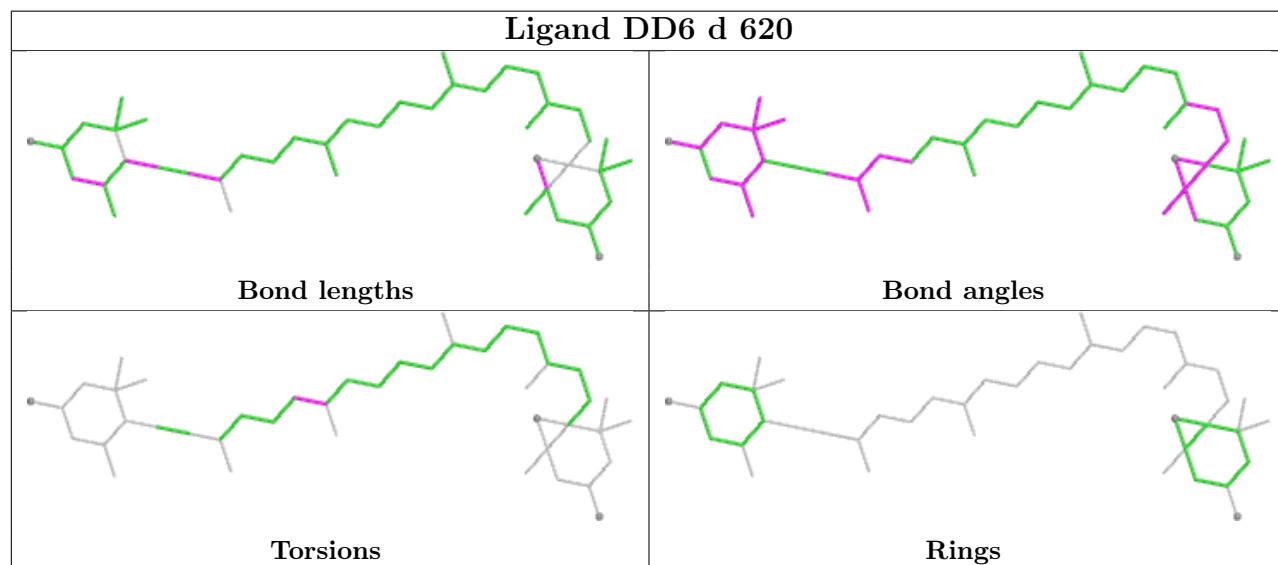
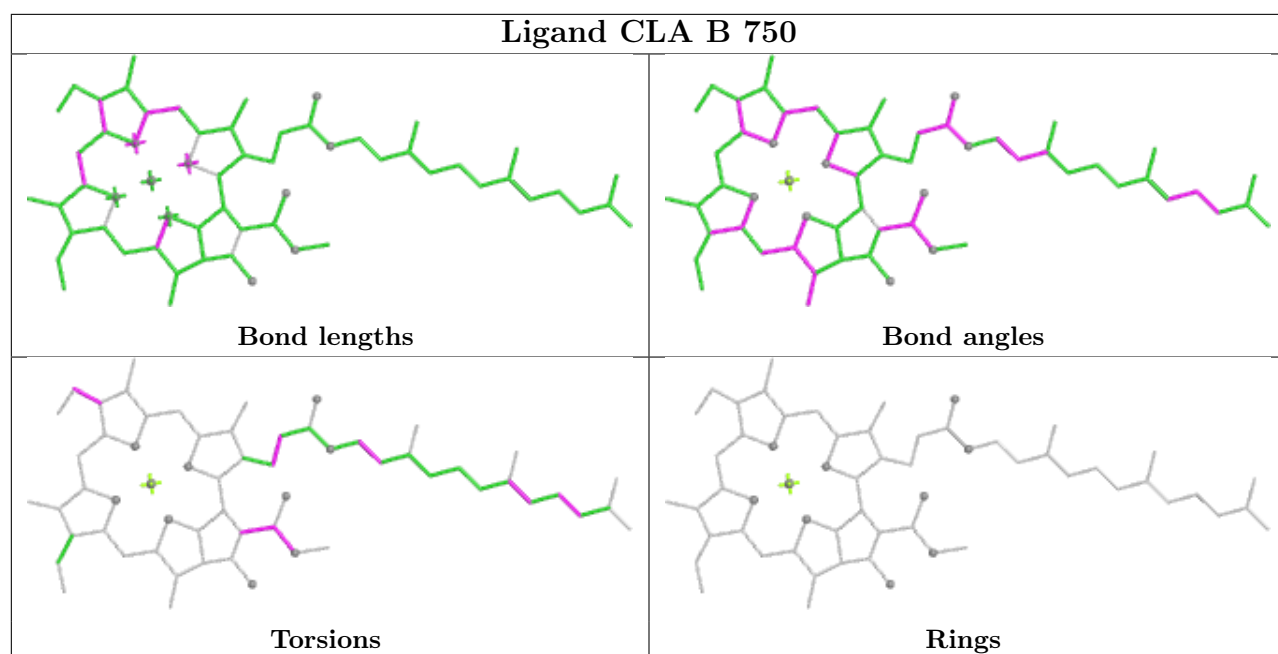
Ligand CLA a 601

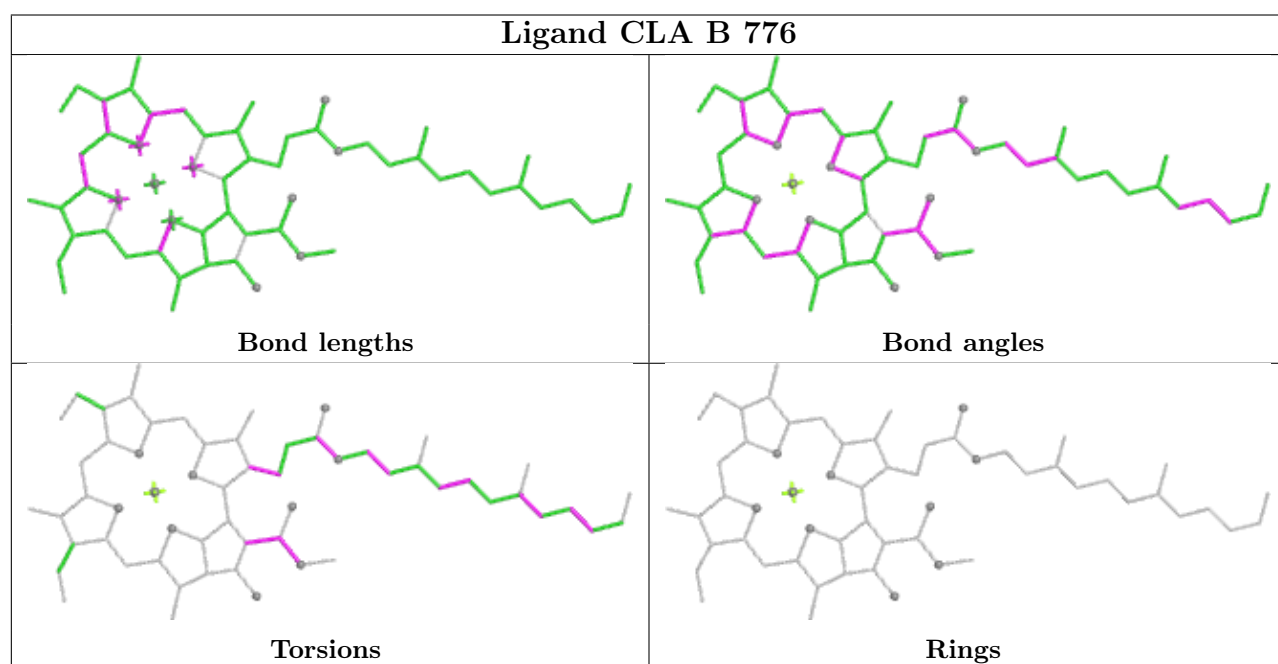
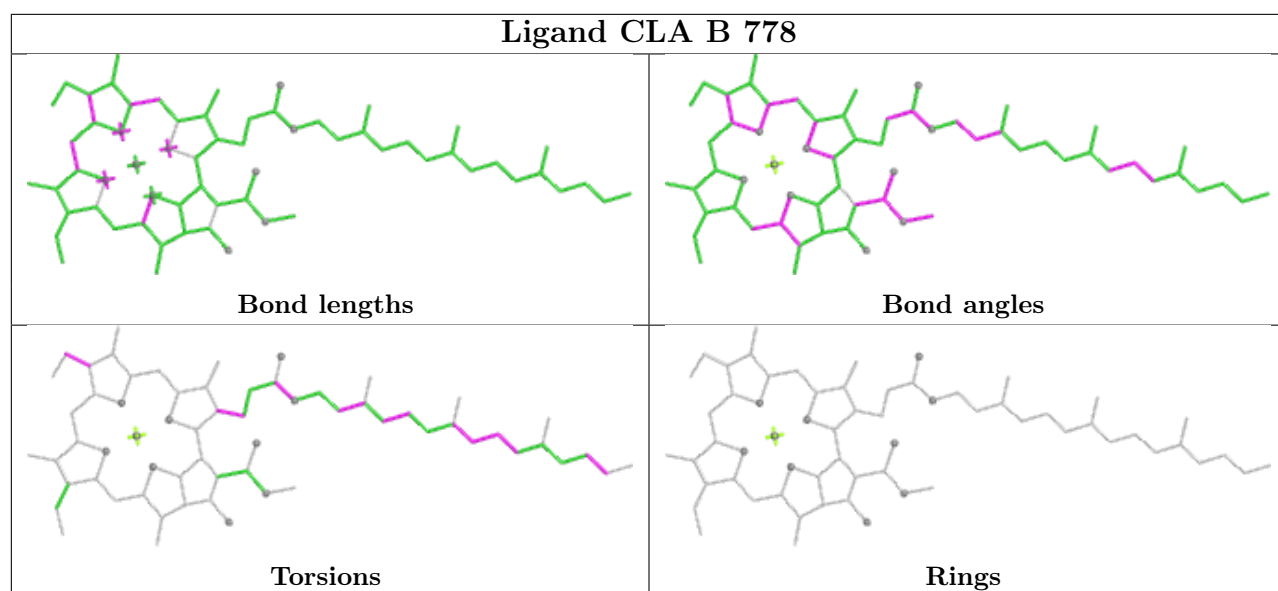


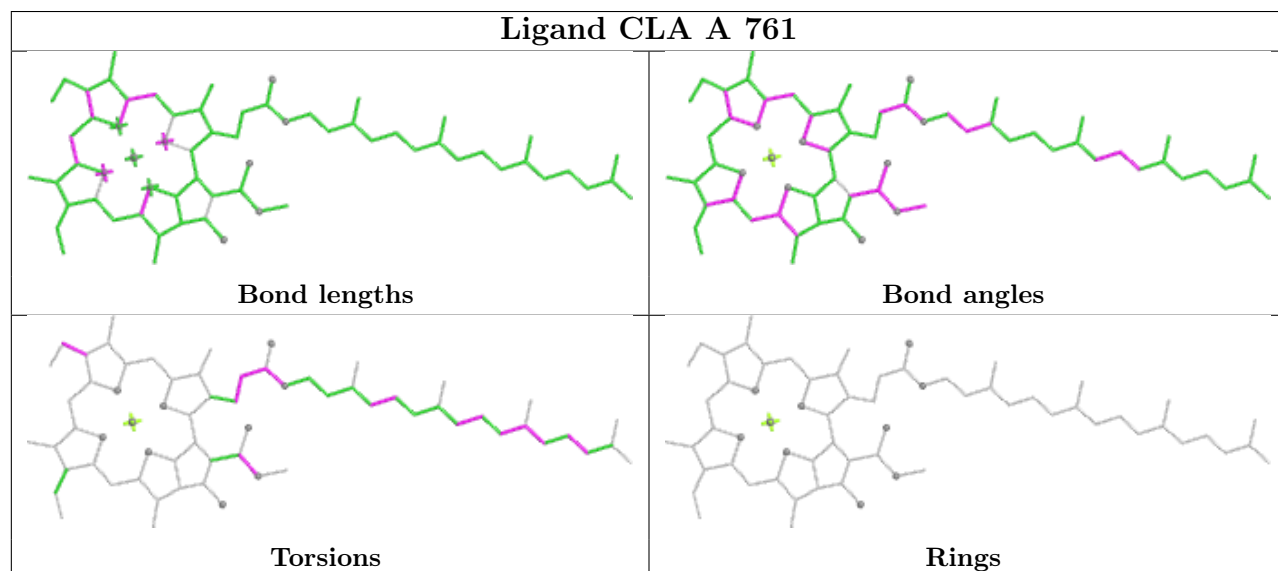
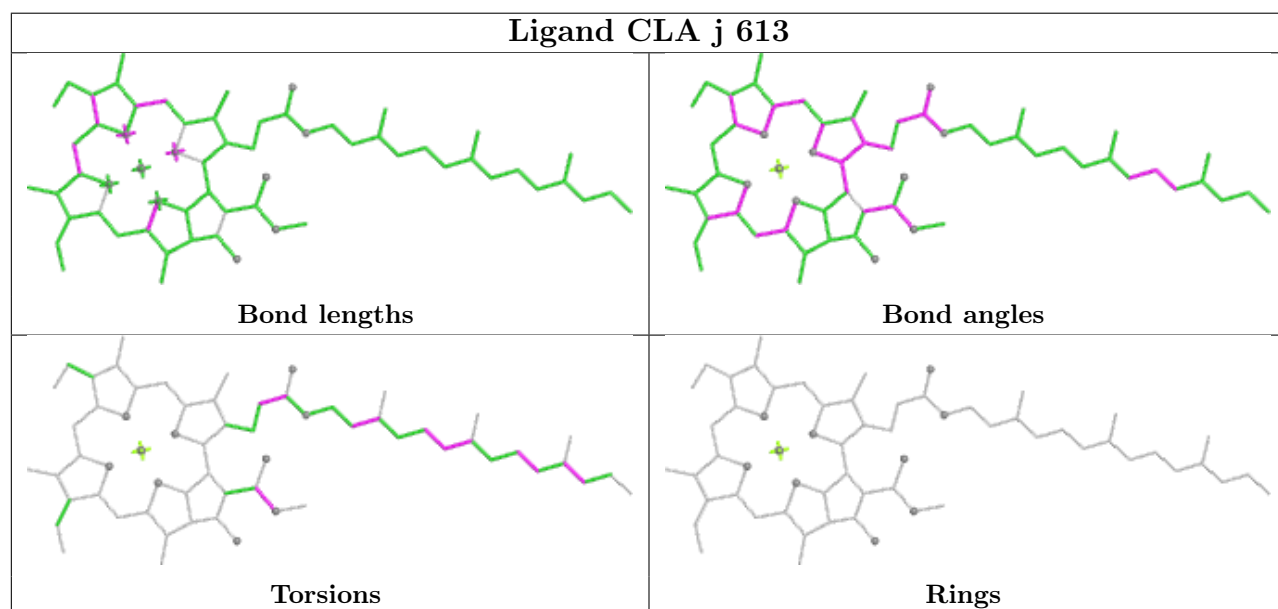
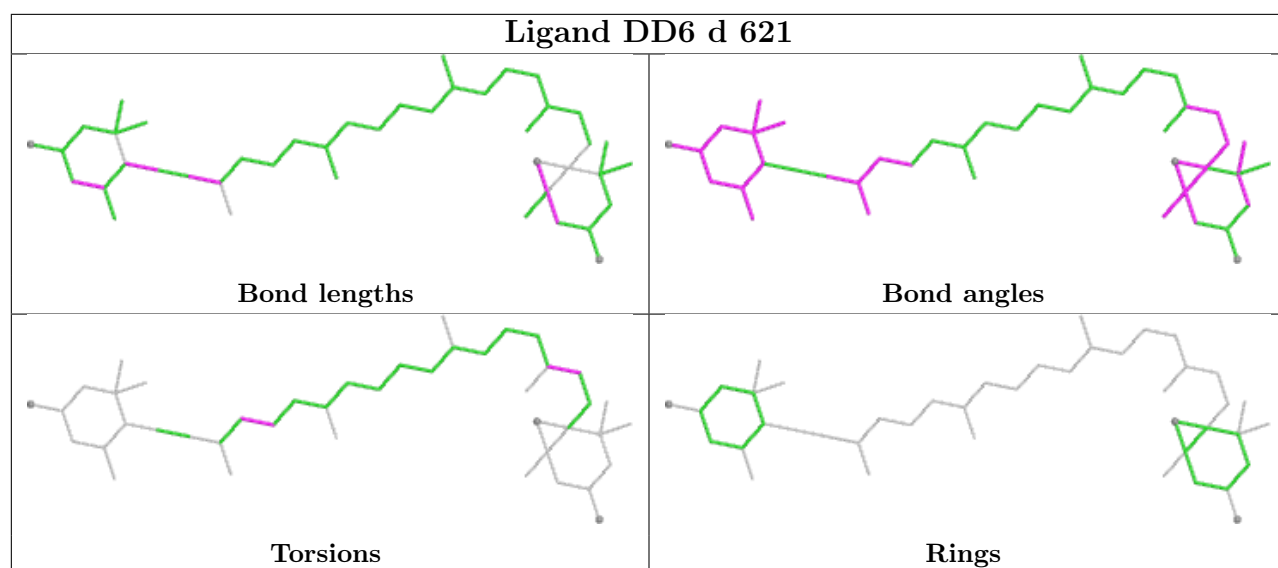
Ligand CLA l 610



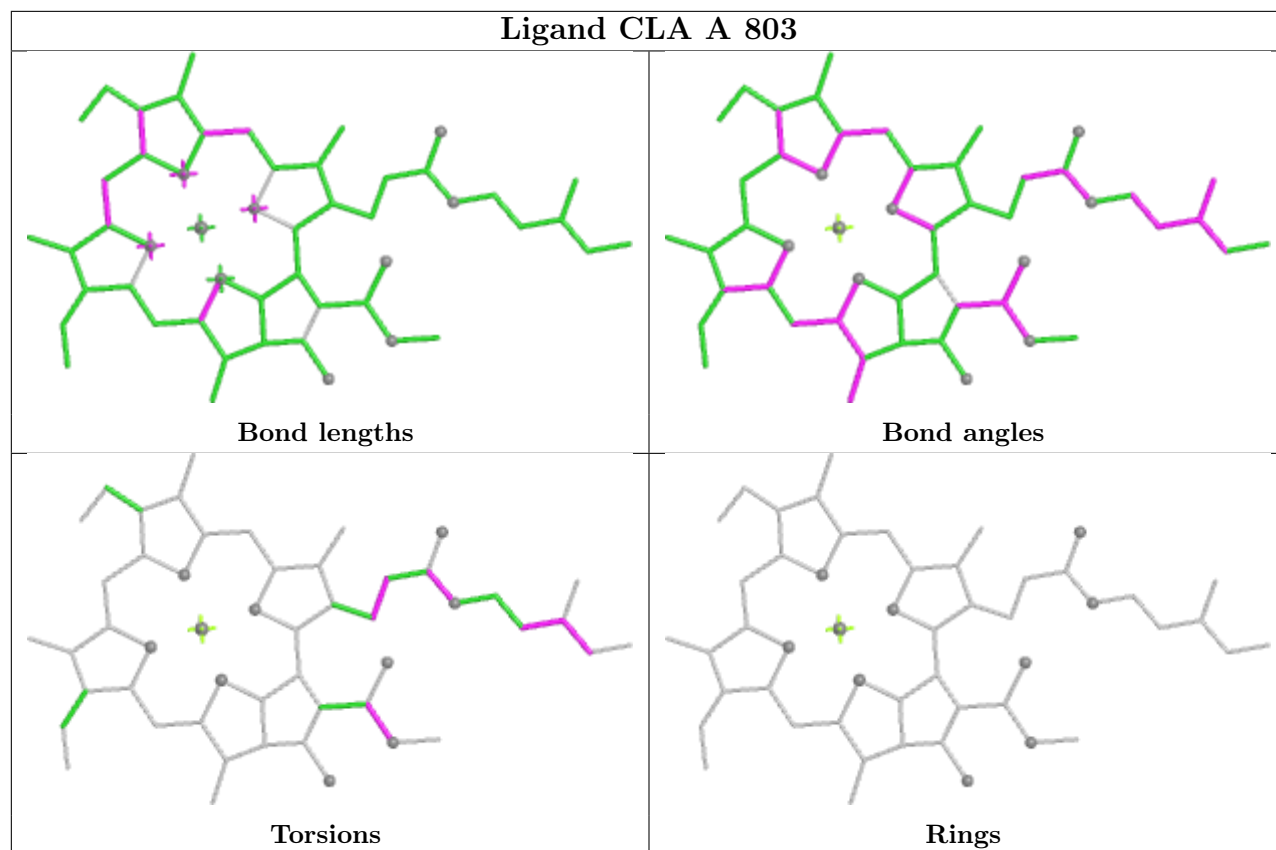




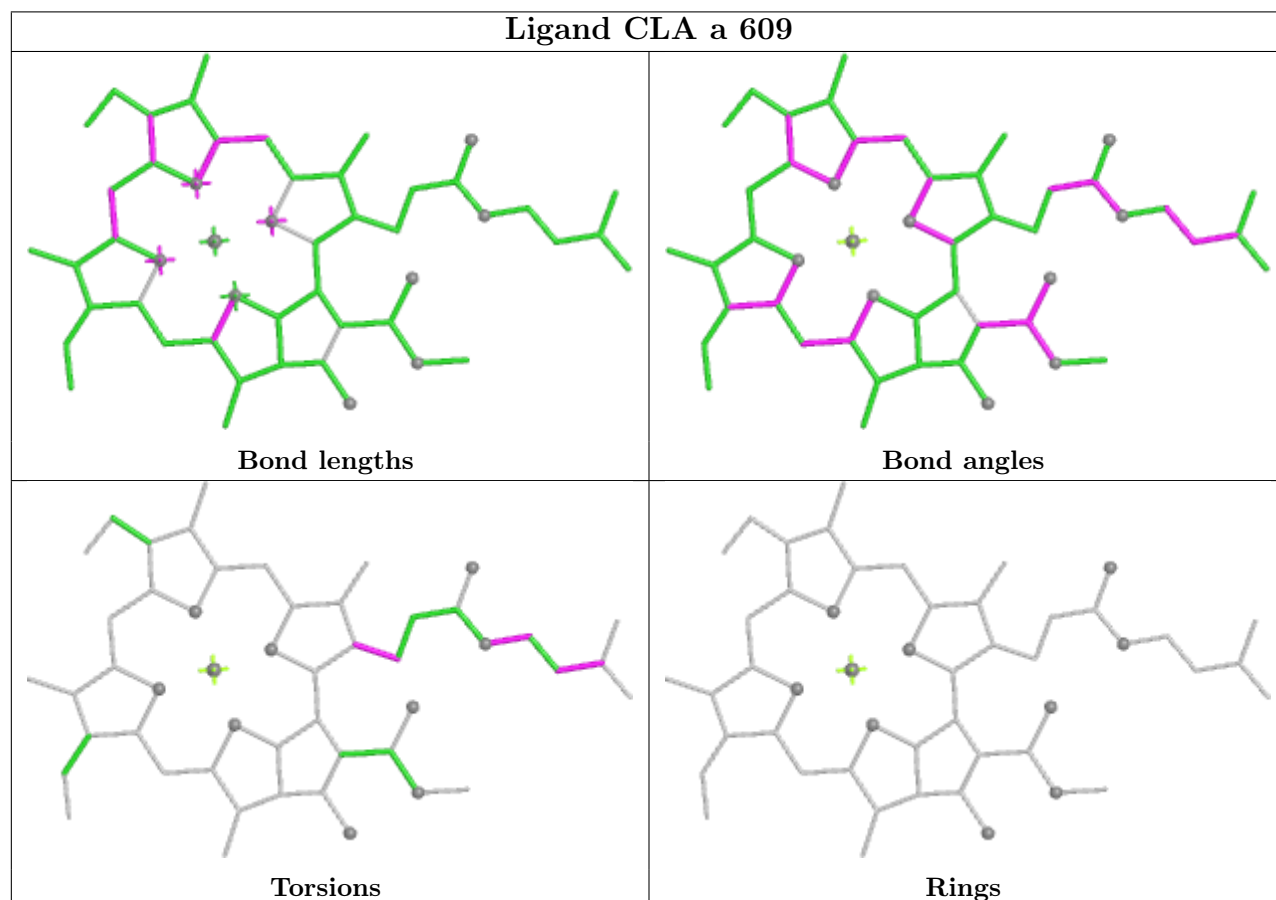




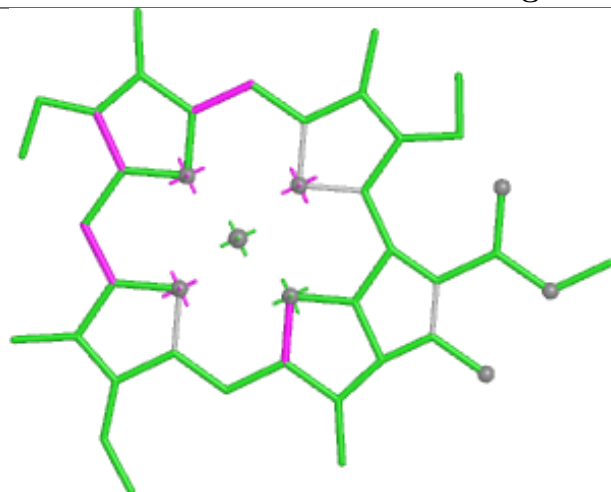
Ligand CLA A 803



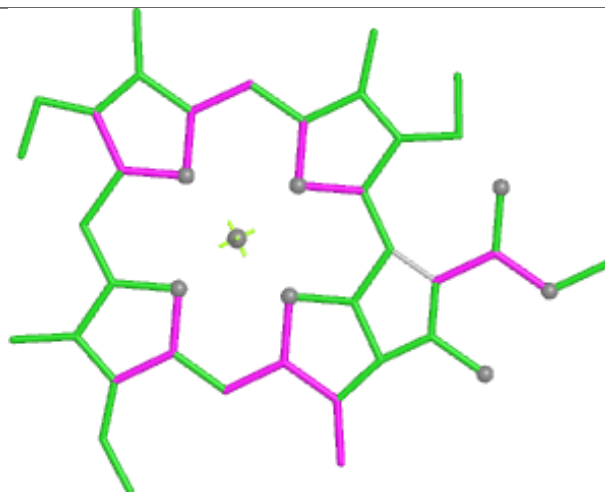
Ligand CLA a 609



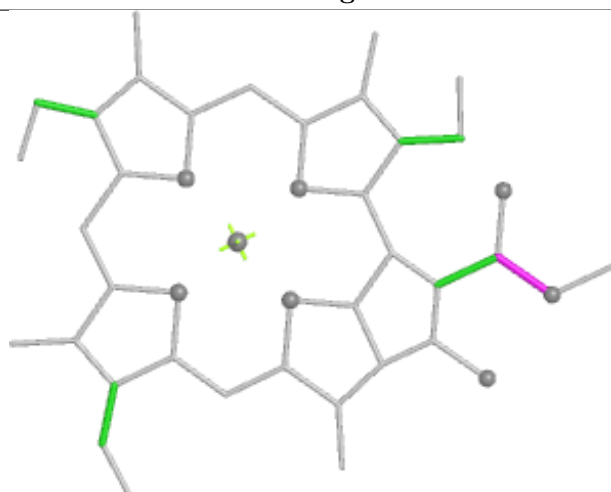
Ligand CLA f 608



Bond lengths



Bond angles

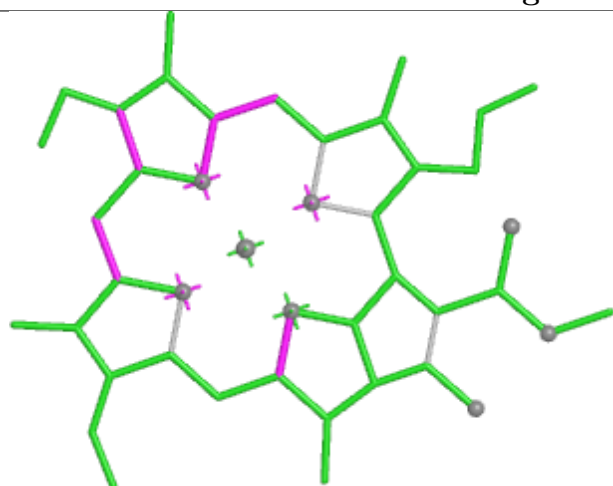


Torsions

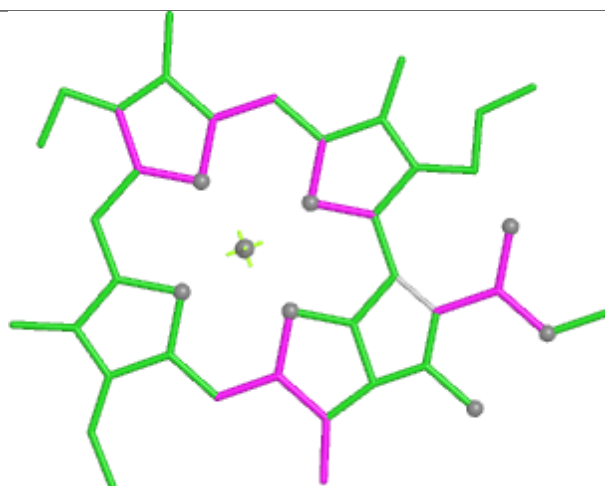


Rings

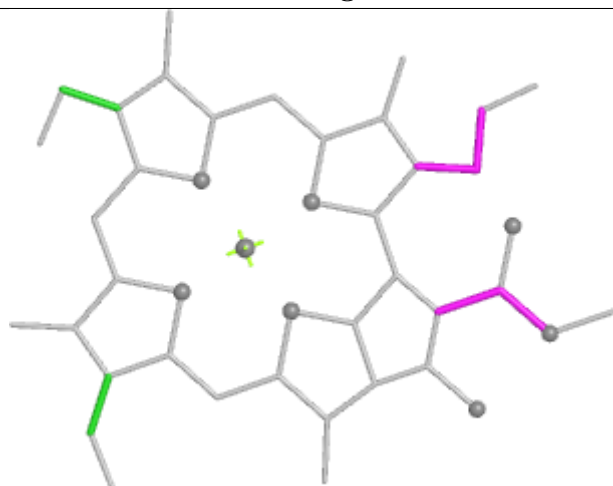
Ligand CLA i 612



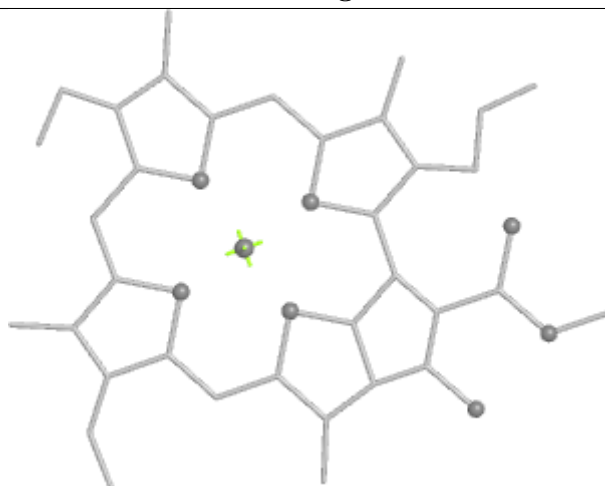
Bond lengths



Bond angles

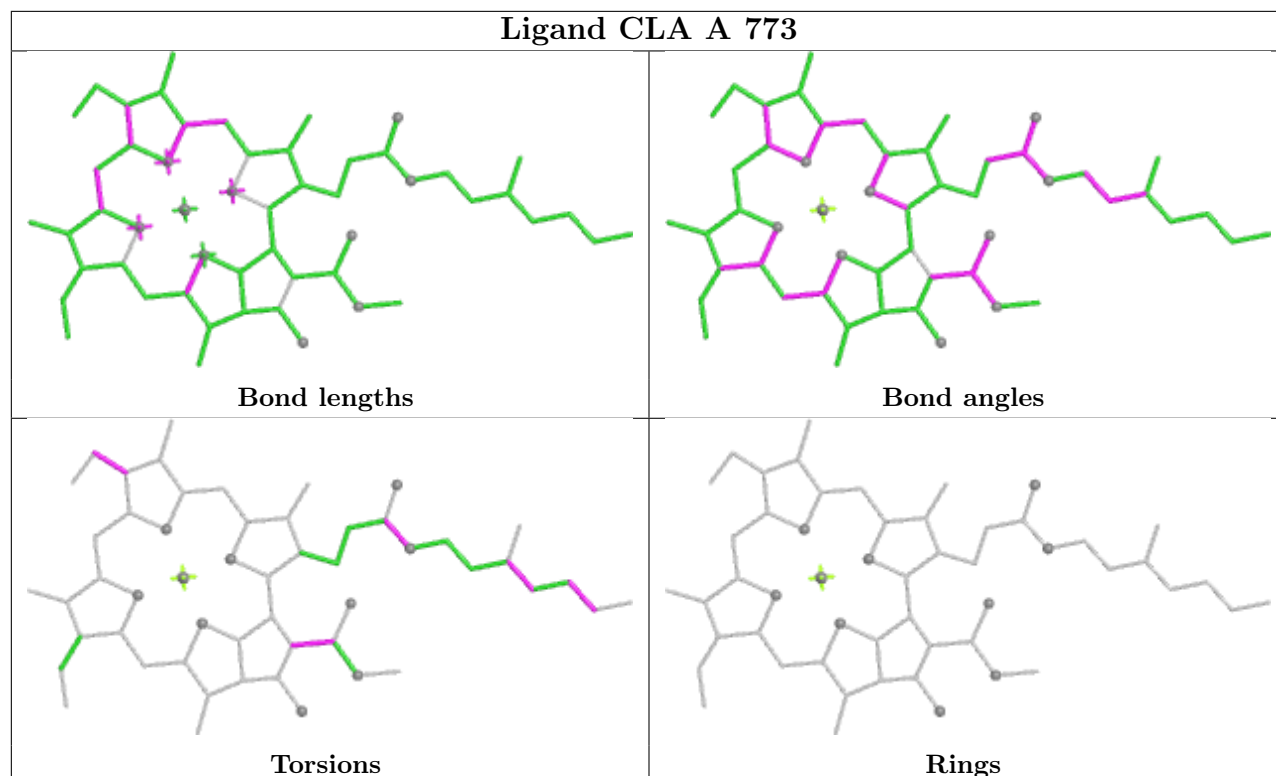


Torsions

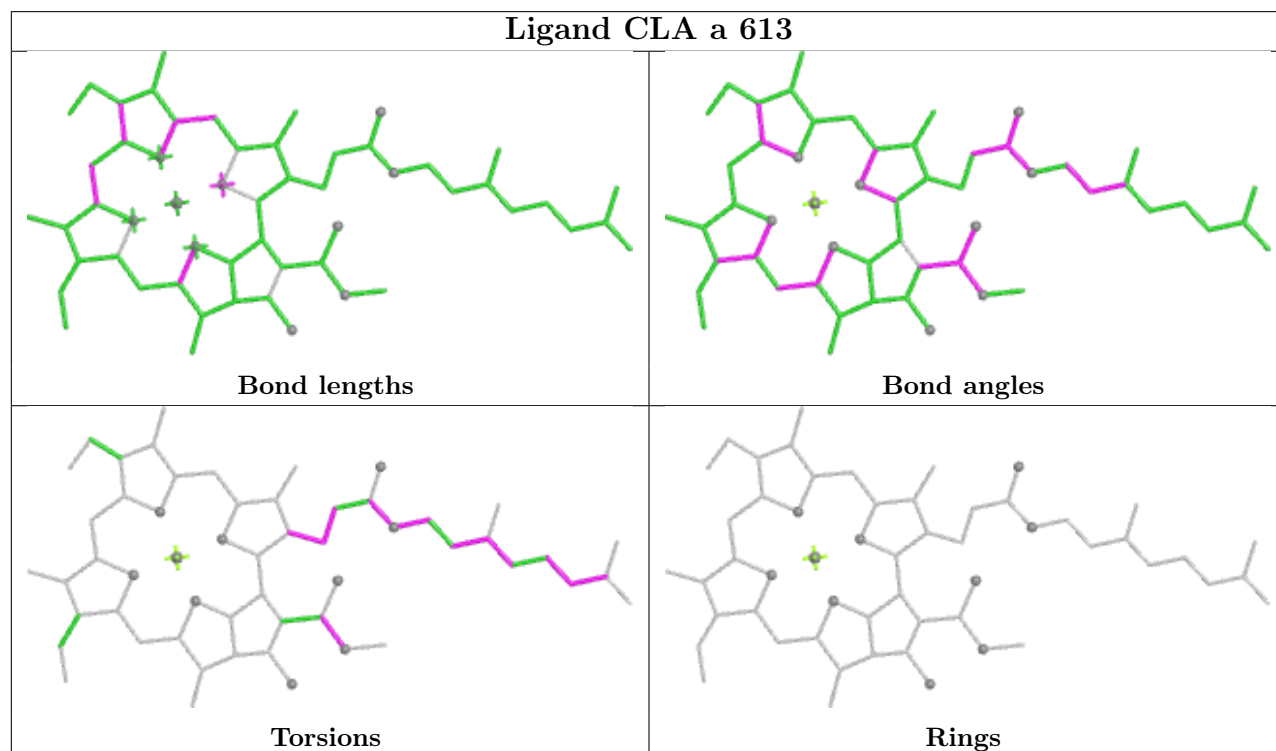


Rings

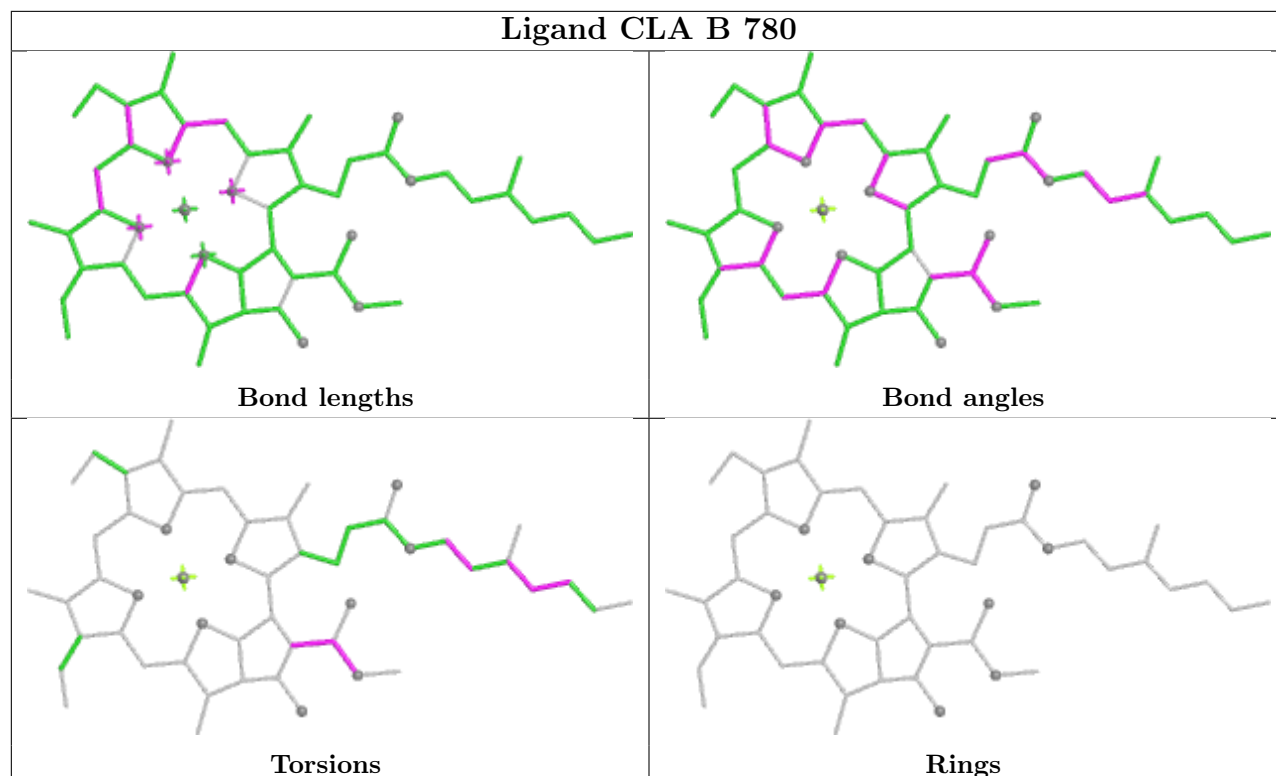
Ligand CLA A 773



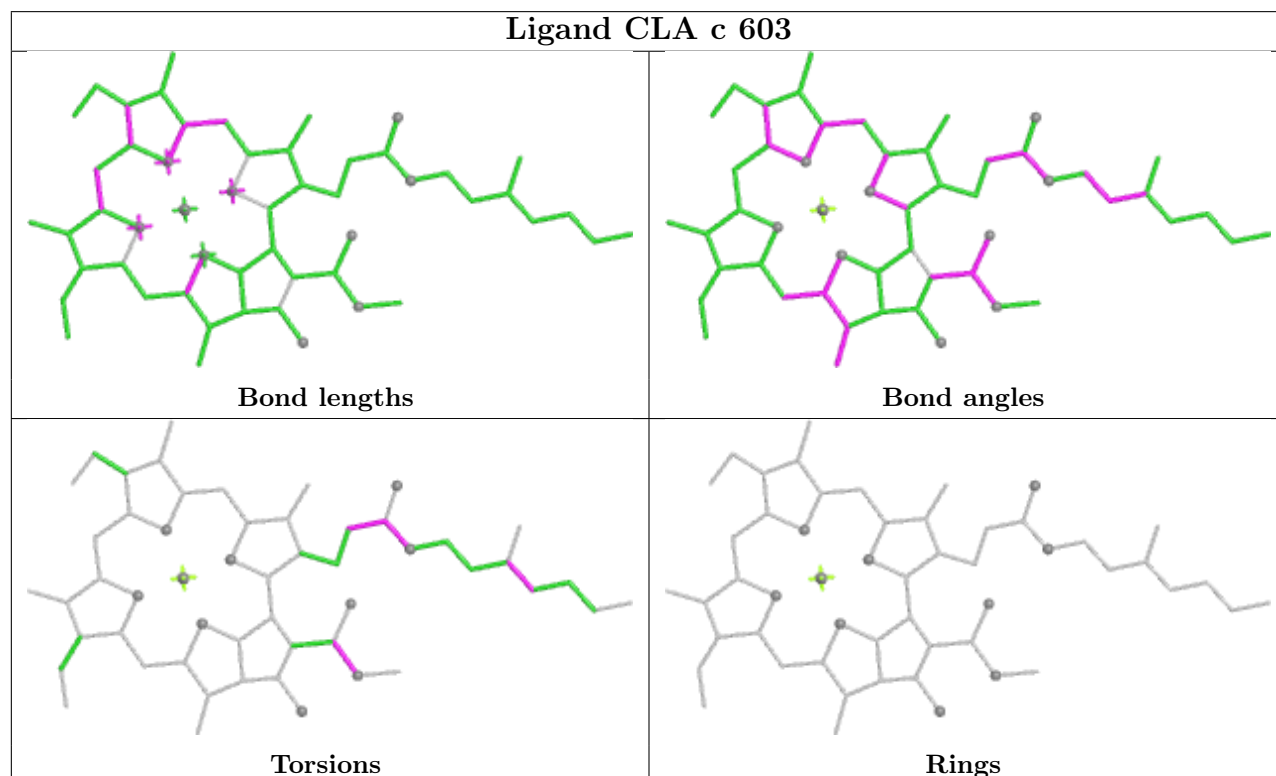
Ligand CLA a 613



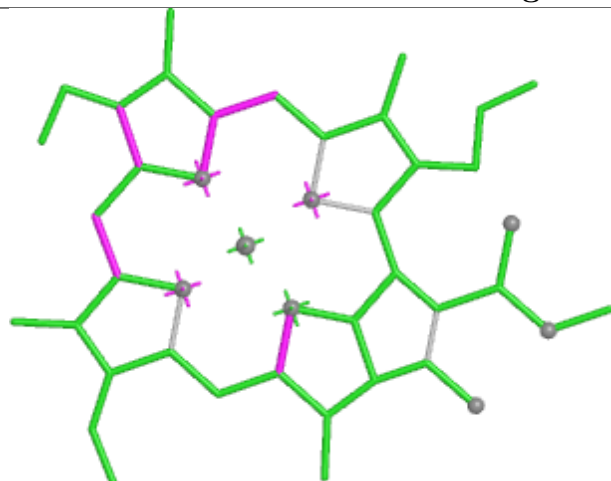
Ligand CLA B 780



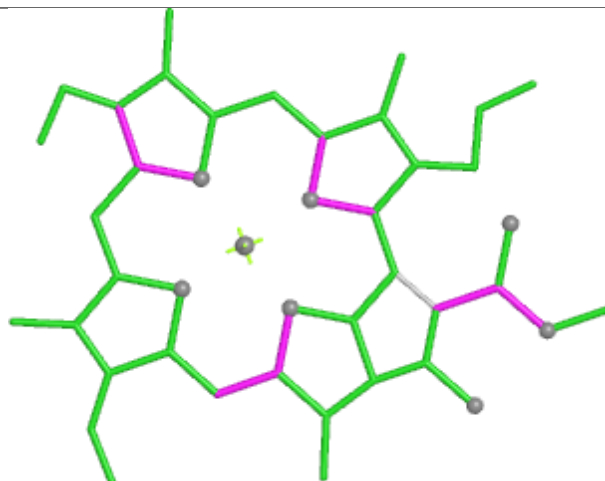
Ligand CLA c 603



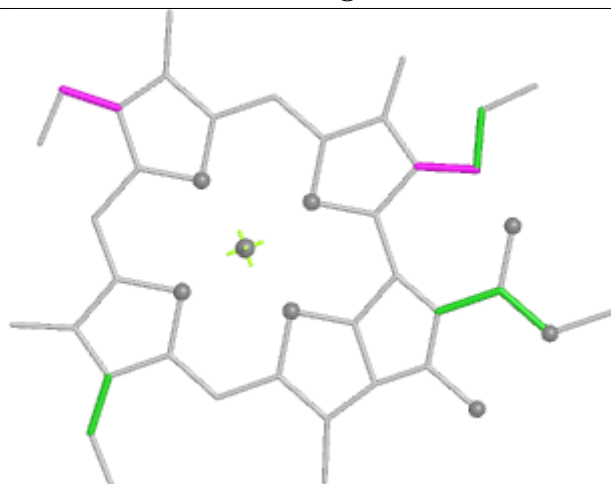
Ligand CLA i 609



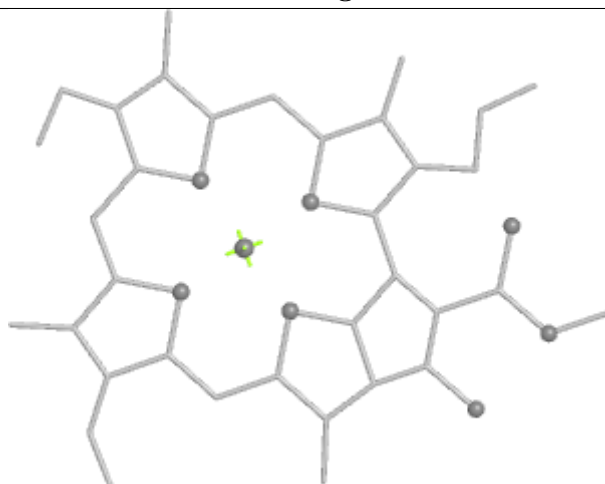
Bond lengths



Bond angles

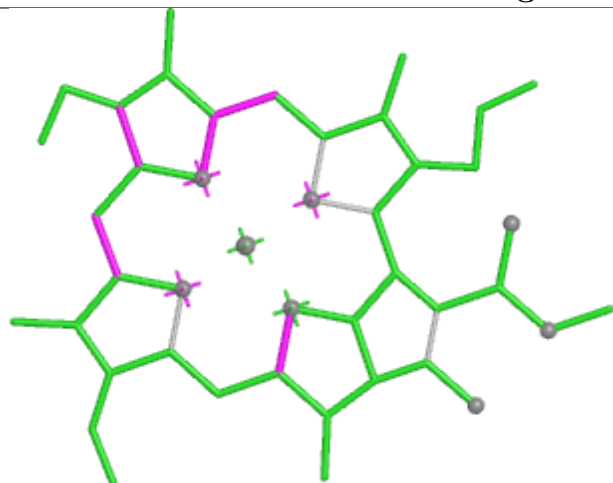


Torsions

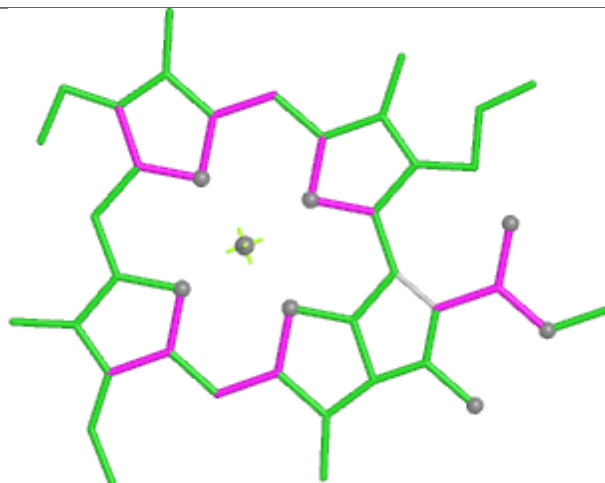


Rings

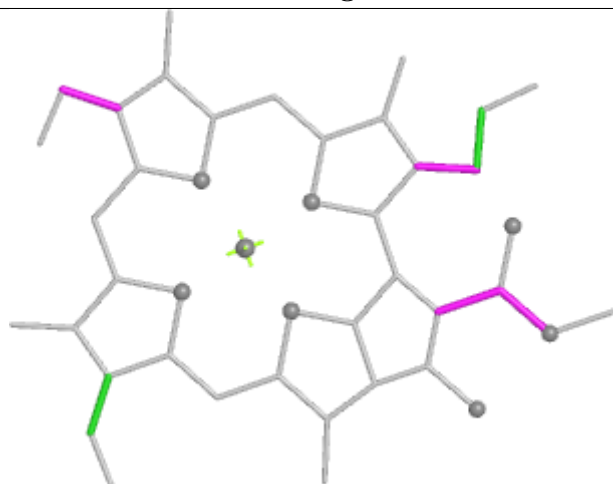
Ligand CLA h 611



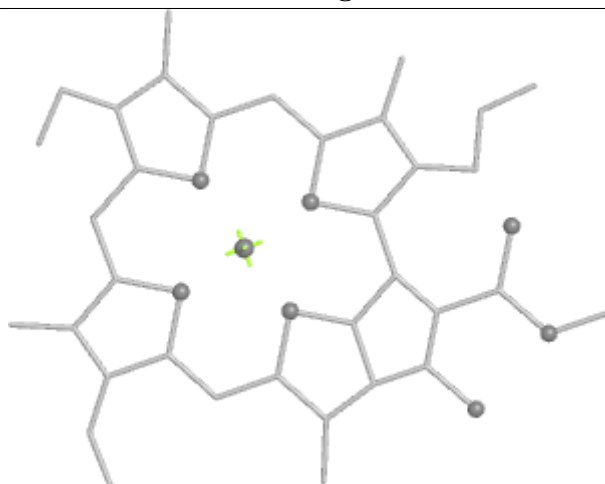
Bond lengths



Bond angles

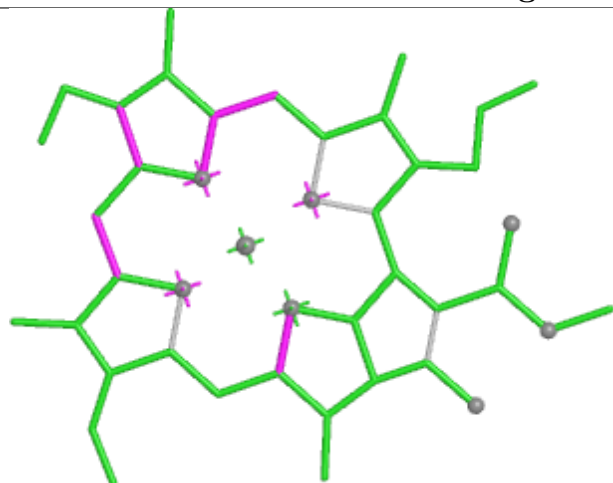


Torsions

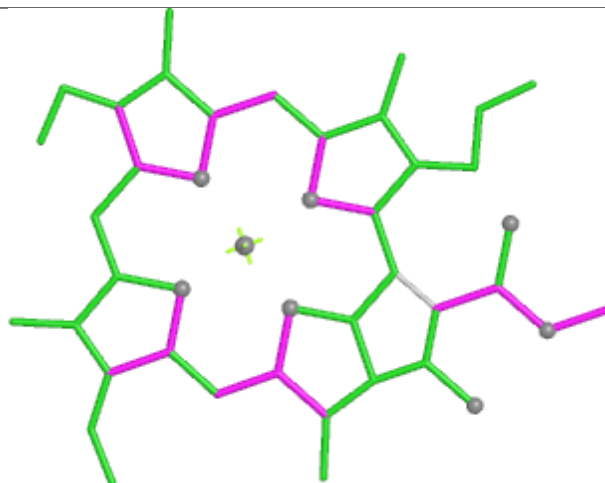


Rings

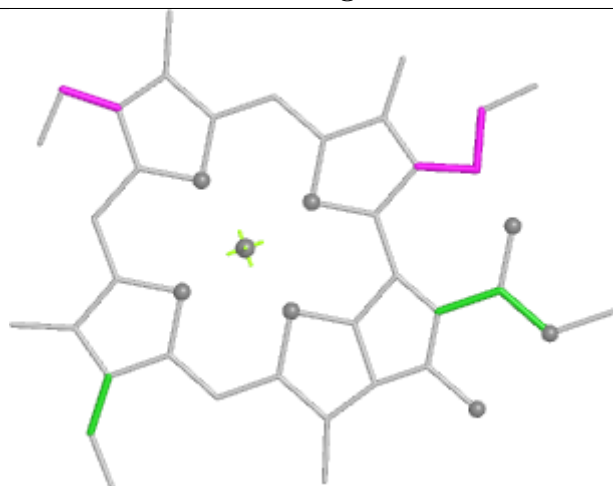
Ligand CLA o 608



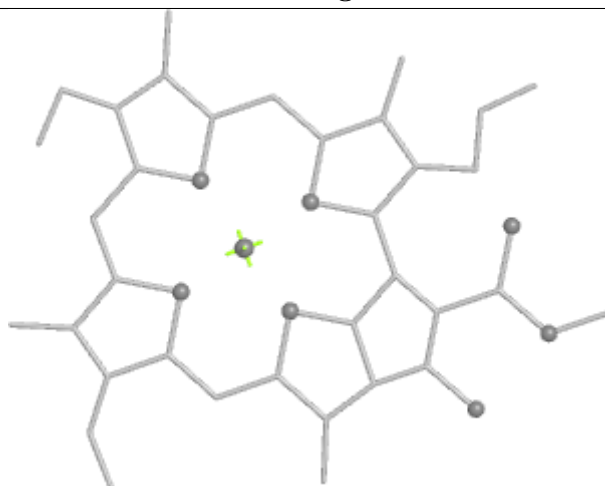
Bond lengths



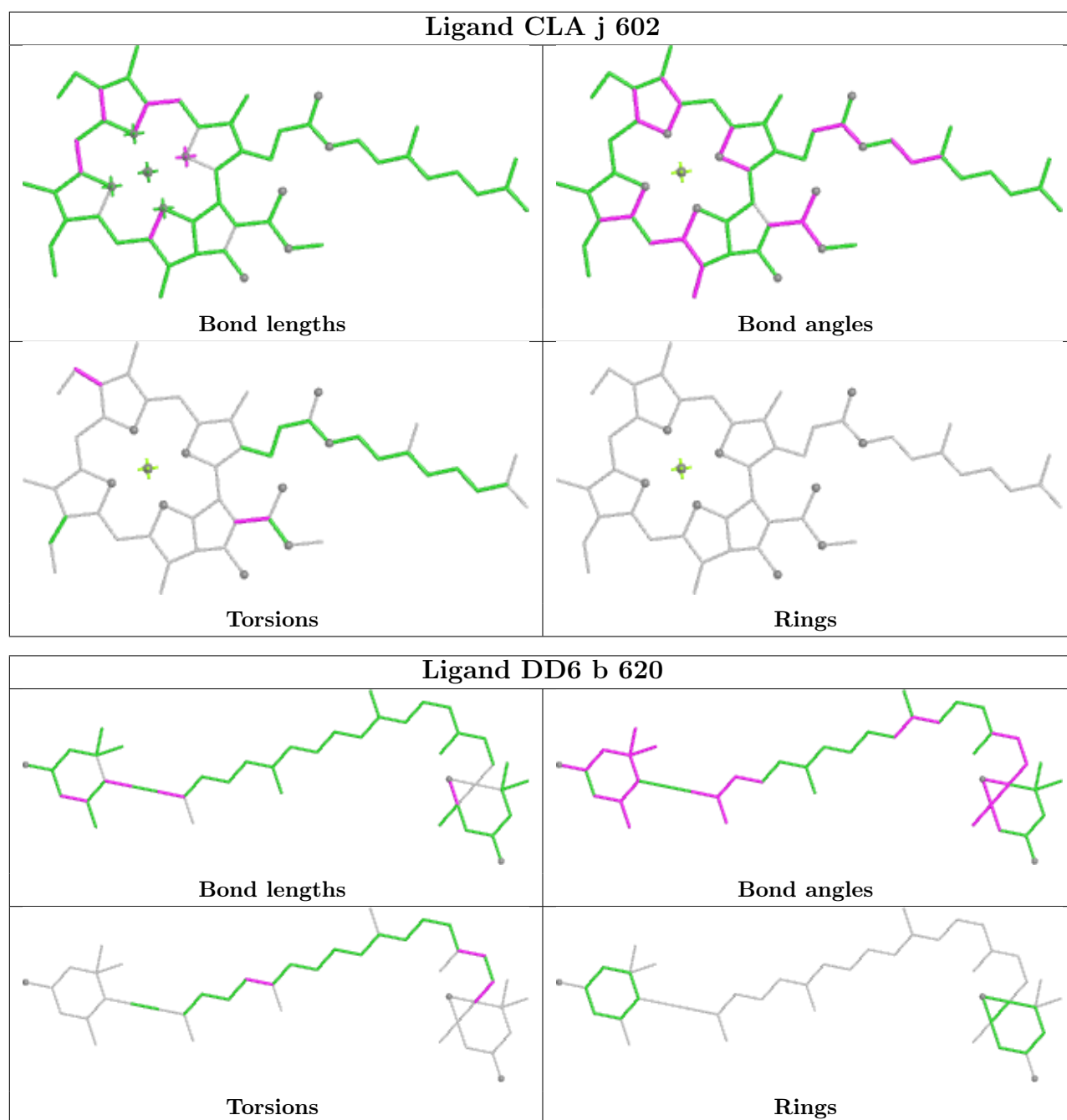
Bond angles



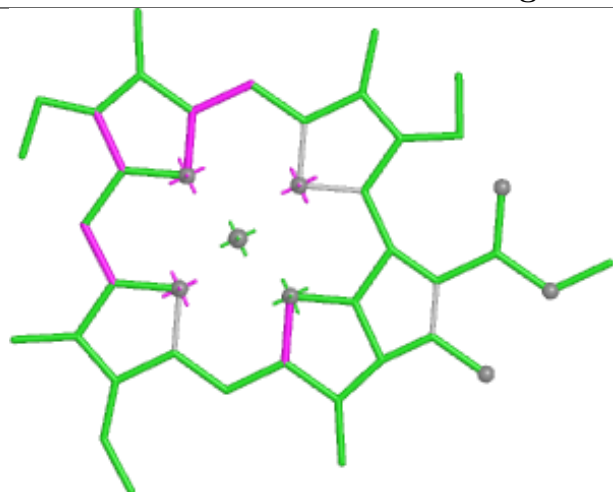
Torsions



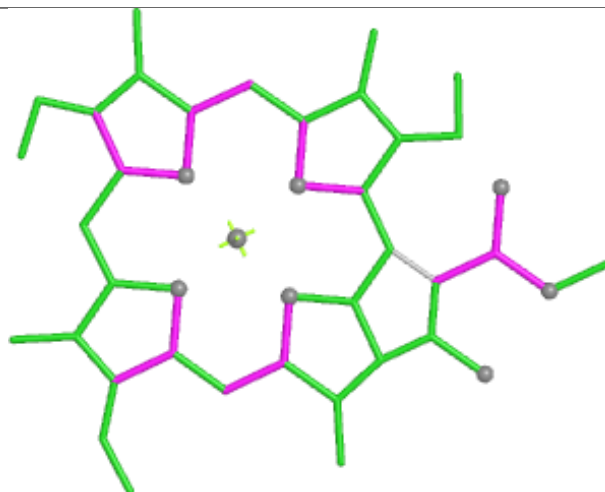
Rings



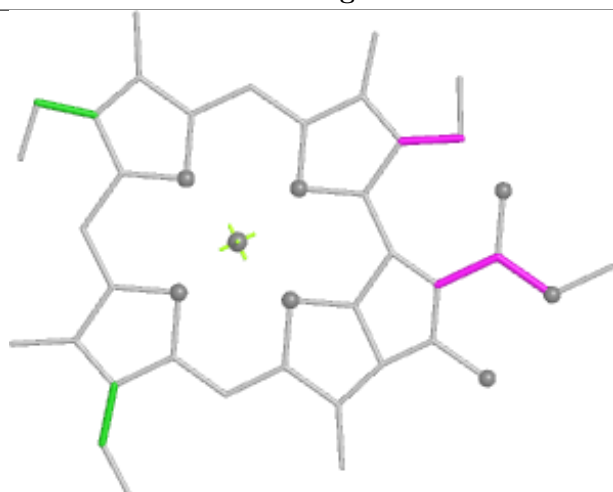
Ligand CLA c 601



Bond lengths



Bond angles

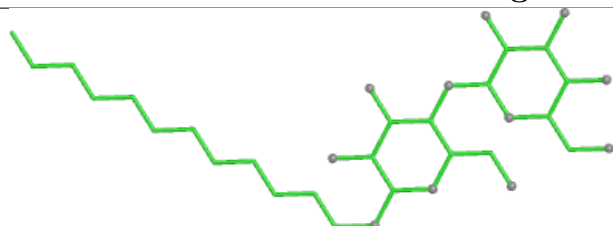


Torsions

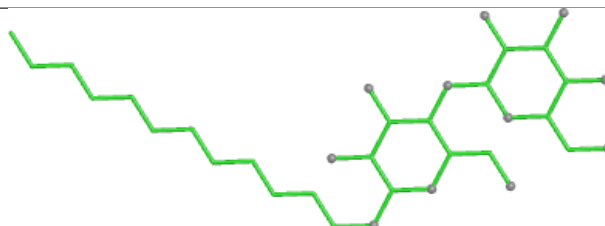


Rings

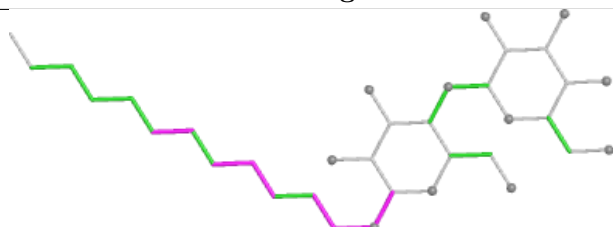
Ligand LMT A 754



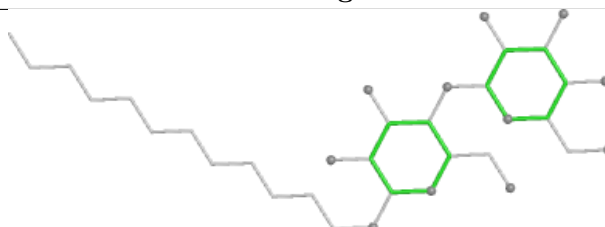
Bond lengths



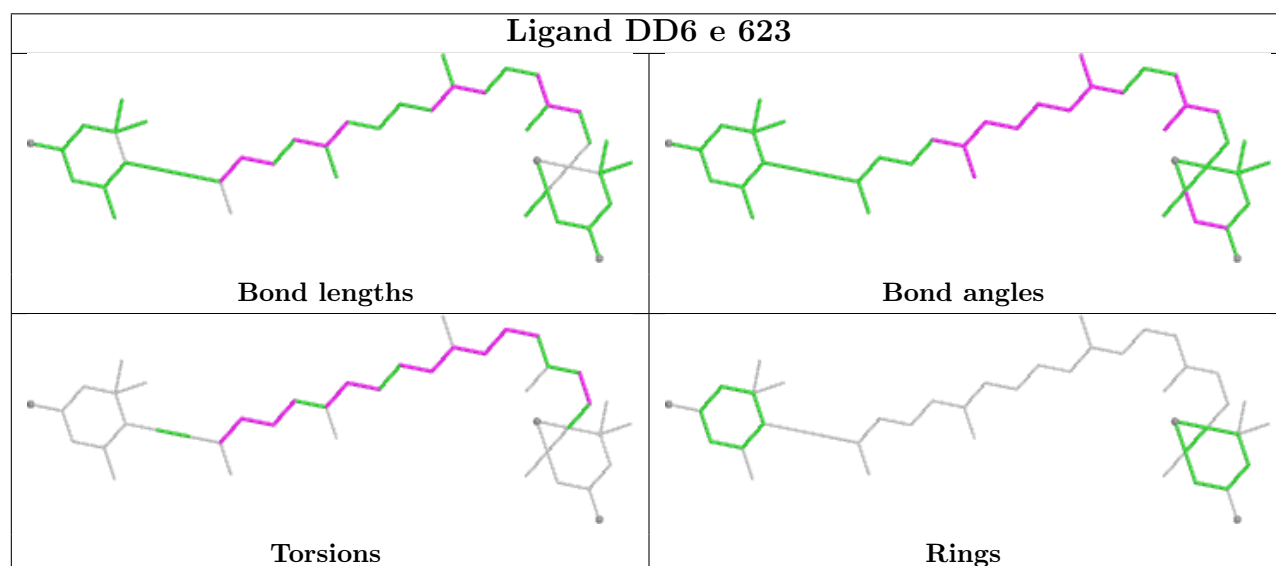
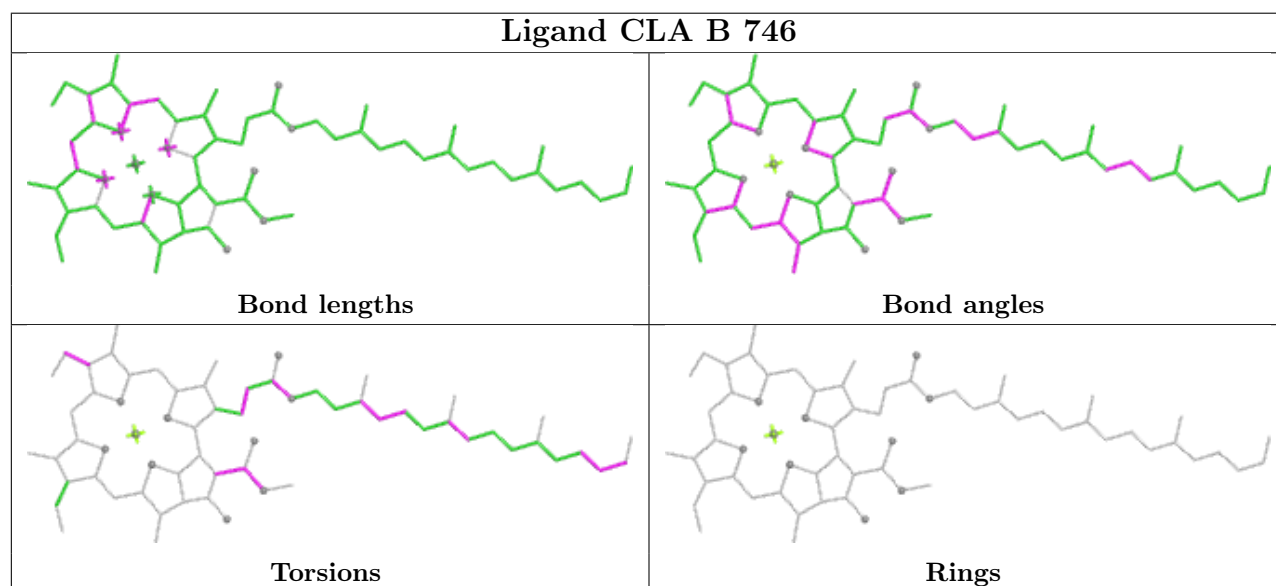
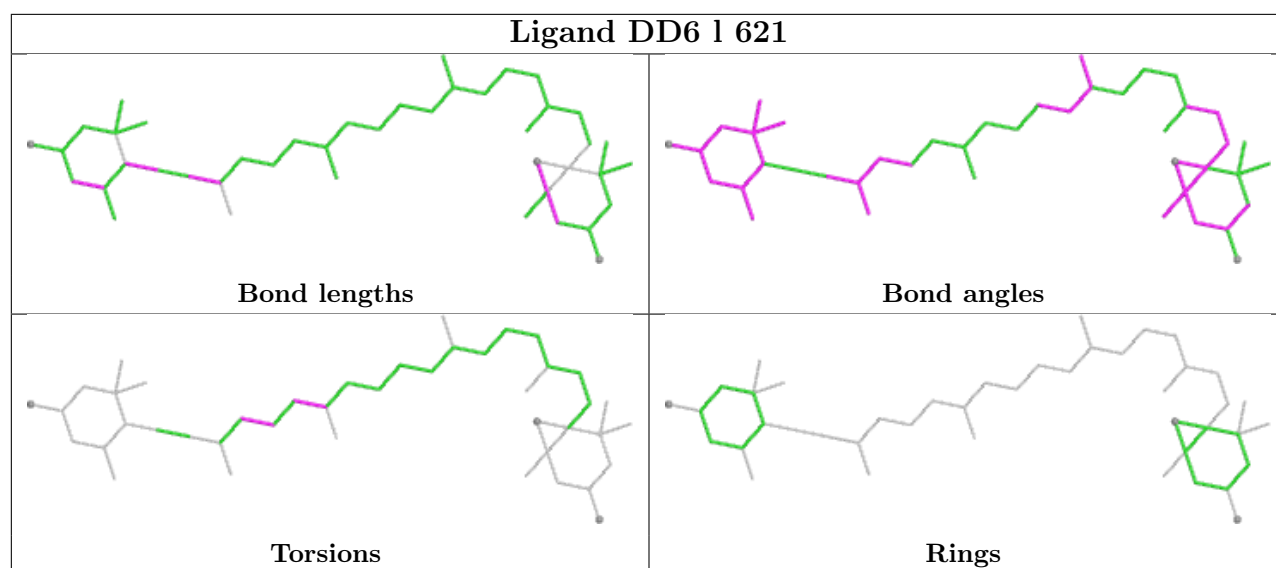
Bond angles



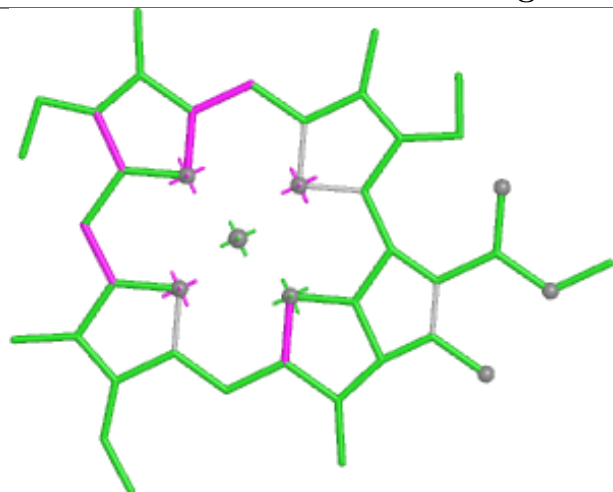
Torsions



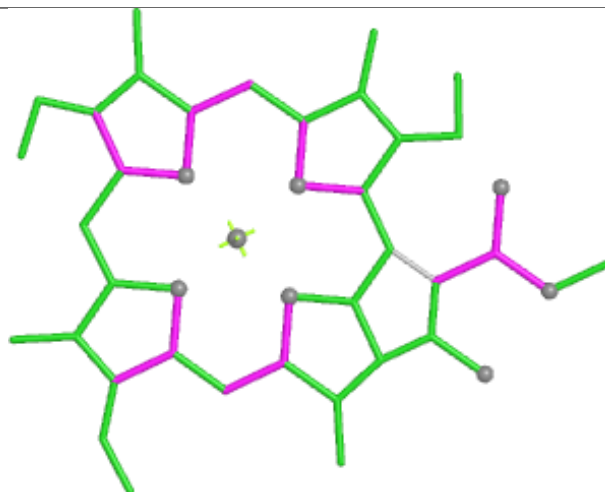
Rings



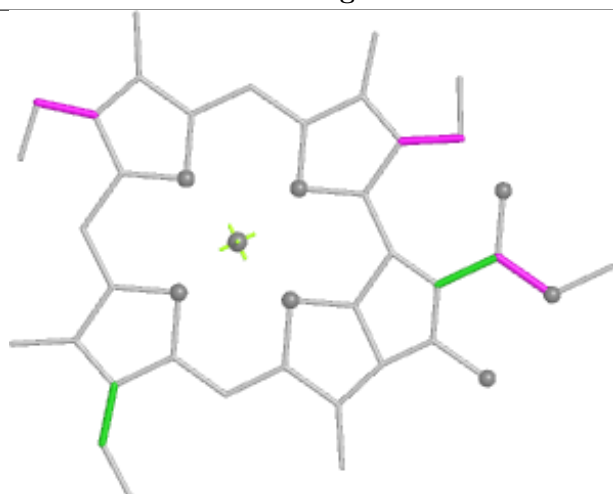
Ligand CLA k 615



Bond lengths



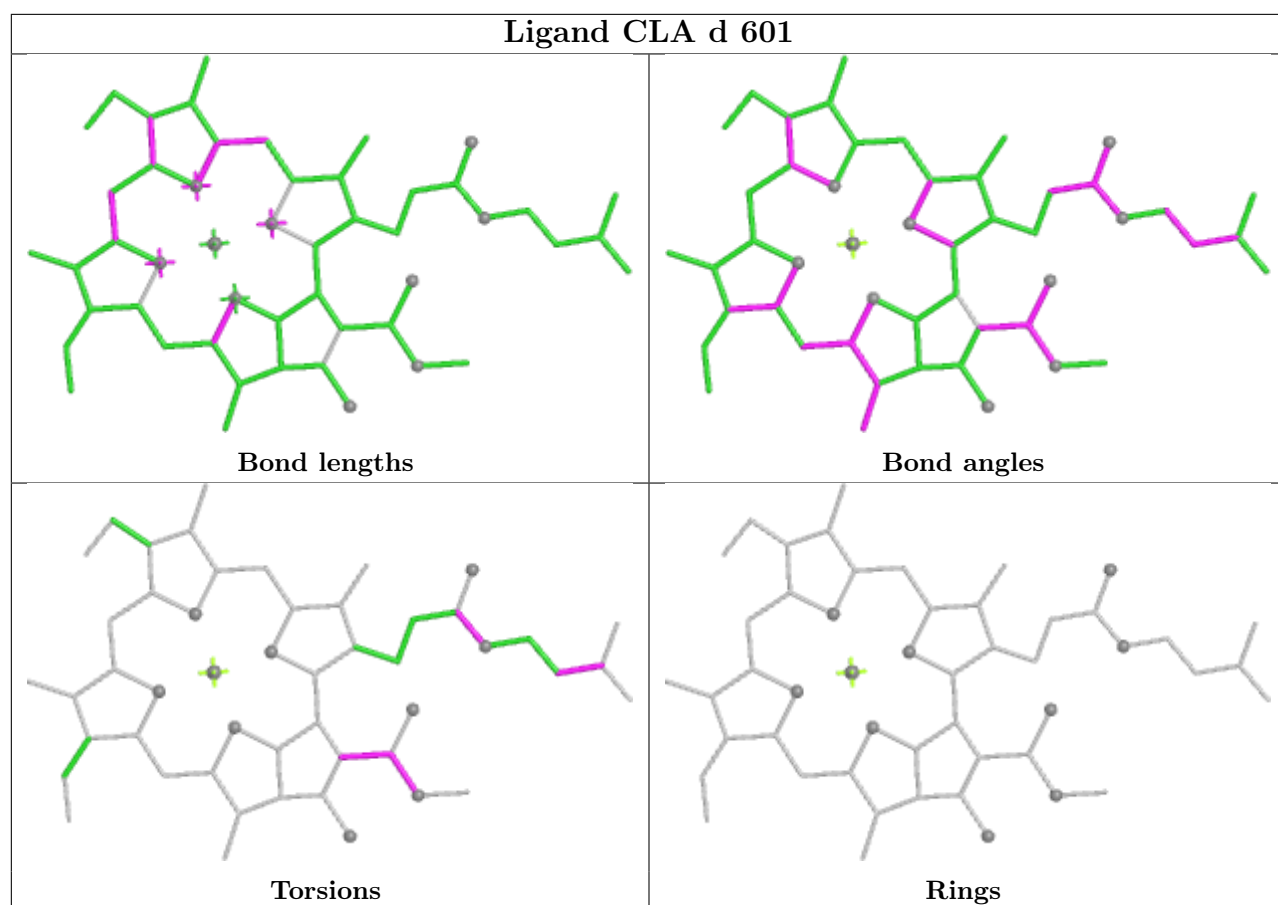
Bond angles

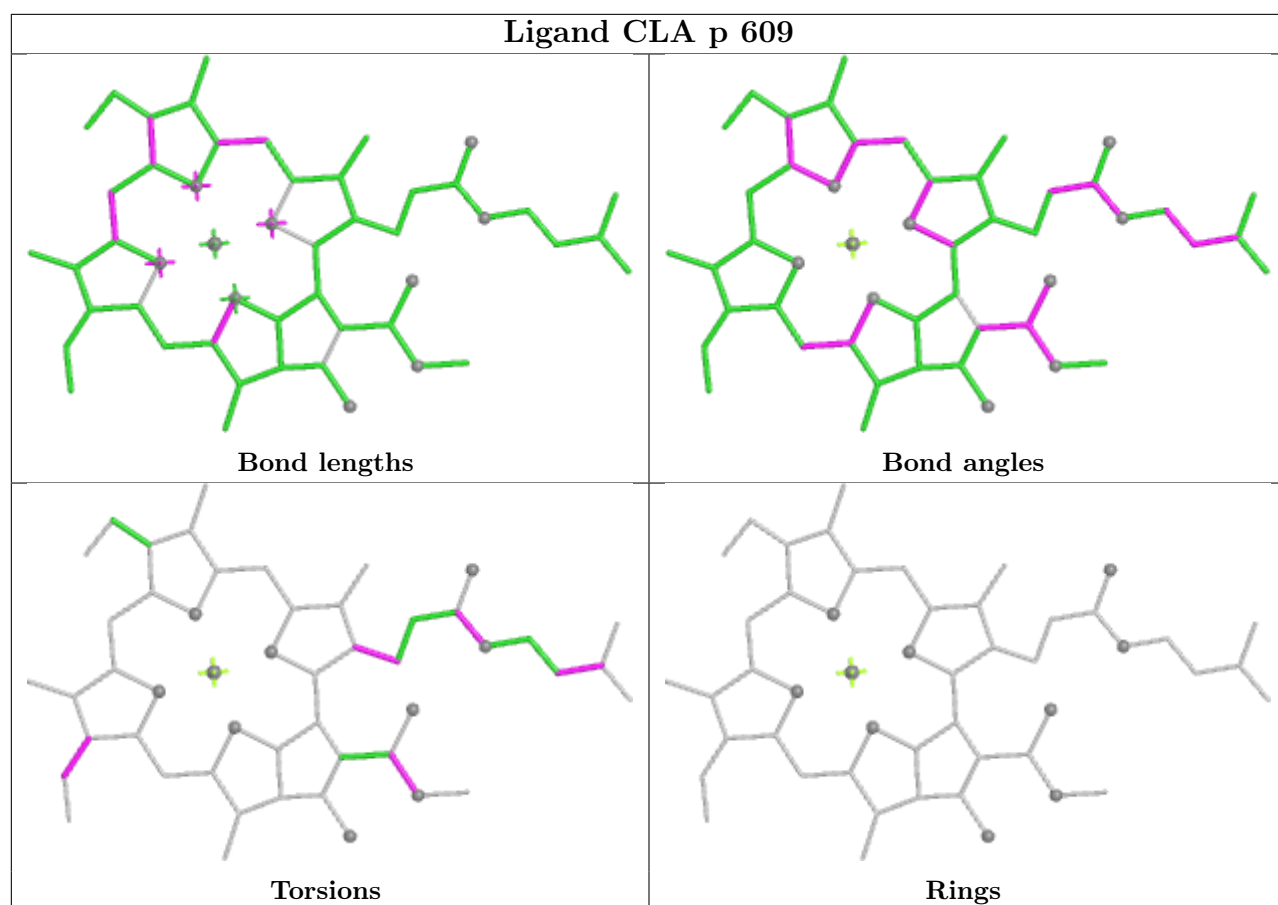


Torsions

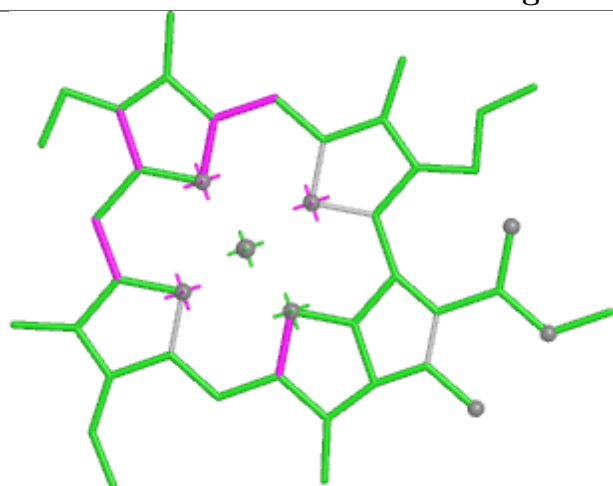


Rings

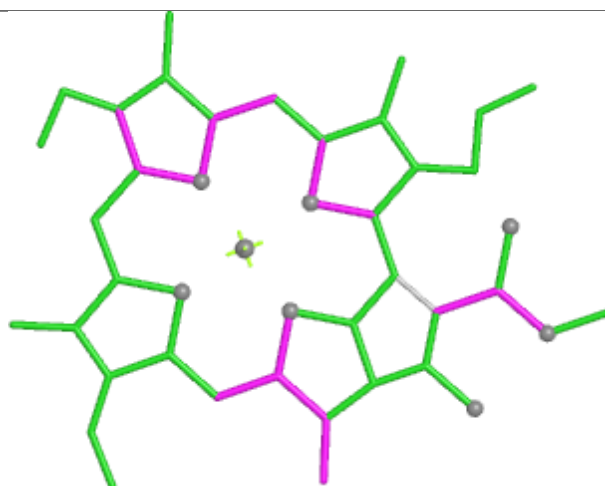




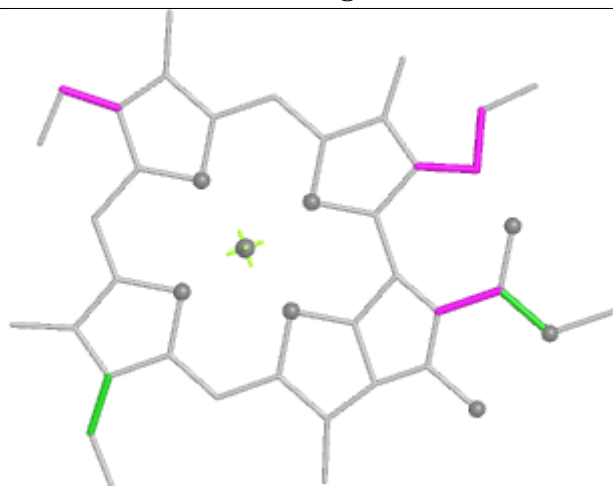
Ligand CLA 1 608



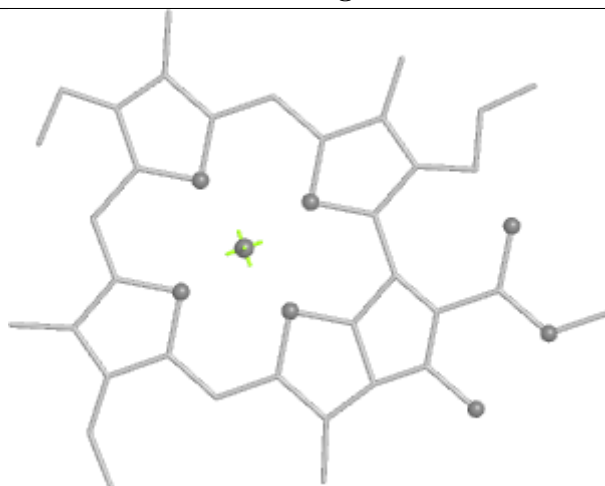
Bond lengths



Bond angles

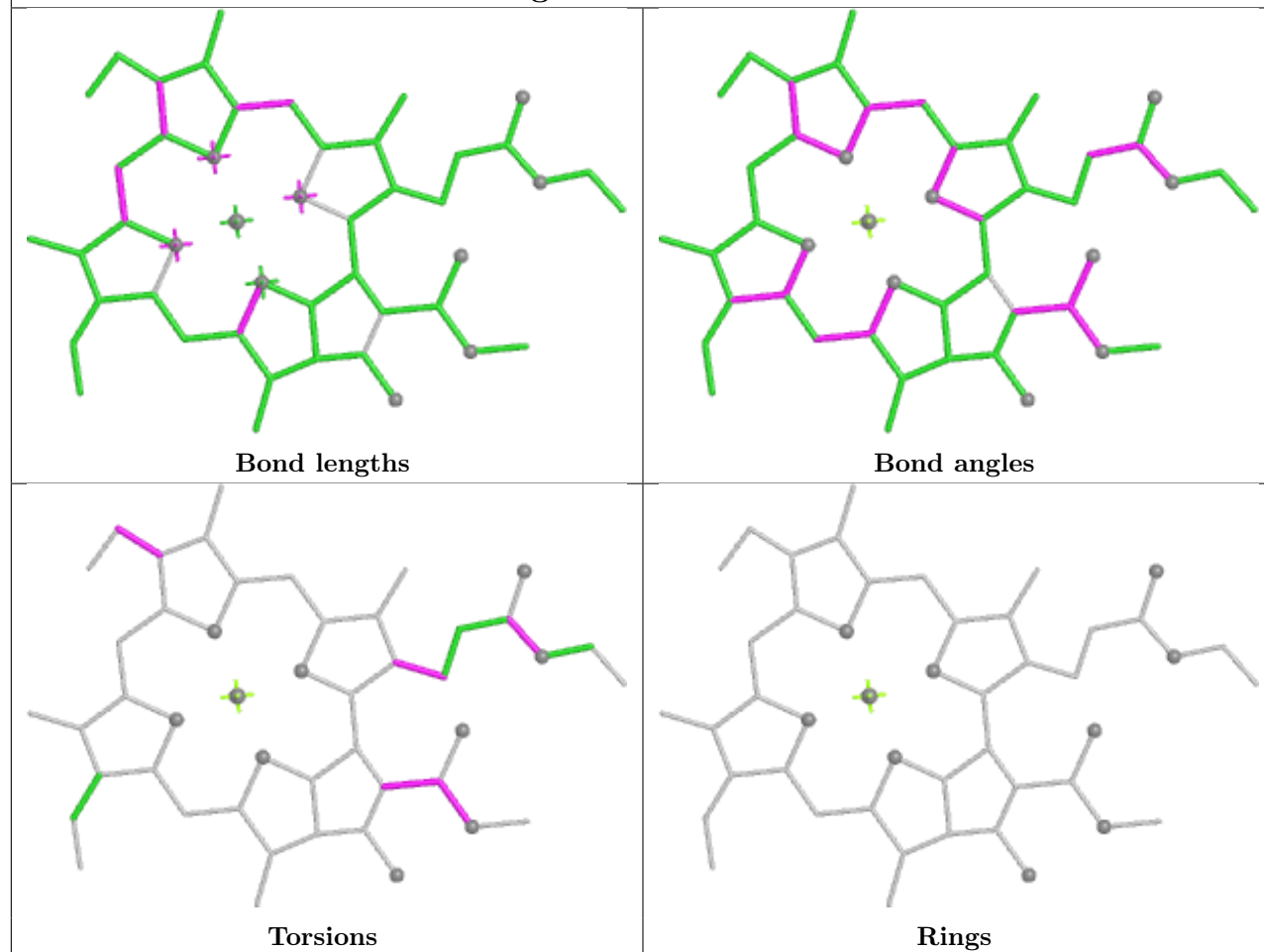


Torsions

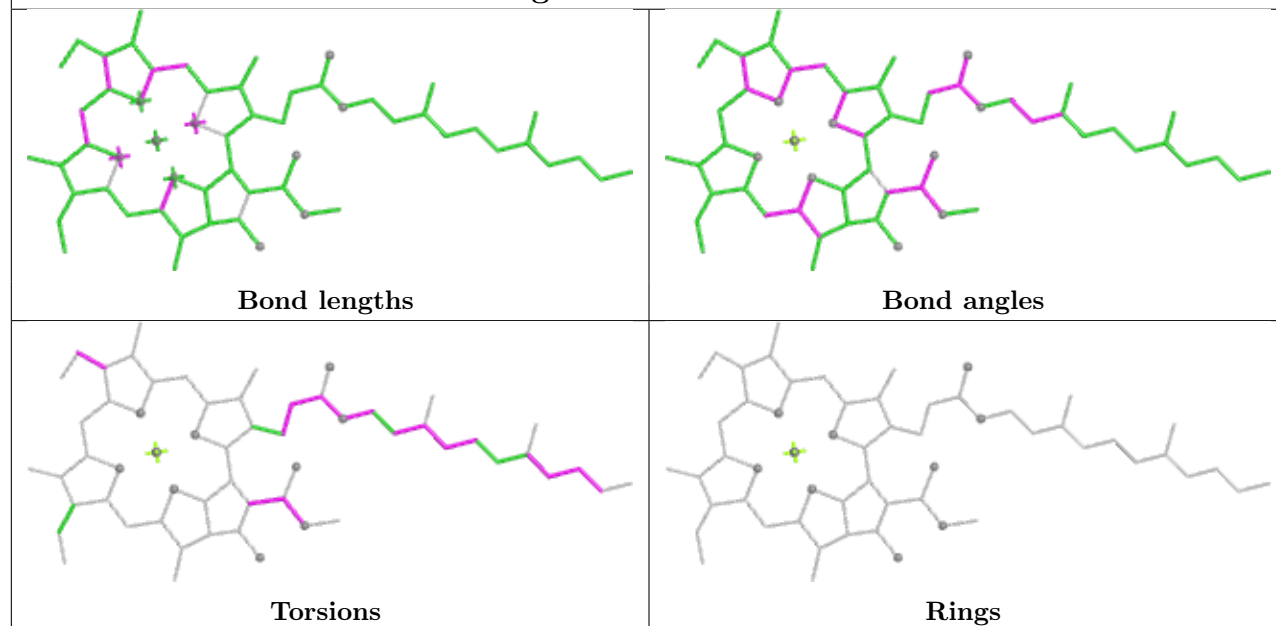


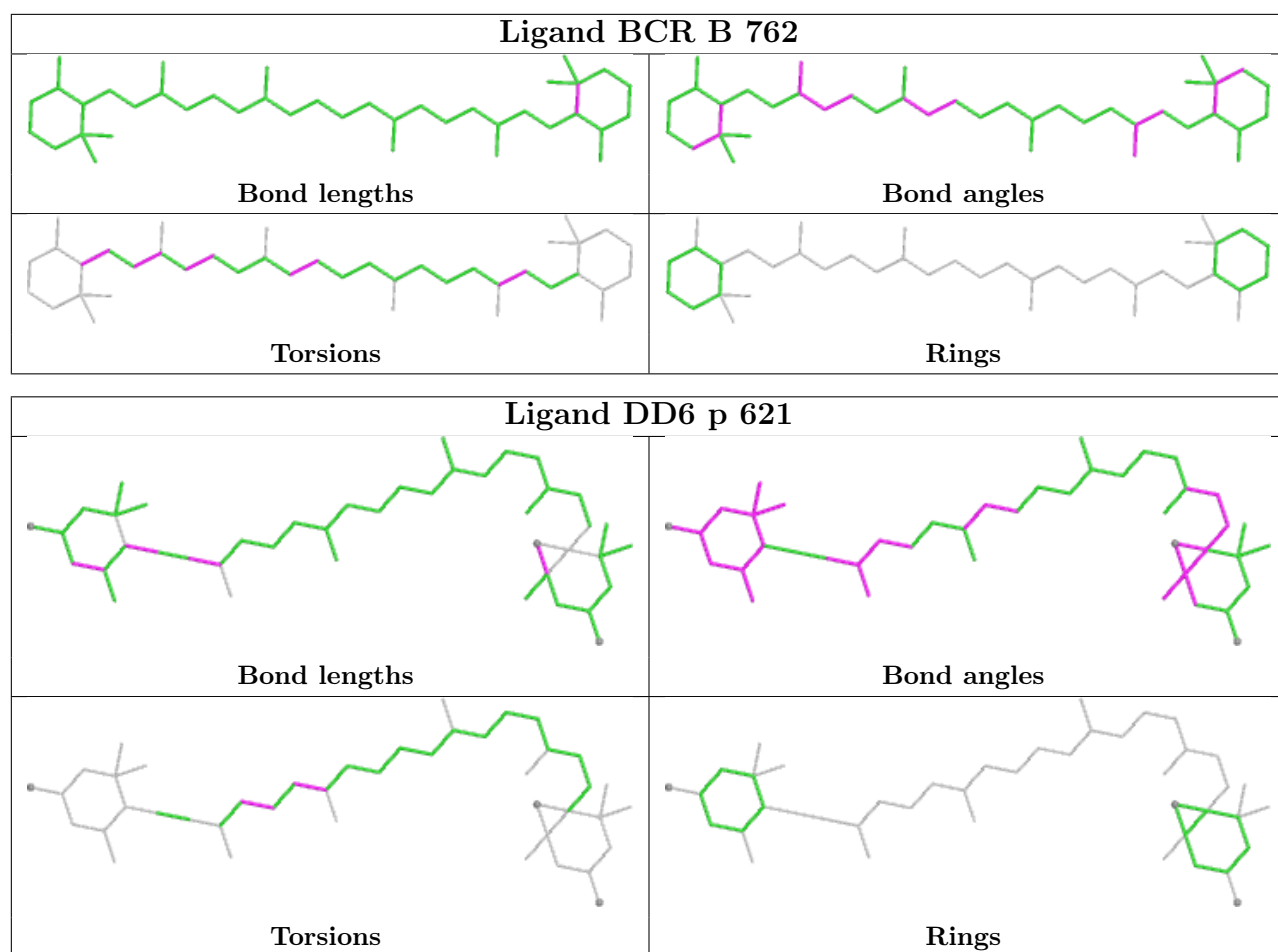
Rings

Ligand CLA o 602

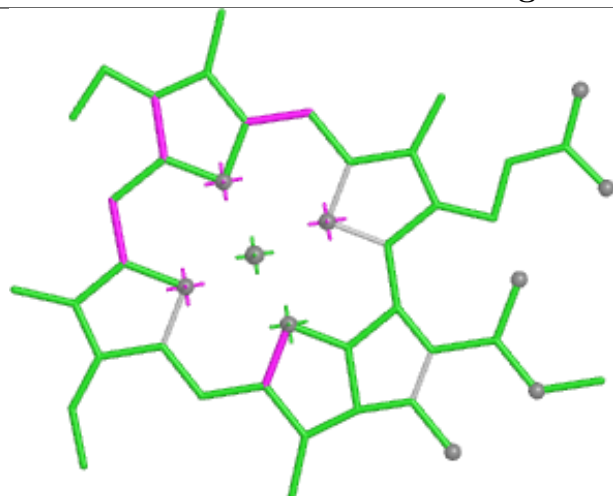


Ligand CLA A 766

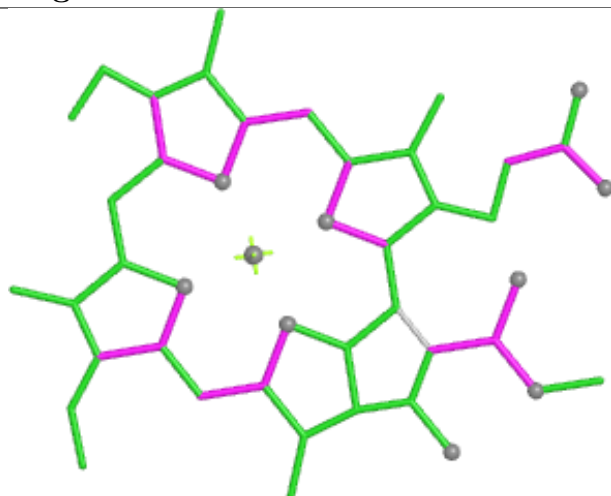




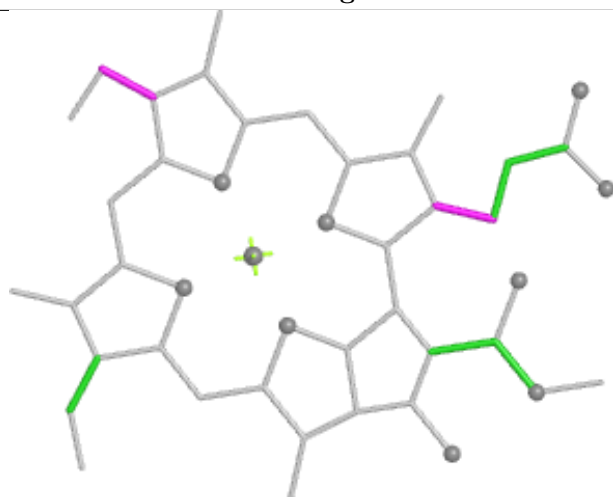
Ligand CLA g 618



Bond lengths



Bond angles

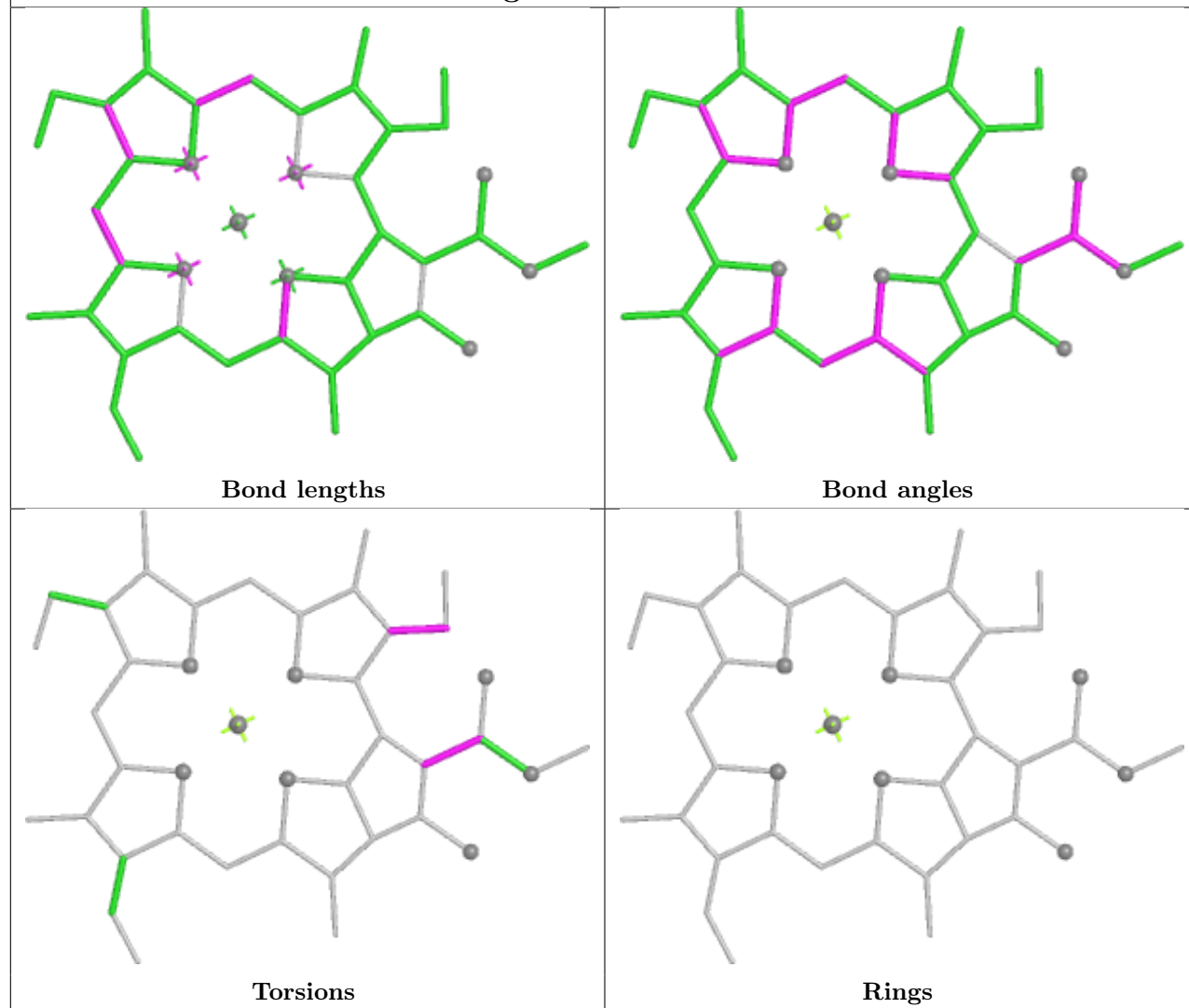


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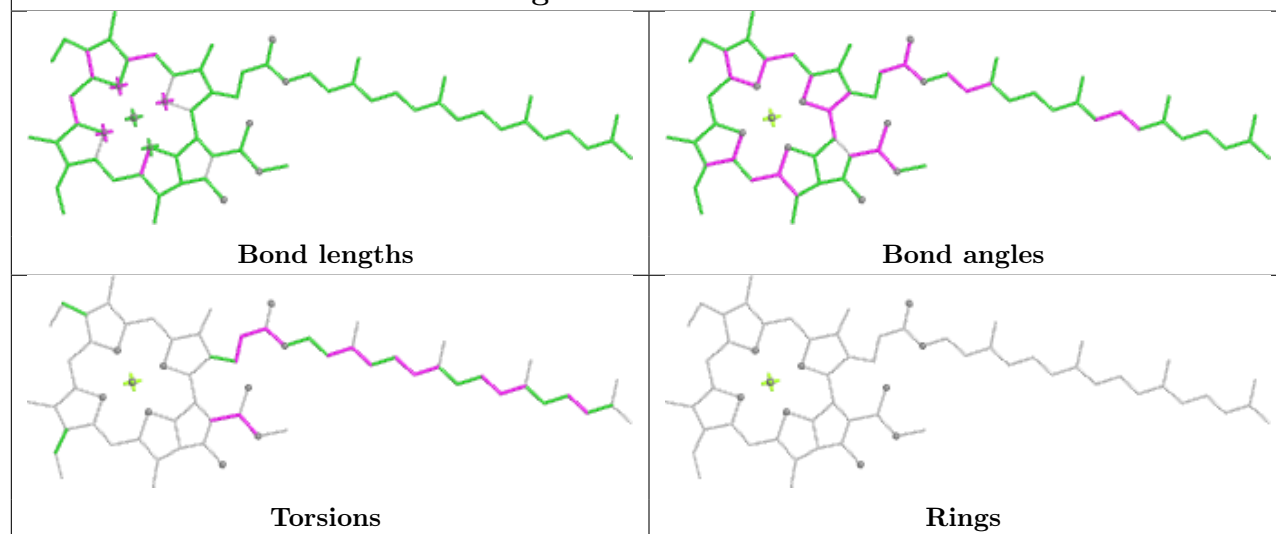


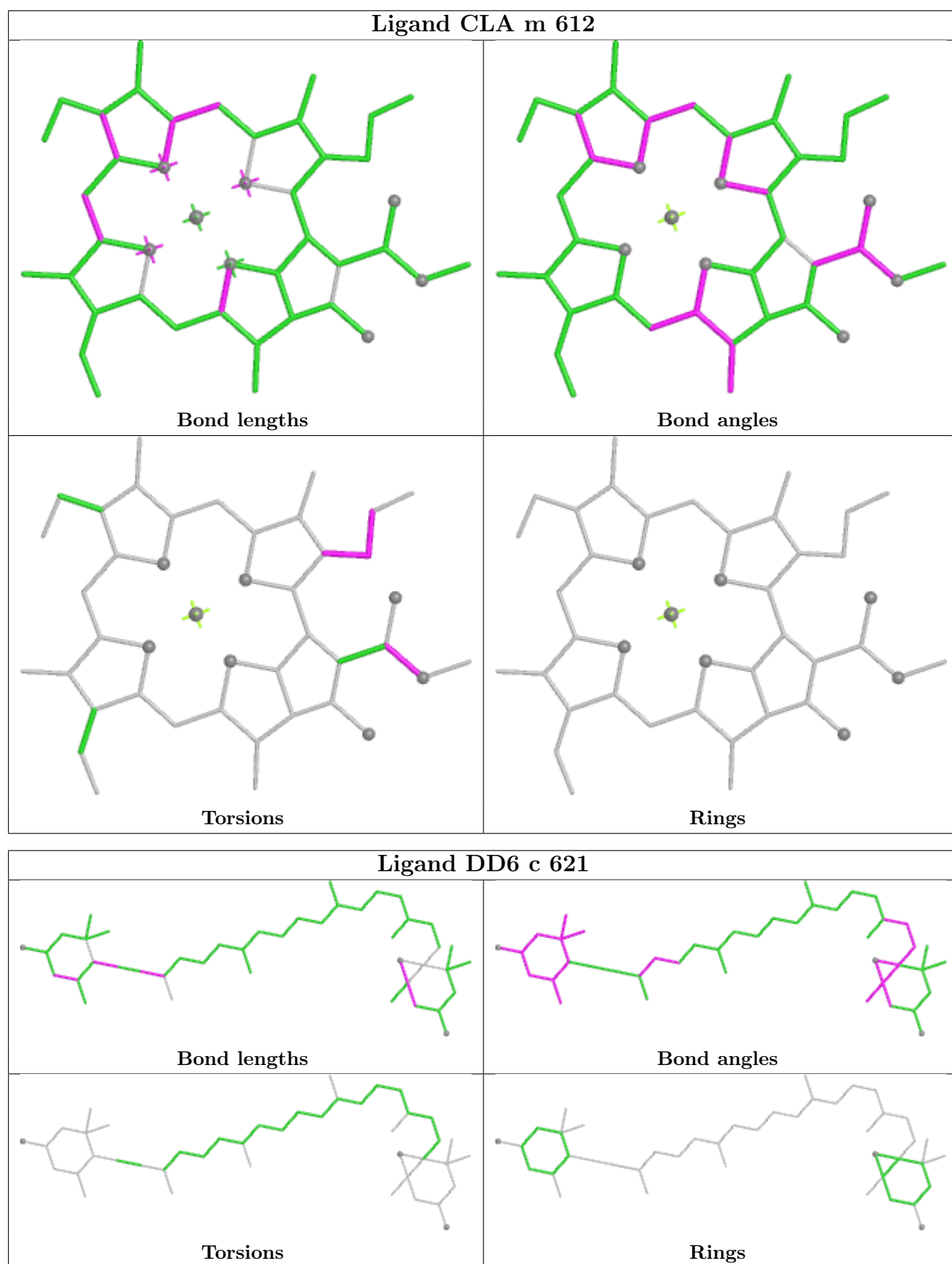
Rings

Ligand CLA i 614

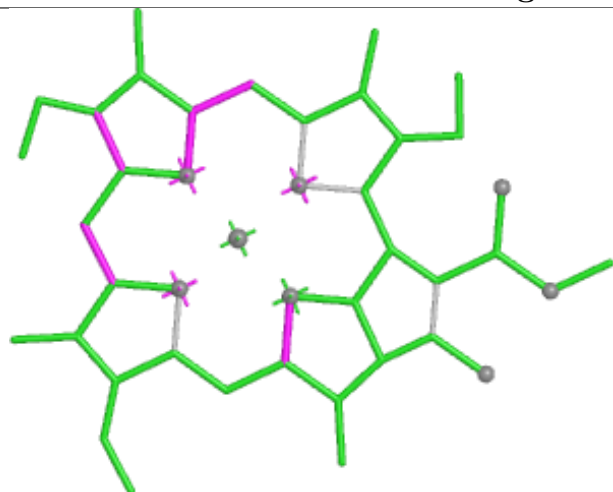


Ligand CLA A 784

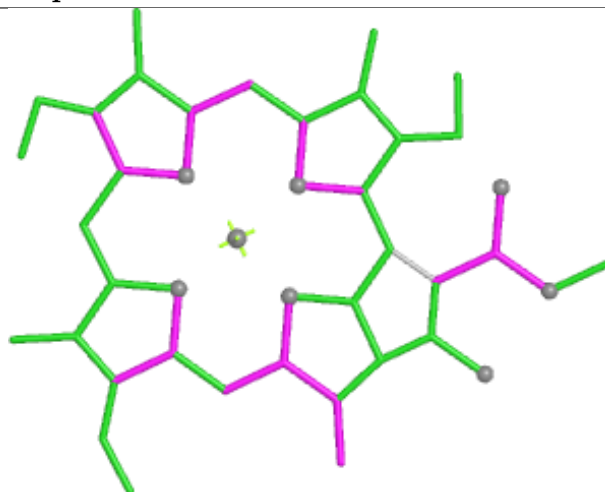




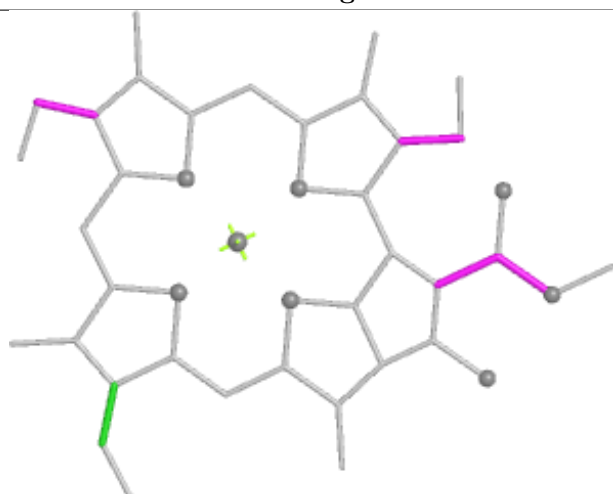
Ligand CLA p 608



Bond lengths



Bond angles

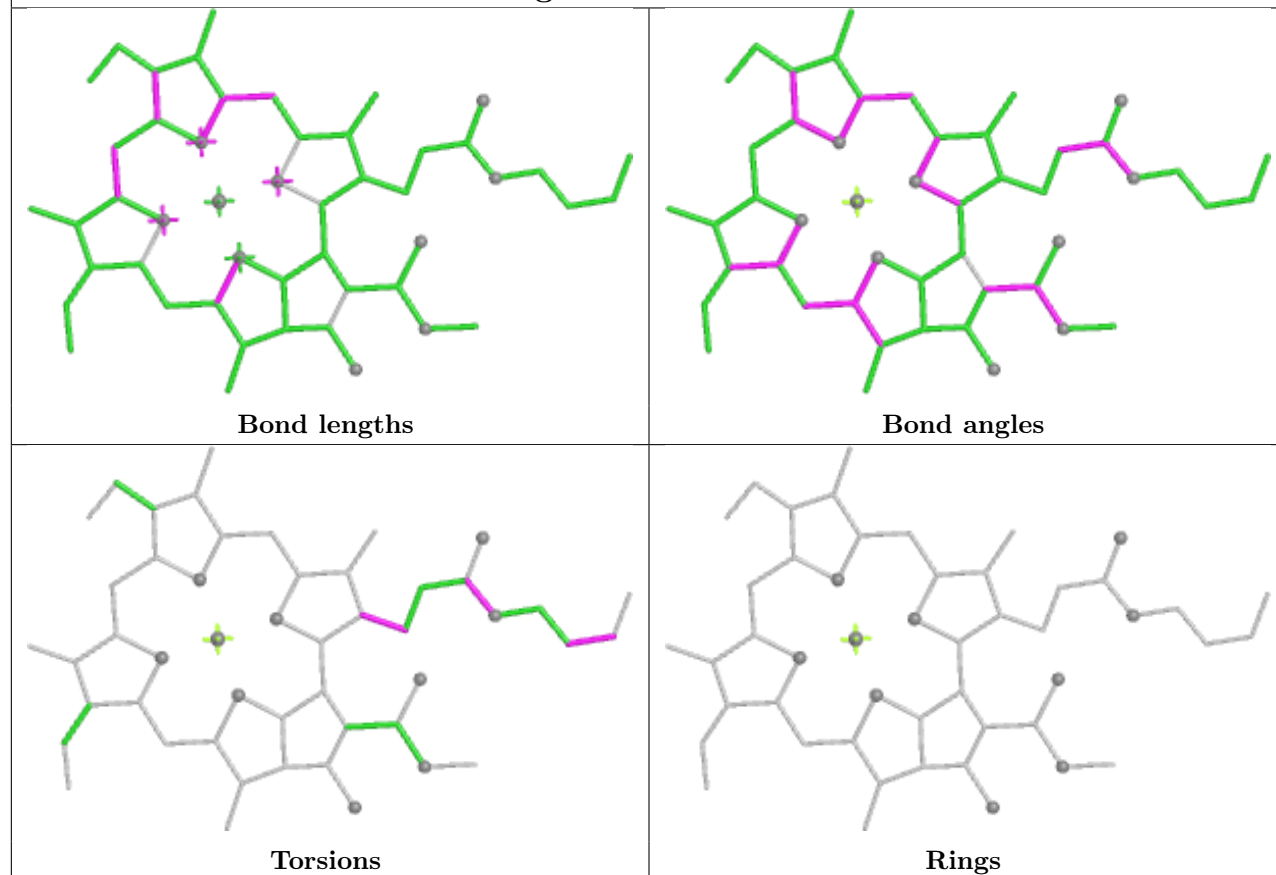


Torsions

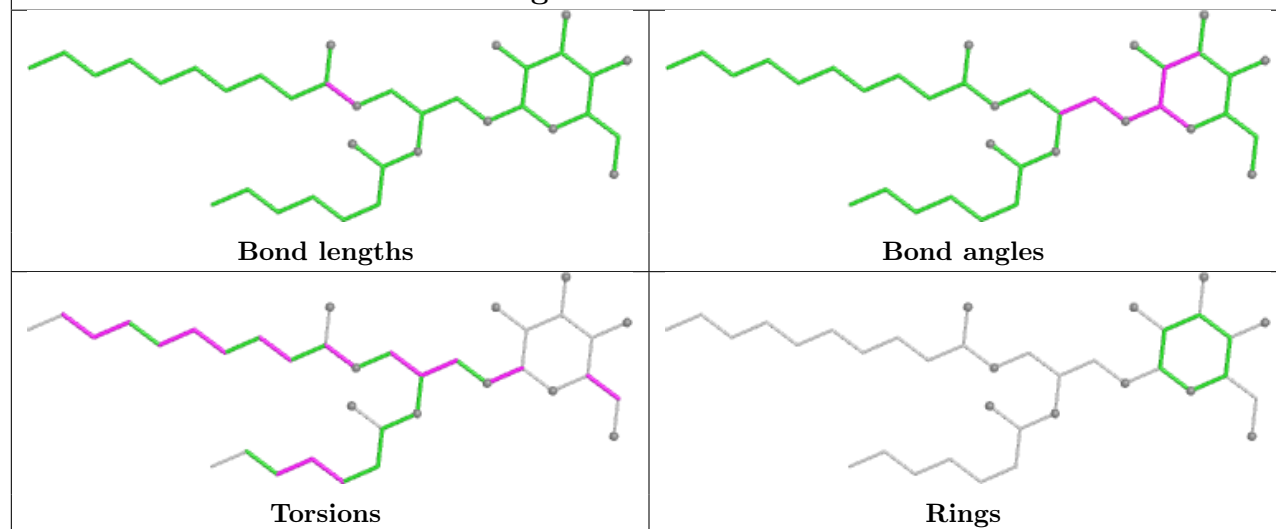


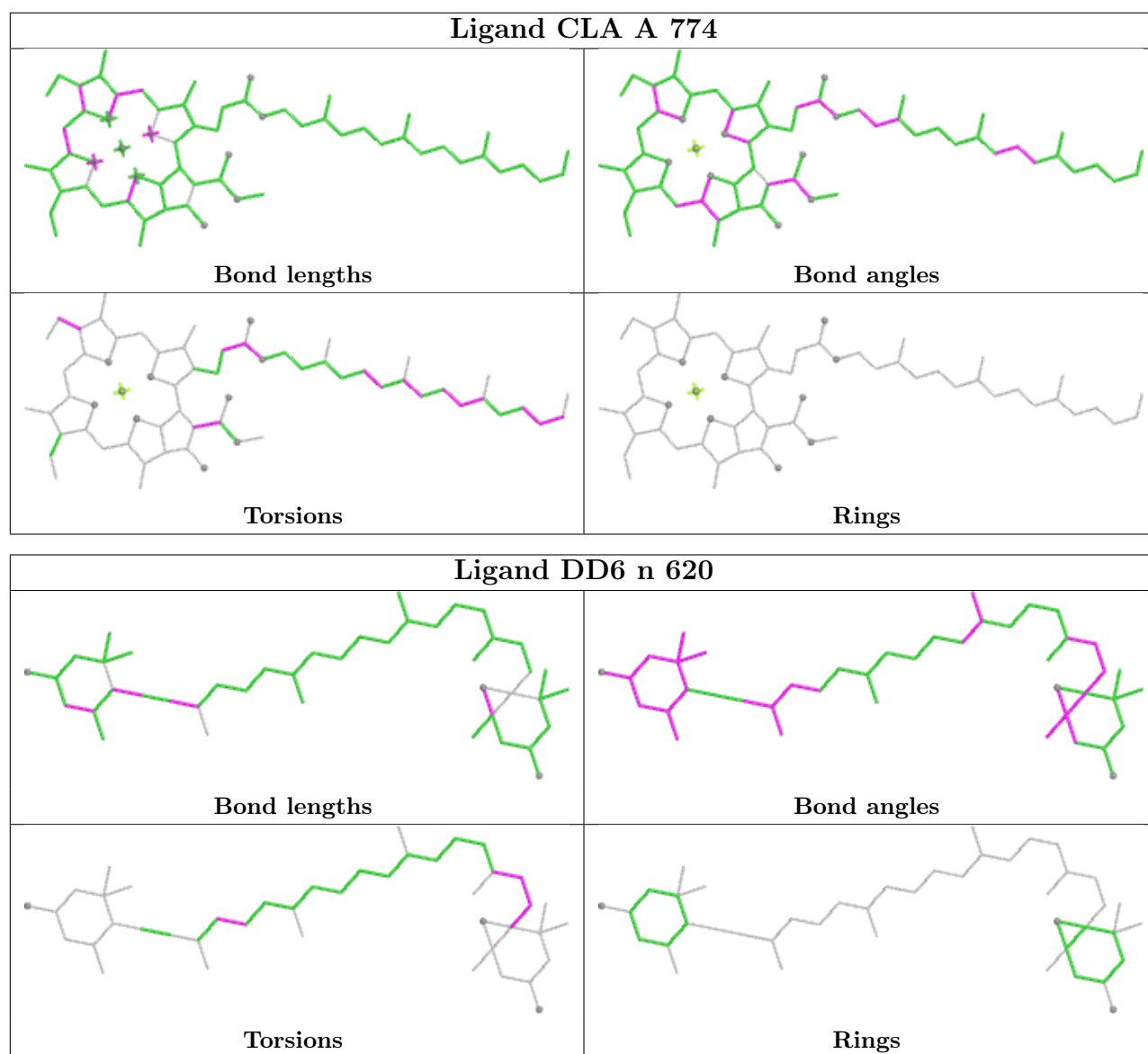
Rings

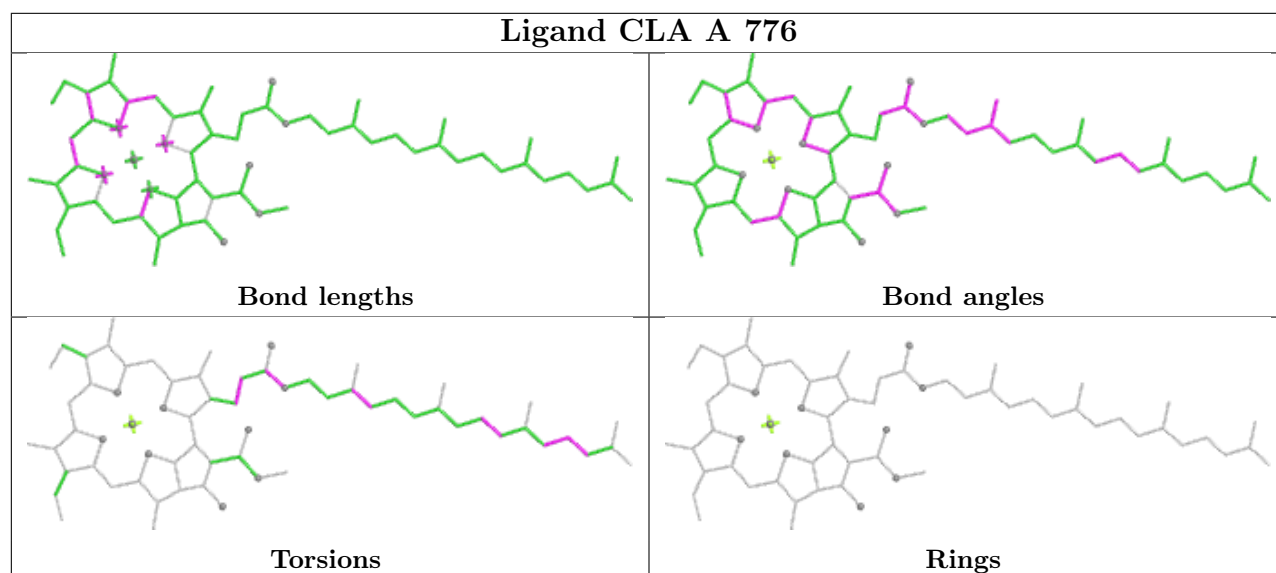
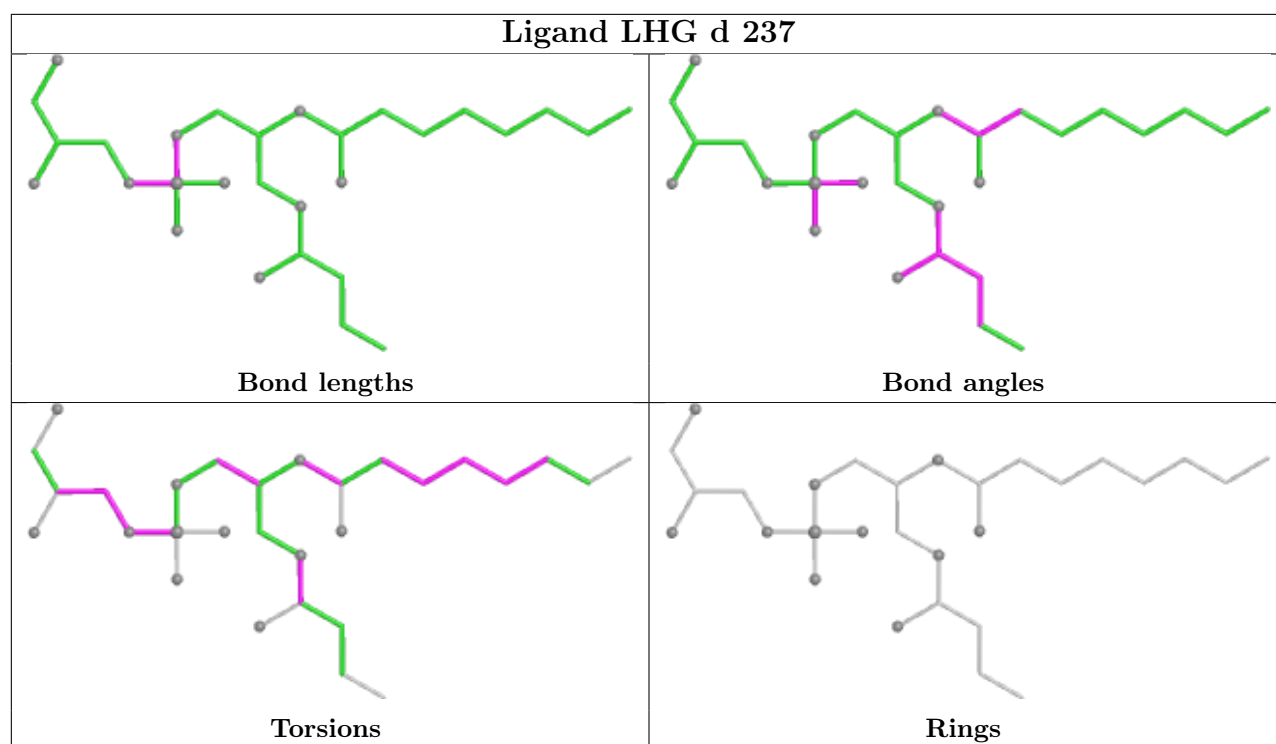
Ligand CLA d 609



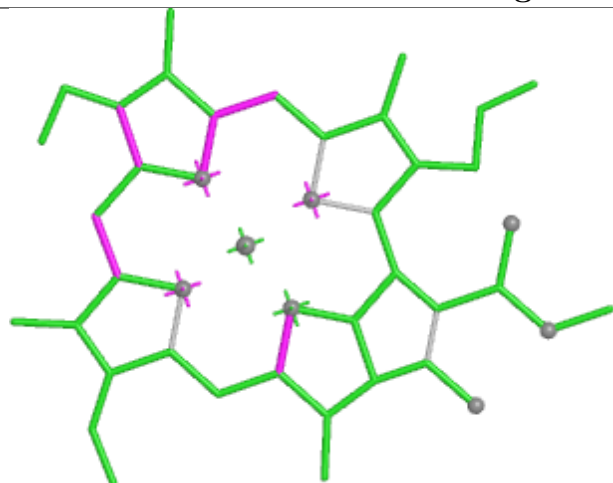
Ligand LMG k 179



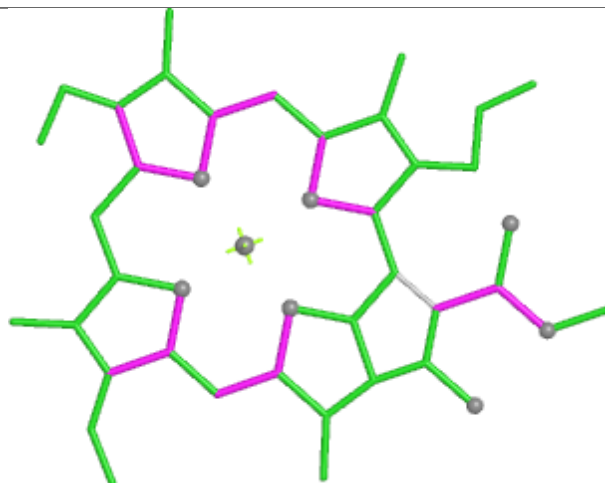




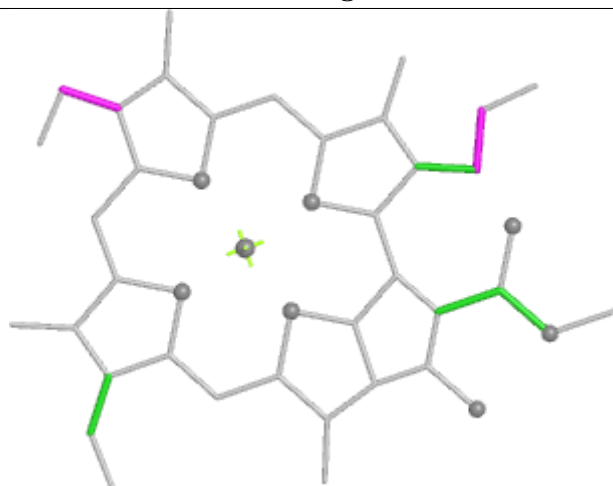
Ligand CLA B 742



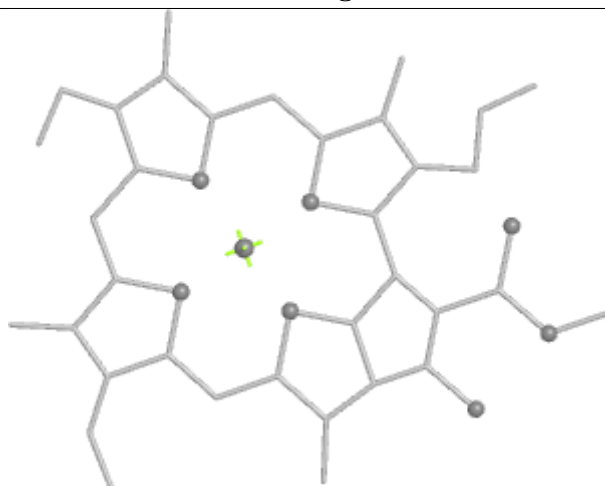
Bond lengths



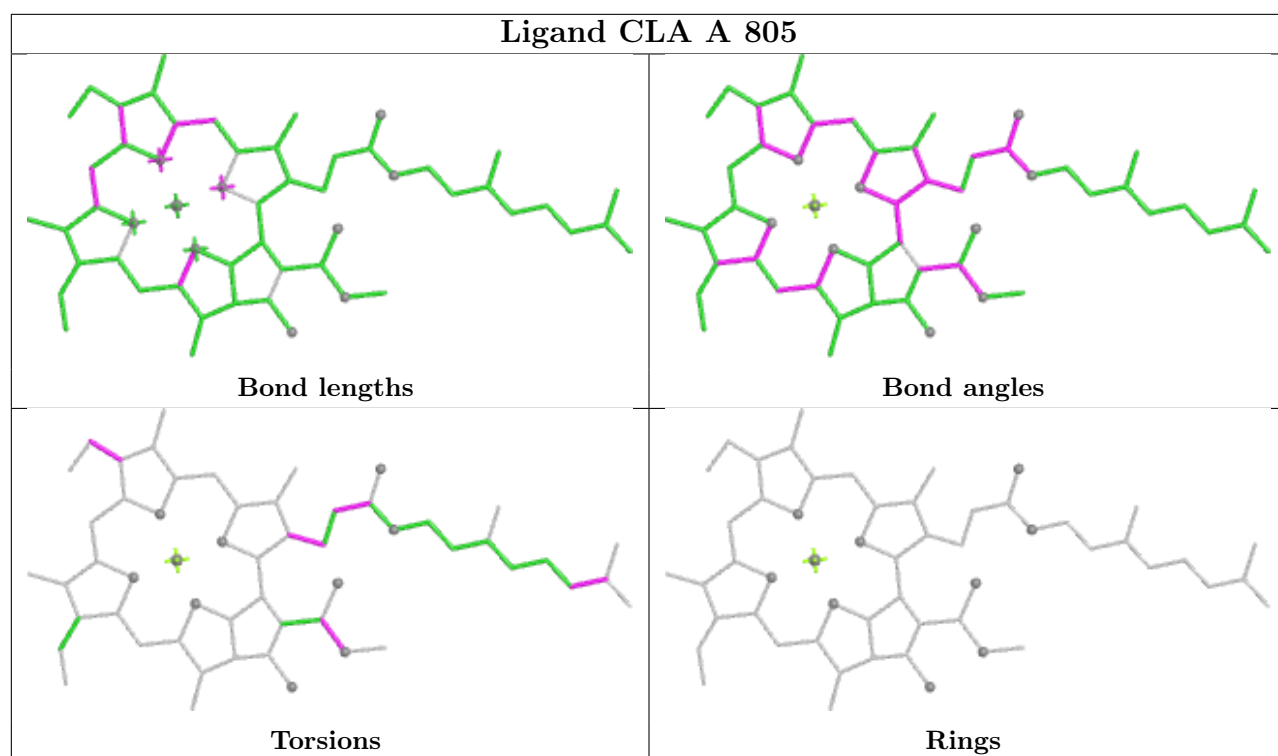
Bond angles



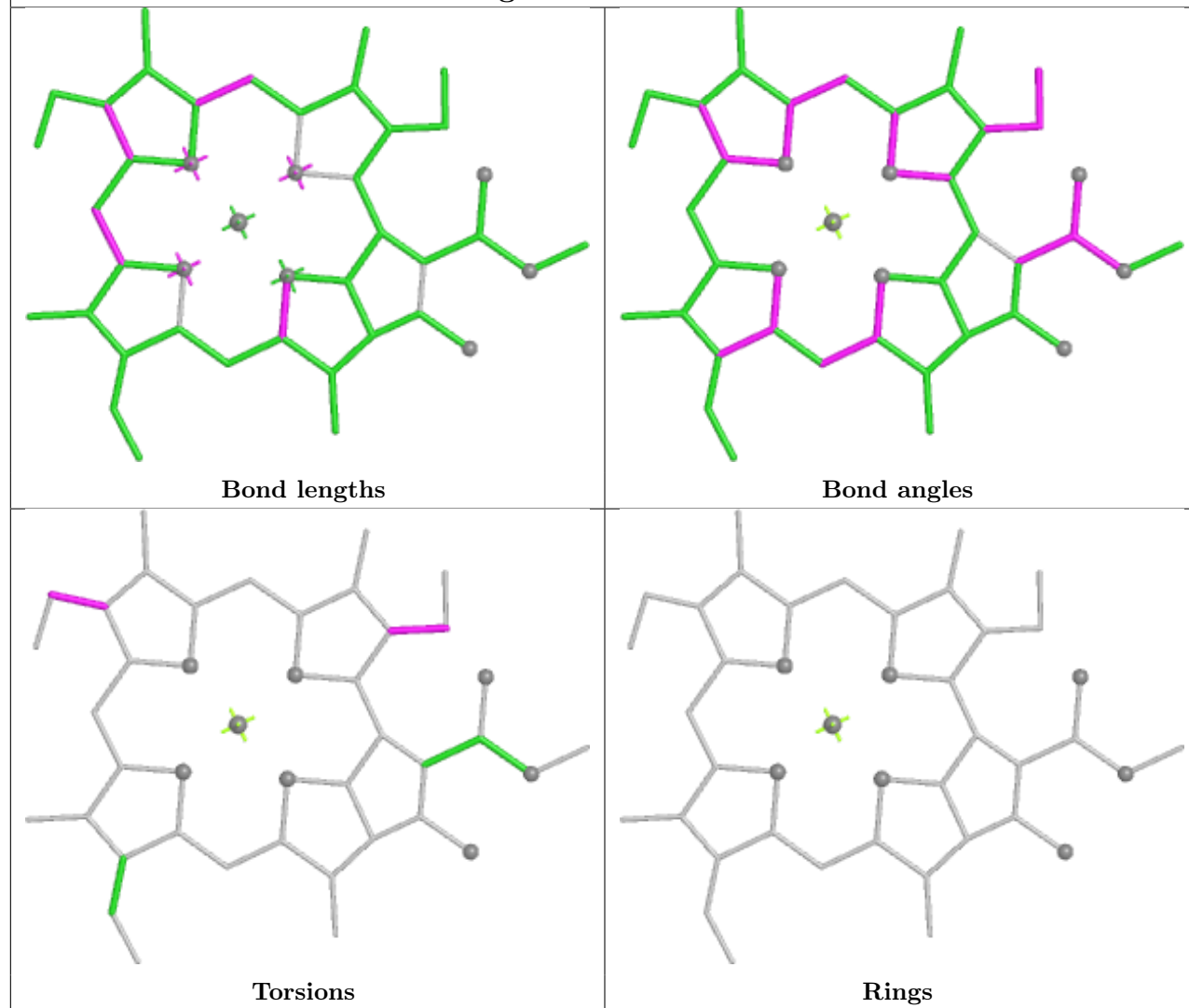
Torsions



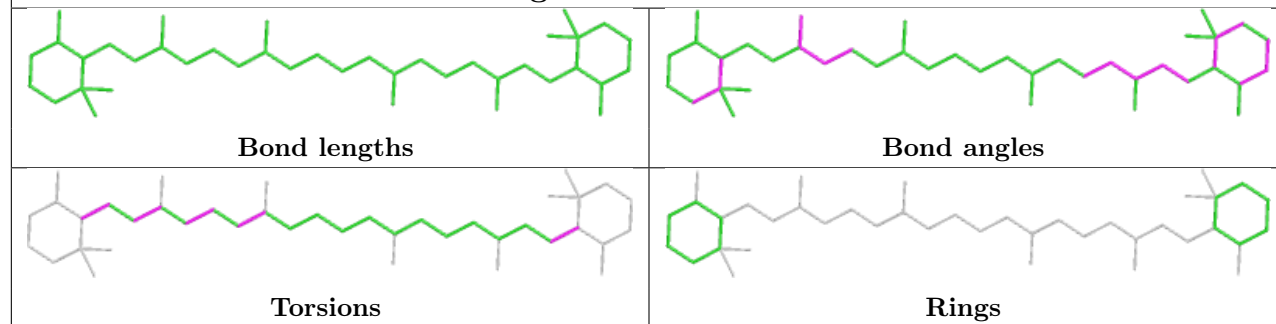
Rings

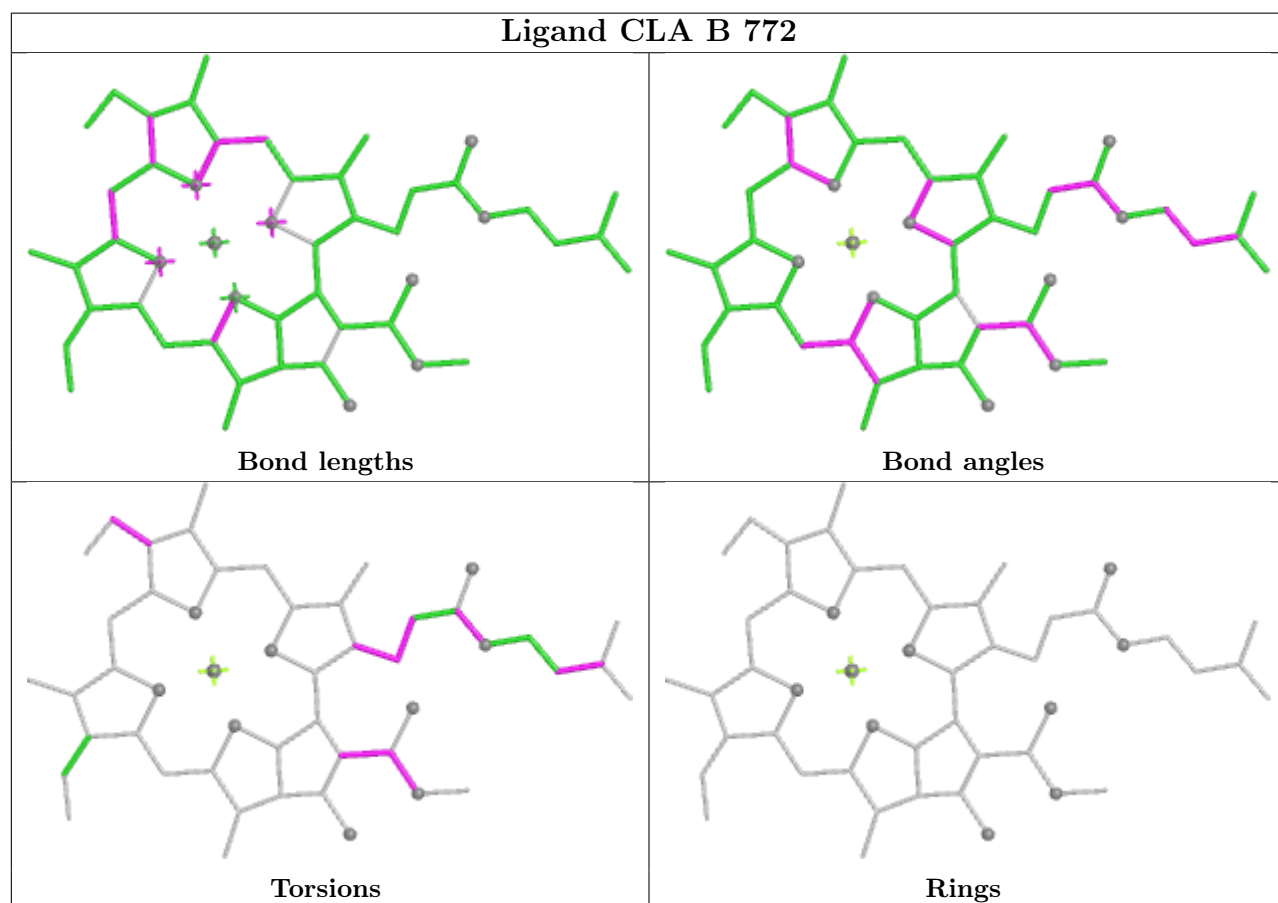
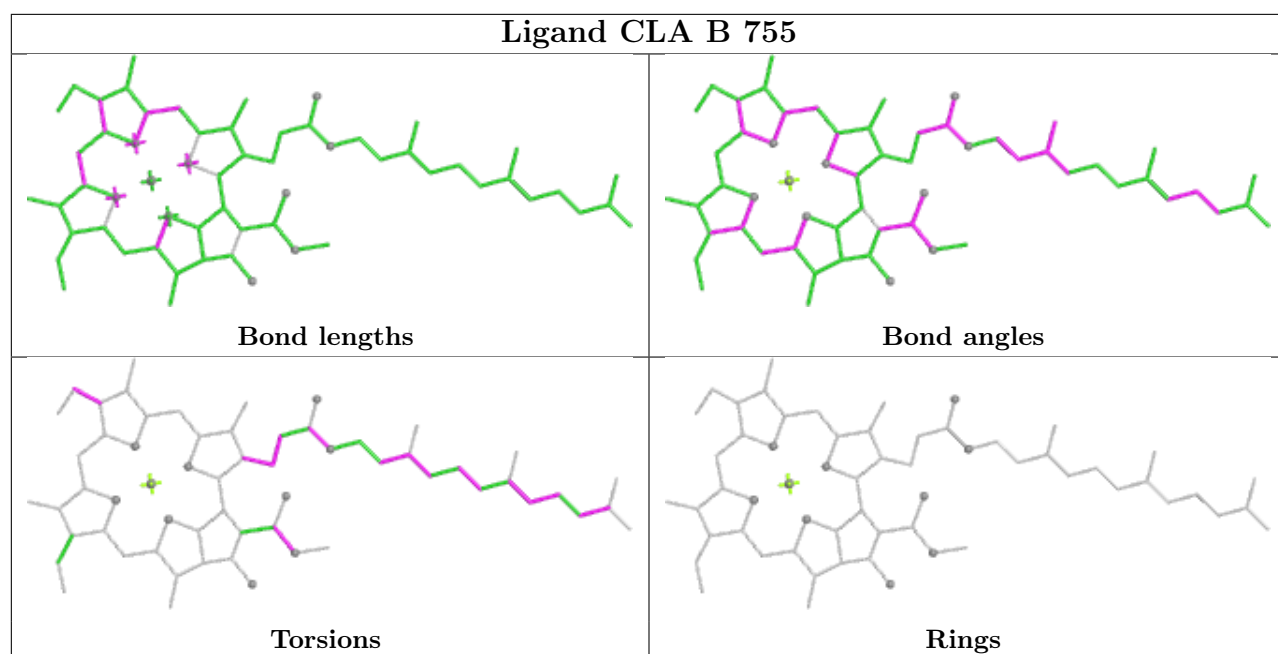


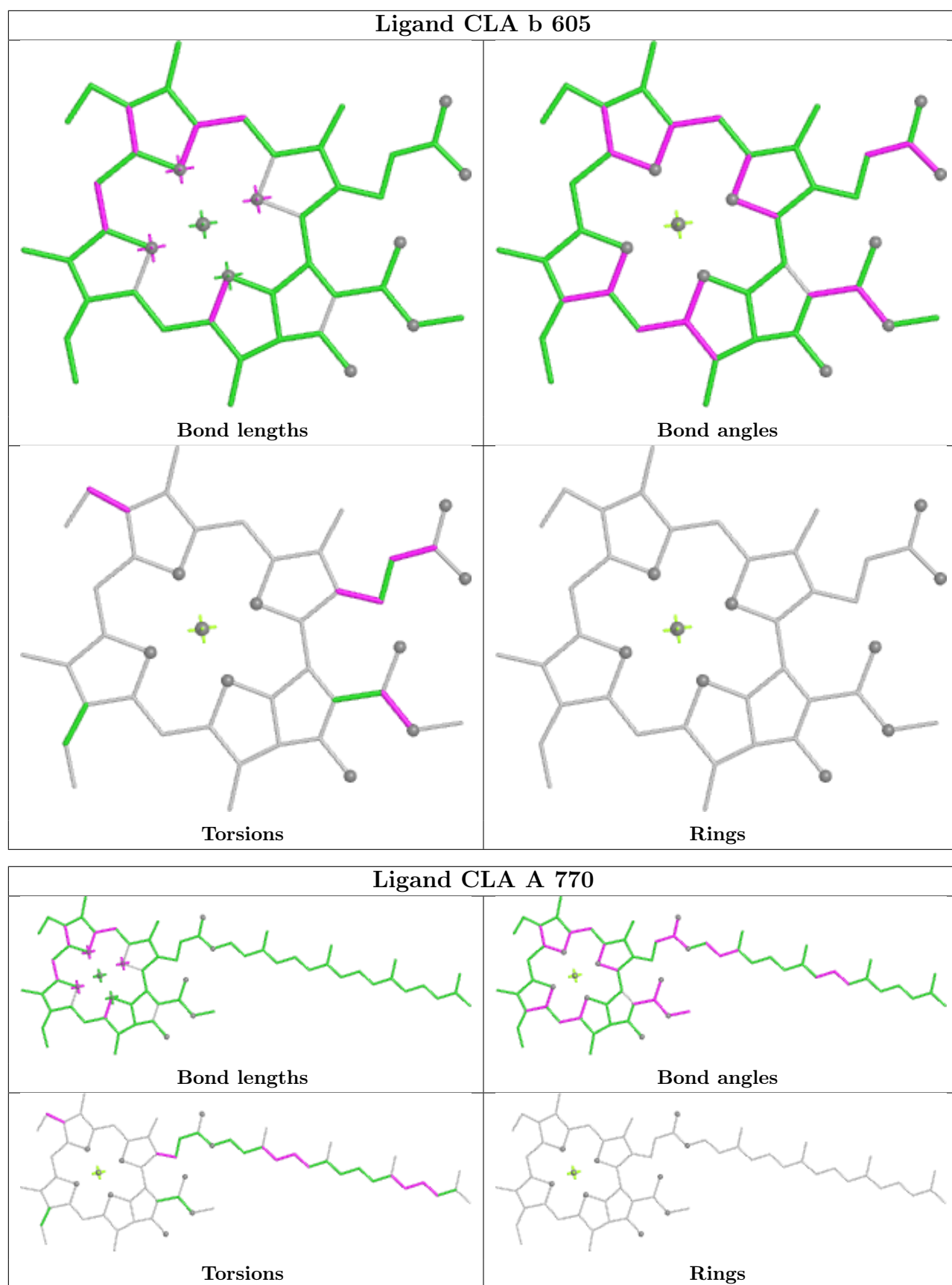
Ligand CLA b 610

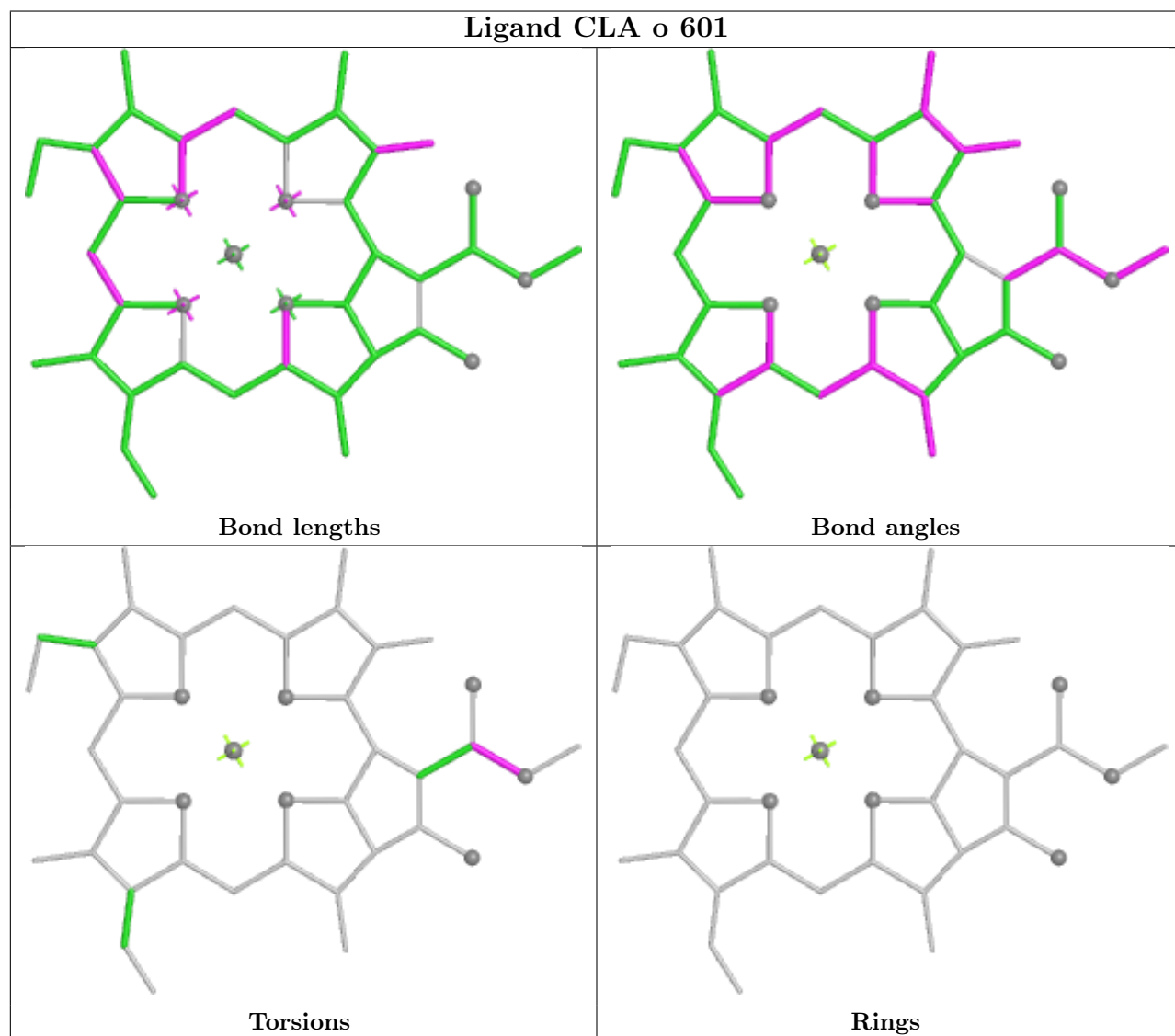
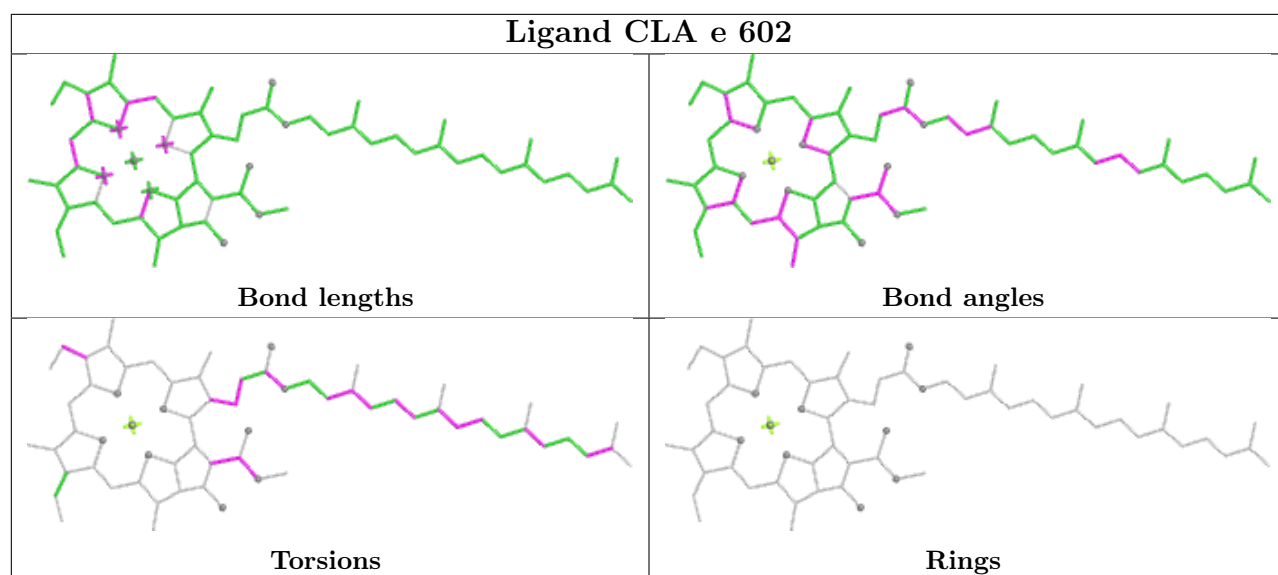


Ligand BCR A 796

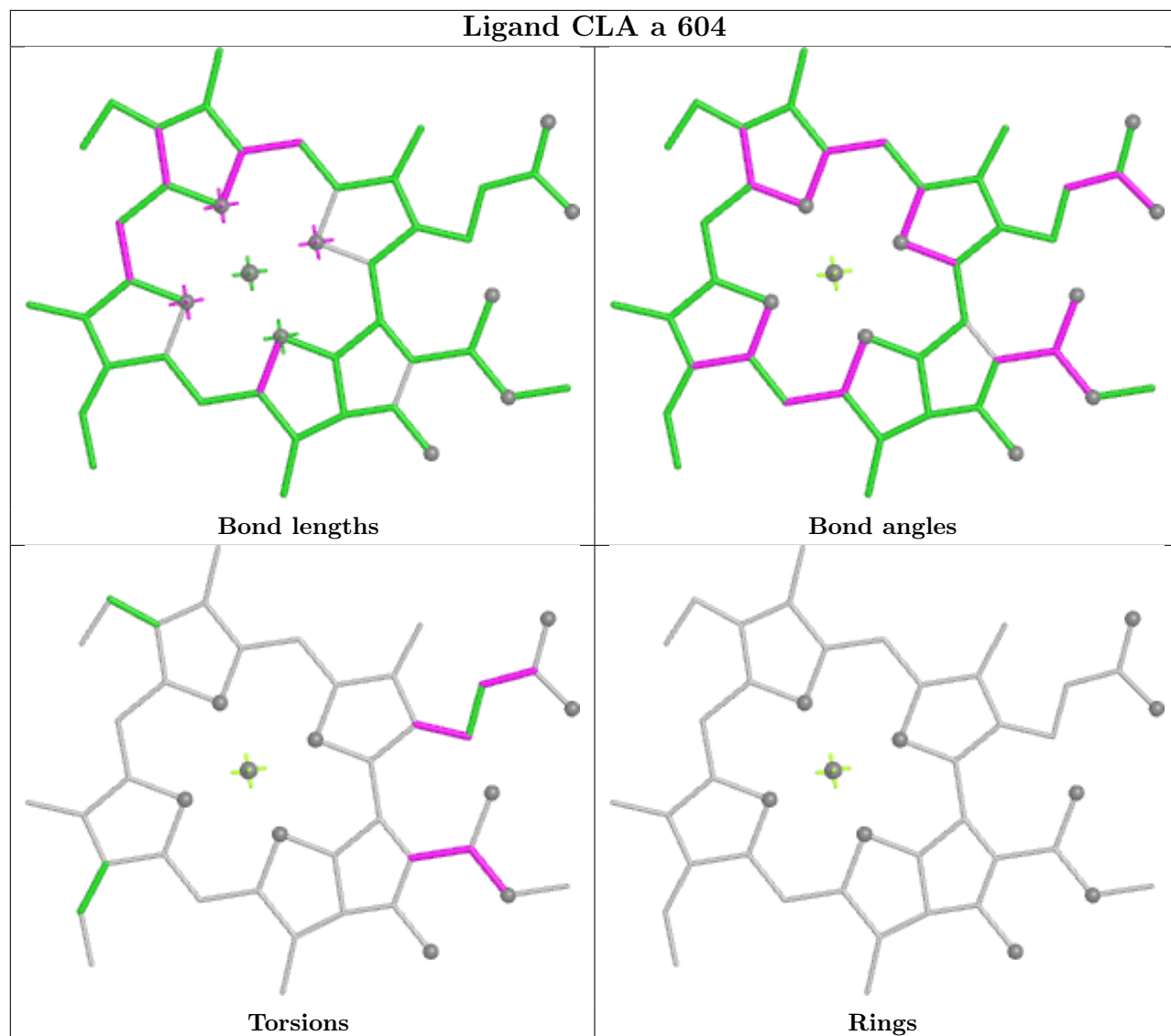




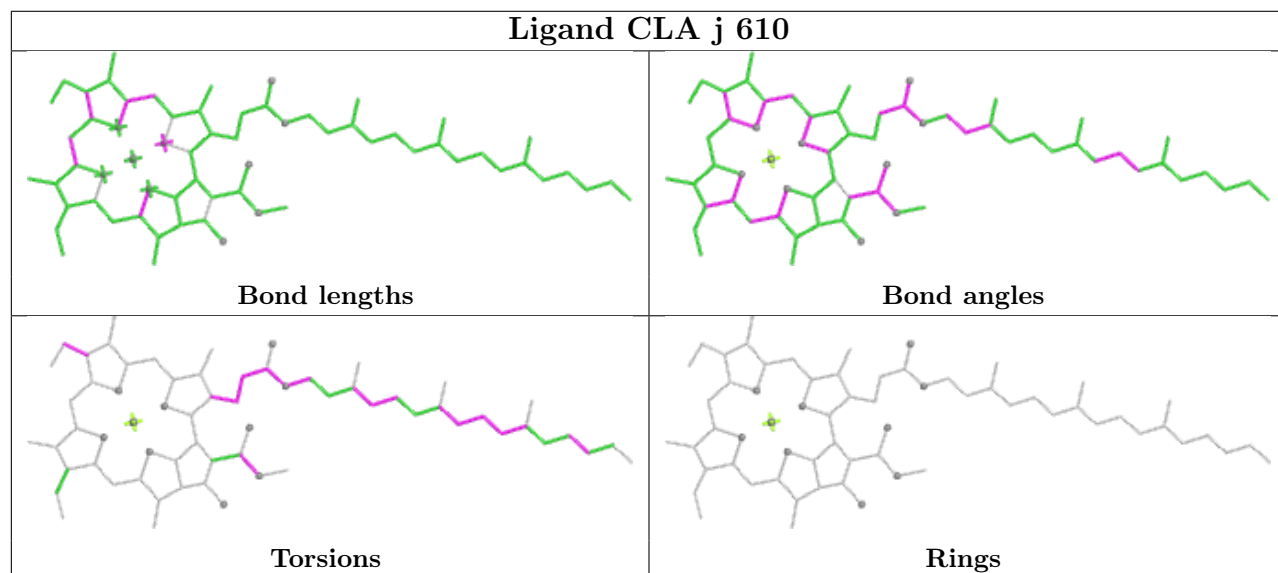




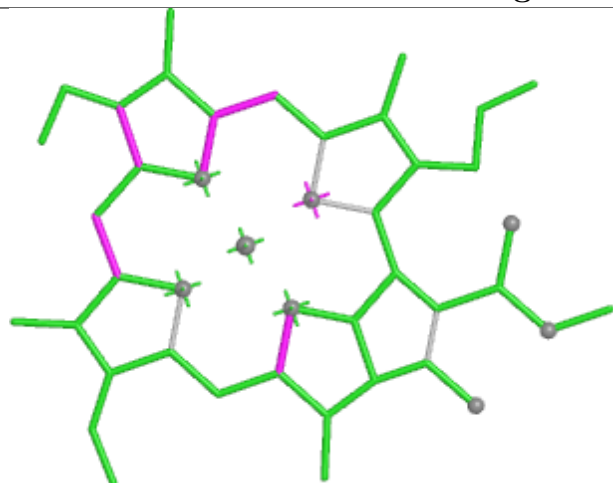
Ligand CLA a 604



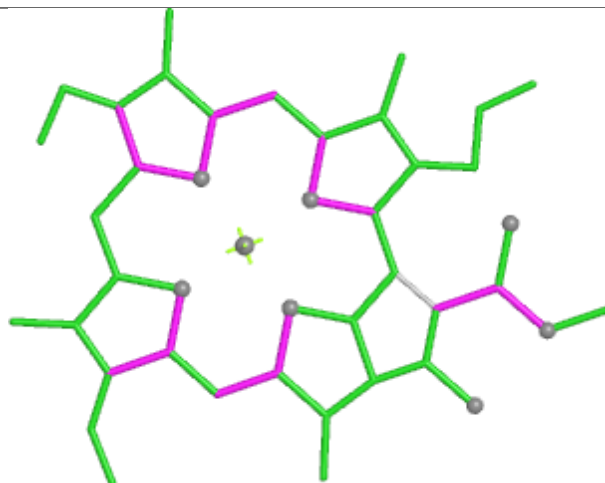
Ligand CLA j 610



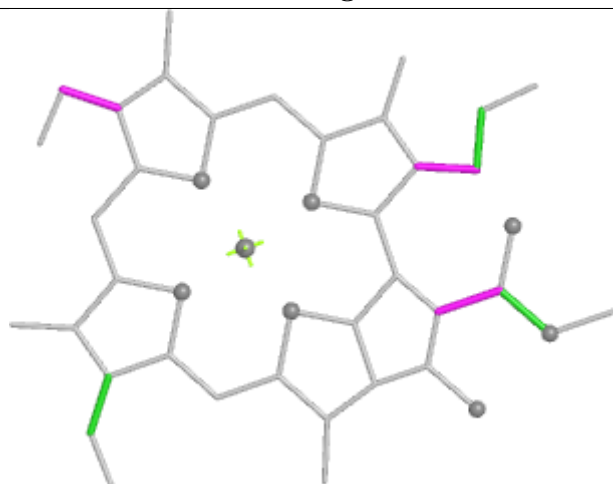
Ligand CLA A 802



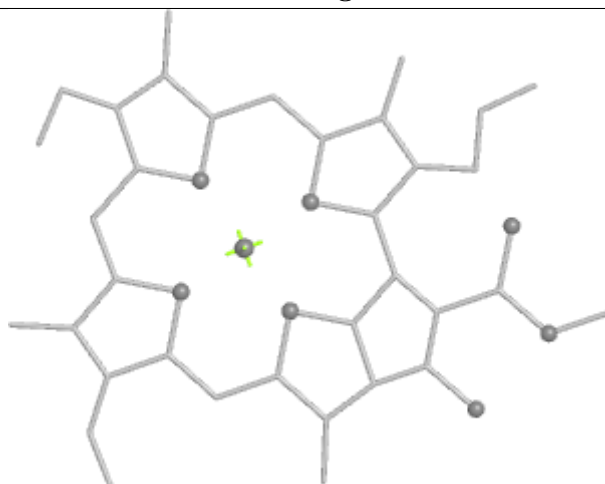
Bond lengths



Bond angles

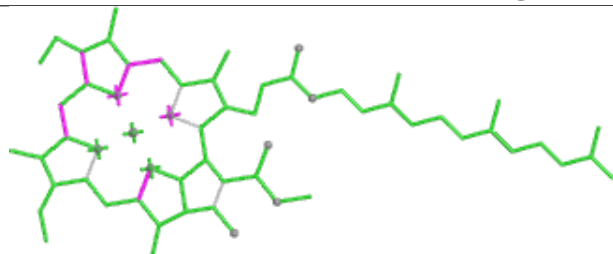


Torsions

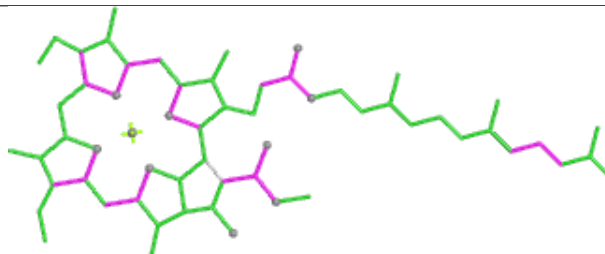


Rings

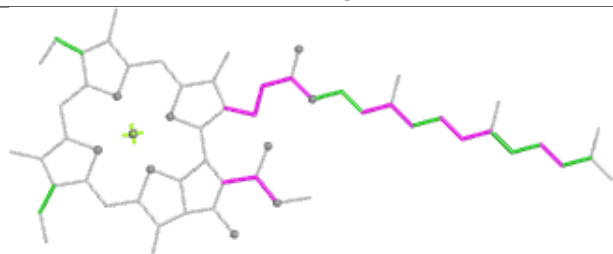
Ligand CLA m 602



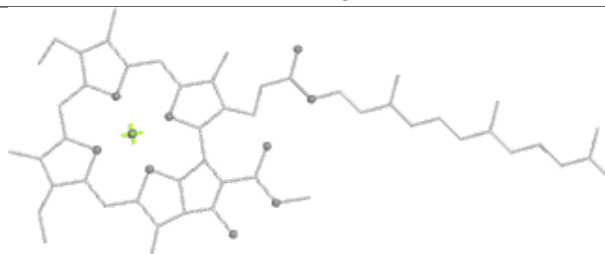
Bond lengths



Bond angles

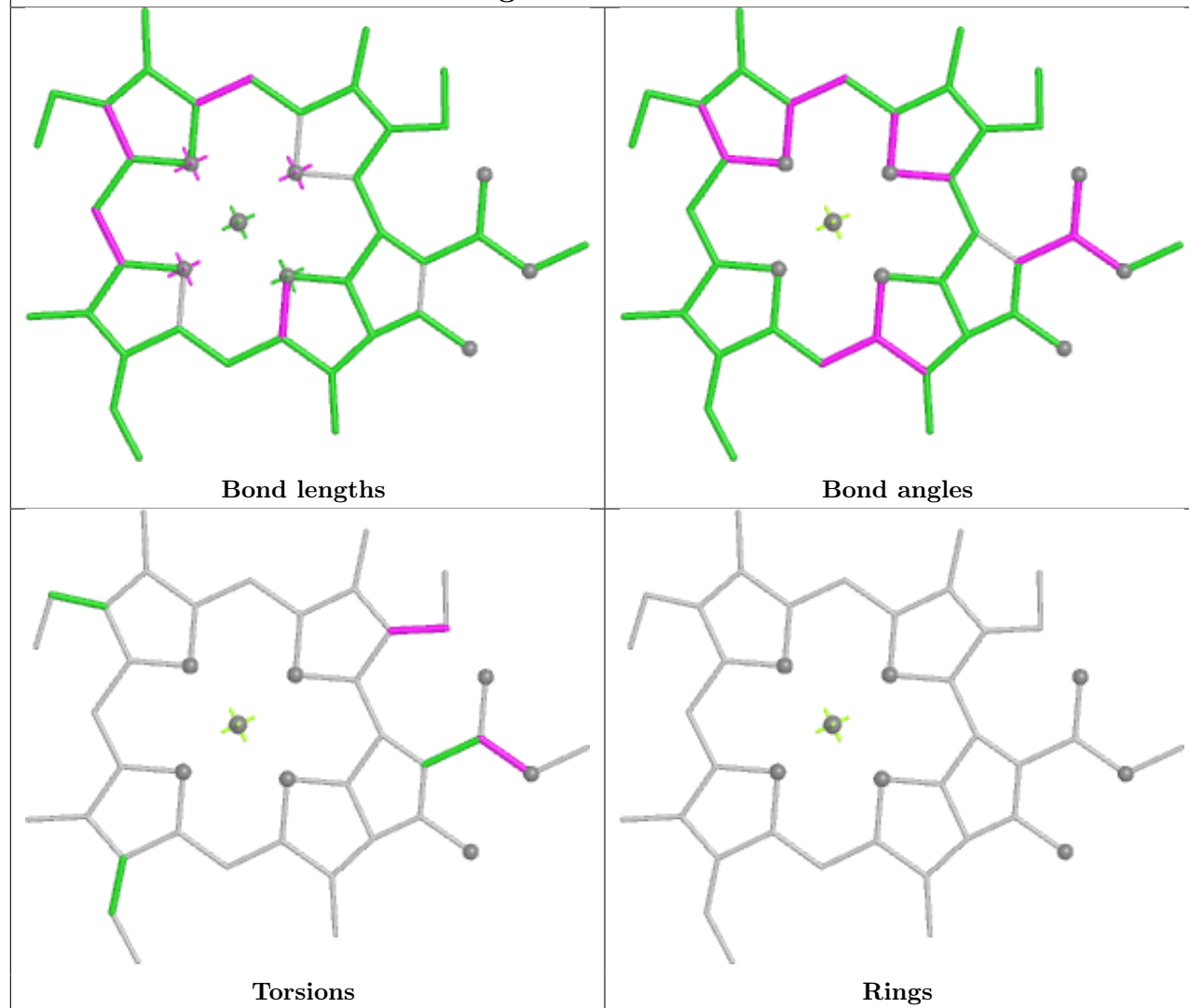


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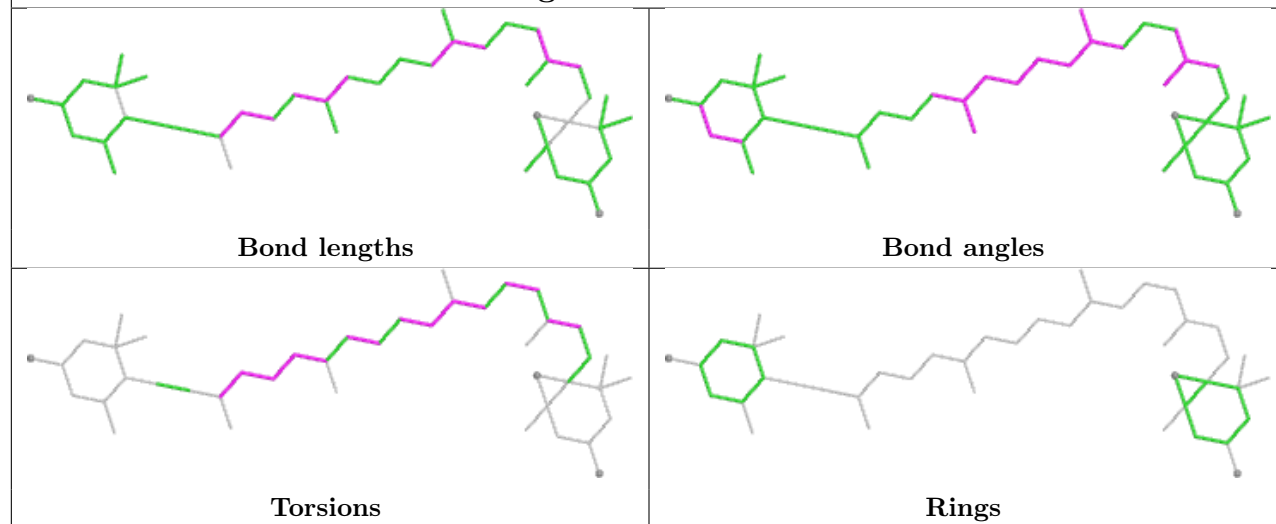


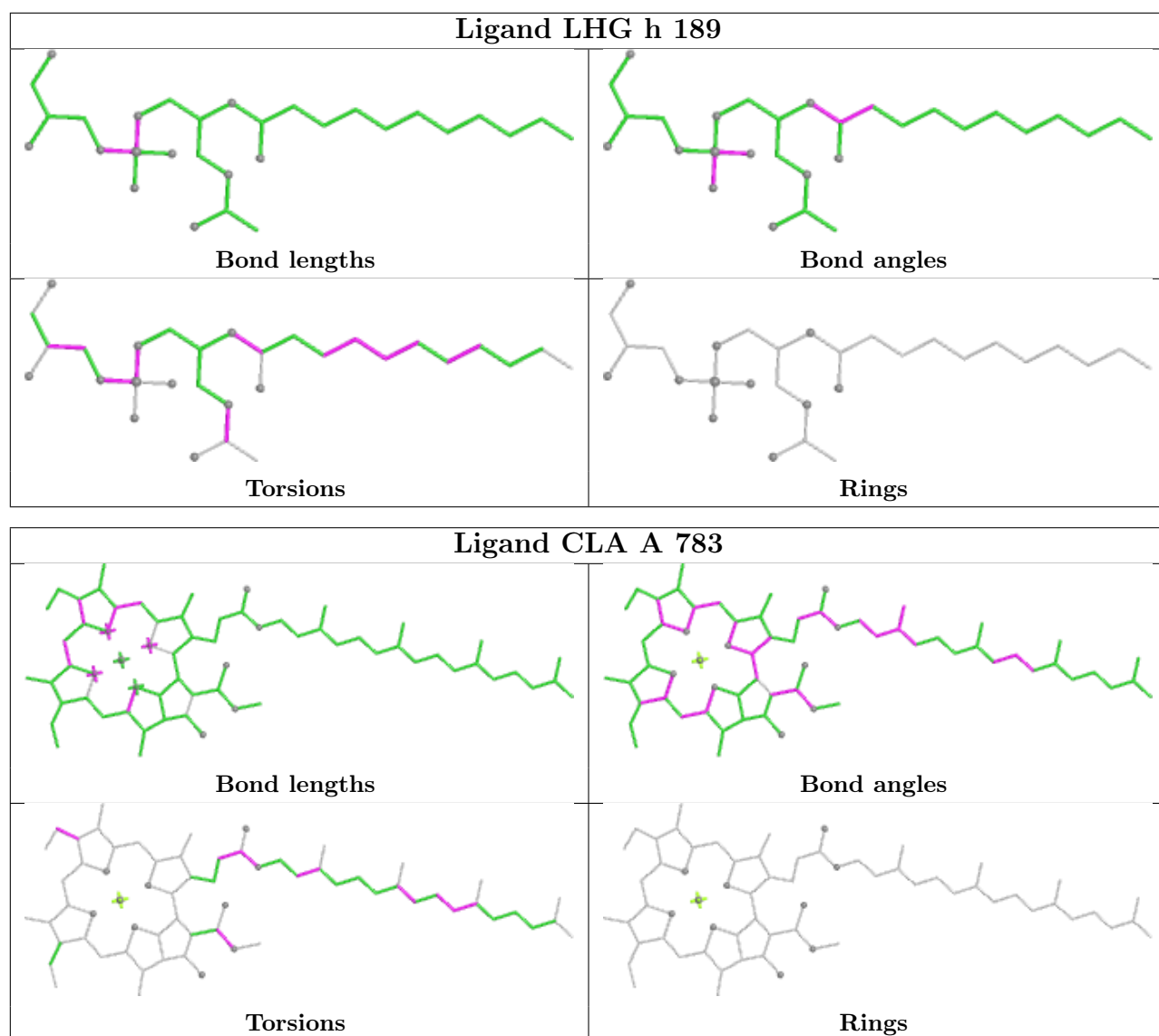
Rings

Ligand CLA d 614

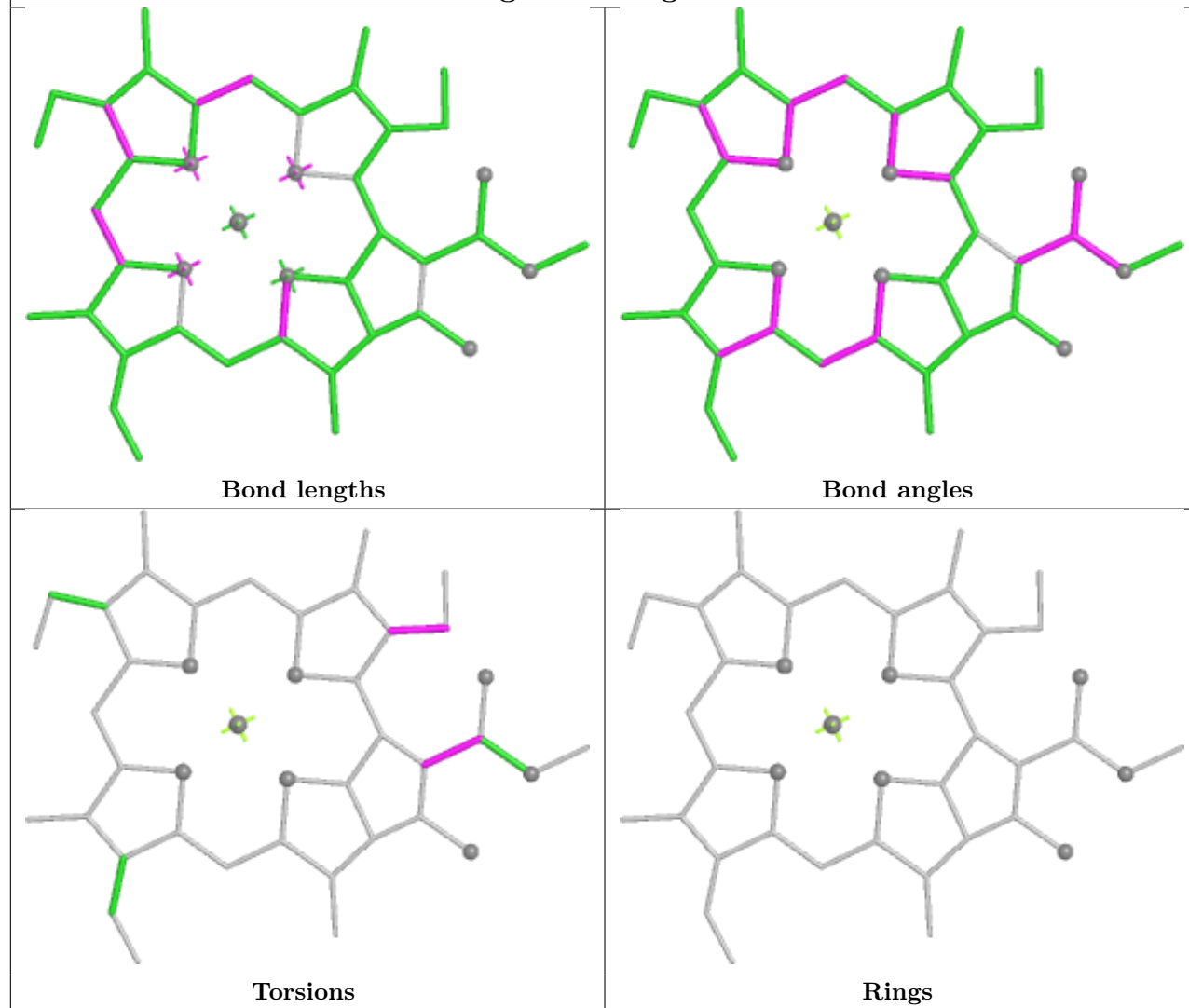


Ligand DD6 c 624

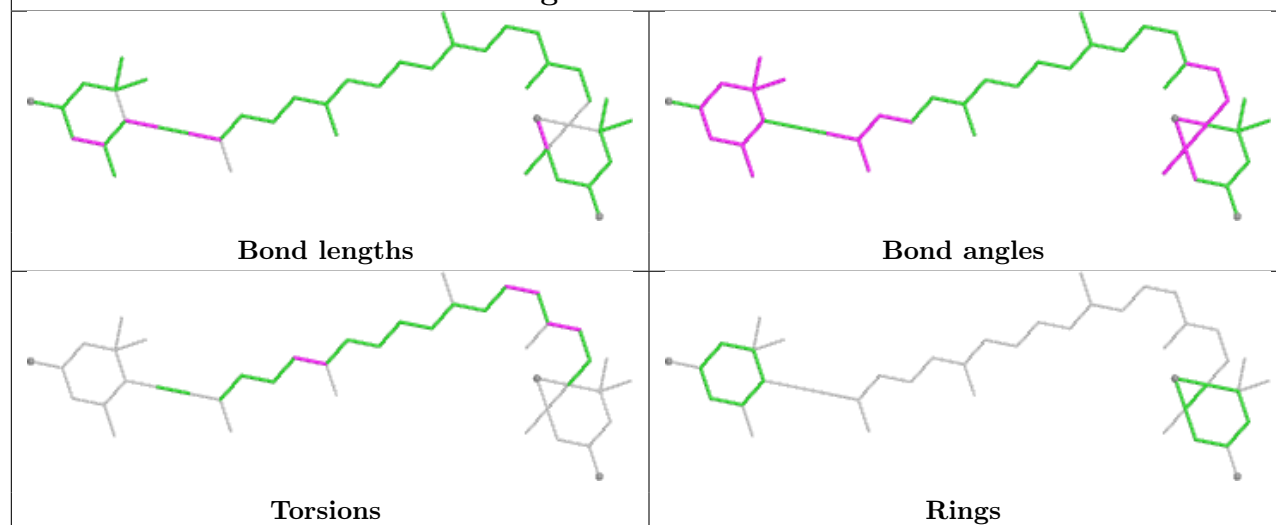


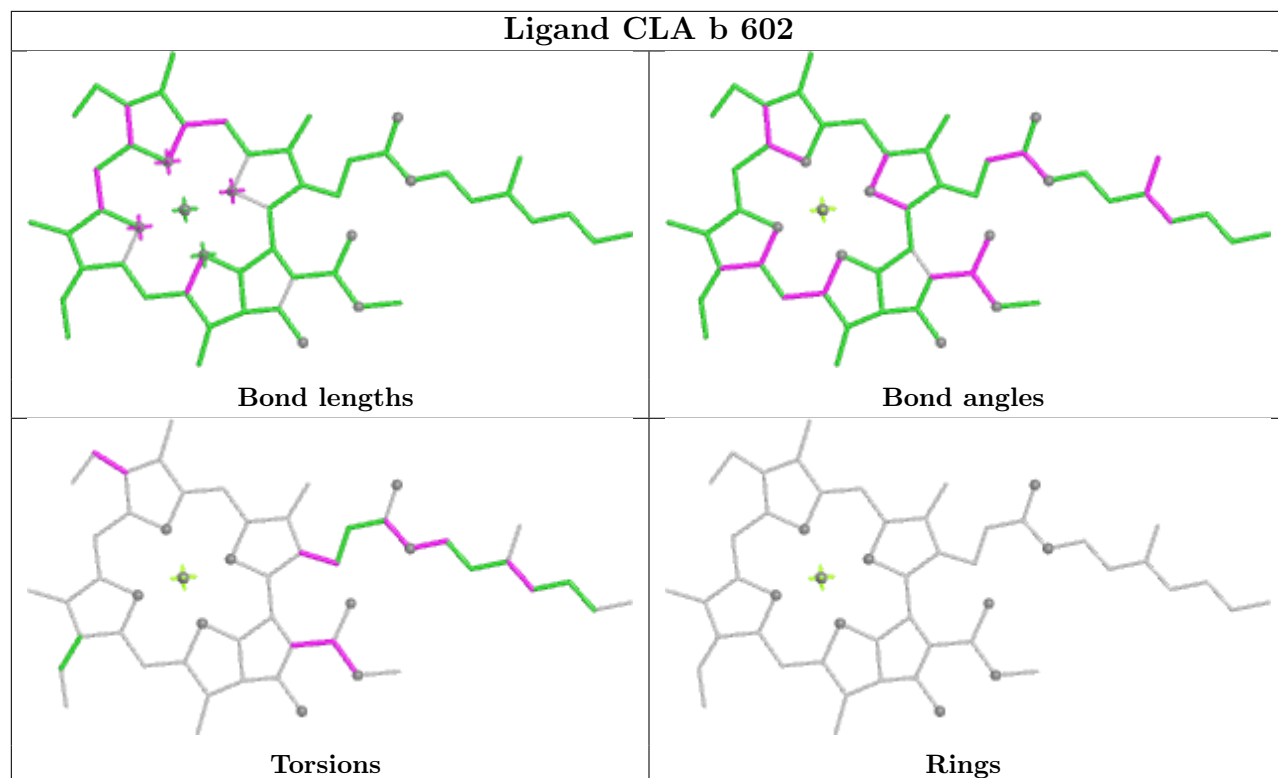


Ligand CLA g 611

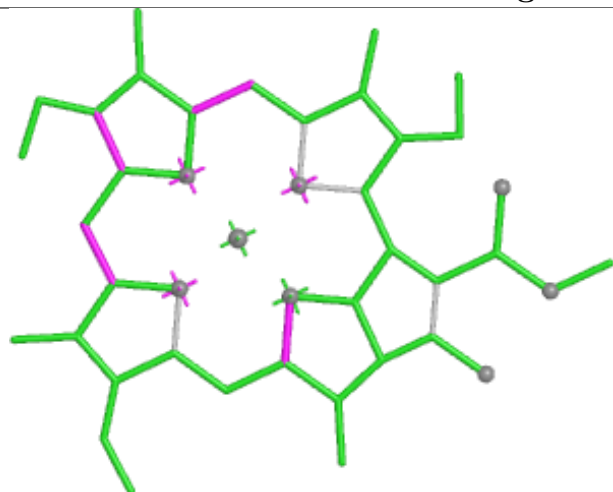


Ligand DD6 f 620

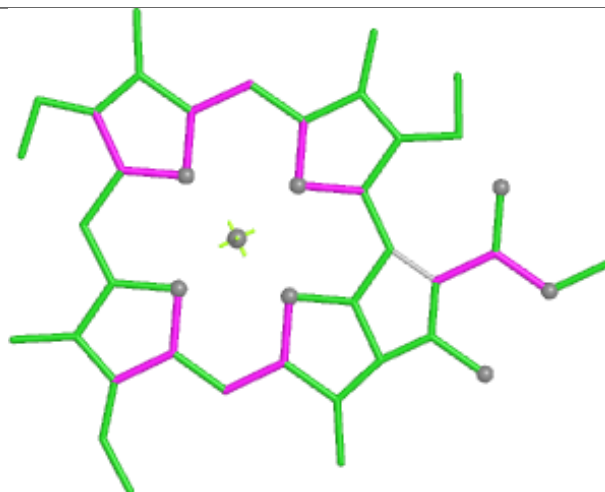




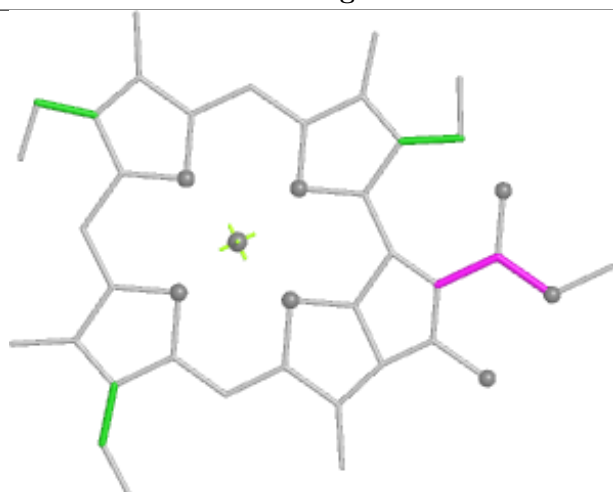
Ligand CLA b 611



Bond lengths



Bond angles

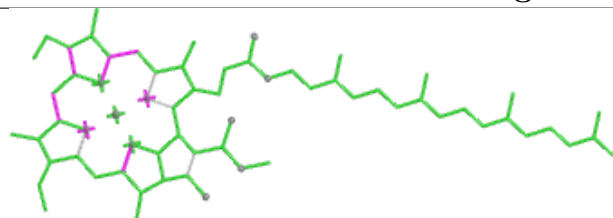


Torsions

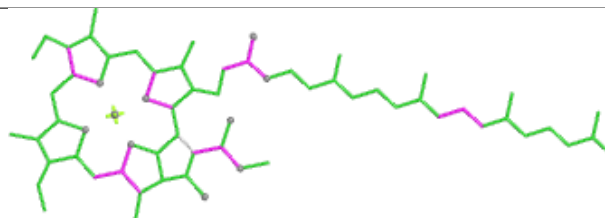


Rings

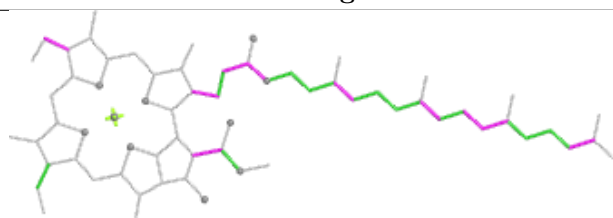
Ligand CLA B 738



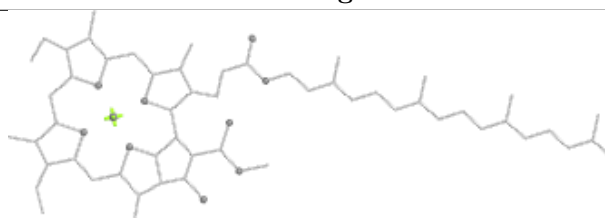
Bond lengths



Bond angles

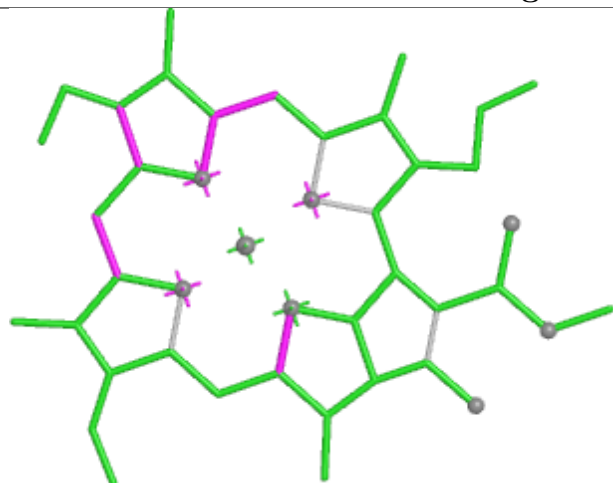


Torsions

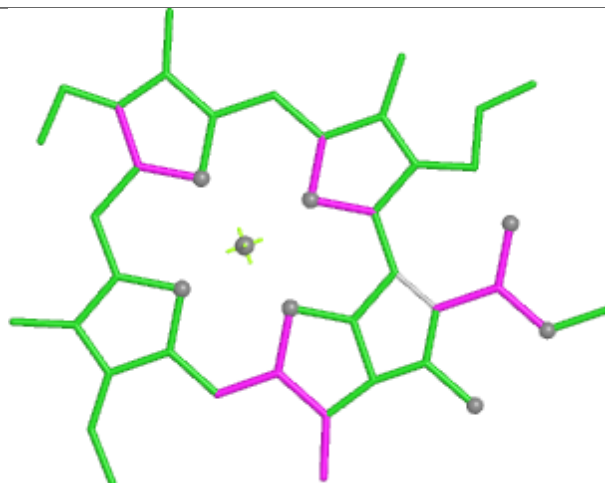


Rings

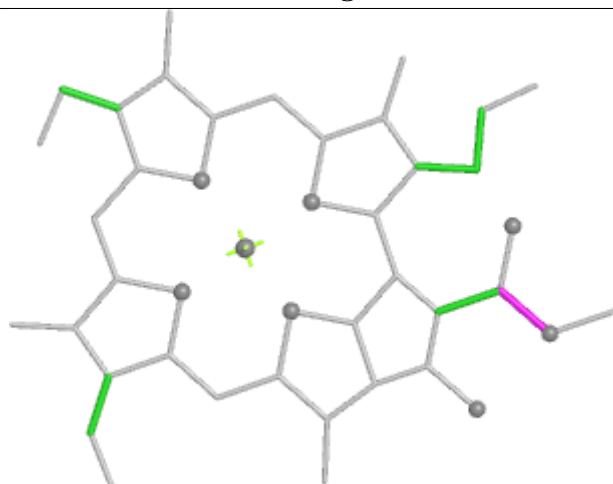
Ligand CLA f 603



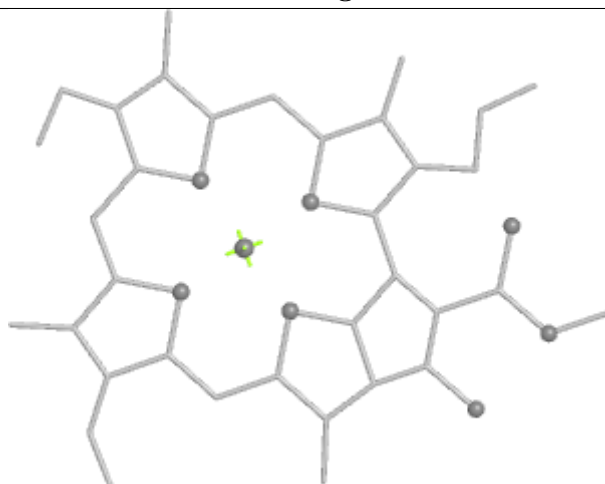
Bond lengths



Bond angles

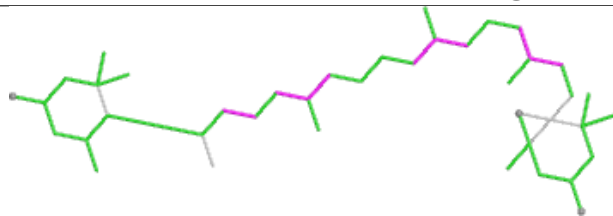


Torsions

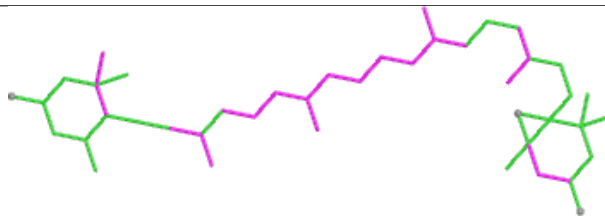


Rings

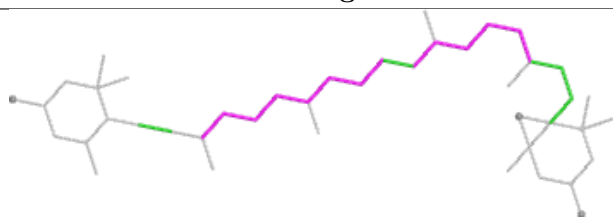
Ligand DD6 F 4002



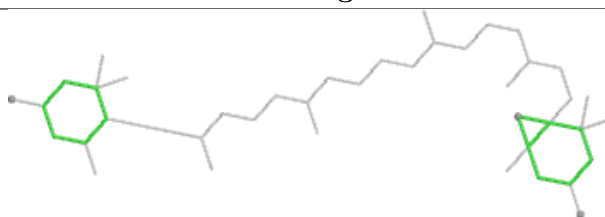
Bond lengths



Bond angles

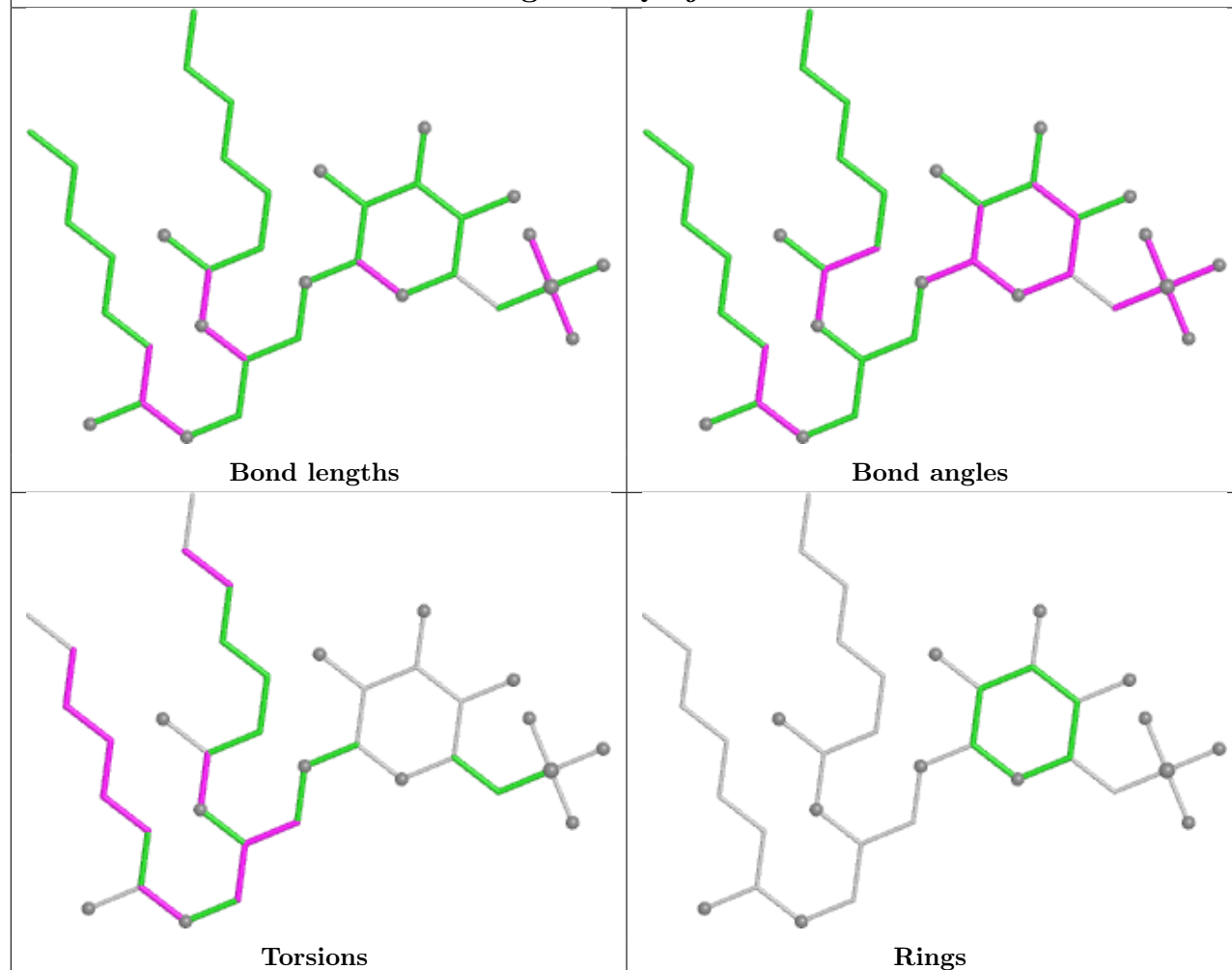


Torsions

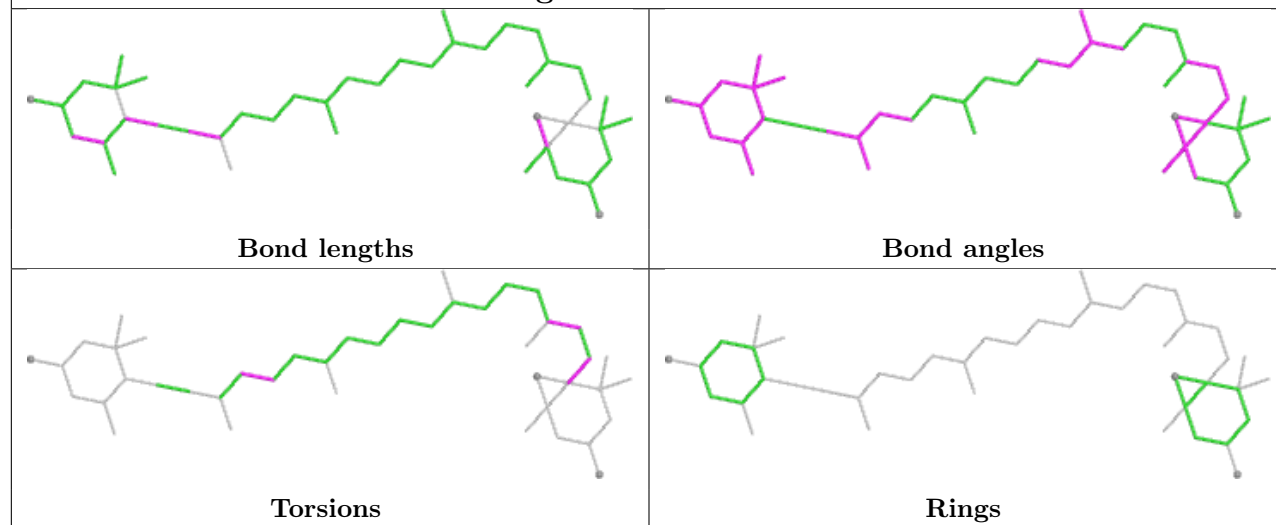


Rings

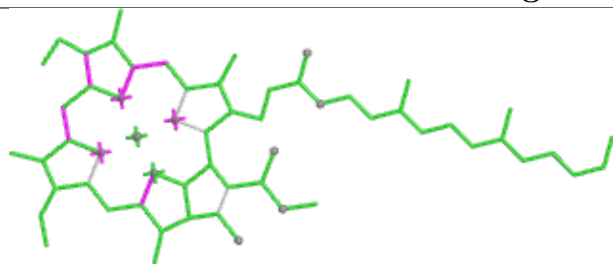
Ligand SQD j 200



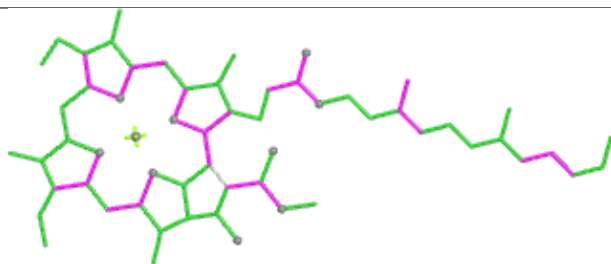
Ligand DD6 d 623



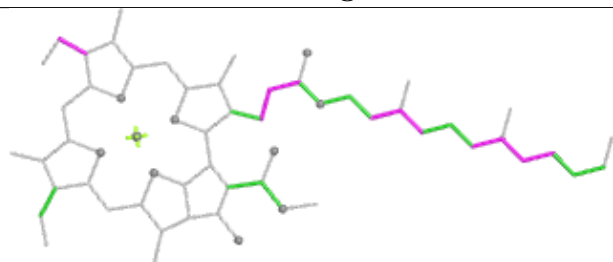
Ligand CLA i 613



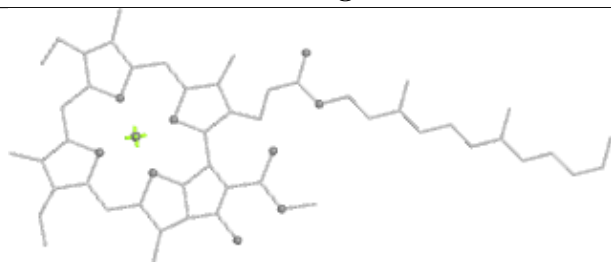
Bond lengths



Bond angles

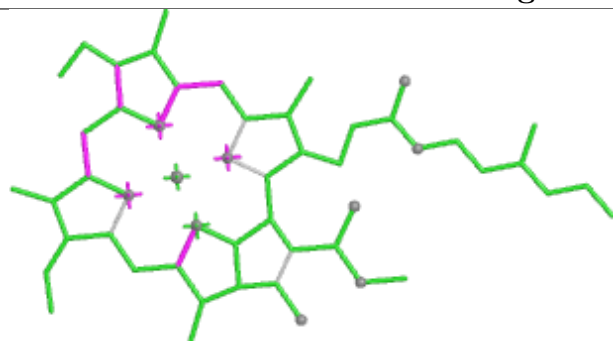


Torsions

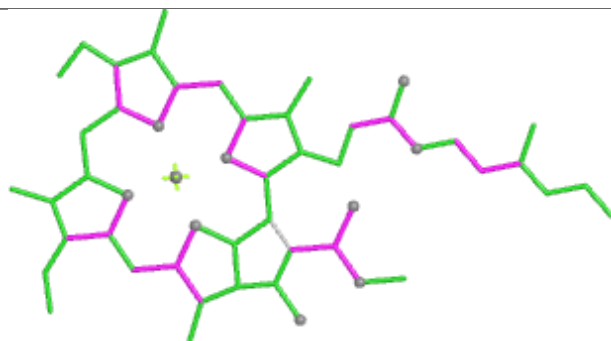


Rings

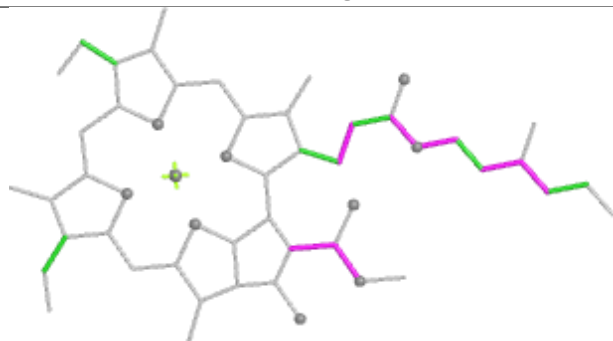
Ligand CLA k 613



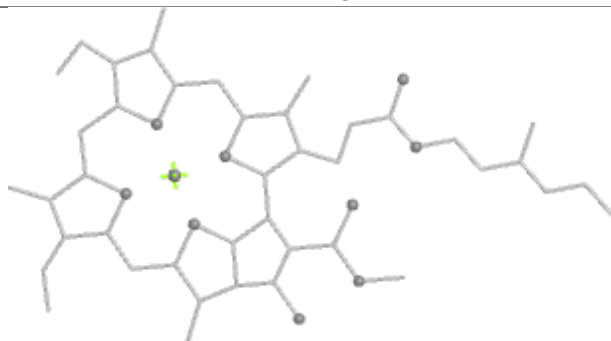
Bond lengths



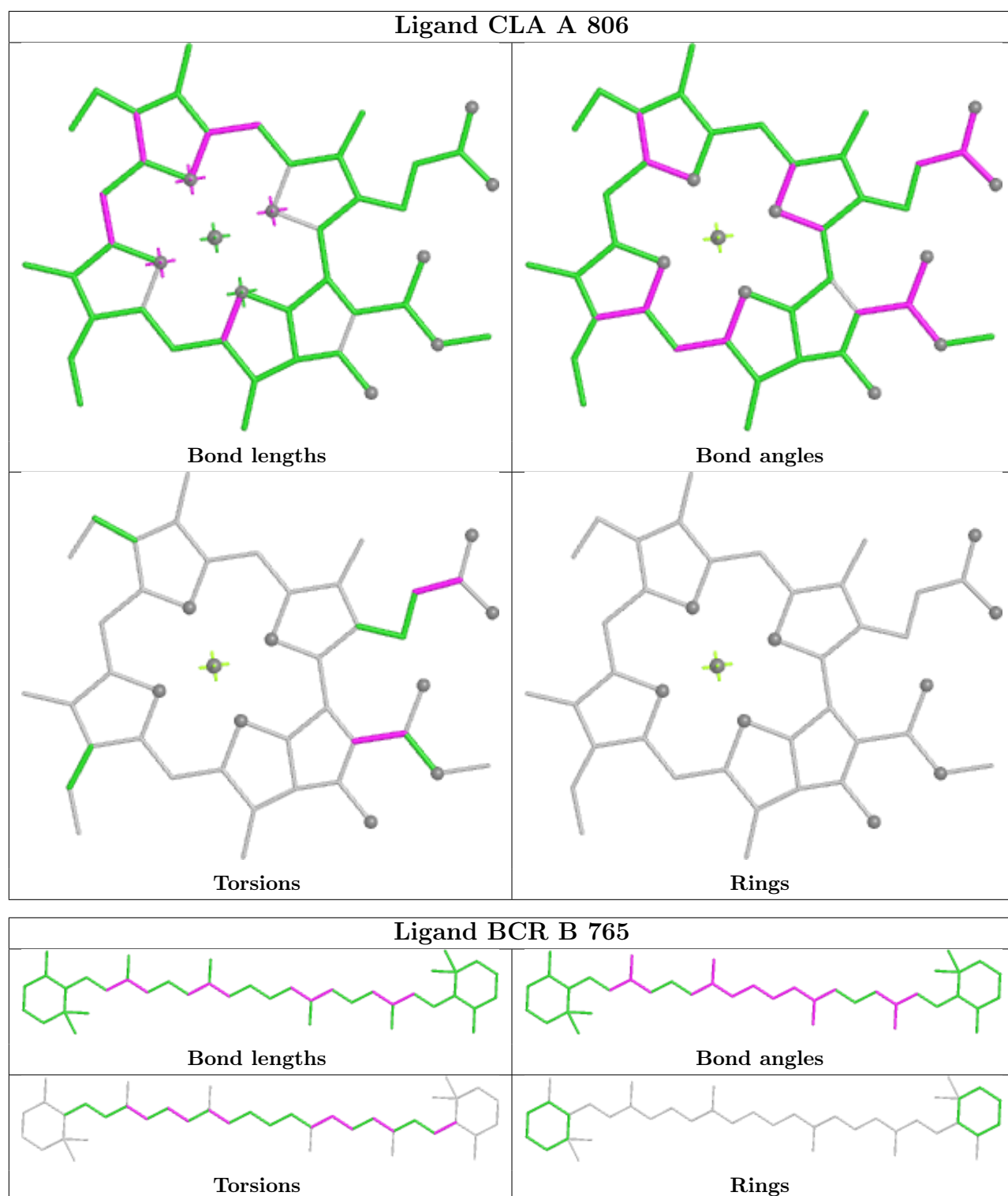
Bond angles

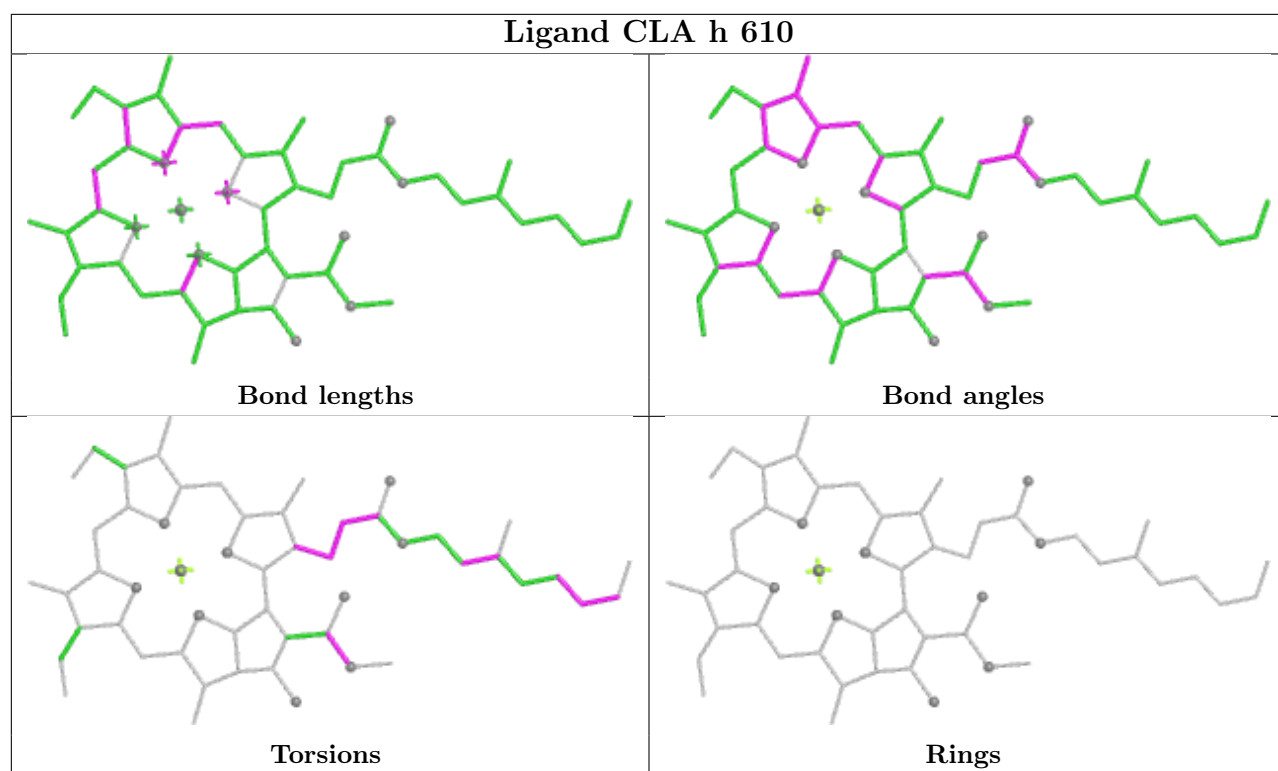


Torsions

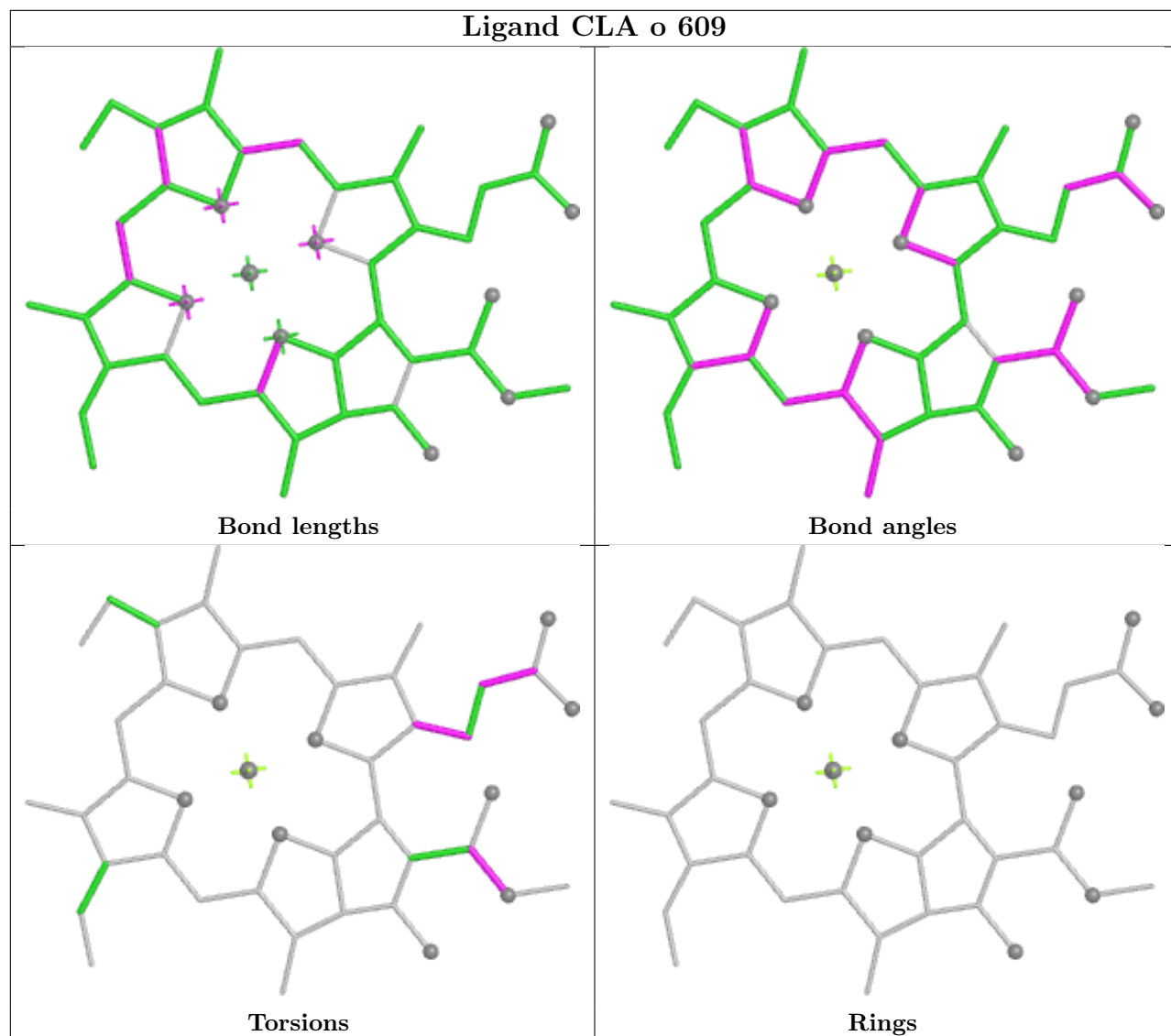


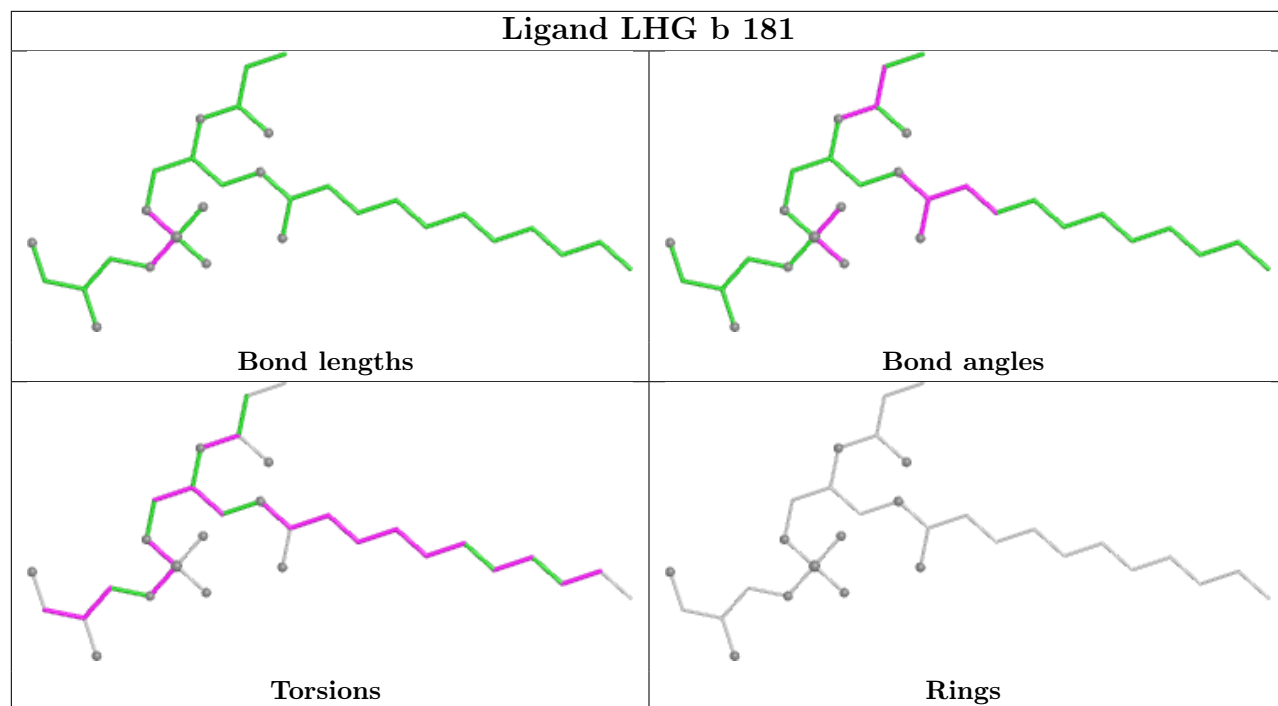
Rings



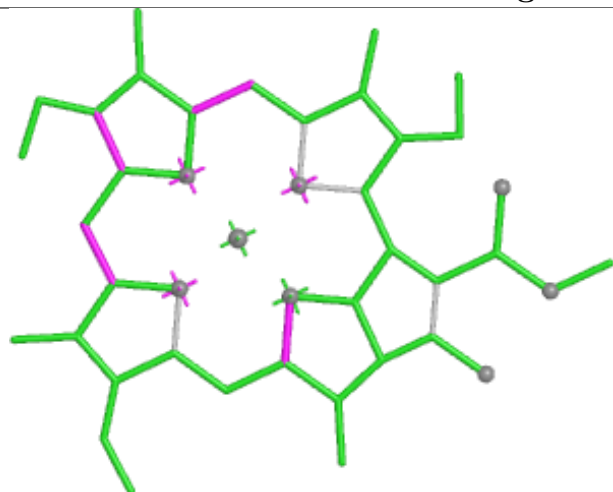


Ligand CLA o 609

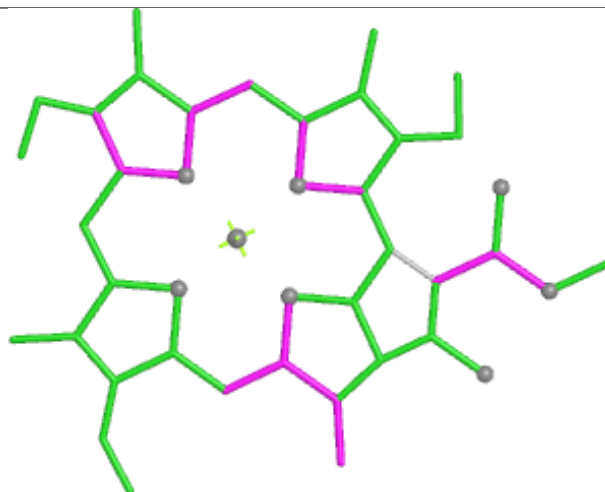




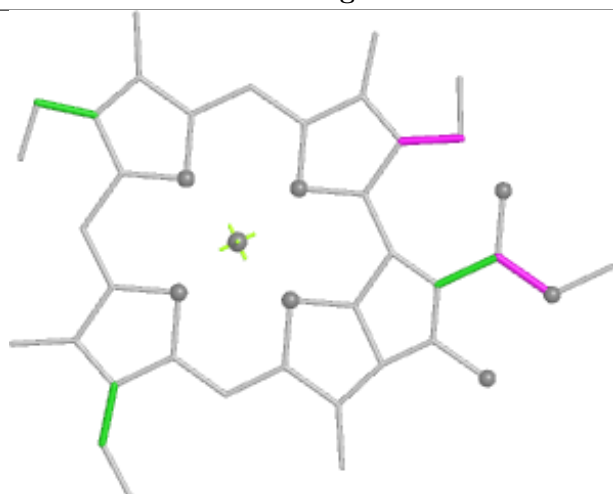
Ligand CLA b 601



Bond lengths



Bond angles

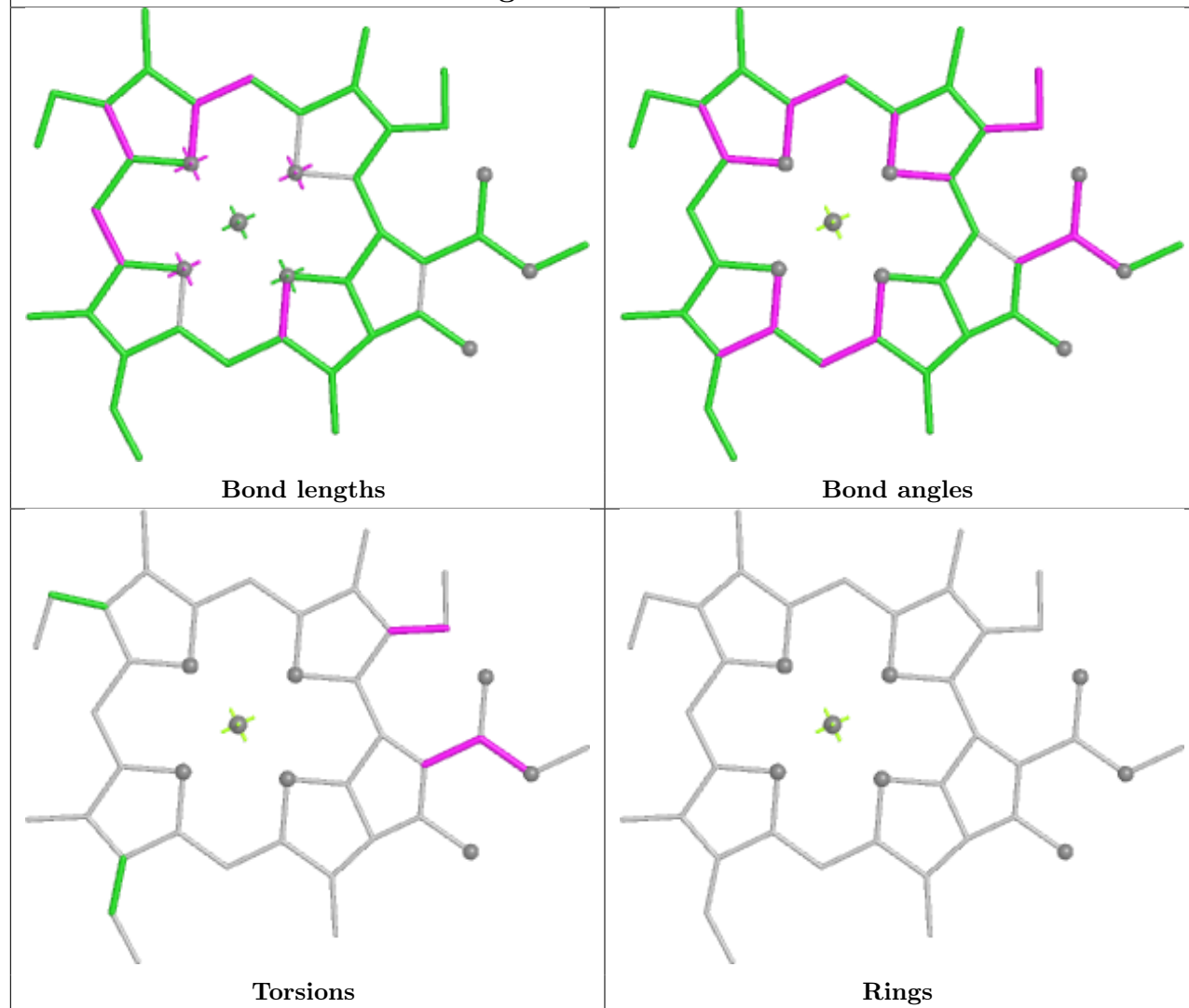


Torsions

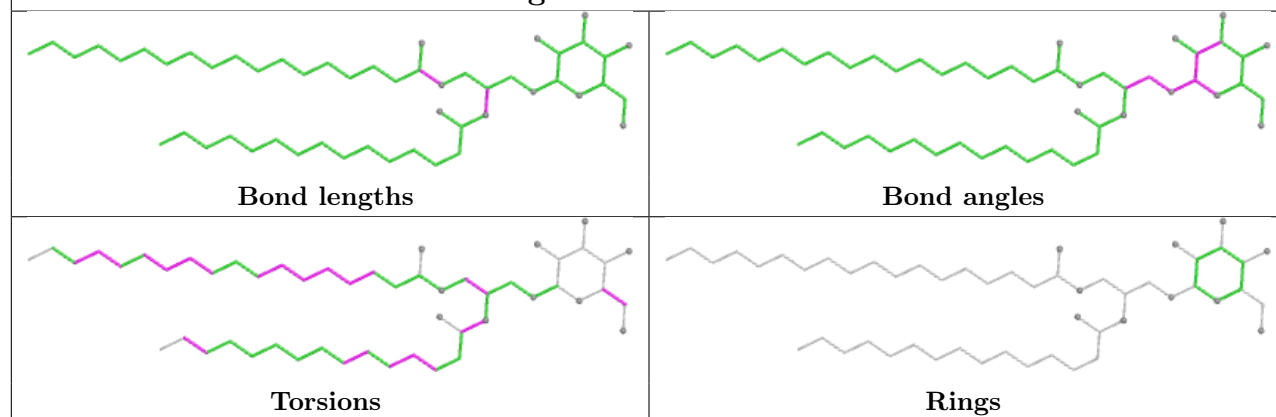


Rings

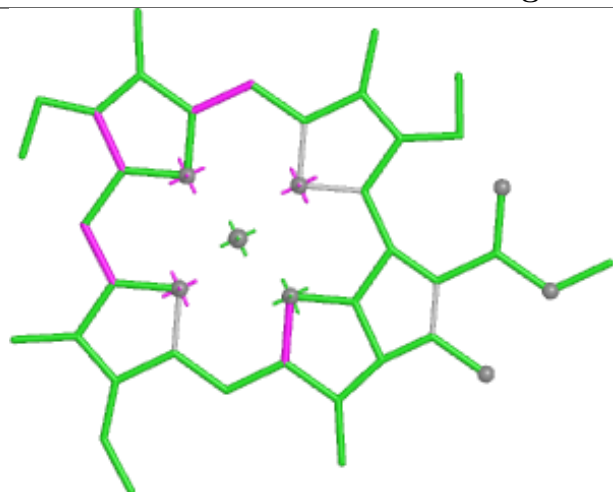
Ligand CLA b 613



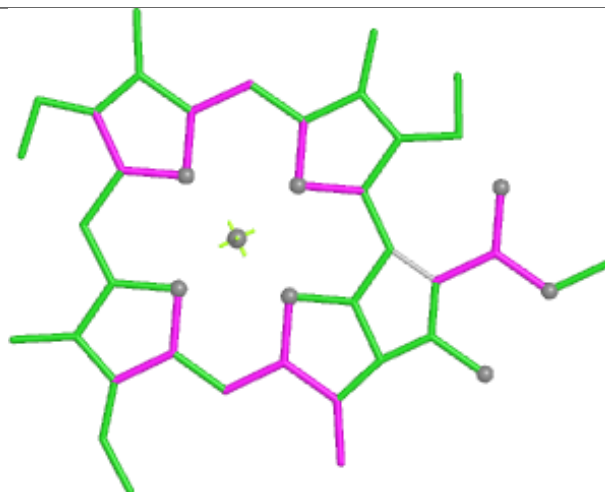
Ligand LMG B 786



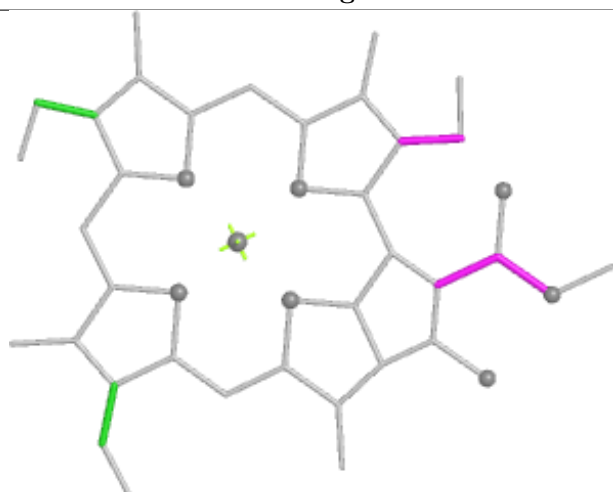
Ligand CLA f 614



Bond lengths



Bond angles

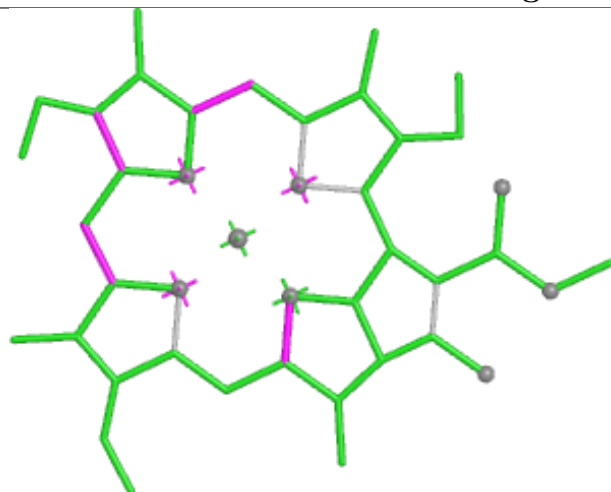


Torsions

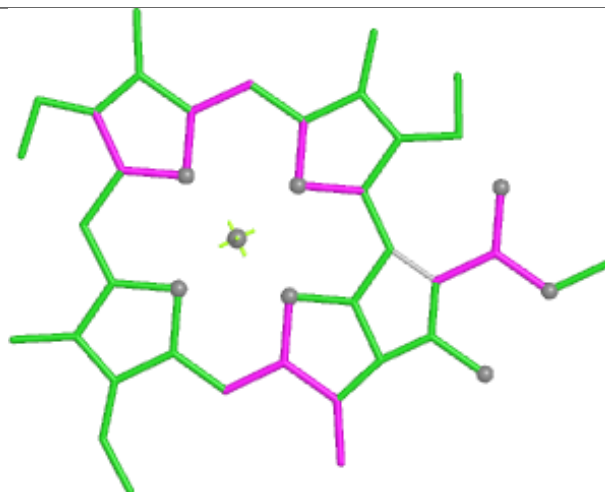


Rings

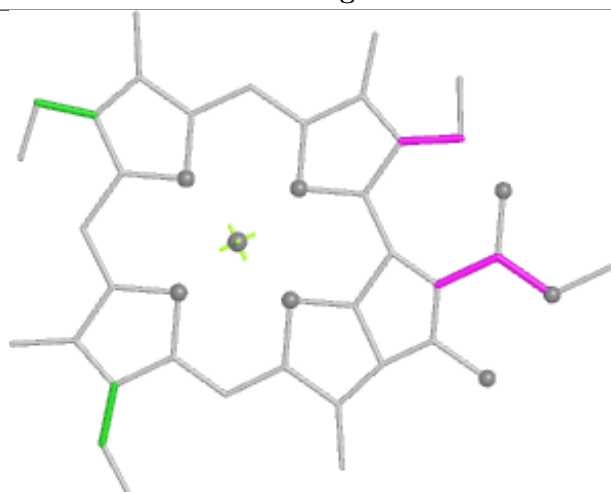
Ligand CLA 1 614



Bond lengths



Bond angles

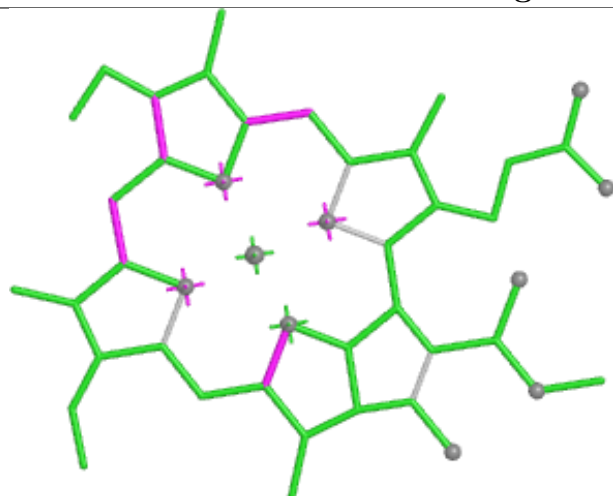


Torsions

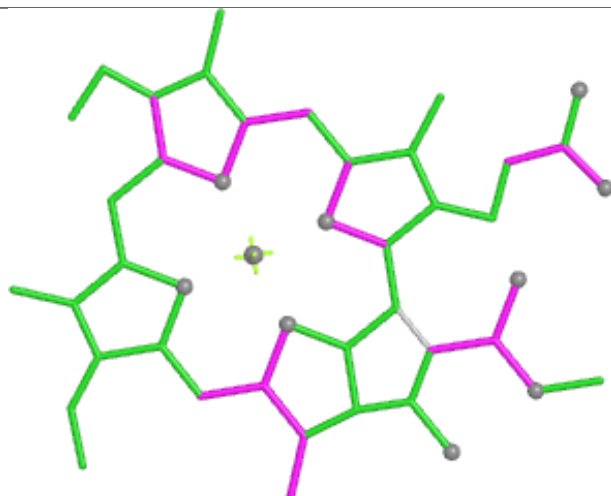


Rings

Ligand CLA B 785



Bond lengths



Bond angles

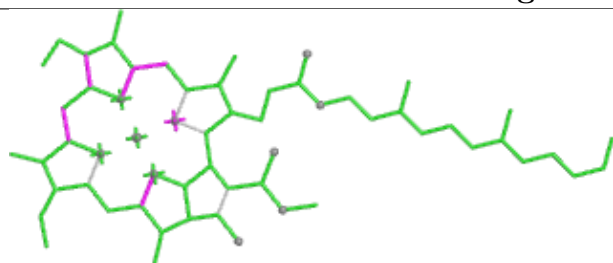


Torsions

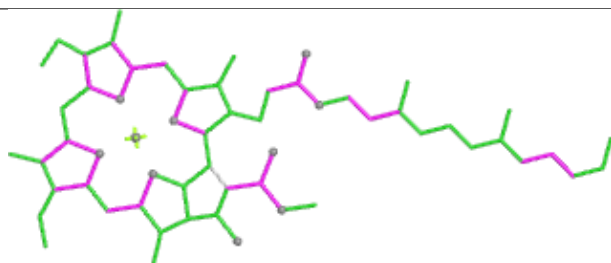


Rings

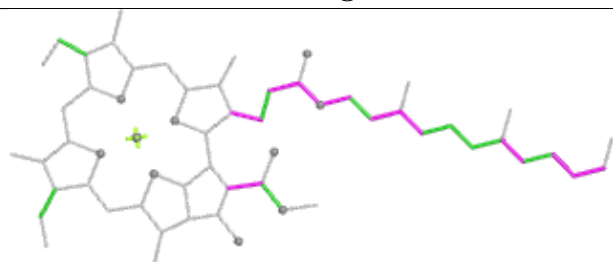
Ligand CLA n 602



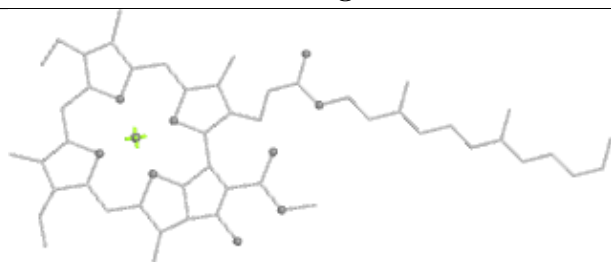
Bond lengths



Bond angles

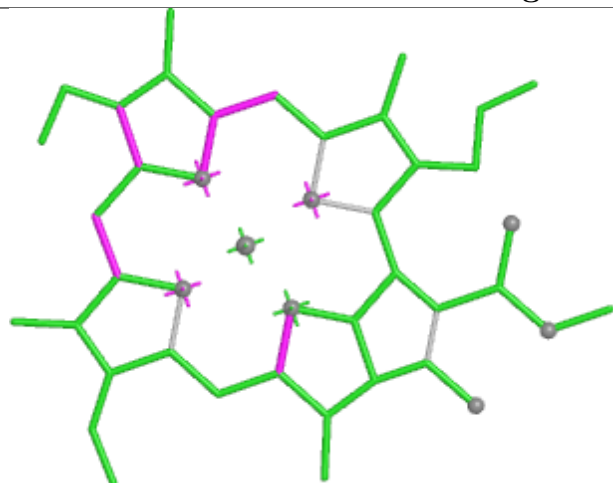


Torsions

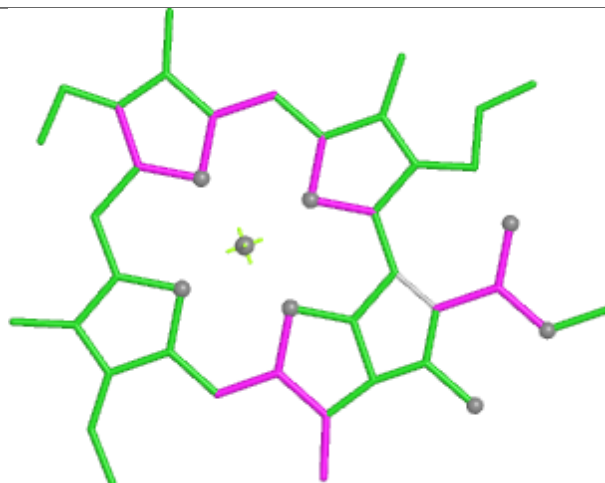


Rings

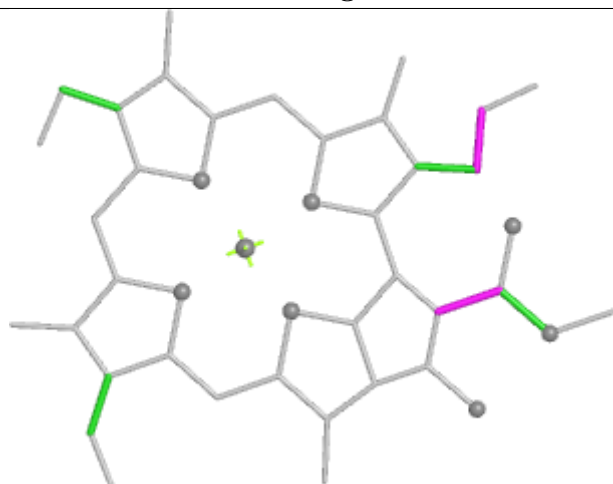
Ligand CLA 1 603



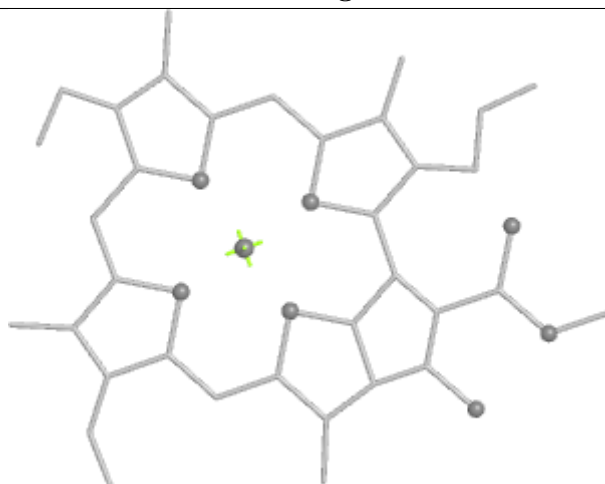
Bond lengths



Bond angles

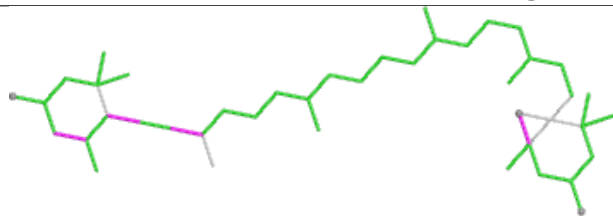


Torsions

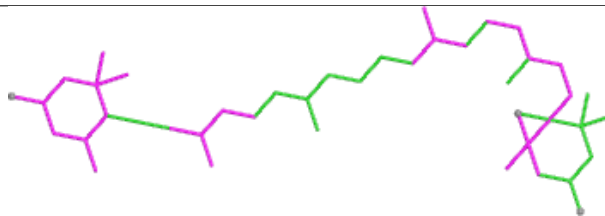


Rings

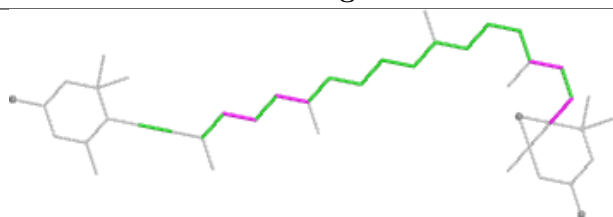
Ligand DD6 f 621



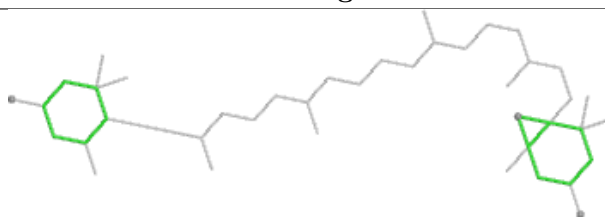
Bond lengths



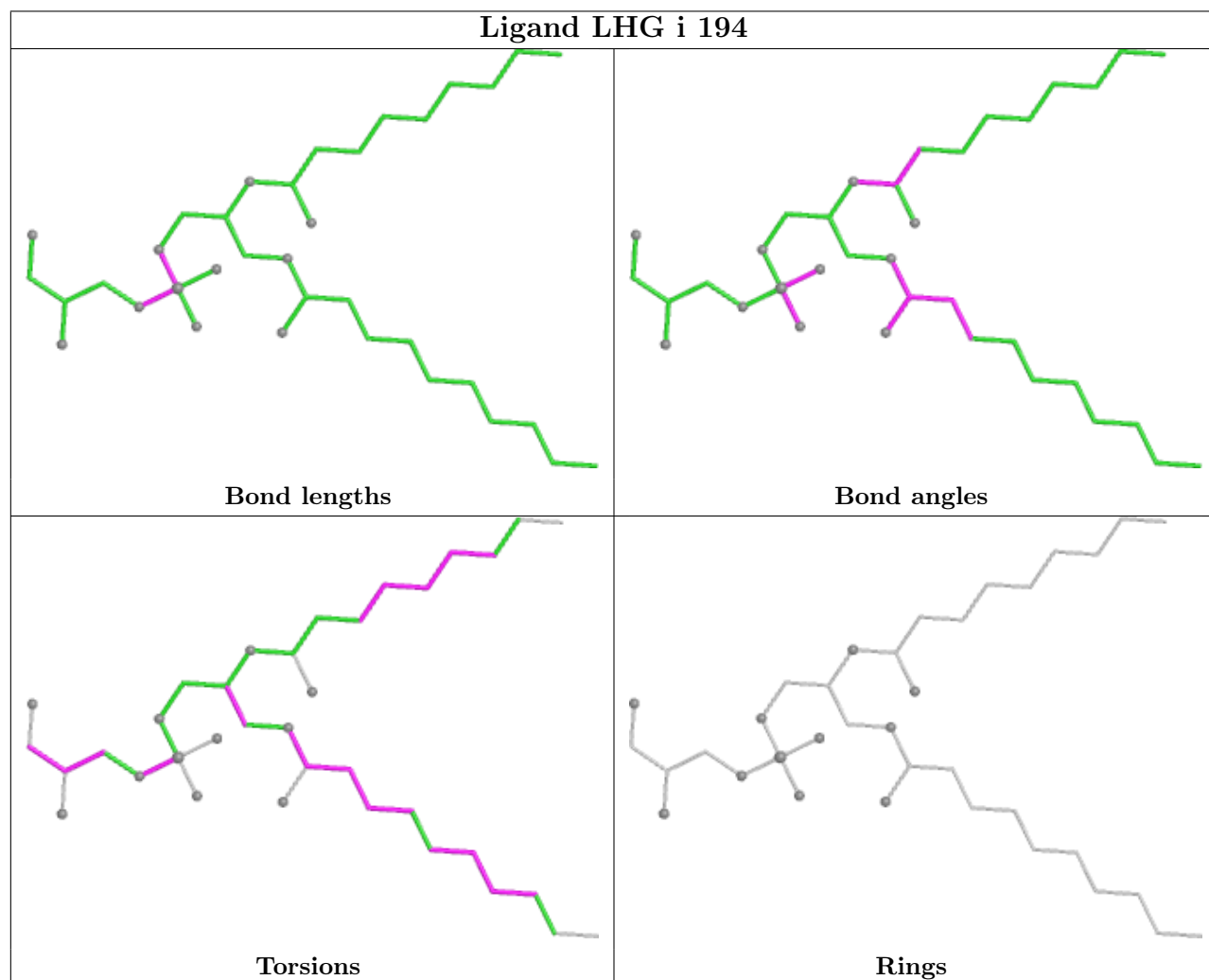
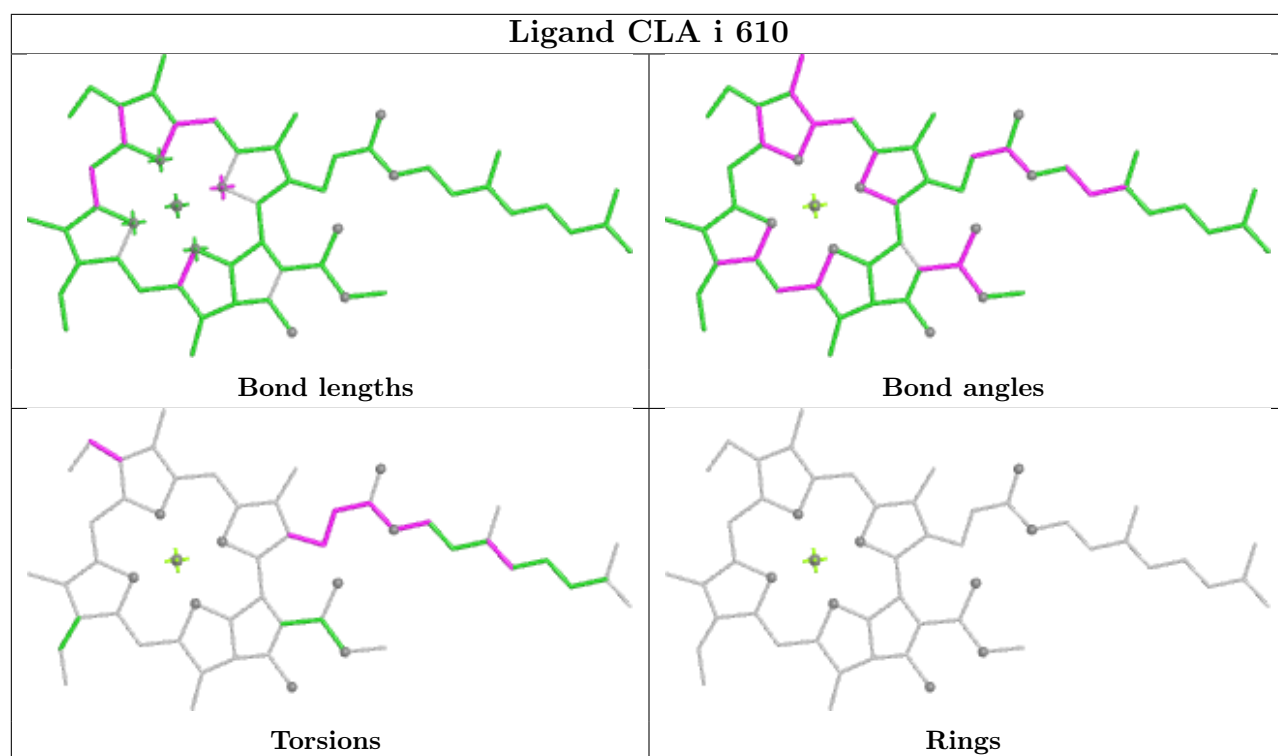
Bond angles

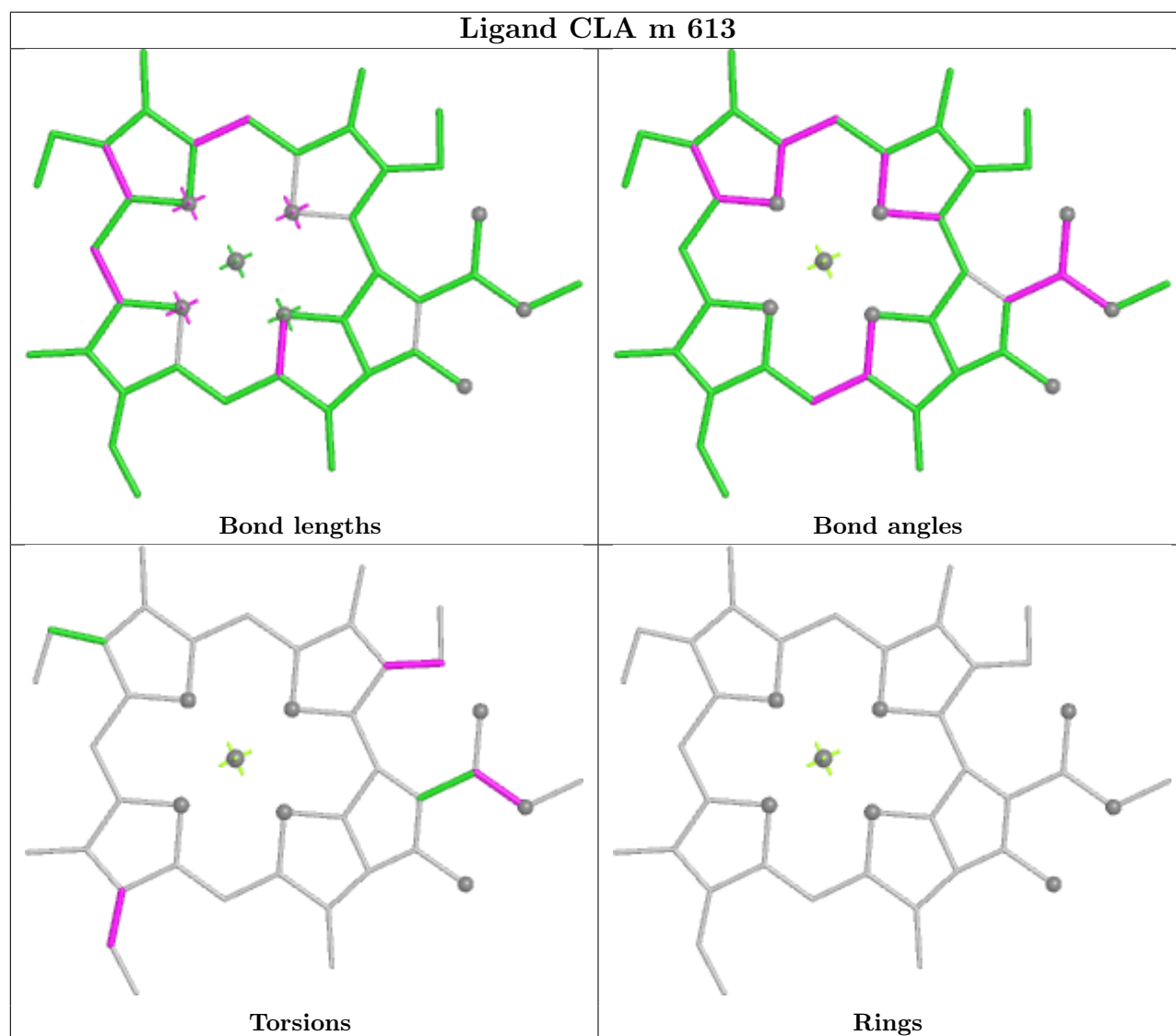
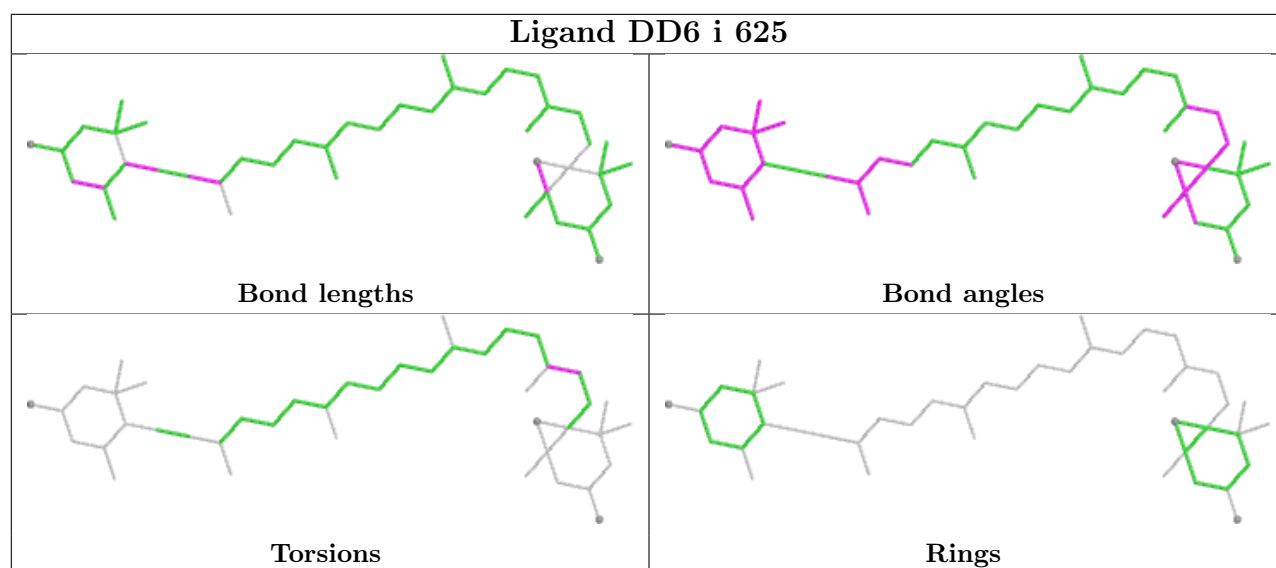


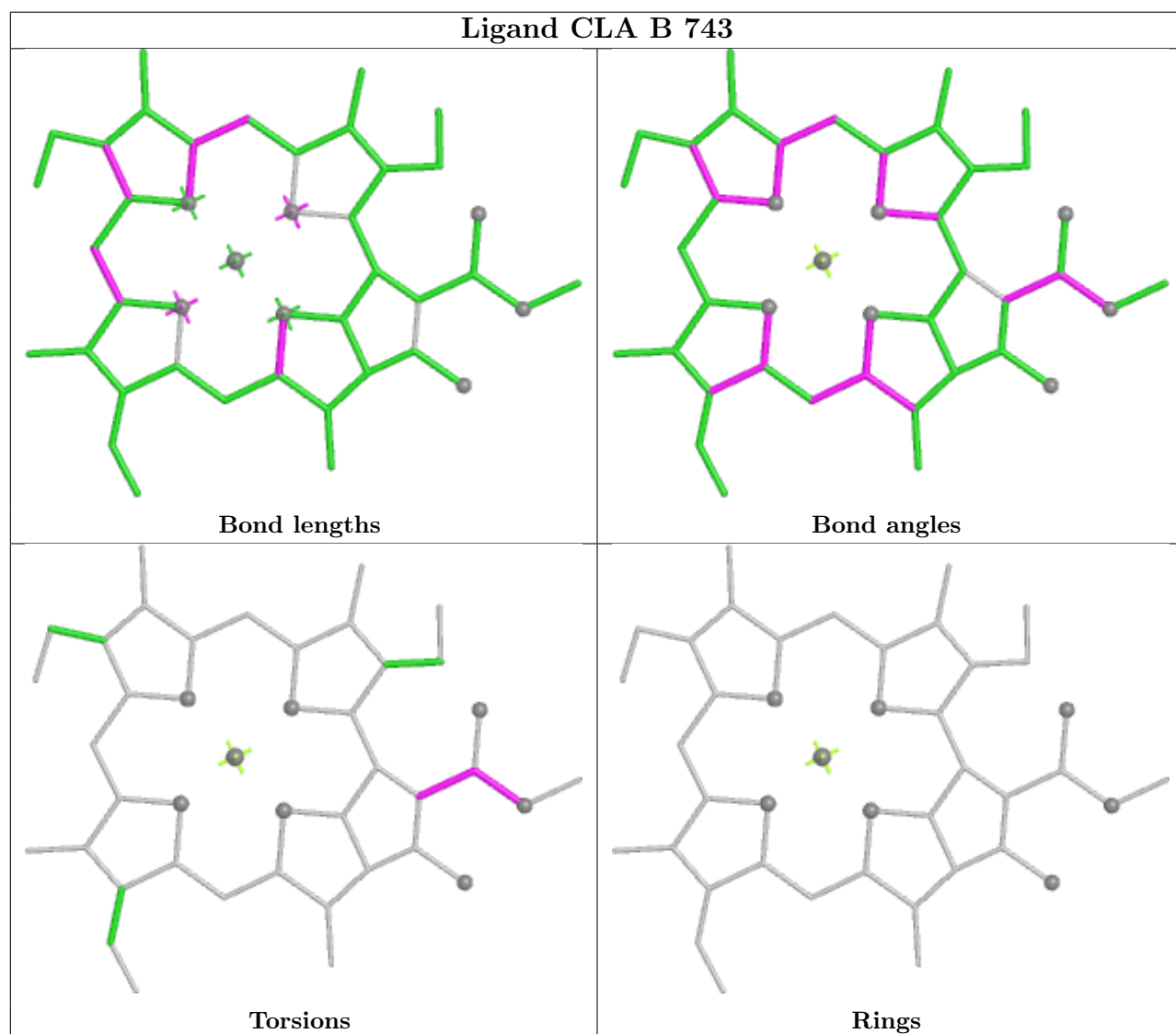
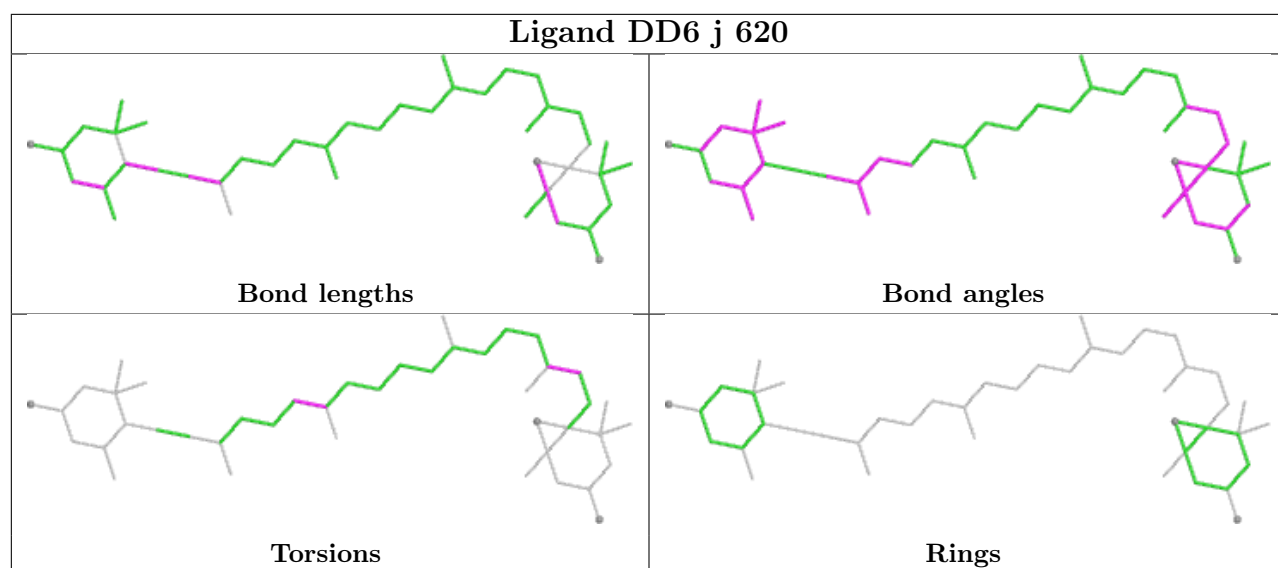
Torsions

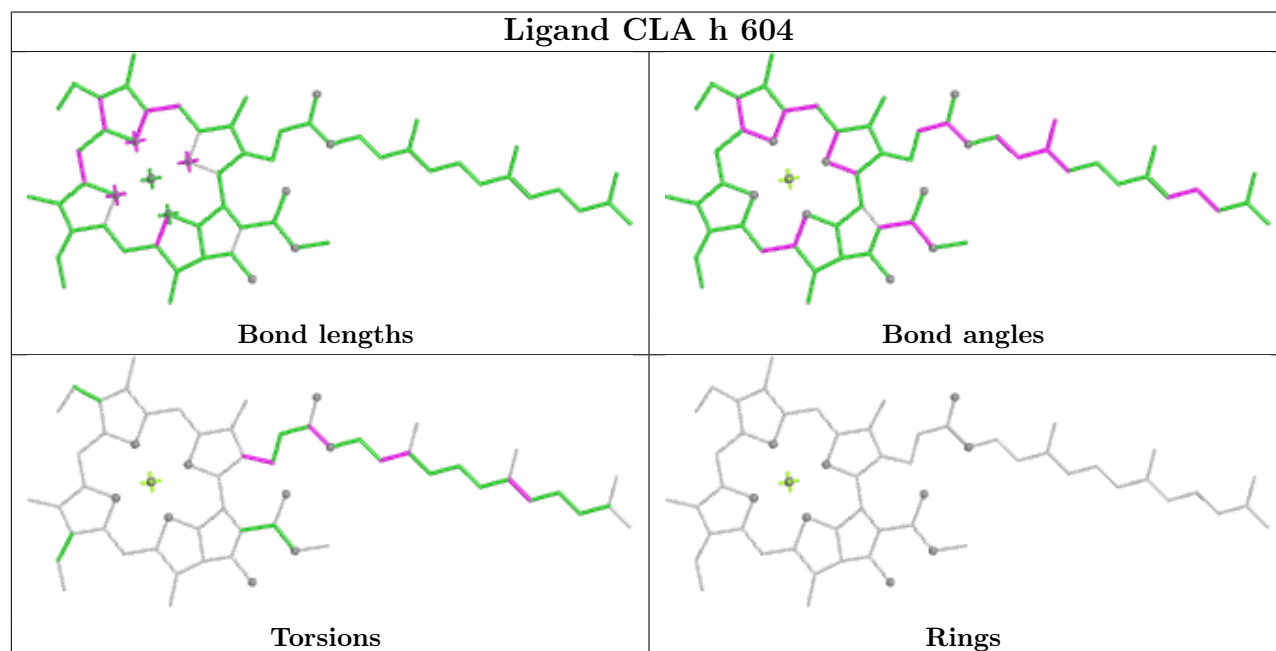
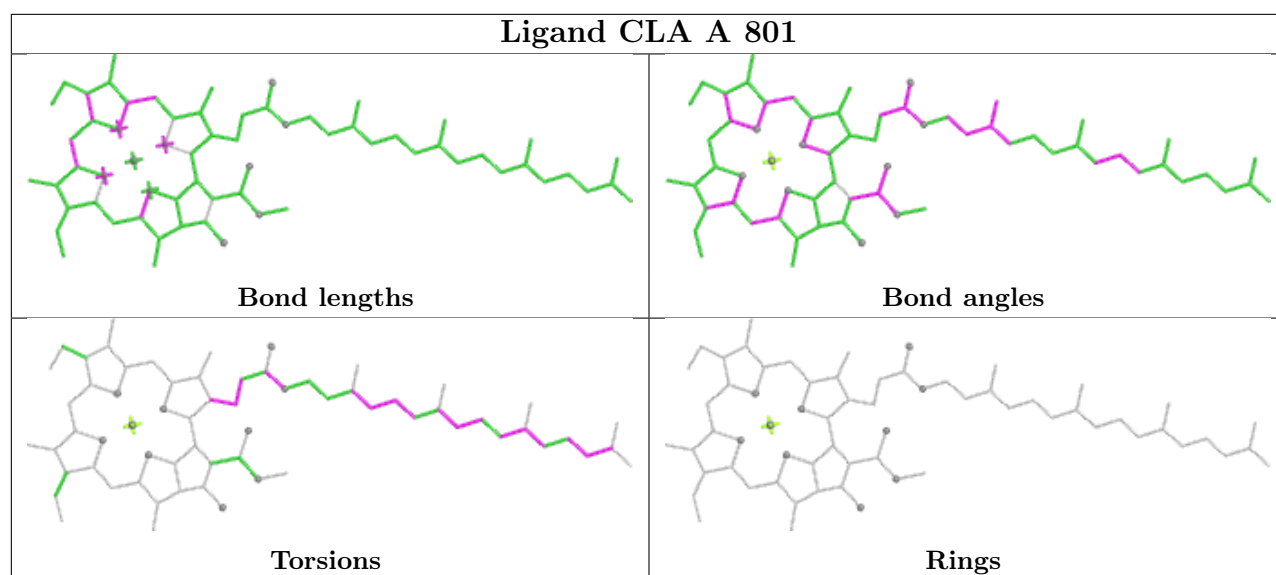


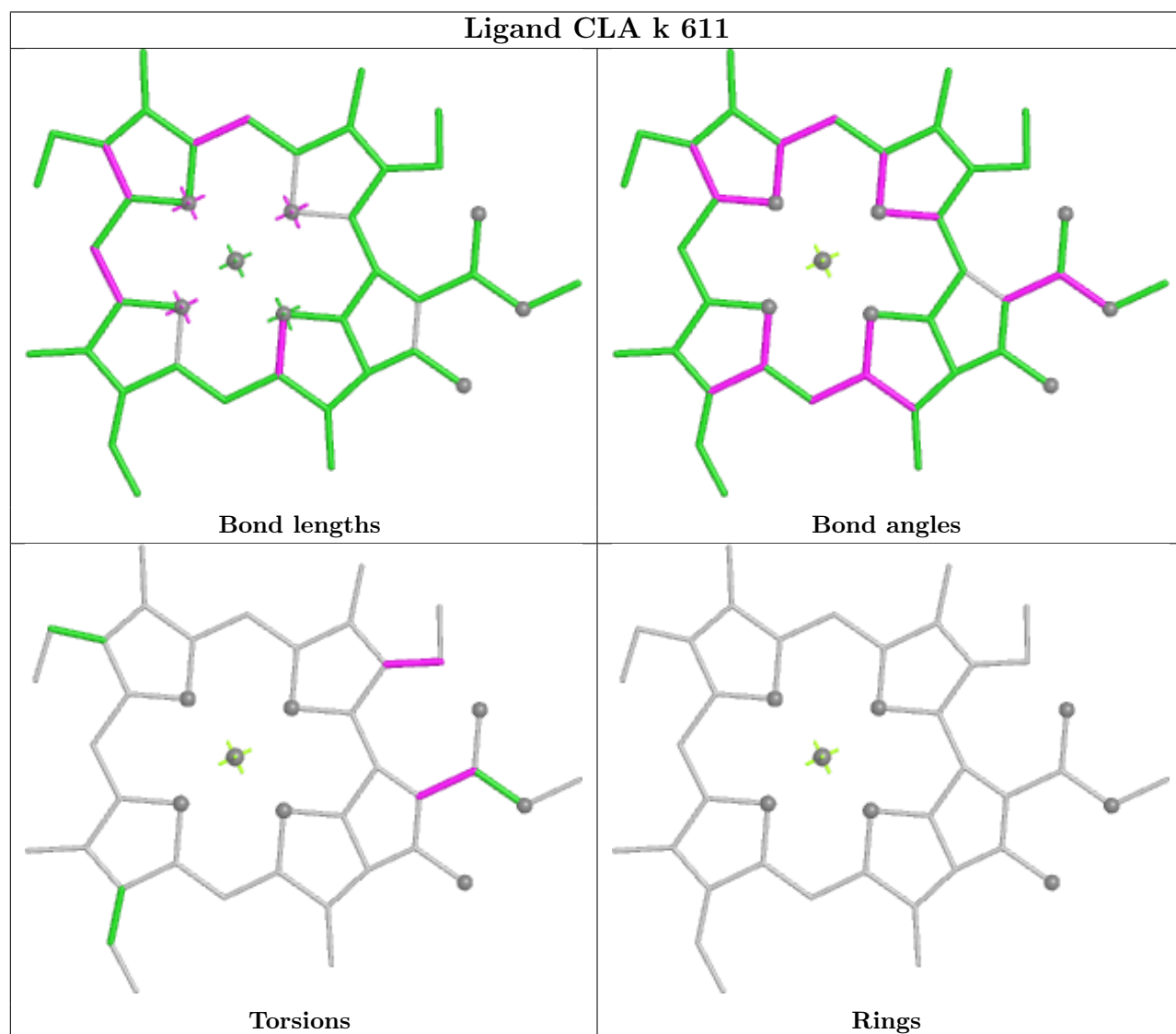
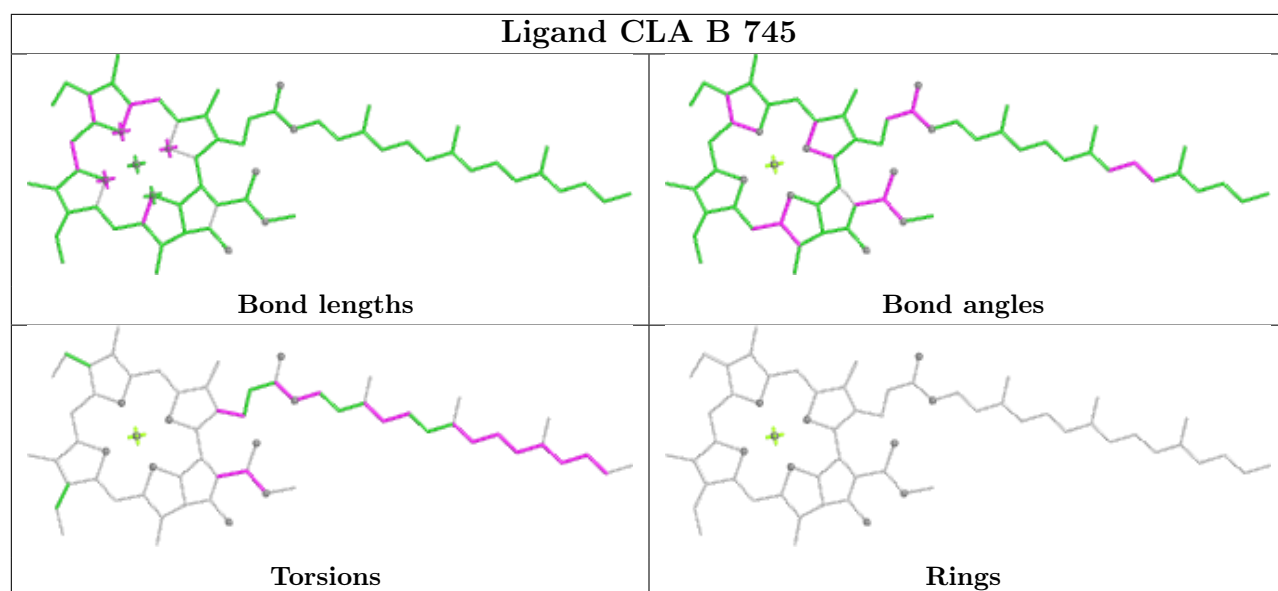
Rings

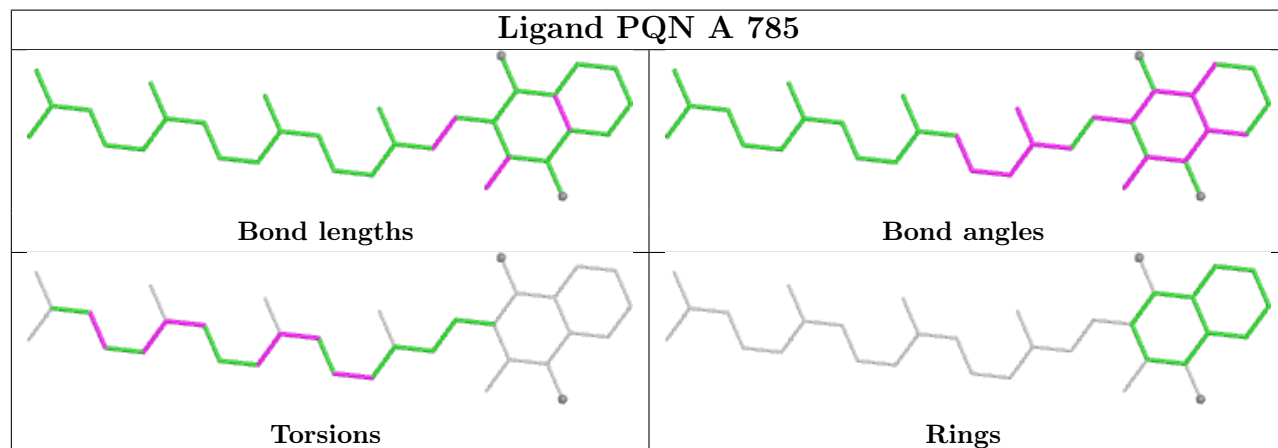
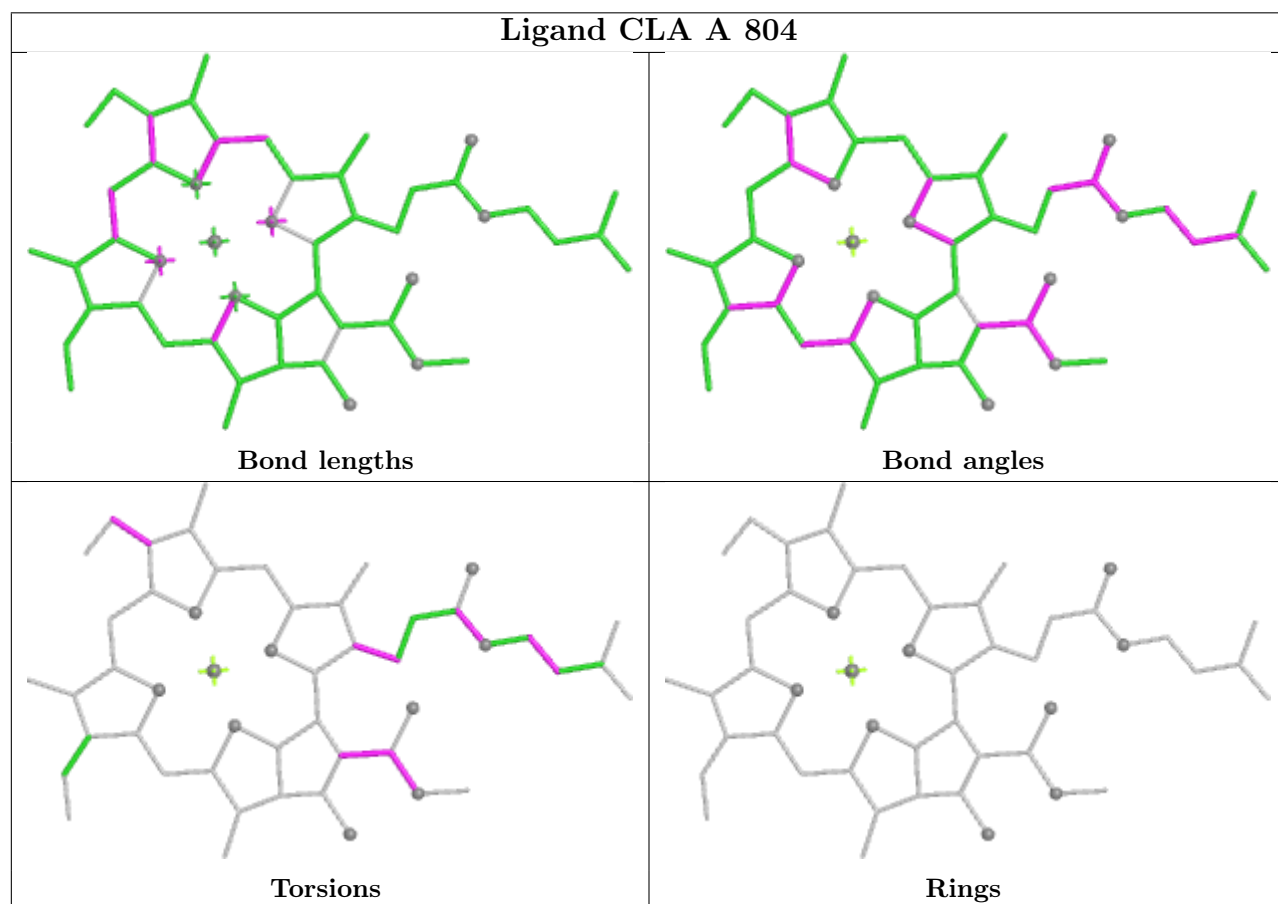
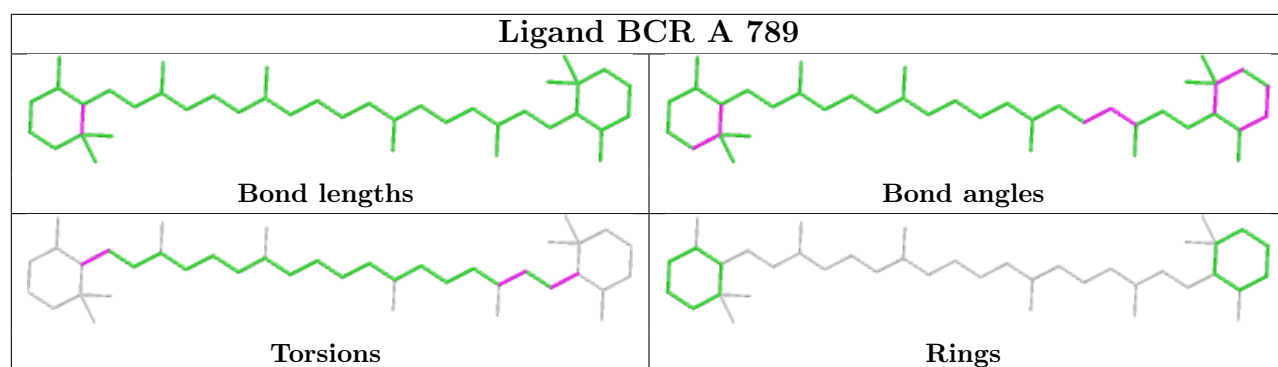




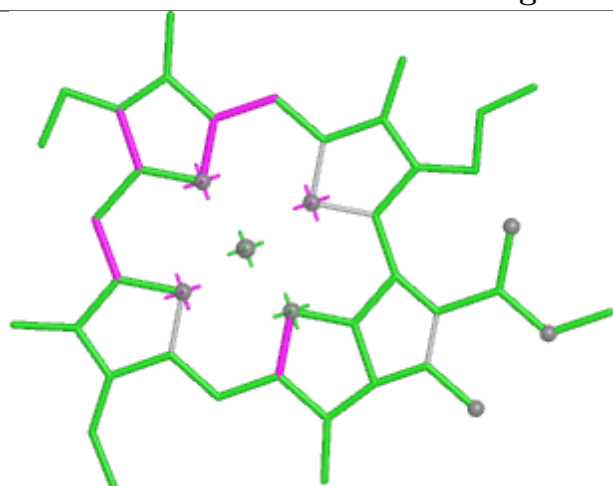




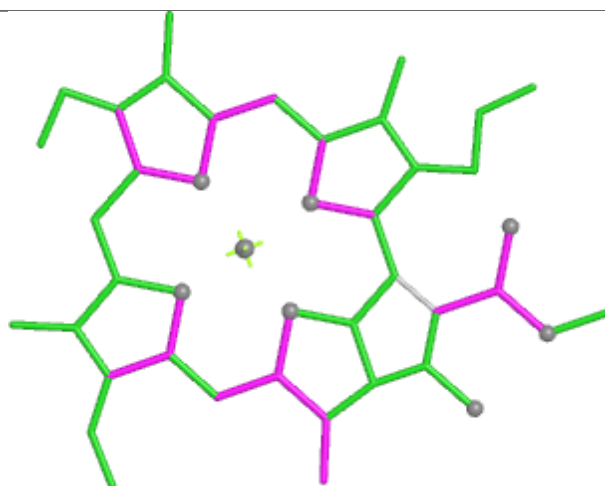




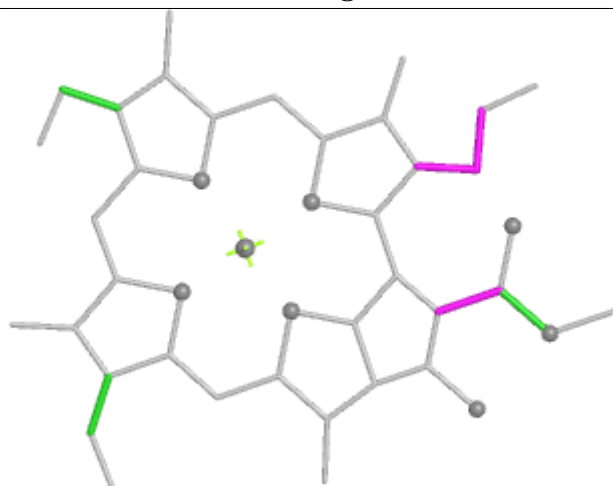
Ligand CLA c 606



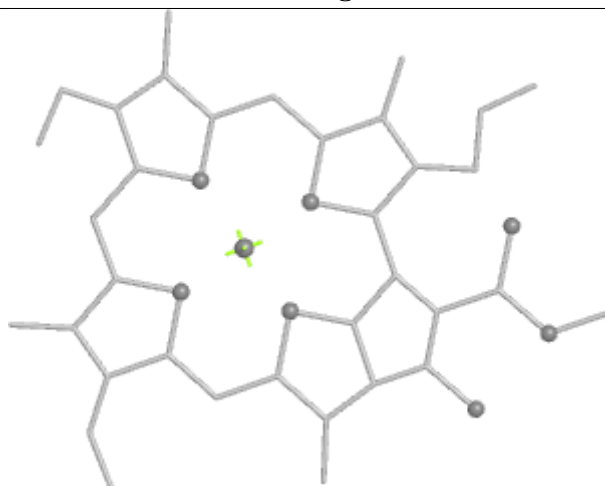
Bond lengths



Bond angles

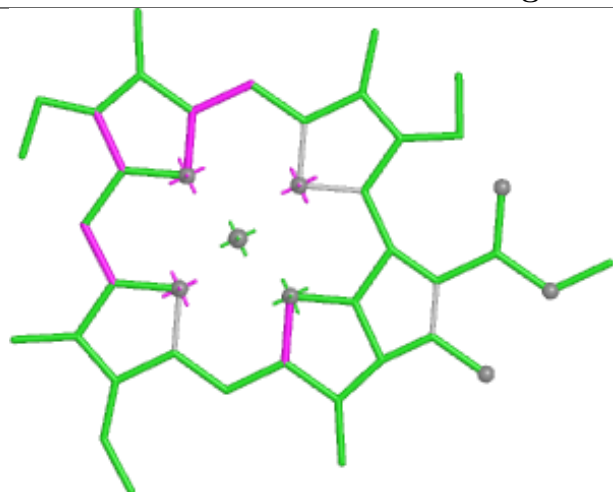


Torsions

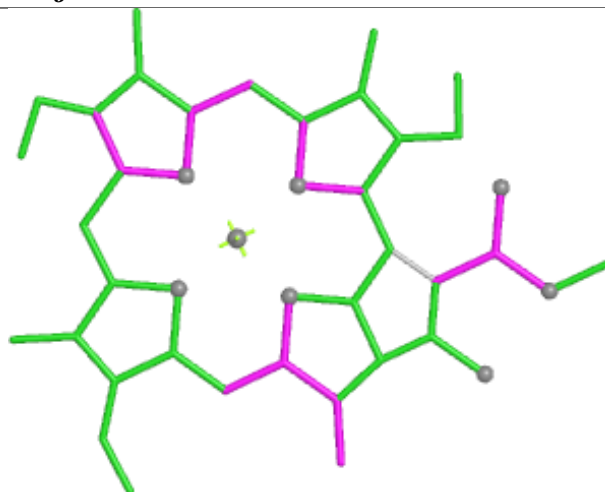


Rings

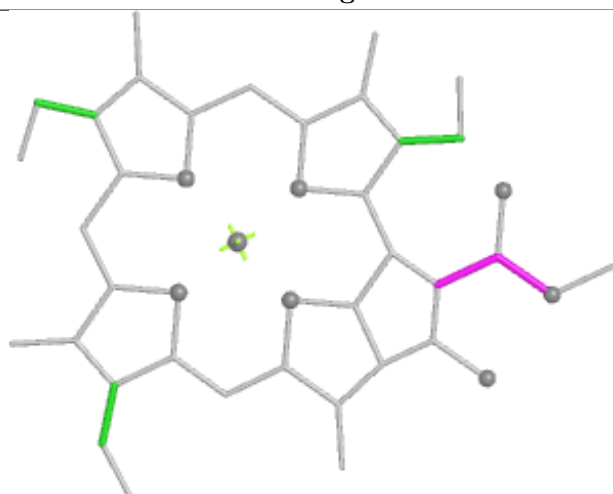
Ligand CLA j 603



Bond lengths



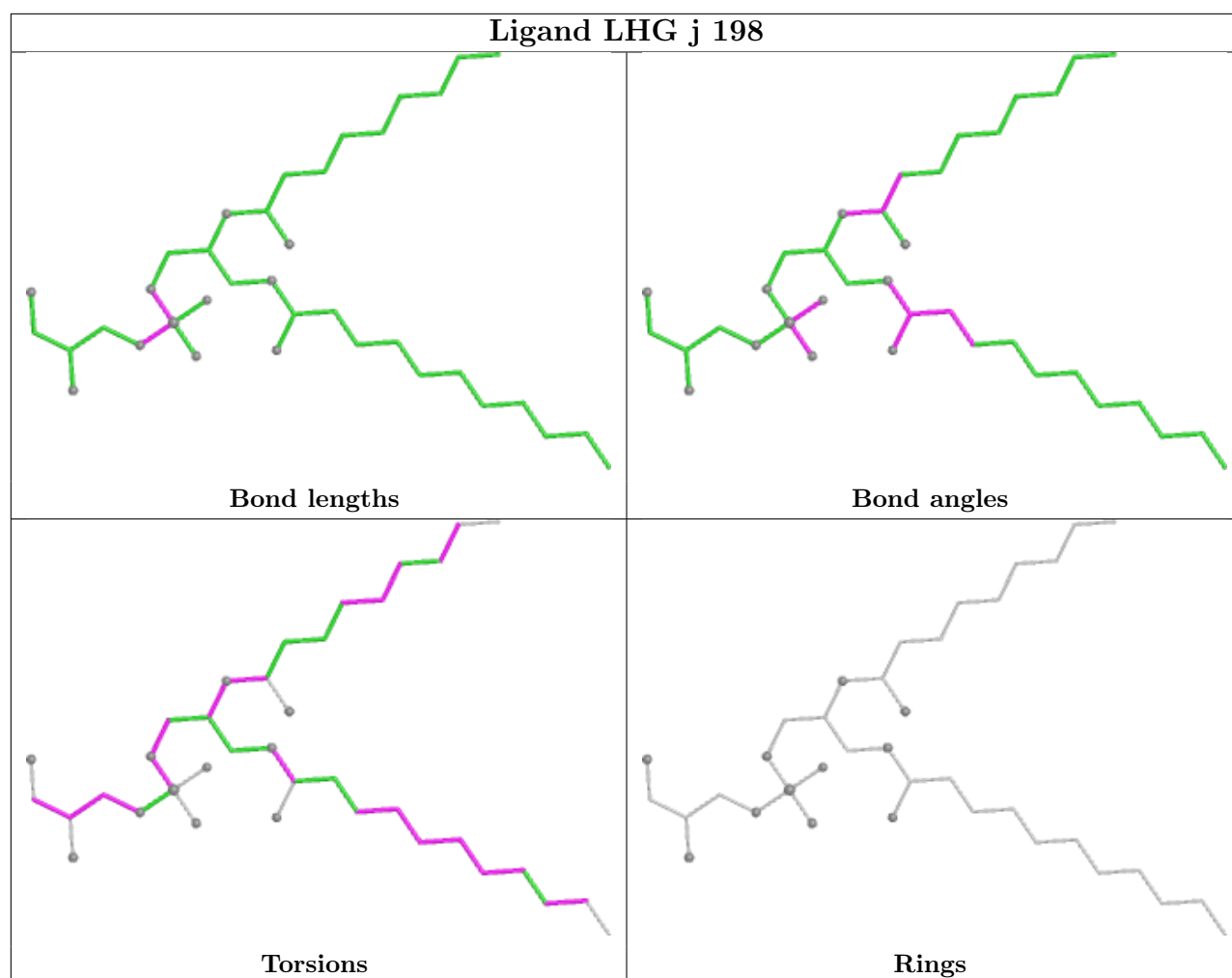
Bond angles

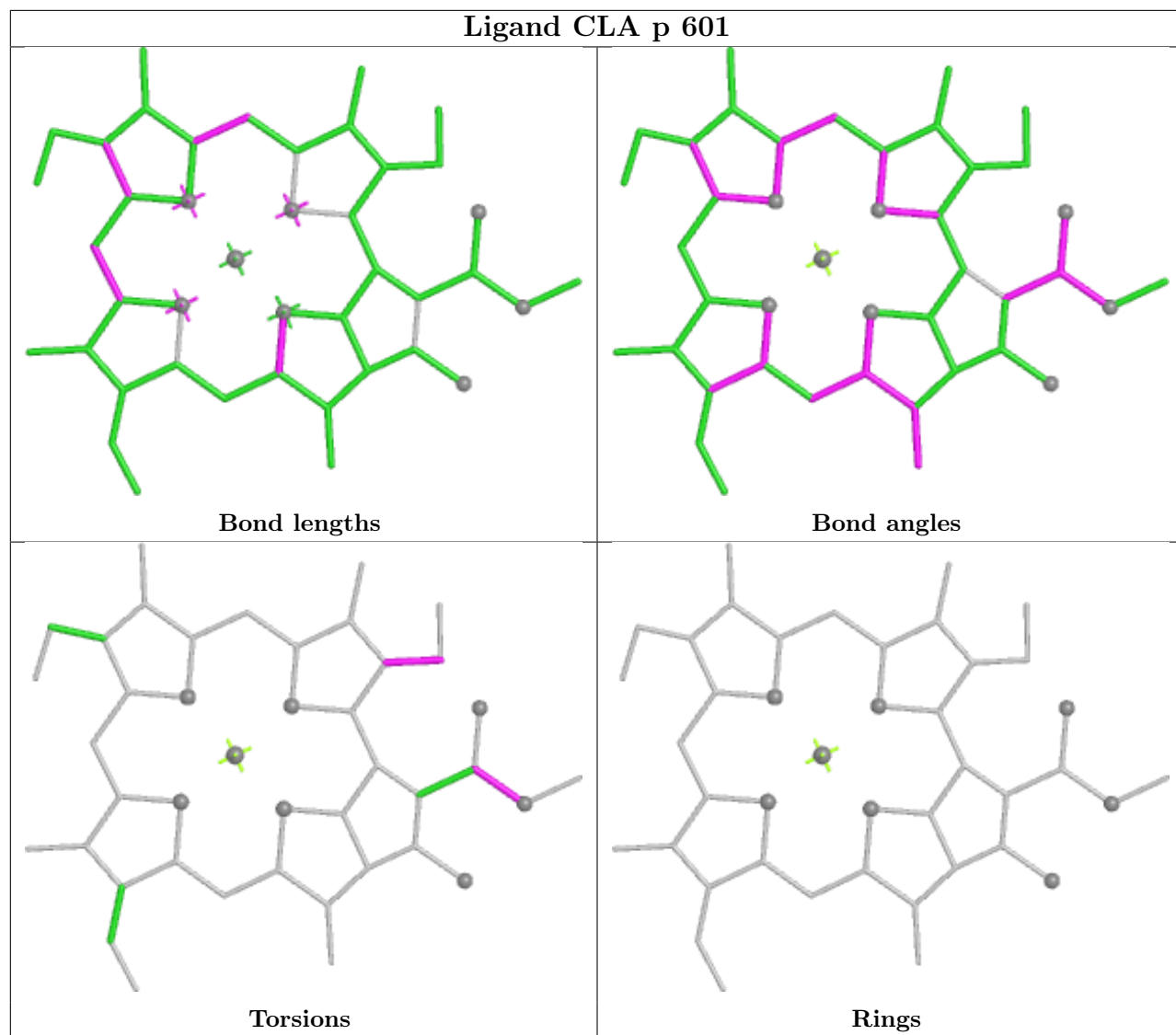


Torsions

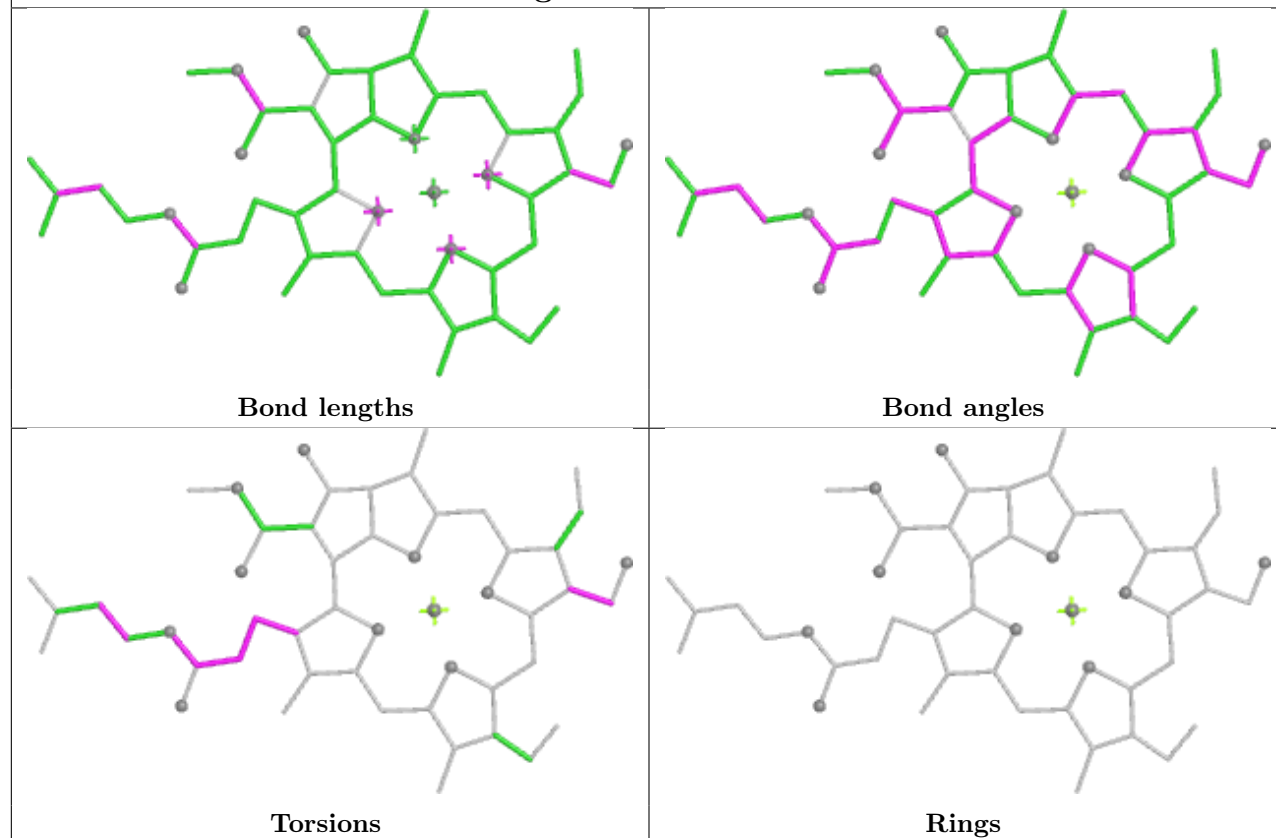


Rings

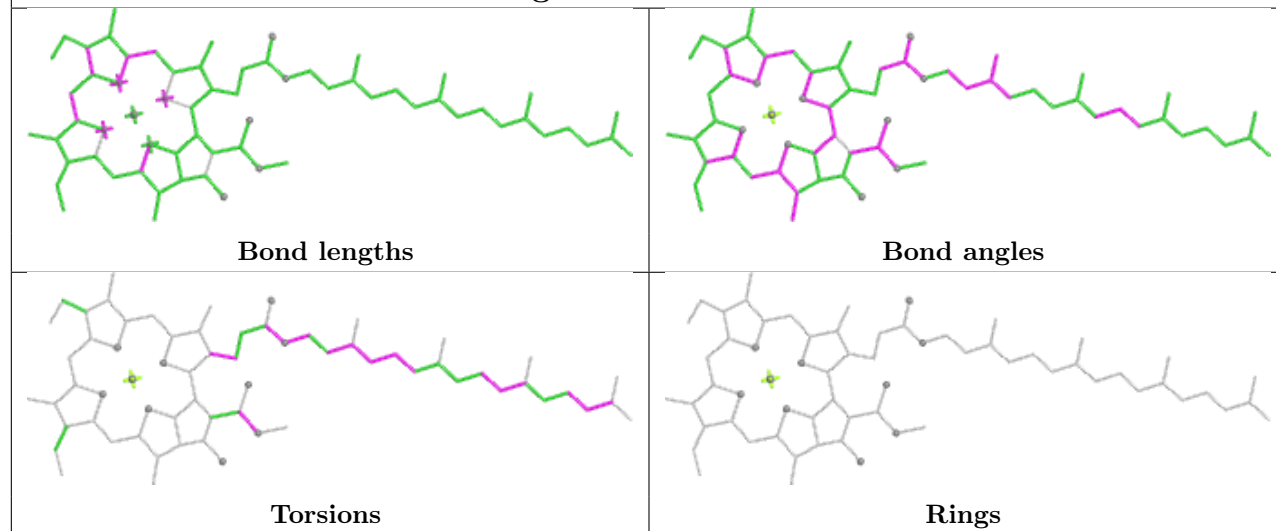




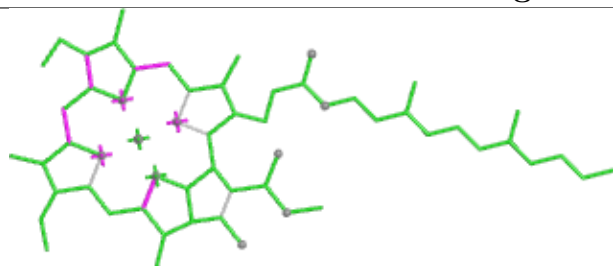
Ligand CHL d 605



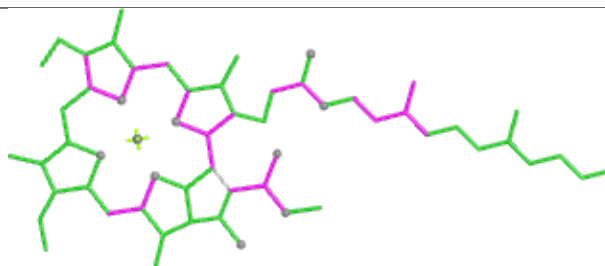
Ligand CLA B 779



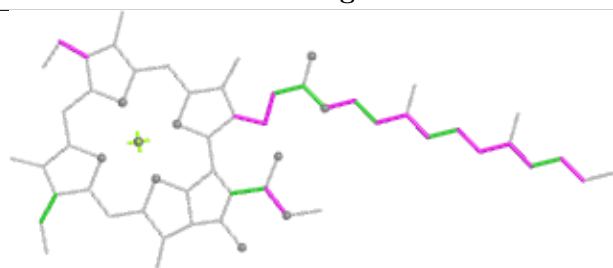
Ligand CLA A 775



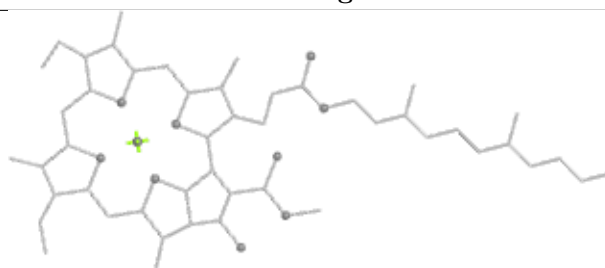
Bond lengths



Bond angles

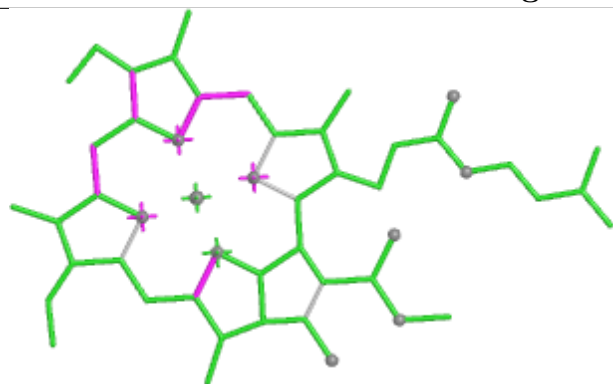


Torsions

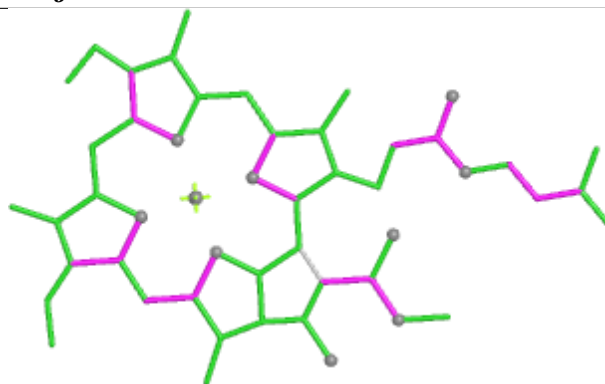


Rings

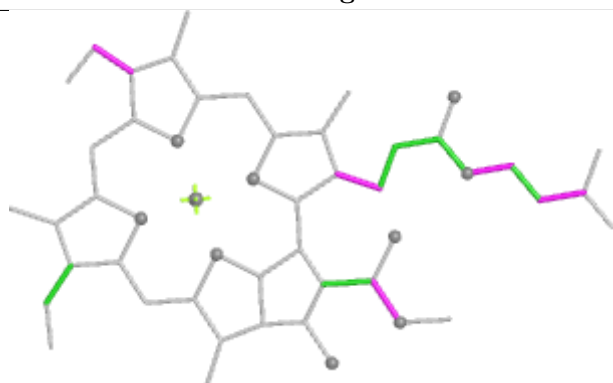
Ligand CLA j 611



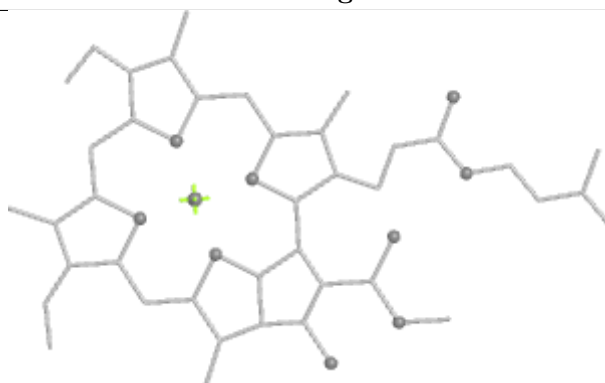
Bond lengths



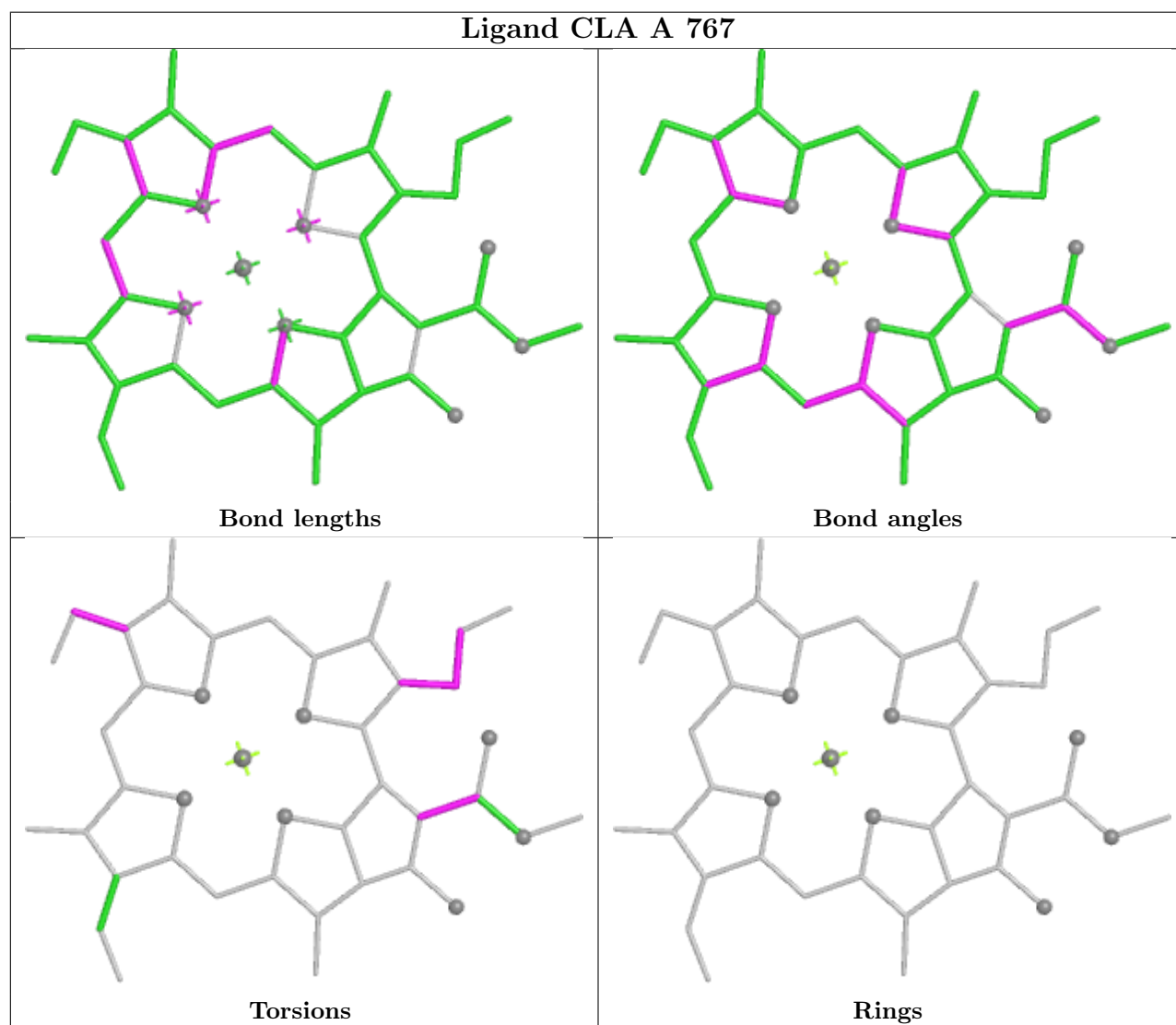
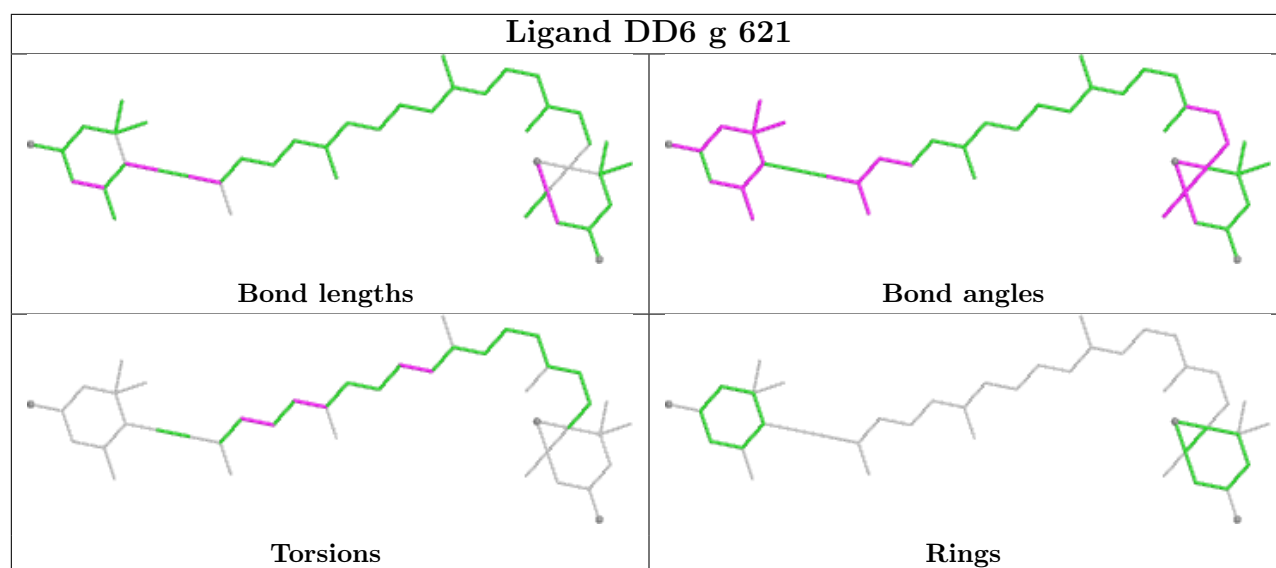
Bond angles

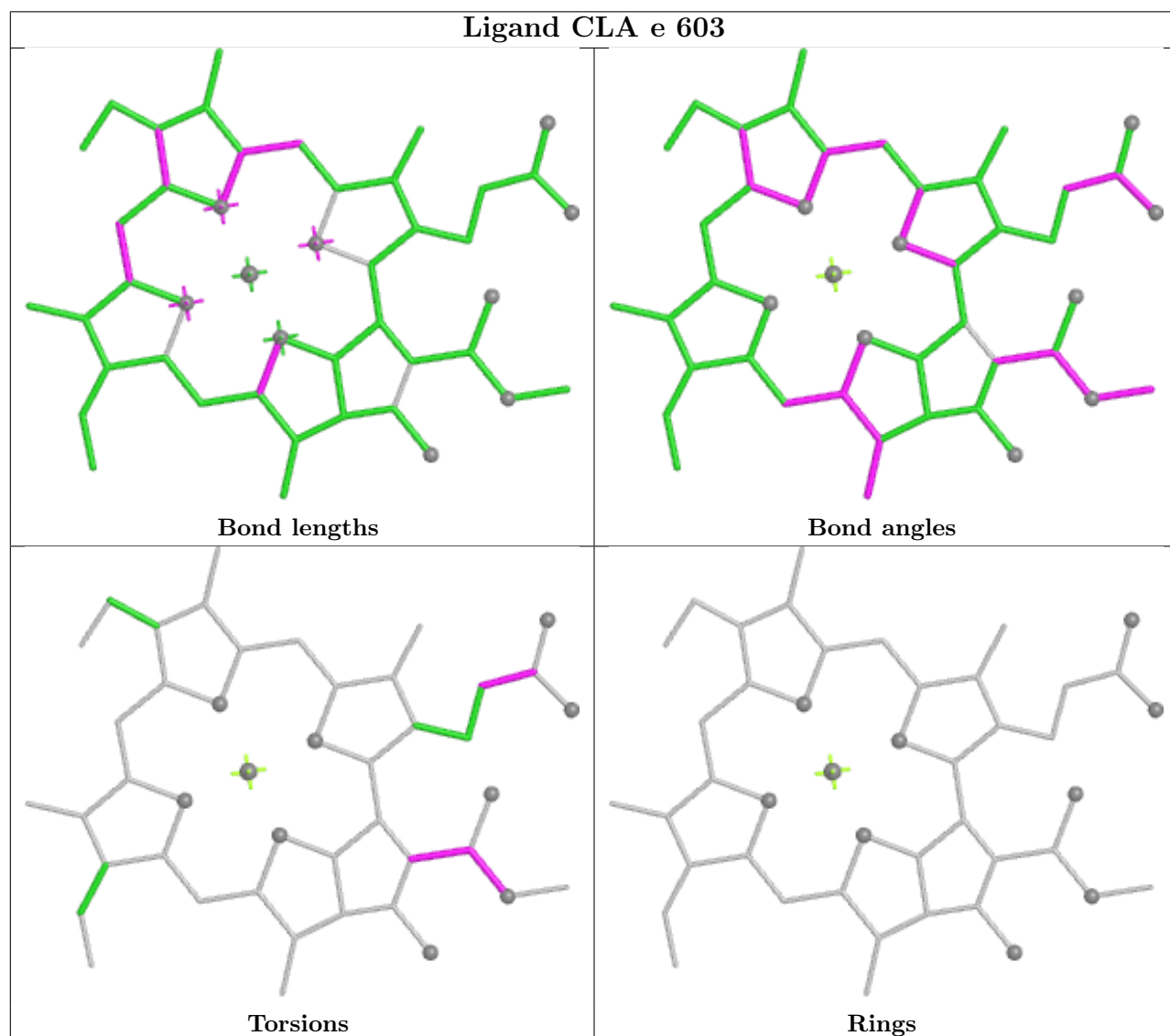
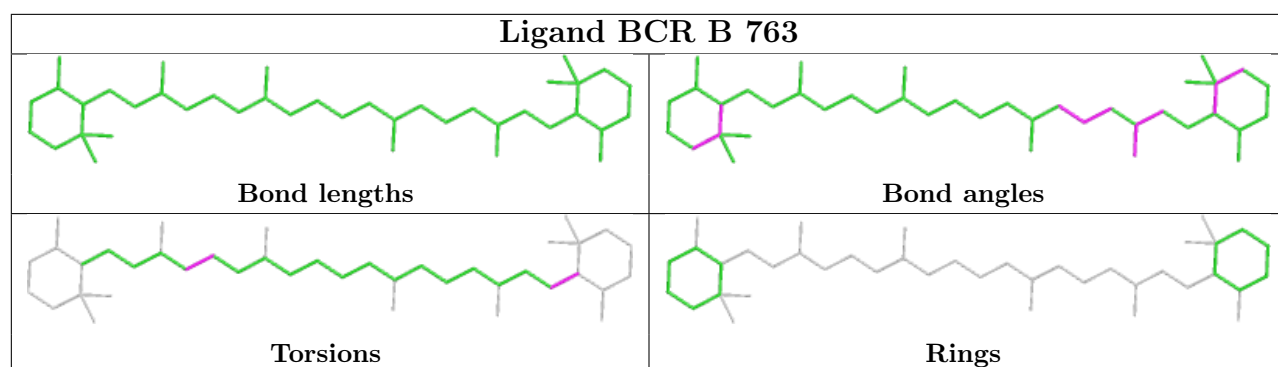


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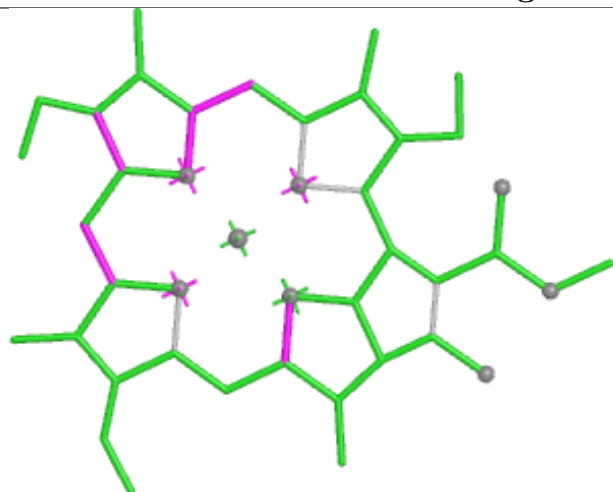


Rings

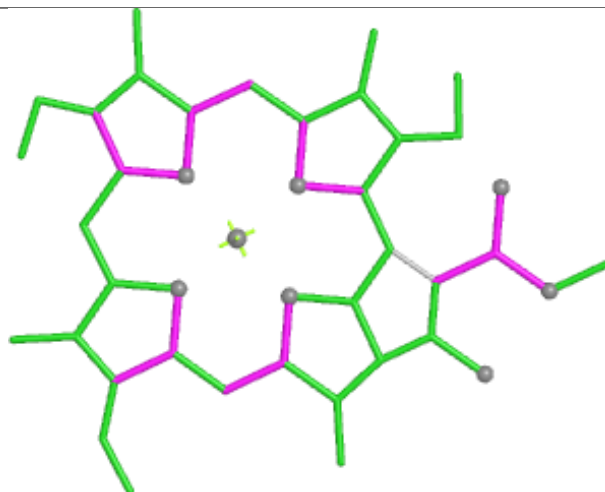




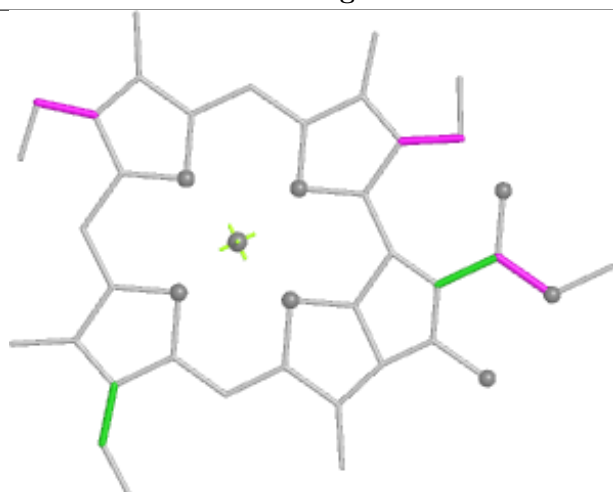
Ligand CLA h 615



Bond lengths



Bond angles

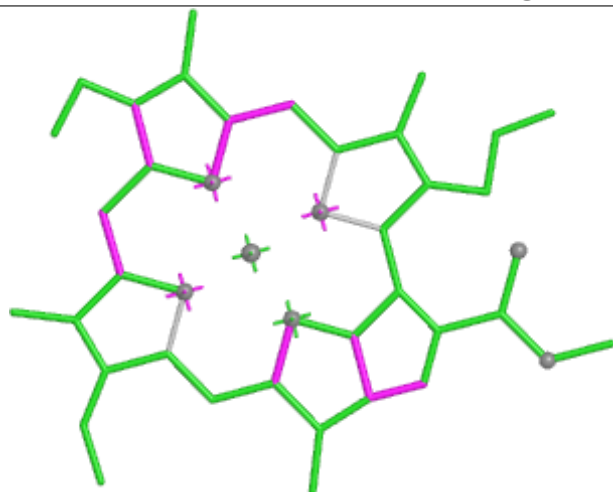


Torsions

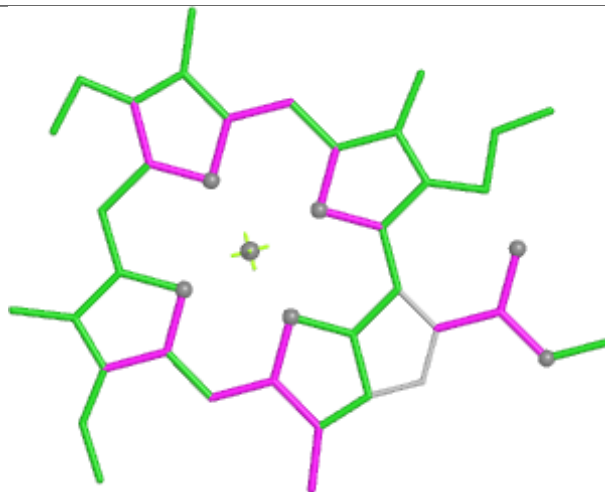


Rings

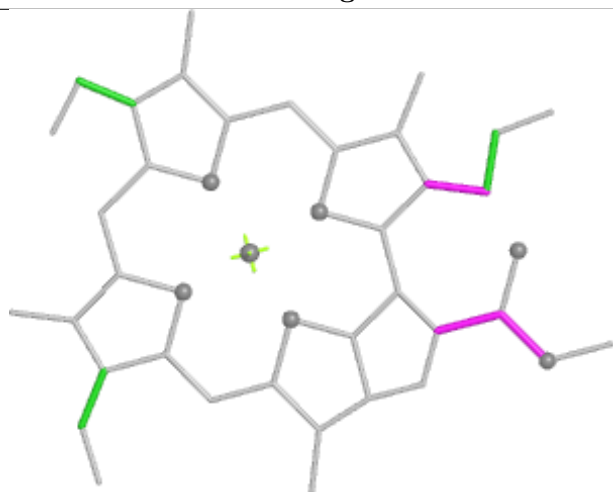
Ligand CLA o 612



Bond lengths



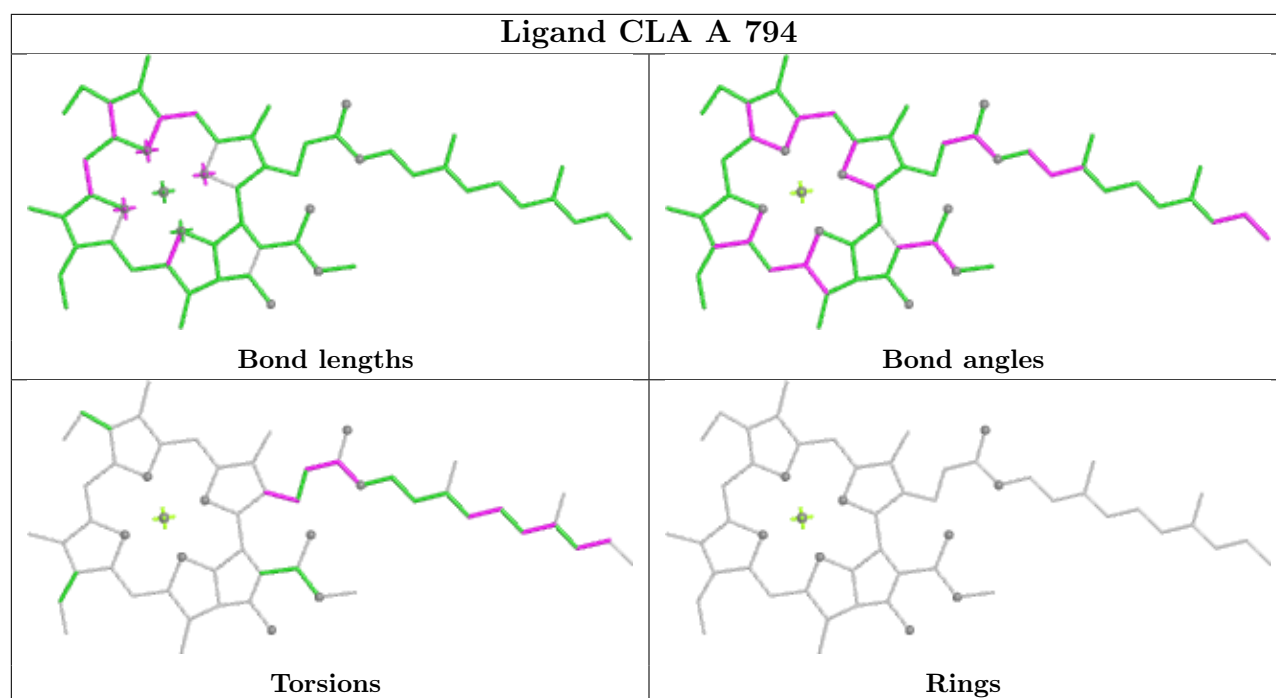
Bond angles



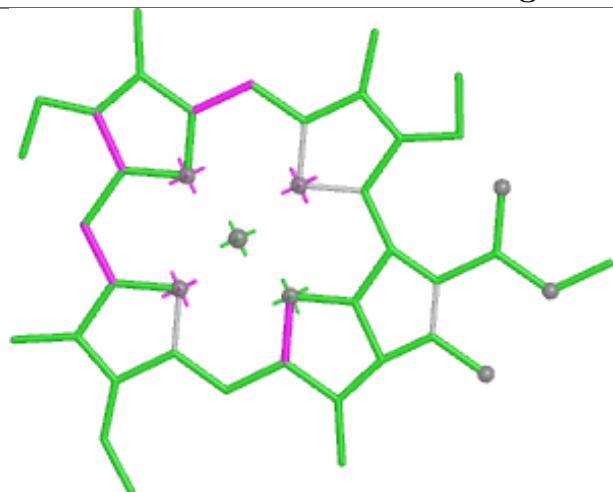
Torsions



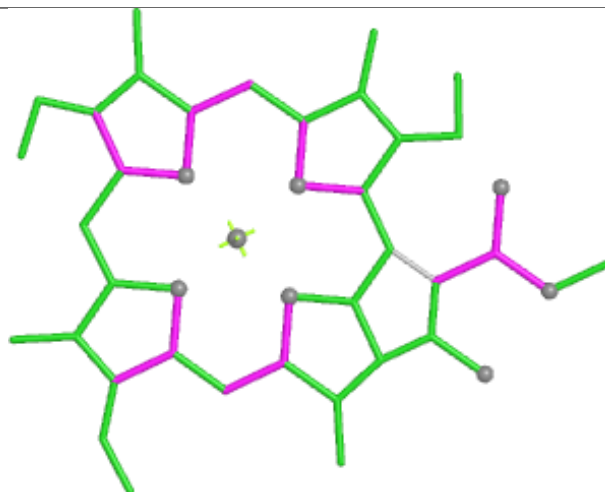
Rings



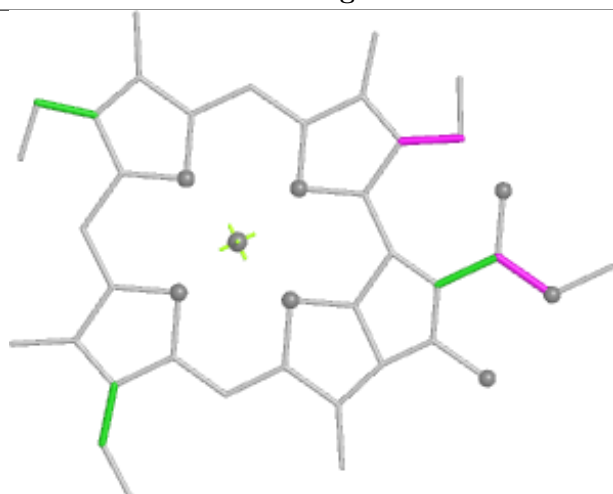
Ligand CLA e 611



Bond lengths



Bond angles

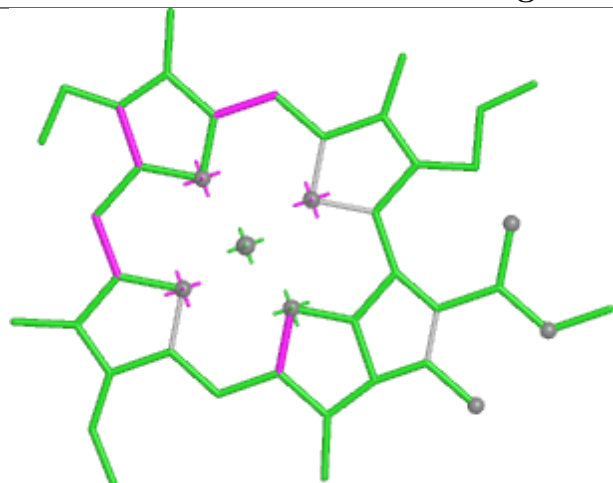


Torsions

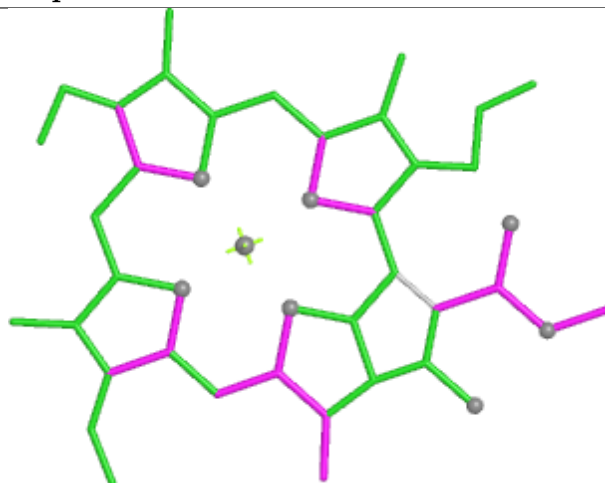


Rings

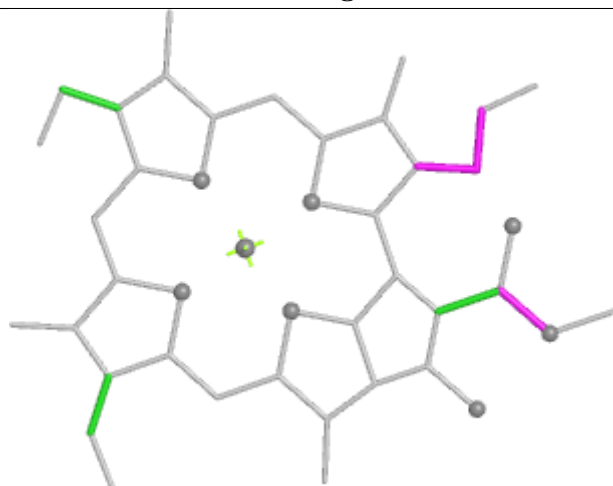
Ligand CLA p 613



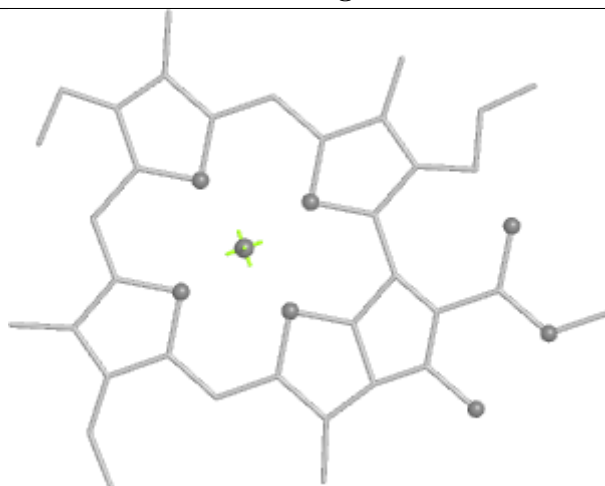
Bond lengths



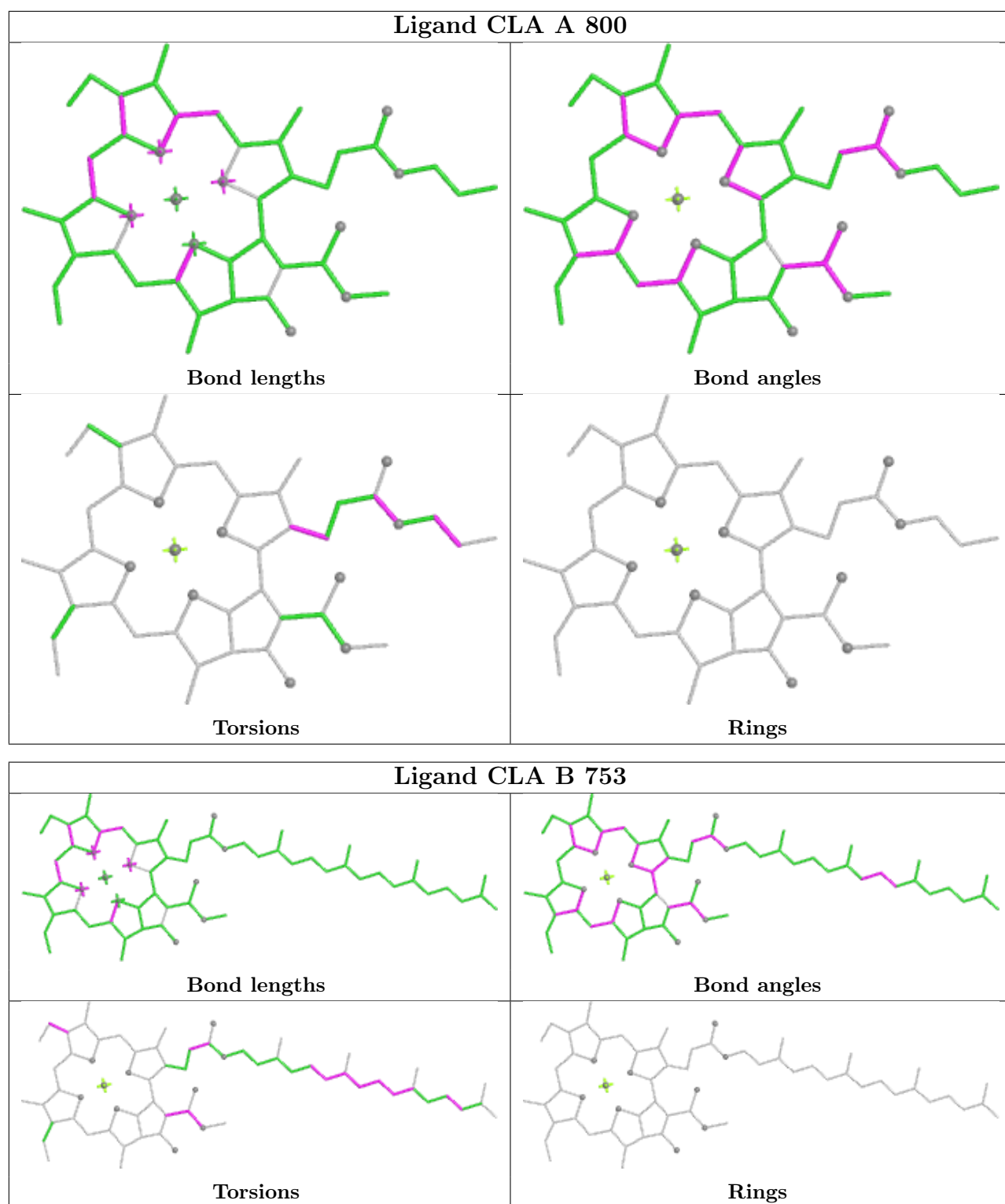
Bond angles



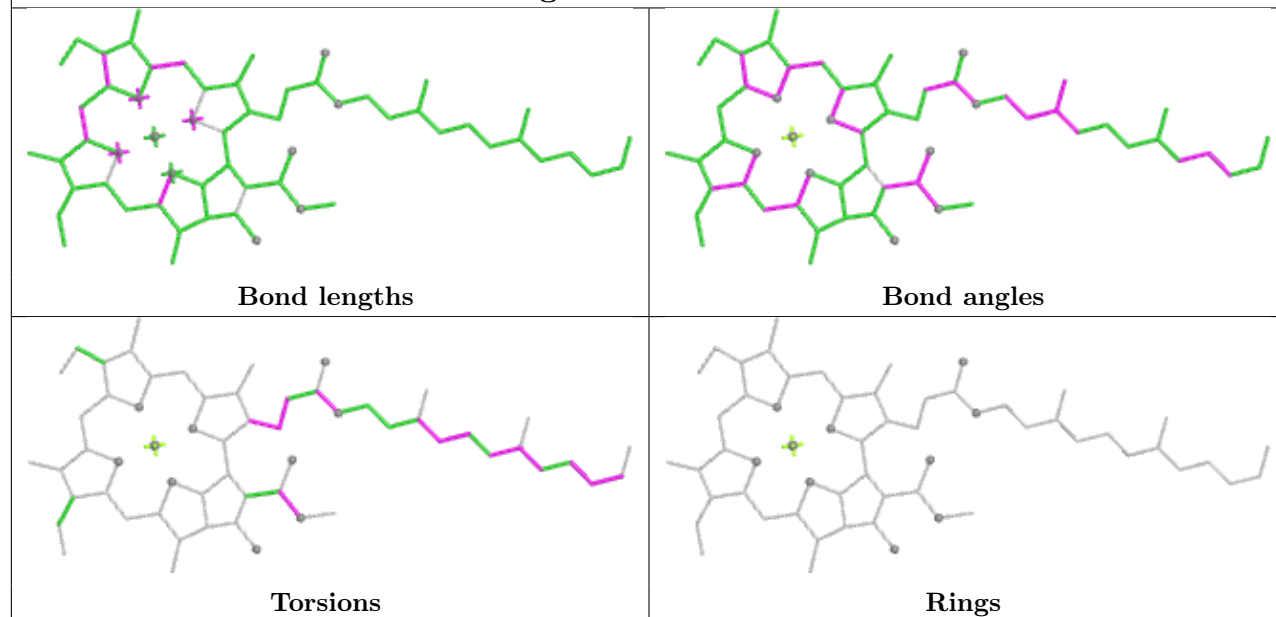
Torsions



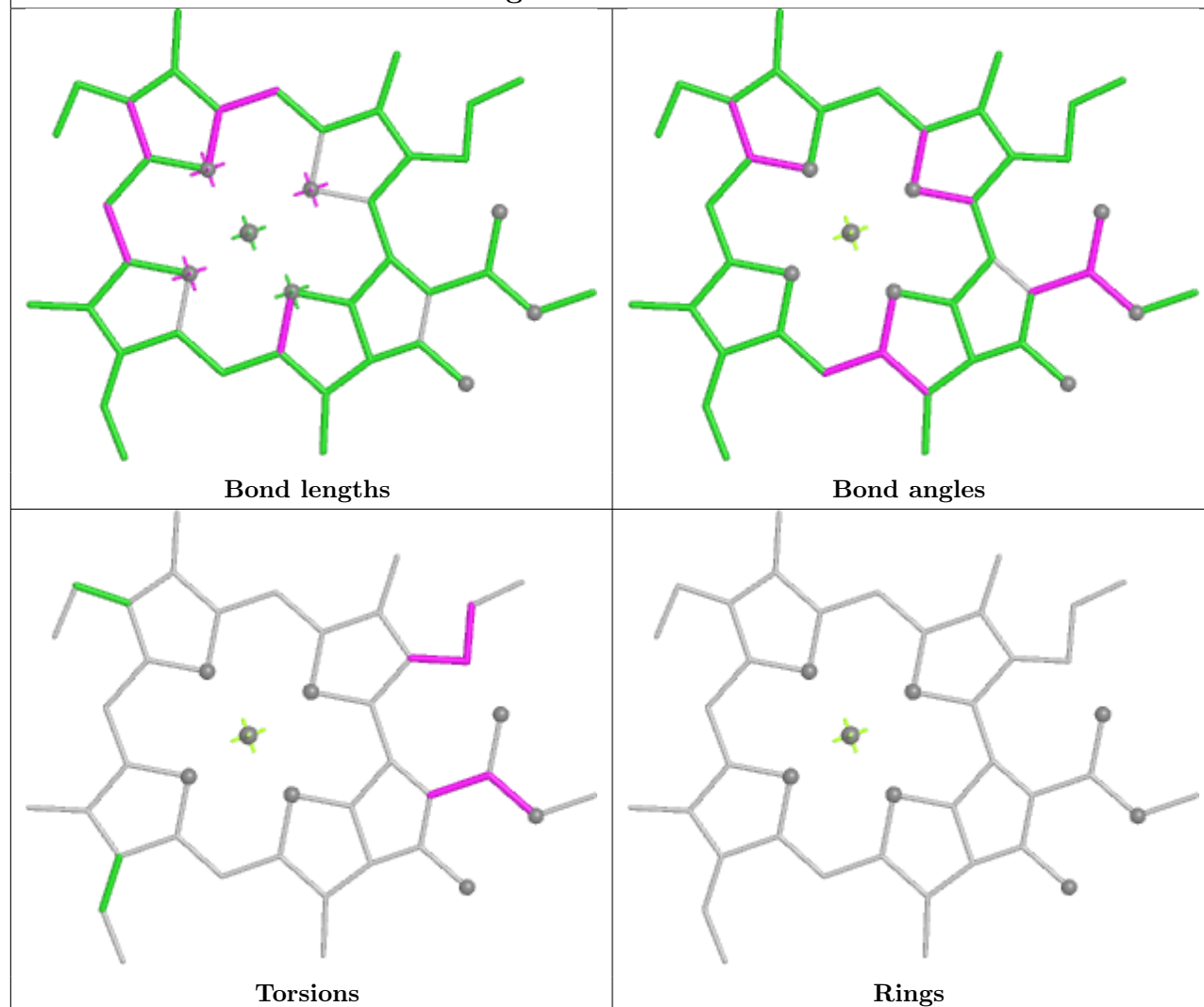
Rings

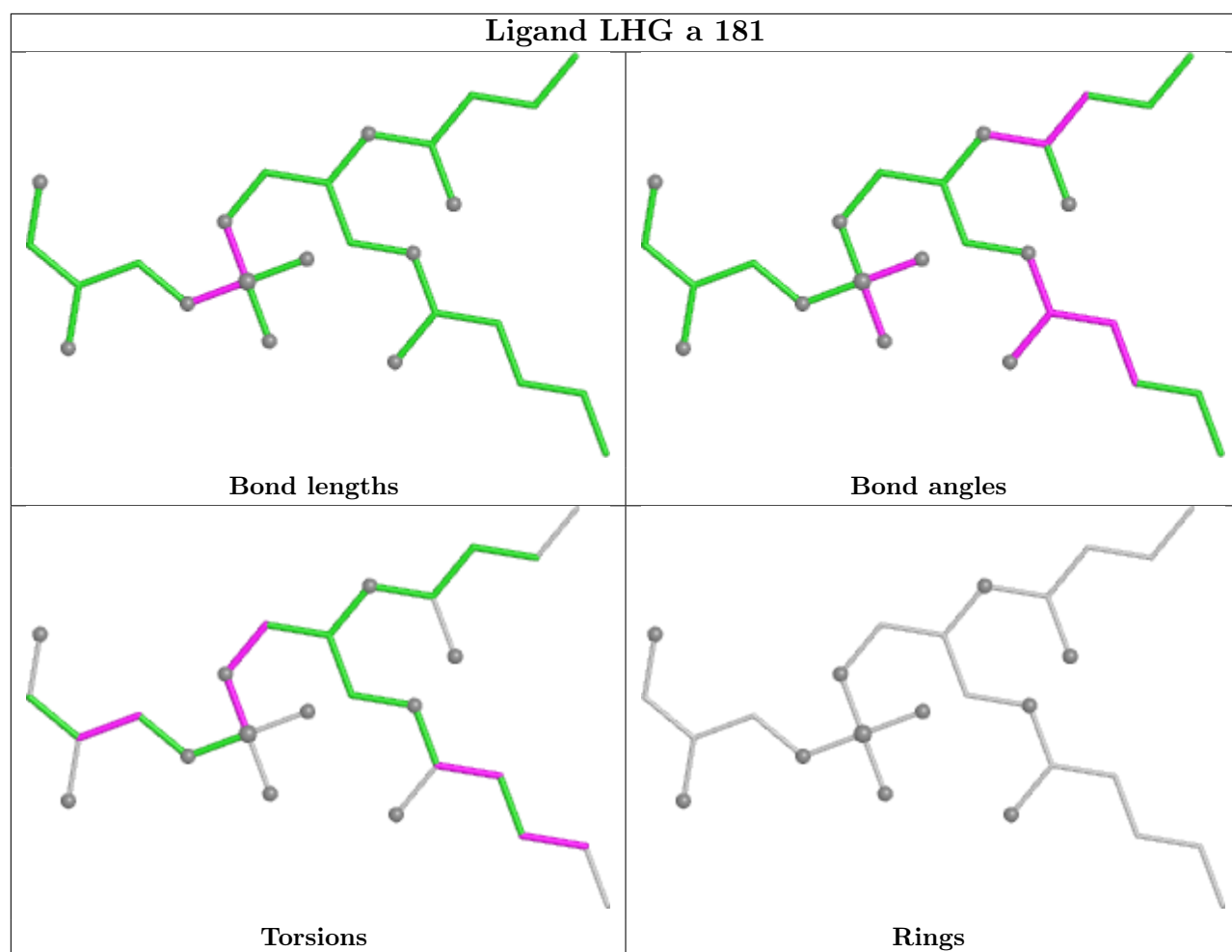


Ligand CLA f 602

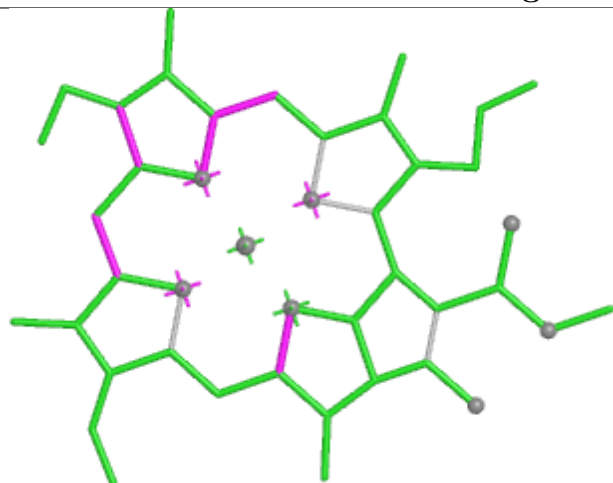


Ligand CLA a 612

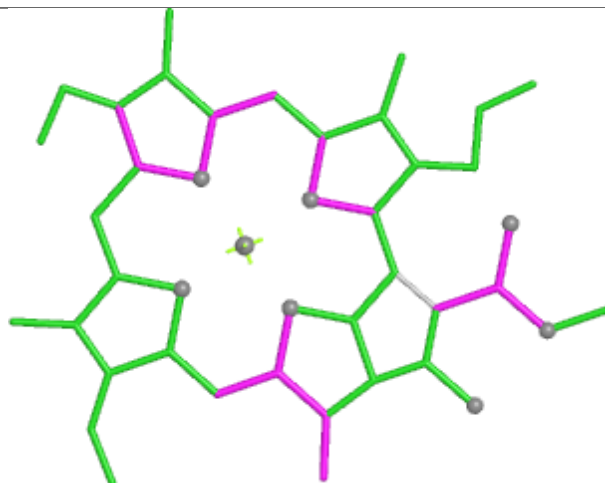




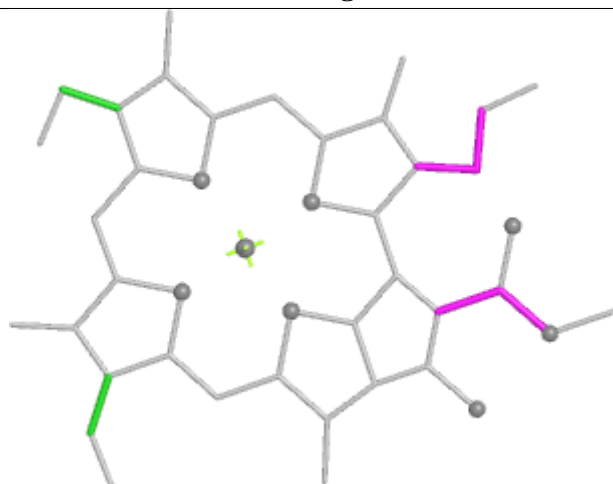
Ligand CLA 1 612



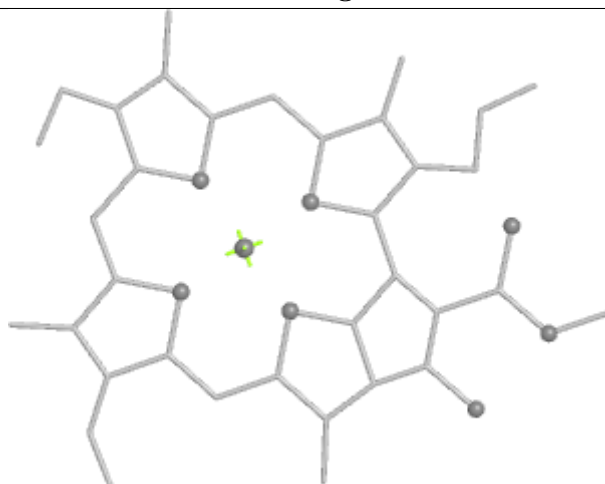
Bond lengths



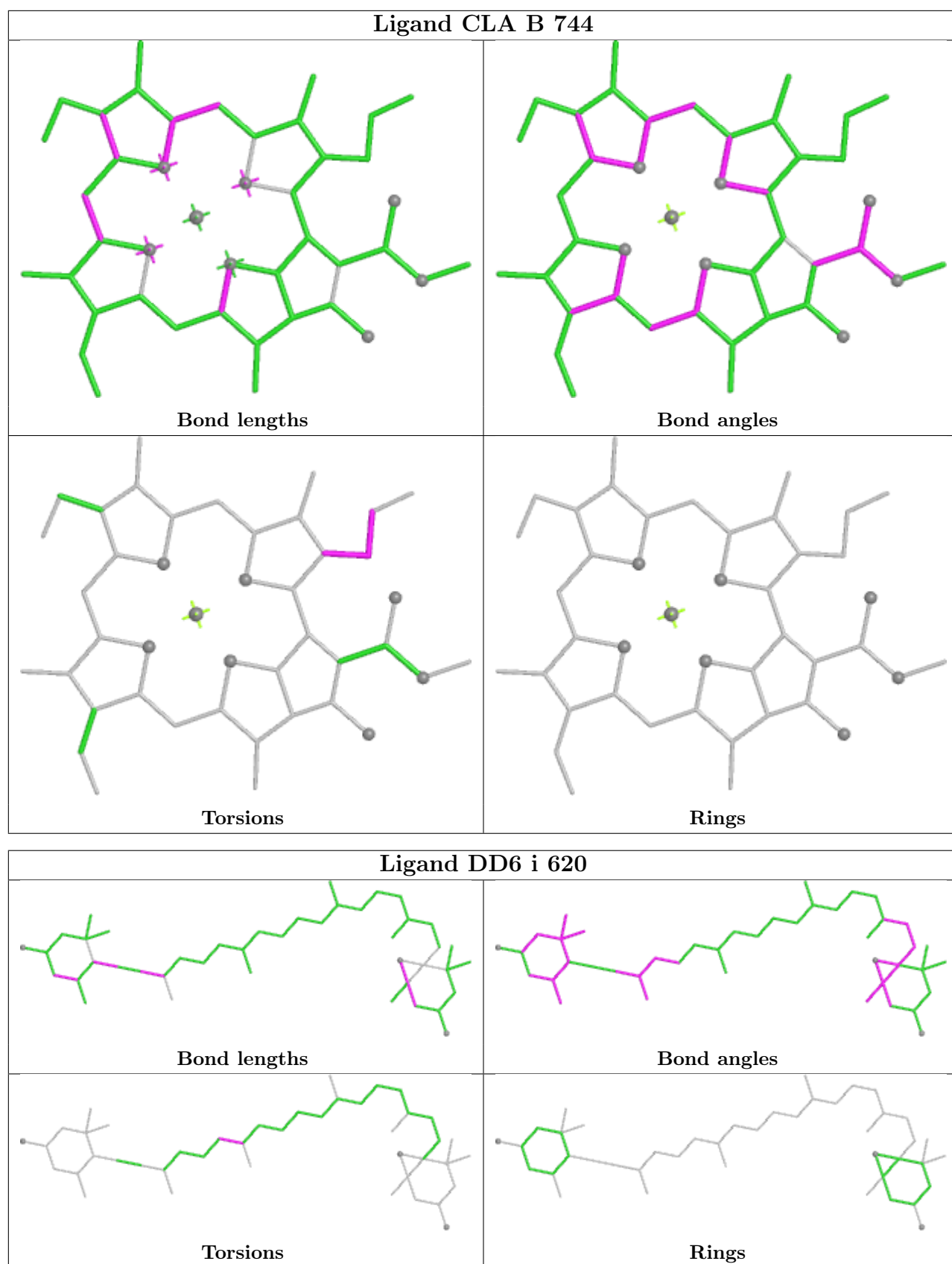
Bond angles

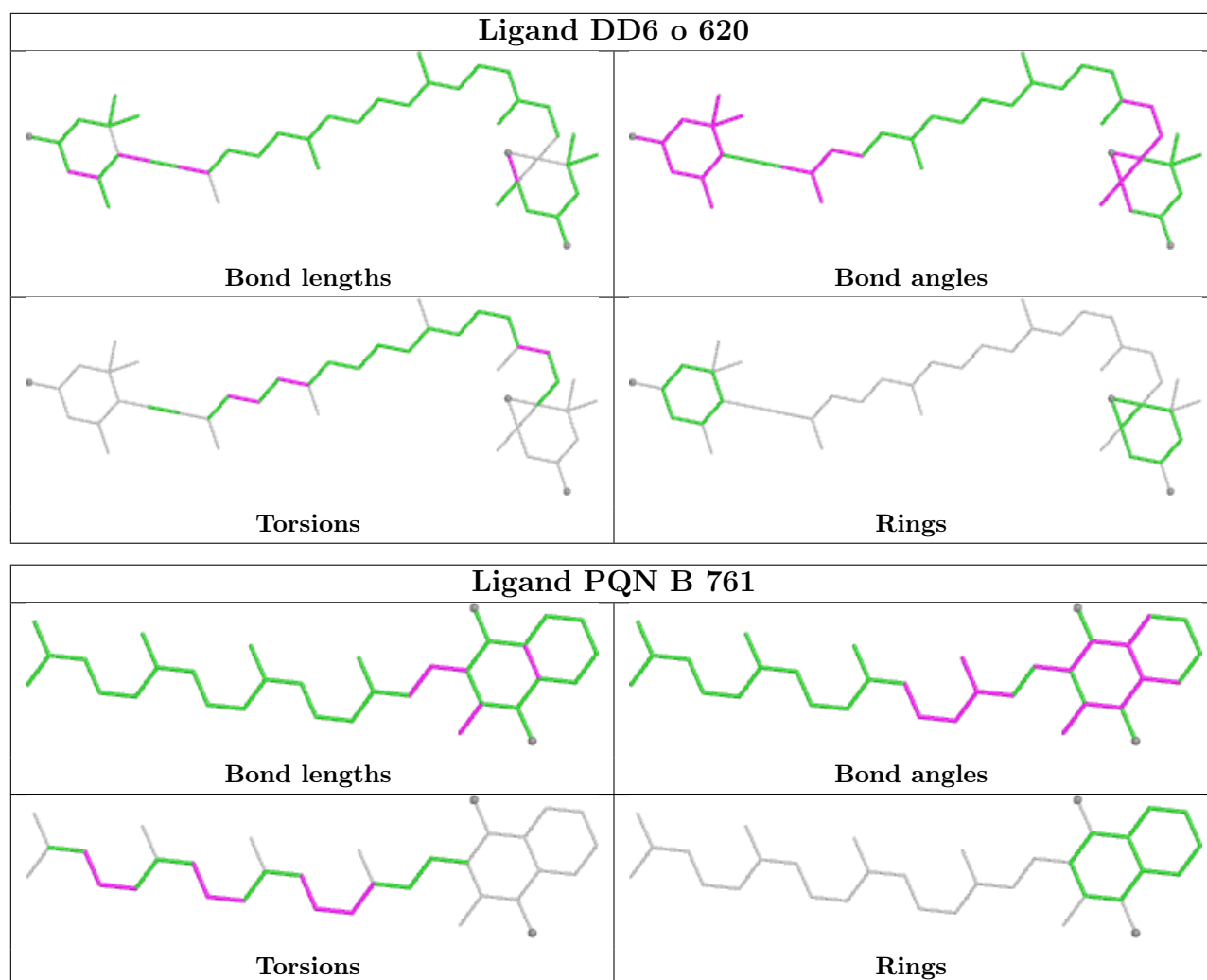


Torsions

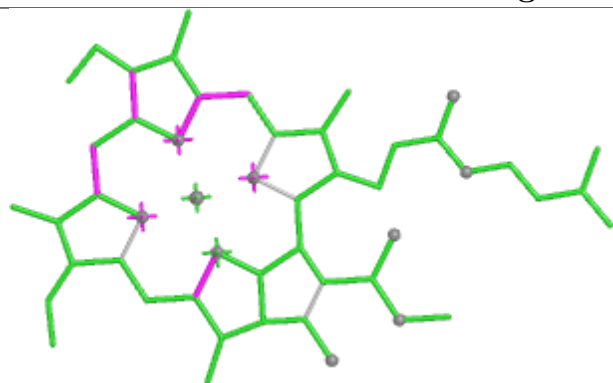


Rings

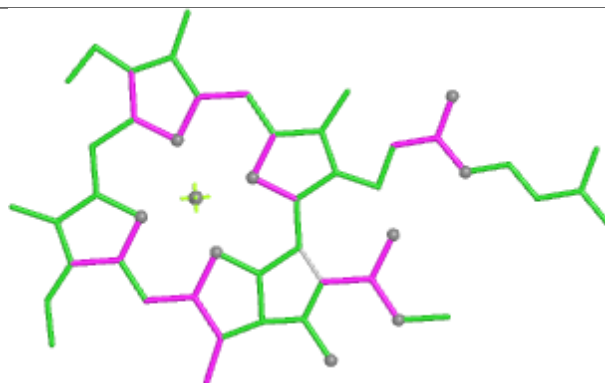




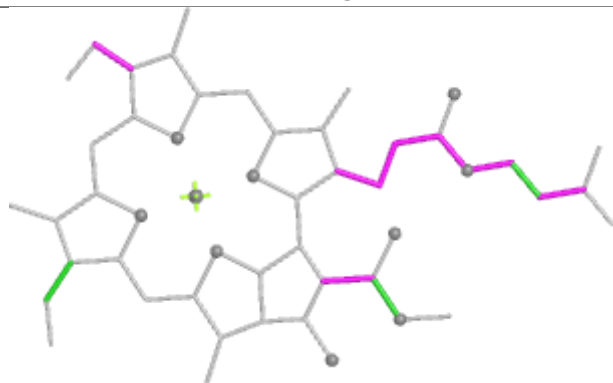
Ligand CLA J 101



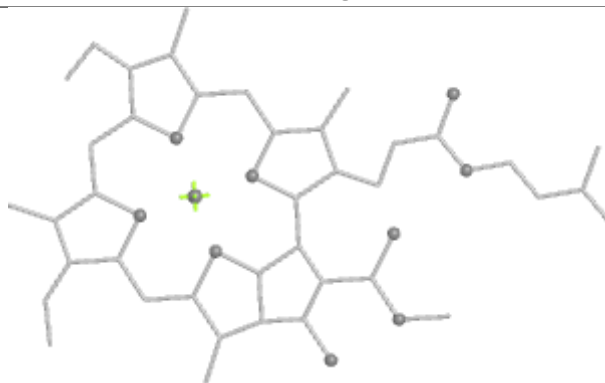
Bond lengths



Bond angles

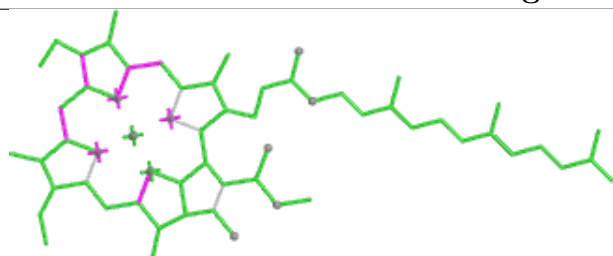


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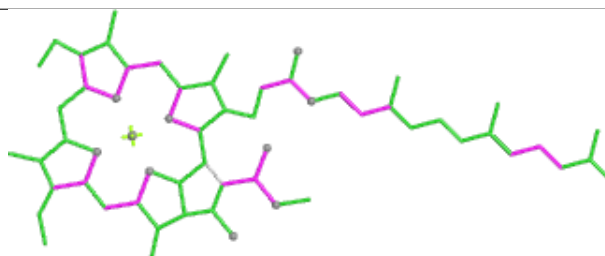


Rings

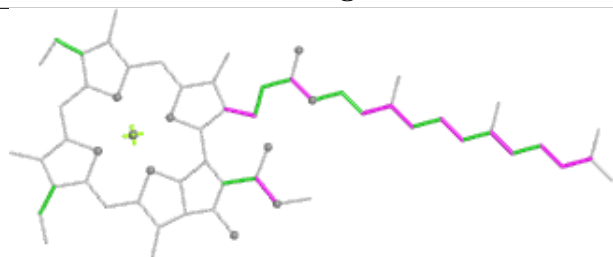
Ligand CLA I 609



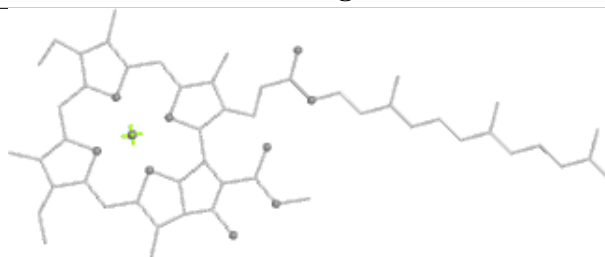
Bond lengths



Bond angles

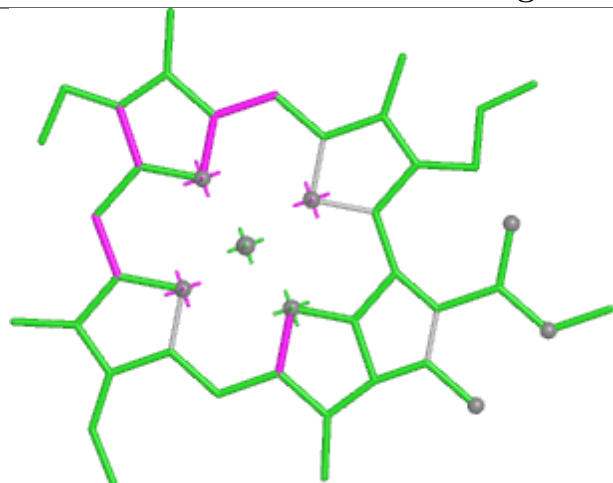


Torsions

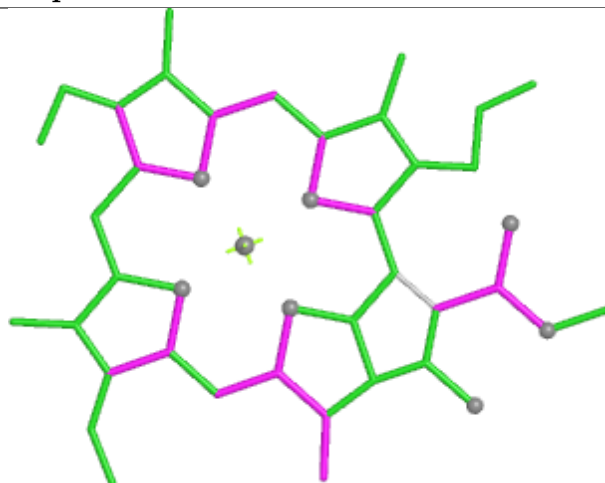


Rings

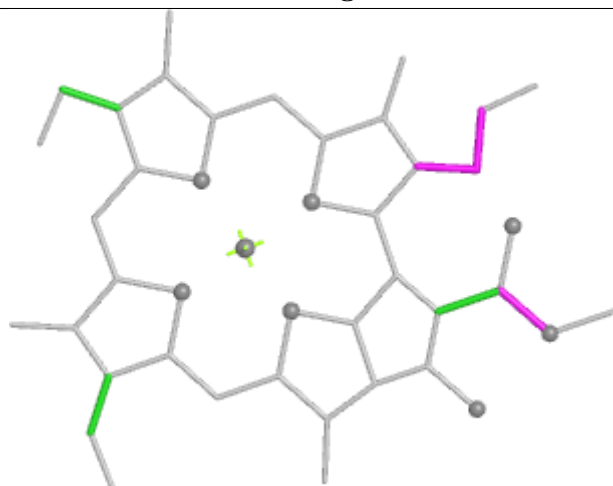
Ligand CLA p 604



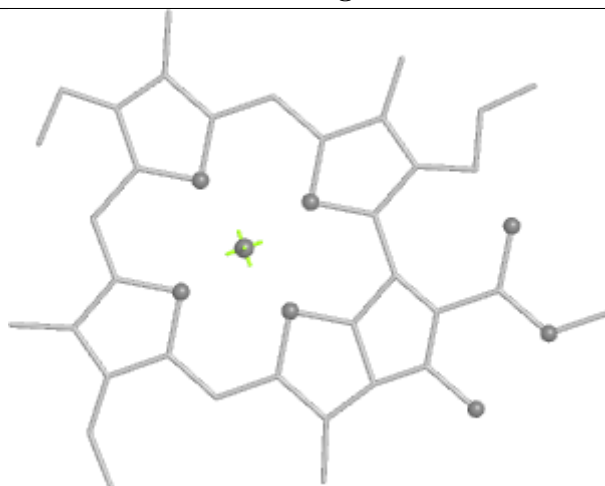
Bond lengths



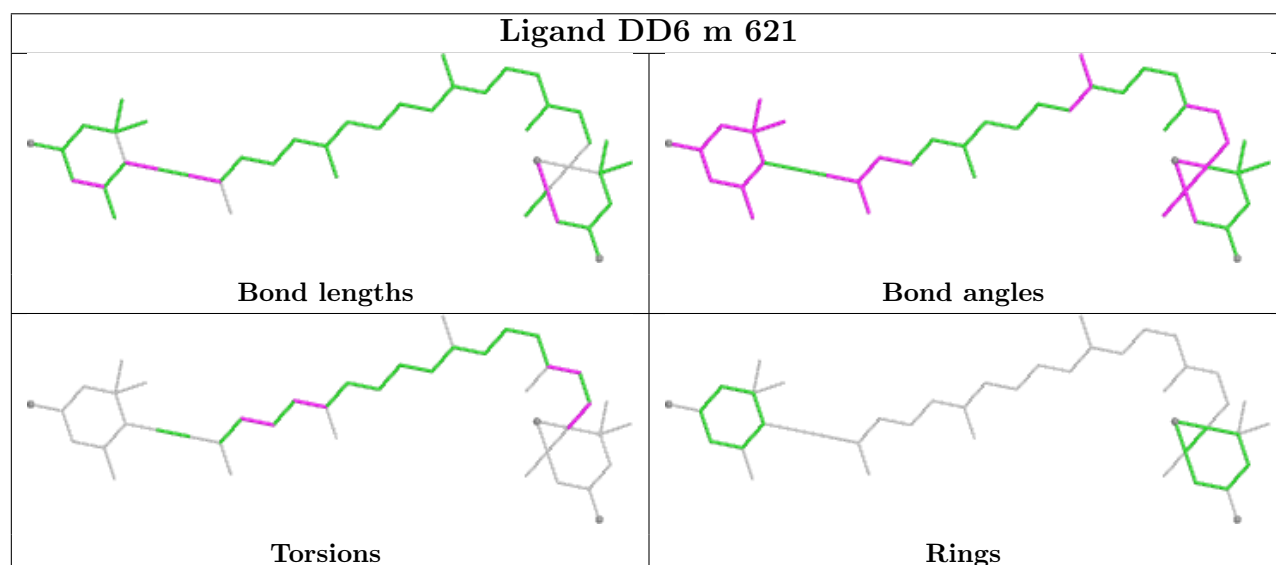
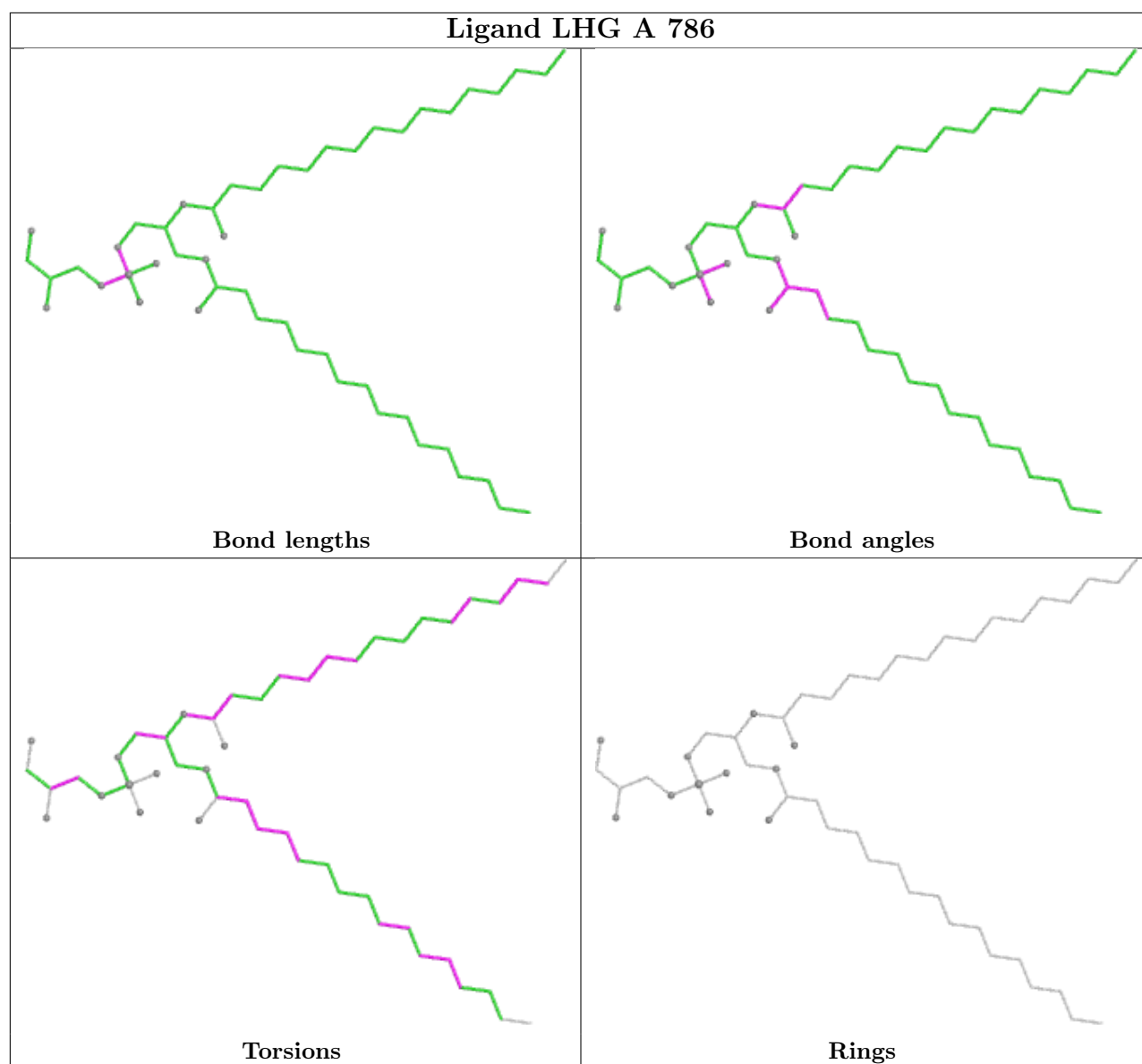
Bond angles

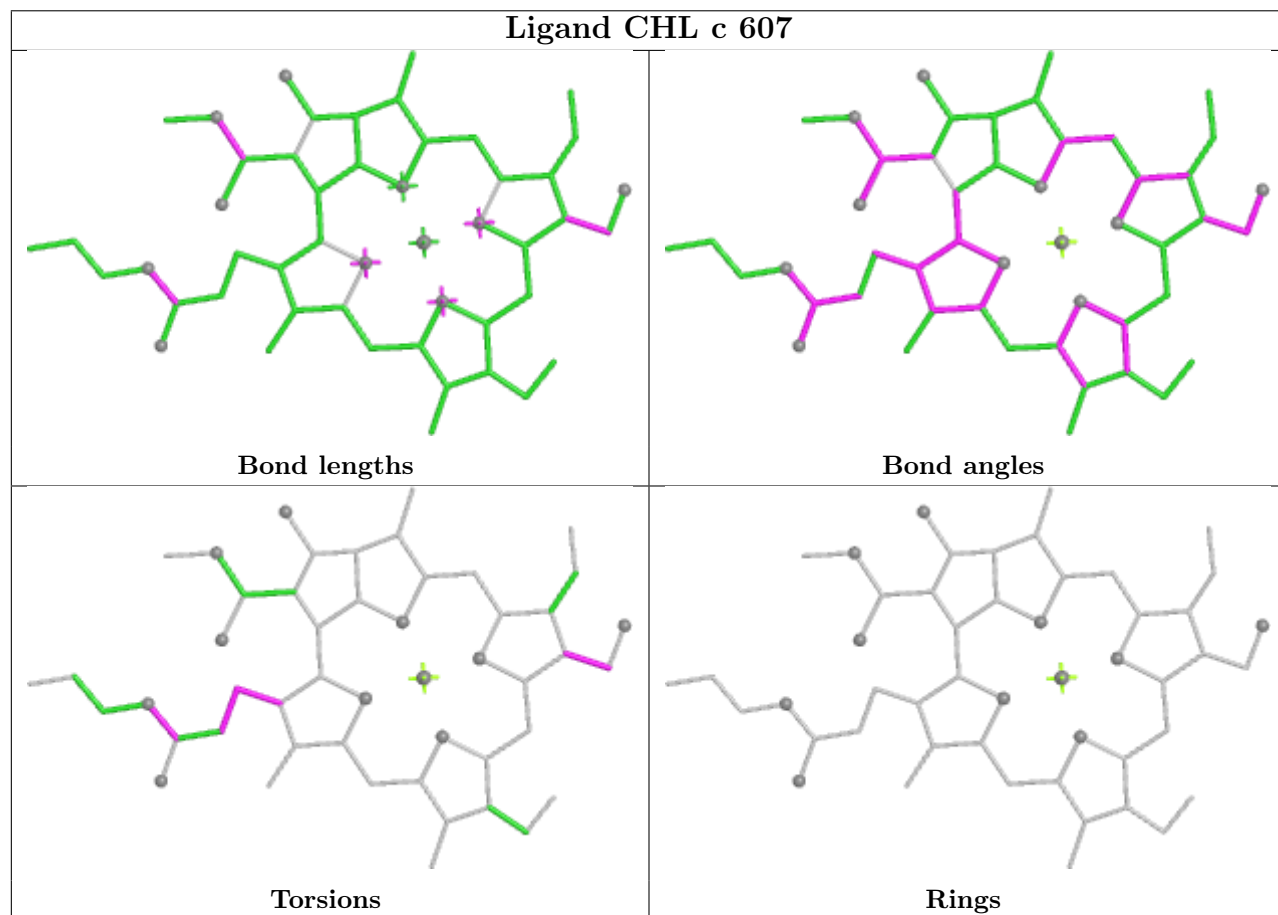
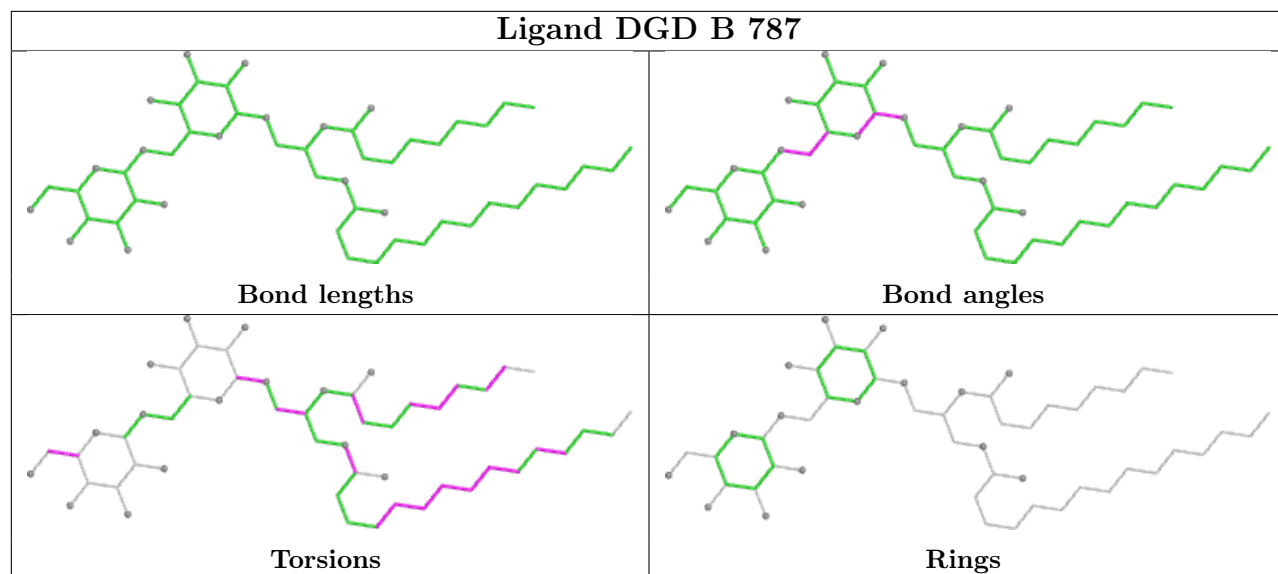


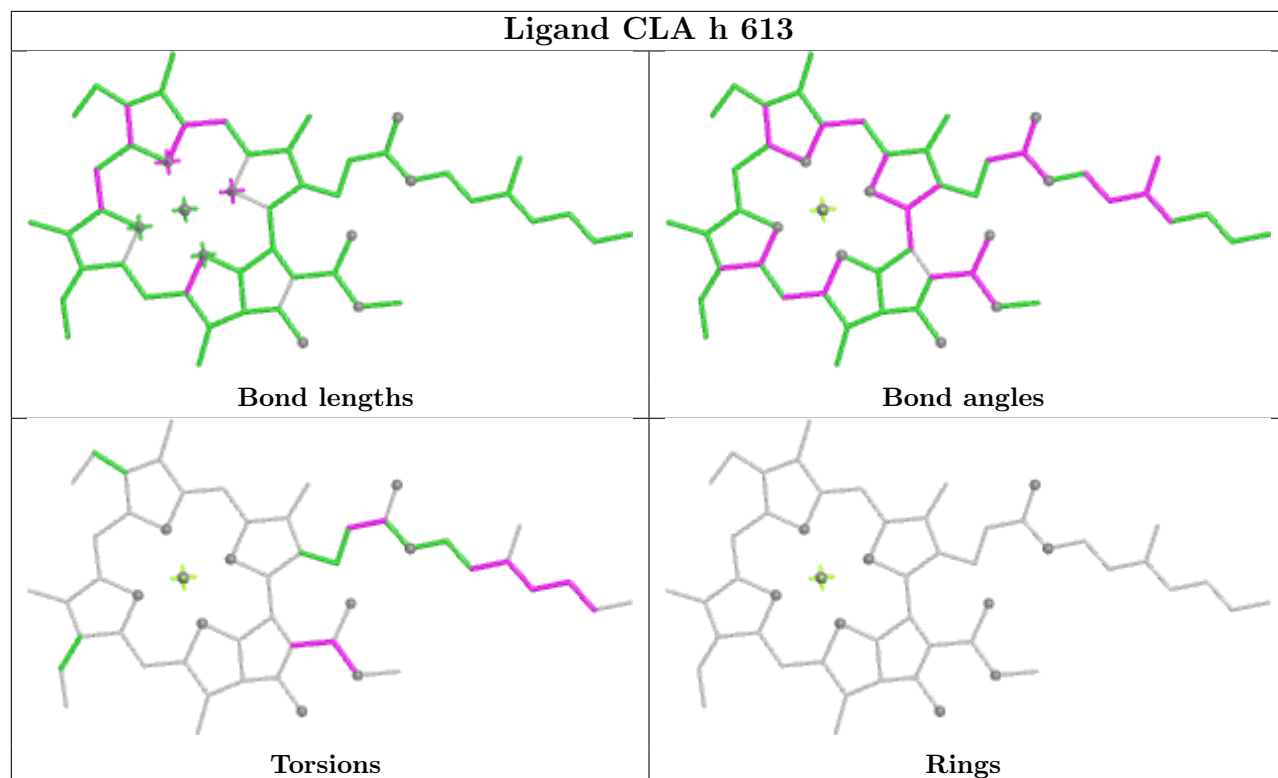
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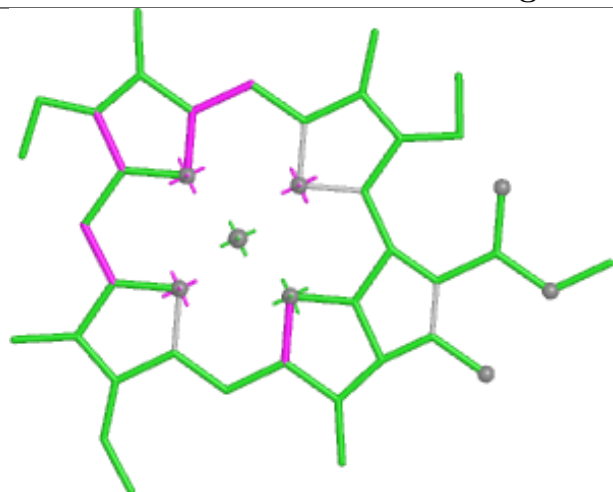
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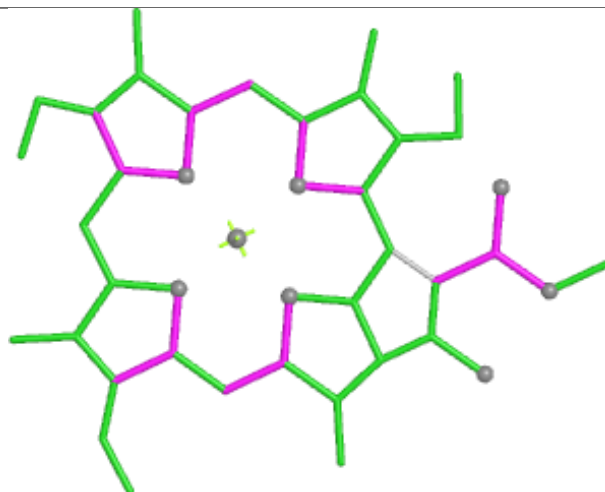




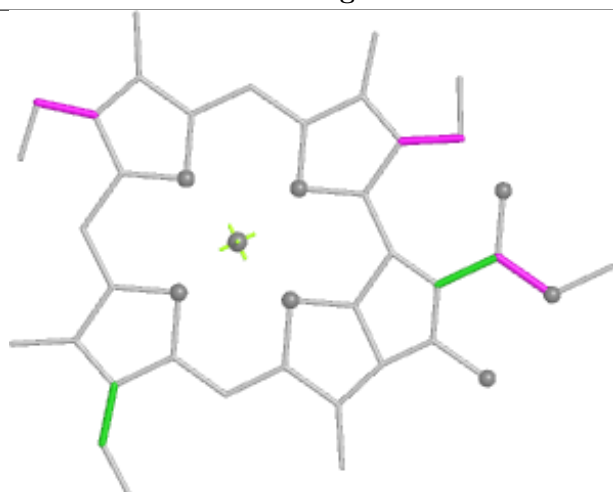
Ligand CLA c 614



Bond lengths



Bond angles

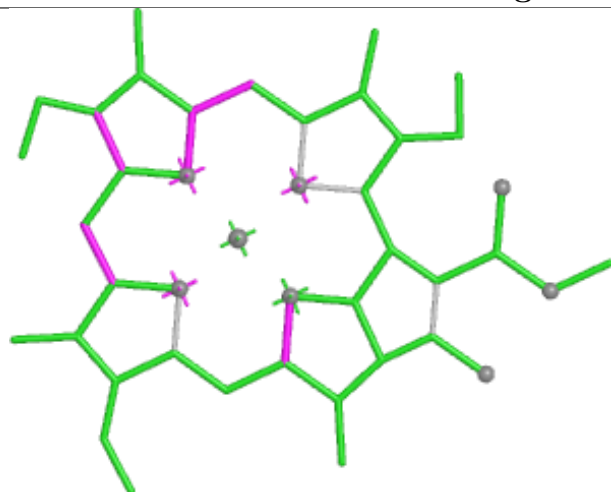


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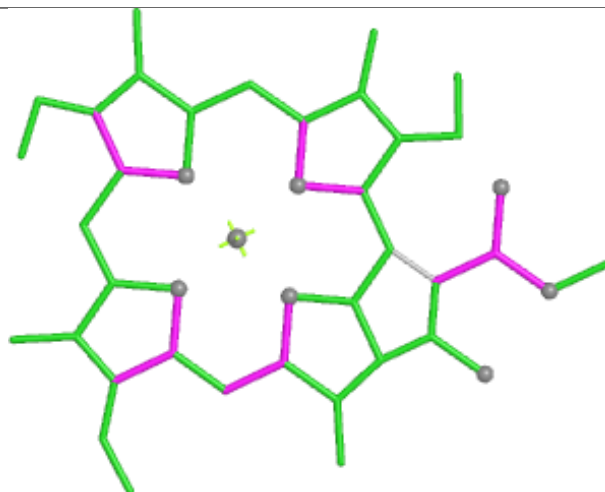


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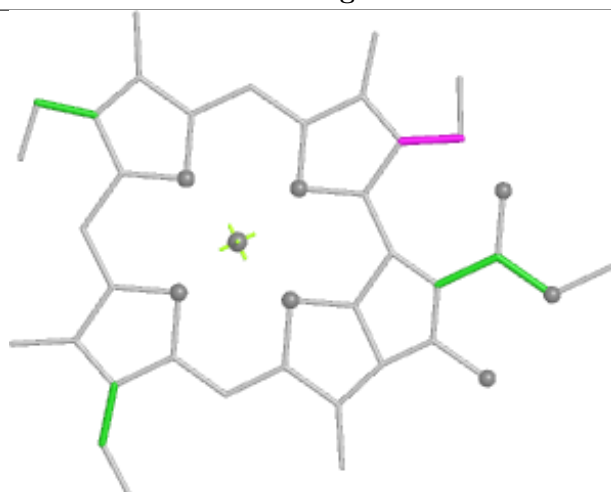
Ligand CLA B 740



Bond lengths



Bond angles

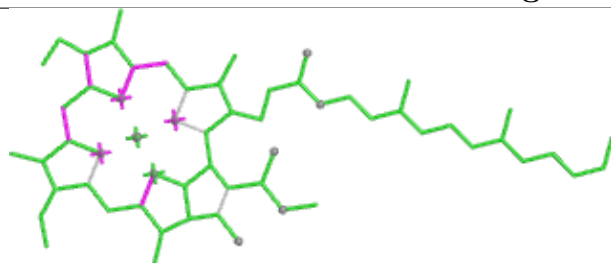


Torsions

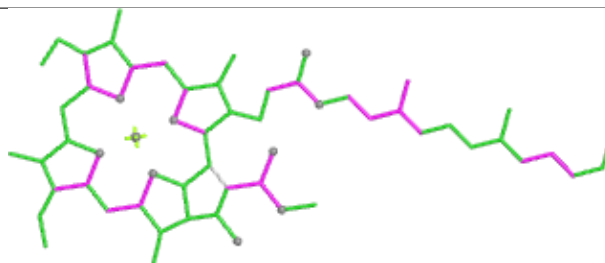


Rings

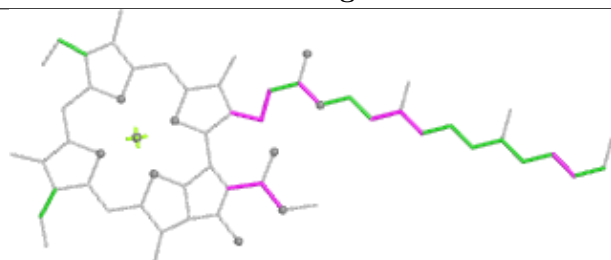
Ligand CLA 1 602



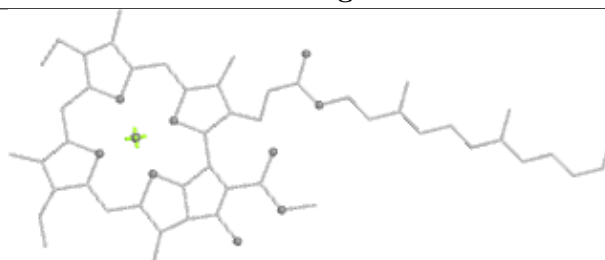
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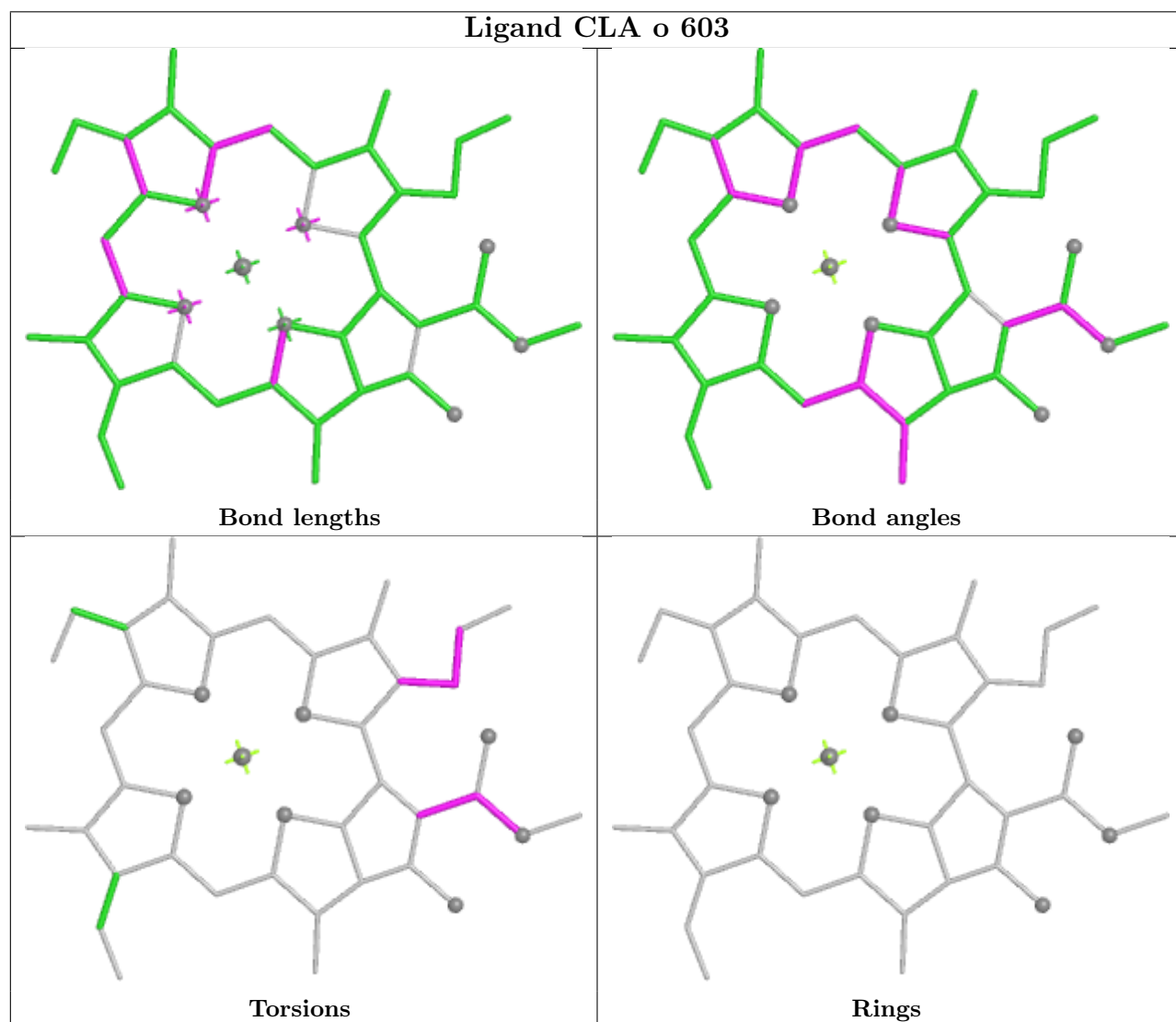
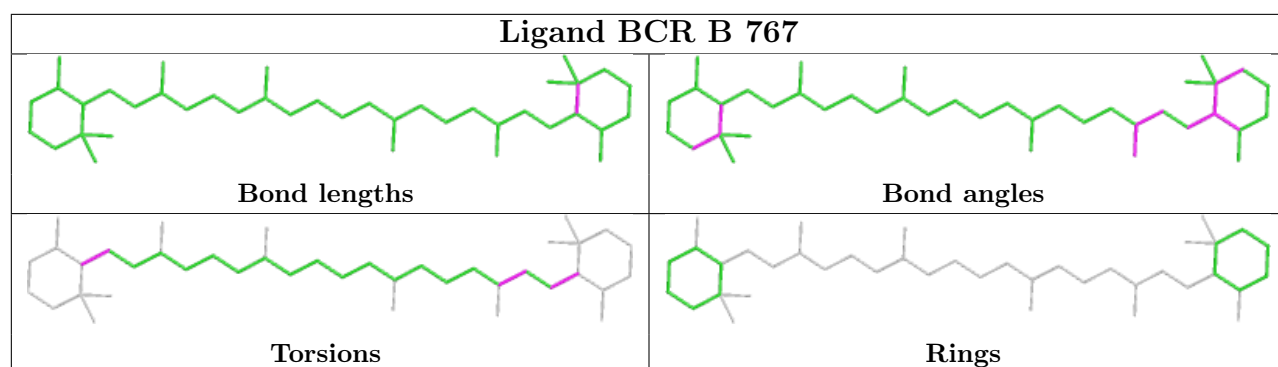
Bond angles



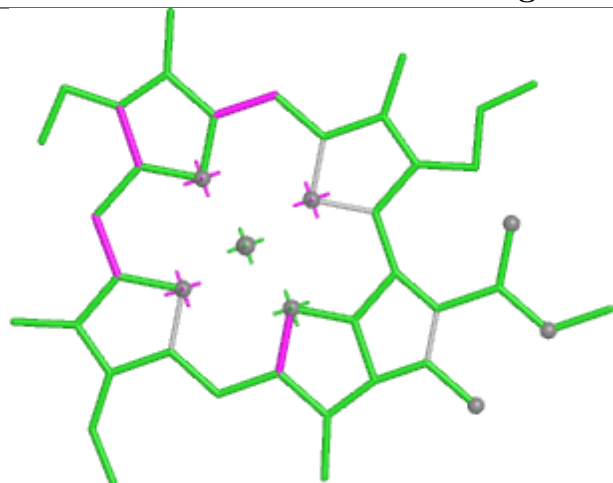
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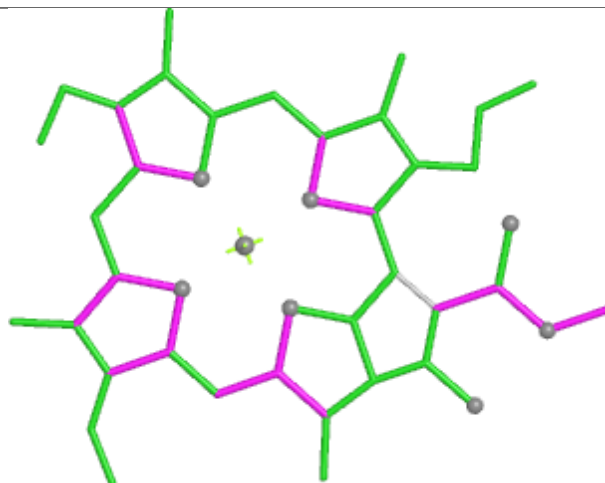
Rings



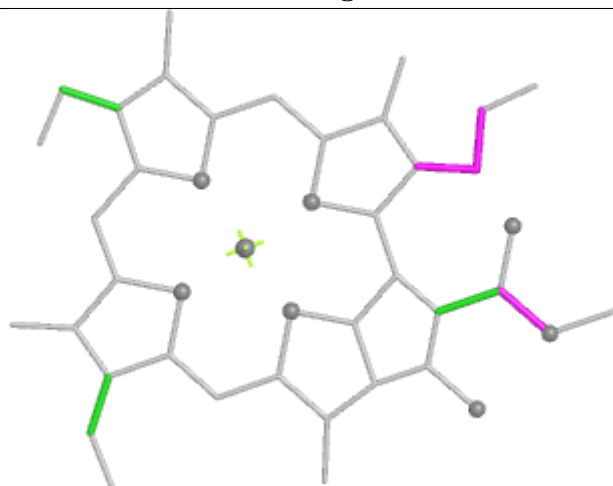
Ligand CLA o 614



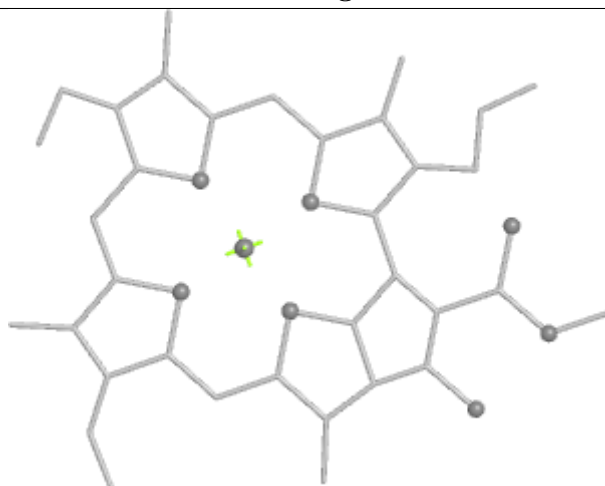
Bond lengths



Bond angles

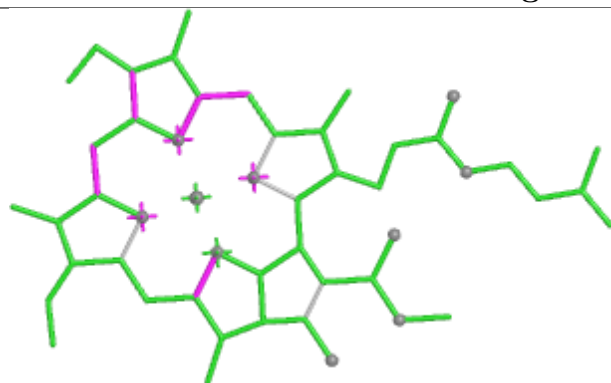


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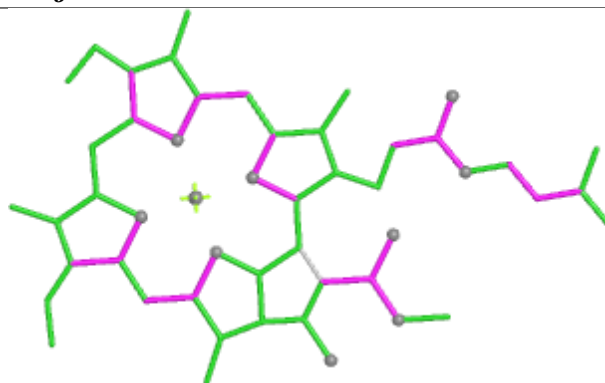


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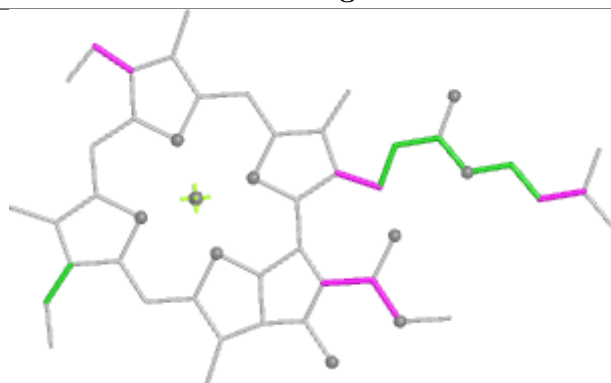
Ligand CLA j 601



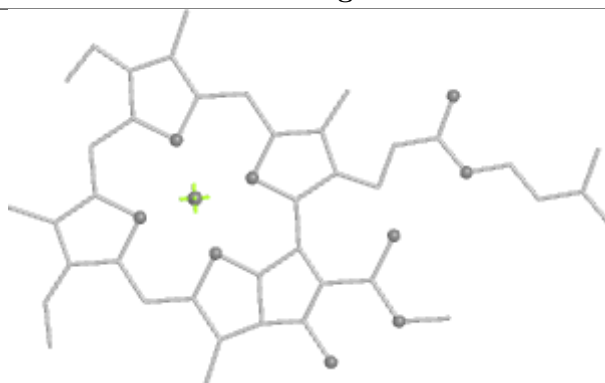
Bond lengths



Bond angles

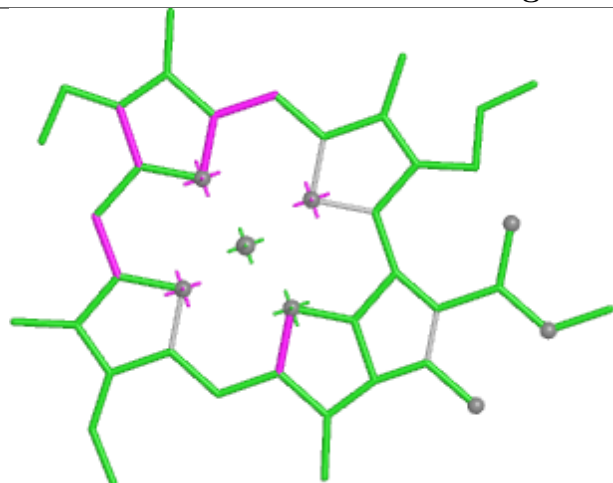


Torsions

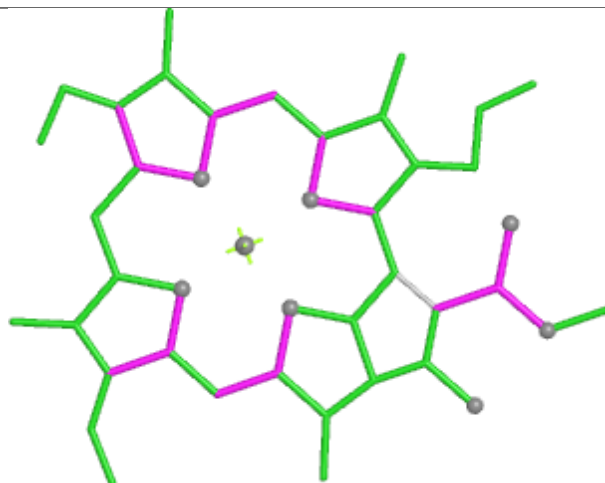


Rings

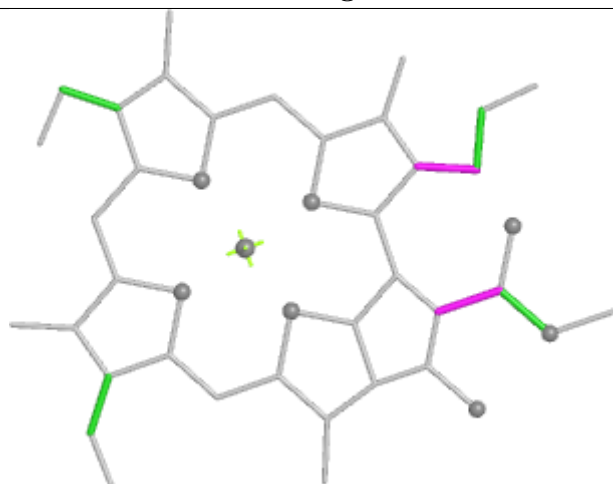
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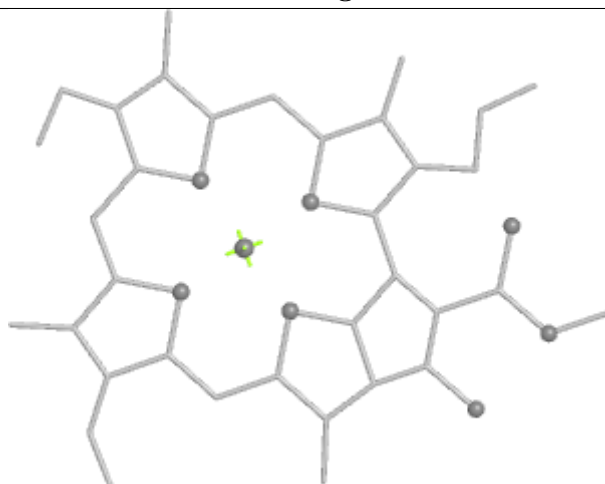
Bond lengths



Bond angles

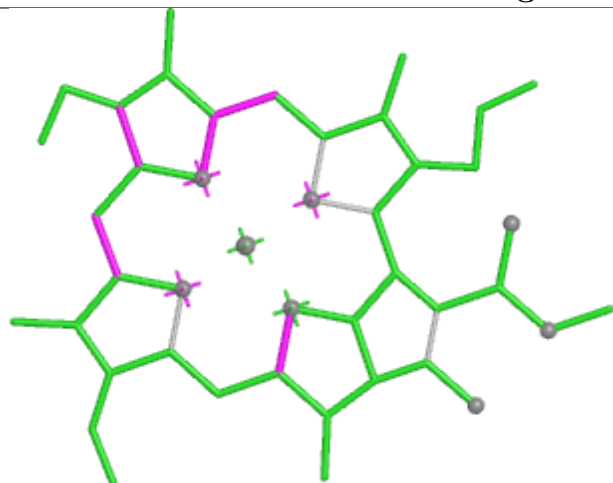


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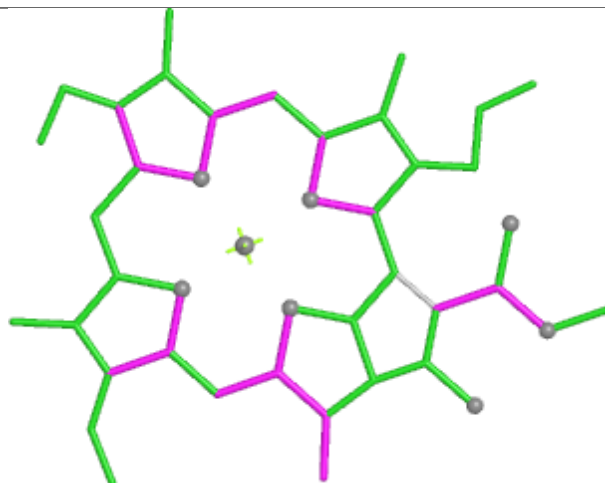


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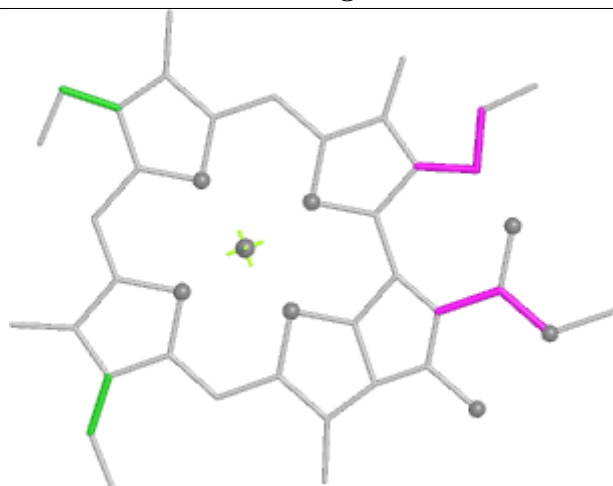
Ligand CLA b 603



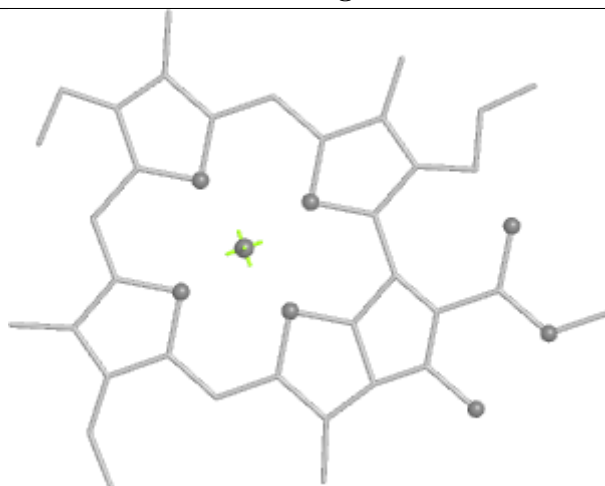
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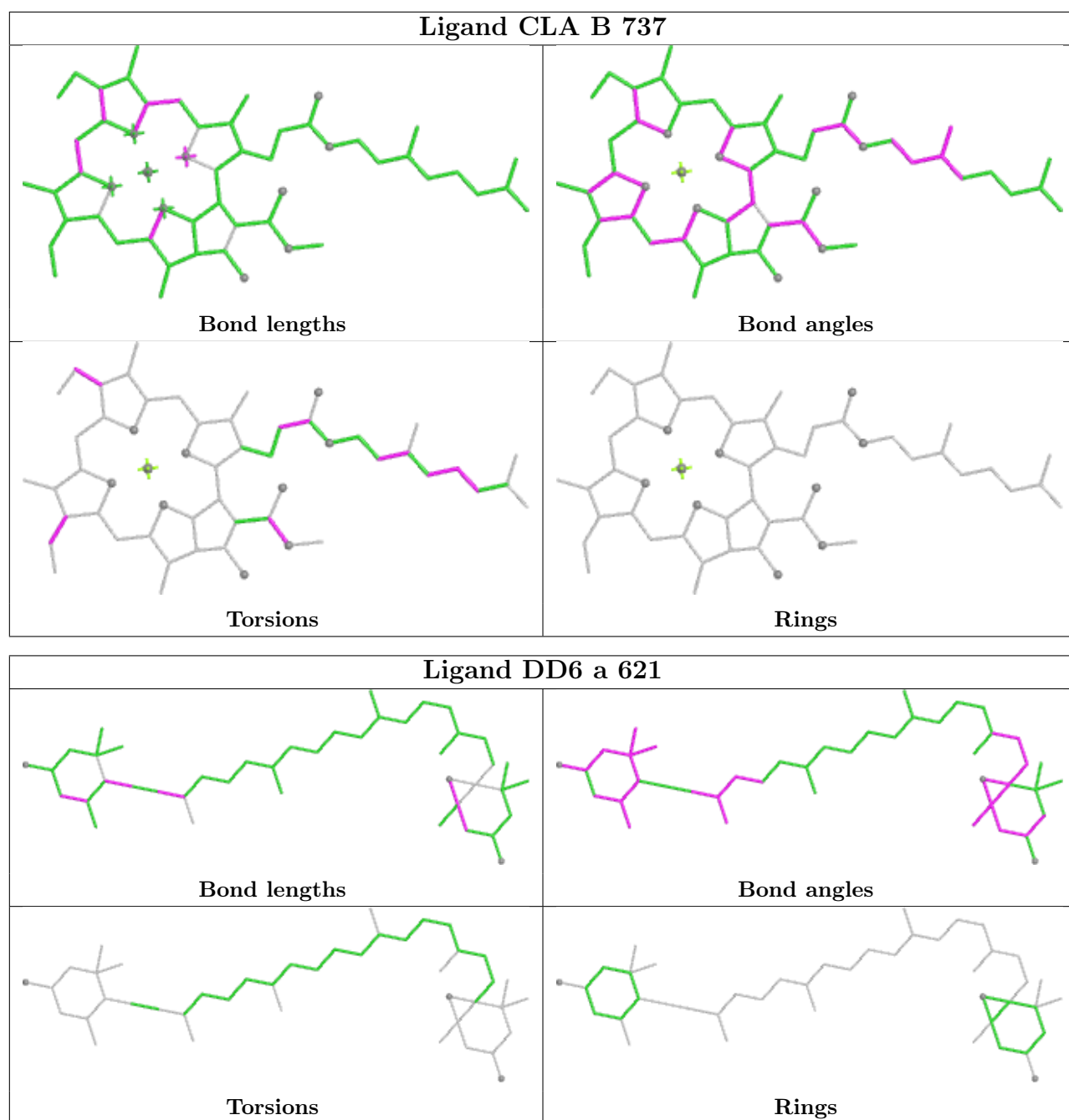
Bond angles



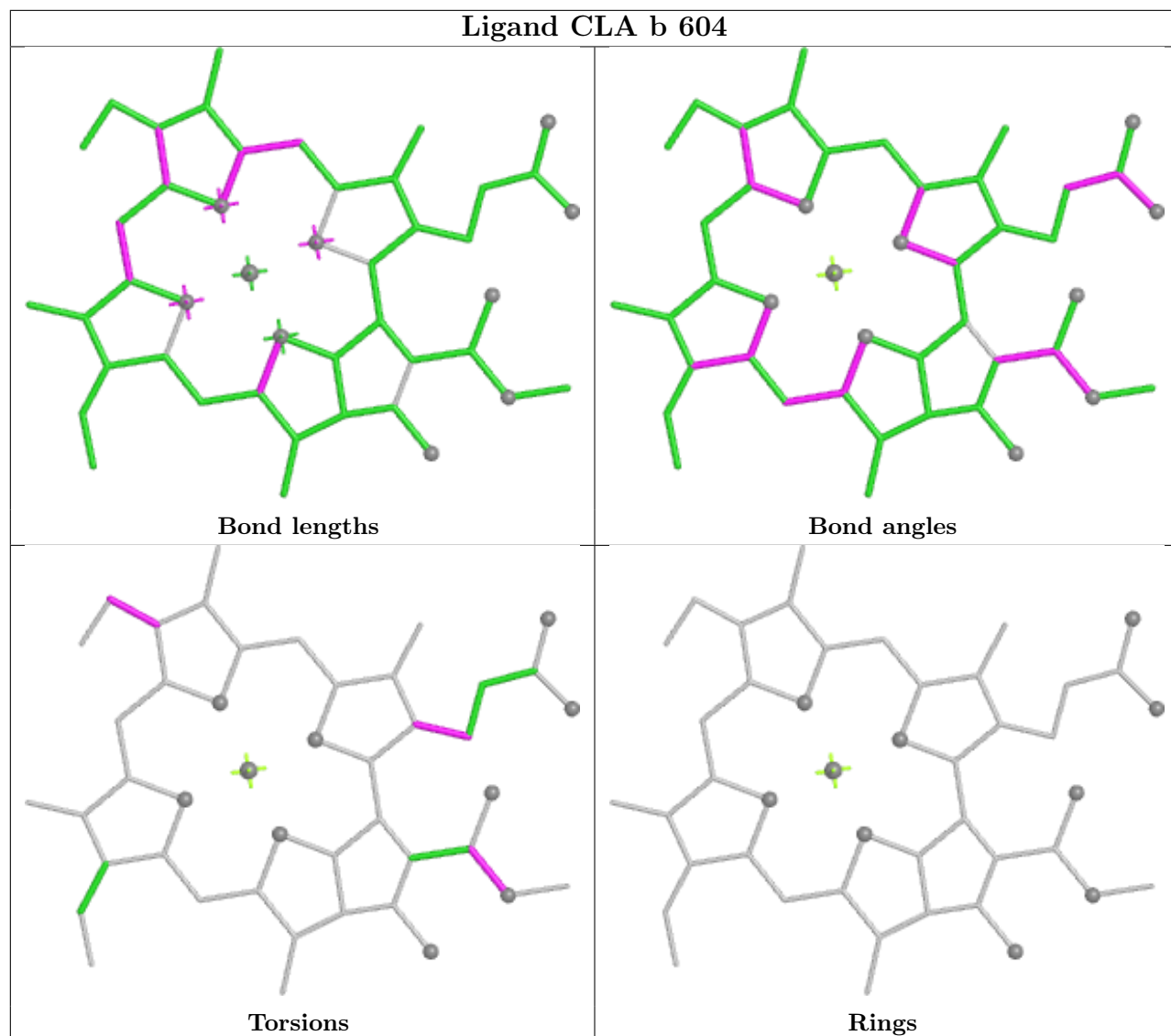
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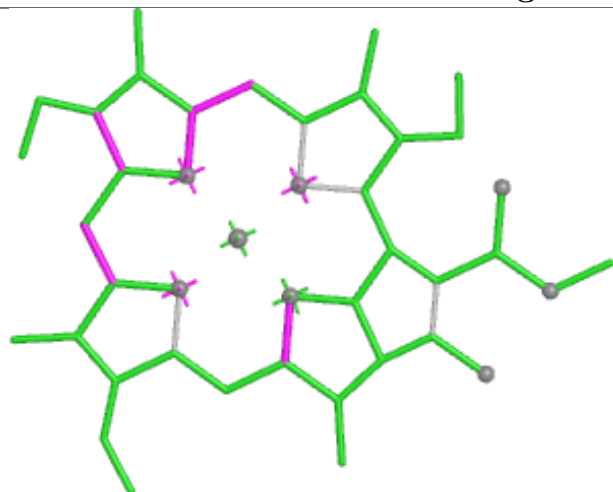
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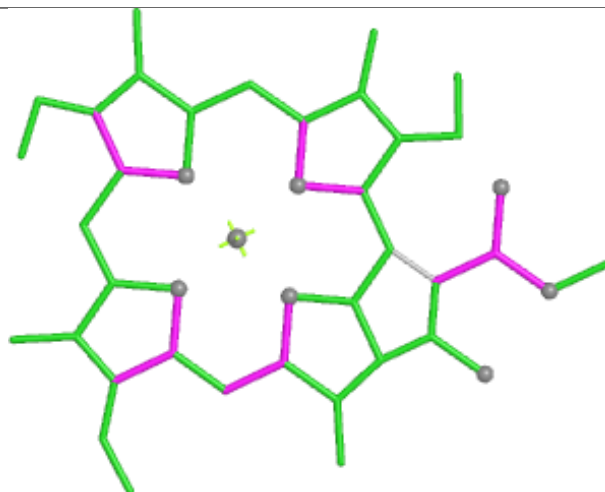
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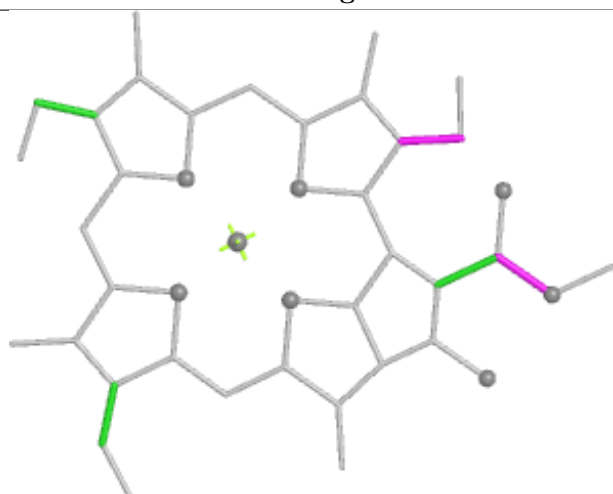
Ligand CLA n 613



Bond lengths



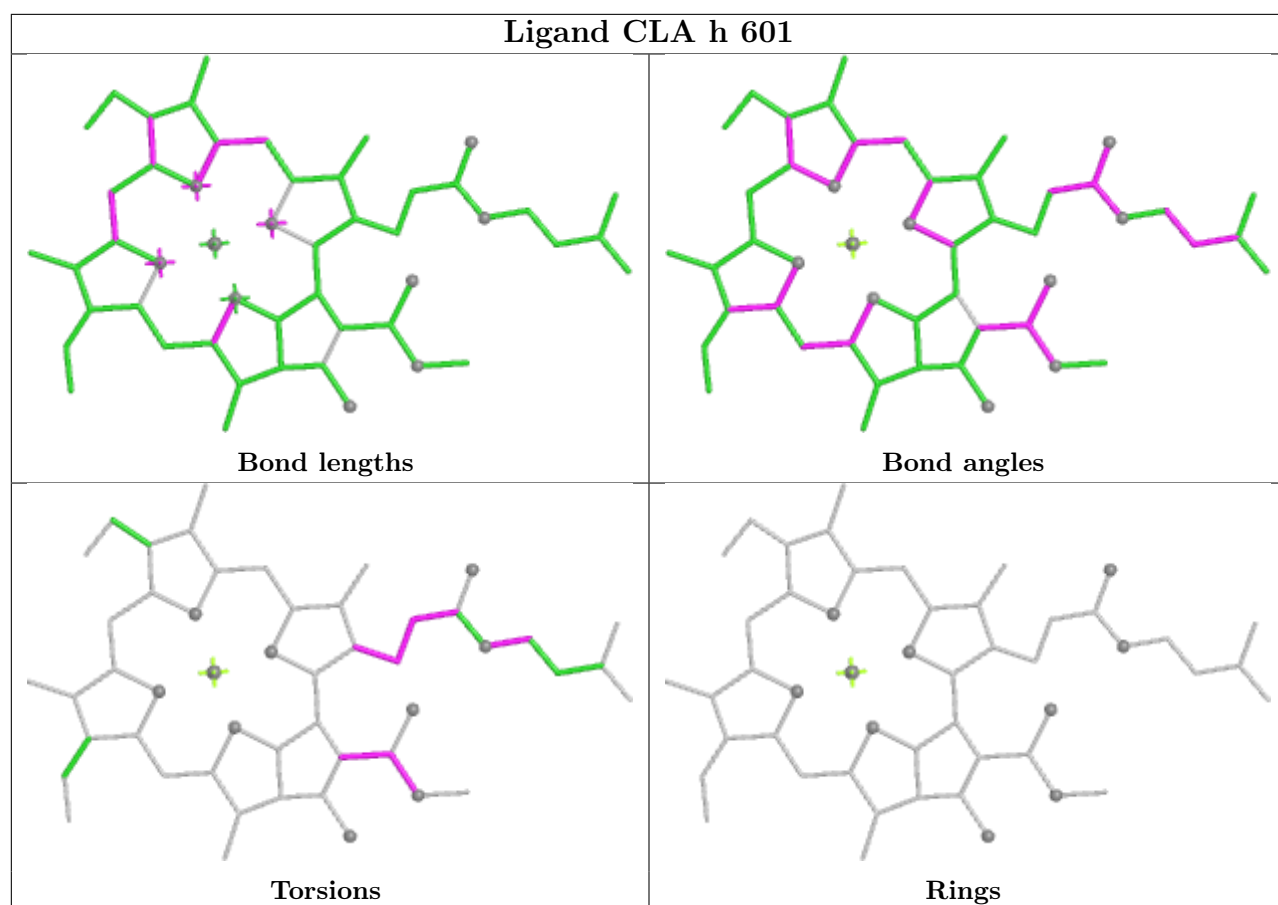
Bond angles



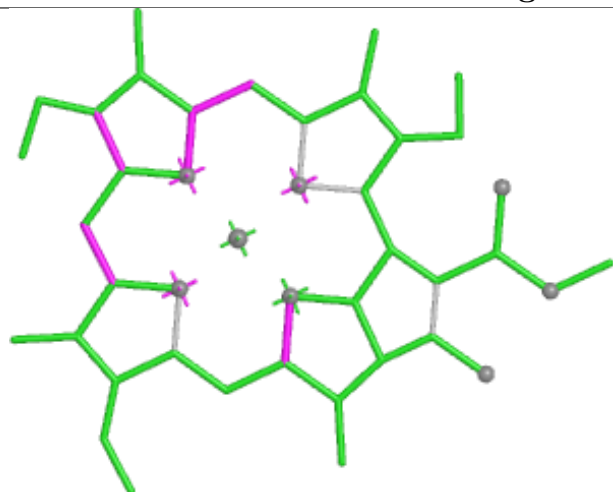
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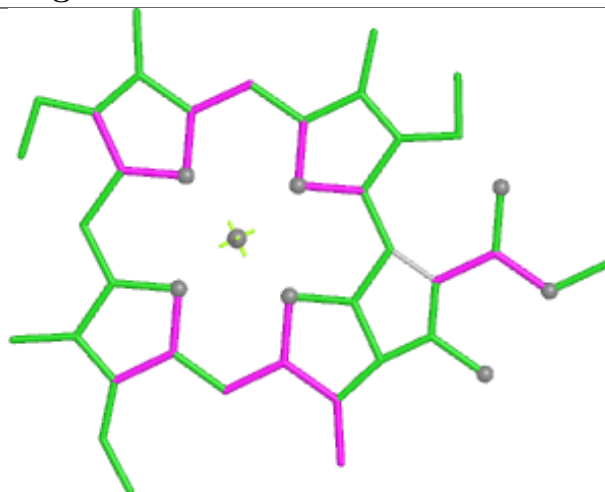
Rings



Ligand CLA g 615



Bond lengths



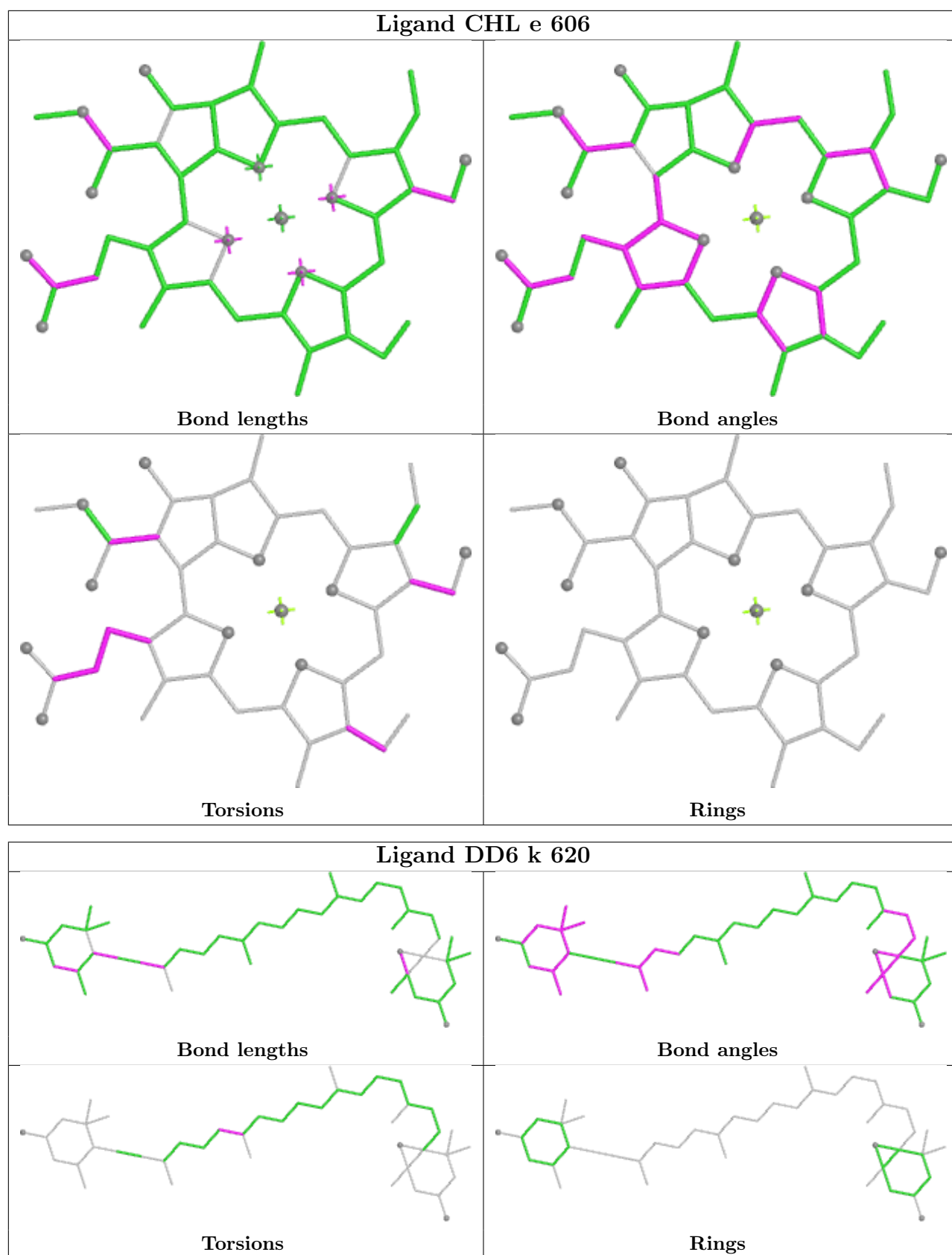
Bond angles



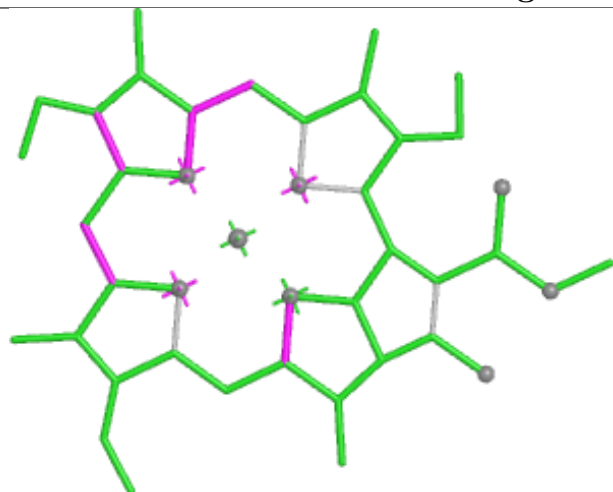
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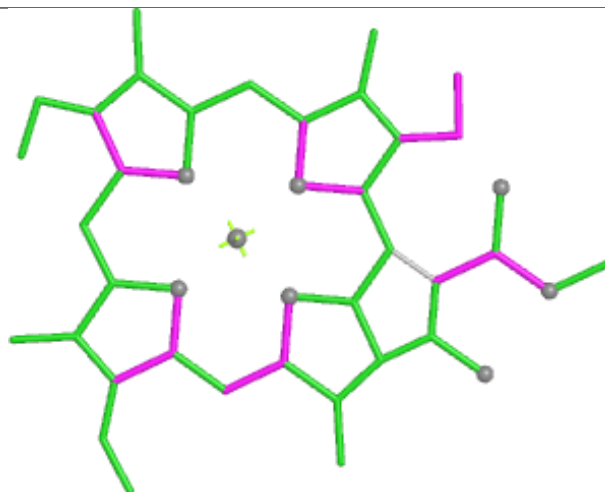
Rings



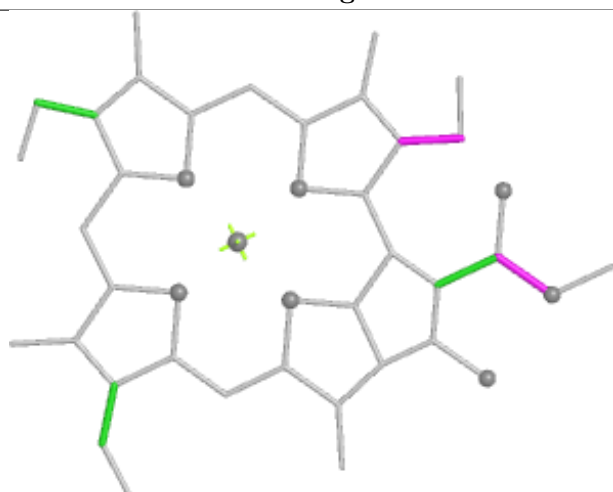
Ligand CLA d 613



Bond lengths



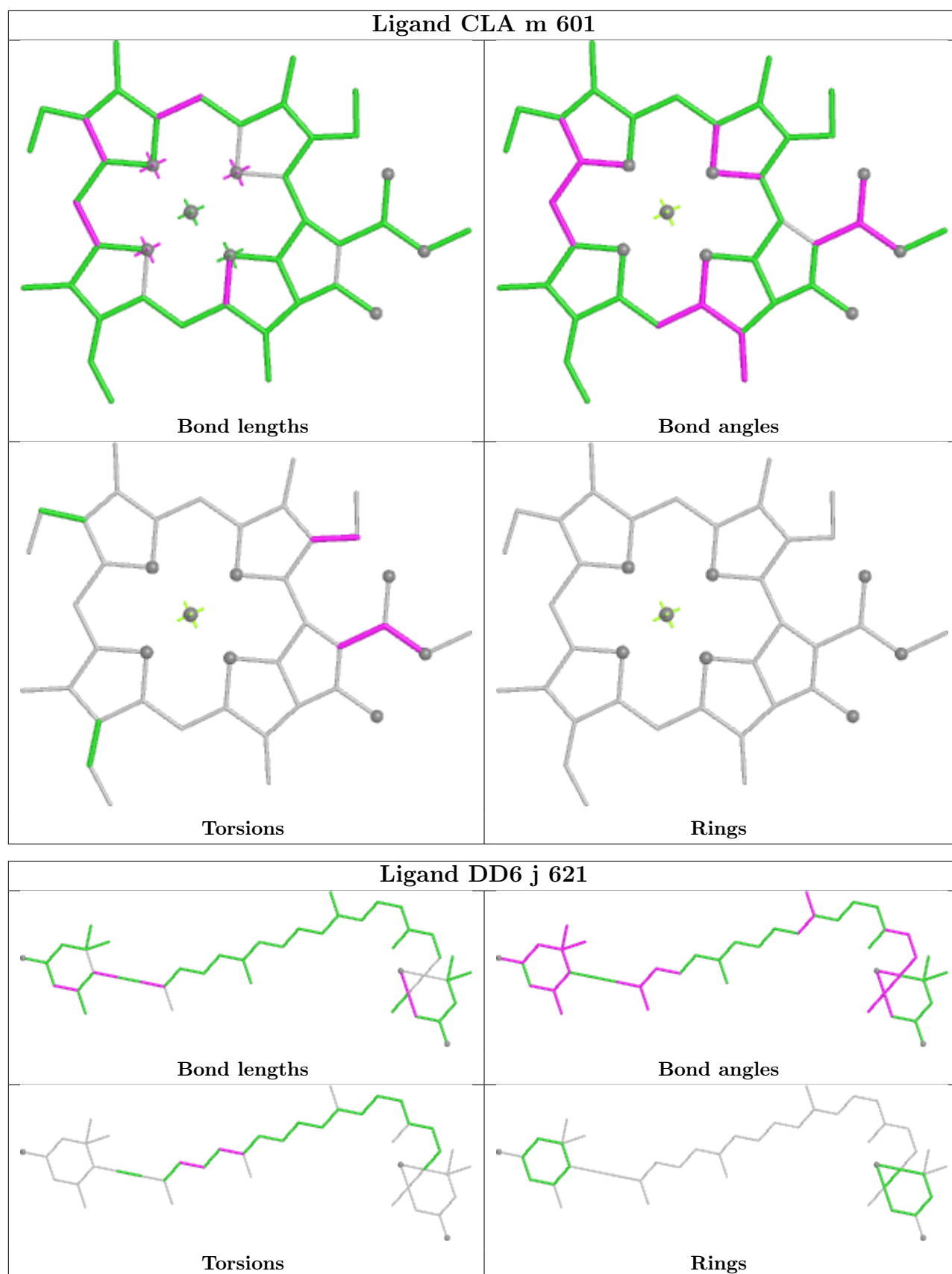
Bond angles

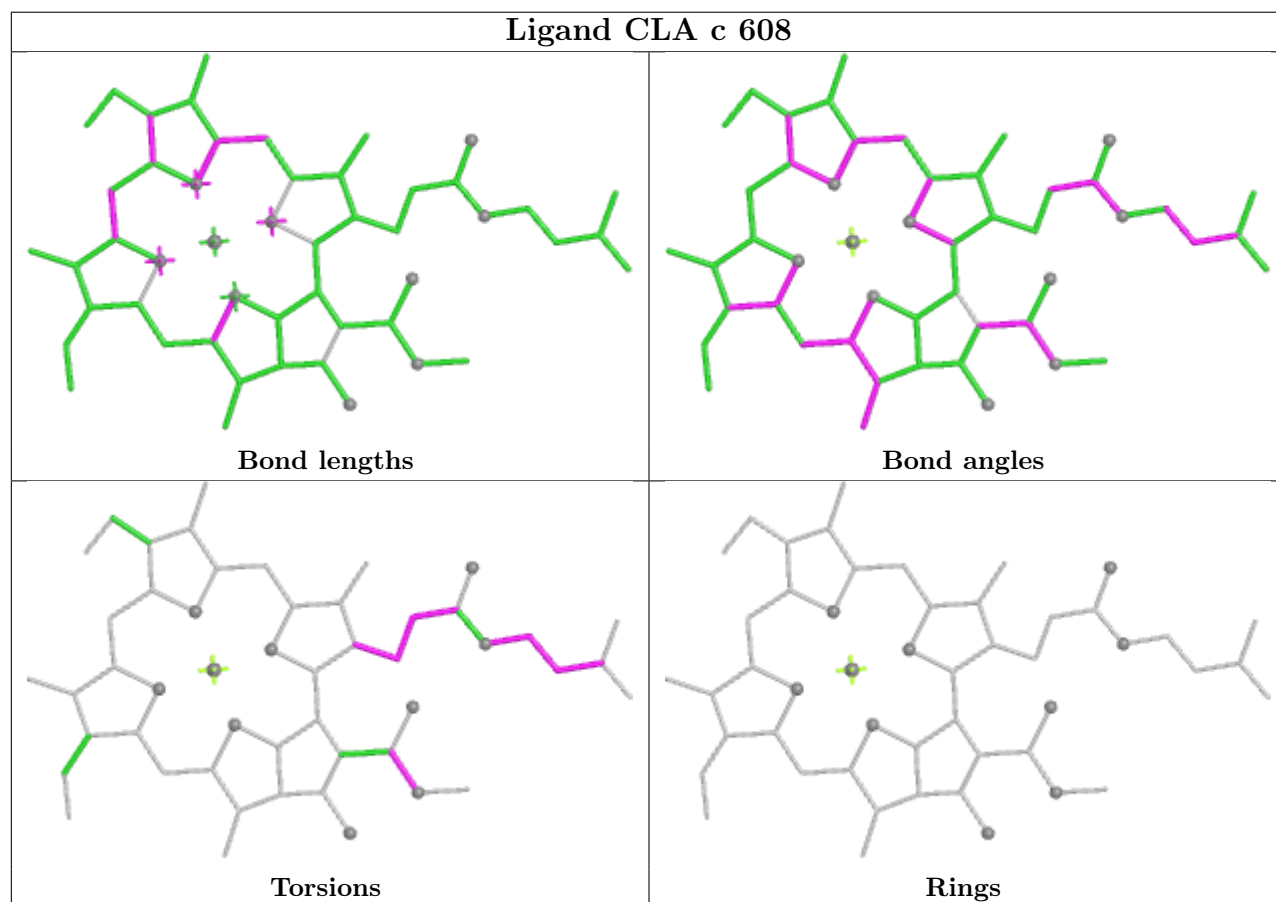
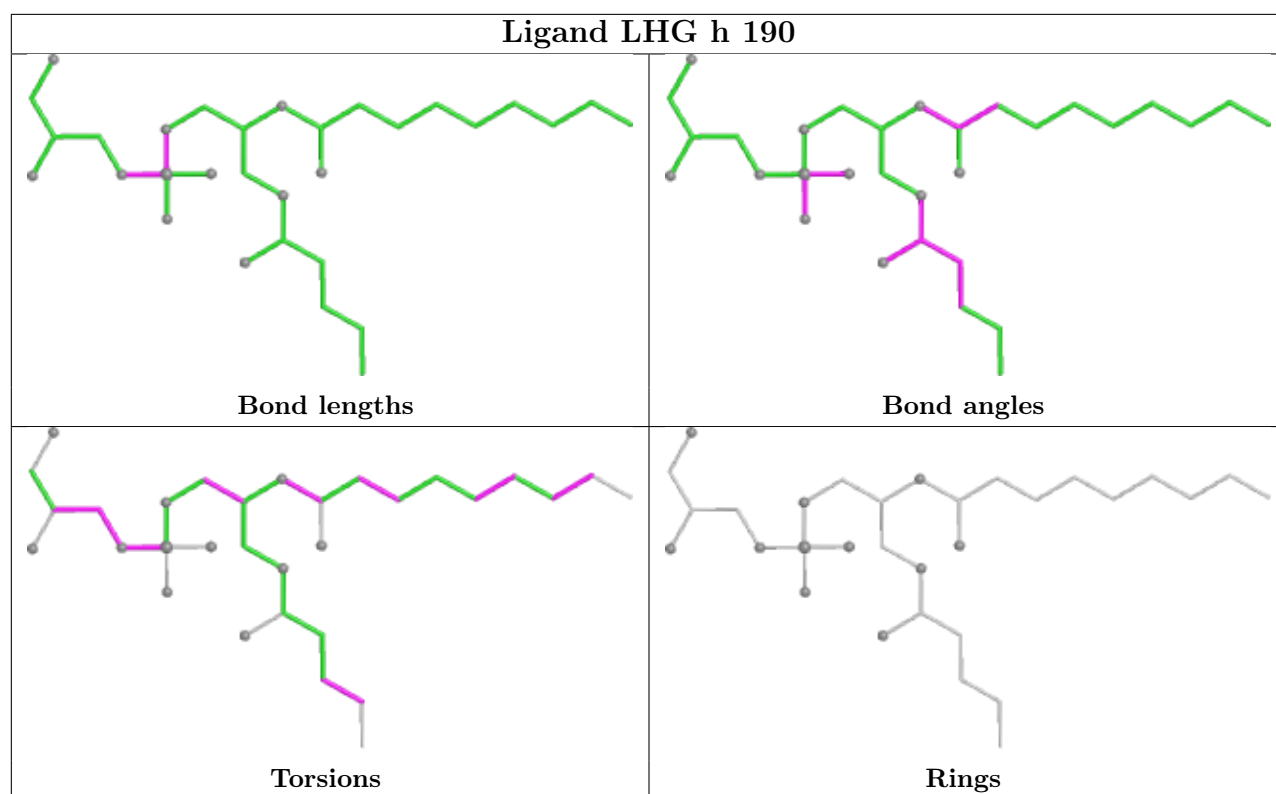


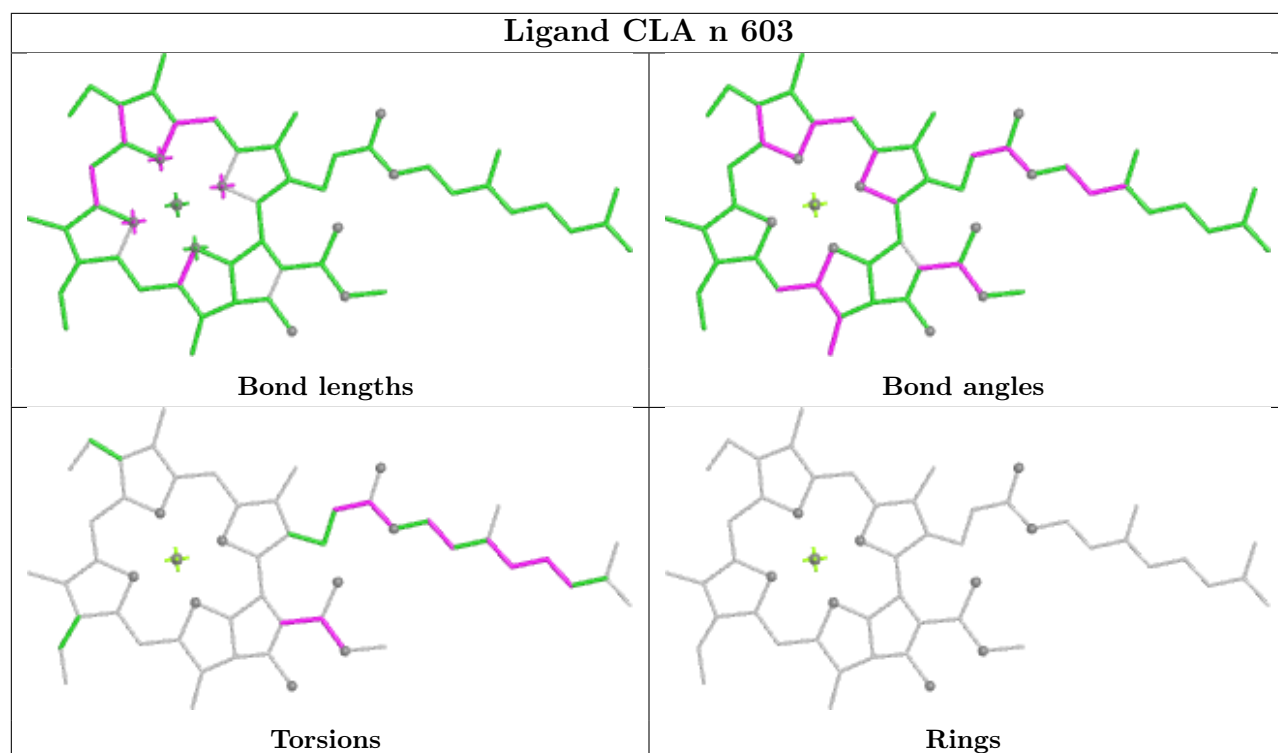
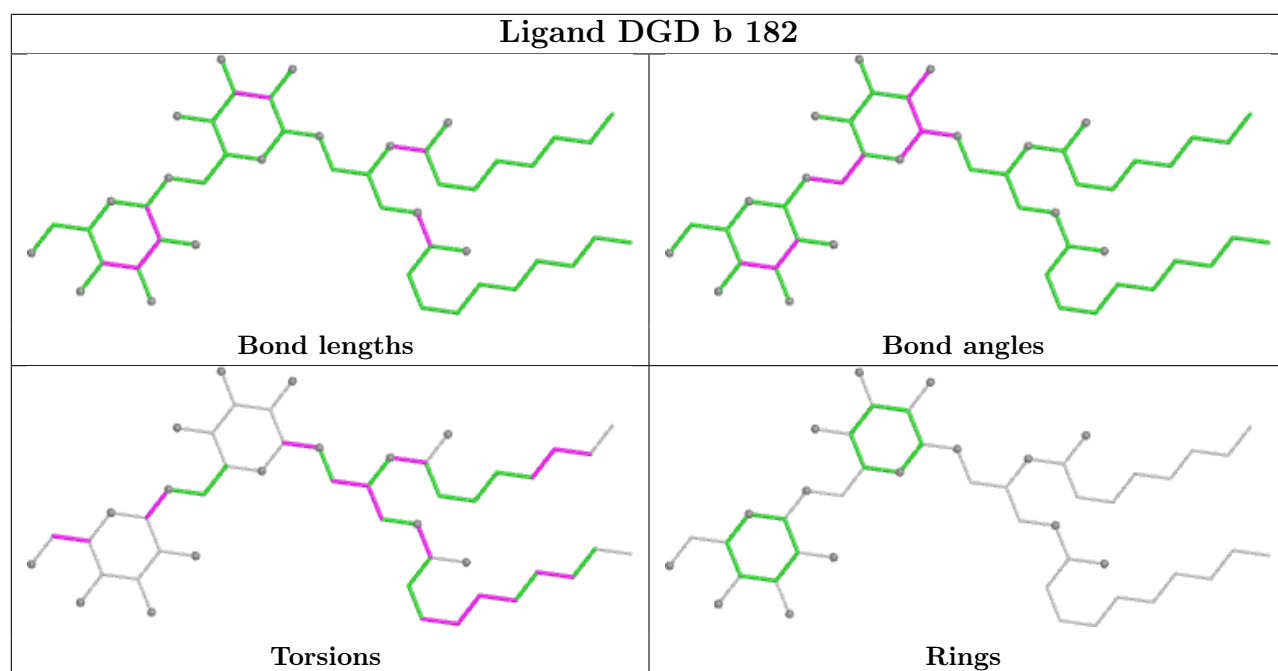
Torsions

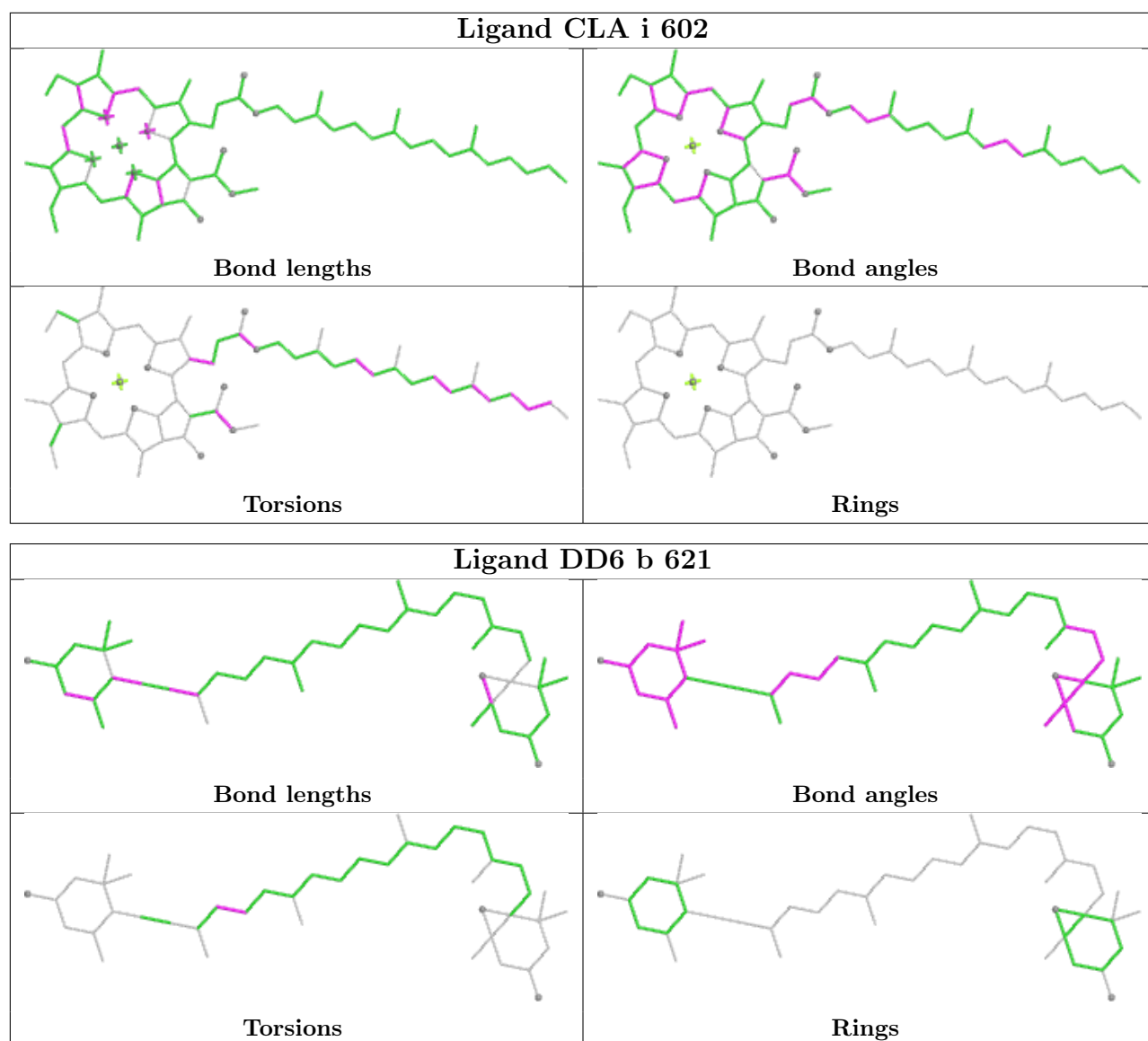


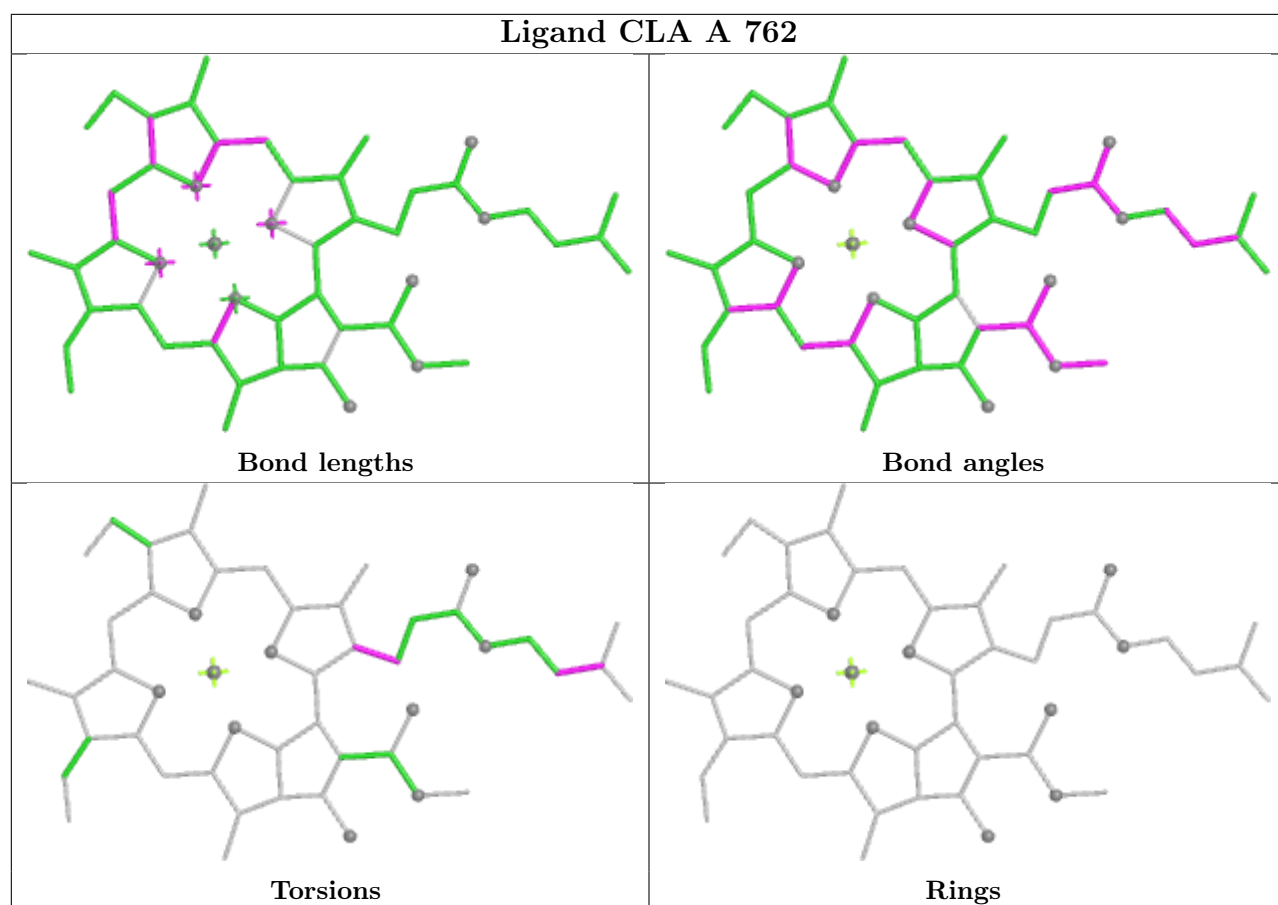
Rings



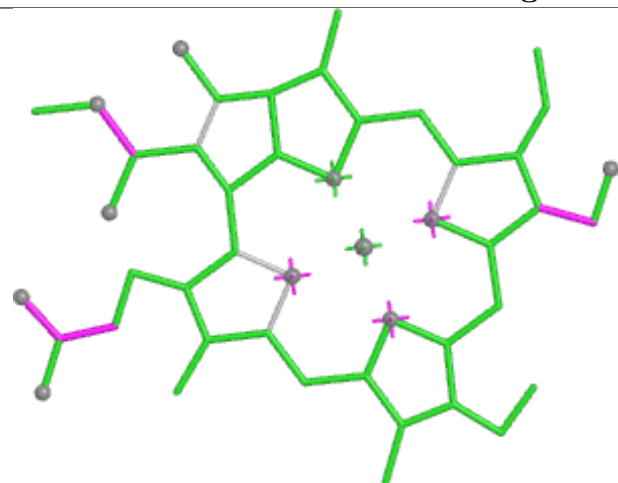




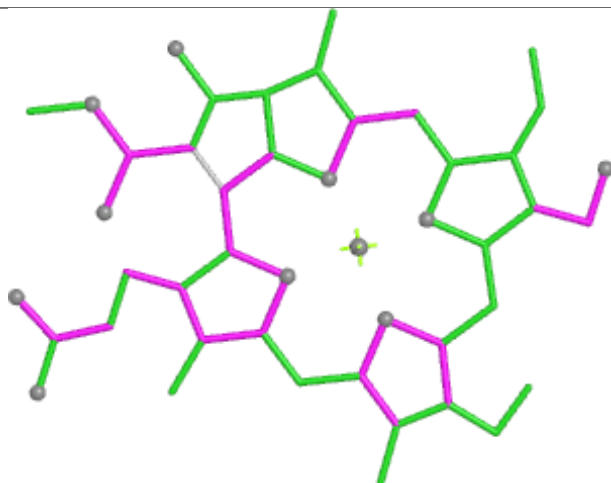




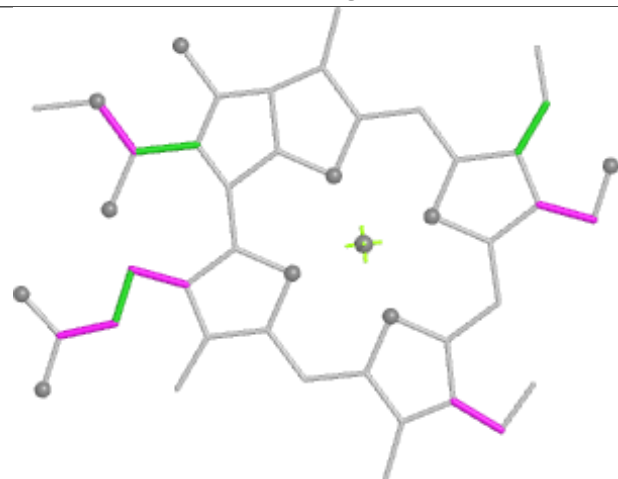
Ligand CHL d 606



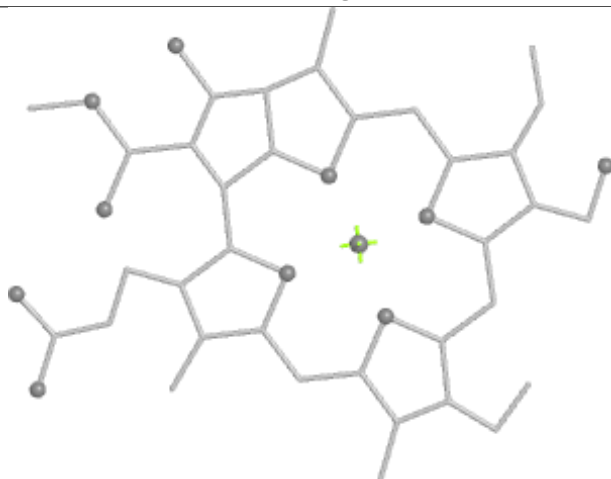
Bond lengths



Bond angles

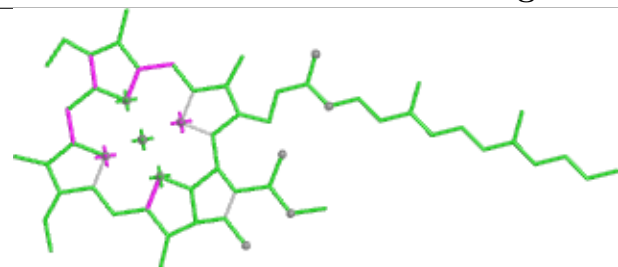


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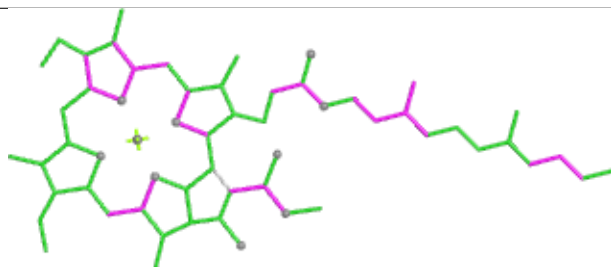


Rings

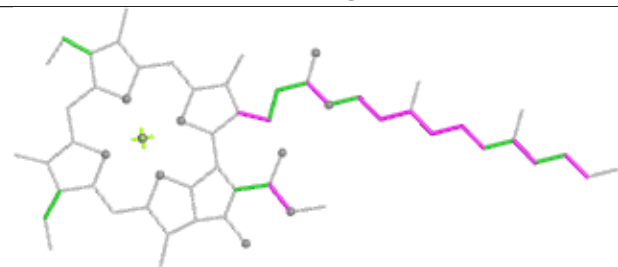
Ligand CLA A 780



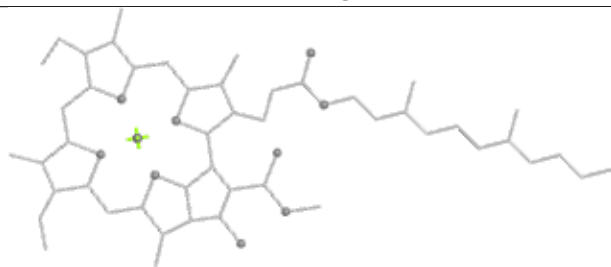
Bond lengths



Bond angles

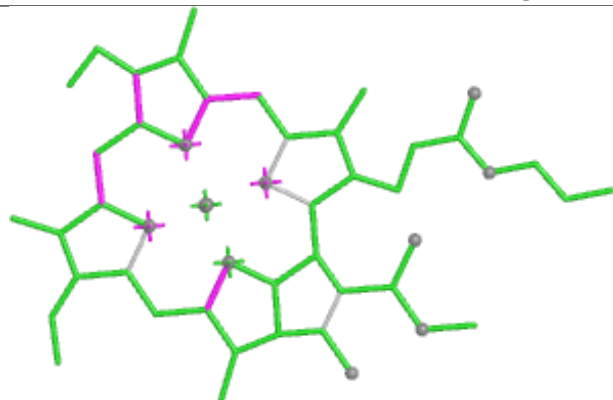


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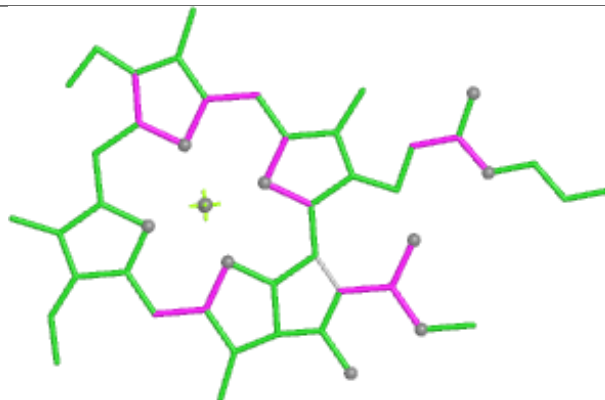


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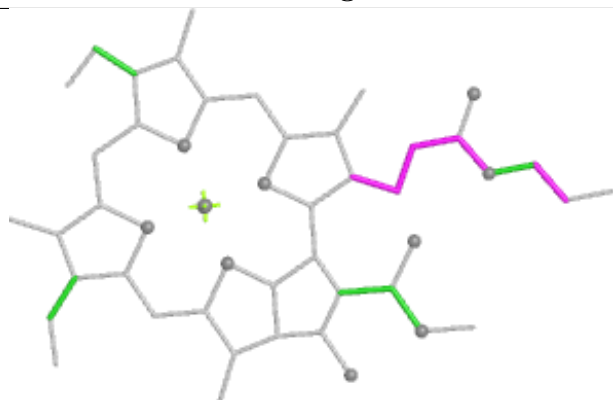
Ligand CLA h 608



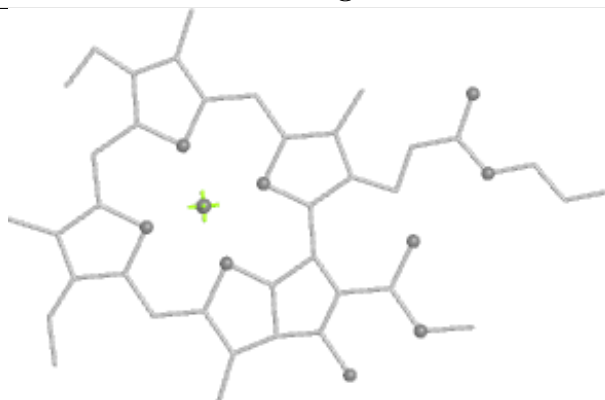
Bond lengths



Bond angles

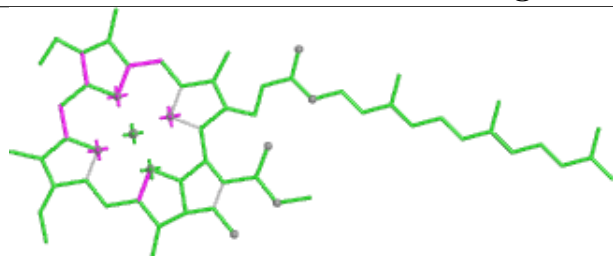


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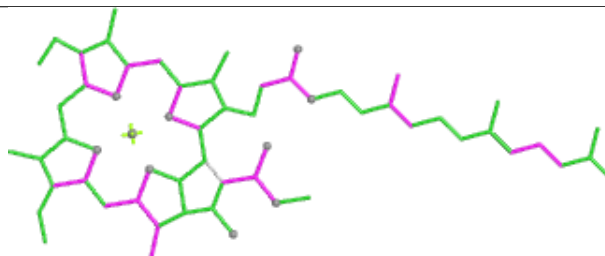


Rings

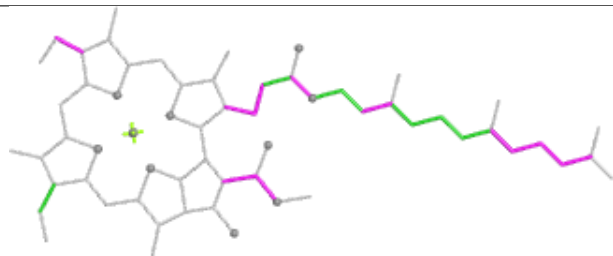
Ligand CLA A 799



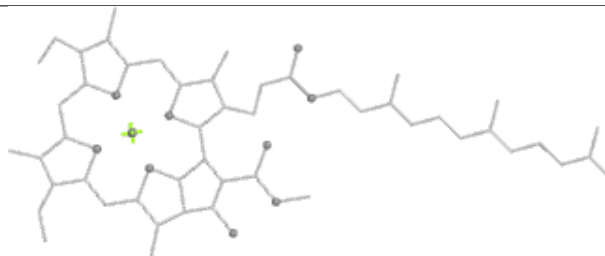
Bond lengths



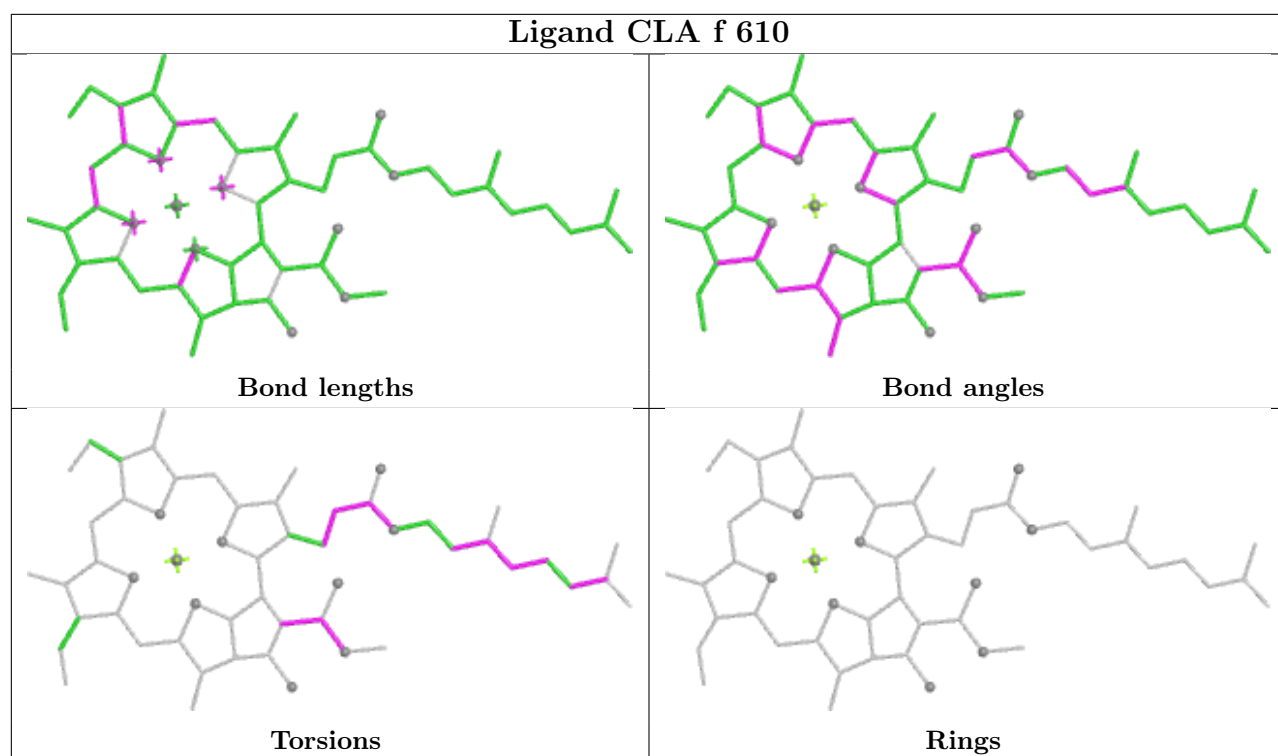
Bond angles

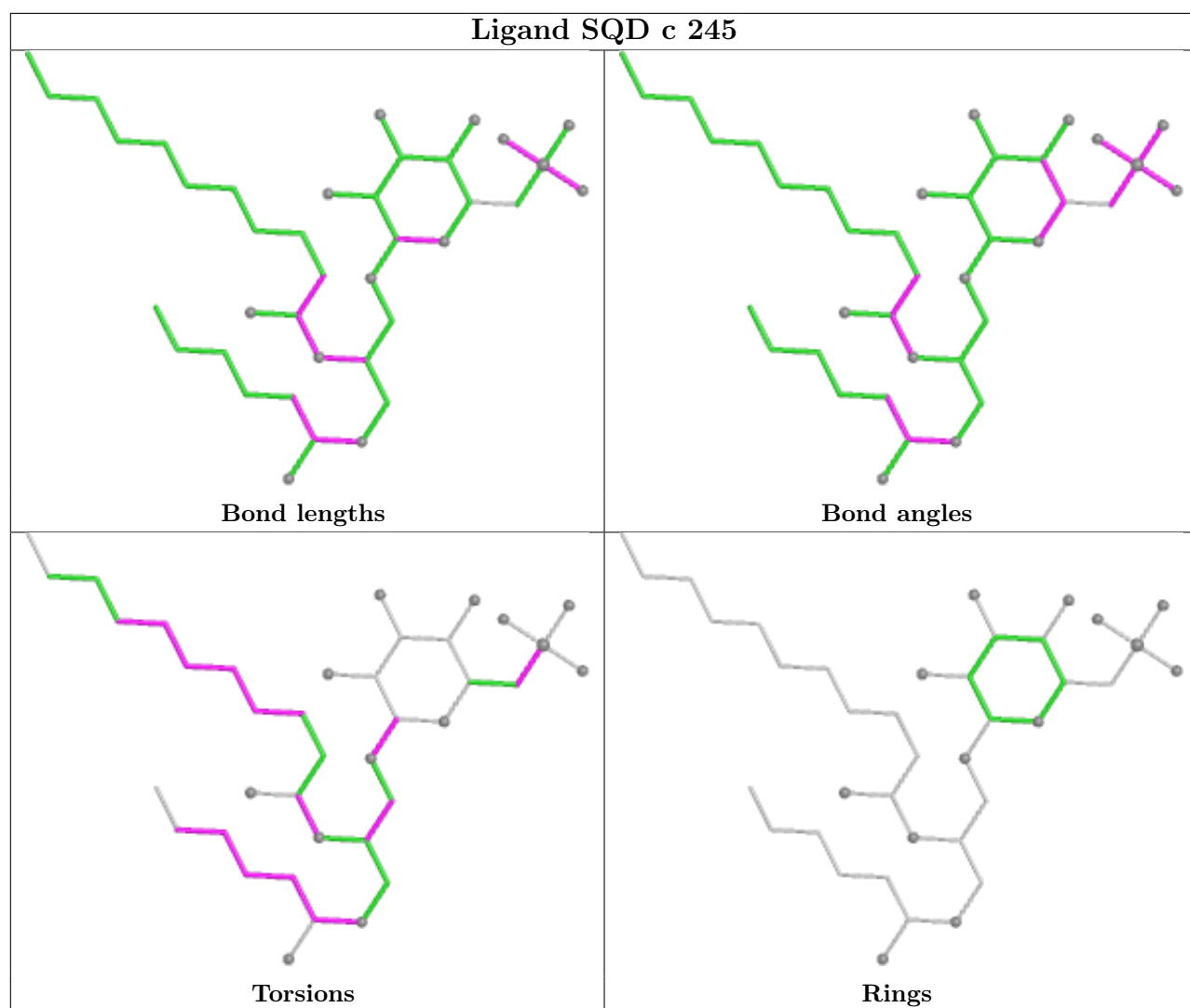


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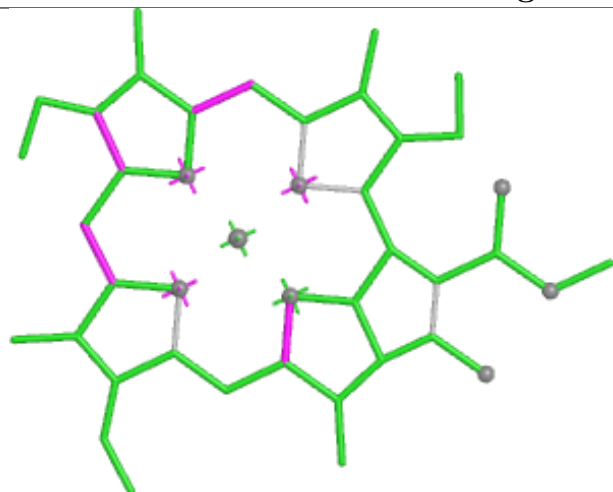


Rings

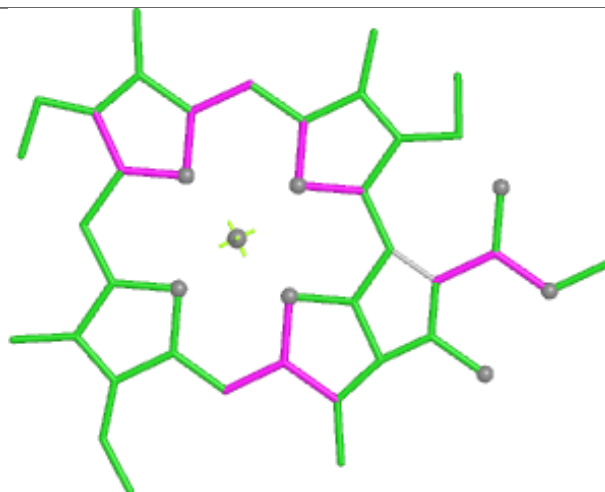




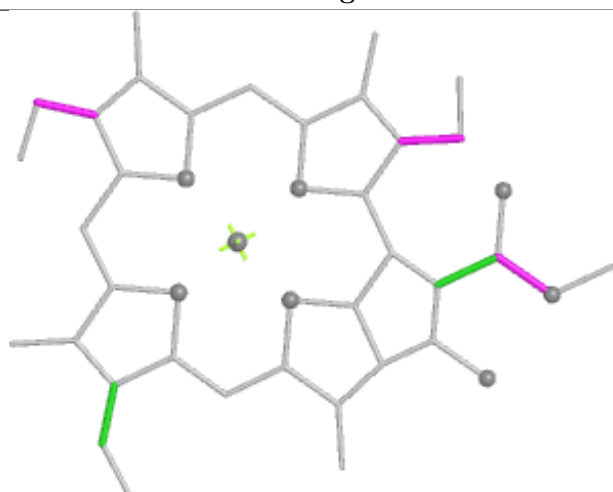
Ligand CLA n 606



Bond lengths



Bond angles

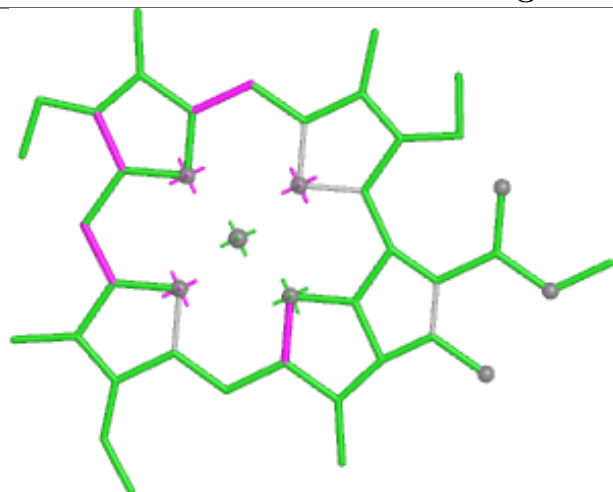


Torsions

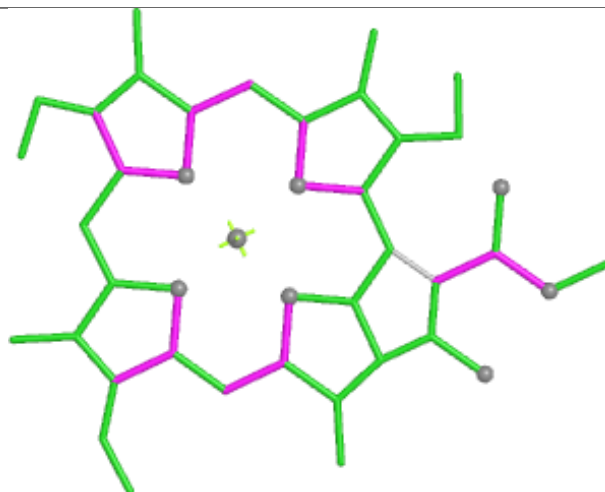


Rings

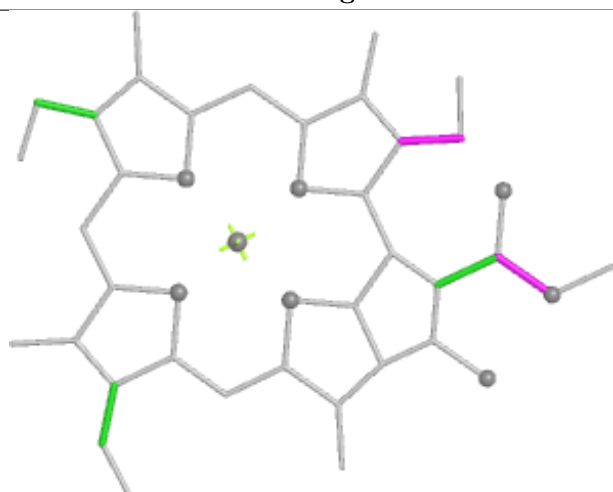
Ligand CLA n 607



Bond lengths



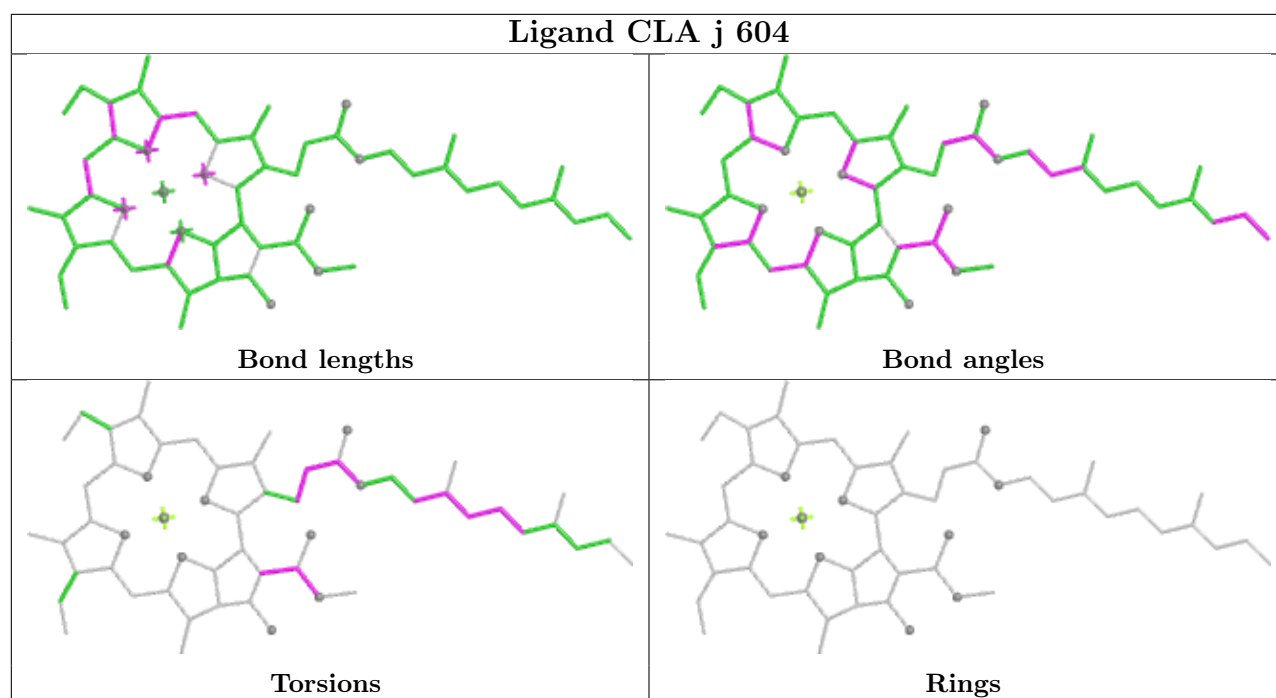
Bond angles



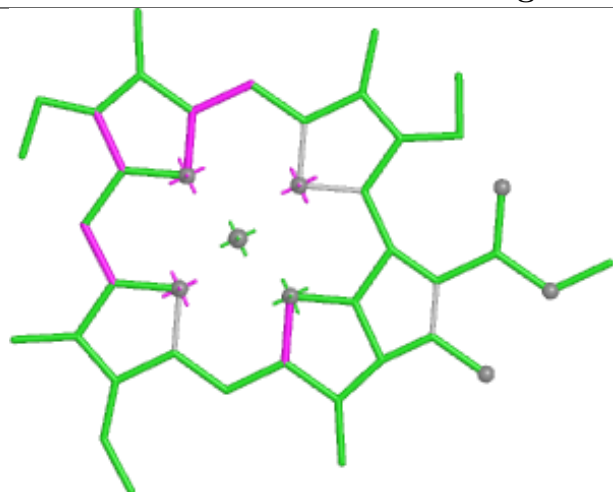
Torsions



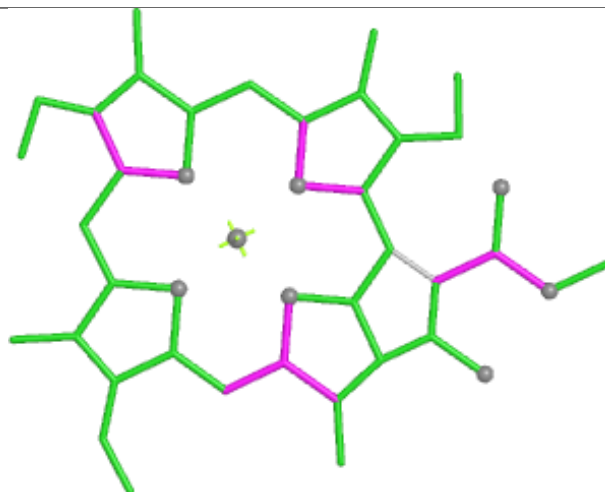
Rings



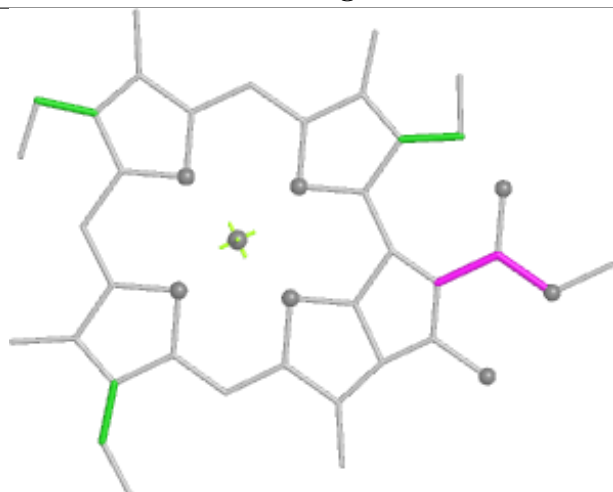
Ligand CLA d 612



Bond lengths



Bond angles

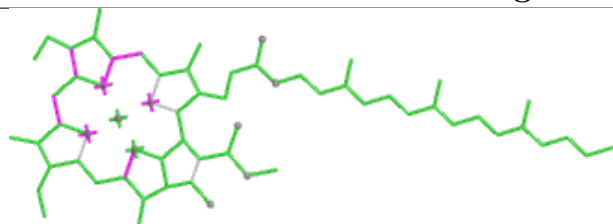


Torsions

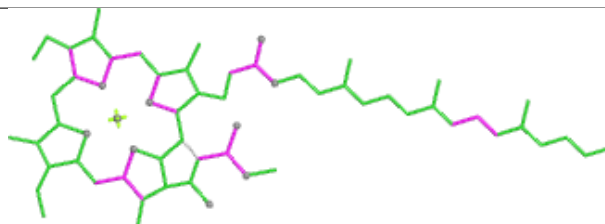


Rings

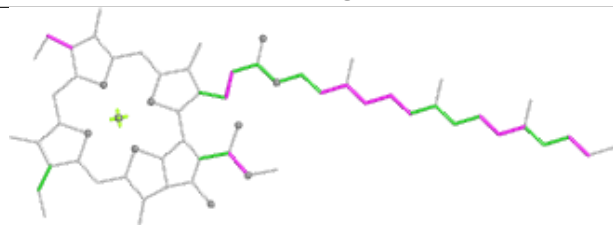
Ligand CLA A 791



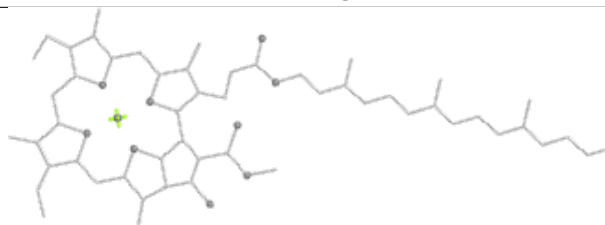
Bond lengths



Bond angles

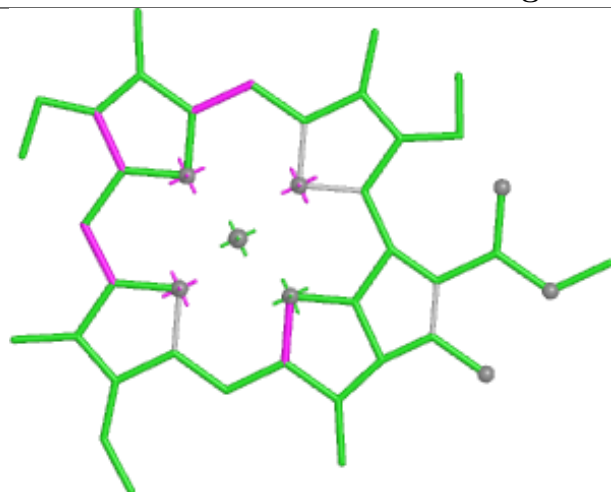


Torsions

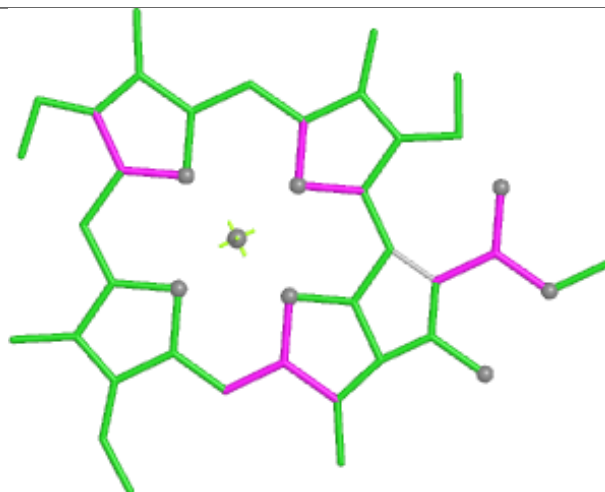


Rings

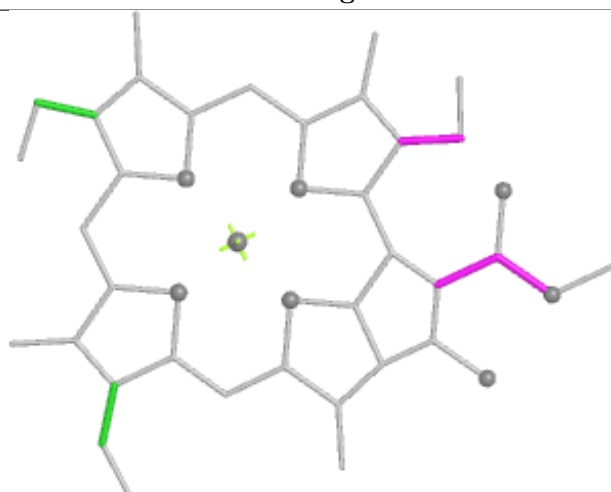
Ligand CLA f 604



Bond lengths



Bond angles

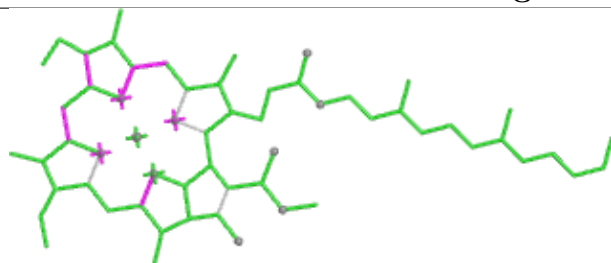


Torsions

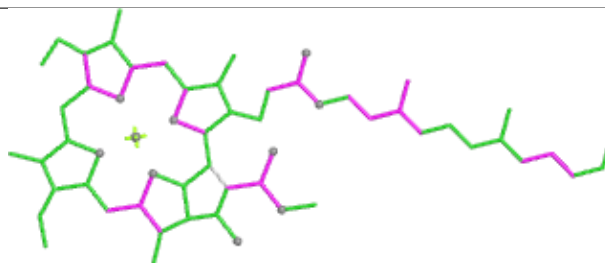


Rings

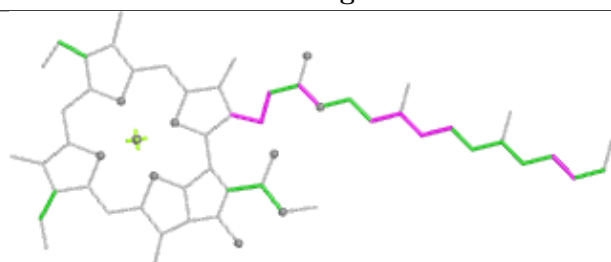
Ligand CLA A 765



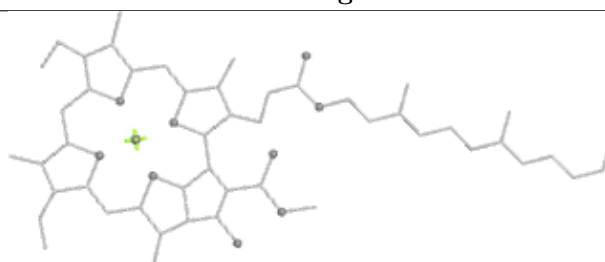
Bond lengths



Bond angles

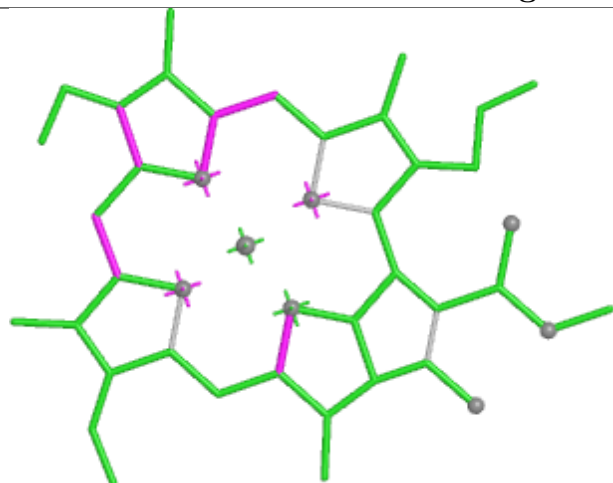


Torsions

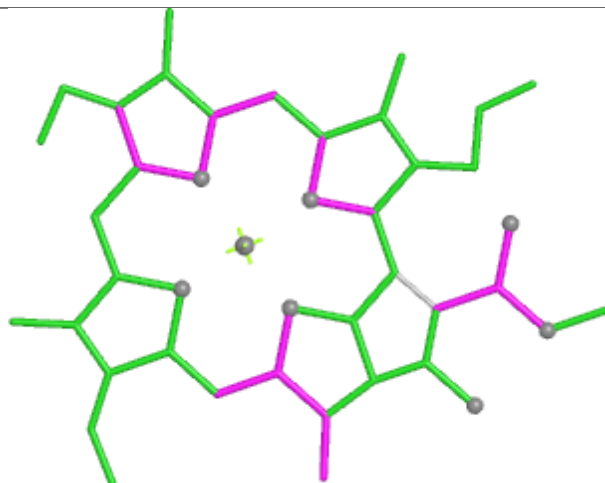


Rings

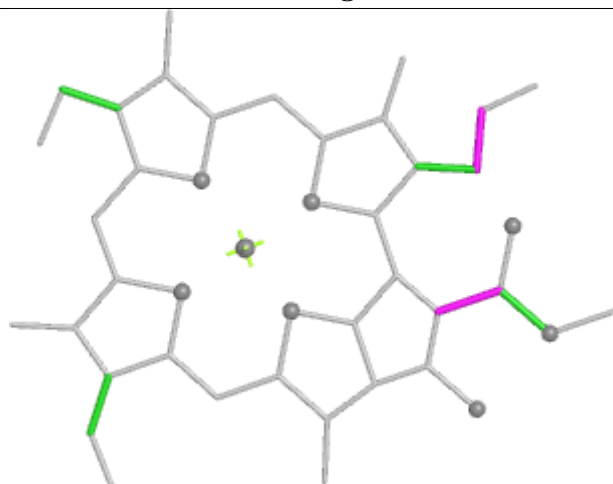
Ligand CLA e 612



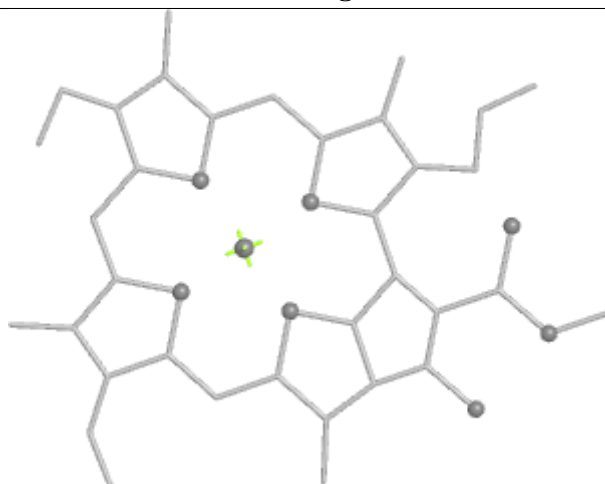
Bond lengths



Bond angles

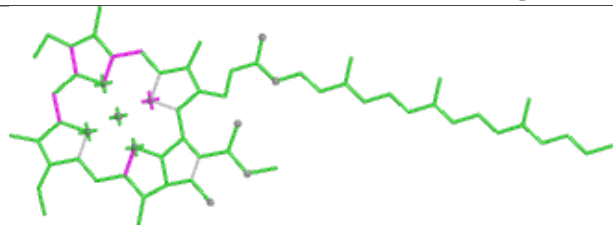


Torsions

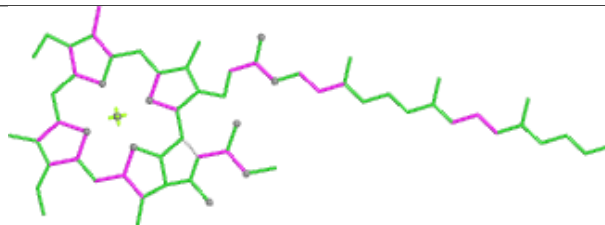


Rings

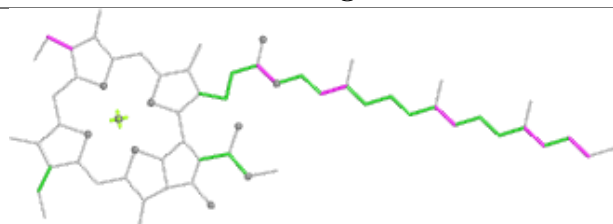
Ligand CLA A 753



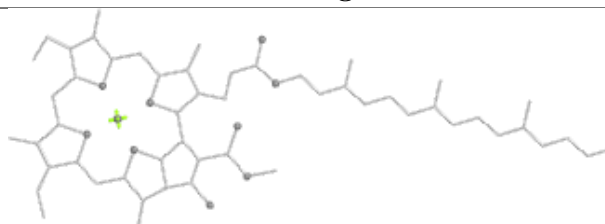
Bond lengths



Bond angles

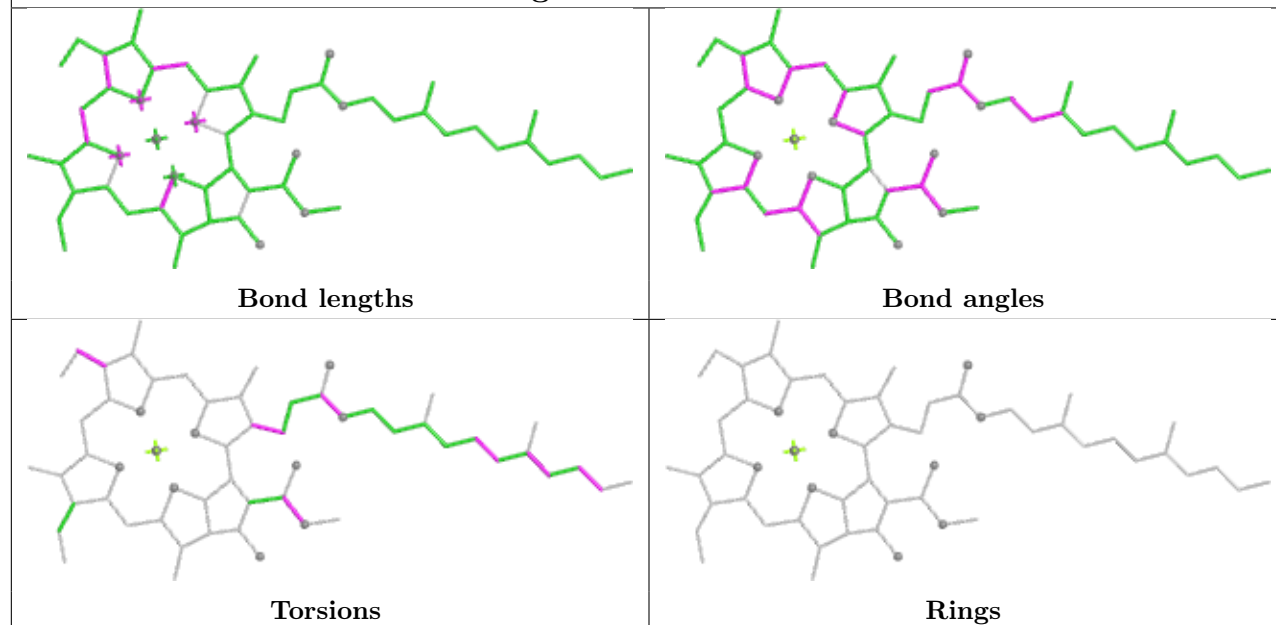


Torsions

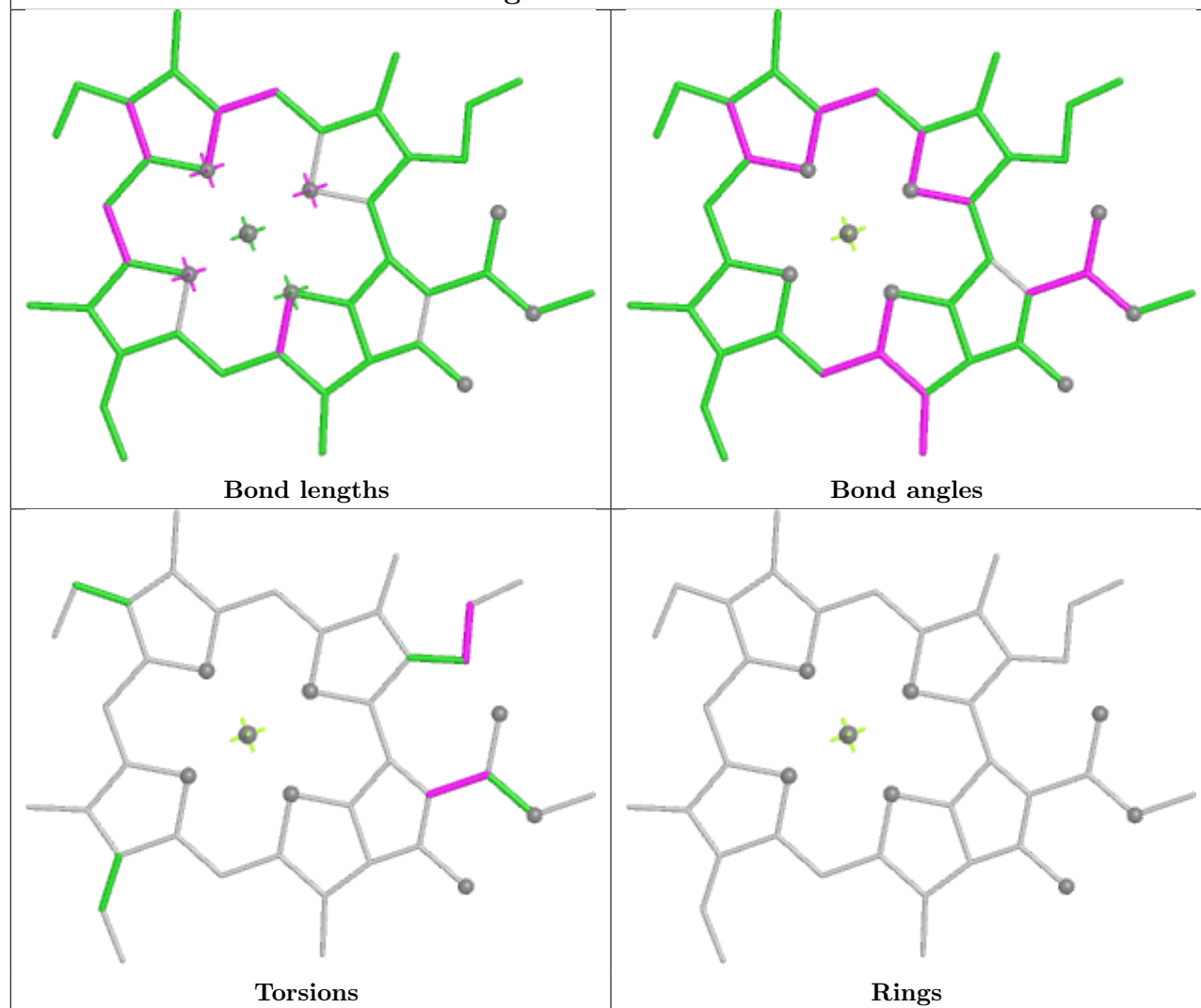


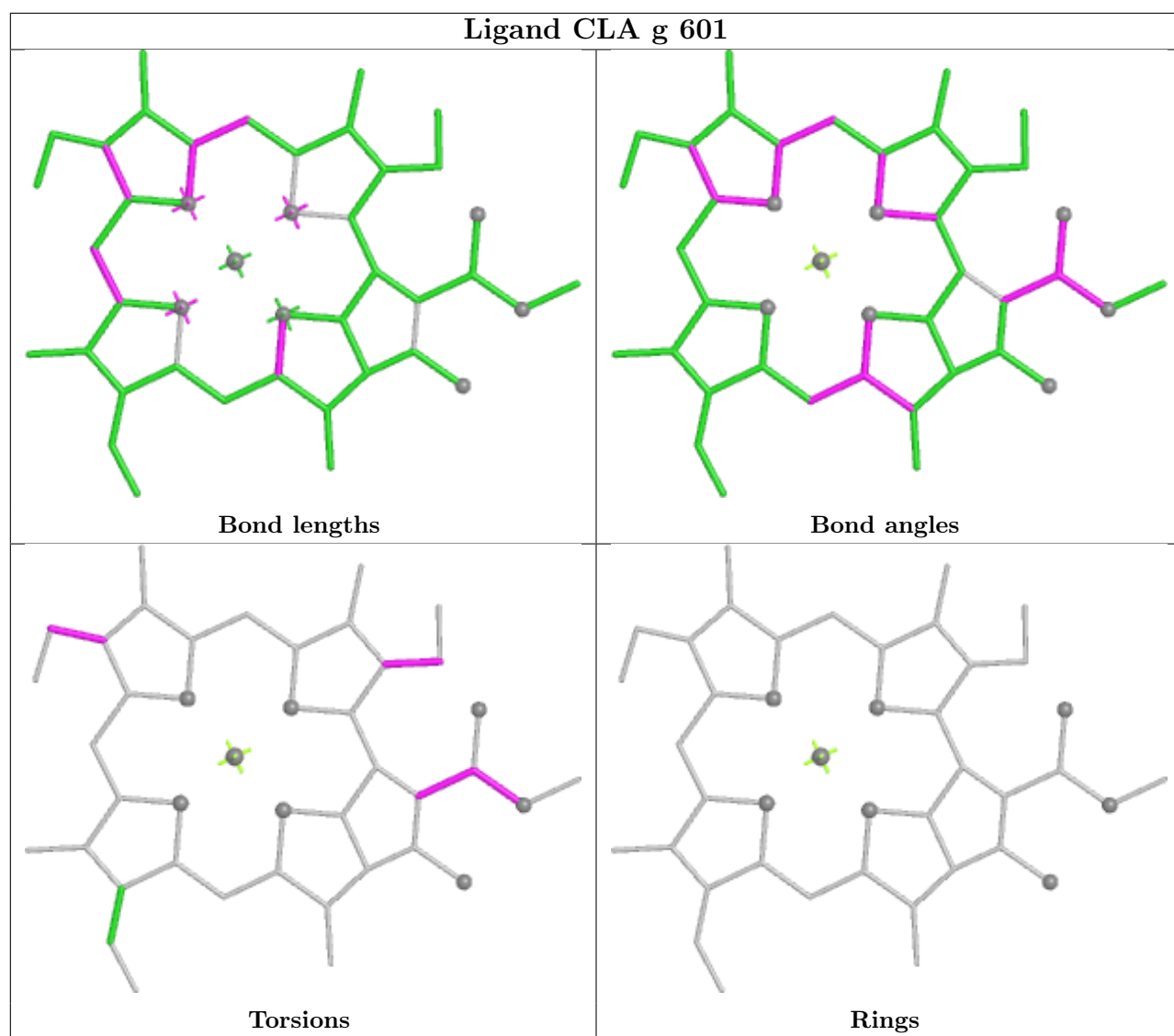
Rings

Ligand CLA A 764

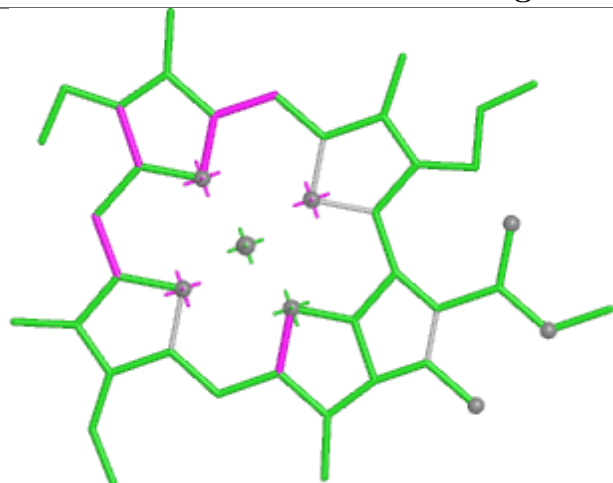


Ligand CLA k 612

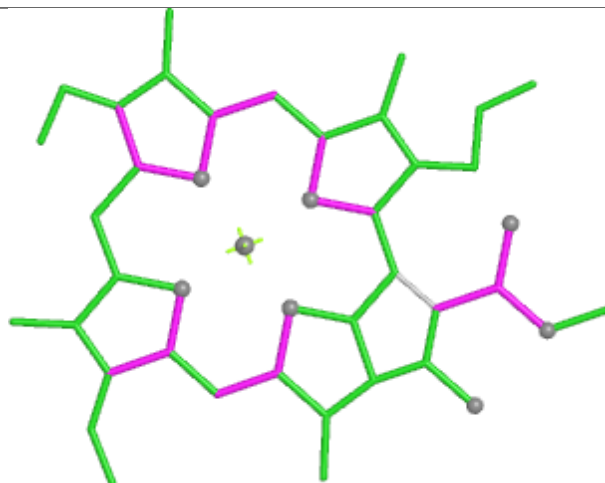




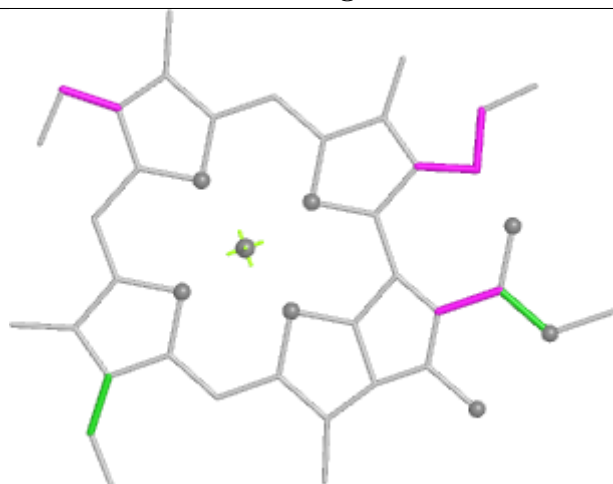
Ligand CLA B 759



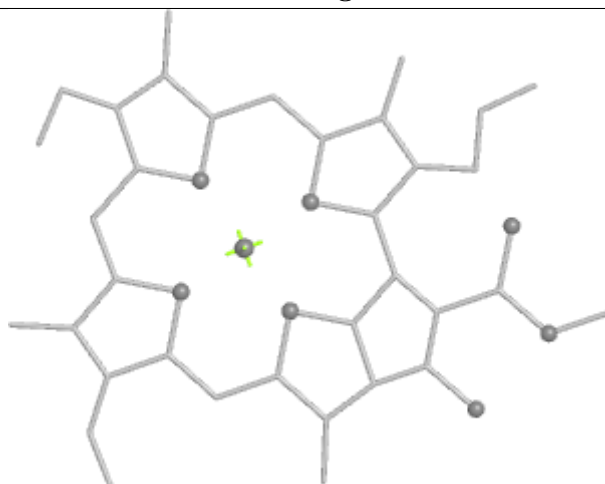
Bond lengths



Bond angles

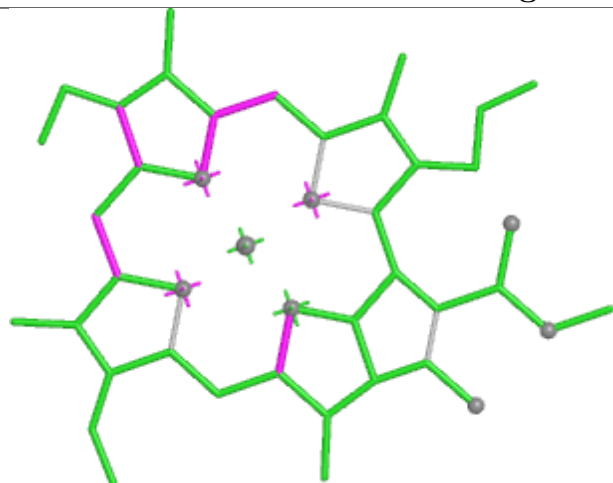


Torsions

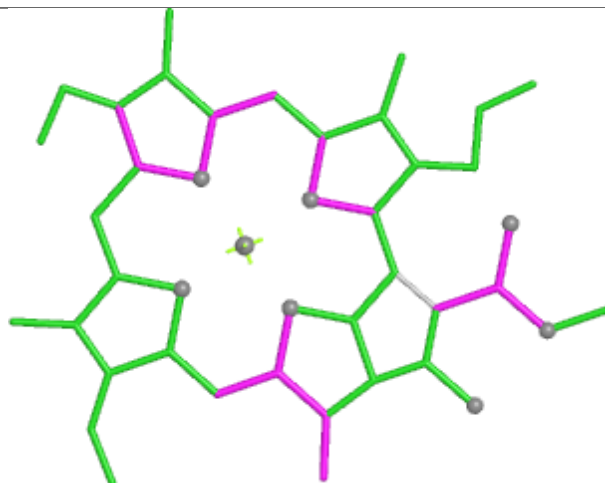


Rings

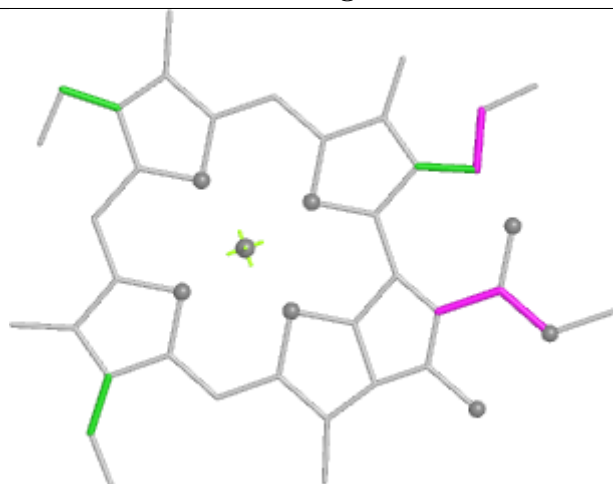
Ligand CLA c 612



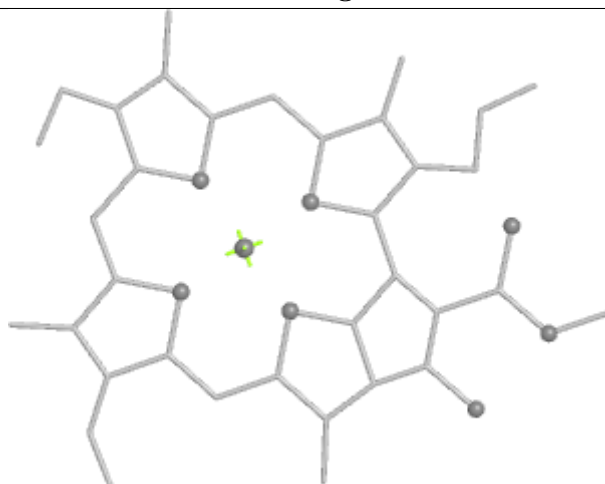
Bond lengths



Bond angles

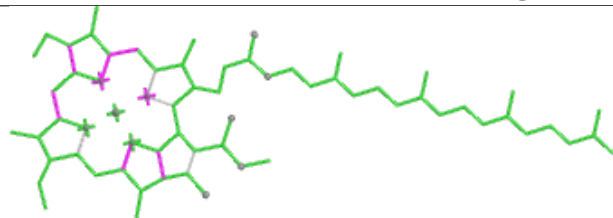


Torsions

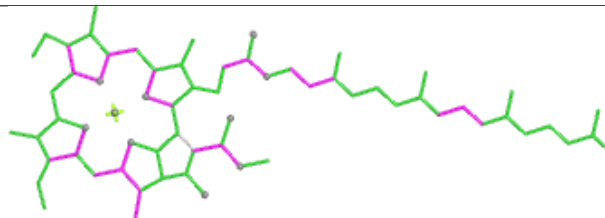


Rings

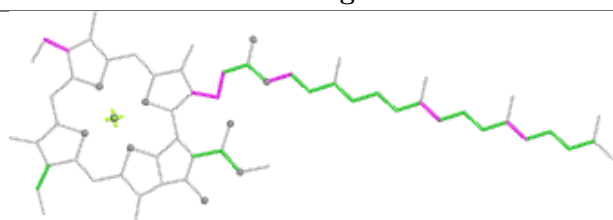
Ligand CLA A 758



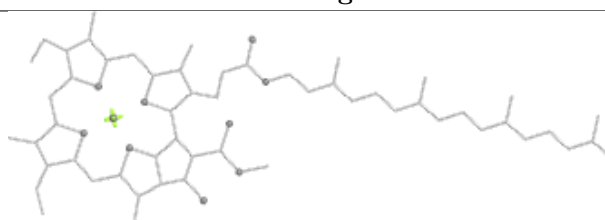
Bond lengths



Bond angles

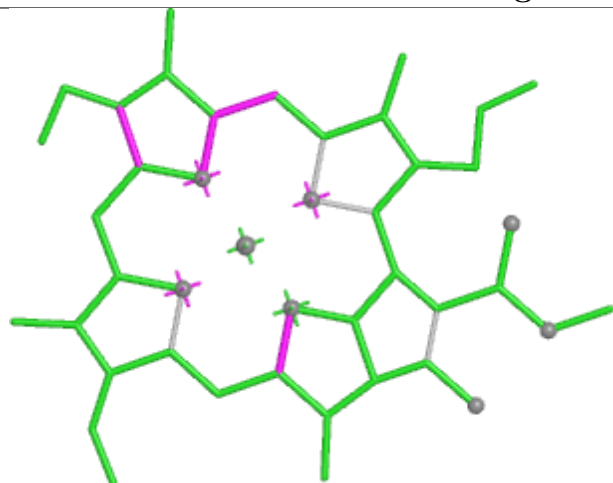


Torsions

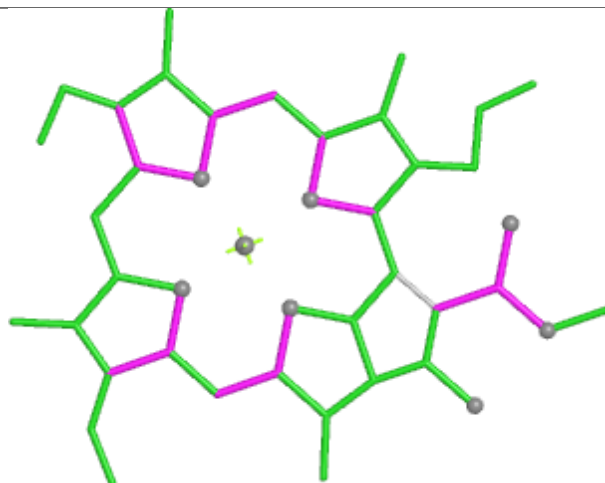


Rings

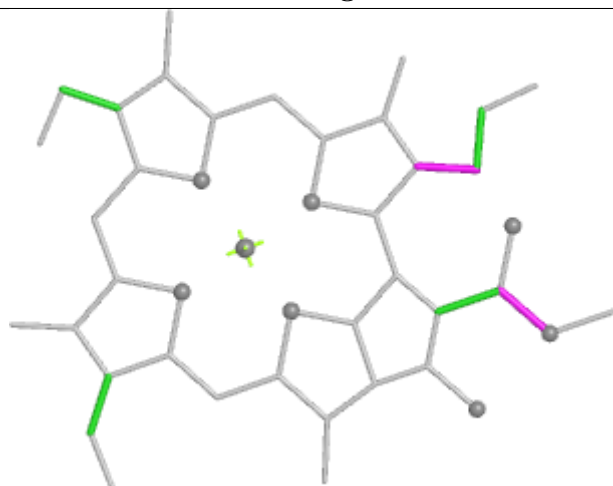
Ligand CLA B 760



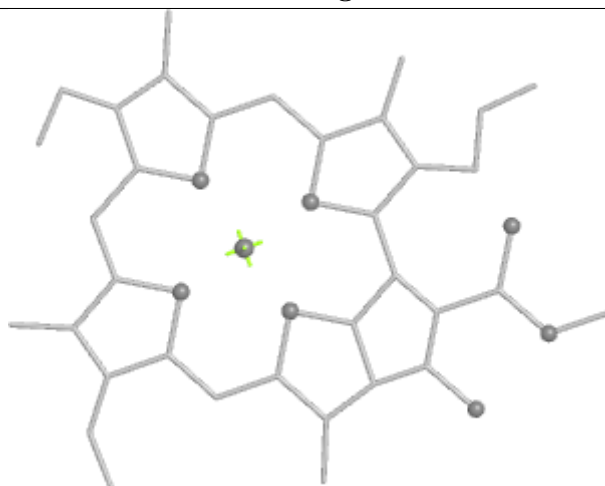
Bond lengths



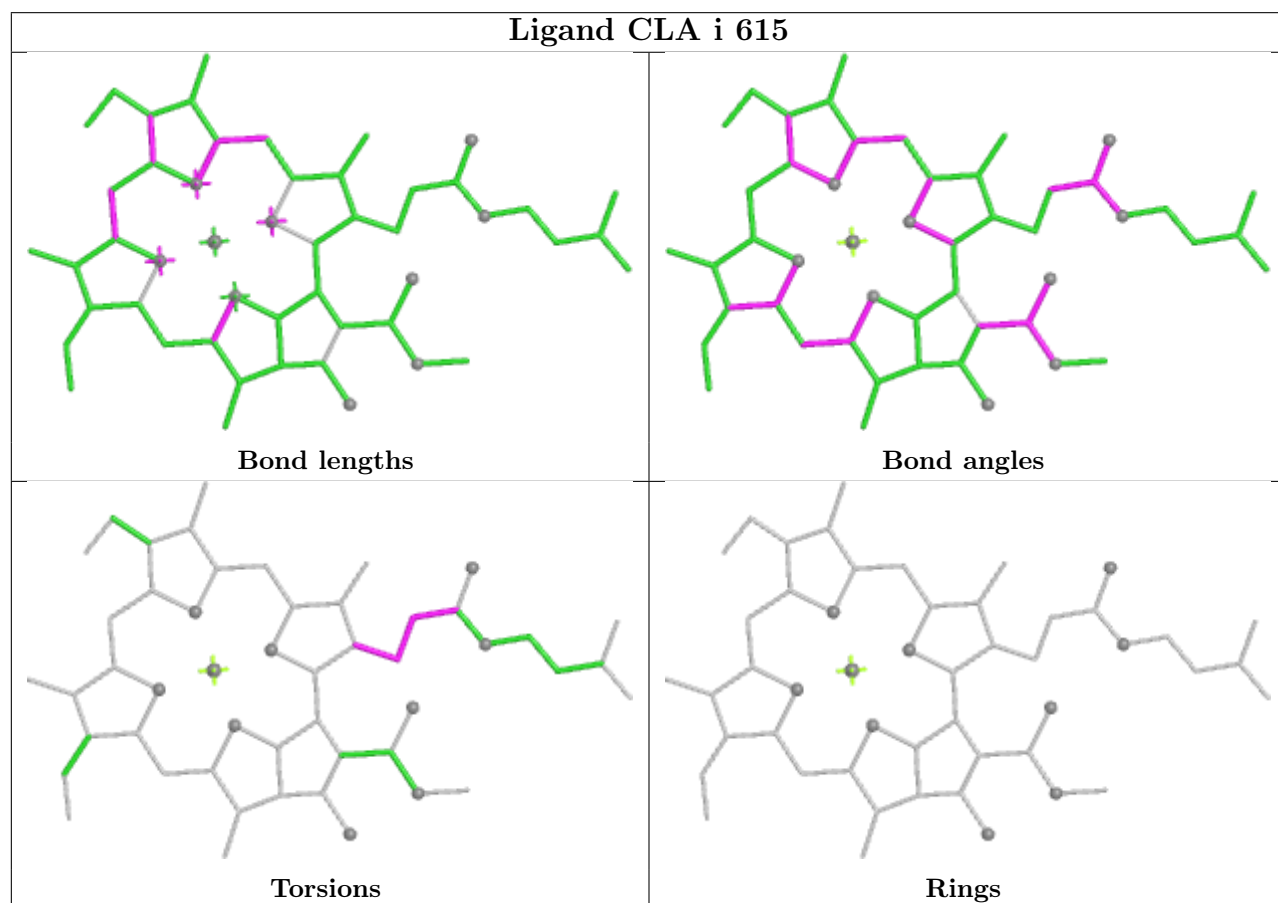
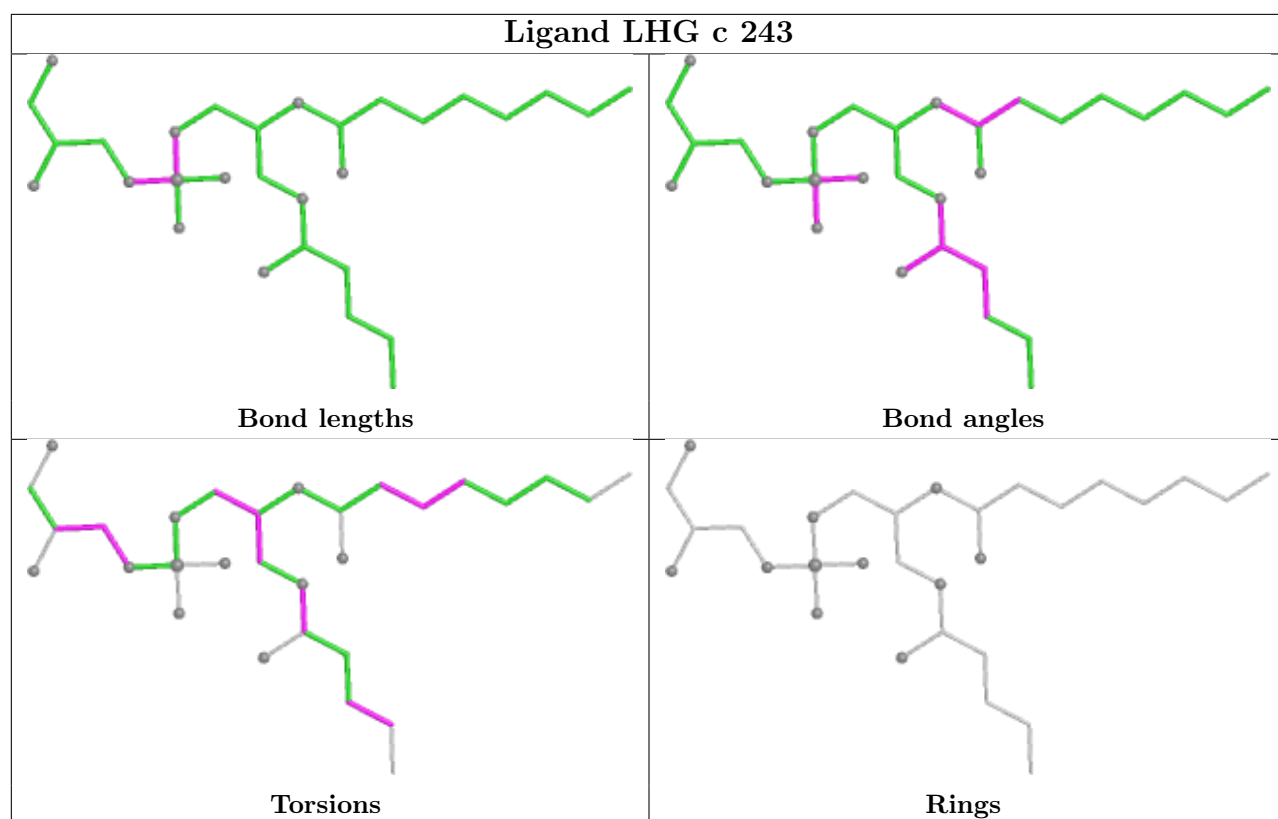
Bond angles

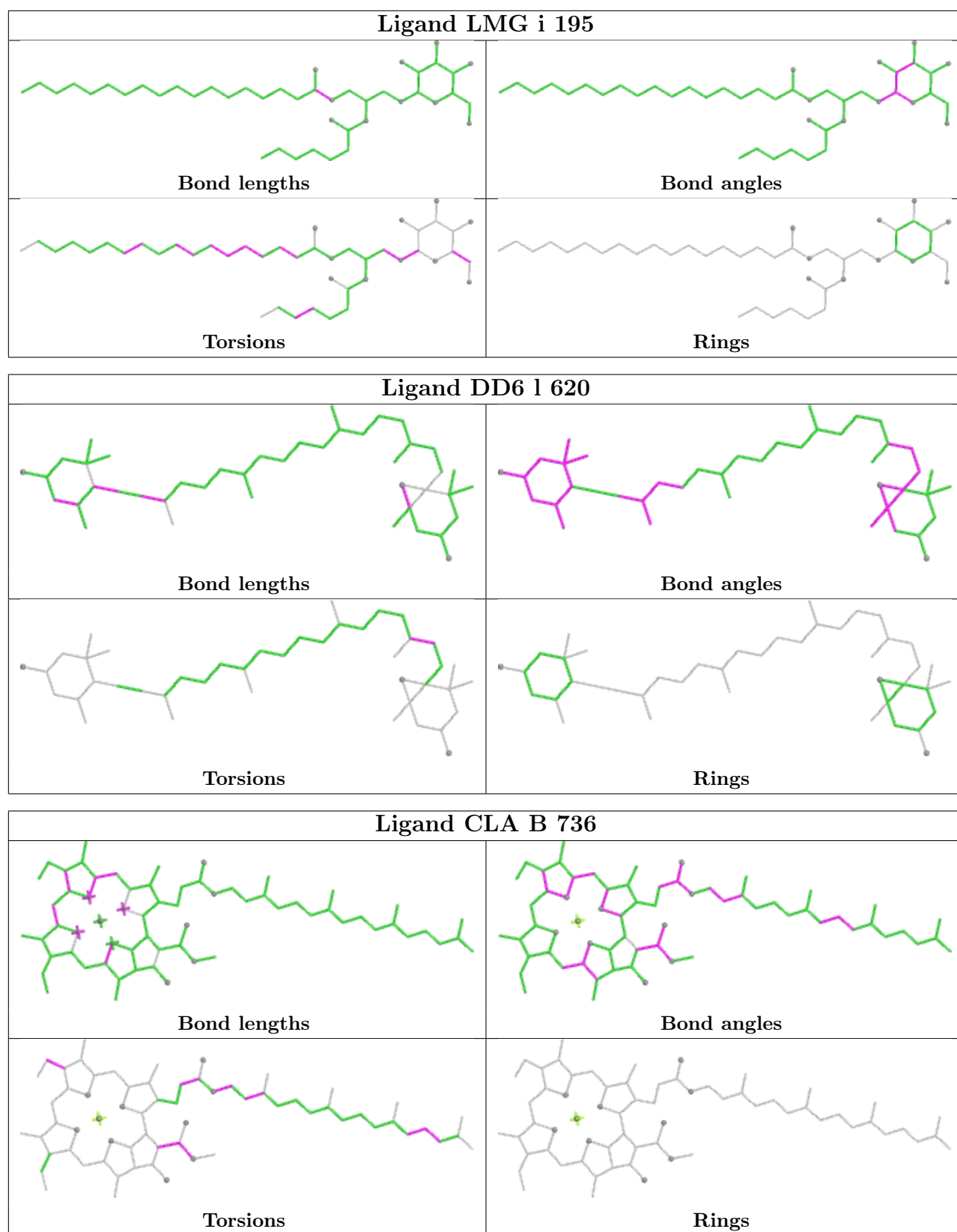


Torsions

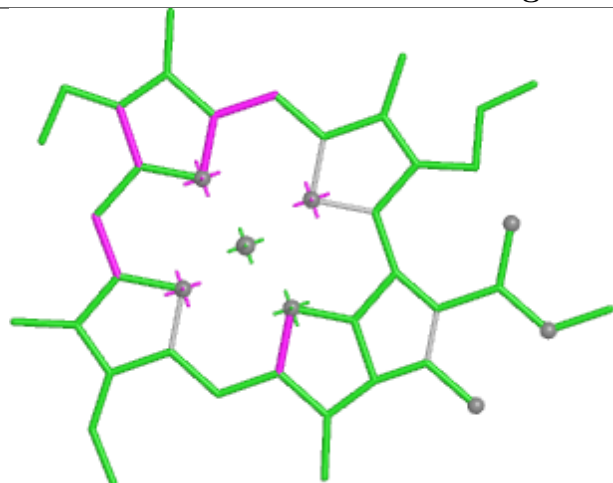


Rings

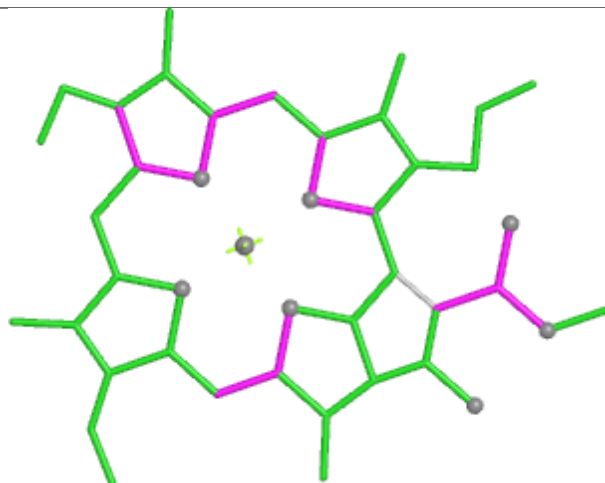




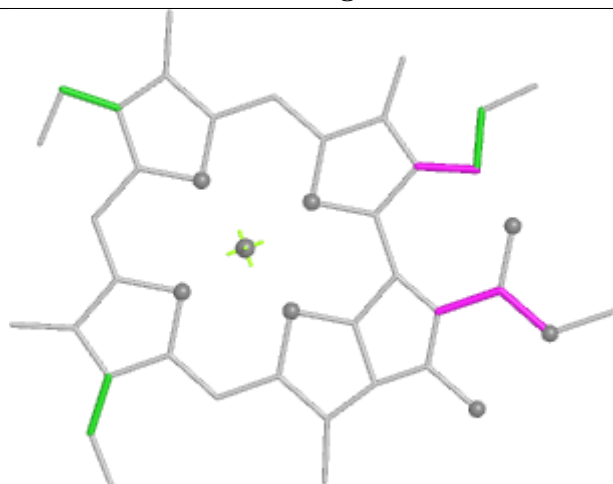
Ligand CLA i 611



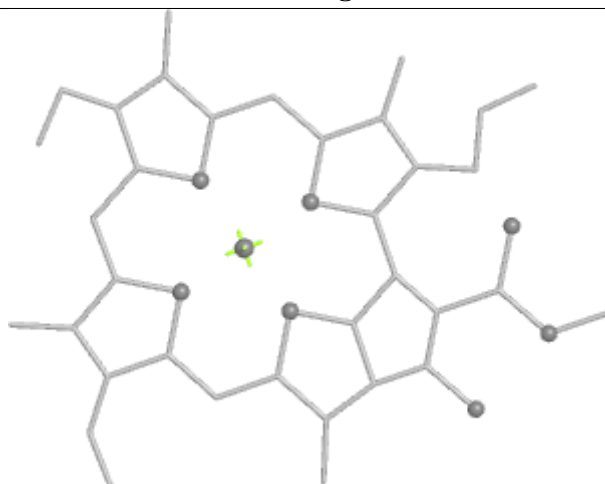
Bond lengths



Bond angles

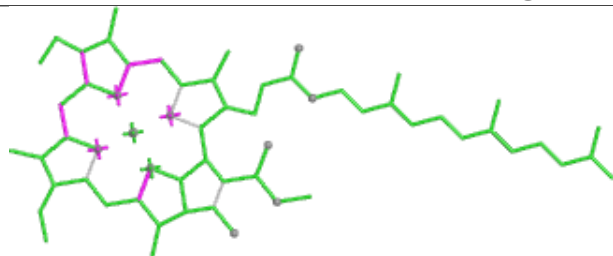


Torsions

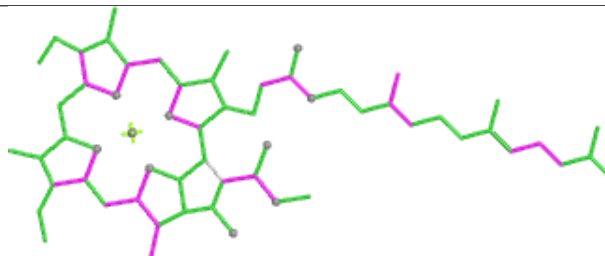


Rings

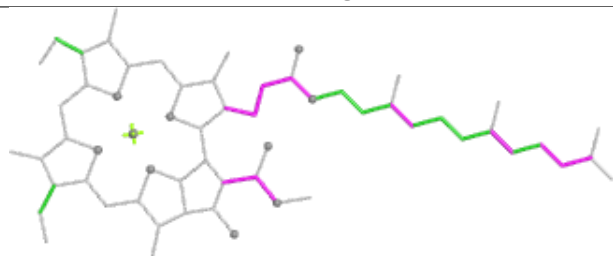
Ligand CLA c 609



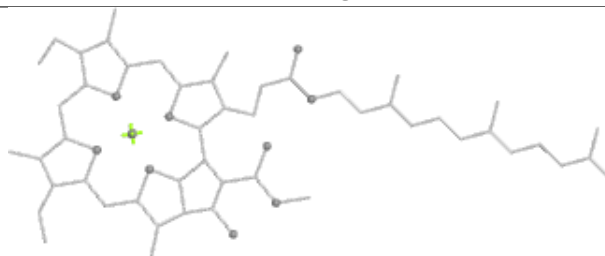
Bond lengths



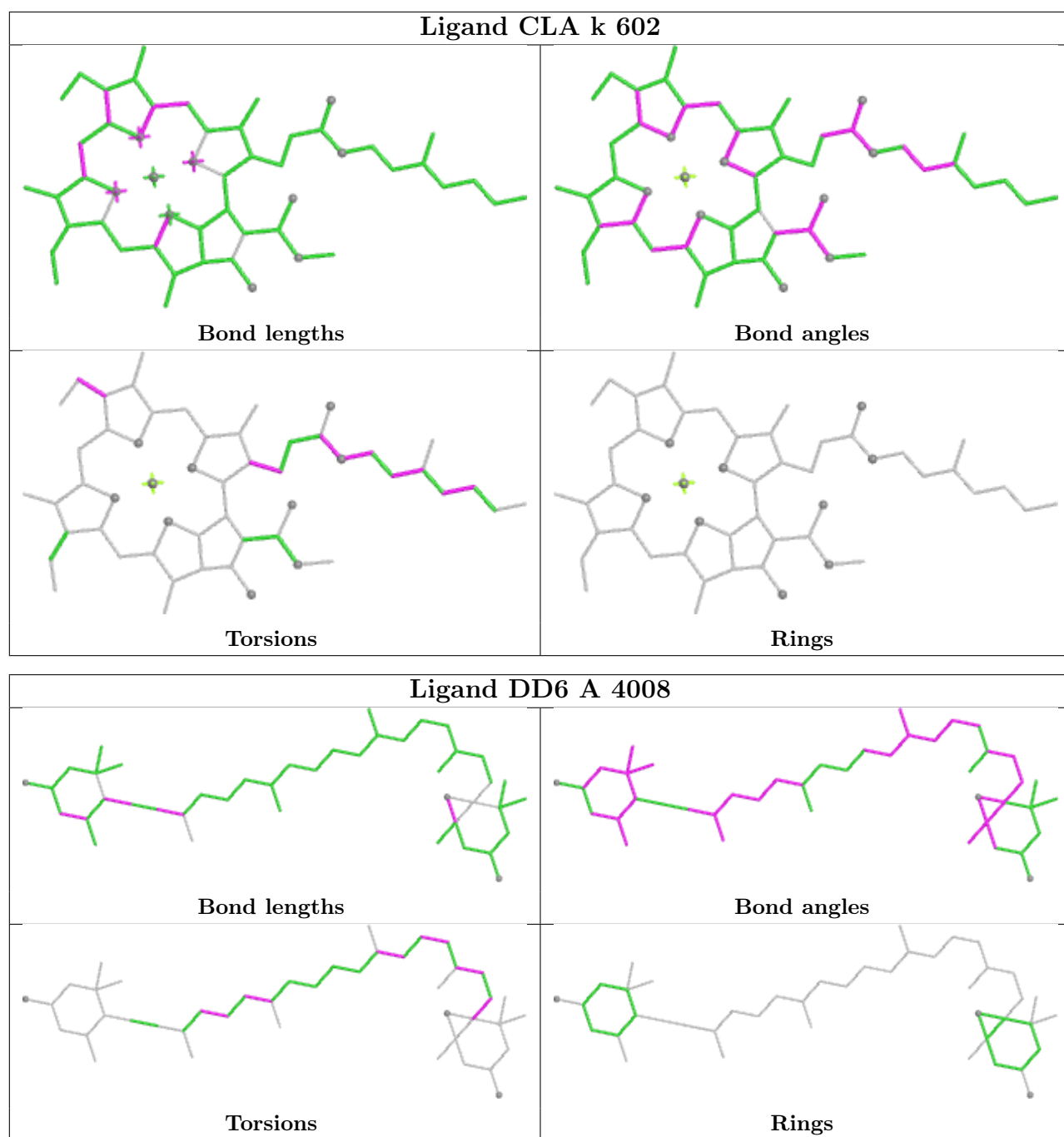
Bond angles

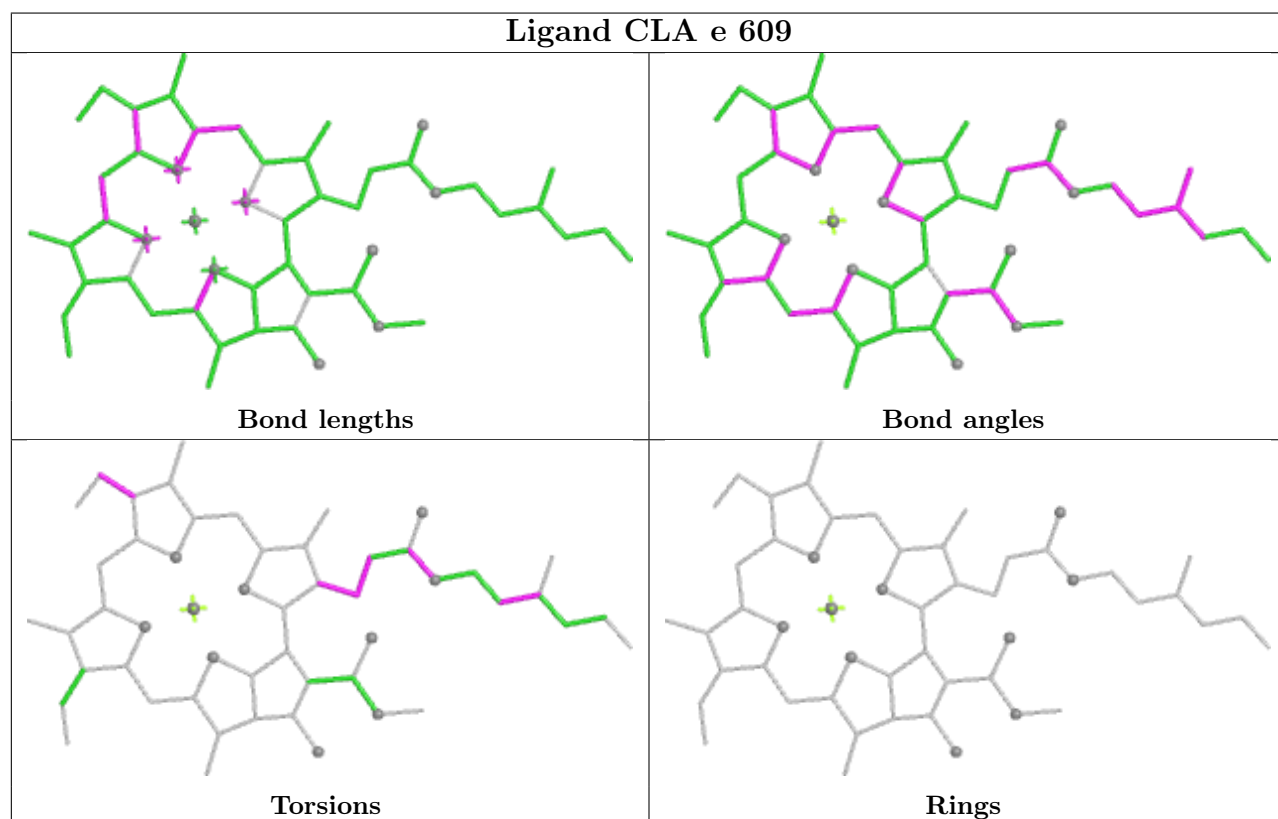
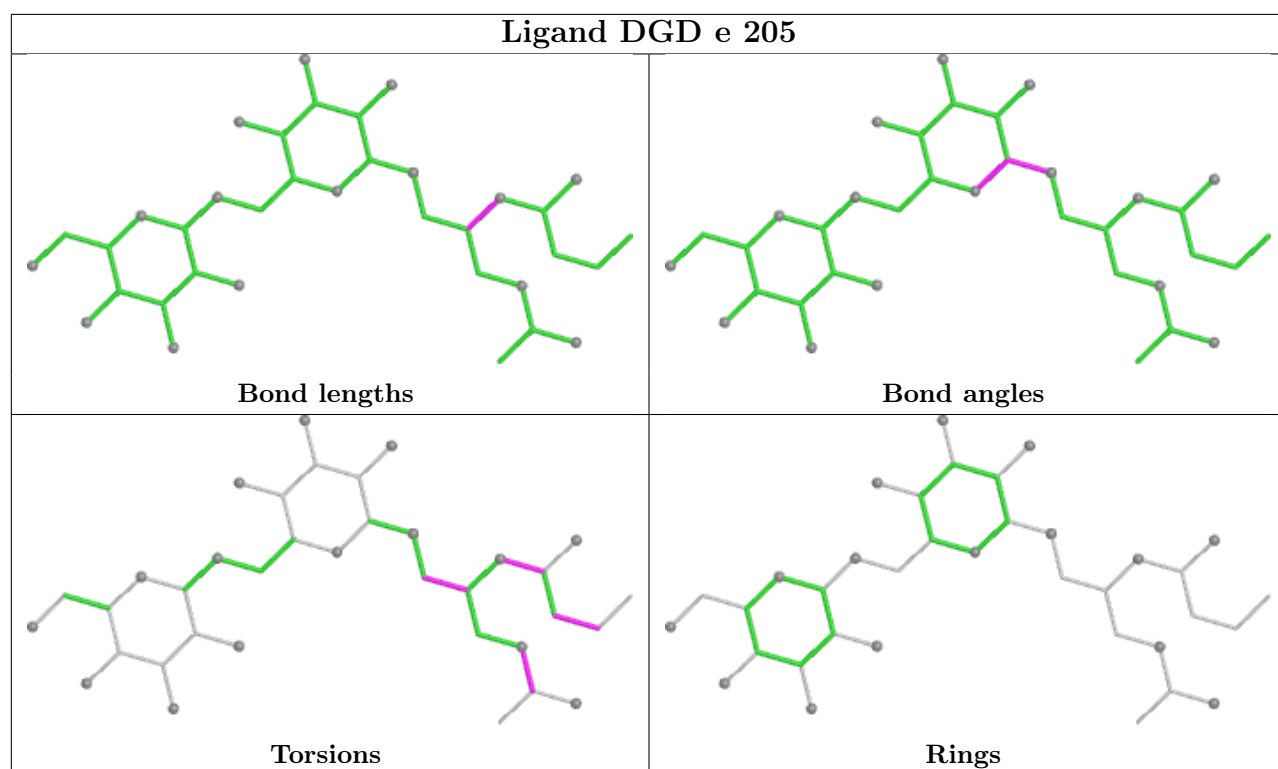


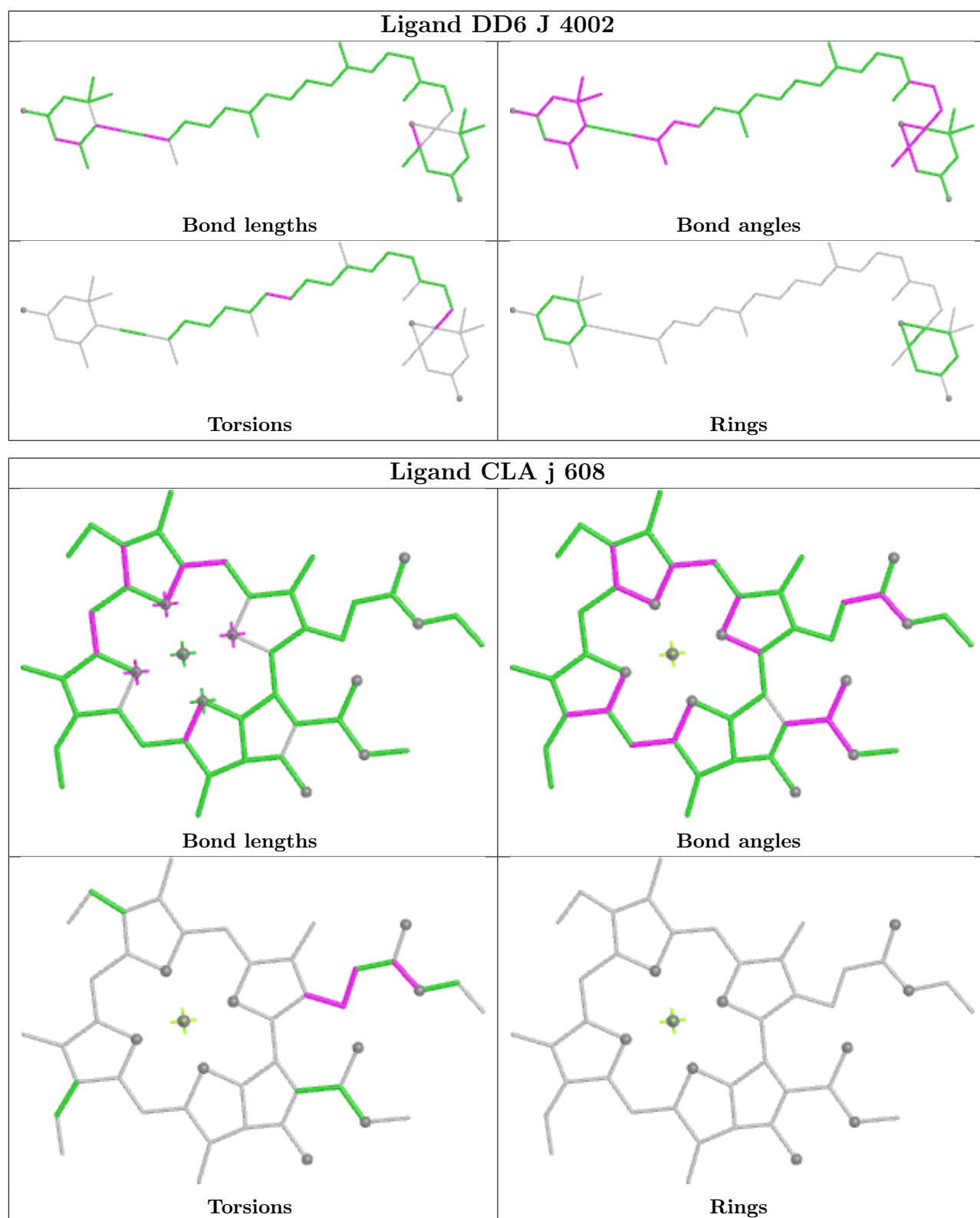
Torsions

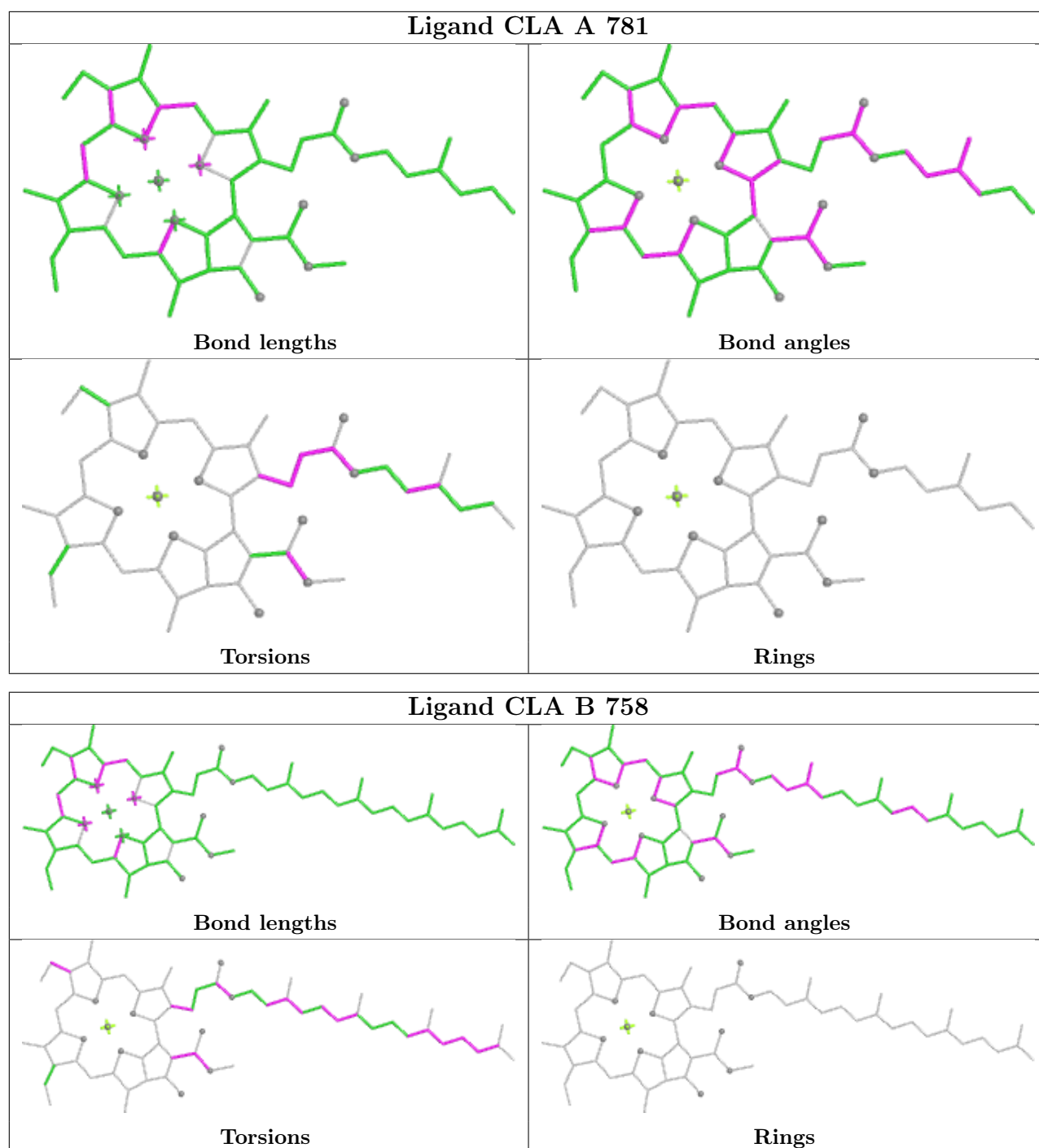


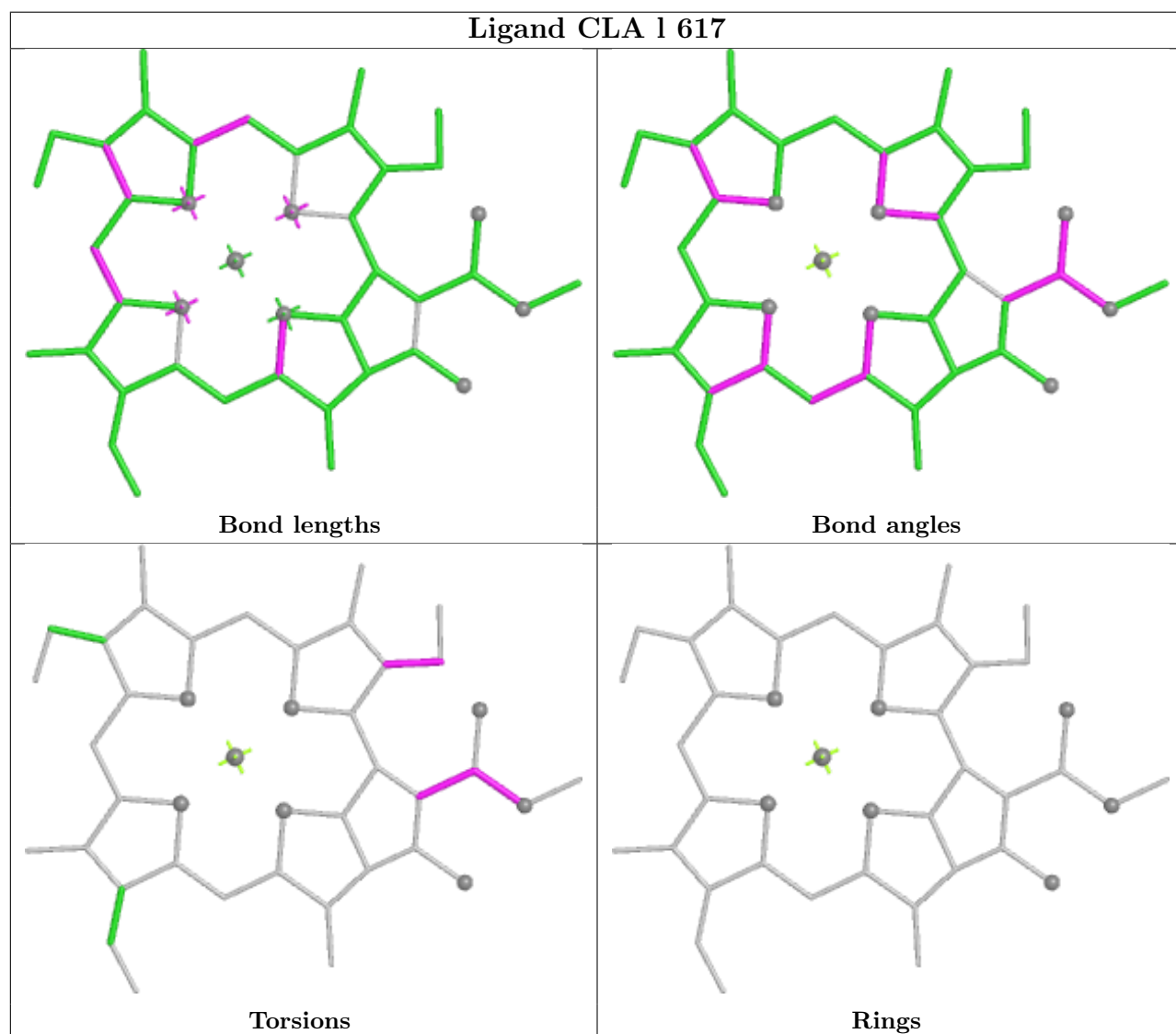
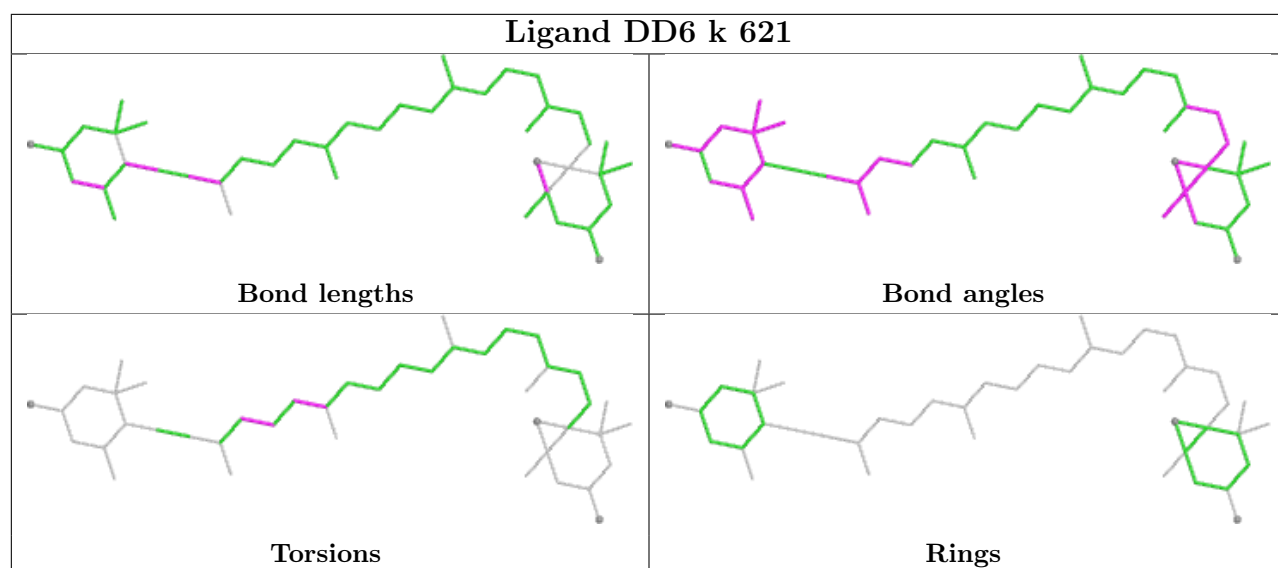
Rings

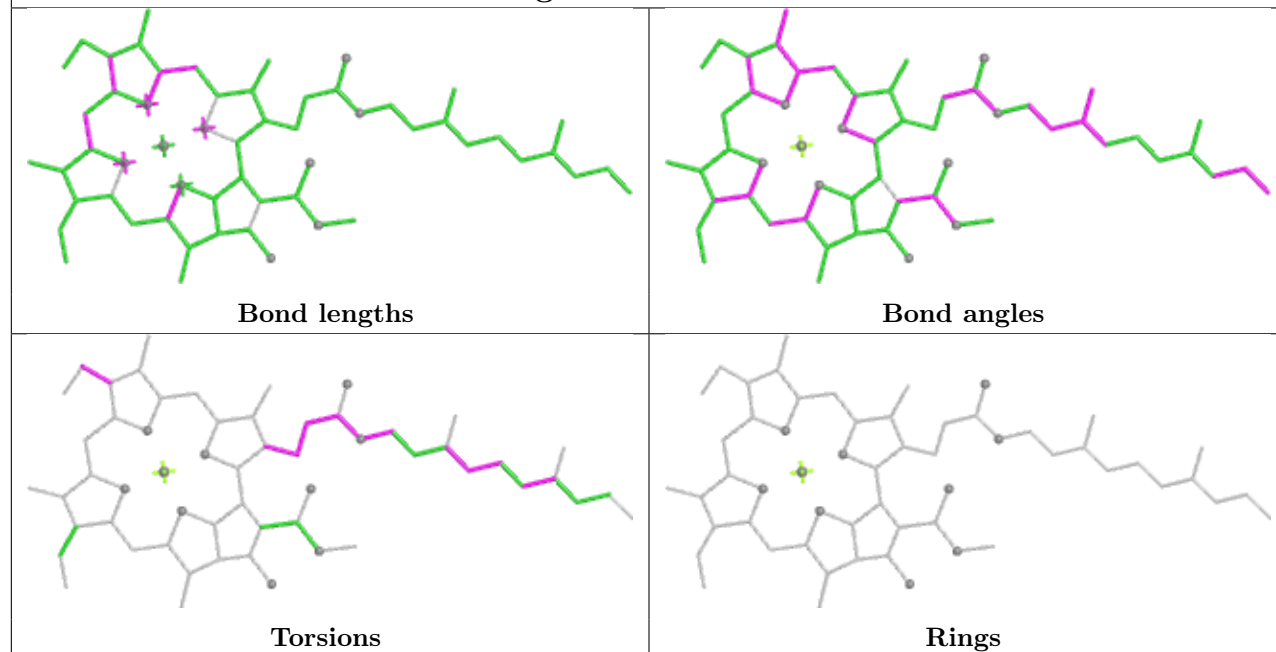
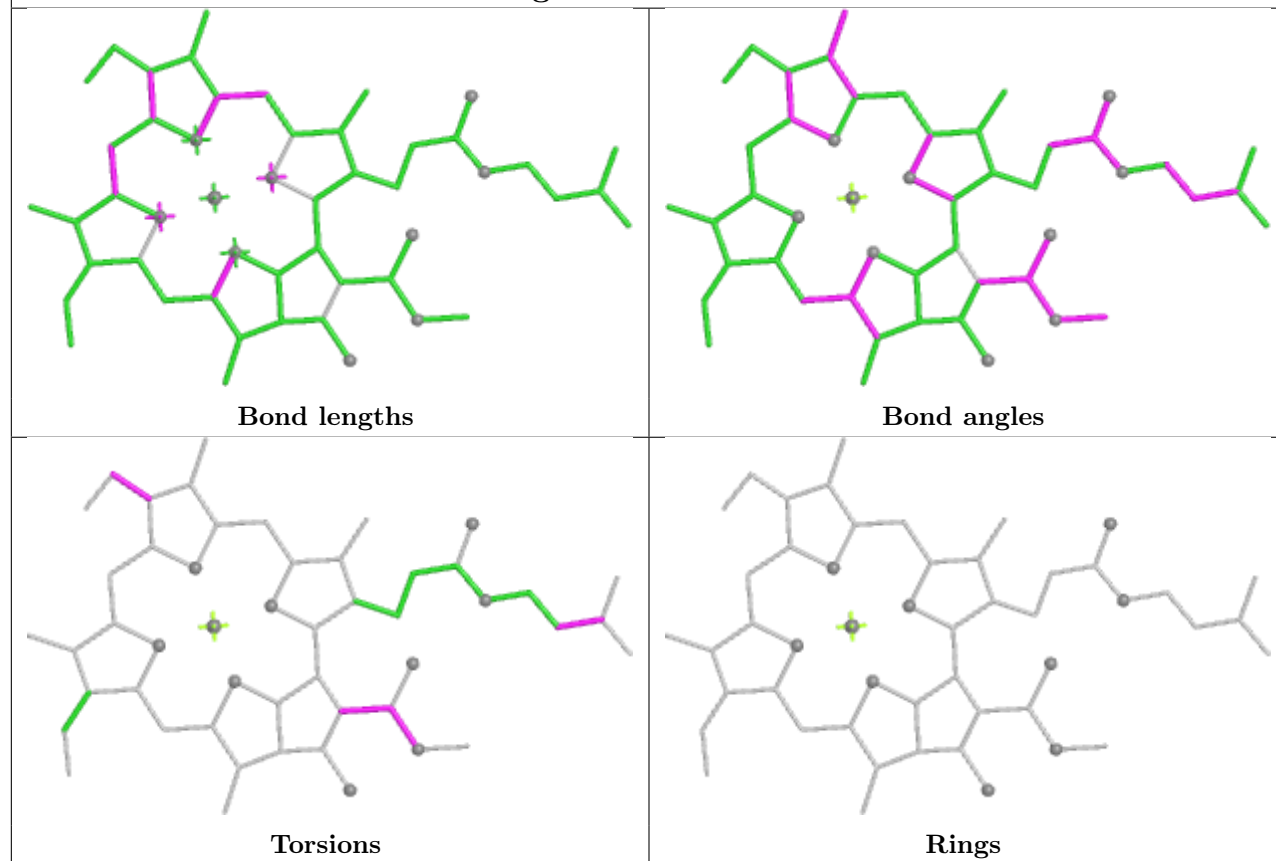




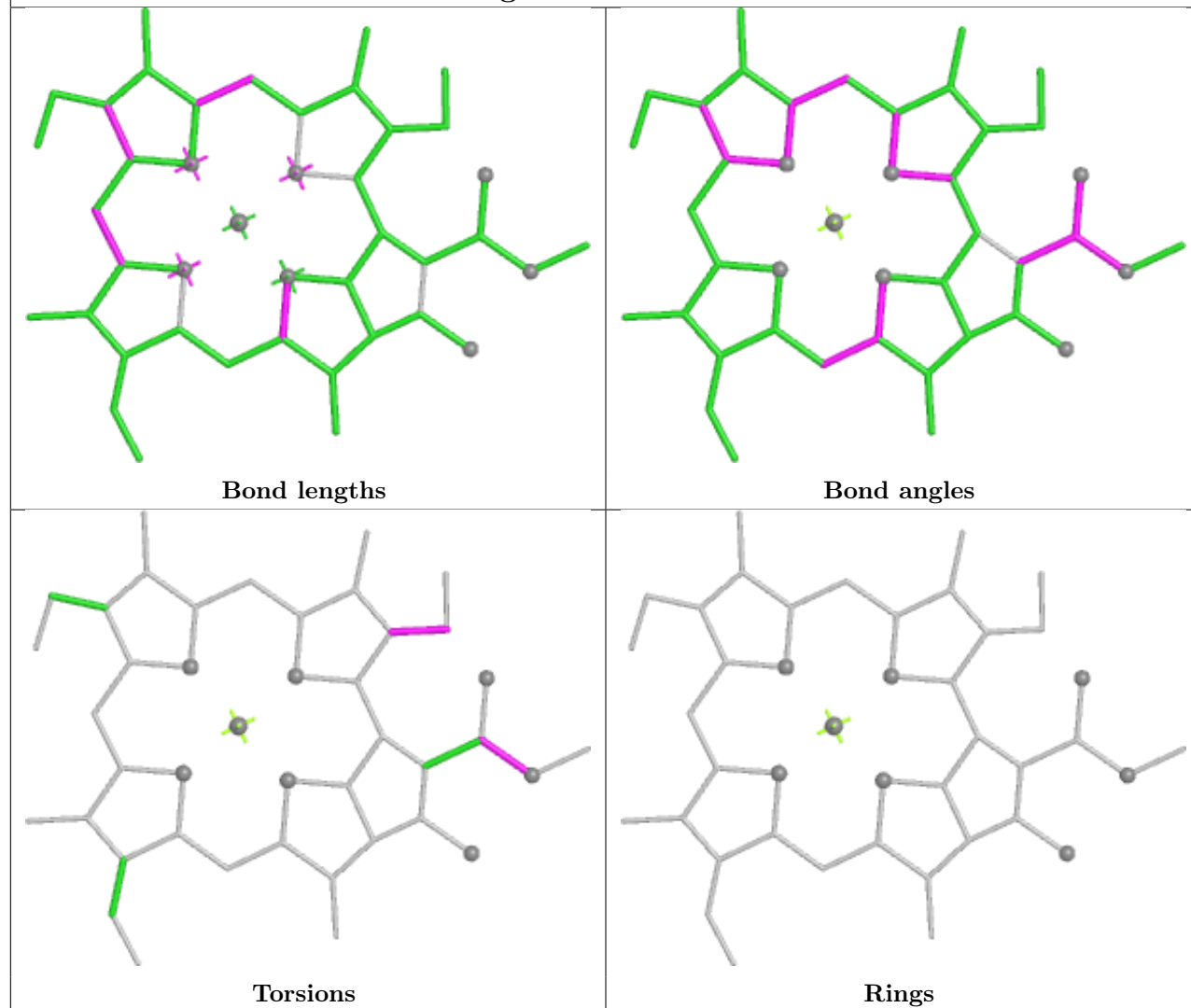




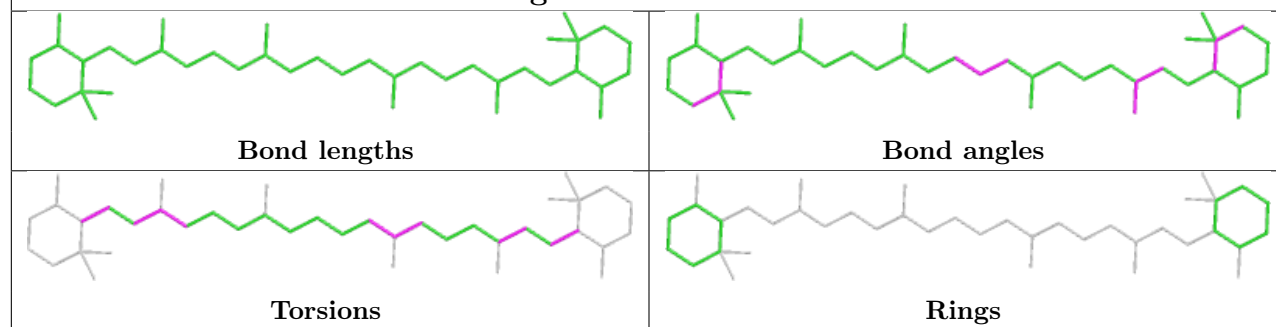


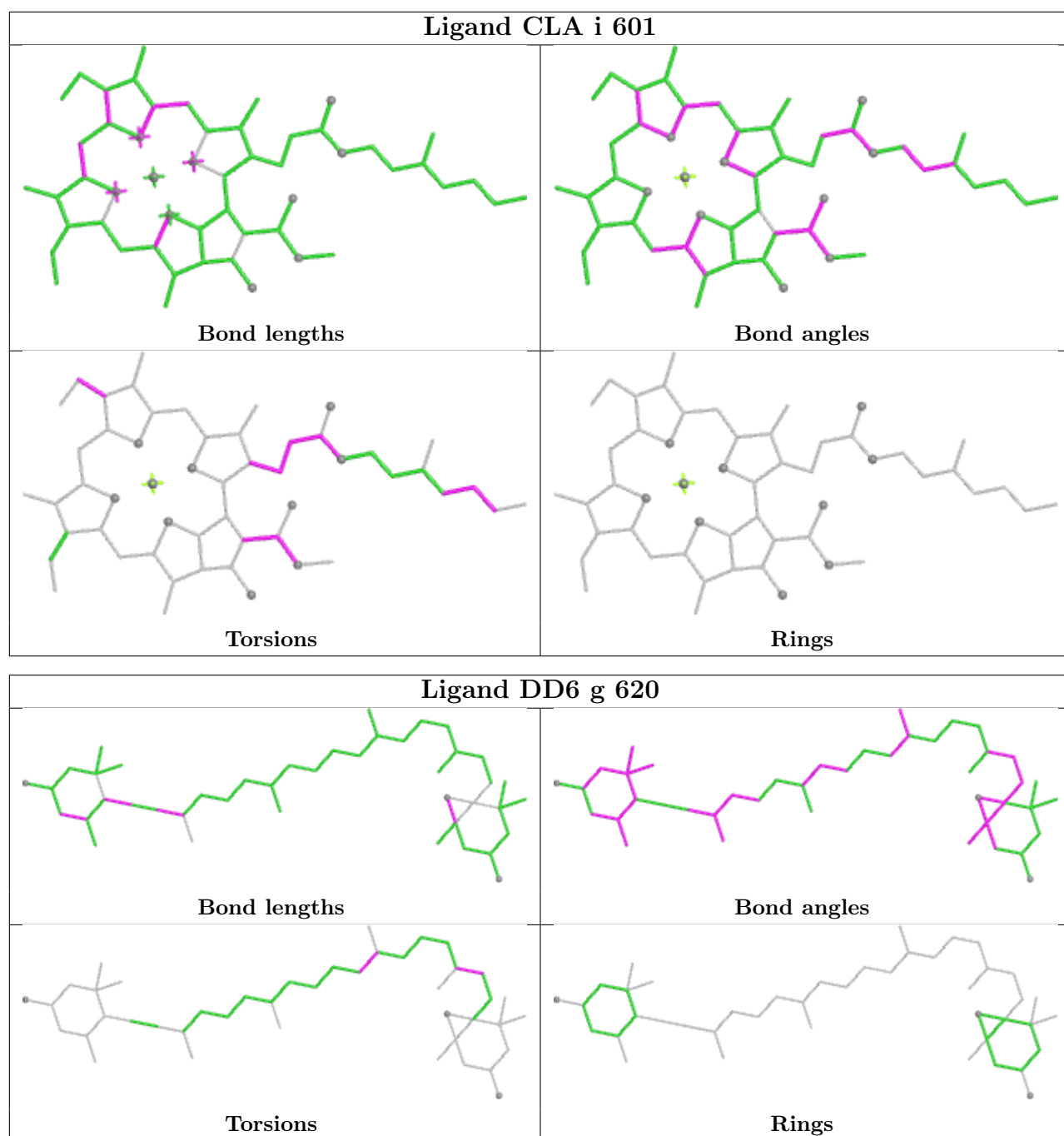
Ligand CLA k 610**Ligand CLA B 782**

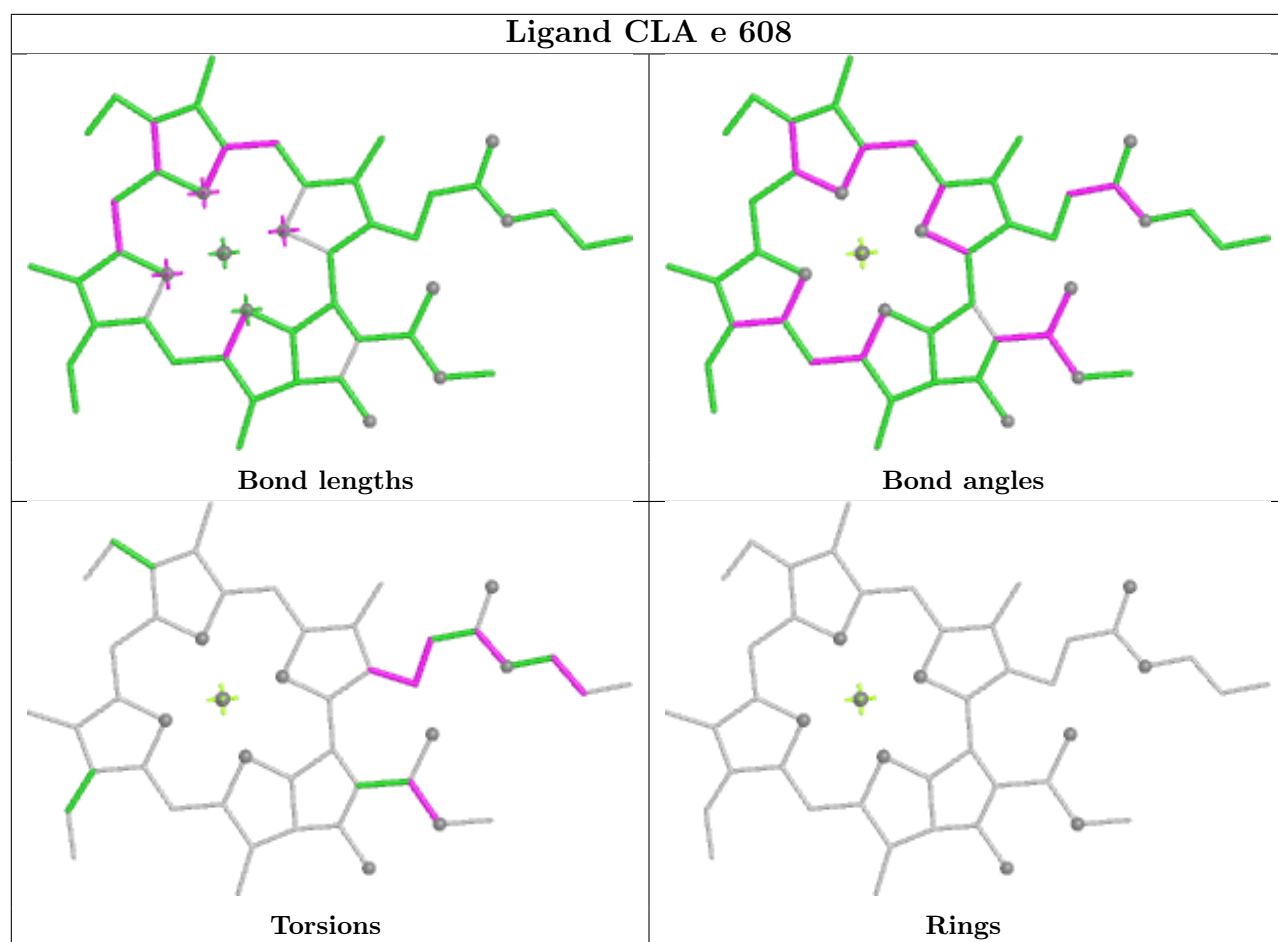
Ligand CLA k 614

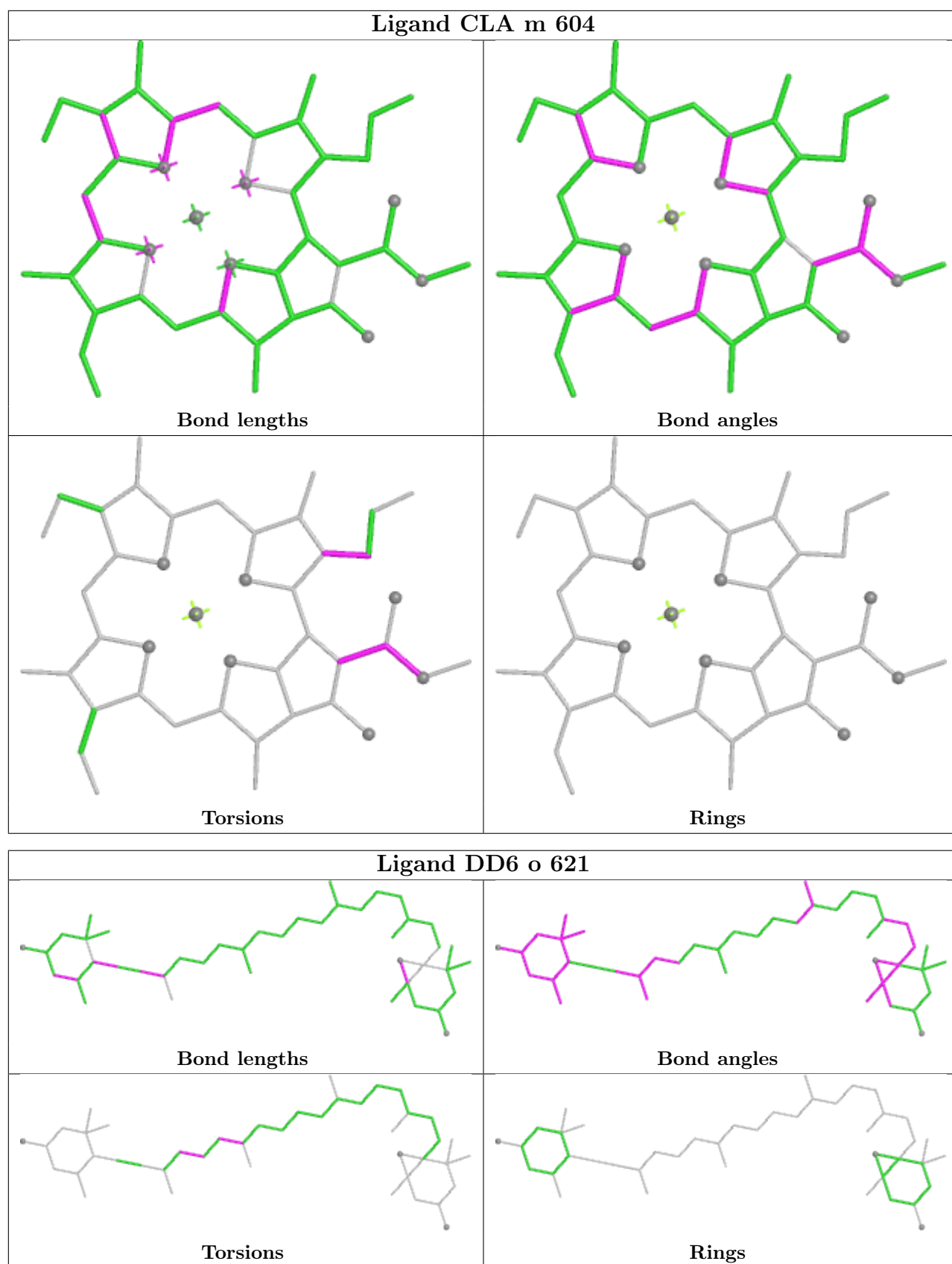


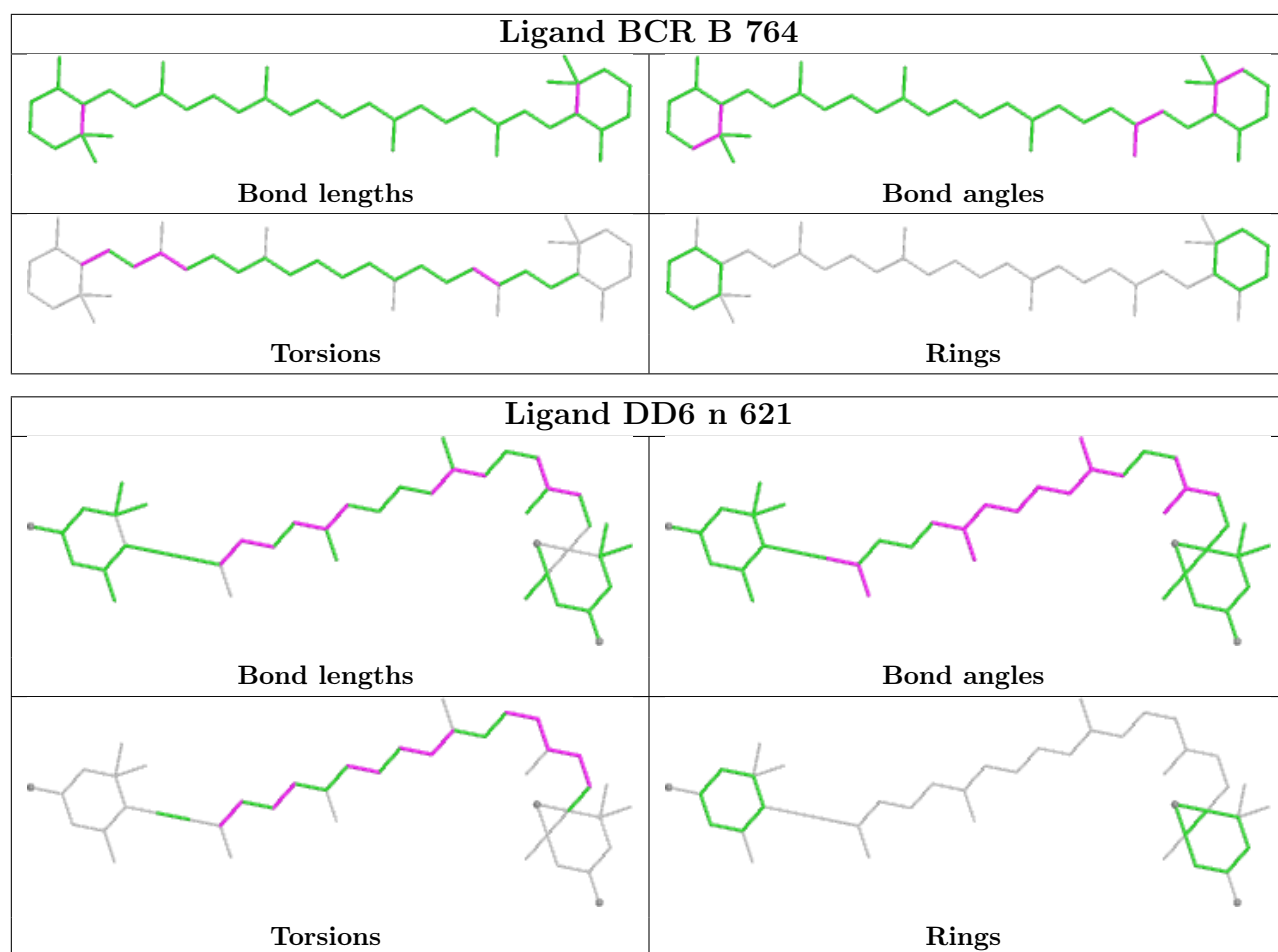
Ligand BCR A 790



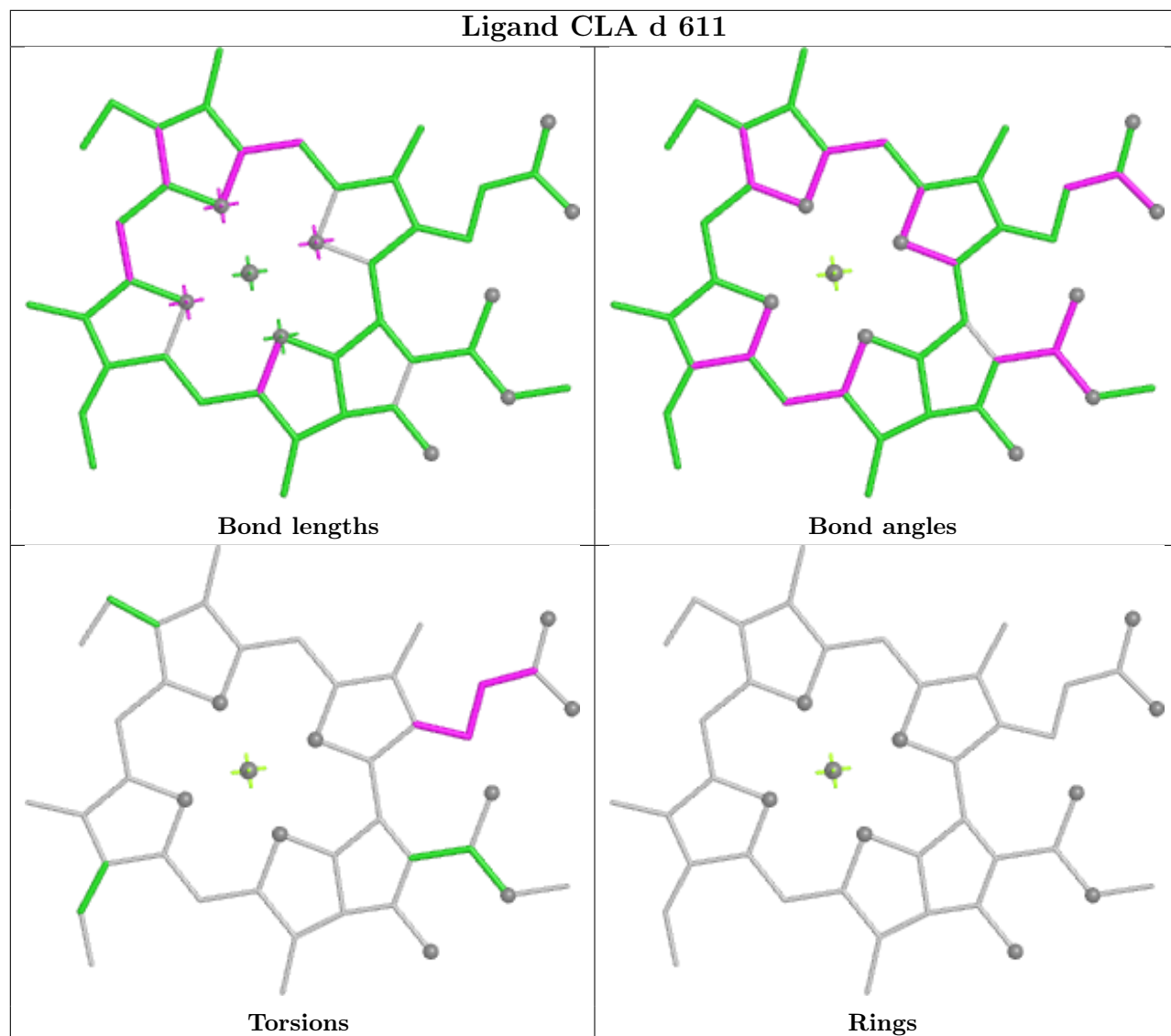




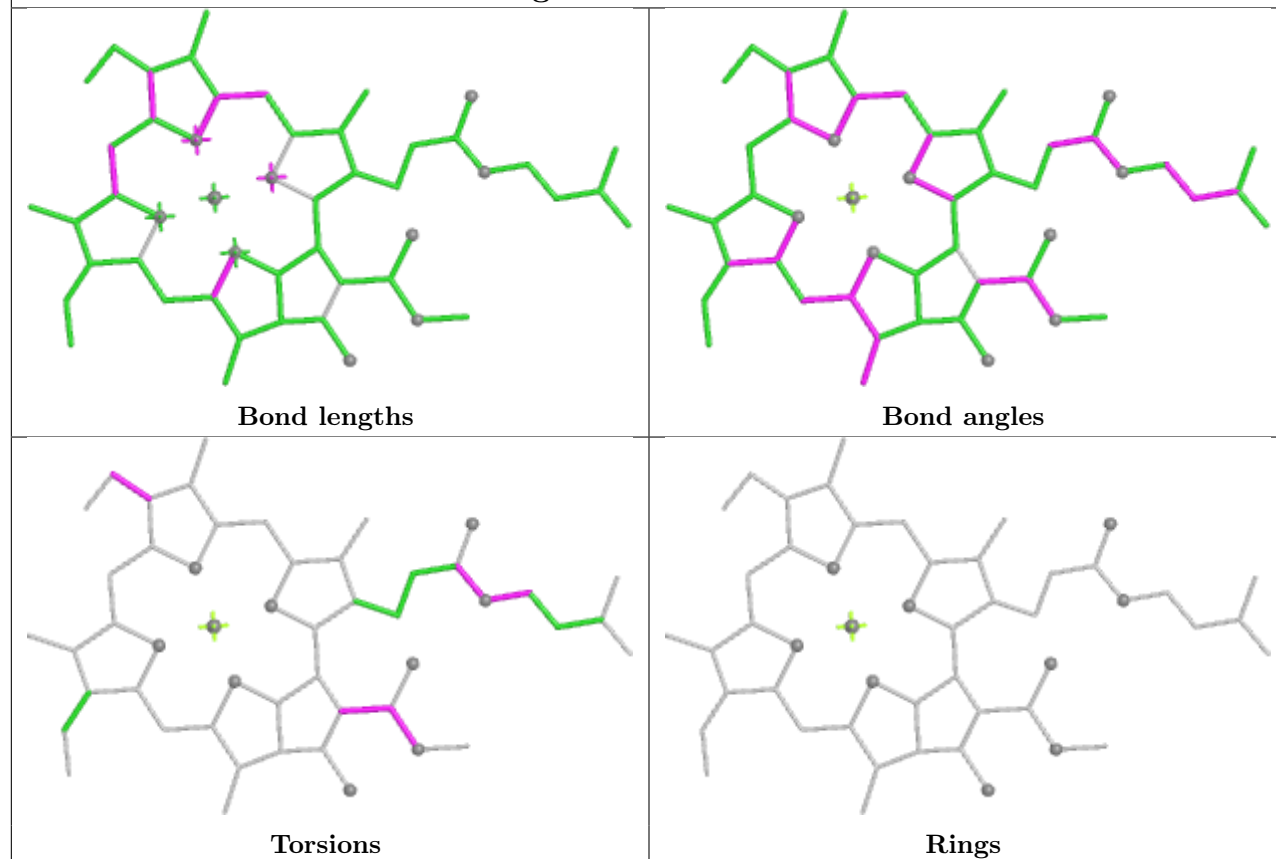




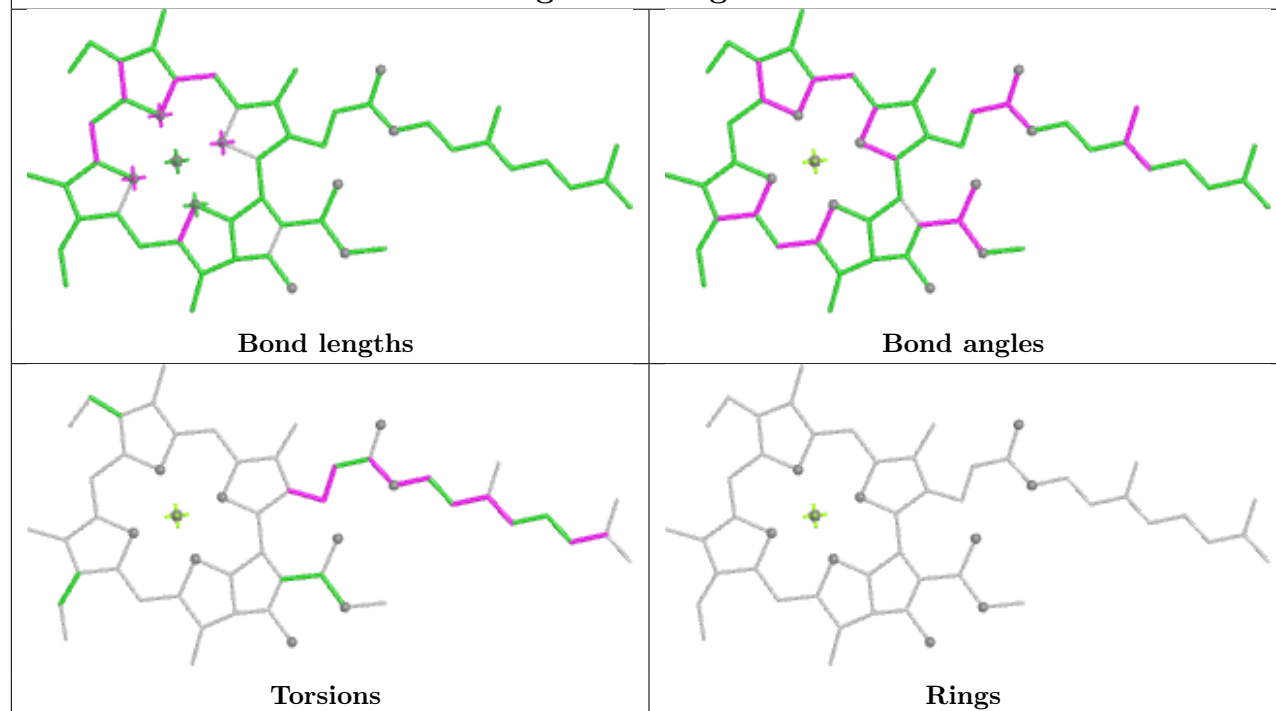
Ligand CLA d 611

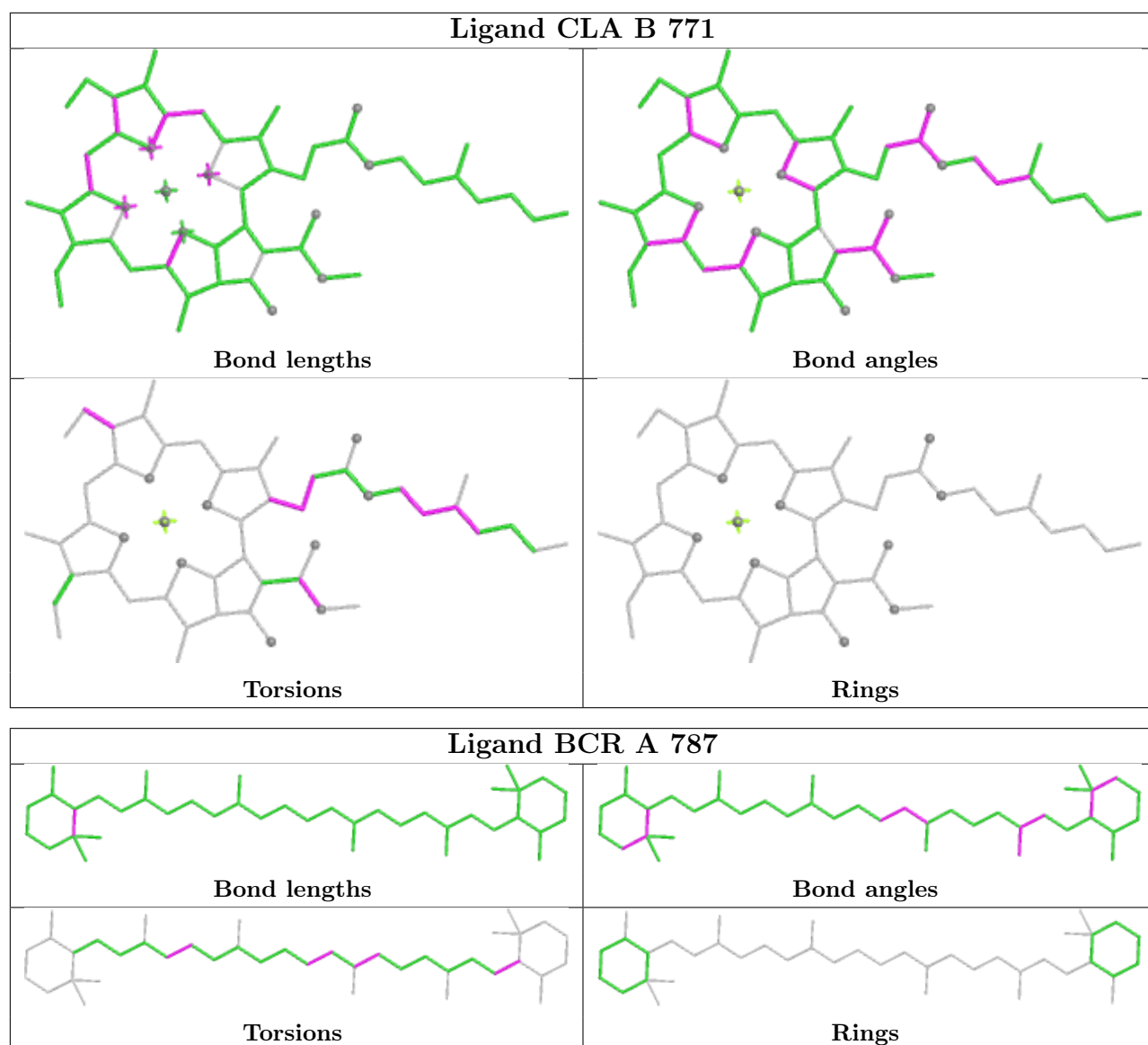


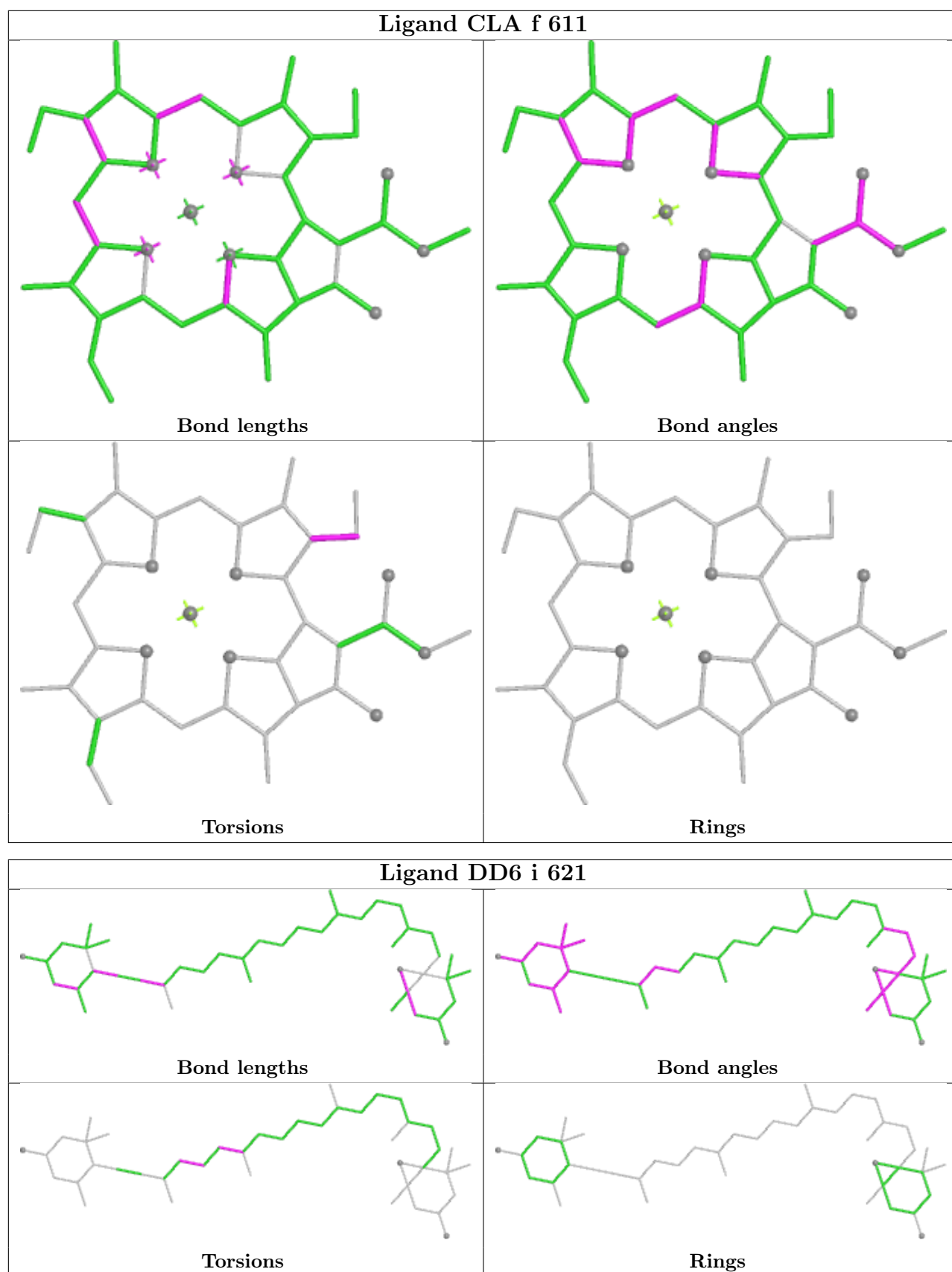
Ligand CLA B 751

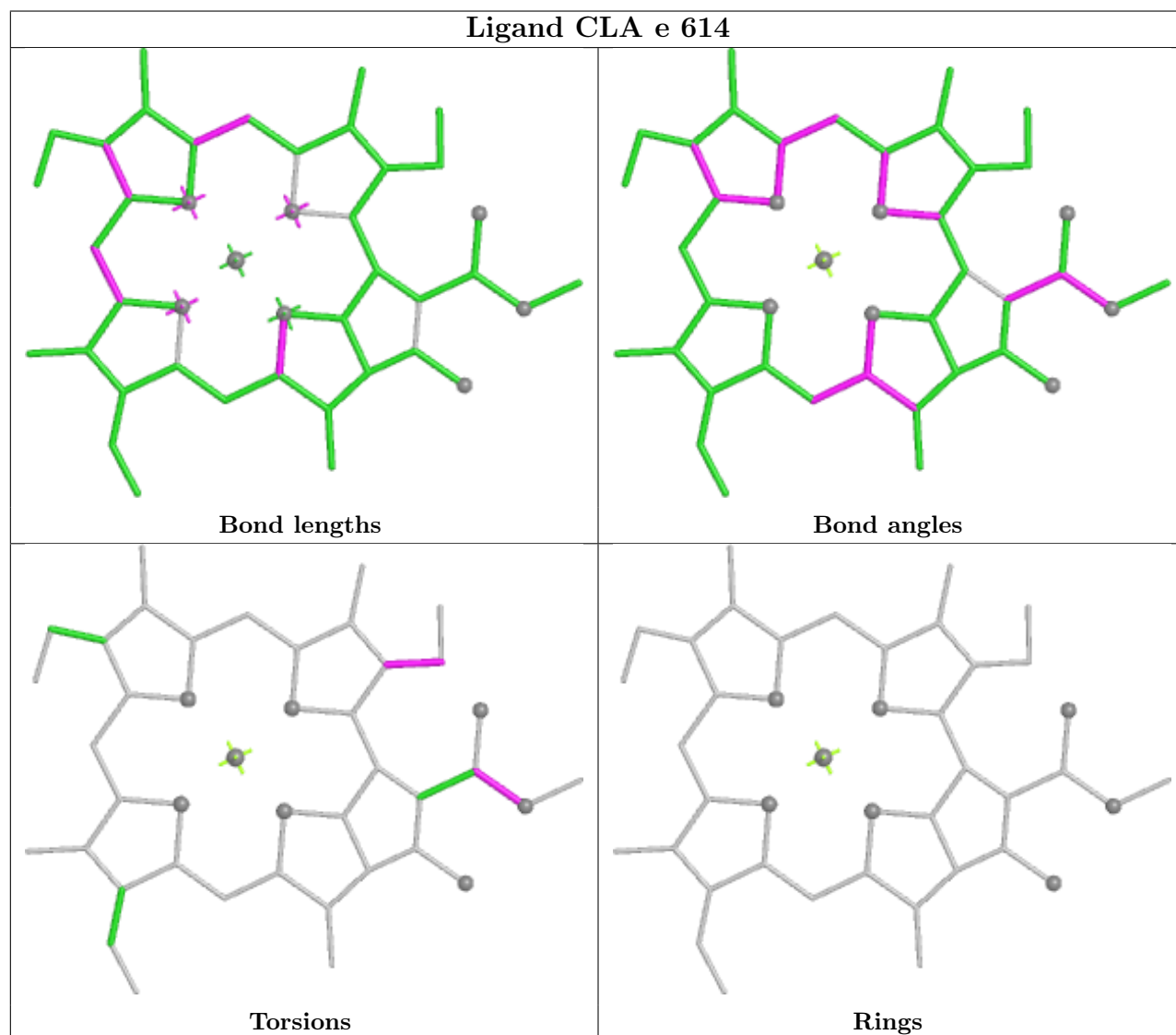
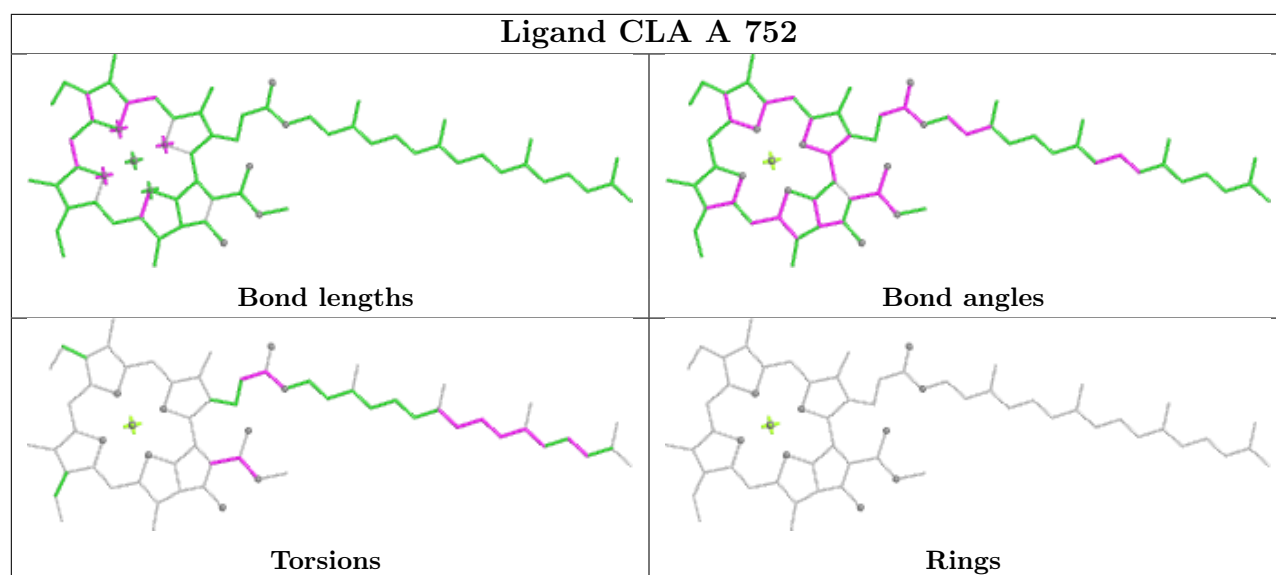


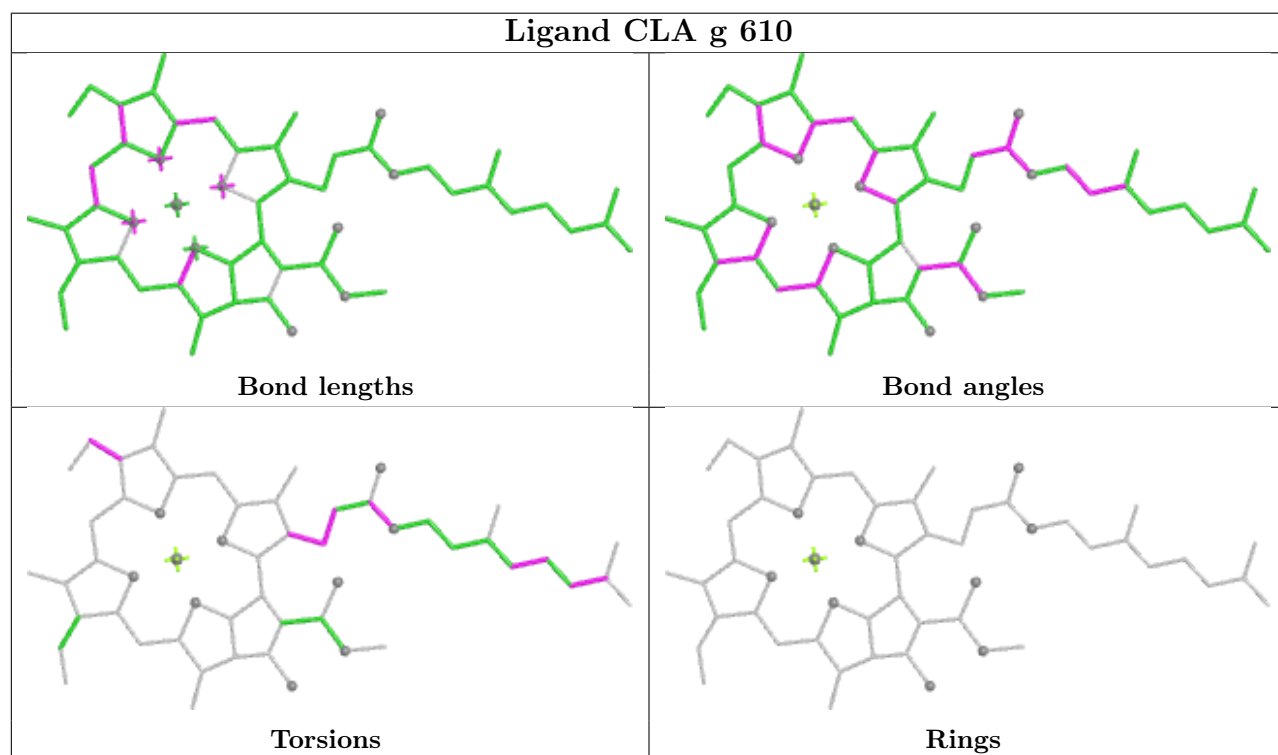
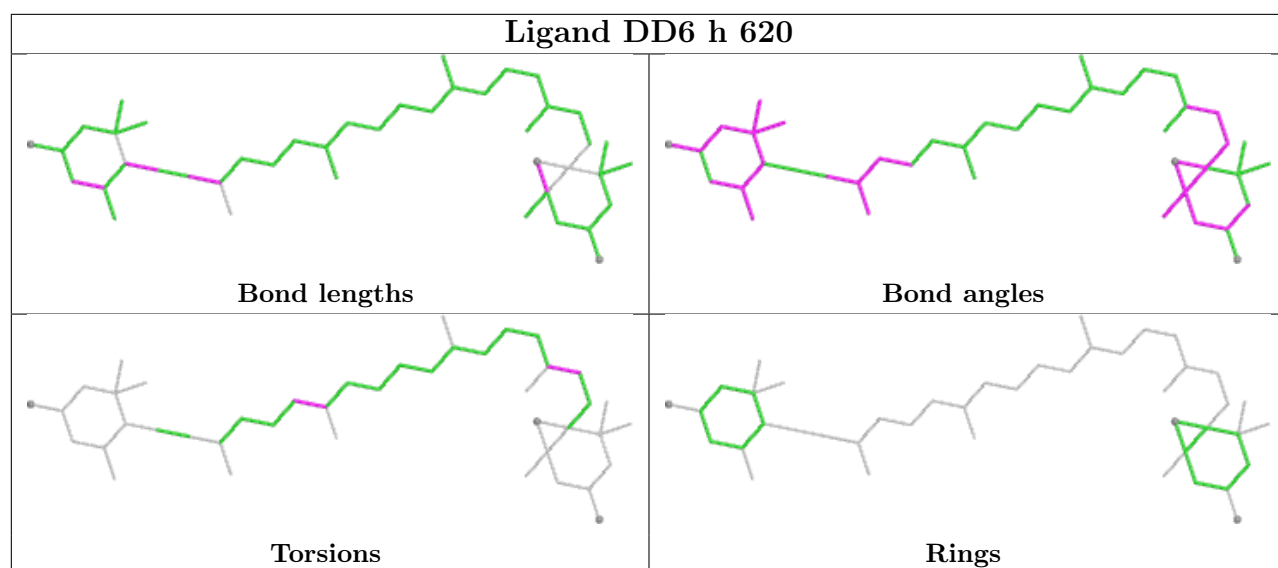
Ligand CLA g 613



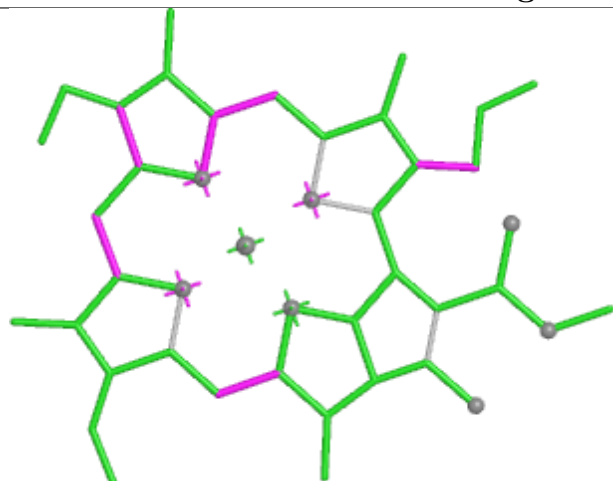




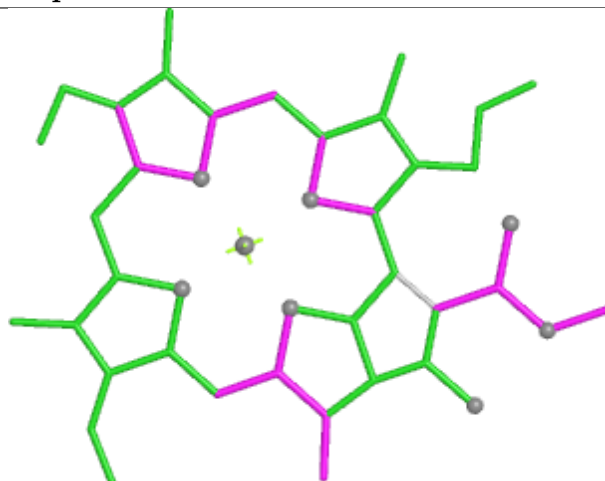




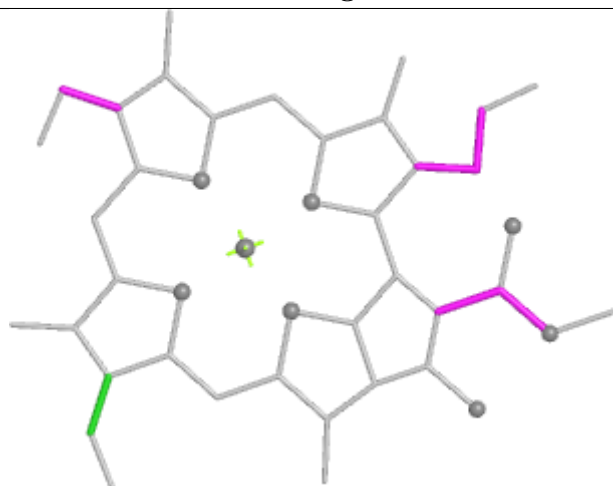
Ligand CLA p 602



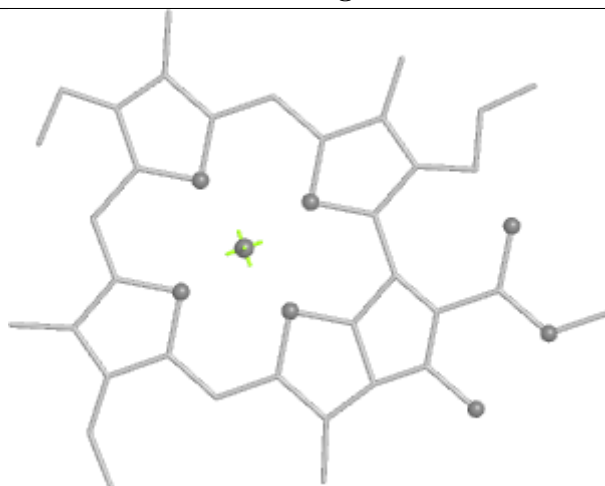
Bond lengths



Bond angles

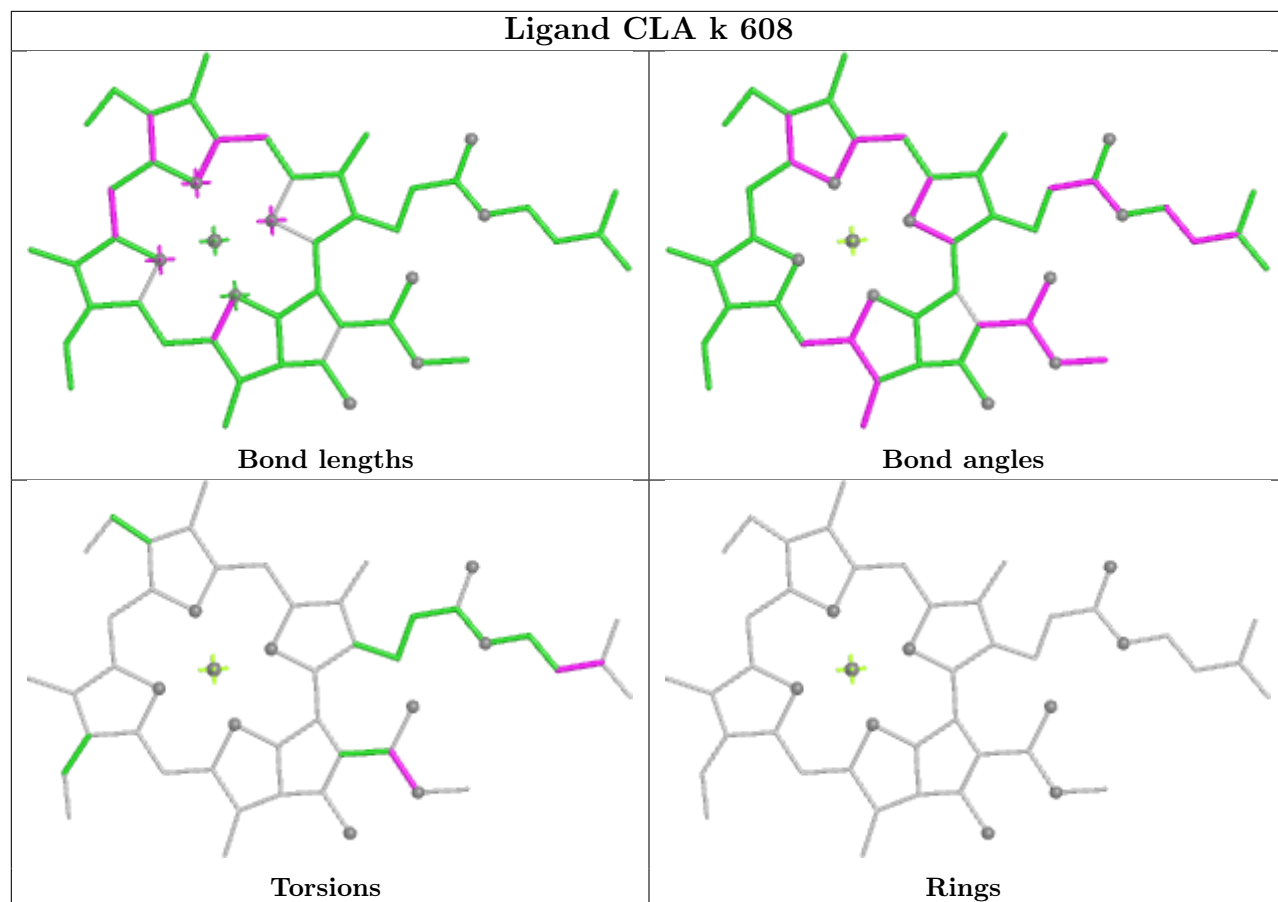


Torsions

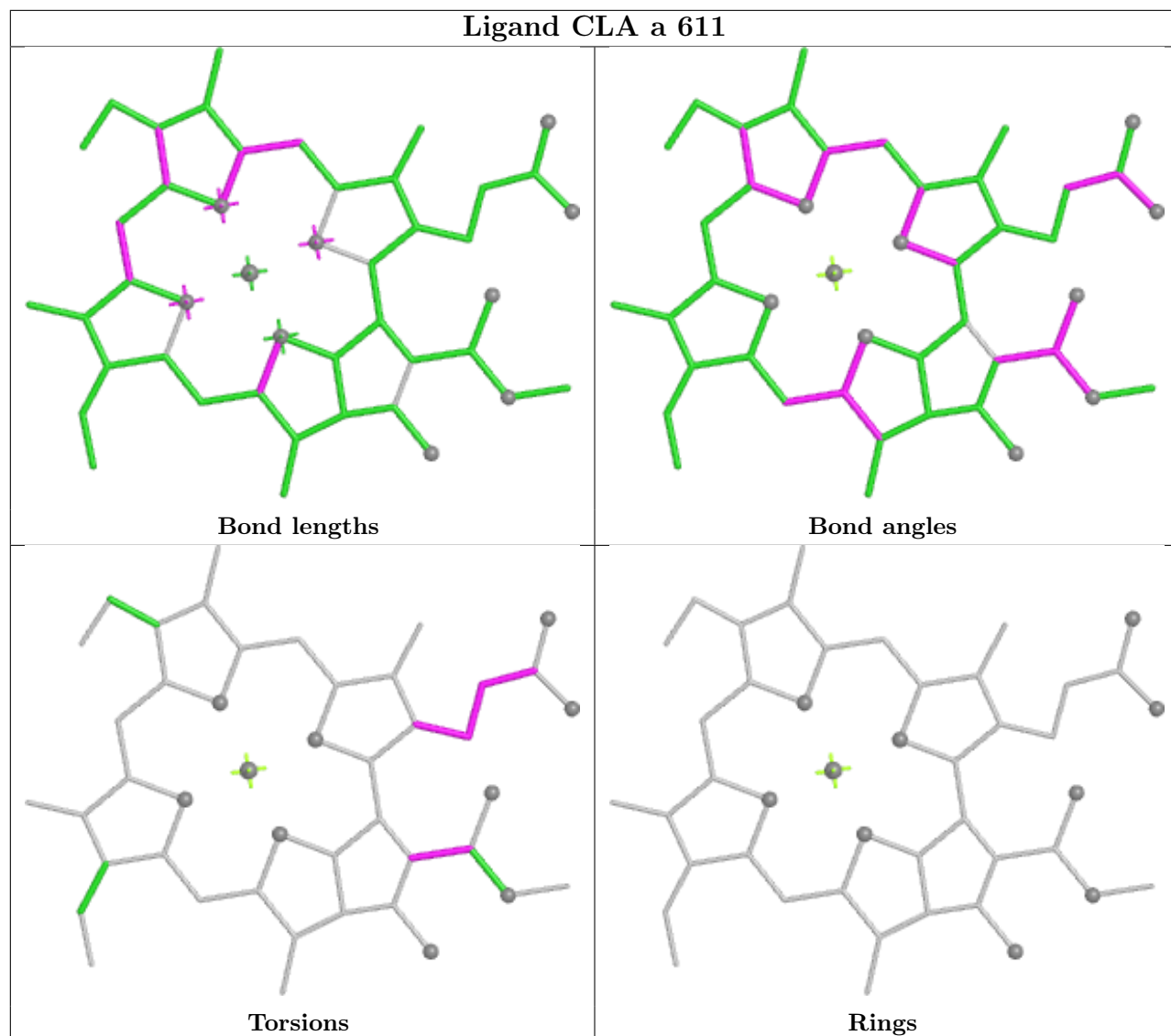


Rings

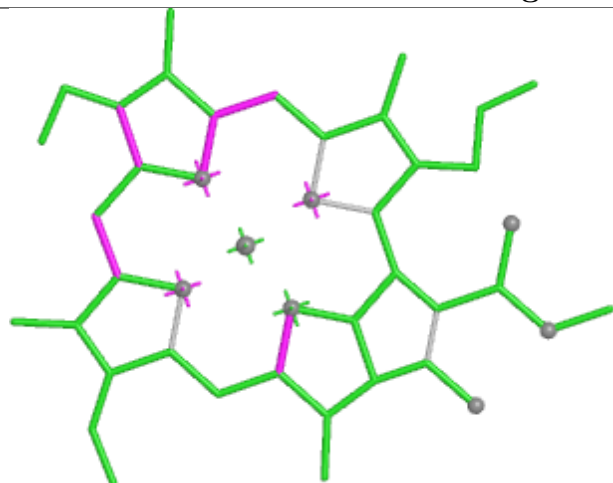
Ligand CLA k 608



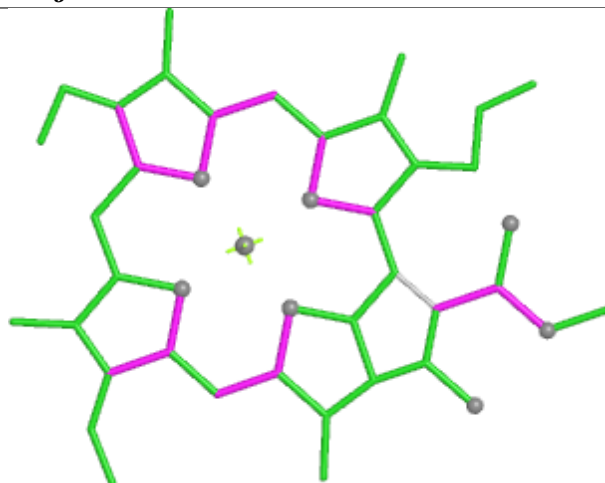
Ligand CLA a 611



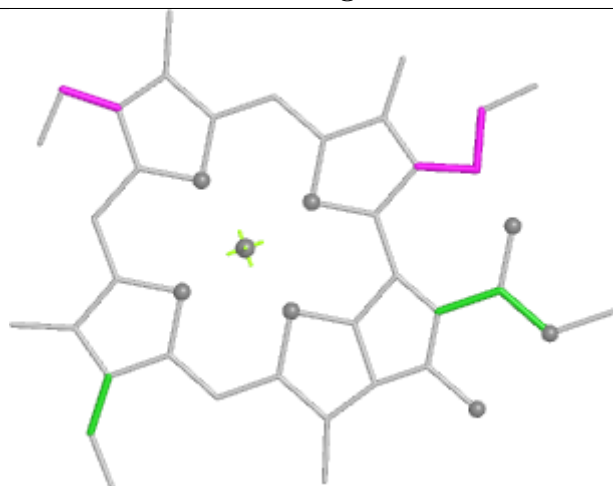
Ligand CLA j 615



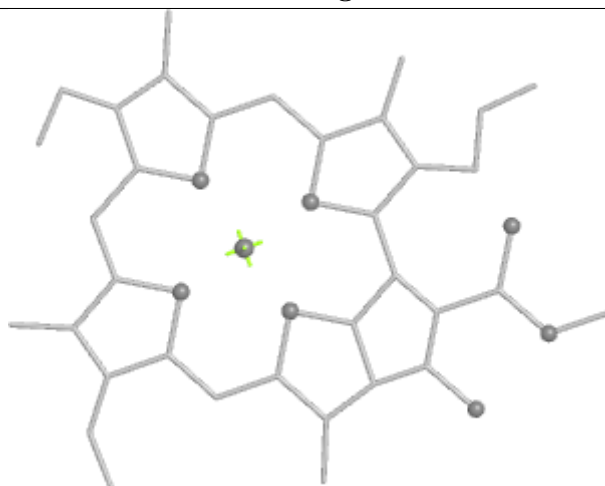
Bond lengths



Bond angles

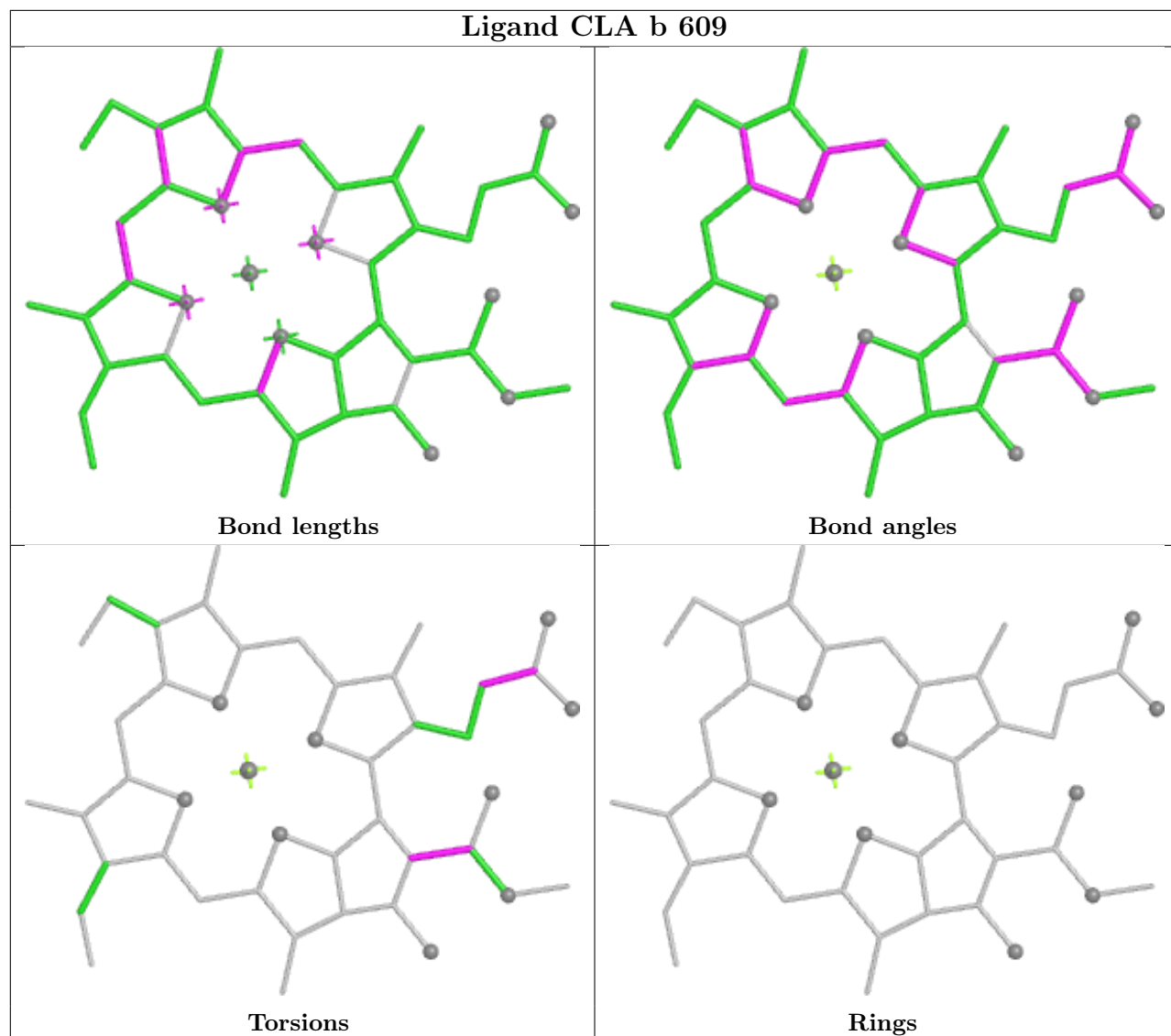


Torsions

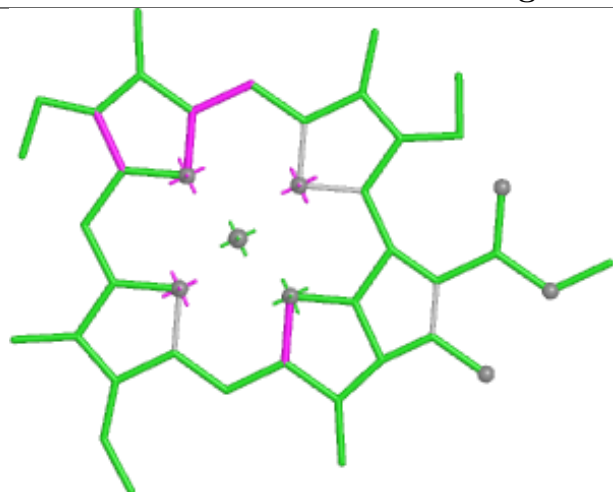


Rings

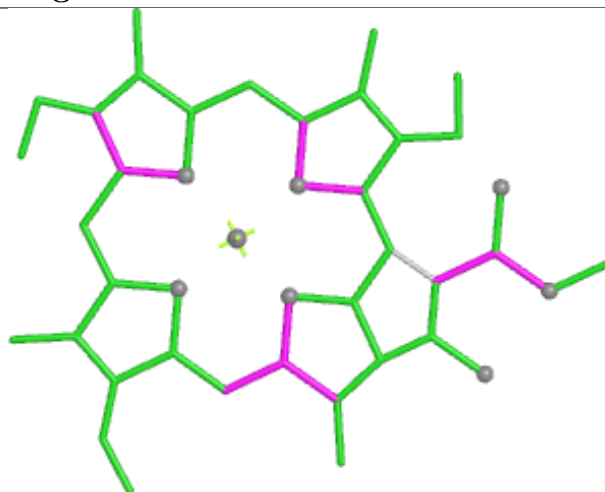
Ligand CLA b 609



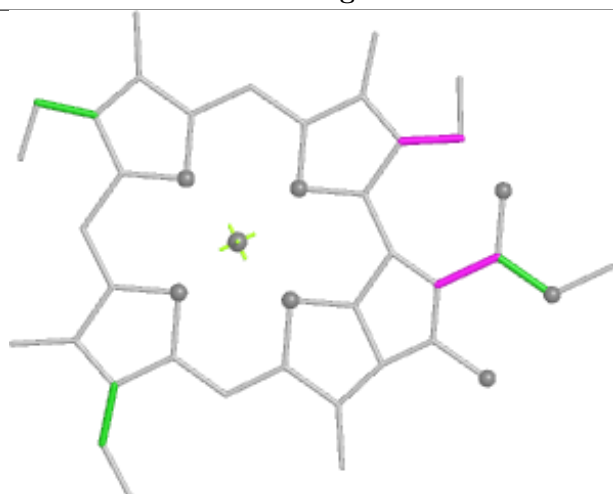
Ligand CLA g 603



Bond lengths



Bond angles

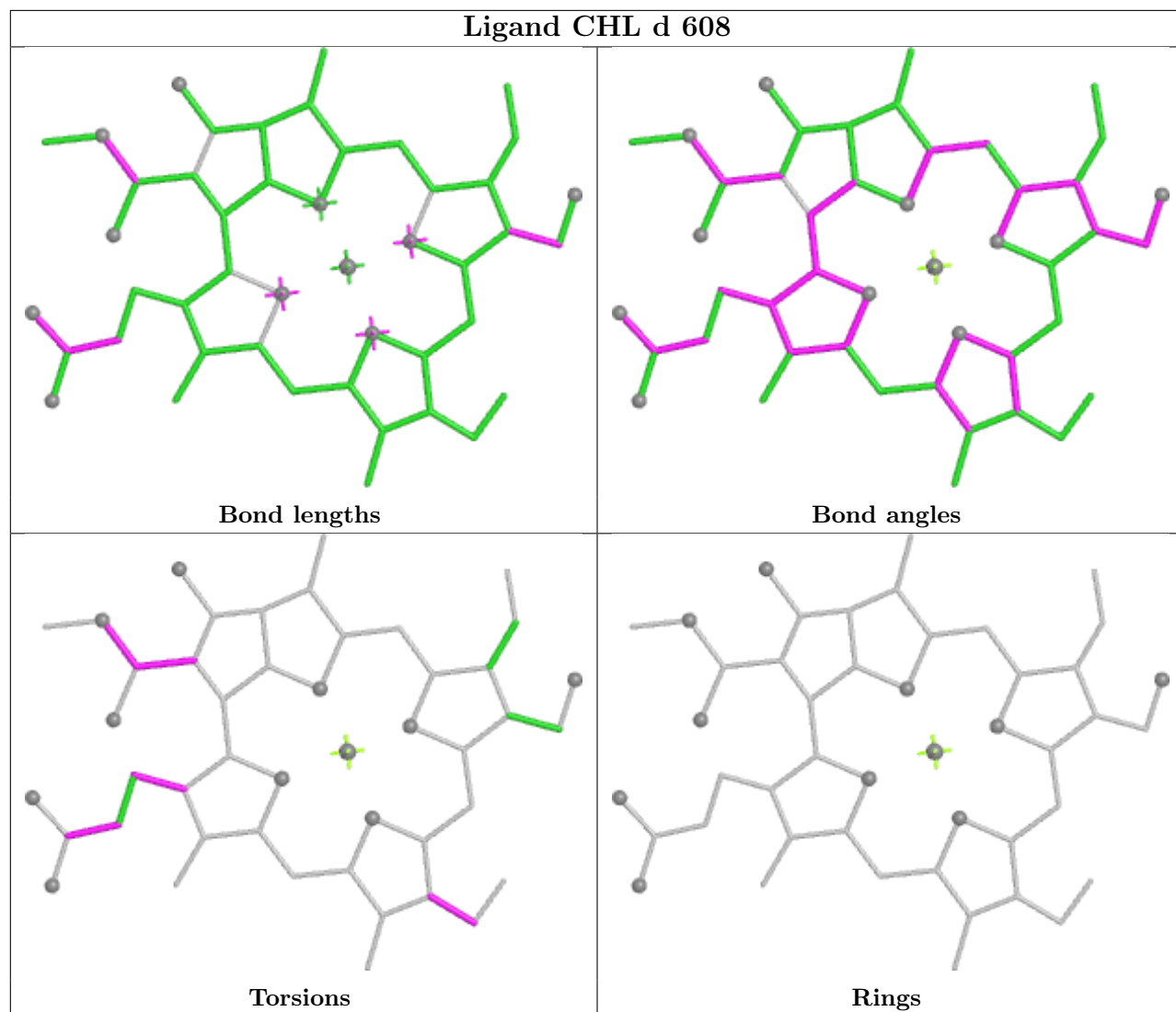


Torsions

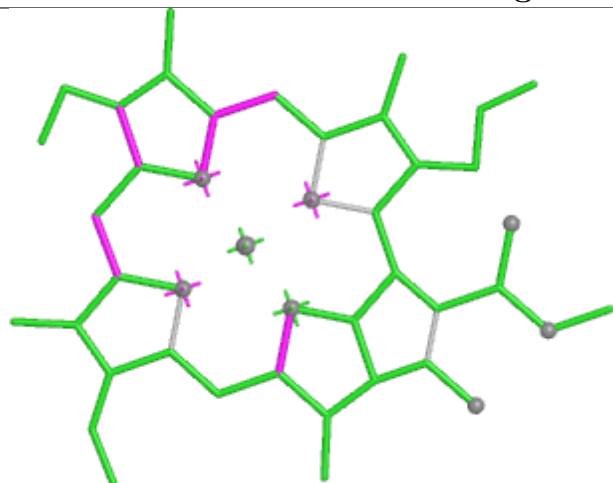


Rings

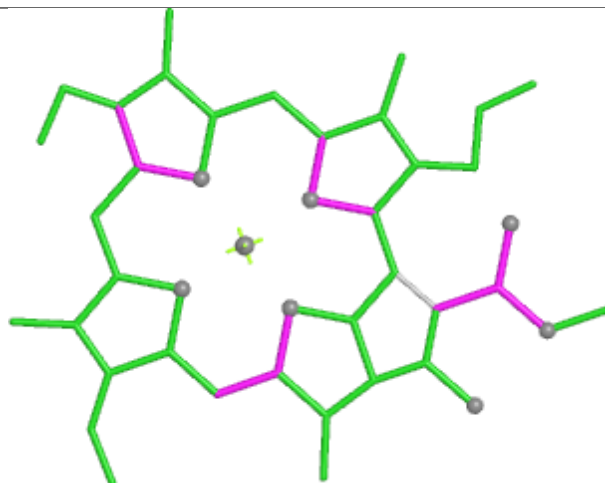
Ligand CHL d 608



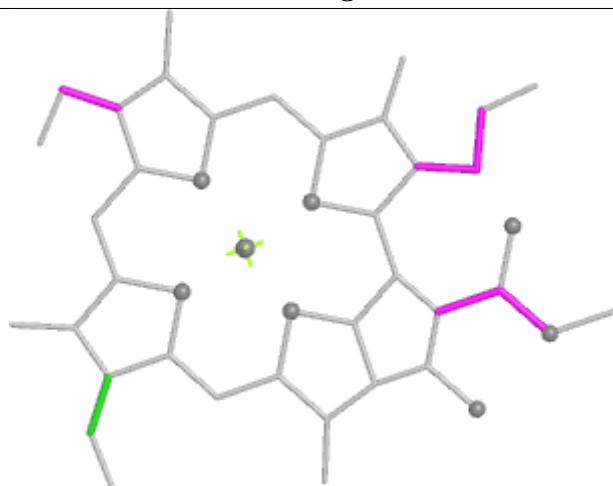
Ligand CLA B 754



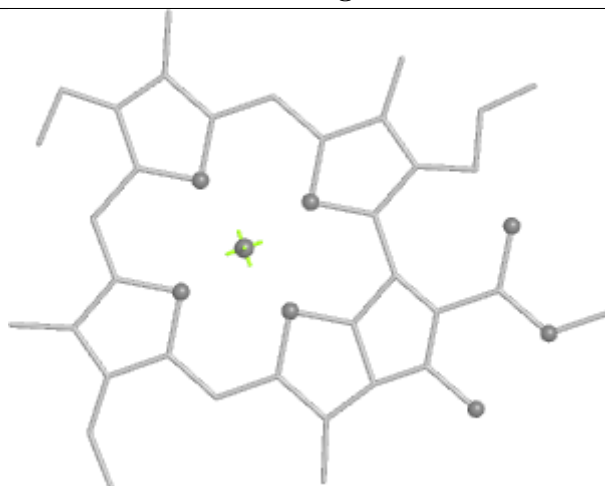
Bond lengths



Bond angles

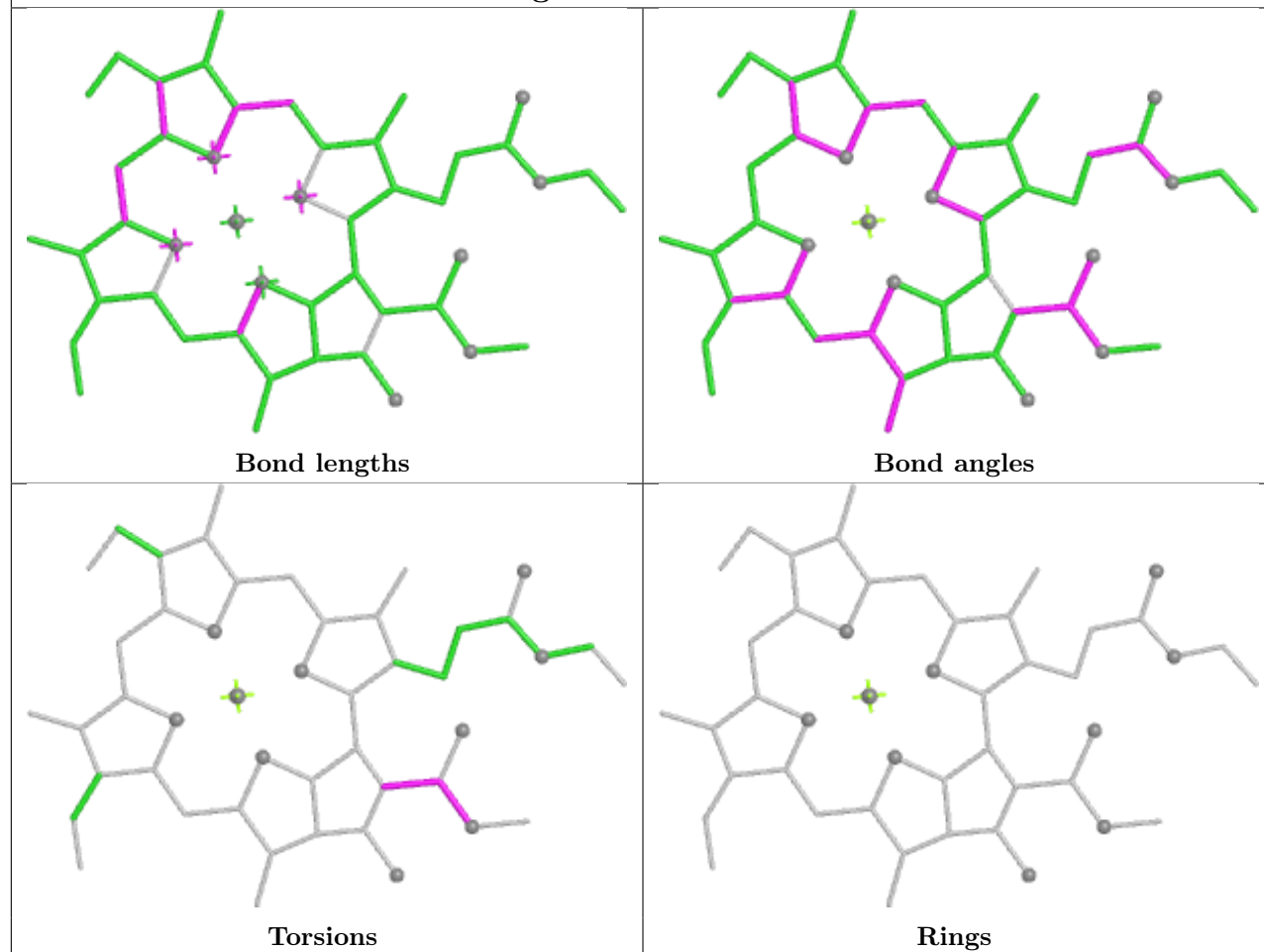


Torsions

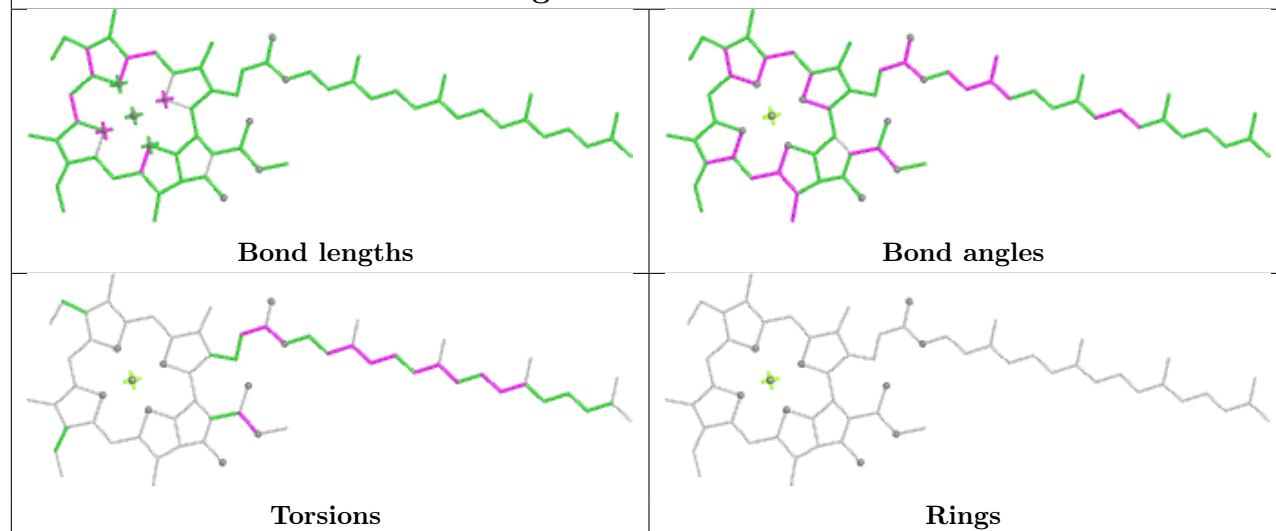


Rings

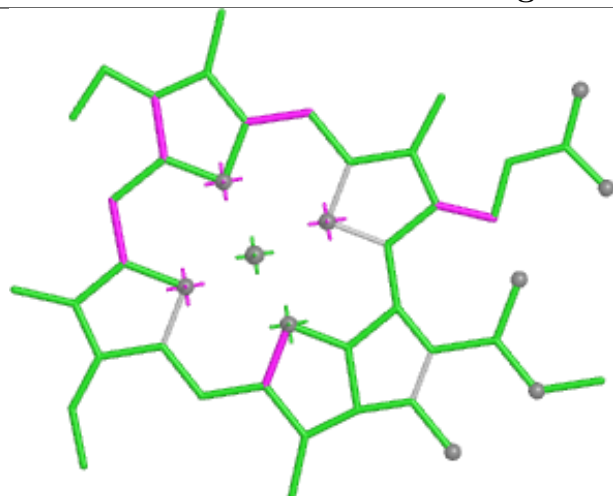
Ligand CLA c 616



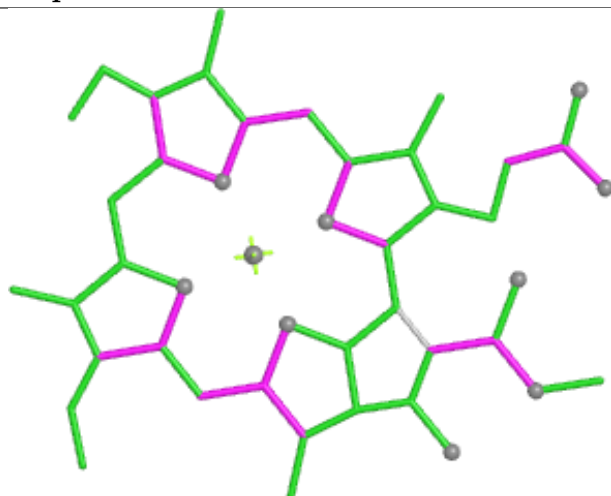
Ligand CLA B 739



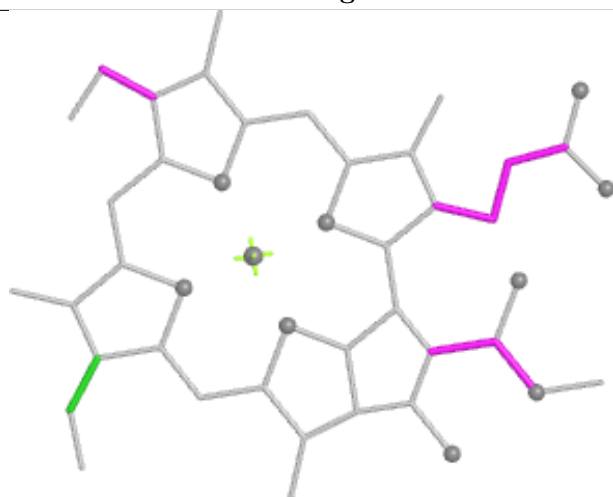
Ligand CLA p 610



Bond lengths



Bond angles

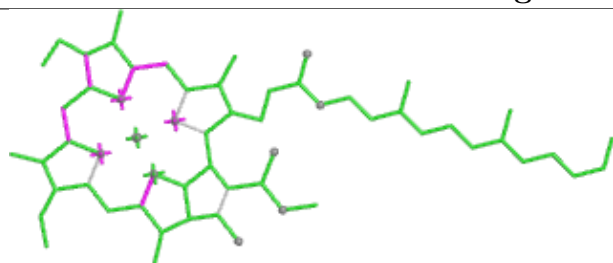


Torsions

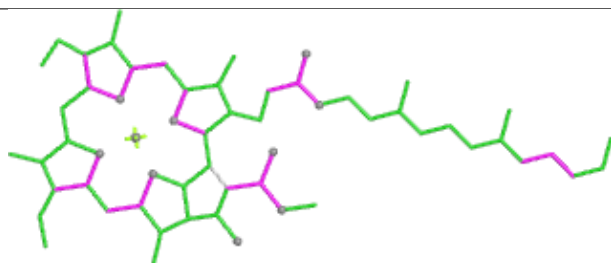


Rings

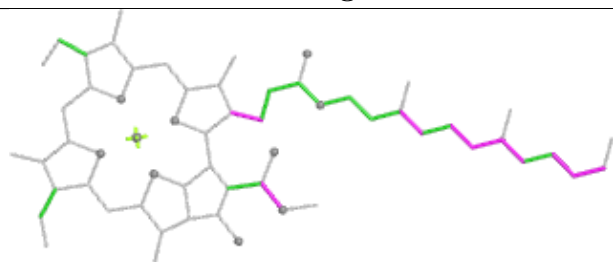
Ligand CLA B 748



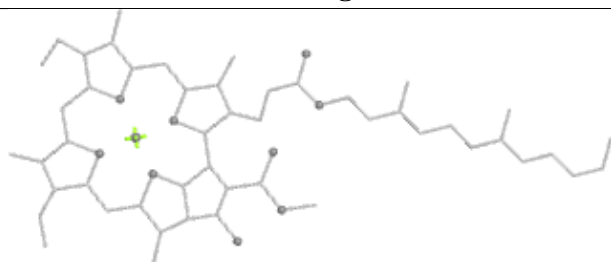
Bond lengths



Bond angles

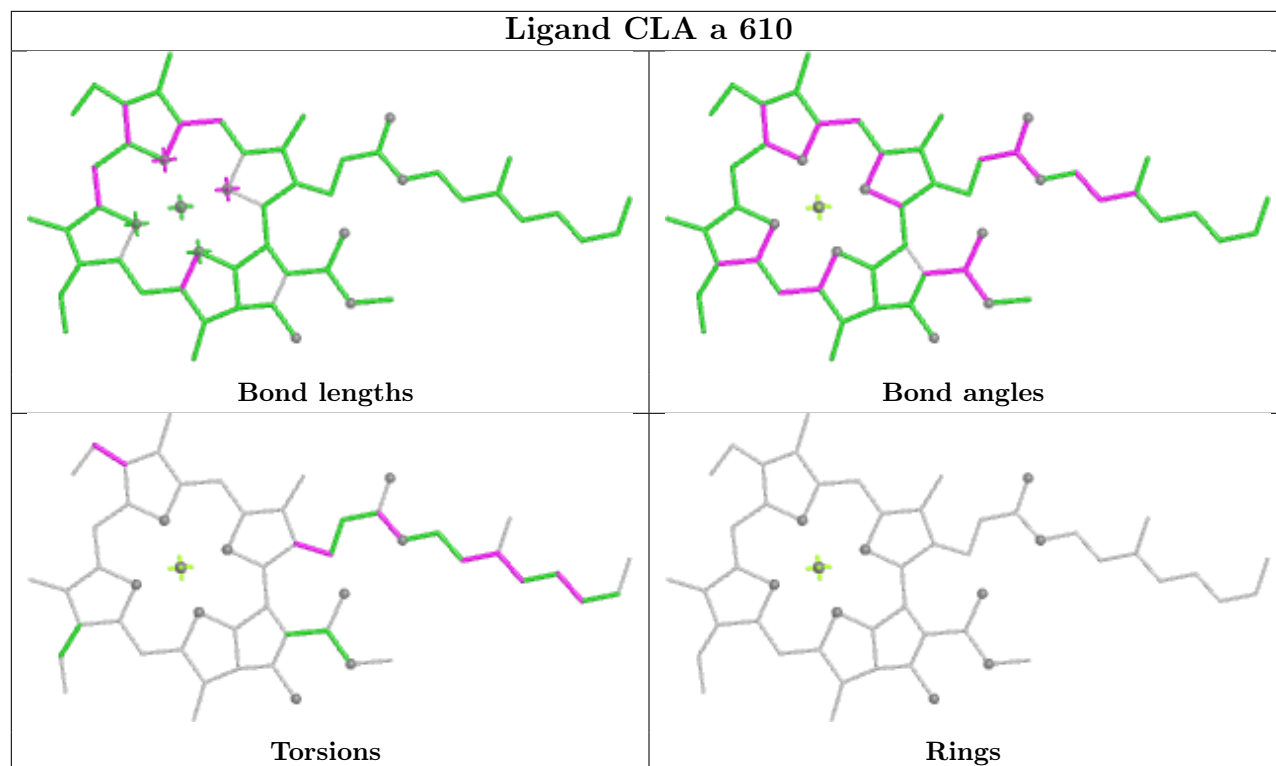


Torsions

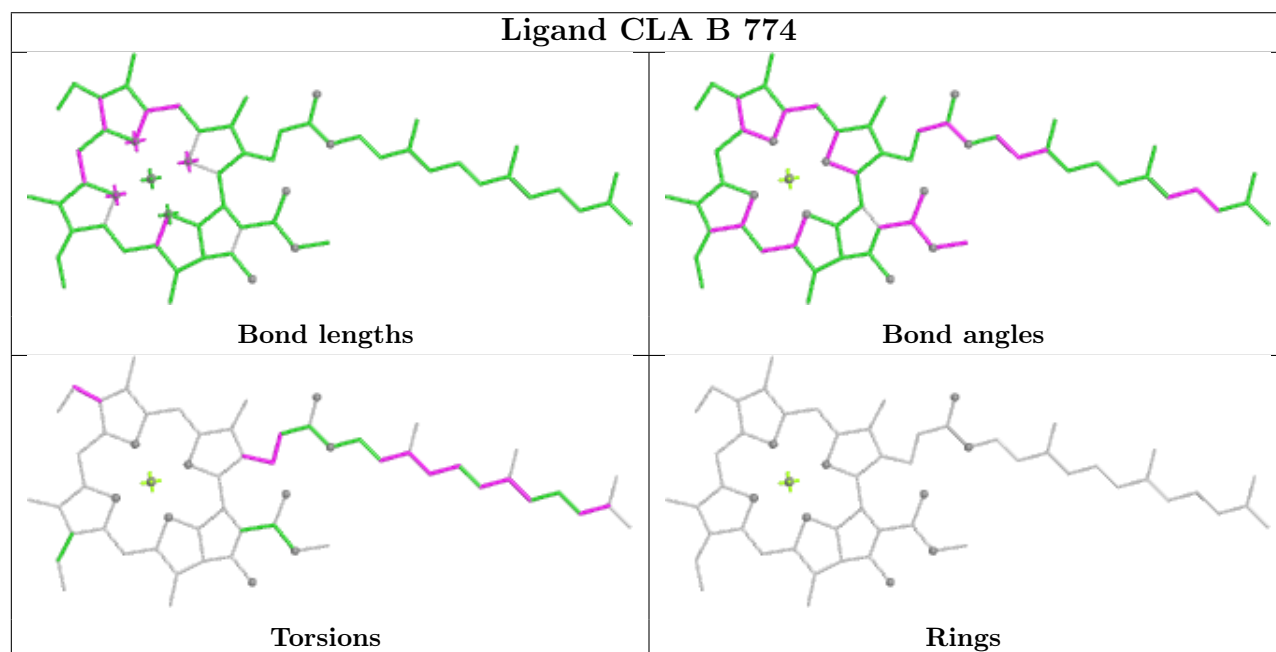


Rings

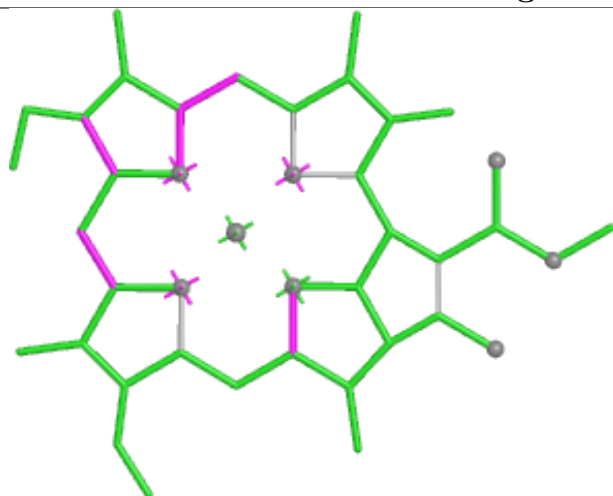
Ligand CLA a 610



Ligand CLA B 774



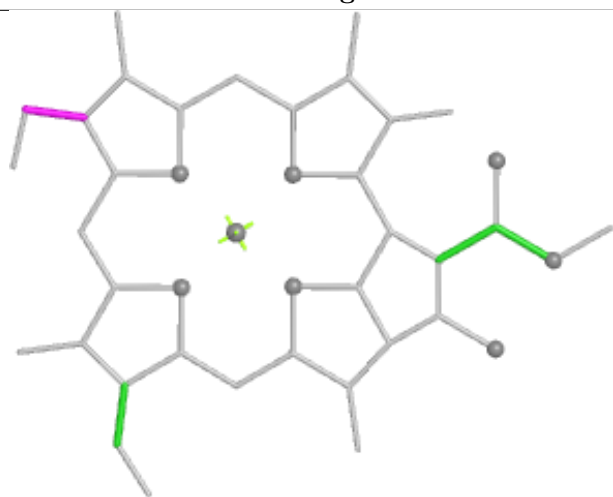
Ligand CLA b 608



Bond lengths



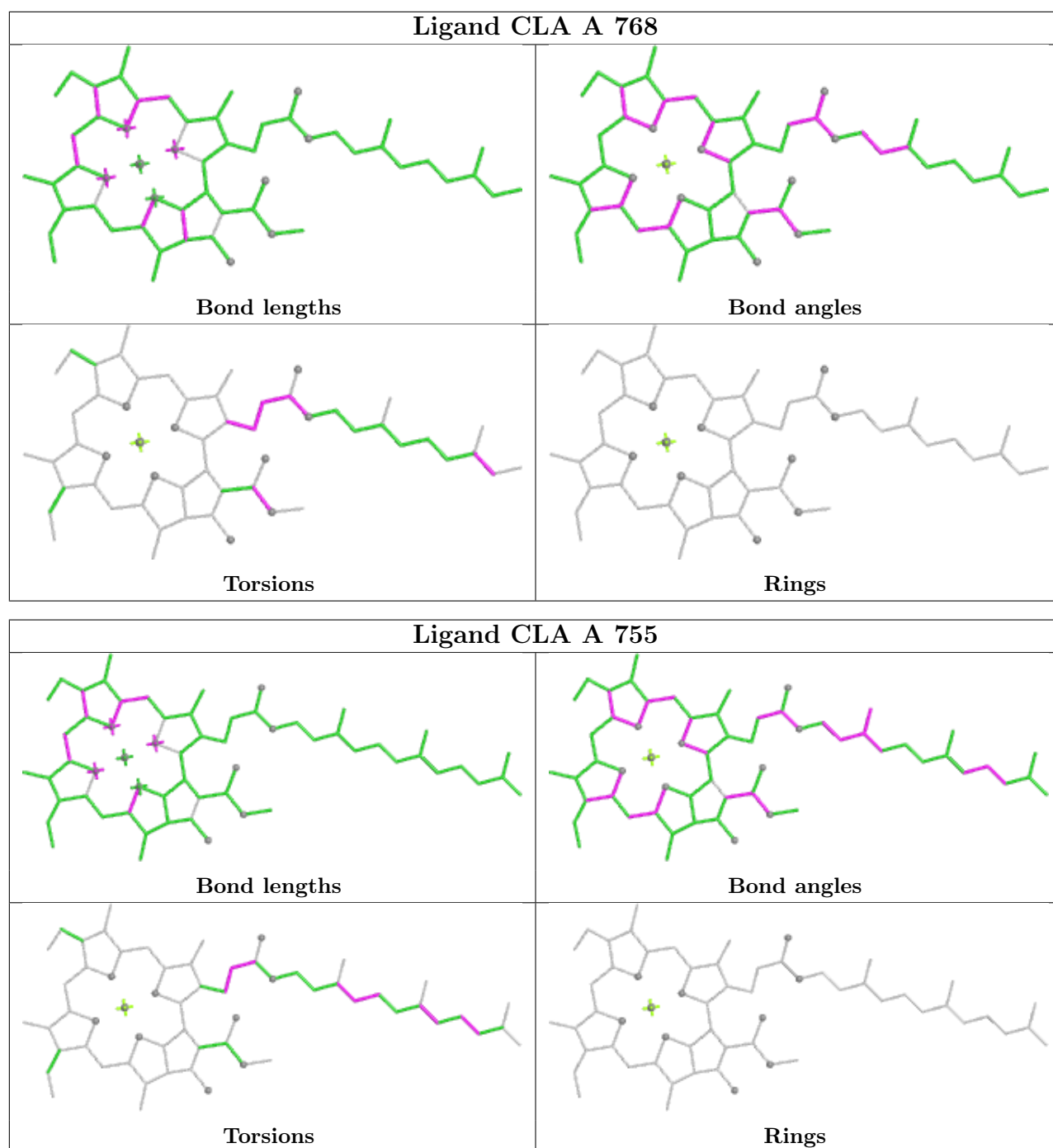
Bond angles

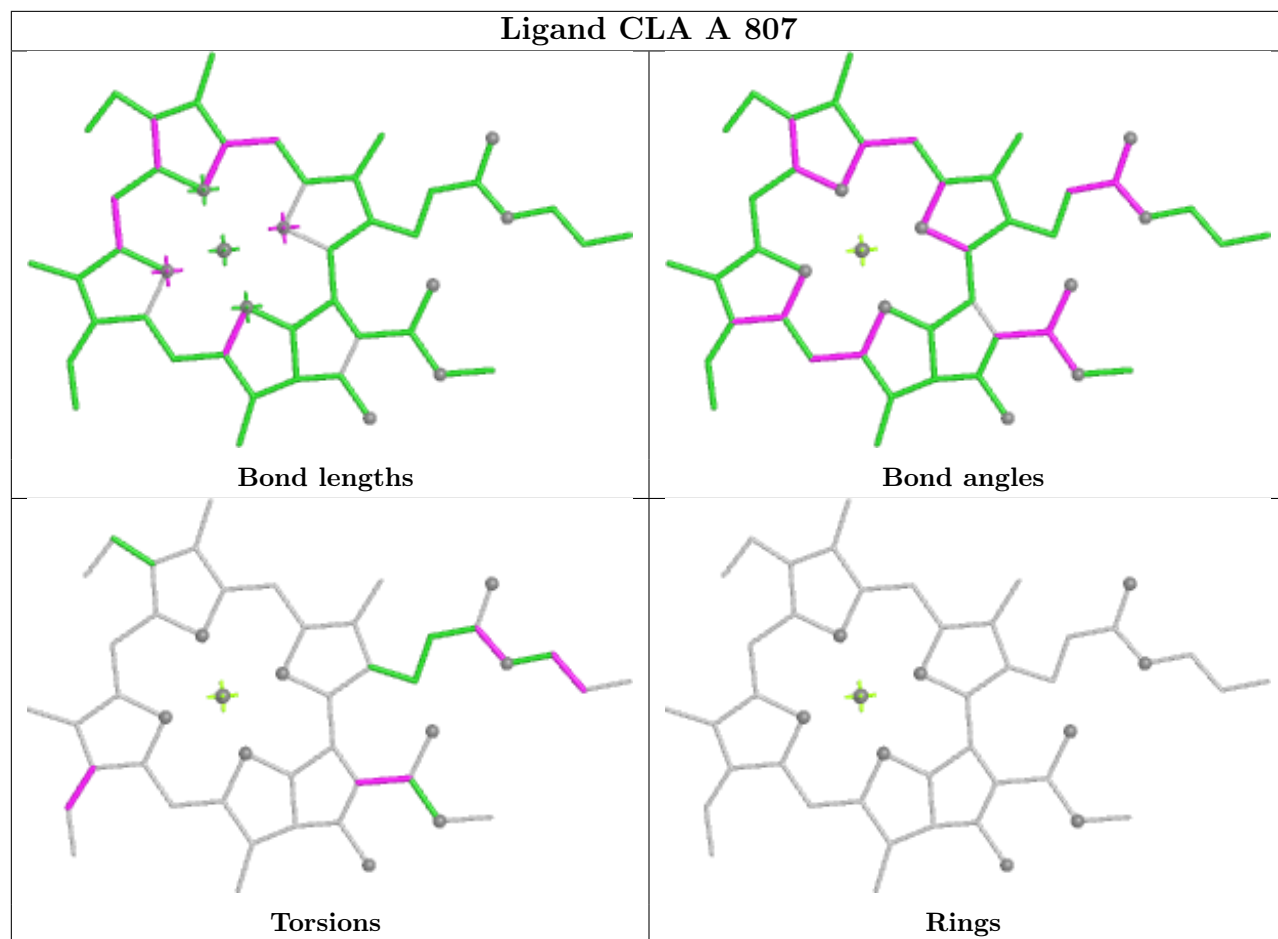


Torsions

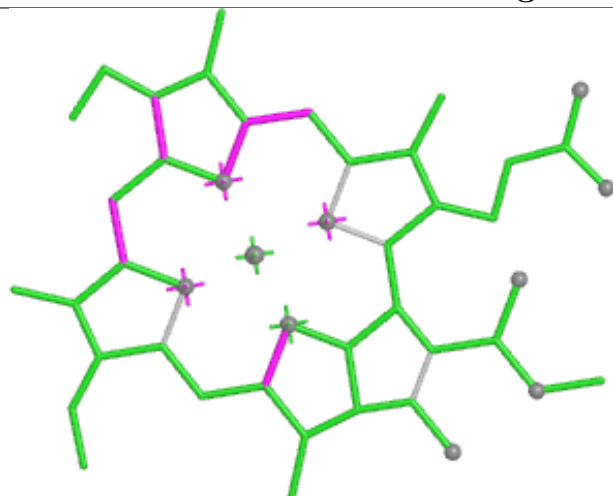


Rings

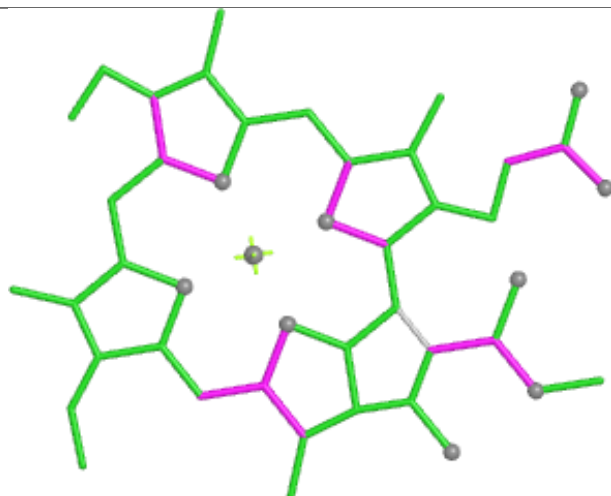




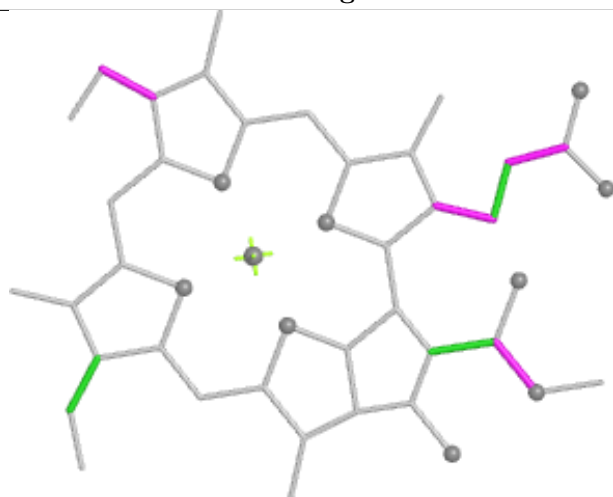
Ligand CLA n 609



Bond lengths



Bond angles

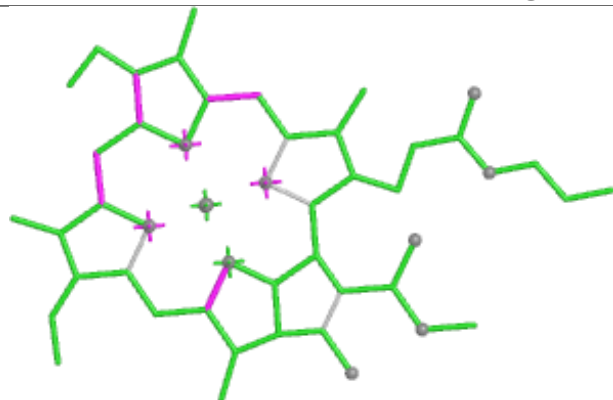


Torsions

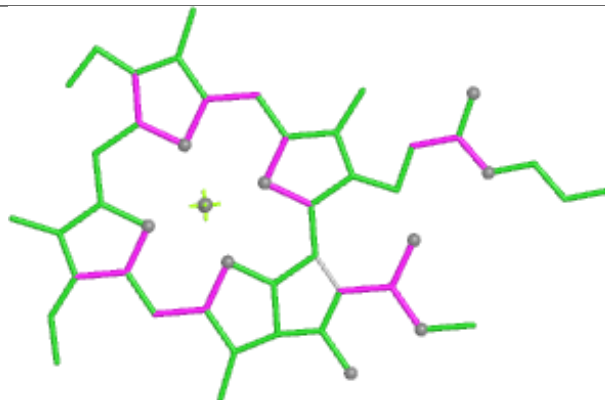


Rings

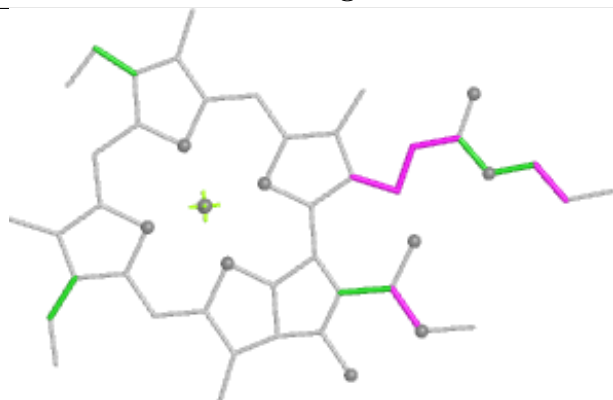
Ligand CLA l 613



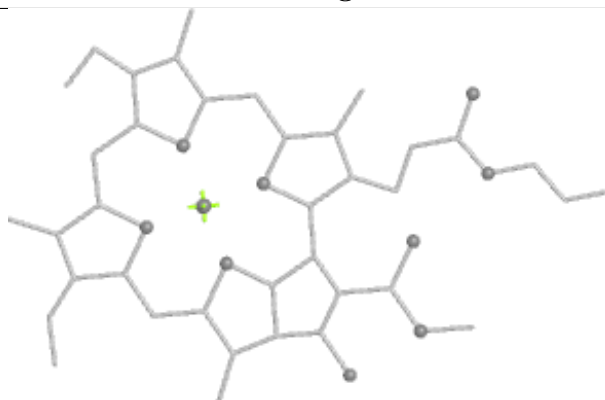
Bond lengths



Bond angles

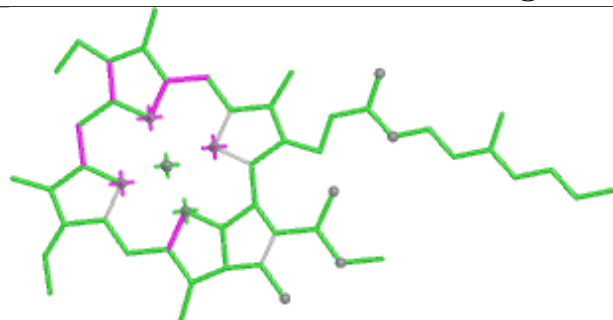


Torsions

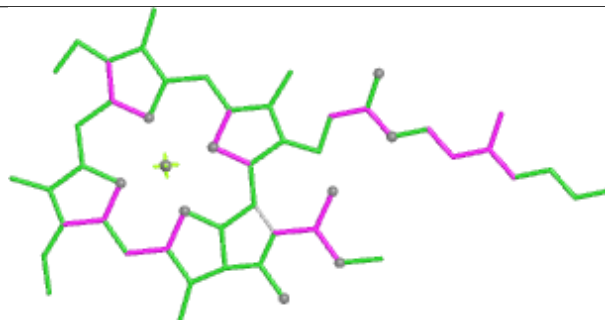


Rings

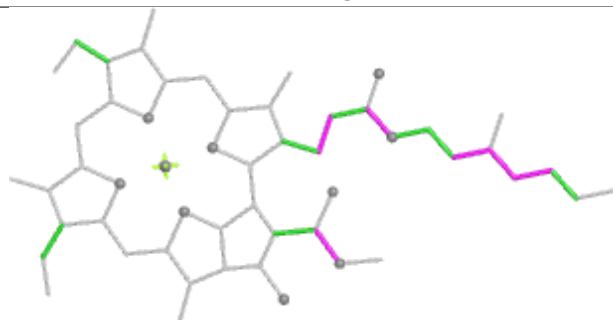
Ligand CLA c 613



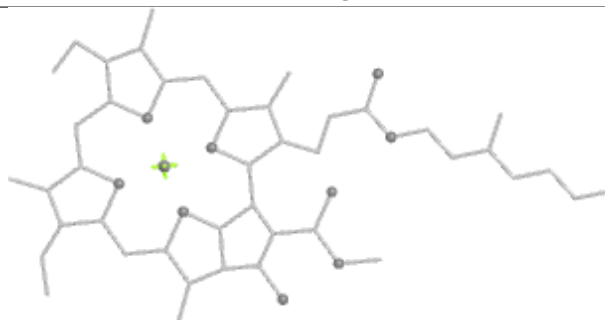
Bond lengths



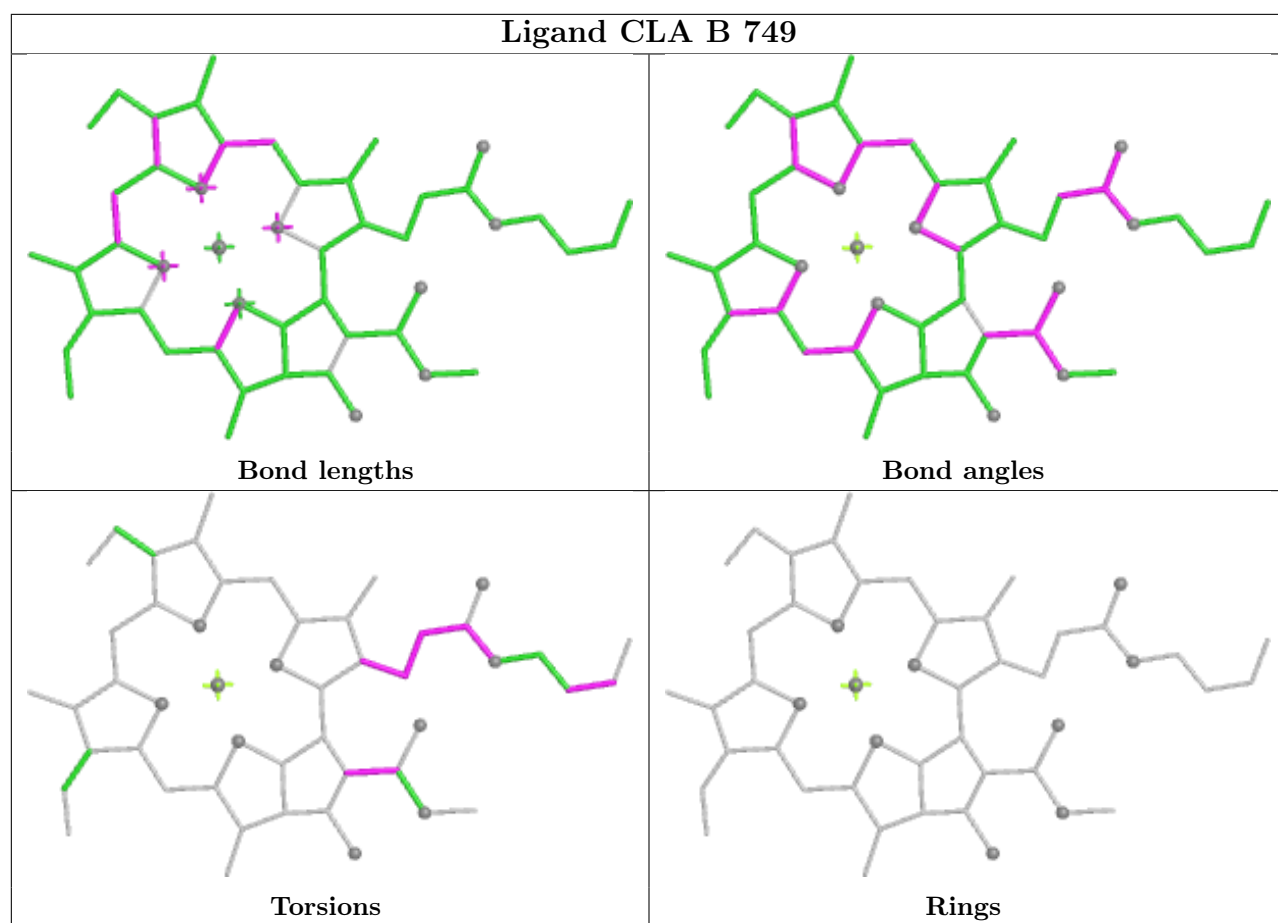
Bond angles



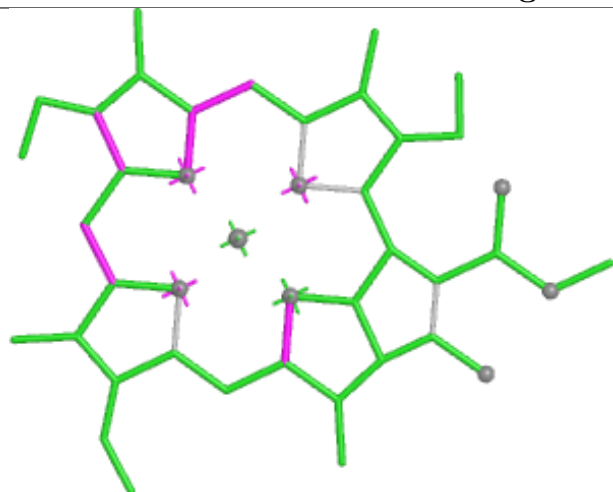
Torsions



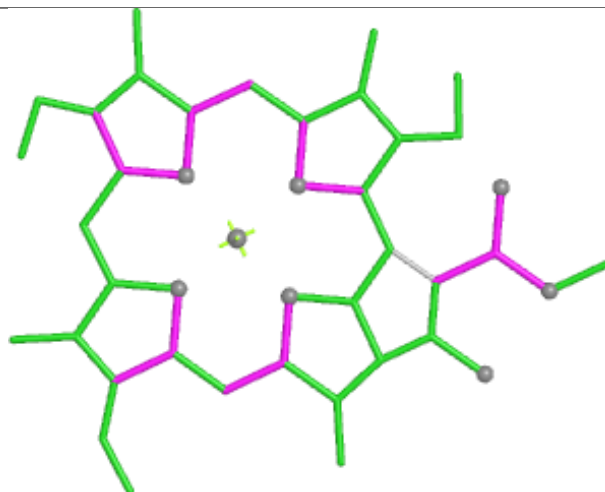
Rings



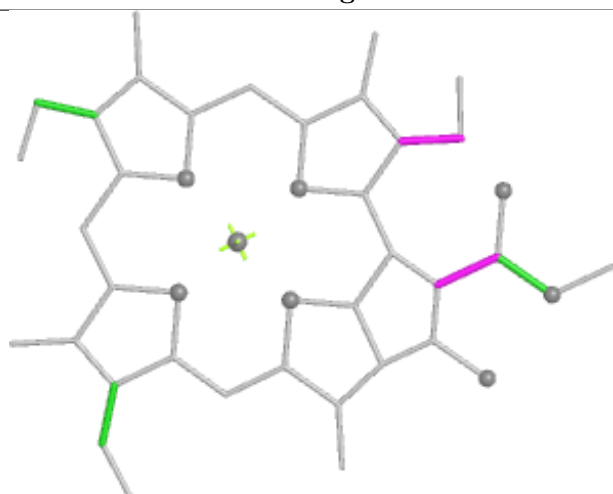
Ligand CLA e 605



Bond lengths



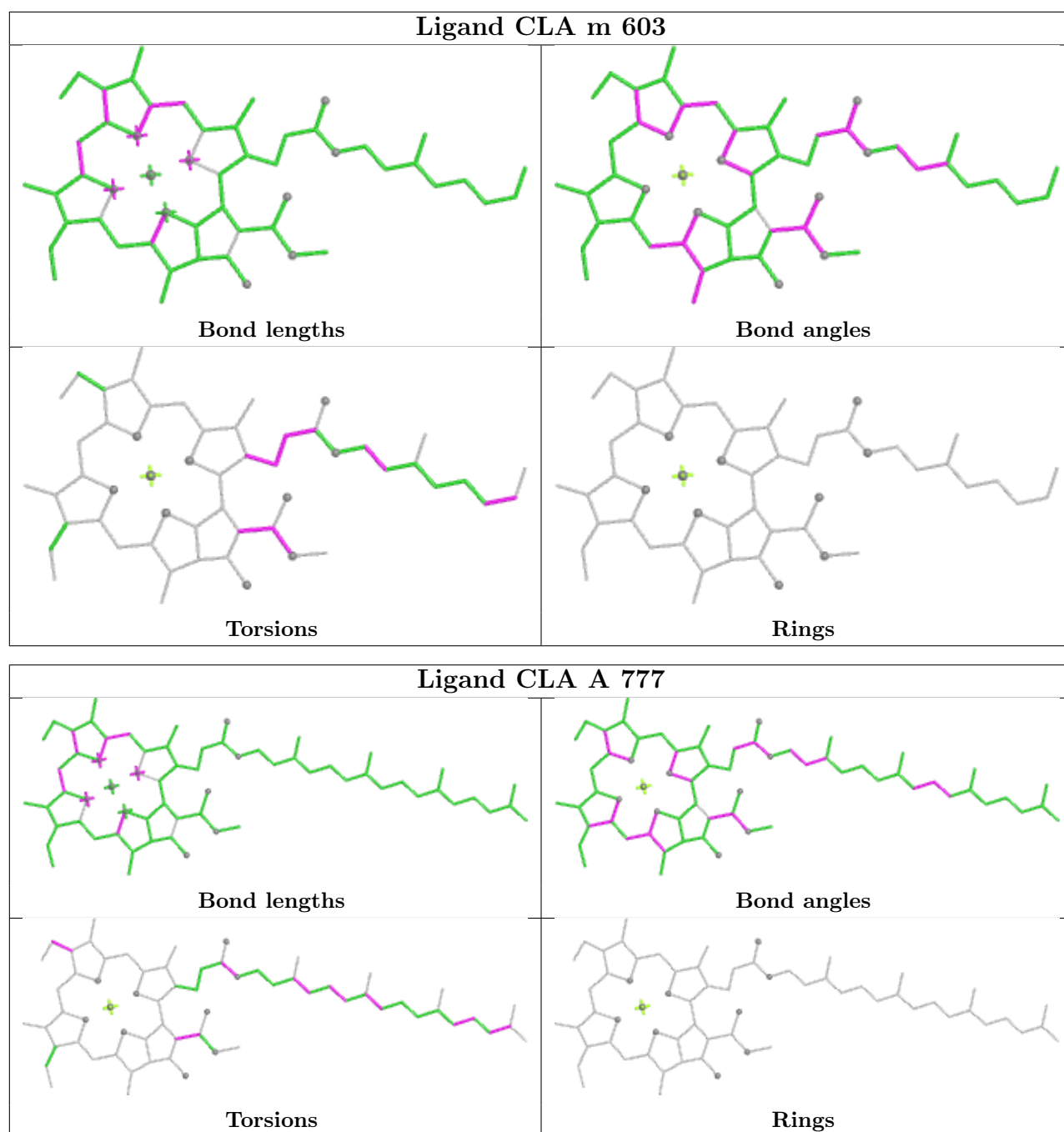
Bond angles

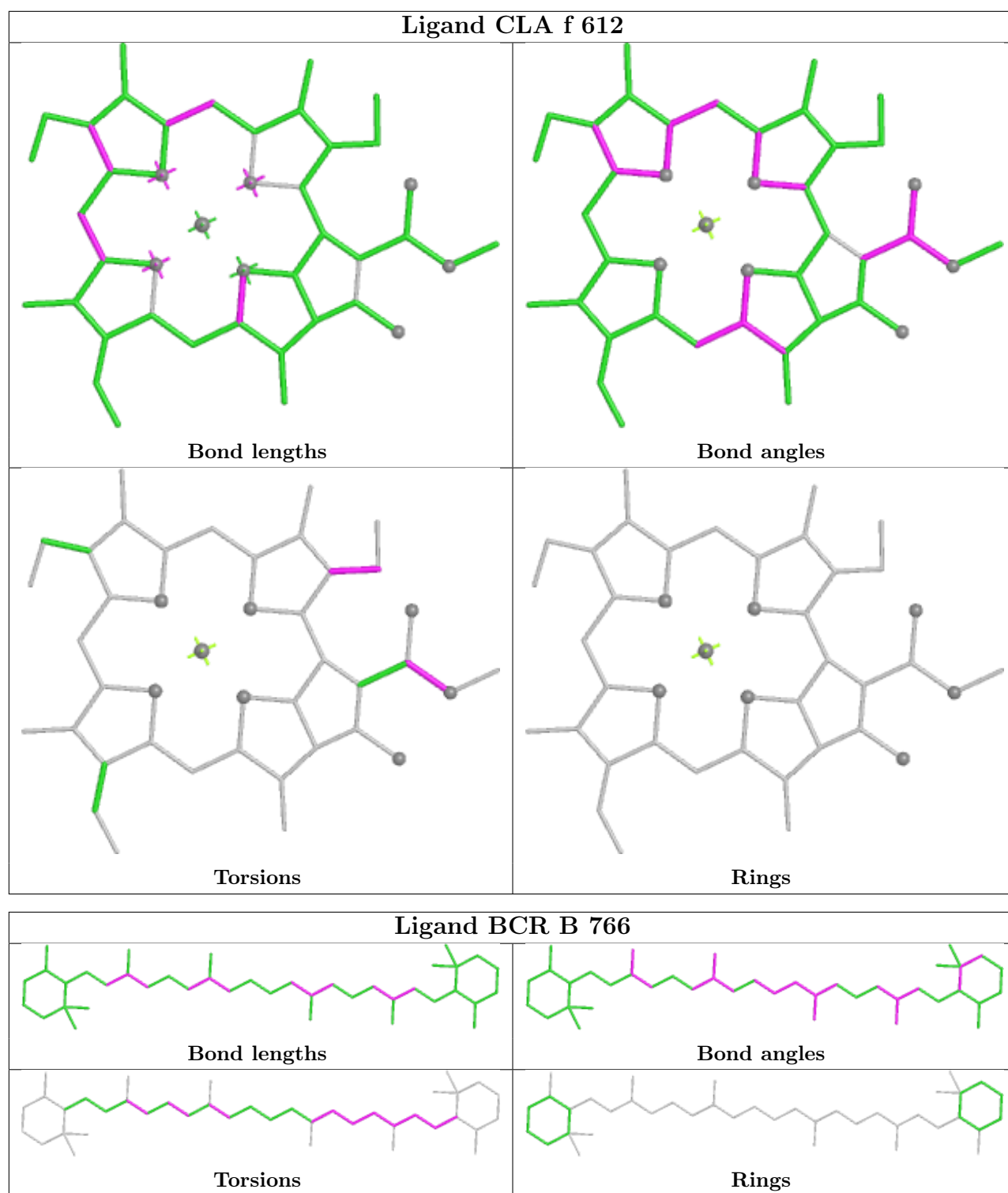


Torsions



Rings





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

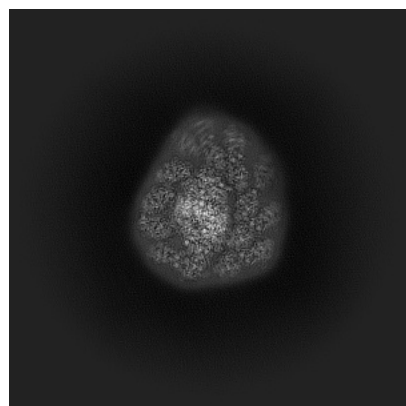
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-64823. These allow visual inspection of the internal detail of the map and identification of artifacts.

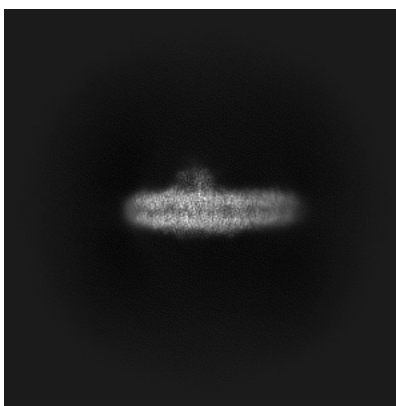
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

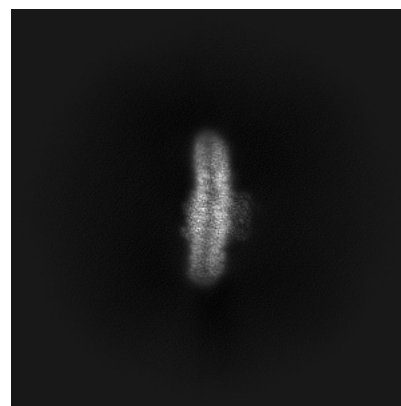
6.1.1 Primary map



X

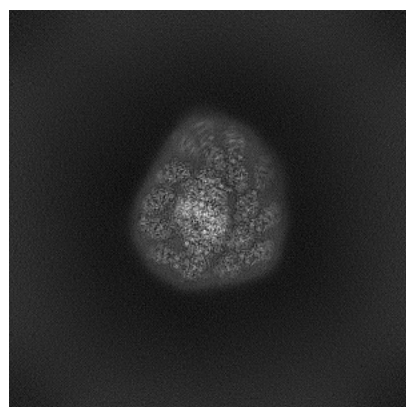


Y

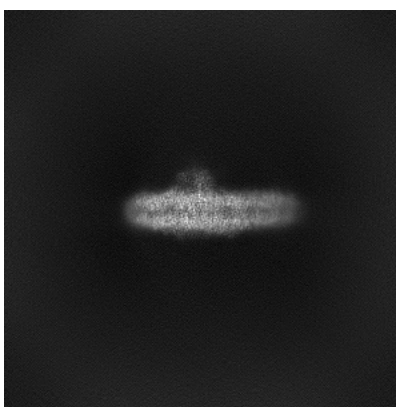


Z

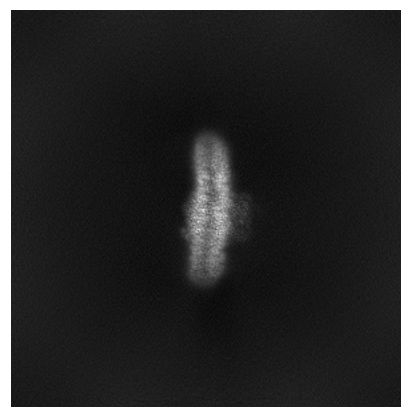
6.1.2 Raw map



X



Y

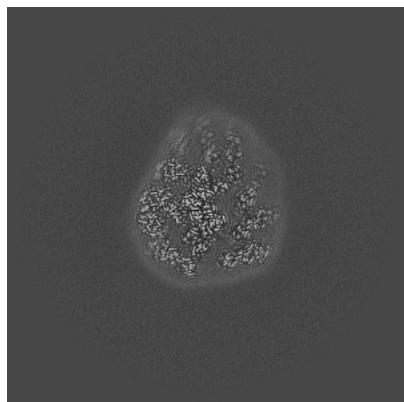


Z

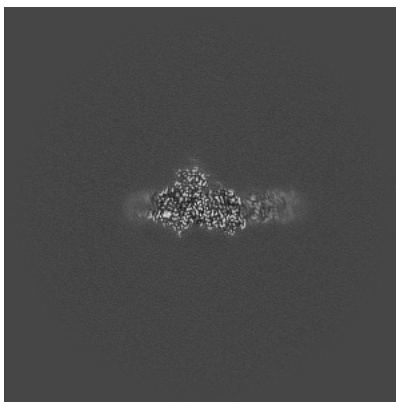
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

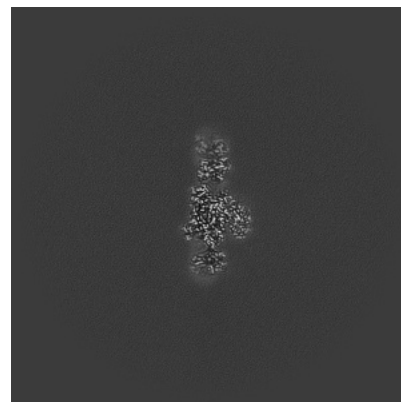
6.2.1 Primary map



X Index: 256

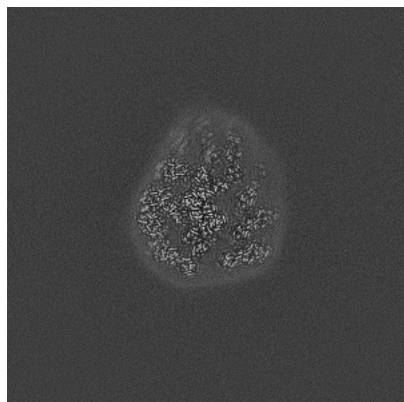


Y Index: 256

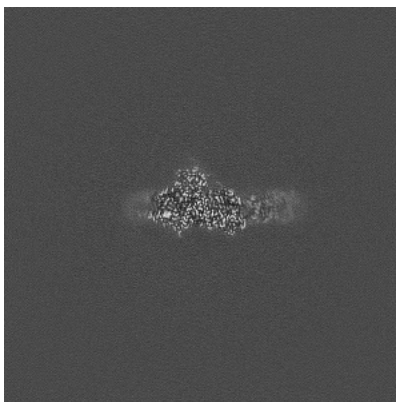


Z Index: 256

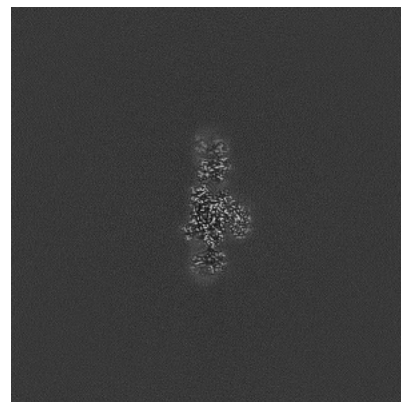
6.2.2 Raw map



X Index: 256



Y Index: 256

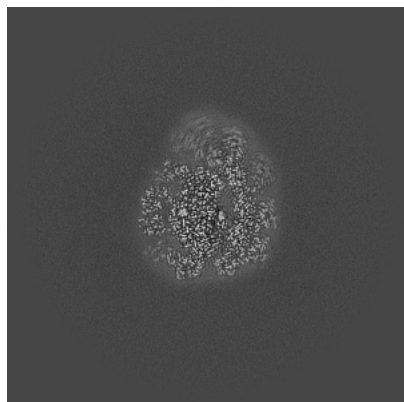


Z Index: 256

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

6.3 Largest variance slices [i](#)

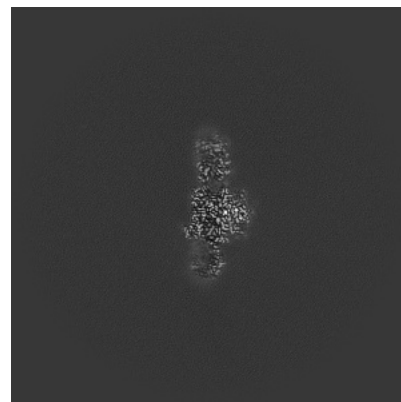
6.3.1 Primary map



X Index: 267

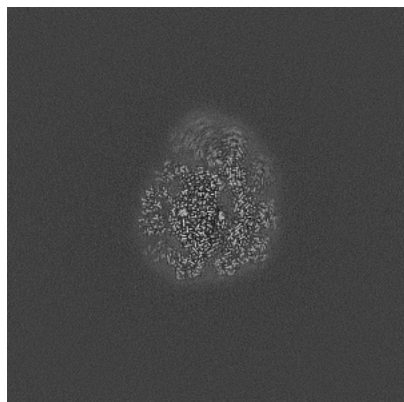


Y Index: 249



Z Index: 250

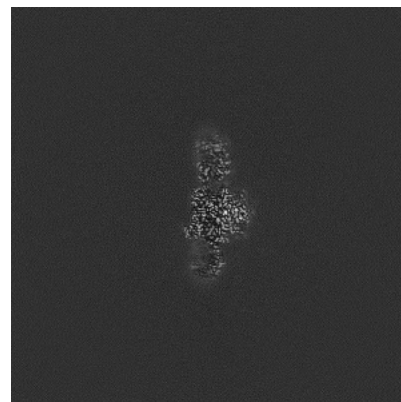
6.3.2 Raw map



X Index: 267



Y Index: 249

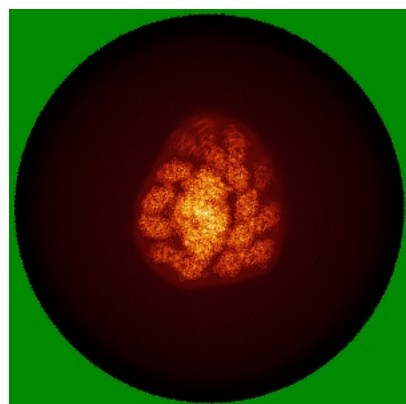


Z Index: 250

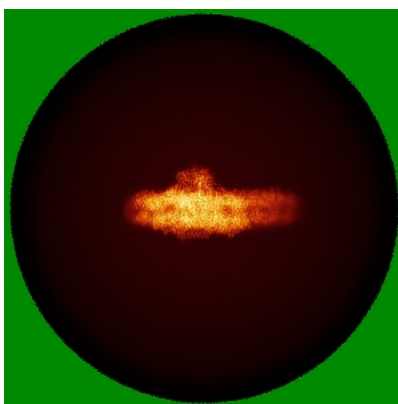
The images above show the largest variance slices of the map in three orthogonal directions.

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

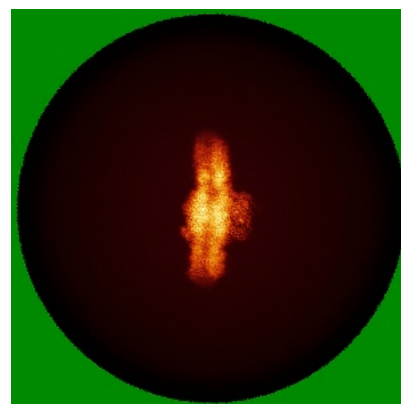
6.4.1 Primary map



X

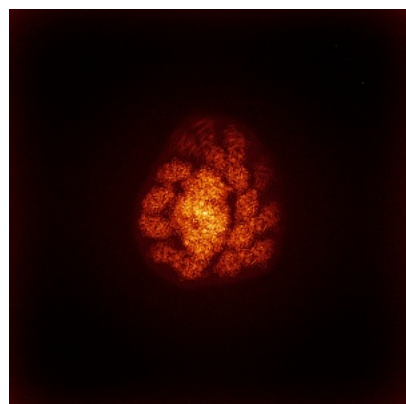


Y

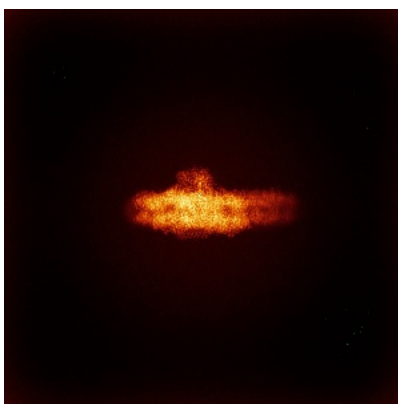


Z

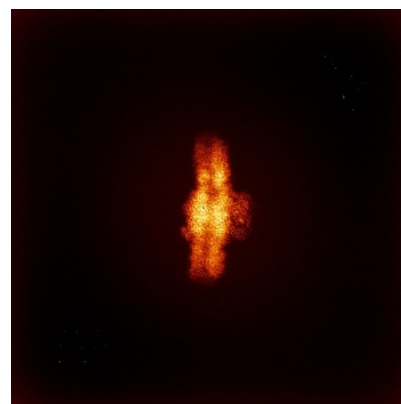
6.4.2 Raw map



X



Y

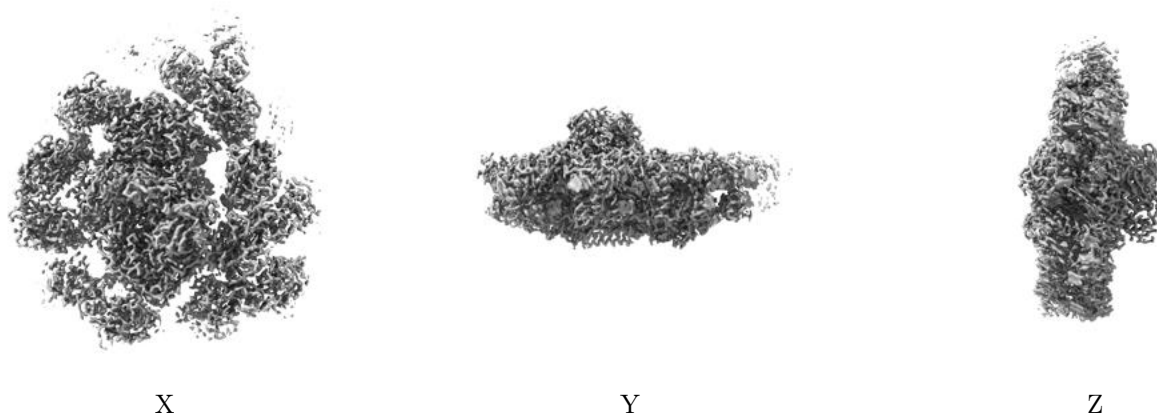


Z

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

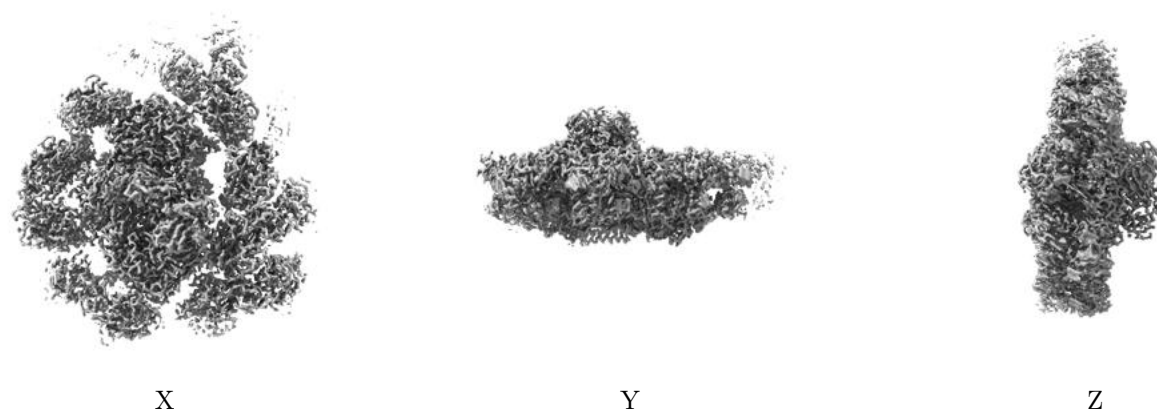
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

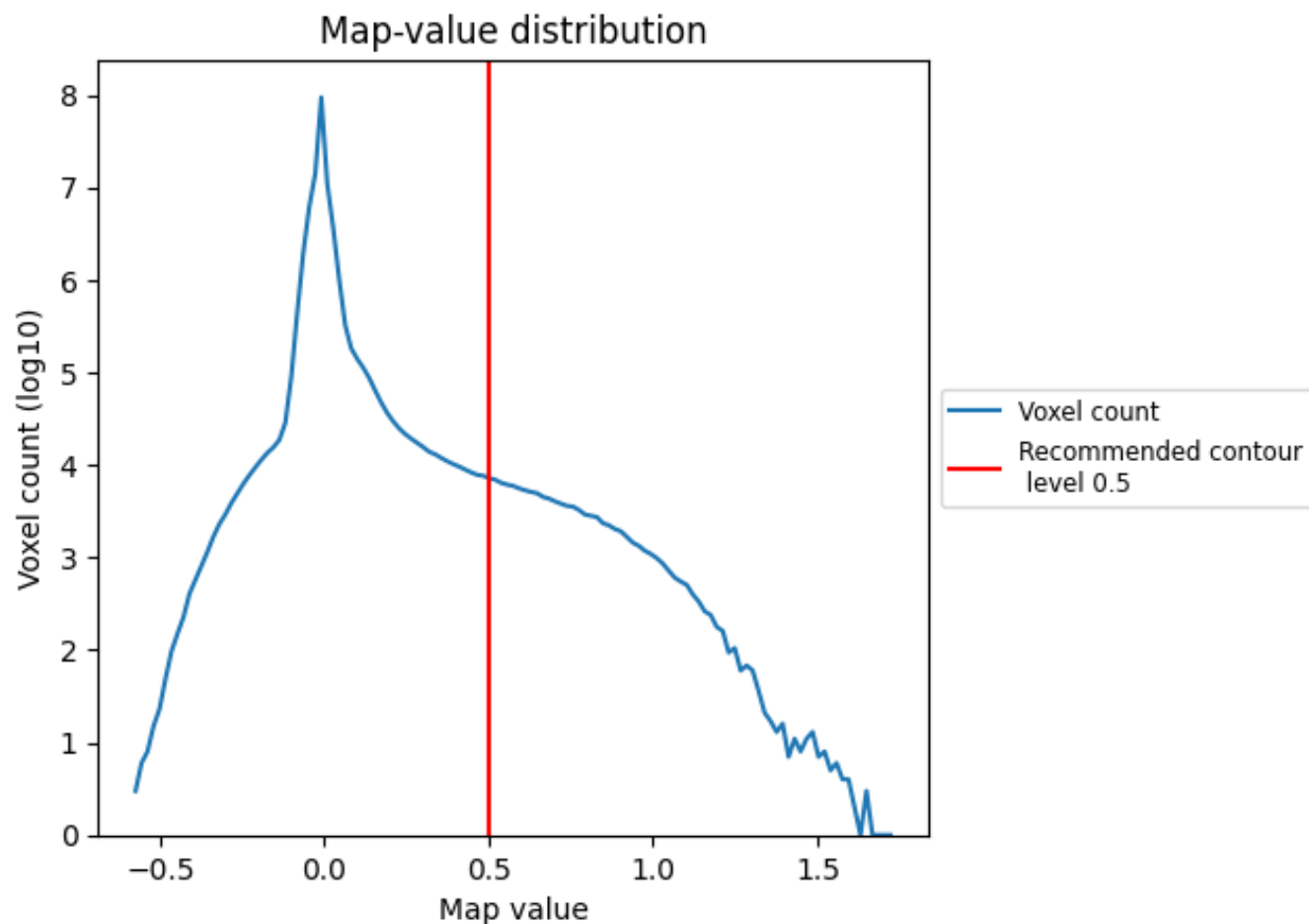
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

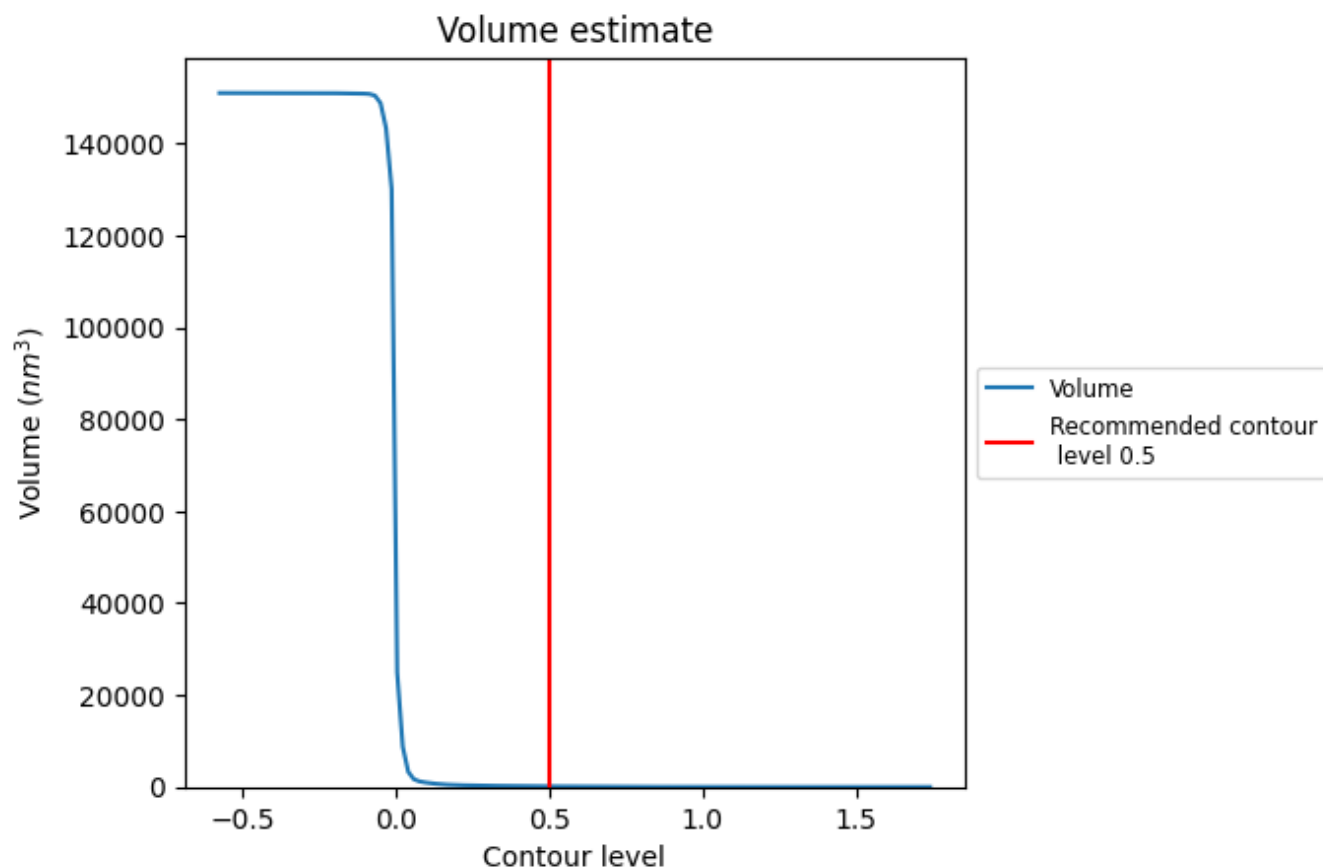
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

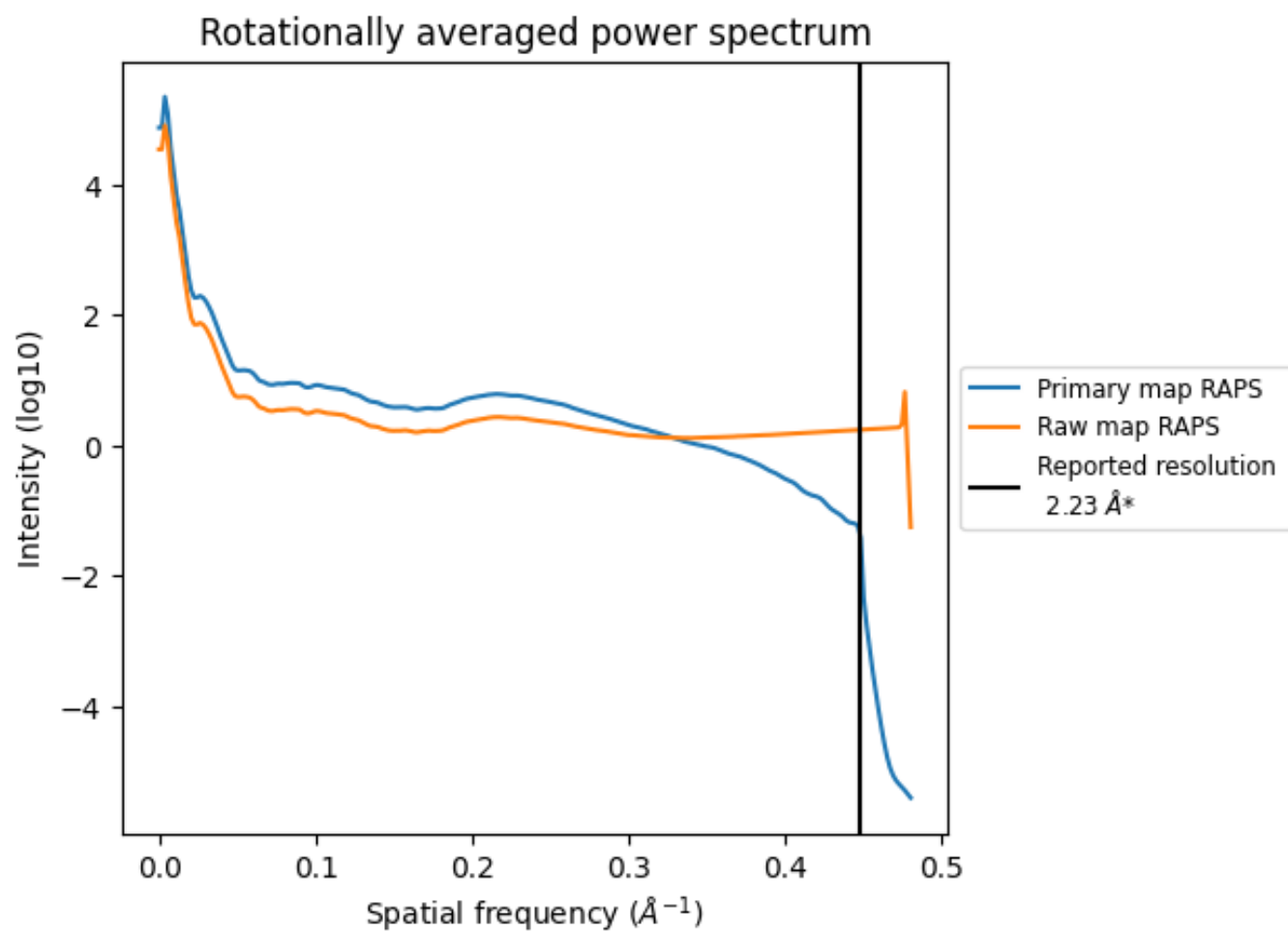
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 125 nm^3 ; this corresponds to an approximate mass of 113 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 ⓘ

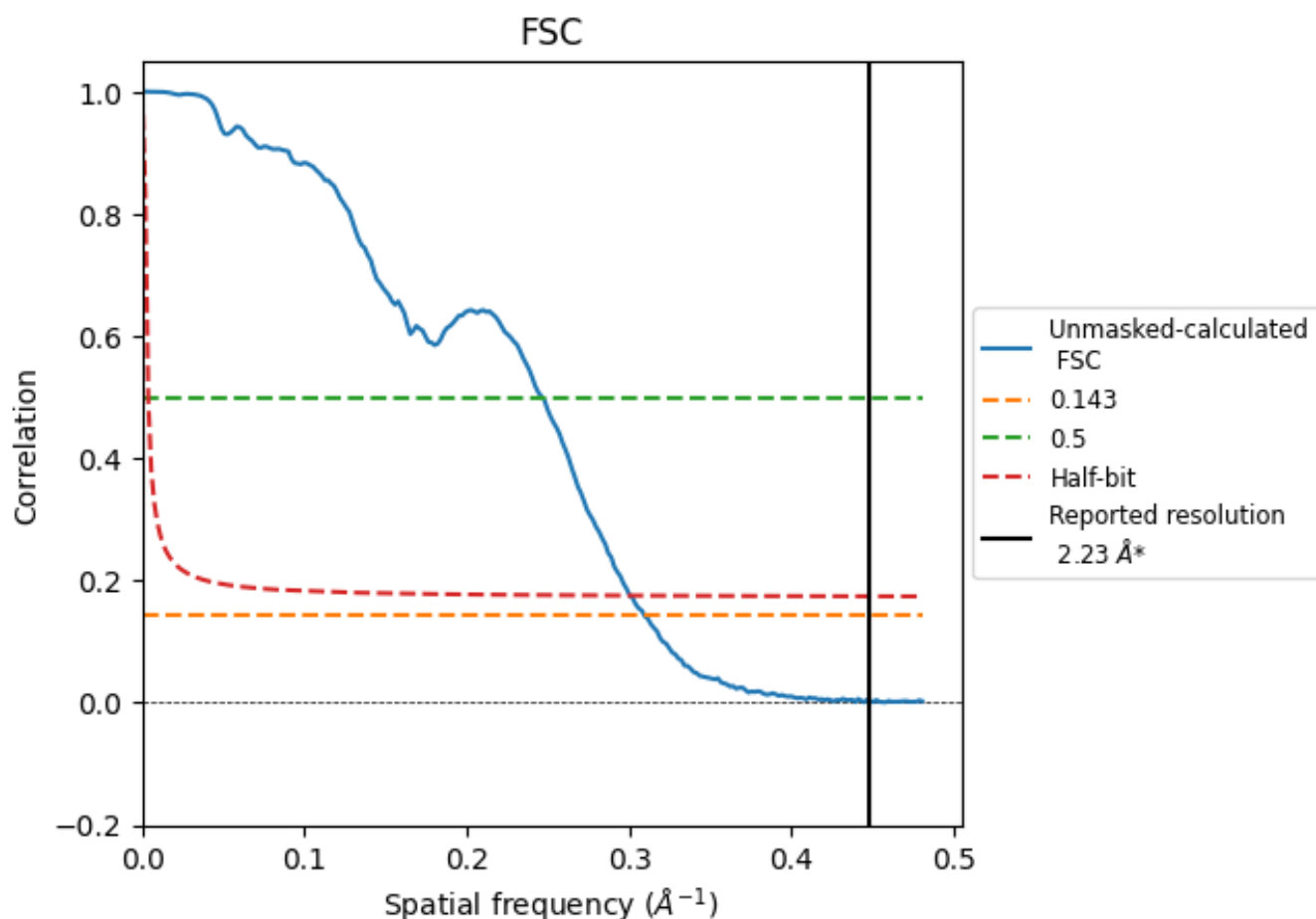


*Reported resolution corresponds to spatial frequency of 0.448 Å⁻¹

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 0.448 Å⁻¹

8.2 Resolution estimates [i](#)

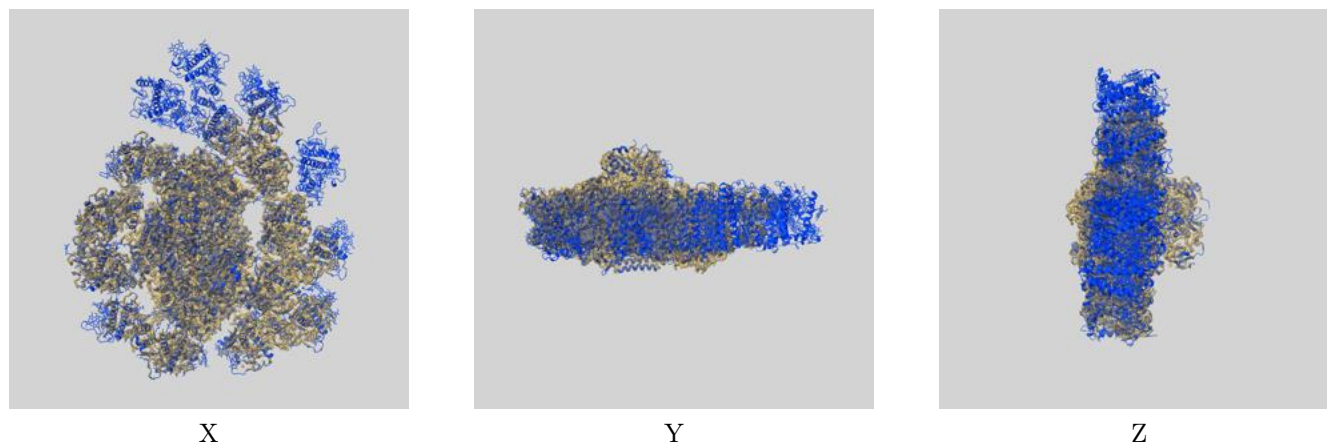
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.23	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.23	4.06	3.33

*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 3.23 differs from the reported value 2.23 by more than 10 %

9 Map-model fit [i](#)

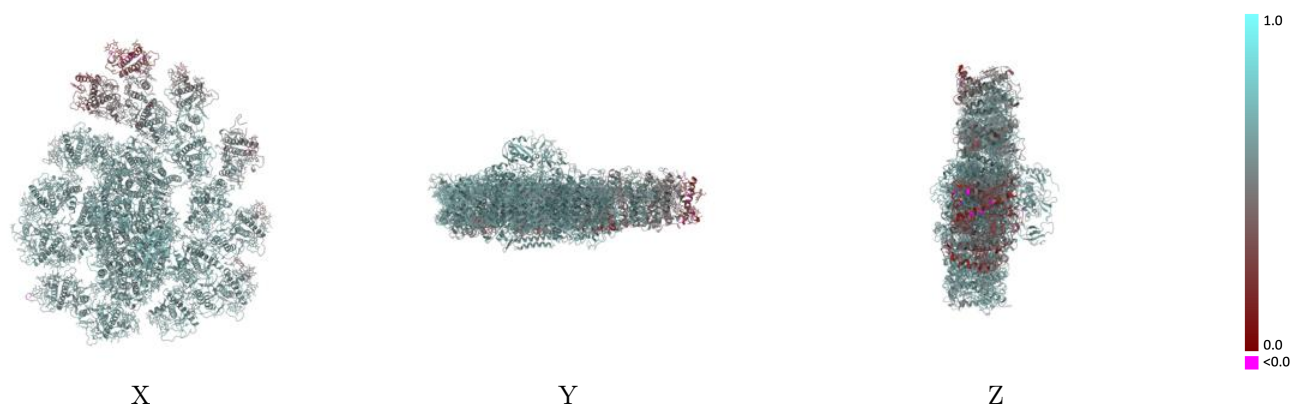
This section contains information regarding the fit between EMDB map EMD-64823 and PDB model 9V7T. Per-residue inclusion information can be found in [section 3](#) on [page 31](#).

9.1 Map-model overlay [i](#)



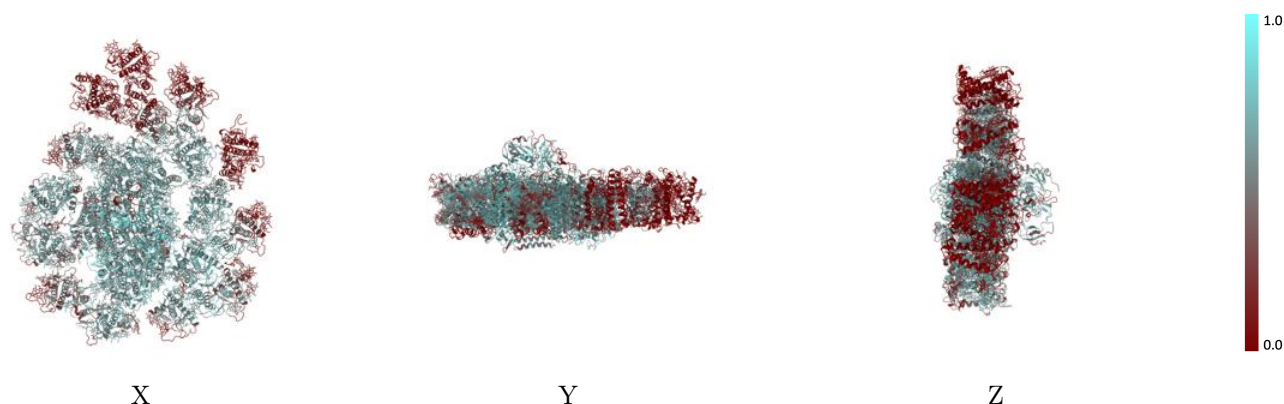
The images above show the 3D surface view of the map at the recommended contour level 0.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



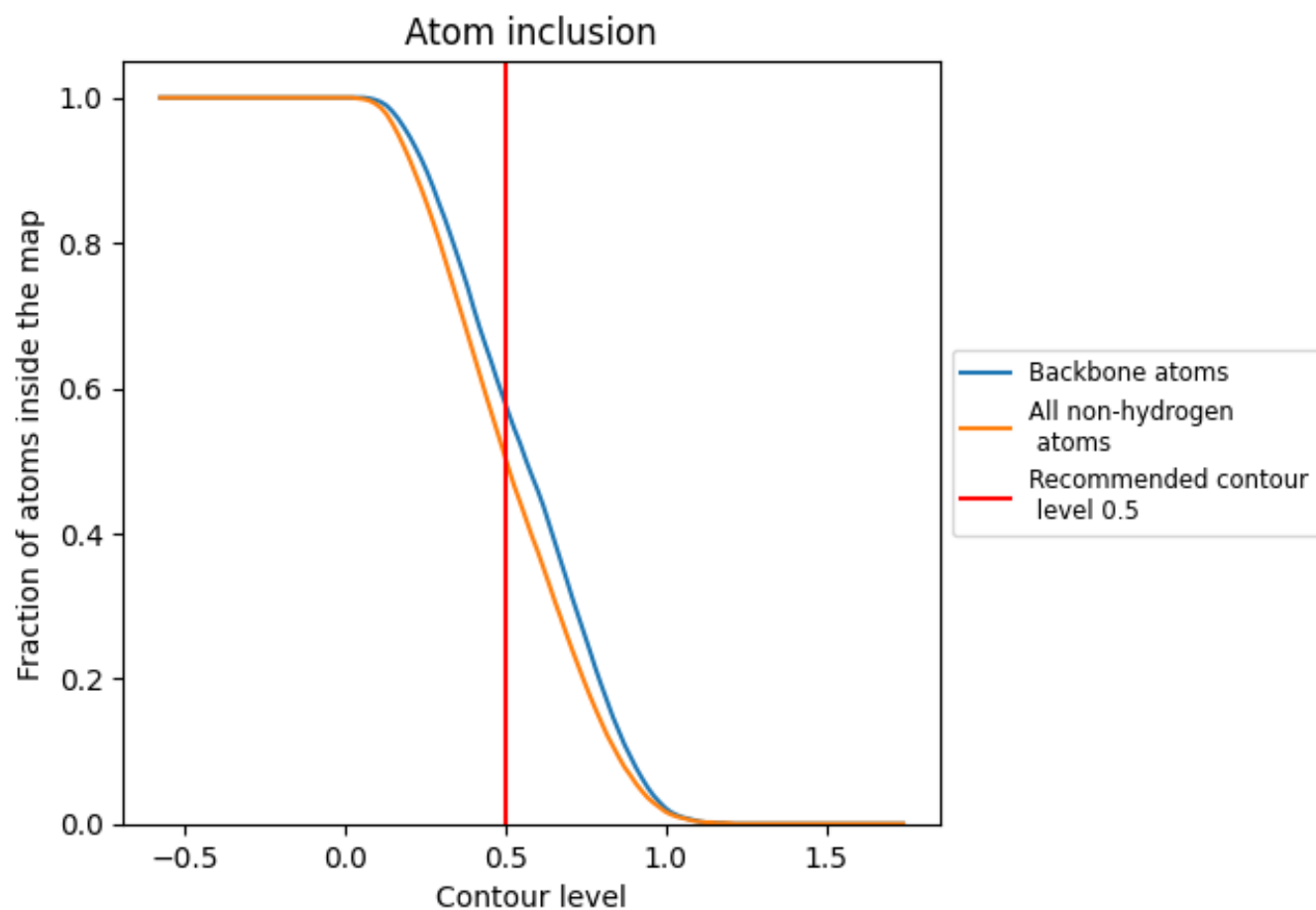
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.5).

9.4 Atom inclusion [i](#)



At the recommended contour level, 58% of all backbone atoms, 50% 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 (0.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5050	 0.6030
A	 0.7370	 0.6620
B	 0.7200	 0.6600
C	 0.7380	 0.6460
D	 0.4870	 0.6250
E	 0.5280	 0.6170
F	 0.5750	 0.6420
J	 0.6550	 0.6550
M	 0.5350	 0.6370
a	 0.5050	 0.6250
b	 0.3480	 0.5970
c	 0.4990	 0.6240
d	 0.5540	 0.6300
e	 0.4480	 0.6170
f	 0.0030	 0.3560
g	 0.2530	 0.5450
h	 0.5780	 0.6320
i	 0.5940	 0.6340
j	 0.6730	 0.6500
k	 0.4950	 0.6240
l	 0.3890	 0.5840
m	 0.2650	 0.5670
n	 0.0050	 0.4830
o	 0.1340	 0.5040
p	 0.0000	 0.2870

